



Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 11:27 AM EDT

PDB ID : 9MGW / pdb_00009mgw
EMDB ID : EMD-48262
Title : Dunaliella salina PSI-LHCI-TIDI1 supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 3.00 Å(reported)
Based on initial model : 6SL5

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

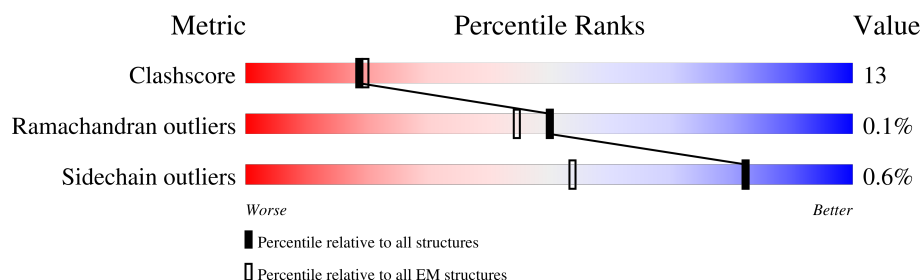
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	228	
1	a	228	
2	2	263	
3	3	320	
4	7	256	
4	c	256	
5	8	254	
5	b	254	

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Mol	Chain	Length	Quality of chain
6	9	222	
7	A	750	
8	B	735	
9	C	81	
10	D	202	
11	E	125	
12	F	232	
13	G	141	
14	H	135	
15	J	41	
16	L	202	
17	O	129	
18	I	109	
19	K	123	
20	T	365	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	301	X	-	-	-
21	CLA	1	302	X	-	-	-
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	307	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	321	X	-	-	-
21	CLA	2	602	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	605	X	-	-	-
21	CLA	2	607	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	-	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	402	X	-	-	-
21	CLA	3	403	X	-	-	-
21	CLA	3	404	X	-	-	-
21	CLA	3	405	X	-	-	-
21	CLA	3	406	X	-	-	-
21	CLA	3	407	X	-	-	-
21	CLA	3	408	X	-	-	-
21	CLA	3	409	X	-	-	-
21	CLA	3	410	X	-	-	-
21	CLA	3	411	X	-	-	-
21	CLA	3	412	X	-	-	-
21	CLA	3	413	X	-	-	-
21	CLA	3	414	X	-	-	-
21	CLA	7	304	X	-	-	-
21	CLA	7	305	X	-	-	-
21	CLA	7	306	X	-	-	-
21	CLA	7	310	X	-	-	-
21	CLA	7	311	X	-	-	-
21	CLA	7	312	X	-	-	-
21	CLA	7	313	X	-	-	-
21	CLA	7	314	X	-	-	-
21	CLA	7	315	X	-	-	-
21	CLA	7	316	X	-	-	-
21	CLA	7	323	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	605	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	8	612	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	8	614	X	-	-	-
21	CLA	8	615	X	-	-	-
21	CLA	8	622	X	-	-	-
21	CLA	9	601	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	605	X	-	-	-
21	CLA	9	607	X	-	-	-
21	CLA	9	608	X	-	-	-
21	CLA	9	609	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	856	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	B	842	X	-	-	-
21	CLA	B	843	X	-	-	-
21	CLA	B	844	X	-	-	-
21	CLA	F	5005	X	-	-	-
21	CLA	F	5006	X	-	-	-
21	CLA	F	5007	X	-	-	-
21	CLA	G	201	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	G	205	X	-	-	-
21	CLA	H	203	X	-	-	-
21	CLA	H	204	X	-	-	-
21	CLA	J	5002	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	202	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	L	301	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	L	305	X	-	-	-
21	CLA	L	306	X	-	-	-
21	CLA	O	2001	X	-	-	-
21	CLA	O	2002	X	-	-	-
21	CLA	O	2003	X	-	-	-
21	CLA	T	603	X	-	-	-
21	CLA	T	604	X	-	-	-
21	CLA	T	605	X	-	-	-
21	CLA	T	607	X	-	-	-
21	CLA	T	608	X	-	-	-
21	CLA	T	609	X	-	-	-
21	CLA	T	610	X	-	-	-
21	CLA	T	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	T	612	X	-	-	-
21	CLA	T	613	X	-	-	-
21	CLA	T	614	X	-	-	-
21	CLA	a	302	X	-	-	-
21	CLA	a	303	X	-	-	-
21	CLA	a	304	X	-	-	-
21	CLA	a	305	X	-	-	-
21	CLA	a	307	X	-	-	-
21	CLA	a	308	X	-	-	-
21	CLA	a	309	X	-	-	-
21	CLA	a	310	X	-	-	-
21	CLA	a	311	X	-	-	-
21	CLA	a	312	X	-	-	-
21	CLA	a	313	X	-	-	-
21	CLA	a	314	X	-	-	-
21	CLA	b	304	X	-	-	-
21	CLA	b	305	X	-	-	-
21	CLA	b	306	X	-	-	-
21	CLA	b	310	X	-	-	-
21	CLA	b	311	X	-	-	-
21	CLA	b	312	X	-	-	-
21	CLA	b	313	X	-	-	-
21	CLA	b	314	X	-	-	-
21	CLA	b	315	X	-	-	-
21	CLA	b	316	X	-	-	-
21	CLA	c	601	X	-	-	-
21	CLA	c	602	X	-	-	-
21	CLA	c	603	X	-	-	-
21	CLA	c	604	X	-	-	-
21	CLA	c	608	X	-	-	-
21	CLA	c	609	X	-	-	-
21	CLA	c	610	X	-	-	-
21	CLA	c	611	X	-	-	-
21	CLA	c	612	X	-	-	-
21	CLA	c	613	X	-	-	-
21	CLA	c	614	X	-	-	-
22	CHL	1	305	X	-	-	-
22	CHL	2	601	X	-	-	-
22	CHL	2	606	X	-	-	-
22	CHL	3	401	X	-	-	-
22	CHL	7	303	X	-	-	-
22	CHL	7	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHL	7	308	X	-	-	-
22	CHL	7	309	X	-	-	-
22	CHL	8	601	X	-	-	-
22	CHL	8	606	X	-	-	-
22	CHL	8	607	X	-	-	-
22	CHL	8	608	X	-	-	-
22	CHL	9	606	X	-	-	-
22	CHL	T	601	X	-	-	-
22	CHL	T	602	X	-	-	-
22	CHL	a	306	X	-	-	-
22	CHL	b	302	X	-	-	-
22	CHL	b	307	X	-	-	-
22	CHL	b	308	X	-	-	-
22	CHL	b	309	X	-	-	-
22	CHL	c	605	X	-	-	-
22	CHL	c	606	X	-	-	-
22	CHL	c	607	X	-	-	-
23	LUT	1	314	X	-	-	-
23	LUT	2	614	X	-	-	-
23	LUT	2	615	X	-	-	-
23	LUT	2	616	X	-	-	-
23	LUT	3	415	X	-	-	-
23	LUT	7	317	X	-	-	-
23	LUT	8	616	X	-	-	-
23	LUT	9	613	X	-	-	-
23	LUT	B	801	X	-	-	-
23	LUT	O	2005	X	-	-	-
23	LUT	T	615	X	-	-	-
23	LUT	a	315	X	-	-	-
23	LUT	b	317	X	-	-	-
23	LUT	c	615	X	-	-	-
36	SF4	A	845	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 53613 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1497	962	253	275	7		
1	a	196	Total	C	N	O	S	0	0
			1490	956	252	275	7		

- Molecule 2 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	221	Total	C	N	O	S	0	0
			1731	1125	285	312	9		

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	230	Total	C	N	O	S	0	0
			1756	1146	287	318	5		

- Molecule 4 is a protein called LHCA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	209	Total	C	N	O	S	0	0
			1609	1039	269	295	6		
4	c	209	Total	C	N	O	S	0	0
			1609	1039	269	295	6		

- Molecule 5 is a protein called LHCA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	226	Total	C	N	O	S	0	0
			1726	1113	288	319	6		
5	b	223	Total	C	N	O	S	0	0
			1707	1103	284	314	6		

- Molecule 6 is a protein called LHCA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	187	Total	C	N	O	S	0	0
			1456	947	244	259	6		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	740	Total	C	N	O	S	0	0
			5807	3795	993	1001	18		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	732	Total	C	N	O	S	0	0
			5803	3813	973	1004	13		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 10 is a protein called PSAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	143	Total	C	N	O	S	0	0
			1133	726	196	205	6		

- Molecule 11 is a protein called PSAE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	64	Total	C	N	O	0	0
			509	323	88	98		

- Molecule 12 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	165	Total	C	N	O	S	0	0
			1303	840	223	238	2		

- Molecule 13 is a protein called PSAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	105	Total	C	N	O	S	0	0
			794	516	136	140	2		

- Molecule 14 is a protein called PSAH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	98	Total	C	N	O	S	0	0
			763	482	131	149	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 16 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	159	Total	C	N	O	S	0	0
			1170	762	192	210	6		

- Molecule 17 is a protein called PSAO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total	C	N	O	S	0	0
			697	464	113	118	2		

- Molecule 18 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	41	Total	C	N	O	S	0	0
			321	219	48	53	1		

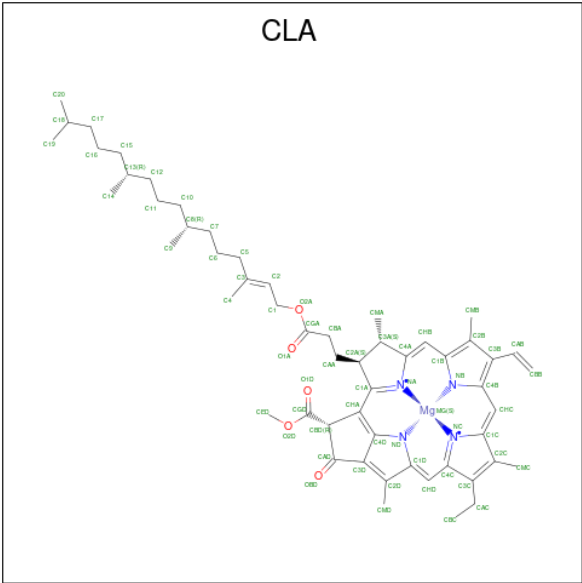
- Molecule 19 is a protein called PSAK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	83	Total	C	N	O	S	0	0
			584	373	101	107	3		

- Molecule 20 is a protein called TIDI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	205	Total	C	N	O	S	0	0
			1612	1048	266	290	8		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	F	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	G	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	a	1	Total 46	C 36	Mg 1	N 4	O 5	0

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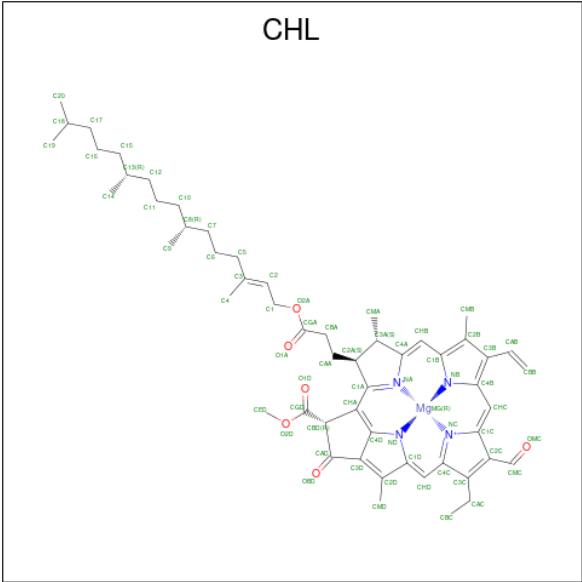
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 22 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



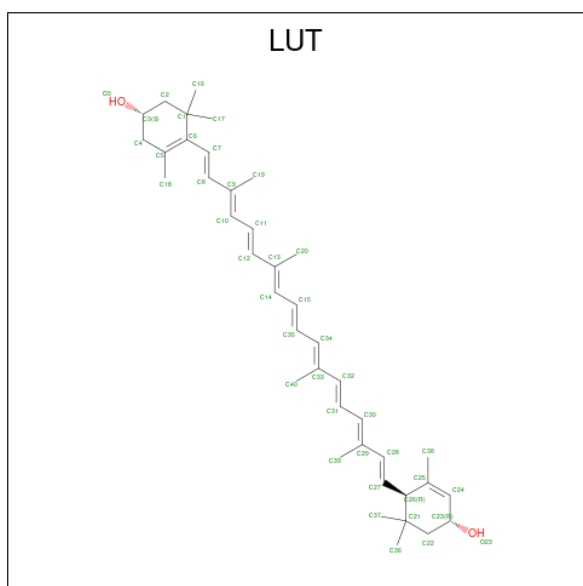
Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
22	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	7	1	Total 48	C 37	Mg 1	N 4	O 6	0
22	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
22	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
22	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
22	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
22	a	1	Total 47	C 36	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
22	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	T	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
22	T	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



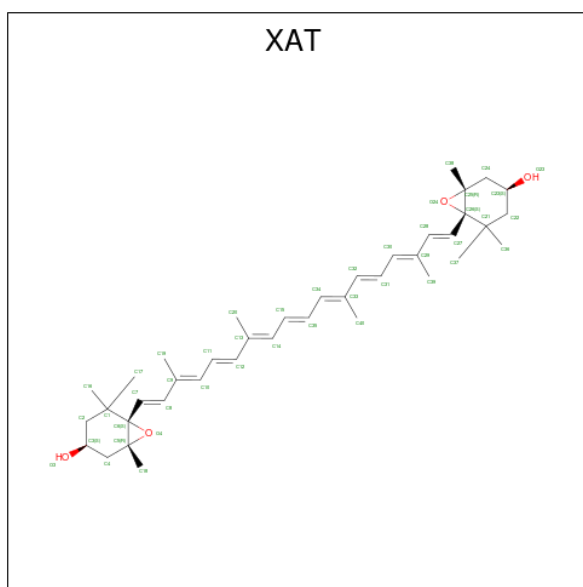
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	

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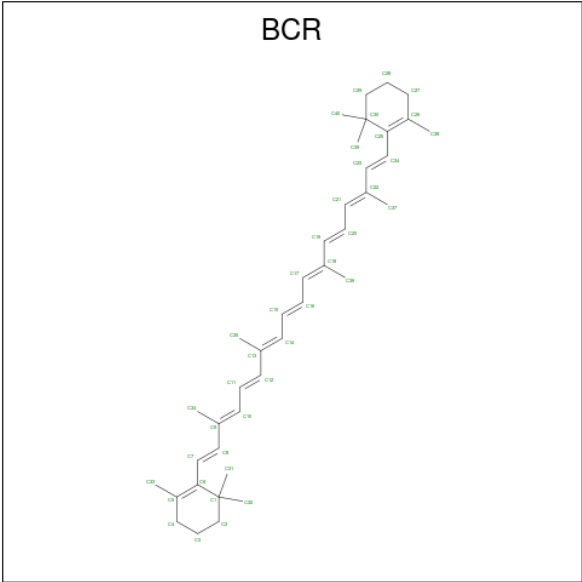
Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	7	1	Total	C	O	0
			42	40	2	
23	8	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	
23	B	1	Total	C	O	0
			42	40	2	
23	O	1	Total	C	O	0
			42	40	2	
23	a	1	Total	C	O	0
			42	40	2	
23	b	1	Total	C	O	0
			42	40	2	
23	c	1	Total	C	O	0
			42	40	2	
23	T	1	Total	C	O	0
			42	40	2	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	7	1	Total	C	O	0
			44	40	4	
24	8	1	Total	C	O	0
			44	40	4	
24	9	1	Total	C	O	0
			44	40	4	
24	9	1	Total	C	O	0
			44	40	4	
24	a	1	Total	C	O	0
			44	40	4	
24	b	1	Total	C	O	0
			44	40	4	
24	c	1	Total	C	O	0
			44	40	4	
24	T	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



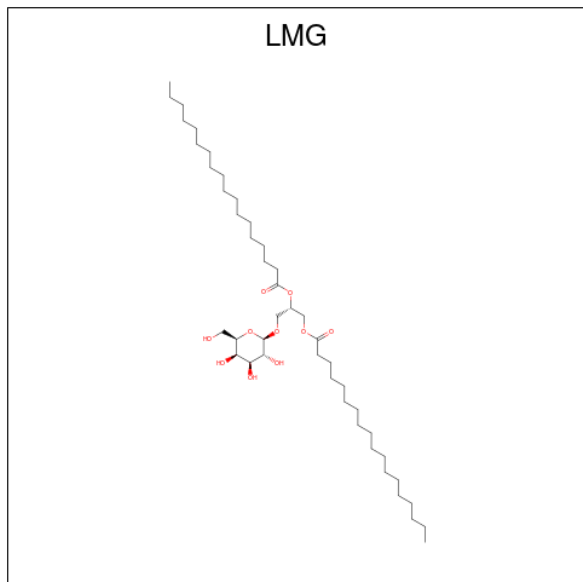
Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	7	1	Total	C	0
			40	40	
25	8	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	

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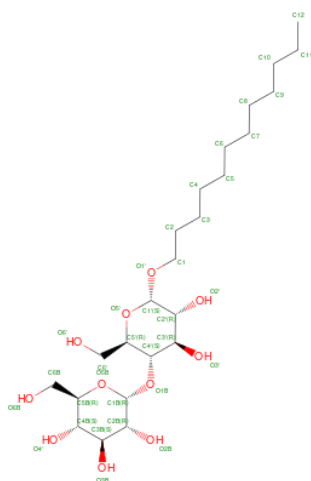
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	T	1	Total C 40 40	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

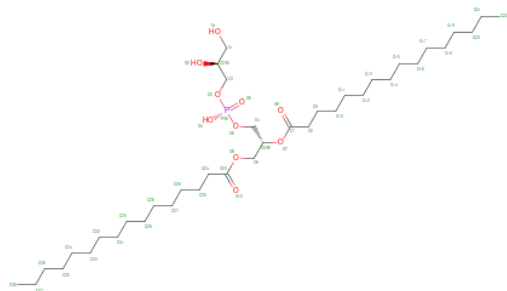


Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			28	19	9	
26	3	1	Total	C	O	0
			40	30	10	
26	7	1	Total	C	O	0
			47	37	10	
26	A	1	Total	C	O	0
			32	22	10	
26	F	1	Total	C	O	0
			39	29	10	
26	G	1	Total	C	O	0
			43	34	9	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



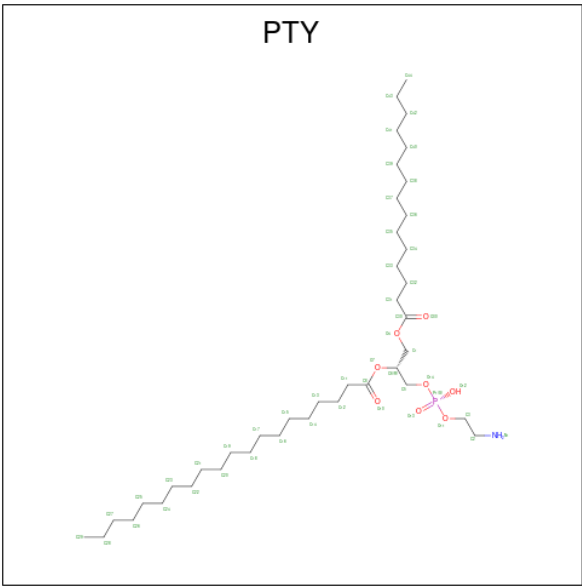
- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			25	14	10	1	
28	1	1	Total	C	O	P	0
			27	16	10	1	
28	1	1	Total	C	O	P	0
			46	35	10	1	
28	2	1	Total	C	O	P	0
			22	13	8	1	
28	3	1	Total	C	O	P	0
			17	8	8	1	
28	3	1	Total	C	O	P	0
			26	15	10	1	
28	7	1	Total	C	O	P	0
			43	32	10	1	
28	7	1	Total	C	O	P	0
			31	20	10	1	
28	8	1	Total	C	O	P	0
			40	29	10	1	
28	9	1	Total	C	O	P	0
			28	17	10	1	
28	A	1	Total	C	O	P	0
			30	20	9	1	
28	A	1	Total	C	O	P	0
			45	34	10	1	
28	B	1	Total	C	O	P	0
			32	21	10	1	
28	F	1	Total	C	O	P	0
			31	20	10	1	
28	F	1	Total	C	O	P	0
			43	32	10	1	
28	H	1	Total	C	O	P	0
			49	38	10	1	
28	a	1	Total	C	O	P	0
			22	11	10	1	
28	a	1	Total	C	O	P	0
			23	12	10	1	
28	b	1	Total	C	O	P	0
			31	20	10	1	
28	b	1	Total	C	O	P	0
			23	13	9	1	
28	c	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 29 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$)

(labeled as "Ligand of Interest" by depositor).



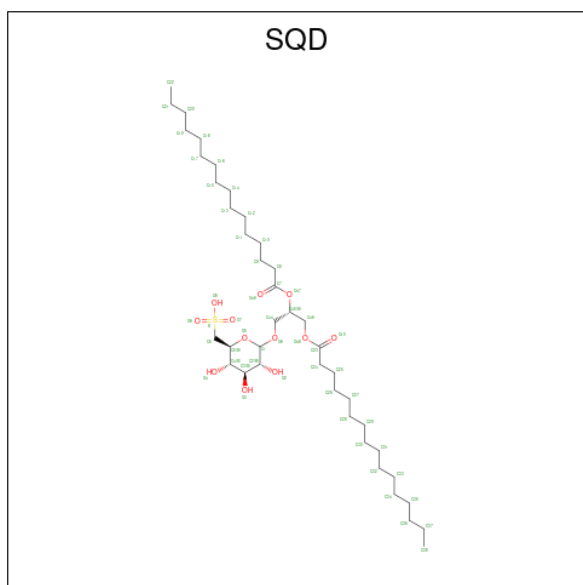
Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	N	O	P	0
			21	11	1	8	1	
29	2	1	Total	C	N	O	P	0
			32	22	1	8	1	
29	3	1	Total	C	O	P		0
			17	9	7	1		
29	7	1	Total	C	N	O	P	0
			26	16	1	8	1	
29	7	1	Total	C	N	O	P	0
			25	15	1	8	1	
29	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
29	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
29	B	1	Total	C	O	P		0
			26	18	7	1		
29	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
29	J	1	Total	C	N	O	P	0
			22	12	1	8	1	
29	L	1	Total	C	N	O	P	0
			20	10	1	8	1	
29	a	1	Total	C	N	O	P	0
			18	8	1	8	1	
29	c	1	Total	C	N	O	P	0
			31	21	1	8	1	

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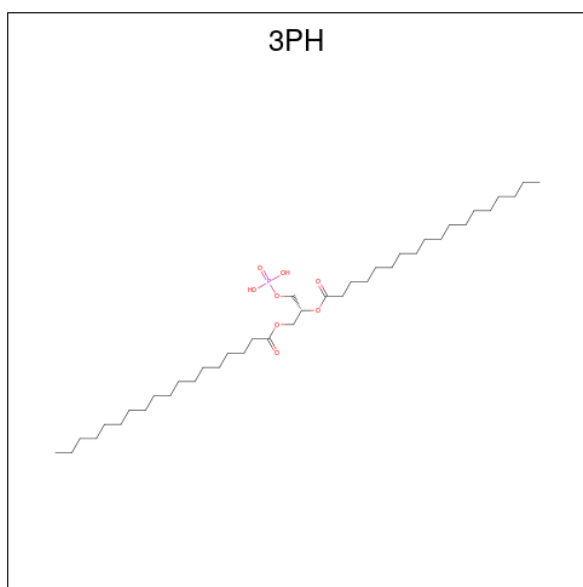
Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total	C	N	O	P	0
			26	16	1	8	1	
29	I	1	Total	C	O	P		0
			38	29	8	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



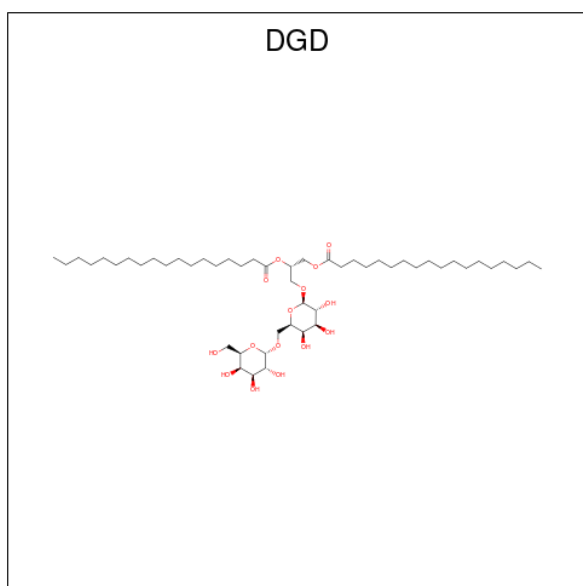
Mol	Chain	Residues	Atoms				AltConf
30	2	1	Total	C	O	S	0
			45	32	12	1	
30	3	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 31 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
31	2	1	Total	C	O	P	0
			43	34	8	1	
31	F	1	Total	C	O	P	0
			26	17	8	1	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



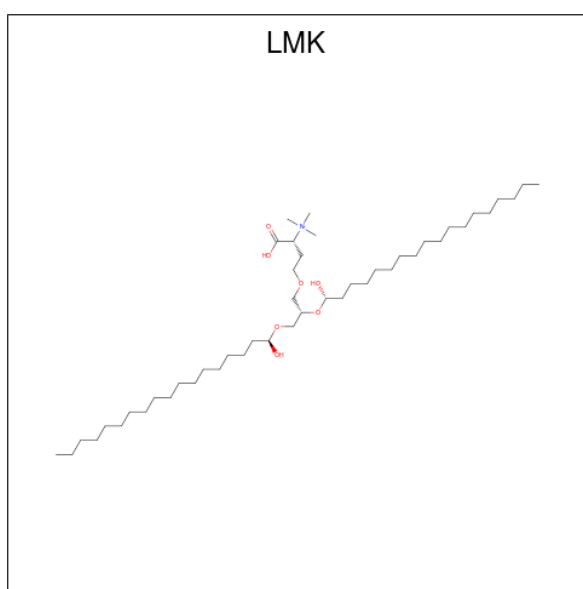
Mol	Chain	Residues	Atoms			AltConf
32	7	1	Total	C	O	0
			39	24	15	

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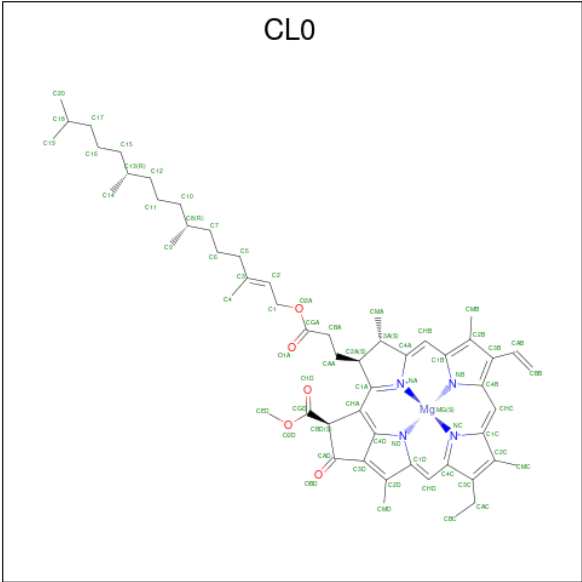
Mol	Chain	Residues	Atoms			AltConf
32	8	1	Total	C	O	0
			47	32	15	
32	A	1	Total	C	O	0
			66	51	15	
32	B	1	Total	C	O	0
			61	46	15	

- Molecule 33 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (CCD ID: LMK) (formula: C₄₆H₉₄NO₇) (labeled as "Ligand of Interest" by depositor).



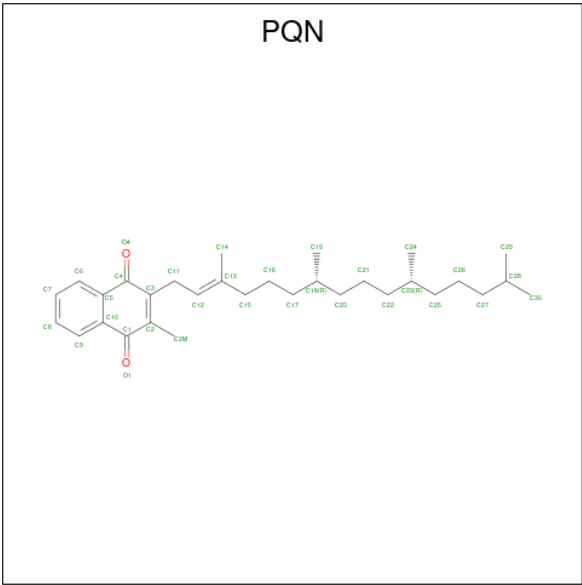
Mol	Chain	Residues	Atoms				AltConf
33	8	1	Total	C	N	O	0
			35	27	1	7	

- Molecule 34 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



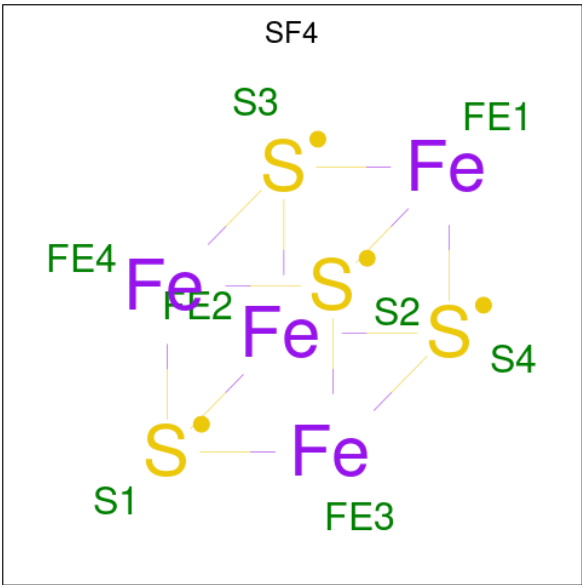
Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 35 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



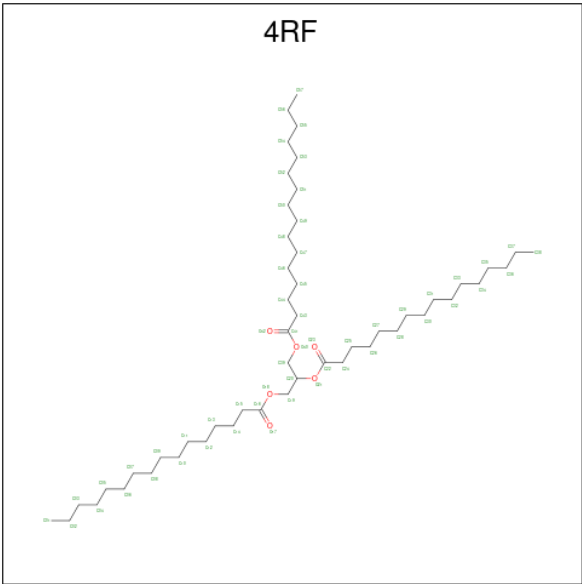
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			33	31	2	
35	B	1	Total	C	O	0
			33	31	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	Fe	S	0
			8	4	4	
36	C	1	Total	Fe	S	0
			8	4	4	
36	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	A	1	Total	C	O	0
			39	33	6	

- Molecule 38 is water.

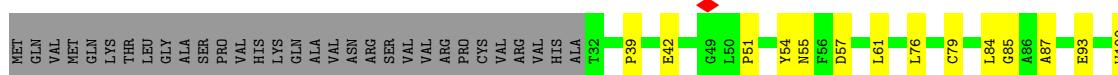
Mol	Chain	Residues	Atoms		AltConf
38	A	1	Total	O	0
			1	1	
38	C	1	Total	O	0
			1	1	
38	F	2	Total	O	0
			2	2	
38	L	1	Total	O	0
			1	1	

3 Residue-property plots

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

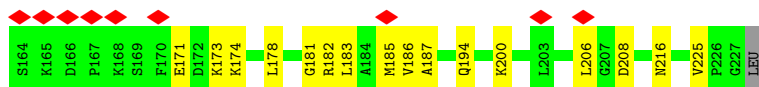
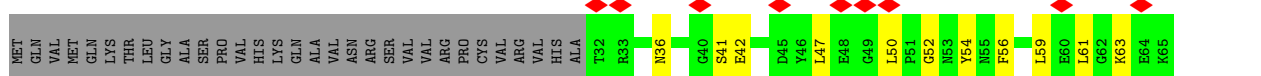
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 



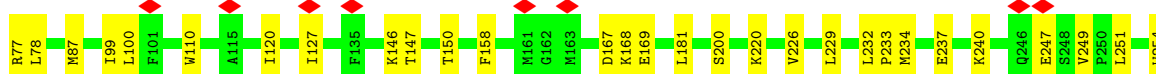
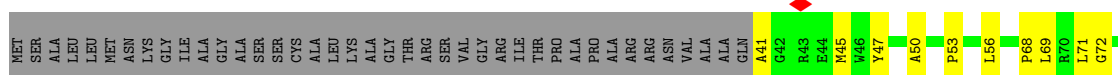
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain a: 



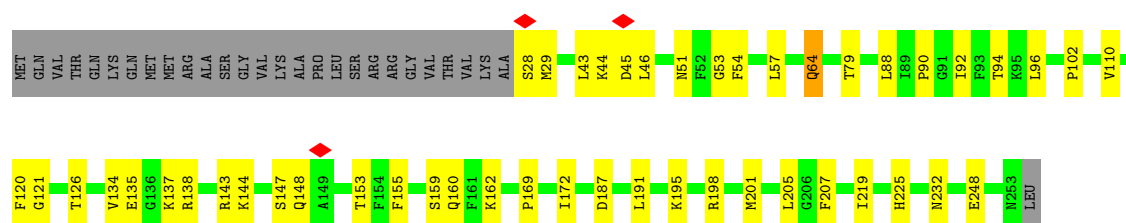
- Molecule 2: LHCA2

Chain 2: 



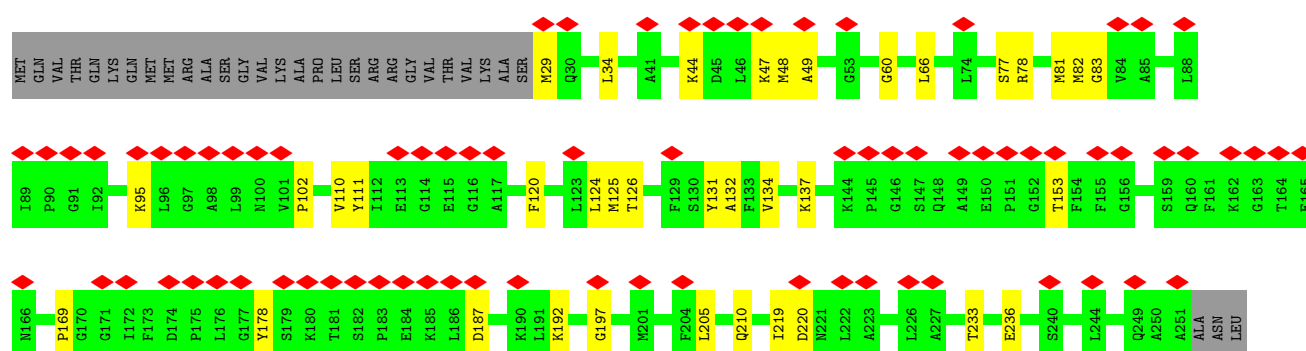


Chain 8: 



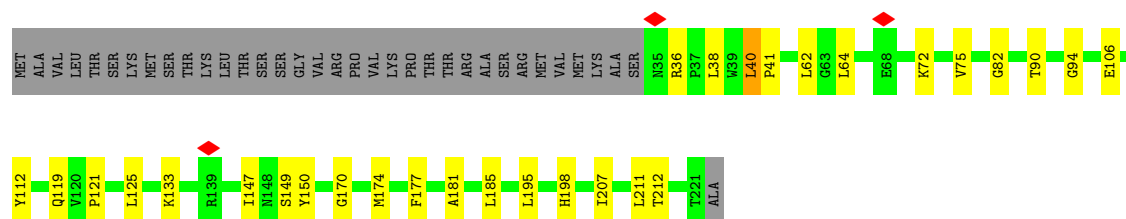
• Molecule 5: LHCA8

Chain b: 



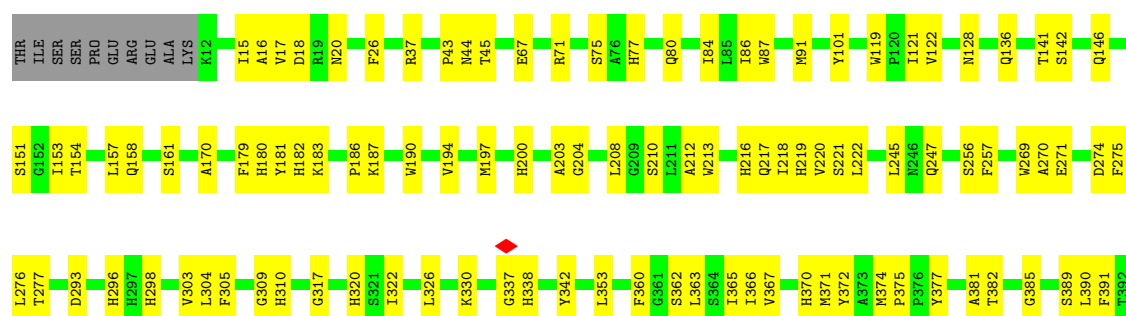
• Molecule 6: LHCA9

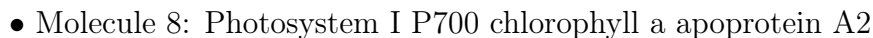
Chain 9: 



• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 





79% 20%



Response	Percentage
Doing a good job	78%
Doing a bad job	21%



Response	Percentage
Yes	52%
No	17%
Don't know	1%
No answer	29%



Chain E: 

MET ALA MET LEU SER SER ARG ILE SER CYS ARG PRO SER VAL SER LYS PRO GLN ARG THR ARG LEU ILE VAL ARG ALA GLU GLY GLU ALA PRO PRO ALA ALA LYS GLN PRO GLN ALA LYS ALA ALA PRO CYS PRO GLY GLU ALA LYS ALA PRO LYS E90

I61 Y77 V98 N112 N113 D117 D121 P122 P123 SER LYS

• Molecule 12: PSAF1

Chain F: 

MET ALA SER LEU THR GLN MET ASN ARG SER ALA PRO VAL ARG ALA PRO ARG ALA ARG VAL ARG ARG THR THR VAL VAL ARG ALA ARG ALA HIS GLN GLU GLN PRO GLN ASN LEU GLY ALA VAL ALA CYS ALA THR ALA LEU ALA THR MET GLY LEU THR ALA

ASP VAL GLN PRO ALA SER MET D68 I69 T73 P74 L92 E100 P101 G102 S103 T112 L129 C130 P136 H137 L138 I139 S140 M149 V154 F155 I156 V164 G172 R173 D182 A183 K188 E189 I190 D193 V194 P195 L196 Q203 L209 A210 S211 I212

Q213 R216 N217 V229 S230 P231 R232

• Molecule 13: PSAG1

Chain G: 

MET ALA LEU SER SER LYS ALA ASN ILE GLN PHE SER ARG GLN THR ALA GLN SER ARG ALA VAL VAL SER PRO ALA SER THR LYS THR ALA L37 L38 V42 S47 T48 V58 R66 T67 E70 P73 G74 K79 T80 T81 G82 D83

P86 L89 Q89 E97 S100 S104 L117 G118 L126 S129 R141

• Molecule 14: PSAH1

Chain H: 

MET ALA LEU LEU ALA LYS THR GLY ALA ALA THR GLN LEU ALA SER ARG ARG PRO ALA ALA CYS ARG ALA L101 F102 K105 G106 L110 L111 L112 P113 P118 R119 M120 E124 L131 R132 S133 ARG ILE Y36 G37 E38 Q39 S40 K41 D44 L45 Q46 D47 L48 E49 N50 G53 A54 W55 D61 E62 K63 R64 R65 Y66

E71 E72 Q75 T78 V81 S82 E85 A86 F90 V91 A92 L93 I99 A100 F101 K105 G106 L110 L111 L112 P113 P118 R119 M120 E124 L131 R132 S133 ARG ILE

• Molecule 15: Photosystem I reaction center subunit IX

Chain J: 

K1 K2 L8 S9 T10 A11 P12 V13 L16 F21 T22 G24 L25 L26 L27 E28 R31 P36 F41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120321	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0128	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LMU, DGD, LHG, PTY, CLA, SQD, LMG, BCR, LMK, LUT, 4RF, CHL, PQN, SF4, CL0, 3PH

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	1	0.15	0/1536	0.37	0/2082
1	a	0.19	0/1529	0.46	0/2073
2	2	0.17	0/1782	0.40	0/2418
3	3	0.17	0/1807	0.41	0/2451
4	7	0.17	0/1659	0.41	0/2254
4	c	0.18	0/1659	0.44	0/2254
5	8	0.15	0/1775	0.41	2/2406 (0.1%)
5	b	0.16	0/1756	0.38	0/2380
6	9	0.27	1/1499 (0.1%)	0.54	2/2043 (0.1%)
7	A	0.15	0/6003	0.35	0/8189
8	B	0.15	0/6016	0.38	0/8225
9	C	0.16	0/610	0.43	0/828
10	D	0.18	0/1163	0.44	0/1571
11	E	0.14	0/521	0.35	0/711
12	F	0.17	0/1332	0.46	2/1801 (0.1%)
13	G	0.19	0/815	0.47	0/1104
14	H	0.22	0/776	0.60	1/1043 (0.1%)
15	J	0.25	0/338	0.70	3/461 (0.7%)
16	L	0.20	0/1201	0.48	0/1643
17	O	0.24	0/723	0.60	0/990
18	I	0.26	0/335	0.66	0/463
19	K	0.29	0/592	0.78	2/801 (0.2%)
20	T	0.22	0/1659	0.64	5/2252 (0.2%)
All	All	0.18	1/37086 (0.0%)	0.44	17/50443 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	D	0	1
12	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	40	LEU	C-N	6.30	1.42	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	149	PRO	N-CA-CB	8.12	111.78	103.25
6	9	40	LEU	CA-CB-CG	7.84	143.74	116.30
6	9	40	LEU	CB-CG-CD2	-6.57	90.98	110.70
20	T	309	LYS	CA-CB-CG	6.03	126.17	114.10
5	8	64	GLN	CB-CG-CD	5.97	122.75	112.60
19	K	85	LEU	CA-CB-CG	5.87	136.83	116.30
20	T	189	MET	CA-CB-CG	5.86	125.82	114.10
5	8	64	GLN	CA-CB-CG	5.46	125.03	114.10
12	F	216	ARG	CB-CG-CD	5.31	123.51	111.30
15	J	1	MET	CB-CG-SD	5.30	128.60	112.70
19	K	66	LEU	CA-CB-CG	5.18	134.45	116.30
15	J	10	THR	CA-C-N	5.15	126.53	120.09
15	J	10	THR	C-N-CA	5.15	126.53	120.09
14	H	120	MET	CA-CB-CG	5.15	124.40	114.10
12	F	216	ARG	CG-CD-NE	5.13	123.29	112.00
20	T	169	ASN	CA-C-N	5.11	131.30	121.54
20	T	169	ASN	C-N-CA	5.11	131.30	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	159	HIS	Peptide
12	F	216	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1497	0	1465	41	0
1	a	1490	0	1453	39	0
2	2	1731	0	1693	35	0
3	3	1756	0	1710	70	0
4	7	1609	0	1564	49	0
4	c	1609	0	1564	36	0
5	8	1726	0	1674	46	0
5	b	1707	0	1662	30	0
6	9	1456	0	1442	34	0
7	A	5807	0	5639	179	0
8	B	5803	0	5554	125	0
9	C	600	0	583	13	0
10	D	1133	0	1141	39	0
11	E	509	0	497	4	0
12	F	1303	0	1327	51	0
13	G	794	0	799	15	0
14	H	763	0	753	33	0
15	J	327	0	328	12	0
16	L	1170	0	1187	37	0
17	O	697	0	678	12	0
18	I	321	0	316	18	0
19	K	584	0	614	15	0
20	T	1612	0	1565	46	0
21	1	683	0	591	33	0
21	2	568	0	492	25	0
21	3	706	0	635	34	0
21	7	598	0	539	22	0
21	8	547	0	429	30	0
21	9	551	0	447	15	0
21	A	2526	0	2620	179	0
21	B	2453	0	2529	138	0
21	F	161	0	146	4	0
21	G	203	0	173	9	0
21	H	106	0	89	1	0
21	J	45	0	33	2	0
21	K	193	0	151	6	0
21	L	267	0	231	13	0
21	O	121	0	69	2	0
21	T	596	0	482	14	0
21	a	619	0	507	23	0
21	b	517	0	430	17	0
21	c	523	0	395	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	1	47	0	31	3	0
22	2	113	0	101	8	0
22	3	66	0	70	8	0
22	7	206	0	165	26	0
22	8	195	0	134	15	0
22	9	47	0	31	5	0
22	T	104	0	80	15	0
22	a	47	0	31	2	0
22	b	211	0	166	23	0
22	c	142	0	97	11	0
23	1	42	0	56	7	0
23	2	126	0	168	6	0
23	3	42	0	56	1	0
23	7	42	0	56	1	0
23	8	42	0	56	0	0
23	9	42	0	56	3	0
23	B	42	0	55	4	0
23	O	42	0	54	1	0
23	T	42	0	54	3	0
23	a	42	0	54	6	0
23	b	42	0	56	2	0
23	c	42	0	56	1	0
24	1	44	0	56	12	0
24	3	44	0	56	6	0
24	7	44	0	56	3	0
24	8	44	0	56	3	0
24	9	88	0	112	7	0
24	T	44	0	56	4	0
24	a	44	0	56	5	0
24	b	44	0	56	3	0
24	c	44	0	56	1	0
25	1	40	0	56	3	0
25	3	120	0	166	8	0
25	7	40	0	53	4	0
25	8	40	0	56	6	0
25	A	240	0	336	31	0
25	B	240	0	336	26	0
25	F	80	0	111	9	0
25	G	80	0	112	4	0
25	I	80	0	112	9	0
25	J	80	0	112	8	0
25	K	40	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	120	0	168	3	0
25	O	40	0	56	1	0
25	T	40	0	56	1	0
25	a	40	0	56	0	0
25	b	40	0	54	6	0
25	c	40	0	56	2	0
26	1	28	0	26	4	0
26	3	40	0	53	2	0
26	7	47	0	64	7	0
26	A	32	0	34	2	0
26	F	39	0	48	3	0
26	G	43	0	55	5	0
27	1	35	0	45	1	0
27	9	35	0	46	4	0
27	A	70	0	92	4	0
28	1	98	0	109	9	0
28	2	22	0	17	0	0
28	3	43	0	32	0	0
28	7	74	0	91	5	0
28	8	40	0	53	3	0
28	9	28	0	26	0	0
28	A	75	0	92	5	0
28	B	32	0	33	0	0
28	F	74	0	91	4	0
28	H	49	0	74	3	0
28	a	45	0	28	2	0
28	b	54	0	43	3	0
28	c	29	0	27	0	0
29	1	21	0	15	0	0
29	2	32	0	37	1	0
29	3	17	0	7	0	0
29	7	51	0	47	0	0
29	8	21	0	17	0	0
29	B	53	0	50	0	0
29	H	42	0	56	1	0
29	I	38	0	49	7	0
29	J	22	0	17	2	0
29	L	20	0	11	1	0
29	a	18	0	9	0	0
29	c	57	0	60	4	0
30	2	45	0	54	4	0
30	3	35	0	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	43	0	62	4	0
31	F	26	0	24	1	0
32	7	39	0	36	2	0
32	8	47	0	52	4	0
32	A	66	0	92	4	0
32	B	61	0	83	3	0
33	8	35	0	0	0	0
34	A	65	0	72	8	0
35	A	33	0	46	1	0
35	B	33	0	46	4	0
36	A	8	0	0	4	0
36	C	16	0	0	1	0
37	A	39	0	53	2	0
38	A	1	0	0	0	0
38	C	1	0	0	0	0
38	F	2	0	0	0	0
38	L	1	0	0	0	0
All	All	53613	0	52599	1344	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 13.

All (1344) 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)
3:3:288:VAL:CG1	21:A:817:CLA:C2	1.82	1.53
3:3:288:VAL:CG1	21:A:817:CLA:H2	1.43	1.38
3:3:288:VAL:HG11	21:A:817:CLA:C2	1.46	1.36
4:7:78:MET:HE3	26:7:320:LMG:O5	1.20	1.34
7:A:584:CYS:SG	36:A:845:SF4:FE4	1.19	1.32
1:1:189:LEU:CD1	24:1:315:XAT:H203	1.61	1.28
3:3:288:VAL:HG13	21:A:817:CLA:C2	1.53	1.24
1:1:189:LEU:CD1	24:1:315:XAT:C20	2.16	1.23
3:3:288:VAL:HG11	21:A:817:CLA:C3	1.66	1.23
12:F:74:PRO:HA	12:F:129:LEU:CD2	1.70	1.20
1:1:189:LEU:HD11	24:1:315:XAT:C20	1.72	1.18
3:3:288:VAL:HG11	21:A:817:CLA:C5	1.75	1.17
21:2:603:CLA:CED	14:H:93:LEU:HD11	1.79	1.13
21:8:604:CLA:H11	12:F:209:LEU:CD1	1.80	1.11
21:2:603:CLA:HED3	14:H:93:LEU:CD1	1.80	1.11
4:7:78:MET:HE3	26:7:320:LMG:C6	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:74:PRO:CA	12:F:129:LEU:HD23	1.82	1.09
12:F:74:PRO:CA	12:F:129:LEU:CD2	2.33	1.07
21:8:604:CLA:H12	12:F:209:LEU:HG	1.37	1.06
10:D:121:LEU:CD2	10:D:123:LEU:HD21	1.85	1.04
10:D:121:LEU:CD2	10:D:132:LEU:HD22	1.90	1.00
3:3:203:GLU:O	3:3:207:ILE:HG22	1.61	0.99
21:8:604:CLA:H11	12:F:209:LEU:HD11	1.43	0.99
10:D:121:LEU:CD2	10:D:132:LEU:CD2	2.43	0.97
12:F:74:PRO:HA	12:F:129:LEU:HD23	0.98	0.96
18:I:86:PRO:O	18:I:90:LEU:HB2	1.64	0.96
4:7:78:MET:CE	26:7:320:LMG:C6	2.45	0.94
1:1:189:LEU:HD12	24:1:315:XAT:C20	1.97	0.94
10:D:121:LEU:HD23	10:D:132:LEU:CD2	1.97	0.94
7:A:204:GLY:O	7:A:208:LEU:HB2	1.68	0.93
21:2:603:CLA:HED3	14:H:93:LEU:HD11	0.94	0.91
10:D:121:LEU:HG	10:D:123:LEU:HD22	1.51	0.91
21:B:804:CLA:C1B	21:B:807:CLA:HBB1	2.00	0.90
4:7:78:MET:CE	26:7:320:LMG:O5	2.16	0.90
3:3:288:VAL:CG2	21:A:817:CLA:H2	2.02	0.89
1:1:189:LEU:HD11	24:1:315:XAT:H203	0.90	0.89
21:8:604:CLA:C1	12:F:209:LEU:CD1	2.50	0.89
4:7:78:MET:CE	26:7:320:LMG:HC62	2.04	0.88
7:A:740:TRP:NE1	7:A:744:LEU:HD11	1.89	0.87
8:B:390:HIS:HE1	21:B:832:CLA:NA	1.73	0.86
21:B:804:CLA:NB	21:B:807:CLA:HBB1	1.88	0.86
3:3:288:VAL:CB	21:A:817:CLA:H2	2.04	0.86
7:A:584:CYS:HG	36:A:845:SF4:FE4	0.90	0.86
10:D:121:LEU:HG	10:D:123:LEU:CD2	2.06	0.86
3:3:288:VAL:CG1	21:A:817:CLA:C3	2.36	0.85
7:A:584:CYS:SG	36:A:845:SF4:S3	2.75	0.85
10:D:121:LEU:HD23	10:D:123:LEU:HD21	1.57	0.84
3:3:280:MET:HE2	24:3:416:XAT:H10	1.58	0.84
21:b:304:CLA:HHD	21:c:601:CLA:HBB2	1.60	0.83
3:3:207:ILE:HD13	21:3:407:CLA:HMC3	1.61	0.82
1:a:76:LEU:HA	1:a:79:CYS:SG	2.20	0.81
3:3:288:VAL:HG13	21:A:817:CLA:C1	2.11	0.81
1:a:182:ARG:HA	1:a:185:MET:HE3	1.63	0.81
21:8:604:CLA:H11	12:F:209:LEU:HD12	1.62	0.81
21:B:822:CLA:H162	21:B:829:CLA:H3A	1.63	0.81
18:I:92:LEU:HD12	29:I:201:PTY:H221	1.61	0.81
16:L:121:VAL:HG12	16:L:193:TYR:CE1	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:288:VAL:HG11	21:A:817:CLA:H2	1.15	0.80
22:7:307:CHL:HBC2	22:7:308:CHL:HAC2	1.64	0.80
3:3:288:VAL:HG11	21:A:817:CLA:H52	1.62	0.79
7:A:182:HIS:HE1	21:A:813:CLA:NA	1.80	0.79
21:3:412:CLA:HAB	21:T:606:CLA:HBB2	1.64	0.79
21:8:604:CLA:H12	12:F:209:LEU:CG	2.13	0.79
7:A:684:MET:HE1	21:A:804:CLA:NA	1.98	0.78
12:F:74:PRO:N	12:F:129:LEU:HD22	1.99	0.78
10:D:121:LEU:HD23	10:D:132:LEU:HD23	1.67	0.77
7:A:121:ILE:HG13	7:A:122:VAL:HG23	1.67	0.76
16:L:121:VAL:HG12	16:L:193:TYR:HE1	1.50	0.76
8:B:685:LYS:HB3	16:L:60:MET:HE1	1.68	0.76
21:K:203:CLA:H3A	25:K:205:BCR:H363	1.67	0.76
1:a:182:ARG:HA	1:a:185:MET:CE	2.15	0.75
4:7:148:LYS:HB3	22:7:309:CHL:HMC	1.68	0.75
3:3:264:LYS:HD3	20:T:169:ASN:HB3	1.67	0.75
10:D:121:LEU:HD22	10:D:132:LEU:HD22	1.67	0.75
21:7:323:CLA:HBB2	21:8:603:CLA:HHD	1.68	0.75
4:7:139:LEU:O	21:7:310:CLA:HBB2	1.87	0.75
3:3:207:ILE:HD13	21:3:407:CLA:CMC	2.17	0.74
21:8:604:CLA:C1	12:F:209:LEU:HD11	2.15	0.74
21:8:622:CLA:HBB2	12:F:209:LEU:HA	1.69	0.74
12:F:74:PRO:CA	12:F:129:LEU:HD22	2.18	0.73
22:8:606:CHL:HBC2	22:8:607:CHL:HHD	1.68	0.73
10:D:121:LEU:HD22	10:D:132:LEU:CD2	2.19	0.73
4:7:78:MET:HE3	26:7:320:LMG:HO5	1.54	0.73
1:1:189:LEU:CD1	24:1:315:XAT:H201	2.17	0.73
7:A:584:CYS:SG	36:A:845:SF4:S2	2.88	0.72
21:A:826:CLA:HBB2	28:A:852:LHG:H242	1.70	0.72
13:G:37:LEU:N	26:G:207:LMG:HO4	1.87	0.72
3:3:288:VAL:CG1	21:A:817:CLA:C5	2.63	0.72
3:3:109:PRO:HB3	3:3:266:LYS:HB3	1.73	0.71
8:B:440:HIS:HE1	21:B:836:CLA:NA	1.88	0.71
6:9:41:PRO:HG2	21:9:601:CLA:HMA3	1.71	0.71
7:A:197:MET:SD	21:A:827:CLA:H122	2.31	0.71
7:A:601:ASN:HD21	34:A:803:CL0:H68	1.54	0.71
6:9:90:THR:HG21	23:9:613:LUT:H401	1.73	0.70
21:1:307:CLA:H3A	28:1:323:LHG:H271	1.73	0.70
10:D:164:VAL:HG12	10:D:164:VAL:O	1.91	0.70
12:F:229:VAL:HG22	12:F:232:ARG:HH22	1.56	0.70
5:8:28:SER:OG	5:8:29:MET:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:811:CLA:HHB	21:B:812:CLA:HMB3	1.74	0.70
4:c:148:LYS:HB3	22:c:607:CHL:HMC	1.72	0.70
21:9:602:CLA:HAB	24:9:614:XAT:H32	1.75	0.69
6:9:82:GLY:CA	6:9:174:MET:HE3	2.23	0.69
12:F:229:VAL:HG22	12:F:232:ARG:NH2	2.08	0.69
21:B:840:CLA:HAC2	25:F:5008:BCR:H322	1.75	0.68
5:8:64:GLN:HE21	21:8:622:CLA:HAA1	1.58	0.68
5:b:126:THR:HG21	22:b:307:CHL:HED1	1.75	0.68
8:B:51:HIS:HB3	21:B:817:CLA:HED3	1.75	0.68
21:A:823:CLA:H101	25:A:850:BCR:H21C	1.76	0.68
22:b:307:CHL:HBC2	22:b:308:CHL:HHH	1.74	0.67
5:b:81:MET:HE3	21:b:311:CLA:HMC3	1.76	0.67
5:8:137:LYS:HE3	22:8:608:CHL:HMC	1.75	0.67
7:A:740:TRP:CE2	7:A:744:LEU:CD1	2.79	0.66
4:c:188:MET:SD	4:c:188:MET:N	2.67	0.66
14:H:124:GLU:HB2	14:H:131:LEU:HD12	1.78	0.66
21:B:825:CLA:HAA1	13:G:66:ARG:HH22	1.61	0.66
21:8:611:CLA:H72	21:8:612:CLA:HBC3	1.77	0.66
21:B:816:CLA:H111	21:B:816:CLA:HBB1	1.78	0.66
1:1:189:LEU:HG	24:1:315:XAT:H201	1.78	0.65
2:2:232:LEU:HD11	31:2:619:3PH:H262	1.78	0.65
21:a:309:CLA:H2	23:a:315:LUT:H382	1.77	0.65
8:B:408:VAL:O	8:B:412:VAL:HG23	1.96	0.65
21:3:409:CLA:HBA1	21:T:603:CLA:H2	1.77	0.65
7:A:678:VAL:HG11	7:A:733:LEU:HD12	1.79	0.65
9:C:77:LEU:HB3	9:C:79:LEU:HD13	1.79	0.65
8:B:525:ALA:HB2	21:B:840:CLA:HMA1	1.78	0.64
1:a:84:LEU:HB3	21:a:304:CLA:HAB	1.80	0.64
7:A:218:ILE:HA	7:A:222:LEU:HD12	1.79	0.64
10:D:121:LEU:HD21	10:D:123:LEU:HD21	1.78	0.64
2:2:169:GLU:HB3	21:2:608:CLA:HMA1	1.78	0.64
21:3:408:CLA:HBB1	21:3:408:CLA:H51	1.80	0.64
3:3:173:THR:HG22	3:3:189:TYR:OH	1.98	0.64
21:8:622:CLA:O1D	12:F:216:ARG:NH1	2.24	0.64
12:F:213:GLN:O	12:F:217:ASN:ND2	2.30	0.64
21:2:603:CLA:HBC1	22:2:606:CHL:HAB	1.79	0.64
8:B:339:LEU:HG	8:B:383:ILE:HG23	1.79	0.64
10:D:121:LEU:CG	10:D:123:LEU:HD21	2.28	0.64
26:1:317:LMG:H311	22:8:601:CHL:HMA2	1.79	0.64
8:B:178:HIS:CE1	21:B:816:CLA:NA	2.66	0.64
5:b:178:TYR:HE2	23:b:317:LUT:H24	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:173:GLY:HA2	4:c:179:PRO:HA	1.80	0.63
5:8:126:THR:HG21	22:8:606:CHL:HED1	1.79	0.63
17:O:64:ILE:HG12	25:O:2004:BCR:HC21	1.81	0.63
4:7:170:GLY:HA2	4:7:181:GLY:HA3	1.78	0.63
1:1:87:ALA:HB2	23:1:314:LUT:H15	1.79	0.63
7:A:448:LEU:HB3	7:A:541:PHE:HB2	1.79	0.63
21:A:834:CLA:HBB2	16:L:109:LEU:HD13	1.79	0.63
21:A:841:CLA:H61	25:F:5004:BCR:H14C	1.81	0.63
25:B:805:BCR:H271	35:B:845:PQN:H142	1.81	0.63
2:2:146:LYS:HG3	2:2:147:THR:HG23	1.81	0.63
4:7:145:VAL:HG13	22:7:309:CHL:C4B	2.16	0.63
22:c:605:CHL:HBC2	22:c:606:CHL:HHD	1.80	0.63
7:A:740:TRP:CE2	7:A:744:LEU:HD12	2.33	0.63
3:3:146:HIS:HB3	3:3:277:MET:HE1	1.81	0.63
7:A:740:TRP:HB2	21:A:830:CLA:HBB1	1.80	0.62
5:b:134:VAL:HG11	22:b:309:CHL:HMA3	1.81	0.62
4:c:84:GLN:HE21	4:c:149:ARG:HD2	1.63	0.62
1:a:52:GLY:HA3	1:a:178:LEU:HD23	1.81	0.62
25:B:805:BCR:H363	21:B:807:CLA:H72	1.81	0.62
7:A:396:TRP:CD1	21:A:830:CLA:HAB	2.35	0.62
20:T:242:THR:HB	20:T:247:LEU:HD12	1.80	0.62
10:D:121:LEU:CG	10:D:123:LEU:CD2	2.77	0.62
5:b:169:PRO:HB3	22:b:309:CHL:HBC2	1.81	0.62
5:8:134:VAL:HG11	22:8:608:CHL:HMA3	1.82	0.62
21:A:824:CLA:CGD	19:K:74:ALA:HB3	2.29	0.62
16:L:93:GLU:HG3	21:L:303:CLA:HMA3	1.82	0.62
21:K:203:CLA:HBB1	25:K:205:BCR:H352	1.81	0.62
7:A:740:TRP:NE1	7:A:744:LEU:CD1	2.62	0.61
1:1:84:LEU:HB3	21:1:303:CLA:HAB	1.82	0.61
4:7:131:LEU:HB3	5:8:248:GLU:HG2	1.82	0.61
6:9:170:GLY:O	6:9:174:MET:HG3	2.00	0.61
16:L:147:GLN:NE2	18:I:105:GLN:O	2.30	0.61
20:T:187:TRP:HD1	21:T:608:CLA:HMD3	1.64	0.61
7:A:708:ARG:HB2	12:F:173:ARG:HH21	1.63	0.61
7:A:440:HIS:CE1	21:A:833:CLA:NA	2.68	0.61
5:8:64:GLN:NE2	21:8:622:CLA:O2A	2.34	0.61
21:A:824:CLA:H2A	19:K:74:ALA:HB3	1.82	0.61
14:H:124:GLU:HB2	14:H:131:LEU:CD1	2.30	0.61
4:7:100:ILE:HG12	4:7:116:TRP:HB2	1.81	0.61
7:A:303:VAL:HA	25:A:846:BCR:H352	1.82	0.61
7:A:605:ILE:HD11	34:A:803:CL0:H38	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:729:ALA:HA	28:A:853:LHG:H352	1.83	0.61
21:B:811:CLA:H42	18:I:84:PHE:CE2	2.36	0.61
1:a:158:PHE:HE2	21:a:307:CLA:NC	1.99	0.60
21:c:604:CLA:C4B	25:c:617:BCR:H281	2.28	0.60
21:B:844:CLA:HBB1	21:B:844:CLA:H71	1.83	0.60
1:1:102:ASP:HA	1:1:105:LEU:HD23	1.84	0.60
3:3:288:VAL:HG21	21:A:817:CLA:H2	1.82	0.60
7:A:180:HIS:HE1	21:A:812:CLA:NC	1.98	0.60
8:B:90:HIS:CD2	21:B:812:CLA:NA	2.70	0.60
1:a:76:LEU:O	1:a:79:CYS:SG	2.57	0.60
21:B:820:CLA:H11	21:G:205:CLA:HED1	1.83	0.60
21:B:844:CLA:H151	25:L:309:BCR:H15C	1.83	0.60
20:T:193:VAL:HG21	23:T:615:LUT:H401	1.82	0.60
20:T:334:VAL:HG21	21:T:612:CLA:HAC2	1.83	0.60
1:a:143:ASN:HA	1:a:151:ARG:HH22	1.65	0.60
14:H:91:VAL:HG11	16:L:136:LEU:HB2	1.83	0.60
1:a:206:LEU:HD13	23:a:315:LUT:H22	1.84	0.60
4:c:63:GLY:HA3	4:c:207:ARG:HH12	1.67	0.60
21:B:842:CLA:HAB	35:B:845:PQN:H141	1.84	0.59
21:A:804:CLA:HBB1	21:A:843:CLA:C4B	2.30	0.59
2:2:72:GLY:HA3	2:2:78:LEU:HD13	1.85	0.59
3:3:183:ILE:HG22	3:3:186:ALA:H	1.67	0.59
21:7:304:CLA:H72	24:7:318:XAT:H10	1.84	0.59
7:A:391:PHE:O	7:A:395:MET:HB2	2.02	0.59
5:8:169:PRO:HD3	22:8:608:CHL:HMD2	1.82	0.59
28:1:323:LHG:H282	21:G:201:CLA:H43	1.85	0.59
12:F:211:SER:HB2	25:F:5008:BCR:H391	1.83	0.59
18:I:69:THR:HG22	18:I:70:GLU:HG3	1.85	0.59
32:7:301:DGD:HE5	26:A:801:LMG:HC1	1.85	0.59
19:K:85:LEU:HD23	19:K:86:GLN:H	1.68	0.59
3:3:244:TYR:HE2	3:3:266:LYS:HG2	1.68	0.59
4:7:211:LEU:HD13	21:7:314:CLA:H102	1.84	0.59
7:A:296:HIS:HE1	21:A:819:CLA:ND	2.01	0.59
7:A:421:ASN:OD1	7:A:422:ASN:ND2	2.36	0.59
20:T:317:LYS:HD3	21:T:611:CLA:HBD	1.84	0.59
22:9:606:CHL:HED1	27:9:616:LMU:H6D	1.85	0.59
21:B:818:CLA:H3A	25:B:847:BCR:H392	1.85	0.59
16:L:62:GLU:HG3	16:L:67:SER:HB3	1.85	0.58
1:a:194:GLN:NE2	1:a:200:LYS:O	2.36	0.58
19:K:48:ASN:ND2	21:K:203:CLA:OBD	2.35	0.58
21:2:603:CLA:HED2	28:H:202:LHG:H191	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:207:ILE:O	6:9:211:LEU:HB2	2.03	0.58
7:A:684:MET:HE1	21:A:804:CLA:C4A	2.33	0.58
8:B:458:PRO:HB3	8:B:518:PHE:HB2	1.86	0.58
21:A:809:CLA:H2A	21:A:811:CLA:HED1	1.84	0.58
25:3:418:BCR:H391	25:A:846:BCR:HC42	1.85	0.58
22:9:606:CHL:HMB2	27:9:616:LMU:H91	1.86	0.58
21:B:804:CLA:C4B	21:B:807:CLA:HBB1	2.33	0.58
5:b:210:GLN:HE21	21:b:314:CLA:C4D	1.96	0.58
1:1:176:LYS:HD3	21:1:310:CLA:HBD	1.84	0.58
21:A:823:CLA:H71	25:A:850:BCR:H19C	1.84	0.58
18:I:92:LEU:HD12	29:I:201:PTY:C22	2.31	0.58
7:A:304:LEU:HD21	21:A:829:CLA:H201	1.85	0.58
21:B:810:CLA:H151	21:B:831:CLA:HBB2	1.86	0.58
8:B:106:THR:HG21	14:H:118:PRO:HG3	1.85	0.58
10:D:73:PRO:HB3	10:D:114:MET:HA	1.84	0.58
8:B:713:HIS:HE1	21:B:843:CLA:ND	2.02	0.57
21:8:611:CLA:C1C	28:8:620:LHG:HC61	2.19	0.57
6:9:195:LEU:HB2	23:9:613:LUT:H21	1.86	0.57
10:D:99:PRO:O	10:D:116:LYS:NZ	2.37	0.57
4:c:90:ALA:HB1	4:c:206:GLY:HA3	1.87	0.57
3:3:215:LEU:HD21	30:3:422:SQD:H82	1.87	0.57
3:3:235:LEU:HA	3:3:248:PRO:HD2	1.85	0.57
7:A:204:GLY:HA3	21:A:815:CLA:HBB1	1.85	0.57
21:B:834:CLA:H2	25:F:5008:BCR:H372	1.86	0.57
21:2:603:CLA:H62	30:2:618:SQD:H152	1.87	0.57
3:3:289:ILE:HG23	3:3:290:THR:HG23	1.86	0.57
21:A:824:CLA:H2A	19:K:74:ALA:CB	2.34	0.57
7:A:363:LEU:HD21	21:A:821:CLA:H71	1.87	0.57
8:B:359:TYR:OH	21:B:831:CLA:OBD	2.22	0.57
21:A:824:CLA:H121	21:K:202:CLA:HBC1	1.85	0.57
31:2:619:3PH:H352	23:B:801:LUT:H30	1.87	0.57
1:1:189:LEU:HD12	24:1:315:XAT:H202	1.84	0.57
7:A:429:ARG:NH2	16:L:47:GLN:OE1	2.38	0.57
7:A:539:HIS:HE1	7:A:605:ILE:HG22	1.70	0.57
31:2:619:3PH:H231	31:2:619:3PH:H322	1.86	0.57
7:A:366:ILE:HG21	21:A:821:CLA:H201	1.87	0.57
21:A:808:CLA:HED3	21:A:832:CLA:H61	1.87	0.57
21:A:826:CLA:H12	25:A:849:BCR:H351	1.87	0.57
5:b:34:LEU:HD13	21:c:601:CLA:HMA3	1.86	0.56
7:A:44:ASN:OD1	7:A:714:GLN:NE2	2.39	0.56
7:A:353:LEU:HD11	21:A:832:CLA:HBB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:152:PHE:HB3	22:T:602:CHL:HMD1	1.87	0.56
22:7:303:CHL:H52	28:7:321:LHG:H142	1.87	0.56
22:8:606:CHL:HBA1	25:8:618:BCR:H19C	1.88	0.56
7:A:338:HIS:CD2	21:A:826:CLA:ND	2.73	0.56
21:A:807:CLA:H72	25:A:848:BCR:H373	1.87	0.56
8:B:659:ALA:HB1	21:B:807:CLA:HAB	1.87	0.56
10:D:160:PRO:HB2	10:D:163:GLY:H	1.71	0.56
17:O:53:ILE:O	17:O:56:VAL:HG22	2.05	0.56
20:T:257:PHE:HD1	22:T:601:CHL:HBD	1.71	0.56
6:9:119:GLN:HE21	21:9:605:CLA:C4D	1.97	0.56
4:c:73:SER:HB2	4:c:79:ARG:HA	1.86	0.56
20:T:326:MET:SD	22:T:602:CHL:HHC	2.45	0.56
8:B:423:LEU:HD13	8:B:533:LEU:HA	1.86	0.56
1:1:189:LEU:CG	24:1:315:XAT:H201	2.34	0.56
14:H:53:GLY:HA3	16:L:58:VAL:HG11	1.86	0.56
14:H:61:ASP:O	14:H:63:LYS:NZ	2.38	0.56
17:O:110:LEU:O	17:O:114:MET:HG3	2.06	0.56
1:1:128:LEU:HD22	26:G:207:LMG:H302	1.88	0.56
4:7:244:ALA:HA	4:7:250:ILE:HG13	1.88	0.56
12:F:74:PRO:CB	12:F:129:LEU:CD2	2.83	0.56
1:1:57:ASP:HB2	21:1:301:CLA:HBA2	1.87	0.56
2:2:150:THR:HG23	2:2:150:THR:O	2.05	0.56
21:8:604:CLA:C1	12:F:209:LEU:CG	2.78	0.56
21:A:824:CLA:HBB1	21:A:825:CLA:H93	1.88	0.56
21:B:804:CLA:C4B	21:B:807:CLA:CBB	2.82	0.56
15:J:21:PHE:HA	21:J:5002:CLA:HBB2	1.88	0.56
1:1:76:LEU:HA	1:1:79:CYS:SG	2.45	0.56
3:3:169:ILE:HD13	21:3:413:CLA:C1C	2.36	0.56
21:T:609:CLA:H12	23:T:615:LUT:H23	1.86	0.56
8:B:226:PHE:HA	8:B:231:TRP:HE1	1.70	0.55
12:F:164:VAL:HG13	21:F:5006:CLA:HAA1	1.87	0.55
14:H:81:VAL:HG13	16:L:179:ALA:HB1	1.87	0.55
8:B:182:GLY:HA2	8:B:186:VAL:HG12	1.87	0.55
28:b:303:LHG:H252	28:b:303:LHG:HC81	1.87	0.55
3:3:97:ASP:HB2	3:3:116:PRO:HA	1.87	0.55
4:7:242:THR:HG23	4:7:244:ALA:H	1.71	0.55
21:B:831:CLA:H142	25:B:847:BCR:H372	1.87	0.55
20:T:257:PHE:CD1	22:T:601:CHL:HBD	2.42	0.55
7:A:212:ALA:HB2	25:A:847:BCR:H16C	1.88	0.55
4:c:142:PHE:HE2	22:c:605:CHL:HHB	1.72	0.55
4:c:233:ASP:HB3	4:c:241:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:158:PHE:N	21:2:608:CLA:OBD	2.40	0.55
5:8:102:PRO:HG3	5:8:110:VAL:HG11	1.89	0.55
7:A:515:VAL:HG23	7:A:522:ALA:HB3	1.88	0.55
21:B:828:CLA:HMA1	25:B:849:BCR:H14C	1.87	0.55
13:G:97:GLU:N	13:G:97:GLU:OE2	2.40	0.55
22:7:308:CHL:HBD	32:8:602:DGD:HG32	1.87	0.55
8:B:352:HIS:ND1	21:B:821:CLA:OBD	2.40	0.55
1:a:135:MET:HE1	21:a:308:CLA:HAB	1.89	0.55
1:1:42:GLU:O	1:1:55:ASN:ND2	2.37	0.55
2:2:256:GLU:OE2	18:I:106:LYS:NZ	2.40	0.55
7:A:245:LEU:HD21	21:A:818:CLA:HAC1	1.89	0.55
7:A:310:HIS:HB3	25:A:846:BCR:H373	1.89	0.55
25:B:852:BCR:H352	15:J:36:PRO:HG2	1.89	0.55
3:3:139:LEU:HD22	22:3:401:CHL:H12	1.89	0.54
5:8:198:ARG:HA	5:8:201:MET:HE2	1.89	0.54
7:A:37:ARG:H	7:A:37:ARG:HD2	1.70	0.54
12:F:230:SER:O	12:F:232:ARG:NH2	2.39	0.54
28:a:318:LHG:HC42	25:b:319:BCR:H312	1.89	0.54
7:A:91:MET:HE1	21:A:810:CLA:H2A	1.88	0.54
8:B:479:LEU:HA	8:B:487:TYR:HB2	1.89	0.54
21:B:829:CLA:HBB1	21:B:837:CLA:HMA2	1.88	0.54
11:E:98:VAL:HG22	11:E:113:ASN:HB3	1.88	0.54
5:b:187:ASP:N	5:b:187:ASP:OD1	2.39	0.54
7:A:418:ASP:OD1	7:A:421:ASN:ND2	2.40	0.54
21:A:833:CLA:H51	21:L:304:CLA:H43	1.88	0.54
8:B:139:SER:HB3	25:B:847:BCR:H401	1.89	0.54
7:A:622:VAL:HG23	7:A:627:VAL:HG22	1.89	0.54
8:B:137:TYR:HB3	18:I:73:PRO:HG2	1.90	0.54
21:B:818:CLA:H111	25:B:847:BCR:H363	1.90	0.54
16:L:112:LEU:HD12	16:L:122:VAL:HG21	1.89	0.54
4:c:89:HIS:HB3	4:c:210:MET:HE1	1.90	0.54
21:3:407:CLA:H2A	21:3:407:CLA:HED2	1.90	0.54
21:3:407:CLA:H203	25:A:848:BCR:H321	1.89	0.54
8:B:229:GLY:HA3	13:G:126:LEU:HB3	1.87	0.54
8:B:175:ARG:HB2	21:B:817:CLA:HBC2	1.90	0.54
1:1:187:ALA:HB2	23:1:314:LUT:H192	1.90	0.54
2:2:251:LEU:HB2	2:2:258:TRP:HB3	1.88	0.54
8:B:143:LEU:HD11	25:B:847:BCR:H292	1.90	0.54
16:L:138:LEU:HD13	25:I:202:BCR:H24C	1.90	0.54
3:3:153:GLY:HA2	24:3:416:XAT:H181	1.89	0.54
25:3:418:BCR:H17C	21:A:817:CLA:H93	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:232:ASN:HB3	21:8:613:CLA:HED1	1.89	0.54
7:A:365:ILE:HD12	7:A:395:MET:HE3	1.90	0.54
7:A:598:TRP:CH2	21:B:804:CLA:HAB	2.43	0.54
21:A:804:CLA:HMD3	8:B:534:ILE:HD12	1.90	0.54
21:A:810:CLA:H13	21:A:856:CLA:H51	1.90	0.54
8:B:269:LEU:HD21	8:B:356:LEU:HB3	1.90	0.54
3:3:310:LEU:HD22	21:3:411:CLA:H2	1.89	0.53
21:c:608:CLA:HBA1	29:c:619:PTY:H321	1.90	0.53
7:A:151:SER:HB3	7:A:213:TRP:HH2	1.73	0.53
37:A:857:4RF:H66	29:L:308:PTY:HC31	1.90	0.53
21:A:843:CLA:HBC2	8:B:586:ASN:HB2	1.89	0.53
12:F:73:THR:C	12:F:129:LEU:HD22	2.34	0.53
12:F:92:LEU:HD21	12:F:112:THR:HG22	1.90	0.53
21:1:304:CLA:HAA1	25:1:316:BCR:H23C	1.91	0.53
4:7:95:LEU:HD13	21:7:306:CLA:HBB2	1.89	0.53
13:G:117:LEU:HG	25:G:202:BCR:H371	1.90	0.53
21:1:310:CLA:HAB	23:1:314:LUT:H12	1.90	0.53
22:2:601:CHL:H42	6:9:125:LEU:HD22	1.90	0.53
3:3:176:ASP:HB2	3:3:179:ARG:HG3	1.90	0.53
8:B:87:PRO:HB2	8:B:117:ALA:HB3	1.90	0.53
8:B:320:HIS:CD2	21:B:826:CLA:ND	2.76	0.53
20:T:154:TRP:HE3	22:T:602:CHL:HMD2	1.72	0.53
4:7:90:ALA:HB1	4:7:206:GLY:HA3	1.91	0.53
25:A:851:BCR:H291	25:F:5004:BCR:H17C	1.90	0.53
8:B:340:ALA:HB2	25:B:849:BCR:H372	1.90	0.53
2:2:229:LEU:HD12	22:2:601:CHL:H3A	1.91	0.53
2:2:233:PRO:HD3	22:2:601:CHL:HMA2	1.90	0.53
7:A:479:LEU:HD21	37:A:857:4RF:H1	1.90	0.53
14:H:105:LYS:HE3	28:H:202:LHG:H241	1.89	0.53
4:c:142:PHE:CE2	22:c:605:CHL:HMA1	2.44	0.53
4:c:201:LYS:HD3	21:c:611:CLA:HBD	1.91	0.53
6:9:82:GLY:N	6:9:174:MET:CE	2.72	0.53
8:B:339:LEU:HB3	8:B:387:ALA:HB2	1.91	0.53
21:A:832:CLA:H143	28:A:853:LHG:H383	1.90	0.53
21:B:829:CLA:H112	25:B:849:BCR:H17C	1.91	0.53
19:K:65:GLY:HA2	19:K:72:LYS:HE3	1.91	0.53
3:3:182:VAL:HG21	24:3:416:XAT:H172	1.91	0.53
5:8:160:GLN:HG3	5:8:172:ILE:HG23	1.90	0.53
7:A:86:ILE:HG13	7:A:170:ALA:HB1	1.91	0.53
7:A:686:LEU:HB3	8:B:666:ILE:HD12	1.90	0.53
10:D:68:PRO:HB3	14:H:44:ASP:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:149:ASN:HB3	29:J:5001:PTY:H112	1.90	0.53
20:T:180:ALA:O	20:T:184:HIS:HB2	2.09	0.53
7:A:219:HIS:HE1	21:A:817:CLA:ND	2.06	0.52
7:A:473:SER:HB2	7:A:640:ASN:HD22	1.74	0.52
21:A:826:CLA:H11	25:A:849:BCR:H362	1.91	0.52
21:B:826:CLA:HAB	21:B:833:CLA:HMD2	1.90	0.52
10:D:93:VAL:HG22	10:D:122:LYS:HG2	1.91	0.52
13:G:129:SER:HA	26:G:207:LMG:HC91	1.91	0.52
29:c:619:PTY:H111	29:c:619:PTY:HC32	1.90	0.52
1:1:76:LEU:O	1:1:79:CYS:SG	2.59	0.52
5:8:64:GLN:NE2	21:8:622:CLA:C1	2.73	0.52
7:A:685:PHE:HA	35:A:844:PQN:H9	1.91	0.52
8:B:508:SER:HA	8:B:511:LEU:HD21	1.91	0.52
16:L:128:ALA:HB2	16:L:189:VAL:HG11	1.92	0.52
21:a:304:CLA:HMA2	21:a:305:CLA:HBC3	1.90	0.52
4:c:179:PRO:HG3	22:c:607:CHL:HHD	1.90	0.52
7:A:441:LEU:HG	7:A:548:LEU:HB2	1.92	0.52
8:B:490:GLY:HA2	8:B:493:LEU:HD12	1.90	0.52
12:F:74:PRO:HG3	12:F:129:LEU:HD21	1.89	0.52
21:1:321:CLA:H71	21:B:826:CLA:HBB2	1.92	0.52
6:9:185:LEU:HD11	25:B:847:BCR:H343	1.90	0.52
1:1:137:VAL:HG12	13:G:58:VAL:HG21	1.91	0.52
4:c:242:THR:OG1	4:c:243:PHE:N	2.43	0.52
1:1:100:TRP:O	24:1:315:XAT:O23	2.27	0.52
4:7:73:SER:HB2	4:7:79:ARG:HA	1.90	0.52
22:7:309:CHL:HMA1	25:7:319:BCR:H361	1.92	0.52
8:B:463:TRP:HZ2	21:F:5007:CLA:H12	1.74	0.52
5:8:195:LYS:HD3	28:8:620:LHG:HC42	1.92	0.52
8:B:601:THR:HG21	8:B:610:PHE:HB2	1.92	0.52
4:c:65:TYR:HB2	21:c:602:CLA:HMD1	1.90	0.52
22:7:309:CHL:H12	23:7:317:LUT:H183	1.91	0.52
7:A:216:HIS:O	7:A:220:VAL:HB	2.10	0.52
21:A:831:CLA:H12	25:A:848:BCR:H24C	1.92	0.52
4:7:45:PRO:HG2	28:7:321:LHG:HC11	1.92	0.52
21:7:304:CLA:HBC1	28:7:321:LHG:H281	1.91	0.52
5:8:159:SER:O	5:8:162:LYS:NZ	2.41	0.52
8:B:442:ASP:OD1	8:B:617:LEU:N	2.42	0.52
10:D:160:PRO:HG3	10:D:165:TYR:HA	1.91	0.52
14:H:99:ILE:HG23	18:I:86:PRO:HB2	1.91	0.52
28:7:321:LHG:H271	28:7:321:LHG:H101	1.91	0.51
21:B:817:CLA:H102	21:B:822:CLA:H71	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:805:CLA:H142	21:A:805:CLA:HED1	1.91	0.51
7:A:247:GLN:NE2	7:A:257:PHE:O	2.44	0.51
7:A:658:ILE:HD12	8:B:622:ARG:HG3	1.92	0.51
7:A:704:HIS:HE1	21:A:841:CLA:ND	2.08	0.51
7:A:719:SER:HB3	7:A:722:GLN:HB2	1.92	0.51
21:A:822:CLA:HBB1	25:A:846:BCR:H16C	1.91	0.51
4:7:173:GLY:HA2	4:7:179:PRO:HA	1.91	0.51
7:A:222:LEU:HD13	7:A:275:PHE:HB2	1.93	0.51
21:A:811:CLA:H91	21:A:811:CLA:H142	1.91	0.51
12:F:194:VAL:HB	26:F:5009:LMG:HC91	1.92	0.51
17:O:107:HIS:CE1	21:O:2001:CLA:ND	2.78	0.51
1:a:56:PHE:HE2	24:a:316:XAT:H173	1.74	0.51
18:I:92:LEU:HD12	29:I:201:PTY:C21	2.40	0.51
3:3:264:LYS:NZ	21:3:410:CLA:O1A	2.44	0.51
21:A:810:CLA:H11	25:J:5003:BCR:H383	1.92	0.51
8:B:103:GLU:HG2	14:H:118:PRO:HA	1.92	0.51
16:L:77:ASN:HA	16:L:82:ARG:HH11	1.75	0.51
1:a:36:ASN:ND2	1:a:41:SER:HG	2.09	0.51
5:b:29:MET:HE3	5:b:44:LYS:HA	1.92	0.51
4:c:148:LYS:HE2	4:c:159:GLN:HG2	1.92	0.51
6:9:195:LEU:HD22	23:9:613:LUT:H172	1.93	0.51
13:G:79:LYS:HE3	13:G:90:GLN:HB3	1.92	0.51
16:L:51:PRO:HA	16:L:61:LEU:HA	1.93	0.51
16:L:77:ASN:HB3	21:L:303:CLA:HAC1	1.93	0.51
18:I:103:TYR:OH	29:I:201:PTY:O13	2.28	0.51
21:A:808:CLA:H2A	21:A:808:CLA:HED2	1.93	0.51
1:a:36:ASN:ND2	1:a:41:SER:OG	2.40	0.51
30:2:618:SQD:H272	14:H:90:PHE:HB2	1.92	0.51
30:3:422:SQD:H242	7:A:179:PHE:HE1	1.76	0.51
8:B:425:TRP:CE2	21:B:834:CLA:HAB	2.46	0.51
21:B:804:CLA:H151	21:B:814:CLA:HBC3	1.93	0.51
21:B:809:CLA:H12	21:B:817:CLA:H11	1.93	0.51
26:G:207:LMG:H312	26:G:207:LMG:H171	1.92	0.51
21:a:311:CLA:HAB	23:a:315:LUT:H12	1.93	0.51
20:T:154:TRP:HZ3	22:T:602:CHL:HBC2	1.76	0.51
28:F:5001:LHG:HC42	31:F:5002:3PH:H2	1.93	0.51
15:J:12:PRO:HB3	25:J:5004:BCR:H391	1.93	0.51
4:7:157:GLY:HA2	4:7:172:LYS:HG3	1.92	0.50
4:7:169:ASP:OD2	1:a:63:LYS:NZ	2.43	0.50
5:8:137:LYS:HD2	5:8:148:GLN:HE21	1.77	0.50
5:8:187:ASP:OD1	5:8:187:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:811:CLA:HBB1	25:J:5003:BCR:HC8	1.93	0.50
2:2:45:MET:HG3	2:2:50:ALA:HB3	1.94	0.50
22:3:401:CHL:H91	21:3:407:CLA:H193	1.92	0.50
21:A:810:CLA:H71	21:A:832:CLA:H162	1.94	0.50
16:L:50:GLN:NE2	17:O:42:ASN:OD1	2.44	0.50
17:O:104:VAL:O	17:O:108:THR:HG23	2.12	0.50
5:b:102:PRO:HG3	5:b:110:VAL:HG21	1.93	0.50
21:c:614:CLA:HAC1	20:T:248:LEU:HD23	1.93	0.50
20:T:191:GLY:HA2	24:T:616:XAT:H181	1.93	0.50
2:2:200:SER:OG	23:2:614:LUT:O3	2.29	0.50
21:2:608:CLA:HMD3	23:2:616:LUT:H373	1.92	0.50
5:8:88:LEU:O	5:8:92:ILE:N	2.36	0.50
6:9:82:GLY:N	6:9:174:MET:HE2	2.26	0.50
20:T:223:SER:O	20:T:223:SER:OG	2.29	0.50
28:1:322:LHG:H242	28:1:322:LHG:H101	1.93	0.50
7:A:200:HIS:HE1	21:A:814:CLA:NA	2.05	0.50
8:B:62:THR:HG23	8:B:143:LEU:HD13	1.93	0.50
18:I:103:TYR:CE2	29:I:201:PTY:HC52	2.47	0.50
21:1:301:CLA:H13	24:1:315:XAT:H193	1.94	0.50
7:A:203:ALA:HB2	7:A:309:GLY:HA3	1.92	0.50
7:A:532:ASP:OD2	7:A:613:LYS:NZ	2.42	0.50
21:A:812:CLA:H72	21:A:815:CLA:H18	1.94	0.50
21:A:820:CLA:HAC1	21:A:836:CLA:H42	1.93	0.50
8:B:561:ASP:OD1	9:C:52:LYS:NZ	2.45	0.50
4:c:144:TRP:HE1	22:c:607:CHL:HBB1	1.76	0.50
4:c:184:ASP:OD1	23:c:615:LUT:O3	2.30	0.50
6:9:212:THR:HG22	8:B:227:TRP:HD1	1.77	0.50
7:A:462:MET:HB2	7:A:471:MET:HG3	1.92	0.50
4:c:46:LEU:HD12	20:T:275:GLN:HE22	1.77	0.50
24:9:614:XAT:H363	21:B:816:CLA:H121	1.92	0.50
7:A:578:PRO:HA	7:A:582:GLY:HA2	1.92	0.50
12:F:130:CYS:HB3	12:F:136:PRO:HA	1.94	0.50
13:G:48:THR:HA	13:G:118:GLY:HA3	1.94	0.50
4:7:146:GLU:HA	4:7:149:ARG:HG2	1.94	0.50
21:A:804:CLA:H3A	21:A:804:CLA:C2	2.42	0.50
8:B:24:TYR:O	8:B:28:THR:OG1	2.27	0.50
21:H:203:CLA:HBB1	21:L:303:CLA:HED1	1.94	0.50
15:J:8:LEU:HD12	15:J:13:VAL:HG11	1.94	0.50
7:A:157:LEU:HD23	27:A:855:LMU:H21	1.93	0.49
21:A:840:CLA:H11	25:A:850:BCR:H14C	1.94	0.49
10:D:82:LEU:HD12	10:D:86:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:69:PRO:HG3	17:O:44:LEU:HD22	1.93	0.49
1:a:59:LEU:HD21	24:a:316:XAT:H41	1.93	0.49
4:c:154:ARG:HH22	29:c:620:PTY:H321	1.76	0.49
20:T:330:LEU:HD22	24:T:616:XAT:H403	1.94	0.49
1:1:206:LEU:HD13	23:1:314:LUT:H21	1.94	0.49
3:3:147:ALA:HB1	3:3:273:GLY:HA3	1.94	0.49
21:8:622:CLA:HBA2	21:8:622:CLA:HBD	1.94	0.49
7:A:407:ALA:HB2	7:A:592:VAL:HG11	1.94	0.49
21:A:815:CLA:HAA2	21:A:827:CLA:H51	1.94	0.49
7:A:45:THR:HB	7:A:716:ARG:HG3	1.93	0.49
21:A:841:CLA:HBB2	12:F:172:GLY:HA3	1.93	0.49
10:D:159:HIS:CG	10:D:160:PRO:HD2	2.48	0.49
5:b:120:PHE:CD1	22:b:308:CHL:HBC2	2.47	0.49
5:b:153:THR:HG22	22:b:302:CHL:HMD3	1.94	0.49
20:T:160:ALA:HB2	22:T:602:CHL:HBA1	1.94	0.49
20:T:344:PHE:HD1	20:T:347:LEU:HD12	1.77	0.49
7:A:146:GLN:HB3	7:A:377:TYR:HB3	1.94	0.49
7:A:322:ILE:HG21	21:A:827:CLA:HAC1	1.93	0.49
21:B:812:CLA:HAB	21:B:813:CLA:HAA2	1.94	0.49
21:a:302:CLA:HAC2	22:b:302:CHL:HBB2	1.94	0.49
2:2:69:LEU:HB3	2:2:254:TRP:HE1	1.76	0.49
6:9:147:ILE:O	6:9:149:SER:N	2.46	0.49
21:A:828:CLA:H2A	21:A:828:CLA:HED2	1.95	0.49
8:B:398:ASP:HA	10:D:190:ILE:HB	1.93	0.49
1:a:171:GLU:HA	1:a:174:LYS:HE3	1.93	0.49
1:a:181:GLY:O	1:a:185:MET:HG3	2.12	0.49
19:K:68:PRO:HB3	19:K:74:ALA:HB2	1.95	0.49
21:3:412:CLA:HAB	21:T:606:CLA:CBB	2.37	0.49
4:7:92:TRP:CE2	22:7:309:CHL:HED2	2.48	0.49
26:F:5009:LMG:H132	15:J:8:LEU:HG	1.95	0.49
13:G:79:LYS:HG3	13:G:80:THR:HG23	1.93	0.49
21:2:603:CLA:H92	21:2:603:CLA:H41	1.93	0.49
4:7:90:ALA:O	4:7:94:MET:HG3	2.12	0.49
4:7:134:LEU:HD23	22:7:307:CHL:HBC3	1.94	0.49
5:8:191:LEU:HD11	5:8:195:LYS:HE3	1.95	0.49
7:A:128:ASN:HB3	7:A:136:GLN:HB2	1.94	0.49
8:B:83:ILE:O	14:H:132:ARG:NH1	2.46	0.49
21:B:844:CLA:H18	16:L:102:LEU:HD11	1.95	0.49
21:1:302:CLA:HED1	25:B:848:BCR:H313	1.95	0.49
3:3:193:TRP:NE1	21:3:404:CLA:OBD	2.42	0.49
21:3:406:CLA:H43	25:3:419:BCR:H17C	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:121:LYS:O	4:7:125:LYS:NZ	2.46	0.49
13:G:86:PHE:HA	13:G:89:LEU:HD12	1.95	0.49
3:3:108:LEU:HD12	22:3:401:CHL:HED3	1.95	0.49
3:3:196:PRO:HA	3:3:199:LEU:HD12	1.95	0.49
22:3:401:CHL:H202	25:A:847:BCR:H401	1.95	0.49
4:7:139:LEU:O	21:7:310:CLA:CBB	2.59	0.49
5:8:88:LEU:HD21	5:8:207:PHE:CZ	2.48	0.49
5:8:205:LEU:HD22	24:8:617:XAT:H403	1.94	0.49
8:B:433:HIS:O	8:B:437:LEU:HD12	2.13	0.49
9:C:15:THR:O	9:C:19:ARG:NE	2.45	0.49
17:O:49:ILE:HA	23:O:2005:LUT:H42	1.94	0.49
2:2:71:LEU:O	2:2:77:ARG:NH1	2.45	0.48
21:3:407:CLA:H192	25:A:848:BCR:H311	1.95	0.48
5:8:64:GLN:NE2	21:8:622:CLA:HAA1	2.26	0.48
7:A:87:TRP:HA	21:A:809:CLA:HBB2	1.94	0.48
21:A:828:CLA:CAD	21:A:838:CLA:HBB1	2.42	0.48
25:A:846:BCR:H353	25:K:205:BCR:HC32	1.94	0.48
21:B:821:CLA:H161	21:G:205:CLA:HMA2	1.95	0.48
13:G:100:SER:OG	13:G:104:SER:O	2.31	0.48
1:a:200:LYS:NZ	1:a:208:ASP:OD2	2.43	0.48
4:c:121:LYS:O	4:c:125:LYS:NZ	2.38	0.48
8:B:617:LEU:HD21	21:B:806:CLA:H171	1.94	0.48
4:c:179:PRO:HD3	22:c:607:CHL:HMD2	1.95	0.48
4:7:246:ASN:ND2	21:7:314:CLA:OBD	2.46	0.48
22:7:307:CHL:HBA1	22:7:307:CHL:HMA2	1.93	0.48
6:9:82:GLY:CA	6:9:174:MET:CE	2.92	0.48
34:A:803:CL0:H51	34:A:803:CL0:H58	1.57	0.48
9:C:81:TYR:HB3	10:D:83:LEU:HD12	1.95	0.48
7:A:615:GLN:OE1	7:A:653:GLN:NE2	2.46	0.48
21:B:844:CLA:H93	25:I:202:BCR:H21C	1.96	0.48
1:1:217:ASN:HA	21:1:311:CLA:HAA1	1.96	0.48
3:3:218:TYR:HE2	30:3:422:SQD:H1	1.79	0.48
21:7:306:CLA:C4B	25:7:319:BCR:H281	2.23	0.48
6:9:82:GLY:HA2	6:9:174:MET:HE3	1.93	0.48
7:A:399:GLY:HA3	7:A:603:LEU:HD11	1.96	0.48
7:A:590:ASP:HA	7:A:593:PHE:HB3	1.94	0.48
8:B:654:GLY:HA3	8:B:721:THR:HB	1.96	0.48
21:B:819:CLA:H2	25:G:202:BCR:HC32	1.94	0.48
21:b:305:CLA:HED2	21:b:305:CLA:H2A	1.96	0.48
20:T:251:MET:HB3	20:T:251:MET:HE3	1.77	0.48
21:2:613:CLA:H61	21:2:613:CLA:H2	1.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:77:HIS:ND1	21:A:815:CLA:OBD	2.40	0.48
34:A:803:CL0:H2	21:B:806:CLA:NC	2.28	0.48
21:B:810:CLA:H43	32:B:850:DGD:HB61	1.95	0.48
9:C:25:VAL:HG11	9:C:48:CYS:HB2	1.95	0.48
20:T:345:GLN:NE2	20:T:349:ASP:OD1	2.46	0.48
21:3:406:CLA:H42	23:3:415:LUT:H27	1.96	0.48
21:A:835:CLA:HMC2	21:B:807:CLA:H111	1.96	0.48
21:B:831:CLA:H172	25:B:847:BCR:H362	1.96	0.48
9:C:21:CYS:HB2	36:C:101:SF4:S4	2.54	0.48
21:1:303:CLA:HMA2	21:1:304:CLA:HBC3	1.94	0.48
2:2:47:TYR:OH	2:2:240:LYS:NZ	2.47	0.48
22:2:601:CHL:HAB	21:2:602:CLA:HHD	1.95	0.48
4:7:80:LYS:HA	4:7:176:ASN:HD21	1.79	0.48
22:7:307:CHL:CBB	22:7:308:CHL:HHC	2.44	0.48
25:7:319:BCR:HC22	28:8:620:LHG:HC82	1.95	0.48
21:B:809:CLA:HBA1	21:B:809:CLA:H3A	1.46	0.48
21:F:5005:CLA:H61	21:F:5005:CLA:H41	1.56	0.48
26:1:317:LMG:HC71	27:1:318:LMU:H82	1.95	0.48
21:3:410:CLA:HBB2	25:3:419:BCR:H311	1.94	0.48
21:8:605:CLA:C4B	25:8:618:BCR:H281	2.32	0.48
7:A:17:VAL:HA	7:A:186:PRO:HA	1.96	0.48
7:A:218:ILE:HD13	21:A:817:CLA:HBC2	1.96	0.48
5:b:219:ILE:HG13	5:b:220:ASP:N	2.28	0.48
22:T:602:CHL:H43	21:T:603:CLA:HMA2	1.96	0.48
21:3:405:CLA:H12	26:3:421:LMG:H132	1.96	0.48
5:8:64:GLN:HE22	21:8:622:CLA:C1	2.27	0.48
7:A:377:TYR:OH	21:A:831:CLA:OBD	2.27	0.48
8:B:416:LYS:HB2	8:B:540:LEU:HD13	1.96	0.48
9:C:52:LYS:HD3	9:C:67:VAL:HB	1.96	0.48
17:O:56:VAL:HG11	21:O:2002:CLA:HMB1	1.96	0.48
21:3:403:CLA:H12	25:3:417:BCR:H391	1.95	0.47
21:7:323:CLA:HBA1	21:7:323:CLA:H3A	1.54	0.47
7:A:452:SER:HB2	7:A:538:ILE:HG12	1.96	0.47
25:B:805:BCR:H383	21:B:844:CLA:HHD	1.96	0.47
21:B:830:CLA:H3A	21:B:830:CLA:HBA2	1.49	0.47
21:b:316:CLA:HAC1	4:c:136:PHE:HE2	1.79	0.47
19:K:74:ALA:HA	19:K:78:LYS:HA	1.94	0.47
1:1:153:TYR:HB3	21:1:308:CLA:HED2	1.94	0.47
5:8:96:LEU:HD13	1:a:125:ALA:HA	1.97	0.47
22:8:606:CHL:HAA2	22:8:606:CHL:HBD	1.96	0.47
7:A:269:TRP:O	21:A:819:CLA:H3A	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:814:CLA:H112	21:A:814:CLA:HBB1	1.96	0.47
8:B:524:ILE:HG12	8:B:591:VAL:HG12	1.96	0.47
10:D:130:LEU:HD12	10:D:133:THR:HB	1.95	0.47
21:K:202:CLA:HBA1	21:K:202:CLA:H3A	1.63	0.47
2:2:181:LEU:HD21	21:2:602:CLA:HAC1	1.97	0.47
3:3:229:PHE:CD1	22:7:303:CHL:HMD1	2.49	0.47
21:B:837:CLA:HBD	21:B:838:CLA:HMA1	1.96	0.47
9:C:30:PRO:HG3	10:D:171:ALA:HA	1.96	0.47
10:D:164:VAL:HB	10:D:170:ASN:HD21	1.78	0.47
4:7:179:PRO:HG3	22:7:309:CHL:HHD	1.95	0.47
21:A:819:CLA:CHD	21:A:820:CLA:HBB2	2.44	0.47
21:A:824:CLA:O1D	19:K:74:ALA:HB3	2.15	0.47
21:A:825:CLA:H11	21:A:825:CLA:H52	1.75	0.47
21:B:835:CLA:HMB1	25:F:5004:BCR:H19C	1.97	0.47
21:a:313:CLA:C3D	22:b:302:CHL:H101	2.44	0.47
1:1:87:ALA:HB2	23:1:314:LUT:H34	1.97	0.47
21:1:303:CLA:HBB1	25:1:316:BCR:H24C	1.97	0.47
6:9:212:THR:HB	8:B:224:THR:HG23	1.96	0.47
7:A:142:SER:HA	21:A:830:CLA:HMA2	1.96	0.47
7:A:161:SER:HA	27:A:855:LMU:H71	1.97	0.47
7:A:714:GLN:OE1	7:A:716:ARG:NH2	2.48	0.47
21:B:826:CLA:HBB1	21:B:833:CLA:H143	1.97	0.47
21:B:835:CLA:HBB2	25:F:5004:BCR:H272	1.96	0.47
4:7:70:LEU:HD22	24:7:318:XAT:H172	1.96	0.47
7:A:712:SER:N	12:F:189:GLU:OE2	2.47	0.47
21:A:833:CLA:HBB2	25:L:309:BCR:H342	1.96	0.47
20:T:154:TRP:CZ3	22:T:602:CHL:HBC2	2.49	0.47
28:1:319:LHG:HC81	25:8:618:BCR:HC41	1.97	0.47
2:2:41:ALA:HB3	2:2:45:MET:HE1	1.96	0.47
2:2:69:LEU:HD12	23:2:615:LUT:H172	1.95	0.47
2:2:234:MET:HE3	21:9:607:CLA:HHB	1.97	0.47
3:3:169:ILE:HD12	21:3:413:CLA:C4C	2.45	0.47
3:3:318:PHE:HE1	7:A:247:GLN:H	1.63	0.47
7:A:84:ILE:HG21	21:A:807:CLA:H61	1.97	0.47
7:A:554:VAL:HG21	25:A:850:BCR:H282	1.95	0.47
7:A:740:TRP:CD1	7:A:744:LEU:HD11	2.48	0.47
8:B:66:LEU:HD21	25:B:847:BCR:H291	1.95	0.47
21:B:812:CLA:H101	21:B:812:CLA:H2	1.96	0.47
14:H:102:PHE:HA	14:H:106:GLY:HA3	1.97	0.47
15:J:28:GLU:OE1	15:J:31:ARG:NH2	2.47	0.47
22:b:307:CHL:HBA1	25:b:319:BCR:C19	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:187:TRP:CD1	21:T:608:CLA:HMD3	2.48	0.47
28:1:322:LHG:HC82	21:B:833:CLA:H71	1.97	0.47
2:2:226:VAL:HG11	6:9:121:PRO:HB3	1.95	0.47
3:3:132:GLY:HA2	7:A:179:PHE:HZ	1.78	0.47
3:3:280:MET:HG3	24:3:416:XAT:H12	1.96	0.47
5:8:137:LYS:HB2	22:8:608:CHL:HH2	1.97	0.47
7:A:154:THR:N	7:A:158:GLN:OE1	2.39	0.47
7:A:374:MET:HE2	21:A:829:CLA:HMC2	1.97	0.47
7:A:582:GLY:HA3	8:B:703:ILE:HD11	1.97	0.47
21:A:807:CLA:H143	25:A:847:BCR:H332	1.96	0.47
28:A:852:LHG:H252	28:A:852:LHG:H102	1.96	0.47
8:B:204:ARG:HH12	8:B:254:ALA:H	1.63	0.47
1:a:182:ARG:HA	1:a:185:MET:HE2	1.95	0.47
1:1:189:LEU:HD21	21:1:302:CLA:HBB2	1.97	0.47
26:1:317:LMG:H291	26:1:317:LMG:HC91	1.36	0.47
30:3:422:SQD:H461	30:3:422:SQD:H241	1.42	0.47
4:7:233:ASP:HB3	4:7:241:VAL:HG11	1.97	0.47
7:A:305:PHE:HZ	21:A:821:CLA:H112	1.80	0.47
7:A:317:GLY:C	19:K:82:ARG:NH2	2.73	0.47
8:B:671:TYR:OH	21:B:807:CLA:OBD	2.33	0.47
21:B:842:CLA:H18	25:I:203:BCR:H353	1.96	0.47
21:a:307:CLA:HBA2	21:a:307:CLA:H3A	1.56	0.47
18:I:88:THR:HA	18:I:92:LEU:HB3	1.95	0.47
20:T:199:GLU:HG3	20:T:213:LEU:HA	1.97	0.47
1:1:212:SER:OG	1:1:216:ASN:OD1	2.32	0.47
6:9:177:PHE:CZ	24:9:614:XAT:H10	2.50	0.47
7:A:270:ALA:HA	21:A:819:CLA:HAA2	1.95	0.47
21:B:824:CLA:HBA2	21:B:824:CLA:H3A	1.57	0.47
21:B:830:CLA:H13	21:B:832:CLA:H162	1.97	0.47
10:D:74:ILE:HD12	10:D:74:ILE:H	1.79	0.47
10:D:96:TRP:HB3	10:D:144:PRO:HB3	1.96	0.47
1:a:183:LEU:HA	1:a:186:VAL:HG22	1.97	0.47
21:b:306:CLA:O1A	22:b:307:CHL:HMD2	2.15	0.47
30:2:618:SQD:H241	30:2:618:SQD:H462	1.35	0.46
7:A:67:GLU:OE2	7:A:71:ARG:NH2	2.49	0.46
7:A:375:PRO:HG2	7:A:381:ALA:HB2	1.97	0.46
21:B:825:CLA:H41	21:B:825:CLA:H62	1.54	0.46
28:a:301:LHG:HC5	28:a:301:LHG:HC82	1.41	0.46
22:b:309:CHL:HMA1	25:b:319:BCR:H362	1.98	0.46
21:1:301:CLA:H41	21:1:321:CLA:HBB2	1.97	0.46
21:1:304:CLA:H3A	25:1:316:BCR:C21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:401:CHL:H101	21:A:814:CLA:H101	1.97	0.46
6:9:133:LYS:O	6:9:150:TYR:OH	2.32	0.46
7:A:119:TRP:HZ2	27:A:854:LMU:H21	1.79	0.46
21:A:823:CLA:H161	21:A:823:CLA:H122	1.60	0.46
8:B:6:PHE:HD1	18:I:103:TYR:CD1	2.33	0.46
25:B:852:BCR:H371	25:B:852:BCR:H24C	1.71	0.46
14:H:49:GLU:HG2	16:L:156:LYS:HB2	1.97	0.46
22:c:606:CHL:HBB1	24:c:616:XAT:H393	1.98	0.46
20:T:320:ARG:NE	21:T:610:CLA:O1D	2.46	0.46
22:1:305:CHL:HBB2	21:1:307:CLA:HBC1	1.96	0.46
7:A:274:ASP:OD1	7:A:274:ASP:N	2.43	0.46
7:A:677:PHE:CG	25:A:851:BCR:H363	2.50	0.46
21:B:838:CLA:HAA1	21:G:205:CLA:HMA1	1.97	0.46
1:a:106:TRP:HE1	21:a:305:CLA:HAC2	1.80	0.46
22:b:307:CHL:HBA1	25:b:319:BCR:H19C	1.97	0.46
2:2:110:TRP:CD1	2:2:110:TRP:H	2.31	0.46
3:3:263:LYS:HE3	3:3:263:LYS:HB3	1.77	0.46
4:7:116:TRP:HE1	4:7:220:HIS:HB2	1.80	0.46
4:7:201:LYS:HD3	21:7:313:CLA:HBD	1.96	0.46
22:7:303:CHL:H51	21:7:314:CLA:H71	1.97	0.46
26:7:320:LMG:HC8	26:7:320:LMG:H111	1.41	0.46
21:A:812:CLA:HBB1	21:A:815:CLA:H142	1.97	0.46
21:A:820:CLA:H41	21:A:820:CLA:H61	1.59	0.46
8:B:396:ILE:HG13	8:B:552:LYS:HA	1.97	0.46
8:B:646:VAL:HG22	21:B:813:CLA:HAC1	1.97	0.46
8:B:663:MET:HE1	21:B:807:CLA:C4D	2.41	0.46
21:B:823:CLA:H111	21:B:826:CLA:H52	1.96	0.46
21:B:825:CLA:O1A	13:G:66:ARG:NH1	2.48	0.46
12:F:156:ILE:HD11	29:J:5001:PTY:HC31	1.98	0.46
21:a:312:CLA:HAB	21:a:312:CLA:H13	1.97	0.46
19:K:73:VAL:HB	19:K:82:ARG:HD3	1.96	0.46
2:2:237:GLU:OE2	2:2:240:LYS:NZ	2.43	0.46
5:8:51:ASN:OD1	5:8:51:ASN:N	2.47	0.46
24:9:615:XAT:H171	24:9:615:XAT:H193	1.97	0.46
7:A:217:GLN:HA	7:A:221:SER:HB2	1.97	0.46
7:A:362:SER:O	7:A:366:ILE:HG13	2.15	0.46
25:B:805:BCR:H24C	25:B:805:BCR:H371	1.71	0.46
21:B:843:CLA:HAC1	35:B:845:PQN:H152	1.97	0.46
5:b:83:GLY:HA2	24:b:318:XAT:H181	1.98	0.46
3:3:155:ALA:O	3:3:159:ALA:HB2	2.16	0.46
21:B:835:CLA:HBC3	25:B:852:BCR:H383	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:50:LEU:HD13	1:a:72:ARG:HD3	1.98	0.46
4:c:170:GLY:HA2	4:c:181:GLY:HA3	1.98	0.46
20:T:222:ASP:OD1	20:T:222:ASP:N	2.45	0.46
21:8:603:CLA:H3A	21:8:603:CLA:HBA2	1.46	0.46
21:8:622:CLA:HBB1	12:F:212:ILE:HB	1.98	0.46
7:A:426:LEU:HD23	21:A:826:CLA:C1C	2.46	0.46
21:A:813:CLA:H161	25:J:5004:BCR:H371	1.98	0.46
3:3:201:PHE:HD2	21:7:315:CLA:HED2	1.80	0.46
3:3:281:PHE:HB3	21:3:411:CLA:HMC2	1.96	0.46
22:8:606:CHL:HBA1	25:8:618:BCR:C19	2.46	0.46
6:9:40:LEU:HB2	6:9:41:PRO:HD2	1.98	0.46
25:B:805:BCR:H15C	21:B:807:CLA:H161	1.98	0.46
16:L:131:VAL:HG11	16:L:185:GLY:HA3	1.98	0.46
21:a:303:CLA:HBC3	24:a:316:XAT:H31	1.97	0.46
4:7:81:TRP:HD1	4:7:82:MET:HE2	1.80	0.46
6:9:41:PRO:HG3	21:9:601:CLA:CGD	2.45	0.46
6:9:62:LEU:HD11	21:B:816:CLA:H122	1.98	0.46
7:A:580:ARG:HG2	9:C:78:GLY:HA3	1.98	0.46
8:B:46:LYS:HD2	21:B:808:CLA:HMA2	1.97	0.46
21:B:832:CLA:H151	21:B:832:CLA:H111	1.80	0.46
15:J:16:LEU:HD21	25:J:5004:BCR:H19C	1.98	0.46
16:L:202:TYR:HB3	16:L:203:SER:H	1.60	0.46
4:c:206:GLY:O	4:c:210:MET:HG2	2.16	0.46
21:3:405:CLA:HMC2	32:A:802:DGD:HAE2	1.97	0.46
6:9:177:PHE:CE2	24:9:614:XAT:H12	2.51	0.46
7:A:488:GLN:HG2	7:A:510:TRP:HE3	1.80	0.46
8:B:411:ARG:NH2	21:B:833:CLA:O1D	2.49	0.46
8:B:669:ARG:NH1	8:B:700:ALA:O	2.49	0.46
8:B:716:VAL:HA	32:B:850:DGD:HBG2	1.98	0.46
21:B:833:CLA:HMC1	21:B:841:CLA:HBB1	1.98	0.46
9:C:6:LYS:HA	9:C:6:LYS:HD3	1.78	0.46
29:c:620:PTY:H111	29:c:620:PTY:HC6	1.66	0.46
31:2:619:3PH:H3B1	23:B:801:LUT:H403	1.98	0.45
22:3:401:CHL:HHC	24:3:416:XAT:H30	1.96	0.45
21:3:412:CLA:H2	21:3:412:CLA:HAA1	1.97	0.45
21:7:311:CLA:HBA2	21:7:311:CLA:H3A	1.43	0.45
5:8:135:GLU:HG2	5:8:138:ARG:HH21	1.81	0.45
7:A:194:VAL:HG13	21:A:827:CLA:HMD3	1.97	0.45
7:A:394:HIS:CD2	21:A:831:CLA:NC	2.84	0.45
21:A:834:CLA:H11	21:B:844:CLA:H43	1.99	0.45
8:B:345:ILE:HG23	21:B:822:CLA:H51	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:400:ASP:HB2	10:D:190:ILE:HD13	1.96	0.45
8:B:657:VAL:HG13	8:B:713:HIS:HD2	1.81	0.45
12:F:188:LYS:HA	12:F:188:LYS:HD3	1.74	0.45
2:2:220:LYS:HB3	23:B:801:LUT:H172	1.98	0.45
21:2:607:CLA:HBA2	21:2:607:CLA:H3A	1.58	0.45
7:A:256:SER:OG	7:A:271:GLU:O	2.29	0.45
7:A:524:MET:SD	7:A:629:HIS:NE2	2.78	0.45
8:B:193:GLY:O	8:B:197:HIS:ND1	2.38	0.45
8:B:416:LYS:HD2	8:B:540:LEU:HB3	1.98	0.45
21:B:826:CLA:HMD1	21:B:827:CLA:HMC1	1.98	0.45
21:B:831:CLA:H3A	21:B:831:CLA:HBA2	1.54	0.45
12:F:74:PRO:N	12:F:129:LEU:CD2	2.68	0.45
22:b:302:CHL:HBA1	22:b:302:CHL:H3A	1.53	0.45
19:K:63:ARG:HH22	19:K:91:PRO:HG2	1.81	0.45
20:T:221:LEU:HB3	21:T:606:CLA:HBC3	1.98	0.45
21:1:311:CLA:HBA1	21:1:311:CLA:H12	1.56	0.45
3:3:204:VAL:O	3:3:208:GLN:HB2	2.16	0.45
4:7:179:PRO:HD3	22:7:309:CHL:HMD2	1.98	0.45
5:8:44:LYS:HB3	5:8:44:LYS:HE2	1.68	0.45
21:9:603:CLA:H2A	21:9:603:CLA:HED2	1.98	0.45
26:A:801:LMG:HC8	26:A:801:LMG:H112	1.48	0.45
21:A:830:CLA:H72	21:A:830:CLA:H111	1.88	0.45
21:A:833:CLA:OBD	21:L:301:CLA:H3A	2.16	0.45
8:B:352:HIS:CD2	21:B:829:CLA:NC	2.83	0.45
14:H:55:TRP:HZ3	16:L:58:VAL:HG21	1.81	0.45
7:A:330:LYS:HA	7:A:337:GLY:HA3	1.98	0.45
7:A:385:GLY:O	7:A:389:SER:OG	2.32	0.45
7:A:443:TRP:CD1	21:A:833:CLA:HAB	2.51	0.45
21:c:602:CLA:H3A	21:c:602:CLA:HBA2	1.63	0.45
3:3:286:GLN:HA	3:3:289:ILE:HG22	1.99	0.45
7:A:218:ILE:HD11	7:A:276:LEU:HD21	1.99	0.45
21:A:836:CLA:H112	21:A:836:CLA:H71	1.69	0.45
25:A:848:BCR:C25	25:A:848:BCR:H371	2.46	0.45
8:B:455:LEU:O	12:F:138:LEU:N	2.47	0.45
9:C:29:VAL:HG12	10:D:173:ARG:HG3	1.99	0.45
10:D:101:GLU:HB3	10:D:113:ILE:HD11	1.99	0.45
1:a:76:LEU:CA	1:a:79:CYS:SG	2.98	0.45
21:b:311:CLA:H11	21:b:311:CLA:H52	1.77	0.45
21:1:308:CLA:H41	21:1:308:CLA:H62	1.71	0.45
2:2:87:MET:HE3	2:2:87:MET:HB3	1.59	0.45
7:A:657:VAL:HG22	7:A:745:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:A:803:CL0:H66	21:B:804:CLA:C2B	2.47	0.45
34:A:803:CL0:H70	21:B:804:CLA:C1B	2.46	0.45
8:B:345:ILE:HG13	21:B:827:CLA:H42	1.98	0.45
21:B:806:CLA:H162	21:B:806:CLA:H122	1.58	0.45
14:H:78:THR:O	14:H:82:SER:N	2.50	0.45
16:L:50:GLN:O	16:L:62:GLU:N	2.50	0.45
17:O:60:LEU:HD21	17:O:64:ILE:HD12	1.97	0.45
3:3:285:ALA:HA	3:3:288:VAL:HG12	1.98	0.45
22:7:303:CHL:HBB2	21:7:304:CLA:HHD	1.99	0.45
8:B:83:ILE:HG23	8:B:364:VAL:HG11	1.99	0.45
8:B:300:HIS:CD2	21:G:201:CLA:ND	2.76	0.45
8:B:300:HIS:HB3	8:B:305:ILE:HD11	1.98	0.45
21:B:833:CLA:H3A	21:B:834:CLA:OBD	2.17	0.45
21:a:313:CLA:ND	22:b:302:CHL:H121	2.32	0.45
22:c:605:CHL:CBB	22:c:606:CHL:HHC	2.46	0.45
23:2:615:LUT:H27	23:2:615:LUT:H381	1.79	0.45
3:3:207:ILE:HD13	21:3:407:CLA:C2C	2.46	0.45
22:7:303:CHL:HBB2	21:7:304:CLA:HMD1	1.99	0.45
5:8:219:ILE:HD13	5:8:219:ILE:HA	1.87	0.45
8:B:9:PHE:HB2	8:B:35:HIS:CG	2.52	0.45
8:B:462:GLN:HG2	8:B:473:TYR:CZ	2.52	0.45
8:B:572:SER:OG	8:B:575:ASP:OD1	2.31	0.45
1:a:141:LEU:HD13	21:a:307:CLA:HMC3	1.75	0.45
22:a:306:CHL:HBB2	21:a:308:CLA:HBC1	1.98	0.45
21:b:304:CLA:HBA2	21:b:304:CLA:H3A	1.61	0.45
22:2:601:CHL:H2	21:2:611:CLA:H102	1.97	0.45
22:7:308:CHL:HAA1	32:8:602:DGD:HB22	1.98	0.45
21:8:611:CLA:H8	21:8:611:CLA:H52	1.60	0.45
7:A:101:TYR:OH	7:A:153:ILE:O	2.35	0.45
7:A:479:LEU:H	7:A:530:THR:HG23	1.82	0.45
21:A:826:CLA:H52	25:A:849:BCR:H15C	1.98	0.45
8:B:349:VAL:O	8:B:353:MET:HG3	2.17	0.45
8:B:462:GLN:NE2	8:B:513:ILE:O	2.50	0.45
5:b:137:LYS:NZ	22:b:302:CHL:HMD1	2.31	0.45
4:7:143:GLY:O	4:7:147:THR:HG23	2.17	0.45
22:9:606:CHL:HMB2	27:9:616:LMU:H111	1.98	0.45
7:A:18:ASP:OD2	7:A:187:LYS:NZ	2.45	0.45
7:A:681:PHE:HZ	21:A:856:CLA:HBC2	1.82	0.45
21:A:819:CLA:H62	21:A:819:CLA:H41	1.53	0.45
14:H:50:ASN:OD1	14:H:55:TRP:NE1	2.40	0.45
16:L:98:HIS:HE1	21:L:304:CLA:ND	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:304:CLA:H51	25:L:309:BCR:HC21	1.97	0.45
21:7:304:CLA:HBA2	21:7:304:CLA:H3A	1.66	0.44
7:A:20:ASN:OD1	7:A:183:LYS:NZ	2.49	0.44
5:b:82:MET:HE1	21:b:311:CLA:HMC2	1.99	0.44
4:c:147:THR:OG1	21:c:601:CLA:O1D	2.26	0.44
19:K:61:ALA:HA	19:K:66:LEU:HG	2.00	0.44
21:A:816:CLA:H72	21:A:818:CLA:HBB1	1.99	0.44
8:B:211:ASP:OD1	8:B:211:ASP:N	2.43	0.44
8:B:353:MET:HE2	8:B:353:MET:HB3	1.84	0.44
8:B:546:LYS:HD2	11:E:77:TYR:HA	1.98	0.44
21:B:815:CLA:HED2	21:B:815:CLA:HBD	1.70	0.44
1:a:128:LEU:HD13	22:a:306:CHL:HAC2	1.99	0.44
25:c:617:BCR:H371	25:c:617:BCR:H24C	1.86	0.44
20:T:260:THR:HG21	22:T:601:CHL:HMA2	1.98	0.44
24:8:617:XAT:H363	28:F:5003:LHG:H151	2.00	0.44
7:A:552:LYS:HZ1	8:B:674:GLU:HB2	1.83	0.44
5:b:132:ALA:HB2	21:b:310:CLA:HAB	1.99	0.44
6:9:94:GLY:HA3	21:9:604:CLA:HBC3	2.00	0.44
7:A:660:SER:HB2	7:A:665:LEU:HG	2.00	0.44
21:A:810:CLA:H111	21:A:810:CLA:H143	1.84	0.44
17:O:64:ILE:HD13	17:O:74:LEU:HD23	1.97	0.44
4:c:244:ALA:HB2	20:T:246:VAL:HG13	1.99	0.44
21:1:308:CLA:CBB	21:1:310:CLA:H3A	2.47	0.44
21:1:321:CLA:H202	21:1:321:CLA:H162	1.82	0.44
21:2:613:CLA:HBA1	29:2:620:PTY:H152	2.00	0.44
4:7:91:ARG:HB3	22:7:309:CHL:HED1	1.99	0.44
21:8:605:CLA:O1A	22:8:606:CHL:HMD2	2.18	0.44
21:9:602:CLA:HBA2	21:9:602:CLA:H3A	1.71	0.44
7:A:330:LYS:HG2	7:A:337:GLY:H	1.81	0.44
7:A:565:ASP:OD1	7:A:565:ASP:N	2.50	0.44
21:A:821:CLA:H203	21:A:829:CLA:H3A	2.00	0.44
8:B:293:ARG:HA	8:B:299:GLY:HA3	1.99	0.44
8:B:375:HIS:HB2	21:B:830:CLA:C1B	2.47	0.44
20:T:257:PHE:CE1	22:T:601:CHL:HBA2	2.52	0.44
1:1:57:ASP:OD2	1:1:61:LEU:N	2.49	0.44
1:1:85:GLY:HA2	24:1:315:XAT:H381	1.99	0.44
2:2:68:PRO:HD2	23:2:615:LUT:H22	1.99	0.44
21:2:602:CLA:H93	21:2:602:CLA:H61	1.76	0.44
6:9:64:LEU:HD13	24:9:614:XAT:H23	2.00	0.44
7:A:43:PRO:HG3	12:F:190:ILE:HD13	1.98	0.44
7:A:80:GLN:HG2	21:A:807:CLA:H3A	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:721:THR:OG1	28:A:853:LHG:O5	2.32	0.44
21:A:829:CLA:H143	21:A:836:CLA:H121	1.98	0.44
10:D:122:LYS:HB2	16:L:57:PHE:HD2	1.83	0.44
1:a:87:ALA:HB2	23:a:315:LUT:H15	1.98	0.44
5:b:95:LYS:HA	5:b:95:LYS:HD3	1.77	0.44
21:b:316:CLA:H3A	21:b:316:CLA:HBA1	1.59	0.44
1:1:158:PHE:CE2	21:1:306:CLA:NC	2.86	0.44
7:A:574:PRO:HB3	7:A:720:ILE:HB	1.98	0.44
12:F:92:LEU:HD12	12:F:92:LEU:HA	1.89	0.44
14:H:131:LEU:HG	14:H:131:LEU:O	2.17	0.44
1:a:173:LYS:HE2	21:a:309:CLA:H3A	1.99	0.44
4:c:135:ILE:O	4:c:139:LEU:HB2	2.18	0.44
18:I:103:TYR:HE2	29:I:201:PTY:HC52	1.82	0.44
3:3:101:LEU:HA	3:3:104:LEU:HD12	1.99	0.44
24:3:416:XAT:H171	21:A:817:CLA:H191	1.99	0.44
4:7:117:TYR:OH	22:7:308:CHL:HBA1	2.18	0.44
4:7:142:PHE:O	4:7:146:GLU:HB2	2.18	0.44
32:7:301:DGD:HA21	32:7:301:DGD:HG12	1.37	0.44
7:A:487:ILE:HD11	21:A:838:CLA:H2	2.00	0.44
8:B:702:SER:O	8:B:706:ALA:N	2.43	0.44
21:B:804:CLA:H141	25:B:805:BCR:H323	1.99	0.44
21:B:821:CLA:HBA2	21:B:821:CLA:H3A	1.67	0.44
1:a:47:LEU:HD23	1:a:50:LEU:HD12	1.99	0.44
20:T:161:ASP:N	20:T:161:ASP:OD1	2.50	0.44
2:2:167:ASP:OD1	2:2:167:ASP:N	2.51	0.44
5:8:57:LEU:HD22	12:F:203:GLN:HA	2.00	0.44
21:A:835:CLA:H62	21:A:835:CLA:H41	1.83	0.44
20:T:347:LEU:HD23	21:T:612:CLA:HMA1	2.00	0.44
22:T:602:CHL:H3A	22:T:602:CHL:HBA2	1.64	0.44
1:1:136:ALA:HB2	21:1:307:CLA:HAB	1.98	0.43
30:2:618:SQD:H442	14:H:86:ALA:HB2	1.99	0.43
21:A:829:CLA:H162	21:A:829:CLA:H121	1.84	0.43
21:A:835:CLA:HMA2	16:L:109:LEU:HB3	1.99	0.43
21:A:840:CLA:HBB2	21:L:301:CLA:HAB	1.99	0.43
21:B:820:CLA:H3A	21:B:820:CLA:HBA2	1.46	0.43
12:F:100:GLU:O	12:F:103:SER:OG	2.31	0.43
5:b:124:LEU:HB2	22:b:308:CHL:HBC3	2.00	0.43
4:c:67:PHE:CG	22:T:601:CHL:HAB	2.53	0.43
21:3:414:CLA:HED3	22:7:303:CHL:H43	2.00	0.43
25:3:418:BCR:H342	26:3:421:LMG:H212	2.00	0.43
6:9:72:LYS:HA	6:9:75:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:580:ARG:O	8:B:669:ARG:NH2	2.48	0.43
21:A:807:CLA:HBC2	21:A:832:CLA:HMA1	2.00	0.43
21:A:835:CLA:H93	21:A:835:CLA:H111	1.88	0.43
21:A:835:CLA:H121	21:L:304:CLA:HBB1	2.00	0.43
8:B:300:HIS:HE1	21:G:201:CLA:NA	2.05	0.43
21:B:837:CLA:HBB1	25:B:849:BCR:H313	2.00	0.43
22:c:605:CHL:CBC	22:c:606:CHL:HAC2	2.48	0.43
21:T:609:CLA:H52	21:T:609:CLA:H11	1.78	0.43
7:A:330:LYS:HB3	7:A:330:LYS:HE2	1.83	0.43
21:A:811:CLA:H92	27:A:854:LMU:H91	2.00	0.43
21:A:839:CLA:H202	21:A:839:CLA:H162	1.80	0.43
8:B:423:LEU:HB3	8:B:533:LEU:HB2	2.00	0.43
8:B:577:PHE:O	8:B:581:VAL:HG23	2.19	0.43
21:F:5005:CLA:H43	21:F:5006:CLA:HBC3	1.99	0.43
1:a:42:GLU:H	28:b:303:LHG:P	2.41	0.43
20:T:242:THR:HG22	20:T:246:VAL:HG23	2.01	0.43
1:1:101:TYR:CE1	22:1:305:CHL:HMA2	2.53	0.43
21:1:309:CLA:NA	28:1:319:LHG:O5	2.52	0.43
2:2:240:LYS:HB2	2:2:240:LYS:HE2	1.82	0.43
3:3:121:ASP:HB3	3:3:124:VAL:HG23	2.00	0.43
4:7:242:THR:OG1	4:7:243:PHE:N	2.48	0.43
5:8:120:PHE:CE1	22:8:607:CHL:HBC2	2.53	0.43
21:A:843:CLA:H61	8:B:439:VAL:HG13	2.00	0.43
8:B:183:LEU:HD13	21:B:817:CLA:HHB	1.99	0.43
8:B:437:LEU:HD23	8:B:454:ILE:HB	2.00	0.43
8:B:559:PRO:HB3	8:B:703:ILE:HD12	2.00	0.43
12:F:195:PRO:HA	28:F:5003:LHG:H271	2.00	0.43
14:H:110:LEU:HB2	14:H:112:LEU:HD23	2.00	0.43
1:a:148:MET:HA	1:a:148:MET:HE3	1.99	0.43
1:1:54:TYR:HE1	22:8:601:CHL:HBC2	1.83	0.43
21:3:412:CLA:H2	21:3:412:CLA:H62	1.69	0.43
4:7:116:TRP:O	24:7:318:XAT:O23	2.26	0.43
7:A:16:ALA:HB1	7:A:187:LYS:HD3	2.00	0.43
7:A:75:SER:OG	7:A:181:TYR:HB2	2.18	0.43
7:A:412:PHE:HD1	7:A:416:ASP:HB2	1.83	0.43
21:A:815:CLA:H61	21:A:815:CLA:H41	1.71	0.43
25:A:850:BCR:H24C	25:A:850:BCR:H371	1.88	0.43
8:B:452:LYS:HB3	21:B:836:CLA:HED1	2.00	0.43
8:B:477:LEU:HD12	8:B:477:LEU:HA	1.88	0.43
12:F:193:ASP:OD1	12:F:196:LEU:HB3	2.19	0.43
21:G:205:CLA:C1A	26:G:207:LMG:H372	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:1:MET:HE2	15:J:1:MET:HA	2.00	0.43
1:a:59:LEU:HD11	1:a:61:LEU:HD22	2.00	0.43
21:3:402:CLA:H112	21:3:402:CLA:H91	1.81	0.43
21:3:411:CLA:H61	21:3:411:CLA:H41	1.82	0.43
4:7:108:LYS:NZ	4:7:229:ASP:OD1	2.49	0.43
7:A:395:MET:HE2	7:A:606:VAL:HG11	2.00	0.43
7:A:524:MET:HG2	7:A:618:VAL:HA	2.01	0.43
7:A:569:LEU:HD12	7:A:569:LEU:HA	1.89	0.43
21:A:830:CLA:H3A	21:A:830:CLA:HBA2	1.73	0.43
21:A:843:CLA:HMB2	21:B:806:CLA:H191	2.01	0.43
21:B:811:CLA:H2A	21:B:813:CLA:HED1	2.01	0.43
21:B:814:CLA:HAC2	25:I:203:BCR:H331	2.01	0.43
21:B:842:CLA:C4D	21:B:844:CLA:HMC2	2.43	0.43
13:G:47:SER:OG	13:G:118:GLY:O	2.34	0.43
14:H:49:GLU:HA	16:L:153:MET:HE2	2.01	0.43
2:2:71:LEU:HB2	21:2:602:CLA:H11	2.00	0.43
2:2:100:LEU:HD12	21:2:610:CLA:HBB2	1.99	0.43
3:3:280:MET:HB3	21:A:817:CLA:H143	2.00	0.43
21:7:310:CLA:HBA1	21:7:310:CLA:H3A	1.91	0.43
21:7:314:CLA:H152	21:7:314:CLA:H112	1.79	0.43
5:8:64:GLN:HE21	21:8:622:CLA:CAA	2.27	0.43
21:B:842:CLA:H51	21:B:842:CLA:H8	1.84	0.43
9:C:61:ASP:O	11:E:112:ASN:ND2	2.47	0.43
10:D:94:THR:HA	10:D:146:PHE:HA	2.00	0.43
25:F:5008:BCR:H24C	25:F:5008:BCR:H371	1.82	0.43
15:J:25:LEU:N	21:J:5002:CLA:HAB	2.34	0.43
5:8:43:LEU:HD23	5:8:46:LEU:HD23	2.01	0.43
5:8:144:LYS:HB2	5:8:147:SER:HB3	2.00	0.43
6:9:112:TYR:HE2	21:9:605:CLA:HAC1	1.82	0.43
21:9:604:CLA:H2	24:9:615:XAT:H203	2.00	0.43
7:A:15:ILE:HA	7:A:190:TRP:HD1	1.83	0.43
21:A:810:CLA:HBA2	21:A:810:CLA:H3A	1.68	0.43
21:B:816:CLA:H202	21:B:824:CLA:H11	2.00	0.43
21:B:828:CLA:H42	21:B:837:CLA:HBB2	2.00	0.43
21:B:830:CLA:H111	21:B:832:CLA:H171	2.01	0.43
12:F:140:SER:HA	12:F:154:VAL:HG21	2.01	0.43
1:a:187:ALA:HB2	23:a:315:LUT:H192	2.00	0.43
1:1:39:PRO:HB3	5:8:153:THR:HG21	2.00	0.43
22:3:401:CHL:H41	22:3:401:CHL:H61	1.63	0.43
7:A:141:THR:OG1	7:A:389:SER:OG	2.33	0.43
7:A:210:SER:OG	7:A:298:HIS:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:811:CLA:HBC3	21:A:843:CLA:H93	2.01	0.43
21:A:812:CLA:H11	21:A:812:CLA:H52	1.79	0.43
8:B:103:GLU:OE2	14:H:119:ARG:NH1	2.52	0.43
10:D:75:PHE:HZ	10:D:110:GLY:H	1.67	0.43
20:T:335:GLN:O	20:T:339:THR:OG1	2.27	0.43
22:2:606:CHL:HMA2	22:2:606:CHL:HAA1	1.82	0.43
3:3:92:LEU:HD12	3:3:96:SER:HB2	2.00	0.43
21:9:608:CLA:HBA2	21:9:608:CLA:H3A	1.61	0.43
21:A:805:CLA:H51	21:A:805:CLA:H8	1.84	0.43
8:B:527:GLY:HA2	8:B:583:TRP:HZ3	1.82	0.43
21:B:842:CLA:H171	16:L:133:ILE:HD13	2.00	0.43
10:D:62:LYS:HB2	10:D:62:LYS:HE2	1.82	0.43
12:F:74:PRO:CG	12:F:129:LEU:CD2	2.97	0.43
25:G:202:BCR:H20C	25:G:202:BCR:H361	1.83	0.43
5:b:77:SER:HB2	5:b:197:GLY:HA3	2.01	0.43
3:3:163:LEU:HB3	3:3:168:VAL:HB	2.01	0.42
22:7:309:CHL:HMA1	25:7:319:BCR:C36	2.49	0.42
28:7:324:LHG:HC62	7:A:26:PHE:HE2	1.84	0.42
5:8:90:PRO:O	5:8:94:THR:OG1	2.34	0.42
5:8:137:LYS:HB3	22:8:608:CHL:HMC	2.02	0.42
32:8:602:DGD:HG11	32:8:602:DGD:HA22	1.39	0.42
7:A:577:GLY:HA2	8:B:563:PRO:HD3	2.00	0.42
21:A:810:CLA:H101	21:A:810:CLA:H61	1.78	0.42
21:A:814:CLA:H143	21:A:814:CLA:H111	1.81	0.42
21:A:825:CLA:HBA1	21:A:825:CLA:HBD	2.00	0.42
21:A:840:CLA:H91	21:A:840:CLA:H112	1.81	0.42
21:B:812:CLA:HBA2	21:B:812:CLA:H141	2.01	0.42
21:B:816:CLA:H2	21:B:816:CLA:H62	1.83	0.42
13:G:67:THR:HA	13:G:70:GLU:HB3	2.00	0.42
14:H:85:GLU:HG3	29:H:201:PTY:HC51	2.01	0.42
21:b:304:CLA:H62	21:b:304:CLA:H41	1.73	0.42
20:T:154:TRP:CE3	22:T:602:CHL:HMD2	2.53	0.42
20:T:331:GLY:O	20:T:335:GLN:HG2	2.19	0.42
3:3:182:VAL:HG13	3:3:183:ILE:HD12	2.00	0.42
25:3:418:BCR:H363	25:A:848:BCR:H313	2.02	0.42
21:8:615:CLA:HBA1	21:8:615:CLA:H3A	1.46	0.42
21:A:814:CLA:H102	21:A:814:CLA:H61	1.75	0.42
21:A:829:CLA:H72	21:A:829:CLA:H112	1.45	0.42
14:H:66:TYR:HB2	14:H:71:GLU:OE1	2.20	0.42
28:b:303:LHG:HC5	28:b:303:LHG:HC82	1.70	0.42
21:c:609:CLA:HBA2	21:c:609:CLA:H3A	1.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:ILE:HD13	2:2:127:ILE:HA	1.93	0.42
3:3:229:PHE:HD1	22:7:303:CHL:HMD1	1.81	0.42
7:A:601:ASN:ND2	34:A:803:CL0:H68	2.26	0.42
21:A:813:CLA:H41	21:A:813:CLA:H61	1.79	0.42
21:A:826:CLA:H43	21:A:840:CLA:H72	2.01	0.42
8:B:712:ALA:HB1	21:B:832:CLA:H122	2.00	0.42
25:B:805:BCR:H20C	25:B:805:BCR:H361	1.64	0.42
16:L:48:VAL:HA	17:O:43:TRP:HZ2	1.84	0.42
3:3:212:LEU:HD23	3:3:212:LEU:HA	1.93	0.42
7:A:393:HIS:HE1	21:A:830:CLA:C1D	2.26	0.42
7:A:598:TRP:HE1	21:B:807:CLA:C1D	2.32	0.42
7:A:620:GLY:HA3	7:A:629:HIS:HA	2.00	0.42
7:A:658:ILE:O	8:B:622:ARG:NH1	2.51	0.42
21:A:823:CLA:H202	25:A:849:BCR:H332	2.01	0.42
21:A:830:CLA:H143	21:A:843:CLA:H101	2.02	0.42
10:D:145:CYS:HA	10:D:159:HIS:CD2	2.54	0.42
14:H:72:GLU:HA	14:H:75:GLN:HB2	2.01	0.42
14:H:101:LEU:O	14:H:106:GLY:N	2.43	0.42
22:b:302:CHL:HAC1	25:b:319:BCR:H313	2.02	0.42
20:T:280:LEU:HD13	20:T:283:LEU:HD23	2.01	0.42
3:3:99:ALA:HA	3:3:102:LYS:HD3	2.01	0.42
22:7:303:CHL:H203	21:7:315:CLA:H42	2.01	0.42
7:A:408:HIS:HA	7:A:411:ILE:HD12	2.00	0.42
21:A:804:CLA:H42	21:A:804:CLA:HHB	2.00	0.42
21:A:816:CLA:HBA1	25:A:847:BCR:HC7	2.00	0.42
21:A:830:CLA:O1D	21:A:831:CLA:HHB	2.19	0.42
25:A:851:BCR:H20C	25:A:851:BCR:H361	1.87	0.42
8:B:23:TRP:CG	8:B:705:GLN:HE22	2.38	0.42
8:B:30:HIS:CG	21:B:809:CLA:HBB2	2.54	0.42
21:B:822:CLA:H161	21:B:822:CLA:H141	1.85	0.42
21:B:822:CLA:H3A	21:B:822:CLA:HBA2	1.44	0.42
16:L:105:PRO:HG3	21:L:305:CLA:HBB1	2.00	0.42
2:2:251:LEU:HD23	2:2:251:LEU:H	1.84	0.42
7:A:158:GLN:H	7:A:158:GLN:HG3	1.49	0.42
7:A:320:HIS:CD2	21:A:824:CLA:ND	2.84	0.42
8:B:103:GLU:HA	14:H:118:PRO:HB3	2.01	0.42
8:B:194:HIS:HB2	21:B:818:CLA:C1C	2.49	0.42
8:B:464:ILE:HD11	21:B:839:CLA:H2	2.01	0.42
21:B:814:CLA:H111	21:B:814:CLA:H72	1.77	0.42
21:B:828:CLA:CAD	21:B:839:CLA:HBB1	2.49	0.42
25:B:852:BCR:H19C	12:F:154:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:164:VAL:O	10:D:164:VAL:CG1	2.62	0.42
12:F:69:ILE:HD11	12:F:139:ILE:HG13	2.02	0.42
5:b:48:MET:SD	5:b:49:ALA:N	2.93	0.42
4:7:210:MET:O	4:7:214:VAL:HG23	2.20	0.42
7:A:360:PHE:HE1	21:A:831:CLA:H161	1.85	0.42
21:A:804:CLA:H42	21:A:804:CLA:HMB1	2.01	0.42
21:A:821:CLA:H111	21:A:821:CLA:H72	1.84	0.42
21:A:823:CLA:O2A	21:A:827:CLA:HBB1	2.20	0.42
8:B:327:VAL:HB	21:B:827:CLA:HBC3	2.00	0.42
21:B:836:CLA:H62	21:B:836:CLA:H41	1.62	0.42
21:B:837:CLA:HBA1	21:B:837:CLA:H3A	1.79	0.42
5:b:78:ARG:NH1	22:b:309:CHL:OBD	2.47	0.42
21:1:311:CLA:H41	21:1:311:CLA:H62	1.89	0.42
2:2:247:GLU:HB3	2:2:249:VAL:HG13	2.02	0.42
21:9:608:CLA:CBB	21:9:610:CLA:H3A	2.49	0.42
7:A:204:GLY:HA2	21:A:822:CLA:HBC1	2.02	0.42
7:A:433:HIS:CE1	21:L:301:CLA:ND	2.87	0.42
21:A:840:CLA:HBD	21:A:840:CLA:HBA1	2.01	0.42
8:B:690:ASN:OD1	8:B:690:ASN:N	2.52	0.42
21:B:829:CLA:H161	21:B:829:CLA:H141	1.71	0.42
28:F:5003:LHG:HC61	28:F:5003:LHG:H242	1.48	0.42
16:L:166:ASP:HB3	16:L:169:MET:HG2	2.02	0.42
5:b:205:LEU:HD22	24:b:318:XAT:H403	2.01	0.42
22:b:302:CHL:HMD2	25:b:319:BCR:H322	2.01	0.42
1:1:93:GLU:HB3	1:1:203:LEU:HG	2.00	0.42
1:1:159:ASP:OD1	23:1:314:LUT:O23	2.35	0.42
3:3:99:ALA:O	3:3:102:LYS:NZ	2.43	0.42
5:8:45:ASP:N	5:8:45:ASP:OD1	2.53	0.42
25:A:846:BCR:H291	19:K:68:PRO:HG2	2.01	0.42
21:B:810:CLA:H193	21:B:810:CLA:H71	2.02	0.42
26:F:5009:LMG:HC5	15:J:2:LYS:NZ	2.35	0.42
25:J:5004:BCR:H20C	25:J:5004:BCR:H361	1.88	0.42
23:a:315:LUT:H31	23:a:315:LUT:H391	1.91	0.42
18:I:106:LYS:HA	18:I:106:LYS:HD3	1.85	0.42
1:1:105:LEU:HD21	22:1:305:CHL:HED3	2.02	0.42
3:3:288:VAL:CG1	21:A:817:CLA:H51	2.49	0.42
7:A:367:VAL:O	7:A:371:MET:HG3	2.19	0.42
8:B:669:ARG:HB2	35:B:845:PQN:H7	2.02	0.42
25:G:202:BCR:H371	25:G:202:BCR:H24C	1.80	0.42
5:b:233:THR:HB	5:b:236:GLU:HG2	2.02	0.42
21:7:311:CLA:H91	21:7:311:CLA:H111	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:198:HIS:CG	21:9:611:CLA:HAA2	2.55	0.41
7:A:390:LEU:HD11	21:A:831:CLA:HED3	2.01	0.41
7:A:441:LEU:HB2	21:A:840:CLA:HBB1	2.01	0.41
21:B:840:CLA:H8	21:B:840:CLA:H122	1.86	0.41
14:H:78:THR:HG21	16:L:88:ASN:HB2	2.02	0.41
16:L:78:LEU:HD22	21:L:304:CLA:HBD	2.02	0.41
5:b:111:TYR:OH	22:b:307:CHL:HMD3	2.20	0.41
20:T:156:PRO:HD2	24:T:616:XAT:H23	2.02	0.41
28:1:323:LHG:HC82	28:1:323:LHG:HC5	1.44	0.41
3:3:216:GLN:HG3	22:7:303:CHL:HED1	2.02	0.41
3:3:268:ASN:ND2	21:3:409:CLA:O2D	2.52	0.41
22:8:606:CHL:H3A	25:8:618:BCR:C21	2.50	0.41
7:A:430:VAL:HA	7:A:433:HIS:CE1	2.55	0.41
8:B:281:ILE:HD13	8:B:281:ILE:HA	1.87	0.41
8:B:588:ILE:HA	8:B:591:VAL:HG22	2.01	0.41
1:a:173:LYS:HB3	21:a:309:CLA:HHB	2.01	0.41
21:a:302:CLA:H2	24:a:316:XAT:H163	2.03	0.41
5:b:47:LYS:HA	5:b:47:LYS:HD2	1.85	0.41
5:b:66:LEU:HD12	5:b:66:LEU:HA	1.92	0.41
22:b:302:CHL:H172	22:b:302:CHL:H13	1.91	0.41
20:T:299:ASN:OD1	23:T:615:LUT:O23	2.37	0.41
21:1:311:CLA:HBB1	23:1:314:LUT:H181	2.01	0.41
21:3:408:CLA:H43	21:3:410:CLA:HBA1	2.02	0.41
32:A:802:DGD:HBN1	25:A:847:BCR:H15C	2.01	0.41
32:A:802:DGD:HBW1	25:A:848:BCR:HC21	2.03	0.41
8:B:331:LEU:HD23	8:B:331:LEU:HA	1.92	0.41
21:a:302:CLA:H112	24:a:316:XAT:H8	2.01	0.41
4:c:237:ASP:HB3	4:c:241:VAL:HG23	2.03	0.41
25:K:205:BCR:H371	25:K:205:BCR:H24C	1.83	0.41
22:T:602:CHL:H92	22:T:602:CHL:H61	1.95	0.41
5:8:79:THR:HG23	24:8:617:XAT:H202	2.02	0.41
7:A:485:GLN:NE2	7:A:528:LEU:O	2.53	0.41
7:A:593:PHE:HA	7:A:596:LEU:HD12	2.02	0.41
21:A:809:CLA:H2	21:A:809:CLA:H62	1.73	0.41
21:A:841:CLA:H3A	21:A:841:CLA:HBA2	1.88	0.41
8:B:173:GLU:HG3	8:B:302:LEU:HG	2.01	0.41
21:B:810:CLA:H2	21:B:810:CLA:H62	1.72	0.41
10:D:148:ARG:HB2	10:D:158:LEU:HD11	2.01	0.41
1:a:225:VAL:HG21	5:b:125:MET:HE2	2.01	0.41
21:a:302:CLA:H93	21:a:302:CLA:H111	1.86	0.41
4:c:135:ILE:HB	22:c:606:CHL:HBC3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:103:TYR:OH	29:I:201:PTY:HC52	2.20	0.41
21:2:611:CLA:H122	21:2:611:CLA:H8	1.93	0.41
6:9:41:PRO:HG2	21:9:601:CLA:CMA	2.45	0.41
7:A:656:GLN:HE22	7:A:746:ARG:HH11	1.69	0.41
7:A:740:TRP:NE1	21:A:830:CLA:O1A	2.54	0.41
21:A:809:CLA:HAB	25:J:5003:BCR:H402	2.01	0.41
21:A:820:CLA:C4D	21:A:829:CLA:HBB1	2.51	0.41
8:B:683:HIS:NE2	8:B:692:VAL:O	2.33	0.41
21:B:810:CLA:H93	21:B:830:CLA:HBC1	2.02	0.41
11:E:121:ASP:OD1	11:E:121:ASP:N	2.53	0.41
21:b:304:CLA:HBA2	21:b:304:CLA:H12	1.85	0.41
4:c:219:GLN:NE2	21:c:612:CLA:C4D	2.74	0.41
25:K:205:BCR:H321	25:K:205:BCR:HC8	2.03	0.41
1:1:148:MET:HE3	1:1:148:MET:HA	2.02	0.41
2:2:168:LYS:HB3	2:2:168:LYS:HE3	1.91	0.41
3:3:301:HIS:HE1	21:3:412:CLA:NA	2.17	0.41
22:3:401:CHL:H171	21:A:814:CLA:H13	2.02	0.41
25:3:417:BCR:H24C	25:3:417:BCR:H371	1.91	0.41
4:7:211:LEU:HD23	4:7:211:LEU:HA	1.90	0.41
21:8:604:CLA:C1	12:F:209:LEU:HG	2.22	0.41
6:9:181:ALA:HB1	27:9:616:LMU:H61	2.03	0.41
8:B:309:HIS:HE1	21:B:825:CLA:ND	2.17	0.41
8:B:528:LEU:HD23	8:B:587:THR:HG21	2.03	0.41
20:T:229:ALA:HB3	21:T:606:CLA:C1C	2.50	0.41
1:1:228:LEU:HD23	5:8:121:GLY:H	1.85	0.41
7:A:371:MET:HE1	21:A:831:CLA:CAD	2.51	0.41
7:A:539:HIS:CD2	21:A:838:CLA:HAB	2.56	0.41
21:A:806:CLA:H92	21:A:806:CLA:H62	1.85	0.41
21:B:826:CLA:HMD1	21:B:827:CLA:HHC	2.02	0.41
21:1:321:CLA:HBA1	21:1:321:CLA:H3A	1.88	0.41
22:2:601:CHL:HMB1	21:2:602:CLA:HBC2	2.02	0.41
7:A:596:LEU:HB3	7:A:732:LEU:HD11	2.03	0.41
7:A:645:TRP:CD2	34:A:803:CL0:H52	2.55	0.41
21:A:822:CLA:HBB2	25:K:205:BCR:H343	2.03	0.41
21:A:823:CLA:CGA	21:A:827:CLA:HBB1	2.51	0.41
8:B:644:LEU:HA	8:B:647:TRP:HD1	1.85	0.41
21:B:808:CLA:HBC2	25:I:202:BCR:HC21	2.02	0.41
21:G:201:CLA:H62	21:G:201:CLA:H92	1.82	0.41
21:2:603:CLA:HBC3	28:H:202:LHG:H152	2.03	0.41
21:2:608:CLA:HBB2	21:2:610:CLA:H3A	2.03	0.41
21:2:611:CLA:H122	21:2:611:CLA:HBB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:613:CLA:H162	21:2:613:CLA:H141	1.75	0.41
3:3:163:LEU:HD22	3:3:168:VAL:HG21	2.03	0.41
21:3:411:CLA:H61	21:3:411:CLA:H93	1.80	0.41
5:8:143:ARG:H	5:8:143:ARG:HG2	1.65	0.41
5:8:225:HIS:CG	21:8:613:CLA:HAA2	2.56	0.41
7:A:141:THR:HG1	7:A:389:SER:HG	1.68	0.41
7:A:187:LYS:HE3	7:A:187:LYS:HB3	1.94	0.41
7:A:397:ILE:HG21	21:A:831:CLA:HHC	2.03	0.41
8:B:27:ALA:HB1	32:B:850:DGD:HB21	2.01	0.41
8:B:70:ALA:HB2	8:B:136:LEU:HB2	2.02	0.41
8:B:240:THR:OG1	8:B:250:GLY:O	2.30	0.41
8:B:414:ASP:HA	12:F:232:ARG:NH1	2.36	0.41
8:B:703:ILE:H	8:B:703:ILE:HG13	1.57	0.41
21:B:804:CLA:C1B	21:B:807:CLA:CBB	2.82	0.41
14:H:112:LEU:HA	14:H:113:PRO:HD3	1.90	0.41
16:L:61:LEU:HD21	21:L:301:CLA:HMA2	2.02	0.41
16:L:108:LYS:HA	16:L:108:LYS:HD3	1.69	0.41
5:b:192:LYS:HD3	21:b:313:CLA:HBD	2.03	0.41
22:b:307:CHL:HAA2	22:b:307:CHL:HBD	2.02	0.41
4:c:53:PRO:HA	4:c:54:PRO:HD3	1.98	0.41
20:T:278:LEU:HD12	25:T:617:BCR:H343	2.03	0.41
21:1:306:CLA:HBA1	21:1:306:CLA:H3A	1.80	0.41
21:1:307:CLA:HAA2	28:1:323:LHG:H241	2.02	0.41
21:1:309:CLA:HAB	5:8:155:PHE:CE1	2.56	0.41
26:1:317:LMG:HC8	26:1:317:LMG:H112	1.40	0.41
2:2:53:PRO:HD2	2:2:56:LEU:HB3	2.03	0.41
3:3:179:ARG:NH1	32:A:802:DGD:O4D	2.54	0.41
21:3:402:CLA:H143	21:3:402:CLA:H111	1.77	0.41
5:8:43:LEU:HD13	5:8:53:GLY:HA2	2.03	0.41
6:9:36:ARG:HB3	6:9:38:LEU:H	1.86	0.41
6:9:106:GLU:HA	22:9:606:CHL:HED3	2.03	0.41
21:9:605:CLA:HBC2	22:9:606:CHL:HBC3	2.03	0.41
7:A:382:THR:HG21	7:A:517:VAL:HB	2.03	0.41
7:A:598:TRP:HE1	21:B:807:CLA:CHD	2.34	0.41
21:A:828:CLA:OBD	21:A:838:CLA:HBB1	2.21	0.41
21:A:834:CLA:H102	21:A:834:CLA:H61	1.88	0.41
21:A:836:CLA:H11	21:A:836:CLA:H51	1.88	0.41
21:B:837:CLA:H92	21:B:837:CLA:H62	1.89	0.41
21:B:837:CLA:H72	21:B:838:CLA:H12	2.03	0.41
25:F:5004:BCR:H24C	25:F:5004:BCR:H371	1.92	0.41
15:J:23:SER:O	15:J:27:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:26:LEU:HD13	25:J:5003:BCR:HC7	2.02	0.41
18:I:100:ALA:HB1	25:I:202:BCR:HC8	2.03	0.41
25:I:203:BCR:H24C	25:I:203:BCR:H371	1.83	0.41
20:T:167:ARG:HH12	20:T:290:PRO:HG3	1.85	0.41
1:1:51:PRO:HB2	1:1:178:LEU:HD12	2.02	0.40
1:1:132:VAL:HG23	21:1:307:CLA:HBB2	2.03	0.40
4:7:148:LYS:O	4:7:159:GLN:NE2	2.54	0.40
6:9:40:LEU:HB2	6:9:41:PRO:CD	2.51	0.40
8:B:183:LEU:HD21	21:B:817:CLA:HAA1	2.03	0.40
9:C:50:GLY:HA2	9:C:67:VAL:HG11	2.02	0.40
4:c:95:LEU:HD13	21:c:604:CLA:HBB2	2.01	0.40
21:1:307:CLA:HBA1	28:1:323:LHG:H292	2.04	0.40
2:2:99:ILE:HD11	23:2:615:LUT:H363	2.02	0.40
21:7:323:CLA:HAB	5:8:54:PHE:CD2	2.57	0.40
7:A:370:HIS:CD2	21:A:829:CLA:NC	2.88	0.40
1:a:54:TYR:HB2	21:a:302:CLA:HMD1	2.03	0.40
21:b:305:CLA:H141	21:b:305:CLA:H162	1.89	0.40
21:b:311:CLA:H13	23:b:317:LUT:H403	2.03	0.40
4:c:116:TRP:HE1	4:c:220:HIS:HB2	1.86	0.40
20:T:338:VAL:HG23	20:T:339:THR:HG23	2.04	0.40
21:1:301:CLA:H62	21:1:302:CLA:HMA3	2.03	0.40
21:3:407:CLA:H62	21:3:407:CLA:H2	1.93	0.40
4:7:183:PHE:CE1	22:7:309:CHL:HBA2	2.56	0.40
7:A:298:HIS:HE1	21:A:821:CLA:NA	2.11	0.40
7:A:537:HIS:HE1	21:A:839:CLA:ND	2.19	0.40
21:A:807:CLA:H8	25:A:848:BCR:H402	2.04	0.40
21:A:811:CLA:HAB	21:B:836:CLA:HMD2	2.03	0.40
23:B:801:LUT:H28	23:B:801:LUT:H361	2.02	0.40
12:F:182:ASP:OD1	12:F:183:ALA:N	2.54	0.40
1:a:128:LEU:HD12	1:a:128:LEU:HA	1.97	0.40
1:a:208:ASP:OD2	1:a:216:ASN:ND2	2.54	0.40
21:a:308:CLA:HBD	21:a:308:CLA:HBA2	2.03	0.40
21:a:313:CLA:C1C	22:b:302:CHL:H151	2.52	0.40
19:K:63:ARG:HG2	21:K:201:CLA:HBB1	2.03	0.40
20:T:157:LEU:HB2	24:T:616:XAT:H241	2.02	0.40
20:T:230:VAL:O	20:T:233:THR:OG1	2.32	0.40
5:8:155:PHE:HE2	25:8:618:BCR:H343	1.87	0.40
21:8:613:CLA:H51	21:8:613:CLA:H11	1.78	0.40
7:A:277:THR:OG1	7:A:293:ASP:OD1	2.39	0.40
7:A:684:MET:HG3	21:A:804:CLA:C4C	2.52	0.40
21:A:811:CLA:H202	21:A:811:CLA:H162	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:841:CLA:H93	21:A:841:CLA:H62	1.83	0.40
21:B:843:CLA:H3A	21:B:843:CLA:HBA2	1.77	0.40
12:F:229:VAL:CG2	12:F:232:ARG:HH22	2.29	0.40
5:b:60:GLY:HA3	5:b:66:LEU:HD13	2.04	0.40
4:c:97:VAL:HG23	4:c:216:PHE:CE2	2.57	0.40
3:3:161:GLU:OE1	3:3:293:GLY:HA3	2.21	0.40
4:7:135:ILE:HD12	32:8:602:DGD:HA52	2.03	0.40
7:A:326:LEU:HD12	7:A:342:TYR:HB2	2.04	0.40
21:A:828:CLA:H62	21:A:828:CLA:H41	1.89	0.40
8:B:400:ASP:OD2	8:B:403:GLN:HG3	2.21	0.40
21:B:804:CLA:H101	25:B:805:BCR:H353	2.03	0.40
21:B:831:CLA:H92	25:B:846:BCR:H21C	2.02	0.40
21:G:201:CLA:H162	21:G:201:CLA:H122	1.79	0.40
21:b:304:CLA:H8	24:b:318:XAT:H371	2.02	0.40
25:I:202:BCR:H20C	25:I:202:BCR:H361	1.89	0.40
25:I:203:BCR:H20C	25:I:203:BCR:H361	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/228 (86%)	188 (96%)	7 (4%)	0	100	100
1	a	194/228 (85%)	182 (94%)	12 (6%)	0	100	100
2	2	219/263 (83%)	208 (95%)	10 (5%)	1 (0%)	25	61
3	3	228/320 (71%)	220 (96%)	8 (4%)	0	100	100
4	7	207/256 (81%)	196 (95%)	11 (5%)	0	100	100
4	c	207/256 (81%)	200 (97%)	7 (3%)	0	100	100
5	8	224/254 (88%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	221/254 (87%)	215 (97%)	6 (3%)	0	100	100
6	9	185/222 (83%)	171 (92%)	14 (8%)	0	100	100
7	A	738/750 (98%)	703 (95%)	35 (5%)	0	100	100
8	B	730/735 (99%)	699 (96%)	31 (4%)	0	100	100
9	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
10	D	141/202 (70%)	134 (95%)	7 (5%)	0	100	100
11	E	62/125 (50%)	59 (95%)	3 (5%)	0	100	100
12	F	163/232 (70%)	154 (94%)	9 (6%)	0	100	100
13	G	103/141 (73%)	95 (92%)	7 (7%)	1 (1%)	13	46
14	H	96/135 (71%)	83 (86%)	13 (14%)	0	100	100
15	J	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
16	L	157/202 (78%)	147 (94%)	10 (6%)	0	100	100
17	O	86/129 (67%)	80 (93%)	6 (7%)	0	100	100
18	I	39/109 (36%)	37 (95%)	2 (5%)	0	100	100
19	K	81/123 (66%)	67 (83%)	14 (17%)	0	100	100
20	T	203/365 (56%)	181 (89%)	20 (10%)	2 (1%)	13	46
All	All	4596/5651 (81%)	4345 (94%)	247 (5%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	149	PRO
2	2	120	ILE
13	G	38	ILE
20	T	298	PHE

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	1	150/178 (84%)	150 (100%)	0	100	100
1	a	150/178 (84%)	150 (100%)	0	100	100
2	2	179/207 (86%)	179 (100%)	0	100	100
3	3	174/236 (74%)	174 (100%)	0	100	100
4	7	166/201 (83%)	166 (100%)	0	100	100
4	c	166/201 (83%)	166 (100%)	0	100	100
5	8	173/196 (88%)	173 (100%)	0	100	100
5	b	171/196 (87%)	170 (99%)	1 (1%)	84	93
6	9	153/183 (84%)	153 (100%)	0	100	100
7	A	599/608 (98%)	597 (100%)	2 (0%)	91	96
8	B	593/594 (100%)	589 (99%)	4 (1%)	81	91
9	C	68/69 (99%)	67 (98%)	1 (2%)	60	83
10	D	123/163 (76%)	122 (99%)	1 (1%)	79	90
11	E	57/101 (56%)	56 (98%)	1 (2%)	54	80
12	F	138/184 (75%)	138 (100%)	0	100	100
13	G	81/110 (74%)	81 (100%)	0	100	100
14	H	78/105 (74%)	77 (99%)	1 (1%)	65	85
15	J	36/36 (100%)	36 (100%)	0	100	100
16	L	122/159 (77%)	122 (100%)	0	100	100
17	O	72/103 (70%)	70 (97%)	2 (3%)	38	70
18	I	32/77 (42%)	31 (97%)	1 (3%)	35	68
19	K	61/94 (65%)	59 (97%)	2 (3%)	33	67
20	T	165/286 (58%)	159 (96%)	6 (4%)	30	64
All	All	3707/4465 (83%)	3685 (99%)	22 (1%)	82	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	372	TYR
7	A	558	ARG
8	B	339	LEU
8	B	395	PHE
8	B	404	ASN
8	B	442	ASP
9	C	12	ILE

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Mol	Chain	Res	Type
10	D	158	LEU
11	E	61	ILE
14	H	112	LEU
17	O	55	PHE
17	O	95	LEU
5	b	131	TYR
18	I	87	LEU
19	K	73	VAL
19	K	88	THR
20	T	184	HIS
20	T	200	ILE
20	T	230	VAL
20	T	242	THR
20	T	333	MET
20	T	351	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	53	ASN
2	2	116	GLN
3	3	216	GLN
3	3	254	ASN
3	3	268	ASN
3	3	286	GLN
4	7	176	ASN
4	7	220	HIS
4	7	221	HIS
4	7	230	ASN
5	8	64	GLN
5	8	103	GLN
5	8	232	ASN
6	9	95	GLN
7	A	225	ASN
7	A	283	ASN
7	A	539	HIS
7	A	653	GLN
7	A	656	GLN
8	B	206	GLN
8	B	295	ASN
8	B	369	GLN
8	B	504	ASN

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Mol	Chain	Res	Type
8	B	521	HIS
8	B	586	ASN
8	B	631	GLN
8	B	634	ASN
10	D	178	GLN
14	H	125	ASN
15	J	30	ASN
16	L	50	GLN
17	O	70	ASN
1	a	36	ASN
5	b	210	GLN
20	T	165	GLN
20	T	321	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](#)

362 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	$\# Z > 2$
21	CLA	B	807	-	63,73,73	1.40	8 (12%)	74,113,113	1.30	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	G	201	8	63,73,73	1.35	4 (6%)	74,113,113	1.26	8 (10%)
21	CLA	3	406	-	53,63,73	1.48	6 (11%)	62,101,113	1.47	8 (12%)
21	CLA	2	602	2	63,73,73	1.35	7 (11%)	74,113,113	1.28	6 (8%)
23	LUT	9	613	-	42,43,43	0.29	0	51,60,60	0.34	0
21	CLA	A	842	28	52,62,73	1.47	6 (11%)	60,99,113	1.38	8 (13%)
29	PTY	1	320	-	20,20,49	0.69	0	23,25,54	0.51	0
21	CLA	3	403	-	48,58,73	1.53	4 (8%)	56,95,113	1.49	7 (12%)
21	CLA	A	812	7	53,63,73	1.47	7 (13%)	62,101,113	1.31	6 (9%)
21	CLA	3	408	3	58,68,73	1.37	5 (8%)	68,107,113	1.28	7 (10%)
21	CLA	a	308	1	48,58,73	1.56	6 (12%)	56,95,113	1.49	10 (17%)
23	LUT	O	2005	-	42,43,43	0.34	0	51,60,60	0.68	2 (3%)
21	CLA	c	611	-	44,54,73	1.62	5 (11%)	51,90,113	1.56	6 (11%)
21	CLA	B	831	8	63,73,73	1.37	6 (9%)	74,113,113	1.27	6 (8%)
21	CLA	3	405	3	48,58,73	1.54	5 (10%)	56,95,113	1.48	7 (12%)
24	XAT	9	615	-	41,47,47	0.17	0	54,74,74	0.72	3 (5%)
21	CLA	A	839	7	63,73,73	1.29	7 (11%)	74,113,113	1.26	8 (10%)
21	CLA	3	404	-	44,54,73	1.58	5 (11%)	51,90,113	1.40	6 (11%)
21	CLA	7	306	-	48,58,73	1.59	5 (10%)	56,95,113	1.50	8 (14%)
21	CLA	c	604	-	48,58,73	1.56	6 (12%)	56,95,113	1.51	8 (14%)
21	CLA	c	603	4	49,59,73	1.54	6 (12%)	56,96,113	1.43	7 (12%)
22	CHL	c	607	-	46,56,74	1.55	4 (8%)	49,92,114	2.43	8 (16%)
21	CLA	T	607	-	48,58,73	1.53	5 (10%)	56,95,113	1.48	8 (14%)
21	CLA	A	824	7	58,68,73	1.40	5 (8%)	68,107,113	1.28	6 (8%)
28	LHG	9	617	21	27,27,48	0.40	0	30,33,54	0.39	0
22	CHL	7	303	-	64,74,74	1.40	4 (6%)	71,114,114	2.10	10 (14%)
21	CLA	b	306	-	48,58,73	1.53	5 (10%)	56,95,113	1.52	6 (10%)
27	LMU	9	616	-	36,36,36	0.27	0	47,47,47	0.63	0
25	BCR	B	848	-	41,41,41	0.15	0	56,56,56	0.26	0
21	CLA	A	838	7	49,59,73	1.53	6 (12%)	56,96,113	1.51	6 (10%)
30	SQD	3	422	-	33,35,54	0.27	0	43,46,65	0.38	0
21	CLA	8	610	5	58,68,73	1.37	6 (10%)	68,107,113	1.21	6 (8%)
21	CLA	A	837	7	45,55,73	1.61	5 (11%)	52,91,113	1.49	6 (11%)
28	LHG	3	424	-	25,25,48	0.39	0	28,31,54	0.36	0
21	CLA	a	303	1	53,63,73	1.51	6 (11%)	62,101,113	1.46	7 (11%)
22	CHL	8	606	-	44,54,74	1.39	5 (11%)	47,90,114	2.37	8 (17%)
21	CLA	A	809	-	58,68,73	1.43	6 (10%)	68,107,113	1.33	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PTY	c	620	-	25,25,49	0.60	0	28,30,54	0.64	0
25	BCR	B	846	-	41,41,41	0.14	0	56,56,56	0.34	0
21	CLA	7	323	5	44,54,73	1.61	6 (13%)	51,90,113	1.52	6 (11%)
22	CHL	7	308	-	44,54,74	1.43	5 (11%)	47,90,114	2.42	11 (23%)
21	CLA	3	413	-	40,50,73	1.67	5 (12%)	45,85,113	1.34	6 (13%)
21	CLA	A	828	-	55,65,73	1.46	6 (10%)	64,103,113	1.44	8 (12%)
21	CLA	B	818	-	63,73,73	1.33	6 (9%)	74,113,113	1.24	7 (9%)
22	CHL	9	606	-	45,55,74	1.51	4 (8%)	48,91,114	2.37	8 (16%)
21	CLA	3	411	3	58,68,73	1.44	7 (12%)	68,107,113	1.33	7 (10%)
21	CLA	B	815	-	53,63,73	1.45	5 (9%)	62,101,113	1.34	6 (9%)
25	BCR	7	319	-	41,41,41	0.20	0	56,56,56	0.42	0
36	SF4	C	101	9	0,12,12	-	-	-	-	-
21	CLA	G	205	-	43,53,73	1.62	4 (9%)	50,89,113	1.42	7 (14%)
21	CLA	A	830	7	63,73,73	1.31	6 (9%)	74,113,113	1.38	9 (12%)
21	CLA	a	311	1	44,54,73	1.66	7 (15%)	51,90,113	1.59	8 (15%)
21	CLA	b	314	5	48,58,73	1.58	6 (12%)	56,95,113	1.45	8 (14%)
21	CLA	9	611	-	44,54,73	1.61	5 (11%)	51,90,113	1.55	6 (11%)
21	CLA	B	834	8	58,68,73	1.41	6 (10%)	68,107,113	1.41	7 (10%)
21	CLA	L	301	7	48,58,73	1.54	6 (12%)	56,95,113	1.45	7 (12%)
26	LMG	7	320	-	47,47,55	0.21	0	55,55,63	0.28	0
21	CLA	7	312	28	43,53,73	1.65	7 (16%)	50,89,113	1.54	6 (12%)
21	CLA	B	810	8	63,73,73	1.33	6 (9%)	74,113,113	1.31	8 (10%)
21	CLA	c	601	5	44,54,73	1.59	5 (11%)	51,90,113	1.49	6 (11%)
21	CLA	b	313	5	48,58,73	1.60	7 (14%)	56,95,113	1.53	10 (17%)
21	CLA	9	607	6	63,73,73	1.36	5 (7%)	74,113,113	1.35	8 (10%)
21	CLA	2	612	2	43,53,73	1.67	6 (13%)	50,89,113	1.46	6 (12%)
21	CLA	1	301	1	59,69,73	1.39	5 (8%)	69,108,113	1.36	7 (10%)
21	CLA	1	304	-	43,53,73	1.64	6 (13%)	50,89,113	1.53	6 (12%)
29	PTY	3	423	-	13,16,49	0.57	0	14,19,54	0.36	0
21	CLA	B	835	8	63,73,73	1.37	6 (9%)	74,113,113	1.54	9 (12%)
21	CLA	B	836	8	53,63,73	1.44	7 (13%)	62,101,113	1.36	8 (12%)
21	CLA	A	816	-	63,73,73	1.33	5 (7%)	74,113,113	1.38	8 (10%)
28	LHG	8	620	21	39,39,48	0.33	0	42,45,54	0.35	0
21	CLA	T	613	-	44,54,73	1.59	5 (11%)	51,90,113	1.37	6 (11%)
21	CLA	A	840	7	58,68,73	1.40	6 (10%)	68,107,113	1.24	7 (10%)
21	CLA	O	2003	-	43,53,73	1.63	6 (13%)	50,89,113	1.44	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	L	307	-	41,41,41	0.12	0	56,56,56	0.28	0
25	BCR	L	309	-	41,41,41	0.19	0	56,56,56	0.44	0
21	CLA	1	307	1	48,58,73	1.53	5 (10%)	56,95,113	1.48	8 (14%)
21	CLA	7	316	4	63,73,73	1.35	6 (9%)	74,113,113	1.34	7 (9%)
21	CLA	H	203	14	58,68,73	1.41	5 (8%)	68,107,113	1.35	6 (8%)
21	CLA	3	414	3	44,54,73	1.63	6 (13%)	51,90,113	1.46	6 (11%)
21	CLA	B	814	8	58,68,73	1.38	6 (10%)	68,107,113	1.39	6 (8%)
28	LHG	A	853	-	44,44,48	0.30	0	47,50,54	0.31	0
29	PTY	7	302	-	25,25,49	0.62	0	28,30,54	0.48	0
22	CHL	b	307	-	45,55,74	1.39	5 (11%)	48,91,114	2.38	8 (16%)
22	CHL	b	309	-	49,59,74	1.33	5 (10%)	53,96,114	2.40	9 (16%)
25	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.52	0
25	BCR	J	5004	-	41,41,41	0.15	0	56,56,56	0.24	0
28	LHG	7	321	21	42,42,48	0.31	0	45,48,54	0.30	0
21	CLA	T	610	-	44,54,73	1.61	5 (11%)	51,90,113	1.48	6 (11%)
21	CLA	K	204	-	46,56,73	1.57	5 (10%)	53,92,113	1.41	7 (13%)
21	CLA	L	306	-	48,58,73	1.53	5 (10%)	56,95,113	1.51	7 (12%)
21	CLA	a	310	28	44,54,73	1.65	6 (13%)	51,90,113	1.47	6 (11%)
22	CHL	b	308	-	45,55,74	1.29	4 (8%)	48,91,114	2.36	8 (16%)
23	LUT	a	315	-	42,43,43	0.21	0	51,60,60	1.48	8 (15%)
26	LMG	1	317	-	28,28,55	0.28	0	35,35,63	0.35	0
25	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.94	4 (7%)
21	CLA	c	608	-	43,53,73	1.64	4 (9%)	50,89,113	1.48	6 (12%)
21	CLA	B	840	8	58,68,73	1.43	6 (10%)	68,107,113	1.31	9 (13%)
21	CLA	A	819	7	58,68,73	1.40	6 (10%)	68,107,113	1.30	7 (10%)
21	CLA	a	312	-	58,68,73	1.39	5 (8%)	68,107,113	1.27	8 (11%)
21	CLA	2	605	-	43,53,73	1.62	5 (11%)	50,89,113	1.44	6 (12%)
35	PQN	B	845	-	34,34,34	0.29	0	43,45,45	0.57	1 (2%)
21	CLA	7	315	4	48,58,73	1.52	5 (10%)	56,95,113	1.47	8 (14%)
21	CLA	8	611	28	53,63,73	1.48	6 (11%)	62,101,113	1.41	8 (12%)
21	CLA	2	609	28	39,49,73	1.67	4 (10%)	46,84,113	1.53	7 (15%)
21	CLA	T	614	-	40,50,73	1.66	4 (10%)	45,85,113	1.37	6 (13%)
29	PTY	J	5001	-	21,21,49	0.67	0	24,26,54	0.54	0
21	CLA	c	602	4	50,60,73	1.51	7 (14%)	57,97,113	1.37	7 (12%)
22	CHL	7	309	-	46,56,74	1.57	5 (10%)	49,92,114	2.16	8 (16%)
25	BCR	1	316	-	41,41,41	0.14	0	56,56,56	0.37	0
21	CLA	F	5006	-	45,55,73	1.57	5 (11%)	52,91,113	1.41	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	7	304	4	58,68,73	1.40	7 (12%)	68,107,113	1.29	8 (11%)
25	BCR	3	419	-	41,41,41	0.22	0	56,56,56	0.28	0
21	CLA	2	604	-	48,58,73	1.51	4 (8%)	56,95,113	1.37	8 (14%)
22	CHL	c	606	-	46,56,74	1.37	4 (8%)	49,92,114	2.05	9 (18%)
21	CLA	G	203	13	45,55,73	1.62	7 (15%)	52,91,113	1.53	7 (13%)
27	LMU	A	855	-	36,36,36	0.19	0	47,47,47	0.33	0
28	LHG	7	324	-	30,30,48	0.40	0	33,36,54	0.61	1 (3%)
28	LHG	3	420	21	16,16,48	0.89	1 (6%)	17,20,54	0.64	0
22	CHL	7	307	-	44,54,74	1.46	5 (11%)	47,90,114	2.33	8 (17%)
21	CLA	B	804	-	63,73,73	1.33	6 (9%)	74,113,113	1.20	7 (9%)
21	CLA	1	309	28	44,54,73	1.61	6 (13%)	51,90,113	1.38	6 (11%)
21	CLA	a	307	-	43,53,73	1.64	5 (11%)	50,89,113	1.49	6 (12%)
21	CLA	a	309	1	58,68,73	1.38	6 (10%)	68,107,113	1.35	7 (10%)
21	CLA	B	824	8	53,63,73	1.48	6 (11%)	62,101,113	1.39	8 (12%)
27	LMU	1	318	-	36,36,36	0.22	0	47,47,47	0.49	0
21	CLA	A	817	7	63,73,73	1.34	5 (7%)	74,113,113	1.28	6 (8%)
25	BCR	3	417	-	41,41,41	0.16	0	56,56,56	0.33	0
24	XAT	3	416	-	41,47,47	0.19	0	54,74,74	0.98	3 (5%)
21	CLA	b	304	5	58,68,73	1.38	4 (6%)	68,107,113	1.24	7 (10%)
23	LUT	T	615	-	42,43,43	0.39	0	51,60,60	0.49	0
21	CLA	L	303	16	50,60,73	1.50	5 (10%)	57,97,113	1.43	6 (10%)
25	BCR	F	5008	-	41,41,41	0.16	0	56,56,56	0.33	0
22	CHL	8	607	-	45,55,74	1.30	4 (8%)	48,91,114	2.34	9 (18%)
28	LHG	1	322	21	26,26,48	0.38	0	29,32,54	0.35	0
21	CLA	7	310	4	43,53,73	1.62	5 (11%)	50,89,113	1.46	6 (12%)
21	CLA	T	612	-	63,73,73	1.34	5 (7%)	74,113,113	1.31	7 (9%)
21	CLA	A	825	7	58,68,73	1.40	5 (8%)	68,107,113	1.23	7 (10%)
21	CLA	9	603	-	53,63,73	1.51	6 (11%)	62,101,113	1.49	8 (12%)
21	CLA	A	822	7	56,66,73	1.40	5 (8%)	65,104,113	1.40	7 (10%)
21	CLA	A	808	7	63,73,73	1.35	5 (7%)	74,113,113	1.37	8 (10%)
22	CHL	1	305	-	45,55,74	1.27	5 (11%)	48,91,114	1.96	11 (22%)
25	BCR	L	302	-	41,41,41	0.24	0	56,56,56	0.57	0
37	4RF	A	857	-	38,38,56	0.42	0	41,41,59	0.40	0
30	SQD	2	618	-	43,45,54	0.24	0	53,56,65	0.48	1 (1%)
21	CLA	c	610	28	43,53,73	1.62	5 (11%)	50,89,113	1.49	6 (12%)
29	PTY	L	308	-	19,19,49	0.71	0	22,24,54	0.64	0
21	CLA	B	823	-	58,68,73	1.44	8 (13%)	68,107,113	1.34	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	SF4	C	102	9	0,12,12	-	-	-		
26	LMG	A	801	-	32,32,55	0.21	0	40,40,63	0.30	0
25	BCR	I	203	-	41,41,41	0.15	0	56,56,56	0.31	0
21	CLA	9	605	6	43,53,73	1.69	7 (16%)	50,89,113	1.69	7 (14%)
21	CLA	T	606	-	44,54,73	1.66	8 (18%)	51,90,113	1.64	8 (15%)
21	CLA	1	311	-	58,68,73	1.42	5 (8%)	68,107,113	1.33	7 (10%)
21	CLA	T	611	20	50,60,73	1.59	7 (14%)	57,97,113	1.57	9 (15%)
23	LUT	2	614	-	42,43,43	0.26	0	51,60,60	0.38	0
29	PTY	a	319	-	17,17,49	0.72	0	18,21,54	0.69	0
21	CLA	O	2002	-	36,46,73	1.86	6 (16%)	45,81,113	1.65	9 (20%)
25	BCR	8	618	-	41,41,41	0.15	0	56,56,56	0.35	0
28	LHG	F	5003	-	42,42,48	0.32	0	45,48,54	0.32	0
21	CLA	8	614	5	44,54,73	1.56	5 (11%)	51,90,113	1.37	6 (11%)
21	CLA	B	820	8	58,68,73	1.47	8 (13%)	68,107,113	1.45	8 (11%)
21	CLA	T	609	20	53,63,73	1.44	6 (11%)	62,101,113	1.43	9 (14%)
21	CLA	A	833	7	53,63,73	1.45	6 (11%)	62,101,113	1.33	7 (11%)
21	CLA	b	310	5	44,54,73	1.58	5 (11%)	51,90,113	1.38	6 (11%)
21	CLA	B	839	-	53,63,73	1.49	5 (9%)	62,101,113	1.52	6 (9%)
24	XAT	7	318	-	41,47,47	0.20	0	54,74,74	0.88	3 (5%)
21	CLA	3	402	3	63,73,73	1.34	6 (9%)	74,113,113	1.32	7 (9%)
21	CLA	9	602	6	45,55,73	1.56	5 (11%)	52,91,113	1.36	7 (13%)
21	CLA	c	612	4	45,55,73	1.67	7 (15%)	52,91,113	1.47	7 (13%)
21	CLA	8	622	-	44,54,73	2.14	10 (22%)	51,90,113	2.35	12 (23%)
21	CLA	9	601	-	44,54,73	2.66	7 (15%)	51,90,113	2.94	13 (25%)
21	CLA	A	841	7	63,73,73	1.34	5 (7%)	74,113,113	1.27	8 (10%)
29	PTY	7	322	-	24,24,49	0.63	0	27,29,54	0.51	0
25	BCR	G	202	-	41,41,41	0.24	0	56,56,56	0.42	0
21	CLA	A	829	7	63,73,73	1.40	7 (11%)	74,113,113	1.36	8 (10%)
21	CLA	B	833	-	63,73,73	1.34	5 (7%)	74,113,113	1.33	8 (10%)
28	LHG	a	301	-	21,21,48	0.44	0	24,27,54	0.52	0
35	PQN	A	844	-	34,34,34	0.28	0	43,45,45	0.57	1 (2%)
24	XAT	9	614	-	41,47,47	0.15	0	54,74,74	0.68	1 (1%)
22	CHL	8	601	-	49,59,74	1.51	4 (8%)	53,96,114	1.95	11 (20%)
25	BCR	a	317	-	41,41,41	0.19	0	56,56,56	0.40	0
28	LHG	F	5001	-	30,30,48	0.36	0	33,36,54	0.33	0
21	CLA	8	603	5	48,58,73	1.52	5 (10%)	56,95,113	1.33	8 (14%)
21	CLA	b	315	5	44,54,73	1.58	5 (11%)	51,90,113	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMK	8	621	-	34,34,53	0.54	0	34,41,60	0.72	1 (2%)
29	PTY	2	620	-	31,31,49	0.57	0	34,36,54	0.46	0
21	CLA	T	604	-	45,55,73	1.56	5 (11%)	52,91,113	1.35	7 (13%)
21	CLA	H	204	-	44,54,73	1.56	4 (9%)	51,90,113	1.40	6 (11%)
21	CLA	a	305	-	43,53,73	1.66	5 (11%)	50,89,113	1.53	7 (14%)
21	CLA	B	828	-	63,73,73	1.33	5 (7%)	74,113,113	1.22	8 (10%)
21	CLA	a	302	1	63,73,73	1.34	4 (6%)	74,113,113	1.25	7 (9%)
21	CLA	J	5002	15	43,53,73	1.66	5 (11%)	50,89,113	1.67	7 (14%)
31	3PH	F	5002	-	25,25,47	0.36	0	28,30,52	0.33	0
21	CLA	F	5005	-	63,73,73	1.33	5 (7%)	74,113,113	1.27	7 (9%)
25	BCR	3	418	-	41,41,41	0.13	0	56,56,56	0.28	0
21	CLA	3	409	28	58,68,73	1.41	5 (8%)	68,107,113	1.37	8 (11%)
28	LHG	b	303	-	22,22,48	0.46	0	25,27,54	0.60	0
21	CLA	1	310	1	44,54,73	1.64	7 (15%)	51,90,113	1.58	9 (17%)
21	CLA	T	603	20	54,64,73	1.45	6 (11%)	63,102,113	1.54	8 (12%)
21	CLA	8	612	5	48,58,73	1.65	8 (16%)	56,95,113	1.59	10 (17%)
31	3PH	2	619	-	42,42,47	0.30	0	45,47,52	0.34	0
21	CLA	9	604	6	48,58,73	1.54	5 (10%)	56,95,113	1.38	7 (12%)
25	BCR	A	846	-	41,41,41	0.25	0	56,56,56	1.39	9 (16%)
24	XAT	T	616	-	41,47,47	0.14	0	54,74,74	0.90	2 (3%)
23	LUT	b	317	-	42,43,43	0.24	0	51,60,60	0.41	0
21	CLA	B	841	-	48,58,73	1.51	5 (10%)	56,95,113	1.52	8 (14%)
22	CHL	2	601	2	64,74,74	1.25	4 (6%)	71,114,114	1.95	8 (11%)
21	CLA	7	314	4	63,73,73	1.41	7 (11%)	74,113,113	1.34	7 (9%)
21	CLA	b	311	5	58,68,73	1.40	7 (12%)	68,107,113	1.33	8 (11%)
21	CLA	B	821	8	63,73,73	1.34	5 (7%)	74,113,113	1.28	6 (8%)
21	CLA	A	807	7	63,73,73	1.32	6 (9%)	74,113,113	1.21	7 (9%)
21	CLA	7	313	-	50,60,73	1.53	5 (10%)	57,97,113	1.53	7 (12%)
23	LUT	1	314	-	42,43,43	0.45	1 (2%)	51,60,60	1.16	5 (9%)
24	XAT	b	318	-	41,47,47	0.16	0	54,74,74	0.65	1 (1%)
24	XAT	c	616	-	41,47,47	0.18	0	54,74,74	0.80	2 (3%)
21	CLA	L	304	16	63,73,73	1.29	5 (7%)	74,113,113	1.28	7 (9%)
21	CLA	O	2001	17	35,46,73	1.84	6 (17%)	39,80,113	1.67	7 (17%)
21	CLA	B	816	8	63,73,73	1.35	5 (7%)	74,113,113	1.19	6 (8%)
21	CLA	B	809	8	63,73,73	1.35	5 (7%)	74,113,113	1.53	8 (10%)
25	BCR	c	617	-	41,41,41	0.16	0	56,56,56	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	312	1	43,53,73	1.64	5 (11%)	50,89,113	1.49	6 (12%)
25	BCR	F	5004	-	41,41,41	0.16	0	56,56,56	0.33	0
22	CHL	T	602	20	54,64,74	1.37	4 (7%)	59,102,114	1.86	8 (13%)
25	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.36	0
21	CLA	A	805	7	63,73,73	1.36	6 (9%)	74,113,113	1.41	8 (10%)
28	LHG	1	323	-	45,45,48	0.32	0	48,51,54	0.34	0
21	CLA	A	835	-	63,73,73	1.33	6 (9%)	74,113,113	1.25	8 (10%)
21	CLA	B	830	-	58,68,73	1.37	5 (8%)	68,107,113	1.30	7 (10%)
21	CLA	G	204	13	44,54,73	1.63	6 (13%)	51,90,113	1.45	6 (11%)
21	CLA	3	410	3	50,60,73	1.53	7 (14%)	57,97,113	1.54	8 (14%)
21	CLA	7	305	4	53,63,73	1.49	6 (11%)	62,101,113	1.46	7 (11%)
21	CLA	B	813	8	63,73,73	1.36	7 (11%)	74,113,113	1.33	7 (9%)
23	LUT	7	317	-	42,43,43	0.32	0	51,60,60	0.55	1 (1%)
26	LMG	3	421	-	40,40,55	0.19	0	48,48,63	0.17	0
21	CLA	A	806	7	58,68,73	1.39	5 (8%)	68,107,113	1.24	8 (11%)
21	CLA	9	609	28	44,54,73	1.57	4 (9%)	51,90,113	1.43	6 (11%)
29	PTY	c	619	-	30,30,49	0.58	0	33,35,54	0.46	0
21	CLA	B	826	8	53,63,73	1.44	6 (11%)	62,101,113	1.24	6 (9%)
23	LUT	c	615	-	42,43,43	0.35	0	51,60,60	0.58	1 (1%)
28	LHG	a	318	21	22,22,48	0.40	0	25,28,54	0.37	0
21	CLA	a	313	1	44,54,73	1.57	5 (11%)	51,90,113	1.43	6 (11%)
21	CLA	B	844	-	63,73,73	1.37	6 (9%)	74,113,113	1.37	6 (8%)
25	BCR	J	5003	-	41,41,41	0.17	0	56,56,56	0.26	0
21	CLA	A	818	-	53,63,73	1.50	6 (11%)	62,101,113	1.46	8 (12%)
21	CLA	1	313	1	43,53,73	1.65	6 (13%)	50,89,113	1.50	6 (12%)
23	LUT	3	415	-	42,43,43	0.29	0	51,60,60	0.54	0
21	CLA	A	815	7	63,73,73	1.32	5 (7%)	74,113,113	1.45	8 (10%)
21	CLA	c	609	4	44,54,73	1.56	5 (11%)	51,90,113	1.34	6 (11%)
25	BCR	A	851	-	41,41,41	0.17	0	56,56,56	0.35	0
21	CLA	1	306	-	48,58,73	1.55	5 (10%)	56,95,113	1.48	8 (14%)
32	DGD	7	301	-	40,40,67	0.25	0	54,54,81	0.37	0
21	CLA	A	823	-	63,73,73	1.34	5 (7%)	74,113,113	1.20	7 (9%)
21	CLA	B	819	-	63,73,73	1.32	6 (9%)	74,113,113	1.22	7 (9%)
21	CLA	A	834	7	63,73,73	1.35	5 (7%)	74,113,113	1.40	8 (10%)
21	CLA	1	308	1	58,68,73	1.37	6 (10%)	68,107,113	1.33	6 (8%)
21	CLA	8	613	5	50,60,73	1.55	6 (12%)	57,97,113	1.44	7 (12%)
32	DGD	8	602	-	48,48,67	0.20	0	62,62,81	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	T	605	-	44,54,73	1.58	6 (13%)	51,90,113	1.44	6 (11%)
26	LMG	G	207	-	43,43,55	0.19	0	51,51,63	0.13	0
21	CLA	1	303	-	48,58,73	1.47	5 (10%)	56,95,113	1.37	8 (14%)
28	LHG	2	617	21	21,21,48	0.59	0	24,26,54	0.89	2 (8%)
21	CLA	A	843	-	63,73,73	1.30	5 (7%)	74,113,113	1.34	8 (10%)
23	LUT	B	801	-	42,43,43	0.39	1 (2%)	51,60,60	0.80	2 (3%)
25	BCR	B	805	-	41,41,41	0.28	0	56,56,56	1.10	7 (12%)
21	CLA	a	314	1	48,58,73	1.51	5 (10%)	56,95,113	1.51	8 (14%)
25	BCR	B	849	-	41,41,41	0.12	0	56,56,56	0.35	0
21	CLA	A	810	7	63,73,73	1.34	5 (7%)	74,113,113	1.25	8 (10%)
21	CLA	2	603	2	58,68,73	1.47	7 (12%)	68,107,113	1.43	7 (10%)
21	CLA	A	811	7	63,73,73	1.38	7 (11%)	74,113,113	1.43	8 (10%)
21	CLA	1	302	1	58,68,73	1.40	6 (10%)	68,107,113	1.38	7 (10%)
21	CLA	A	832	7	63,73,73	1.36	6 (9%)	74,113,113	1.31	7 (9%)
21	CLA	1	321	28	63,73,73	1.38	6 (9%)	74,113,113	1.50	11 (14%)
21	CLA	A	836	-	58,68,73	1.39	5 (8%)	68,107,113	1.30	7 (10%)
29	PTY	I	201	-	37,37,49	0.63	1 (2%)	40,42,54	0.99	2 (5%)
22	CHL	b	302	-	64,74,74	1.37	4 (6%)	71,114,114	1.71	10 (14%)
21	CLA	A	821	7	63,73,73	1.34	6 (9%)	74,113,113	1.30	9 (12%)
21	CLA	2	610	2	44,54,73	1.61	7 (15%)	51,90,113	1.60	6 (11%)
32	DGD	A	802	-	67,67,67	0.17	0	81,81,81	0.15	0
25	BCR	b	319	-	41,41,41	0.16	0	56,56,56	0.32	0
23	LUT	2	616	-	42,43,43	0.25	0	51,60,60	0.37	0
21	CLA	B	812	8	63,73,73	1.33	6 (9%)	74,113,113	1.21	8 (10%)
25	BCR	A	847	-	41,41,41	0.32	0	56,56,56	0.88	2 (3%)
23	LUT	8	616	-	42,43,43	0.25	0	51,60,60	0.36	0
22	CHL	3	401	3	64,74,74	1.17	4 (6%)	71,114,114	1.85	7 (9%)
21	CLA	2	613	-	63,73,73	1.34	5 (7%)	74,113,113	1.28	7 (9%)
21	CLA	A	826	7	58,68,73	1.43	6 (10%)	68,107,113	1.30	7 (10%)
21	CLA	A	814	7	60,70,73	1.40	6 (10%)	70,109,113	1.23	8 (11%)
21	CLA	L	305	-	48,58,73	1.56	6 (12%)	56,95,113	1.51	6 (10%)
21	CLA	b	312	-	44,54,73	1.60	5 (11%)	51,90,113	1.45	6 (11%)
21	CLA	3	412	3	53,63,73	1.45	6 (11%)	62,101,113	1.21	6 (9%)
21	CLA	B	806	-	63,73,73	1.37	7 (11%)	74,113,113	1.32	8 (10%)
25	BCR	I	202	-	41,41,41	0.13	0	56,56,56	0.43	0
21	CLA	B	822	8	63,73,73	1.30	5 (7%)	74,113,113	1.26	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	608	2	43,53,73	1.61	5 (11%)	50,89,113	1.46	6 (12%)
22	CHL	T	601	4	46,56,74	1.64	4 (8%)	49,92,114	2.39	10 (20%)
21	CLA	B	811	8	53,63,73	1.47	6 (11%)	62,101,113	1.36	6 (9%)
22	CHL	c	605	-	44,54,74	1.53	5 (11%)	47,90,114	2.51	8 (17%)
21	CLA	B	832	8	63,73,73	1.39	7 (11%)	74,113,113	1.29	8 (10%)
21	CLA	B	842	-	63,73,73	1.40	7 (11%)	74,113,113	1.33	7 (9%)
21	CLA	K	202	-	53,63,73	1.46	5 (9%)	62,101,113	1.28	8 (12%)
28	LHG	B	802	-	31,31,48	0.35	0	34,37,54	0.34	0
29	PTY	H	201	-	41,41,49	0.50	0	44,46,54	0.48	0
29	PTY	8	619	-	20,20,49	0.65	0	21,24,54	0.55	0
25	BCR	T	617	-	41,41,41	0.13	0	56,56,56	0.28	0
26	LMG	F	5009	-	39,39,55	0.18	0	47,47,63	0.15	0
21	CLA	B	825	8	58,68,73	1.40	5 (8%)	68,107,113	1.35	7 (10%)
21	CLA	B	817	8	63,73,73	1.37	6 (9%)	74,113,113	1.38	7 (9%)
21	CLA	b	305	5	61,71,73	1.40	6 (9%)	71,110,113	1.42	9 (12%)
28	LHG	1	319	21	24,24,48	0.40	0	27,30,54	0.37	0
21	CLA	3	407	3	63,73,73	1.37	6 (9%)	74,113,113	1.26	7 (9%)
21	CLA	B	808	8	46,56,73	1.56	5 (10%)	53,92,113	1.39	7 (13%)
25	BCR	G	206	-	41,41,41	0.19	0	56,56,56	0.56	0
21	CLA	8	604	5	49,59,73	1.53	6 (12%)	56,96,113	1.50	8 (14%)
29	PTY	B	803	-	26,26,49	0.61	0	29,31,54	0.48	0
22	CHL	a	306	-	45,55,74	1.45	5 (11%)	48,91,114	2.06	10 (20%)
21	CLA	A	856	7	59,69,73	1.40	6 (10%)	69,108,113	1.35	7 (10%)
21	CLA	B	837	-	58,68,73	1.41	5 (8%)	68,107,113	1.37	7 (10%)
25	BCR	B	847	-	41,41,41	0.19	0	56,56,56	0.40	0
21	CLA	c	614	4	43,53,73	1.63	4 (9%)	50,89,113	1.43	6 (12%)
21	CLA	B	843	8	63,73,73	1.37	7 (11%)	74,113,113	1.17	7 (9%)
21	CLA	K	203	19	43,53,73	1.69	8 (18%)	50,89,113	1.65	8 (16%)
21	CLA	A	804	-	63,73,73	1.42	8 (12%)	74,113,113	1.26	6 (8%)
29	PTY	B	851	-	22,25,49	0.46	0	23,28,54	0.27	0
32	DGD	B	850	-	62,62,67	0.18	0	76,76,81	0.22	0
21	CLA	8	609	5	44,54,73	1.63	7 (15%)	51,90,113	1.37	6 (11%)
21	CLA	a	304	-	48,58,73	1.49	5 (10%)	56,95,113	1.41	8 (14%)
21	CLA	8	605	-	44,54,73	1.61	6 (13%)	51,90,113	1.58	6 (11%)
28	LHG	A	852	21	29,29,48	0.35	0	33,35,54	0.47	0
24	XAT	1	315	-	41,47,47	0.16	0	54,74,74	0.98	3 (5%)
21	CLA	2	607	-	44,54,73	1.62	5 (11%)	51,90,113	1.41	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	K	205	-	41,41,41	0.31	0	56,56,56	0.77	2 (3%)
28	LHG	H	202	-	48,48,48	0.29	0	51,54,54	0.29	0
21	CLA	b	316	5	43,53,73	1.65	5 (11%)	50,89,113	1.44	6 (12%)
25	BCR	B	852	-	41,41,41	0.24	0	56,56,56	1.28	6 (10%)
21	CLA	A	831	7	63,73,73	1.36	7 (11%)	74,113,113	1.31	7 (9%)
28	LHG	b	301	-	30,30,48	0.35	0	33,36,54	0.34	0
21	CLA	A	827	-	63,73,73	1.40	6 (9%)	74,113,113	1.44	7 (9%)
21	CLA	7	311	4	63,73,73	1.30	5 (7%)	74,113,113	1.22	8 (10%)
21	CLA	c	613	4	48,58,73	1.55	5 (10%)	56,95,113	1.48	8 (14%)
28	LHG	c	618	21	28,28,48	0.37	0	31,34,54	0.34	0
21	CLA	B	838	-	48,58,73	1.53	5 (10%)	56,95,113	1.49	8 (14%)
22	CHL	2	606	-	45,55,74	1.36	5 (11%)	48,91,114	2.30	8 (16%)
23	LUT	2	615	-	42,43,43	0.25	0	51,60,60	0.43	0
21	CLA	A	813	7	63,73,73	1.34	6 (9%)	74,113,113	1.20	7 (9%)
21	CLA	F	5007	-	47,57,73	1.55	5 (10%)	53,93,113	1.50	7 (13%)
24	XAT	a	316	-	41,47,47	0.20	0	54,74,74	1.09	6 (11%)
21	CLA	9	610	6	43,53,73	1.71	7 (16%)	50,89,113	1.59	8 (16%)
24	XAT	8	617	-	41,47,47	0.17	0	54,74,74	0.65	1 (1%)
21	CLA	2	611	-	58,68,73	1.40	6 (10%)	68,107,113	1.39	6 (8%)
27	LMU	A	854	-	36,36,36	0.18	0	47,47,47	0.35	0
21	CLA	K	201	-	43,53,73	1.66	6 (13%)	50,89,113	1.60	6 (12%)
21	CLA	8	615	5	43,53,73	1.63	5 (11%)	50,89,113	1.35	6 (12%)
34	CL0	A	803	7	63,73,73	1.09	4 (6%)	74,113,113	1.83	10 (13%)
36	SF4	A	845	8,7	0,12,12	-	-	-		
25	BCR	O	2004	-	41,41,41	0.20	0	56,56,56	0.73	2 (3%)
21	CLA	B	827	-	63,73,73	1.31	6 (9%)	74,113,113	1.45	10 (13%)
21	CLA	B	829	8	63,73,73	1.41	6 (9%)	74,113,113	1.34	7 (9%)
21	CLA	9	608	6	58,68,73	1.38	5 (8%)	68,107,113	1.26	7 (10%)
21	CLA	A	820	7	59,69,73	1.42	6 (10%)	69,108,113	1.40	7 (10%)
21	CLA	T	608	20	43,53,73	1.67	6 (13%)	50,89,113	1.62	6 (12%)
21	CLA	9	612	6	44,54,73	1.61	6 (13%)	51,90,113	1.44	6 (11%)
22	CHL	8	608	-	49,59,74	1.35	5 (10%)	53,96,114	2.39	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	807	-	1/1/15/20	15/37/115/115	-
21	CLA	G	201	8	1/1/15/20	14/37/115/115	-
21	CLA	3	406	-	1/1/13/20	6/25/103/115	-
21	CLA	2	602	2	1/1/15/20	13/37/115/115	-
23	LUT	9	613	-	3/3/12/27	1/29/67/67	0/2/2/2
21	CLA	A	842	28	1/1/12/20	7/24/102/115	-
29	PTY	1	320	-	-	9/23/23/53	-
21	CLA	3	403	-	1/1/12/20	5/19/97/115	-
21	CLA	A	812	7	1/1/13/20	7/25/103/115	-
21	CLA	3	408	3	1/1/14/20	11/31/109/115	-
21	CLA	a	308	1	1/1/12/20	11/19/97/115	-
23	LUT	O	2005	-	3/3/12/27	4/29/67/67	0/2/2/2
21	CLA	c	611	-	1/1/11/20	4/15/93/115	-
21	CLA	B	831	8	1/1/15/20	23/37/115/115	-
21	CLA	3	405	3	1/1/12/20	5/19/97/115	-
24	XAT	9	615	-	-	4/31/93/93	0/4/4/4
21	CLA	A	839	7	1/1/15/20	9/37/115/115	-
21	CLA	3	404	-	1/1/11/20	5/15/93/115	-
21	CLA	7	306	-	1/1/12/20	4/19/97/115	-
21	CLA	c	604	-	1/1/12/20	4/19/97/115	-
21	CLA	c	603	4	1/1/12/20	5/21/99/115	-
22	CHL	c	607	-	2/2/16/26	4/18/116/137	-
21	CLA	T	607	-	1/1/12/20	7/19/97/115	-
21	CLA	A	824	7	1/1/14/20	10/31/109/115	-
28	LHG	9	617	21	-	10/32/32/53	-
22	CHL	7	303	-	3/3/20/26	11/39/137/137	-
21	CLA	b	306	-	1/1/12/20	7/19/97/115	-
27	LMU	9	616	-	-	6/21/61/61	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	838	7	1/1/12/20	7/21/99/115	-
30	SQD	3	422	-	-	11/30/50/69	0/1/1/1
21	CLA	8	610	5	1/1/14/20	12/31/109/115	-
21	CLA	A	837	7	1/1/11/20	5/16/94/115	-
28	LHG	3	424	-	-	9/30/30/53	-
21	CLA	a	303	1	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHL	8	606	-	1/1/16/26	6/15/113/137	-
21	CLA	A	809	-	1/1/14/20	7/31/109/115	-
29	PTY	c	620	-	-	7/29/29/53	-
25	BCR	B	846	-	-	2/29/63/63	0/2/2/2
21	CLA	7	323	5	1/1/11/20	6/15/93/115	-
22	CHL	7	308	-	1/1/16/26	4/15/113/137	-
21	CLA	3	413	-	1/1/10/20	4/10/88/115	-
21	CLA	A	828	-	1/1/13/20	10/28/106/115	-
21	CLA	B	818	-	1/1/15/20	14/37/115/115	-
22	CHL	9	606	-	1/1/16/26	6/17/115/137	-
21	CLA	3	411	3	1/1/14/20	8/31/109/115	-
21	CLA	B	815	-	1/1/13/20	6/25/103/115	-
25	BCR	7	319	-	-	4/29/63/63	0/2/2/2
36	SF4	C	101	9	-	-	0/6/5/5
21	CLA	G	205	-	1/1/11/20	4/13/91/115	-
21	CLA	A	830	7	1/1/15/20	17/37/115/115	-
21	CLA	a	311	1	1/1/11/20	6/15/93/115	-
21	CLA	b	314	5	1/1/12/20	5/19/97/115	-
21	CLA	9	611	-	1/1/11/20	3/15/93/115	-
21	CLA	B	834	8	1/1/14/20	7/31/109/115	-
21	CLA	L	301	7	1/1/12/20	2/19/97/115	-
26	LMG	7	320	-	-	3/42/62/70	0/1/1/1
21	CLA	7	312	28	1/1/11/20	4/13/91/115	-
21	CLA	B	810	8	1/1/15/20	12/37/115/115	-
21	CLA	c	601	5	1/1/11/20	6/15/93/115	-
21	CLA	b	313	5	1/1/12/20	8/19/97/115	-
21	CLA	9	607	6	1/1/15/20	16/37/115/115	-
21	CLA	2	612	2	1/1/11/20	3/13/91/115	-
21	CLA	1	301	1	1/1/14/20	10/33/111/115	-
21	CLA	1	304	-	1/1/11/20	4/13/91/115	-
29	PTY	3	423	-	-	1/16/18/53	-
21	CLA	B	835	8	1/1/15/20	11/37/115/115	-
21	CLA	B	836	8	1/1/13/20	12/25/103/115	-
21	CLA	A	816	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	8	620	21	-	11/44/44/53	-
21	CLA	T	613	-	1/1/11/20	8/15/93/115	-
21	CLA	A	840	7	1/1/14/20	5/31/109/115	-
21	CLA	O	2003	-	1/1/11/20	9/13/91/115	-
25	BCR	L	307	-	-	0/29/63/63	0/2/2/2
25	BCR	L	309	-	-	4/29/63/63	0/2/2/2
21	CLA	1	307	1	1/1/12/20	6/19/97/115	-
21	CLA	7	316	4	1/1/15/20	8/37/115/115	-
21	CLA	H	203	14	1/1/14/20	10/31/109/115	-
21	CLA	3	414	3	1/1/11/20	3/15/93/115	-
21	CLA	B	814	8	1/1/14/20	9/31/109/115	-
28	LHG	A	853	-	-	10/49/49/53	-
29	PTY	7	302	-	-	10/29/29/53	-
22	CHL	b	307	-	1/1/16/26	7/17/115/137	-
22	CHL	b	309	-	2/2/17/26	5/21/119/137	-
25	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	BCR	J	5004	-	-	2/29/63/63	0/2/2/2
28	LHG	7	321	21	-	11/47/47/53	-
21	CLA	T	610	-	1/1/11/20	3/15/93/115	-
21	CLA	K	204	-	1/1/11/20	8/17/95/115	-
21	CLA	L	306	-	1/1/12/20	9/19/97/115	-
21	CLA	a	310	28	1/1/11/20	6/15/93/115	-
22	CHL	b	308	-	1/1/16/26	2/17/115/137	-
23	LUT	a	315	-	3/3/12/27	8/29/67/67	0/2/2/2
26	LMG	1	317	-	-	5/23/40/70	1/1/1/1
25	BCR	A	848	-	-	3/29/63/63	0/2/2/2
21	CLA	c	608	-	1/1/11/20	4/13/91/115	-
21	CLA	B	840	8	1/1/14/20	7/31/109/115	-
21	CLA	A	819	7	1/1/14/20	14/31/109/115	-
21	CLA	a	312	-	1/1/14/20	9/31/109/115	-
21	CLA	2	605	-	1/1/11/20	6/13/91/115	-
35	PQN	B	845	-	-	9/23/43/43	0/2/2/2
21	CLA	7	315	4	1/1/12/20	7/19/97/115	-
21	CLA	8	611	28	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	609	28	1/1/10/20	2/8/86/115	-
21	CLA	T	614	-	1/1/10/20	4/10/88/115	-
29	PTY	J	5001	-	-	6/25/25/53	-
21	CLA	c	602	4	1/1/12/20	7/22/100/115	-
22	CHL	7	309	-	2/2/16/26	7/18/116/137	-
25	BCR	1	316	-	-	4/29/63/63	0/2/2/2
21	CLA	F	5006	-	1/1/11/20	6/16/94/115	-
21	CLA	7	304	4	1/1/14/20	11/31/109/115	-
25	BCR	3	419	-	-	5/29/63/63	0/2/2/2
21	CLA	2	604	-	1/1/12/20	7/19/97/115	-
22	CHL	c	606	-	1/1/16/26	4/18/116/137	-
21	CLA	G	203	13	1/1/11/20	5/16/94/115	-
27	LMU	A	855	-	-	7/21/61/61	0/2/2/2
28	LHG	7	324	-	-	15/35/35/53	-
28	LHG	3	420	21	-	11/19/19/53	-
22	CHL	7	307	-	1/1/16/26	5/15/113/137	-
21	CLA	B	804	-	1/1/15/20	13/37/115/115	-
21	CLA	1	309	28	1/1/11/20	7/15/93/115	-
21	CLA	a	307	-	1/1/11/20	4/13/91/115	-
21	CLA	a	309	1	1/1/14/20	14/31/109/115	-
21	CLA	B	824	8	1/1/13/20	9/25/103/115	-
27	LMU	1	318	-	-	9/21/61/61	0/2/2/2
21	CLA	A	817	7	1/1/15/20	18/37/115/115	-
25	BCR	3	417	-	-	4/29/63/63	0/2/2/2
24	XAT	3	416	-	-	2/31/93/93	0/4/4/4
21	CLA	b	304	5	1/1/14/20	12/31/109/115	-
23	LUT	T	615	-	3/3/12/27	1/29/67/67	0/2/2/2
21	CLA	L	303	16	1/1/12/20	6/22/100/115	-
25	BCR	F	5008	-	-	4/29/63/63	0/2/2/2
22	CHL	8	607	-	1/1/16/26	6/17/115/137	-
28	LHG	1	322	21	-	9/31/31/53	-
21	CLA	7	310	4	1/1/11/20	4/13/91/115	-
21	CLA	T	612	-	1/1/15/20	14/37/115/115	-
21	CLA	A	825	7	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	603	-	1/1/13/20	5/25/103/115	-
21	CLA	A	822	7	1/1/13/20	12/29/107/115	-
21	CLA	A	808	7	1/1/15/20	14/37/115/115	-
22	CHL	1	305	-	2/2/16/26	7/17/115/137	-
25	BCR	L	302	-	-	12/29/63/63	0/2/2/2
37	4RF	A	857	-	-	10/41/41/59	-
30	SQD	2	618	-	-	13/40/60/69	0/1/1/1
21	CLA	c	610	28	1/1/11/20	5/13/91/115	-
29	PTY	L	308	-	-	11/22/22/53	-
21	CLA	B	823	-	1/1/14/20	8/31/109/115	-
36	SF4	C	102	9	-	-	0/6/5/5
26	LMG	A	801	-	-	10/26/46/70	0/1/1/1
25	BCR	I	203	-	-	4/29/63/63	0/2/2/2
21	CLA	9	605	6	1/1/11/20	4/13/91/115	-
21	CLA	T	606	-	-	6/15/93/115	-
21	CLA	1	311	-	1/1/14/20	9/31/109/115	-
21	CLA	T	611	20	1/1/12/20	5/22/100/115	-
23	LUT	2	614	-	3/3/12/27	2/29/67/67	0/2/2/2
29	PTY	a	319	-	-	12/19/19/53	-
21	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
25	BCR	8	618	-	-	4/29/63/63	0/2/2/2
28	LHG	F	5003	-	-	14/47/47/53	-
21	CLA	8	614	5	1/1/11/20	5/15/93/115	-
21	CLA	B	820	8	1/1/14/20	7/31/109/115	-
21	CLA	T	609	20	1/1/13/20	7/25/103/115	-
21	CLA	A	833	7	1/1/13/20	4/25/103/115	-
21	CLA	b	310	5	1/1/11/20	4/15/93/115	-
21	CLA	B	839	-	1/1/13/20	8/25/103/115	-
24	XAT	7	318	-	-	2/31/93/93	0/4/4/4
21	CLA	3	402	3	1/1/15/20	14/37/115/115	-
21	CLA	9	602	6	1/1/11/20	9/16/94/115	-
21	CLA	c	612	4	1/1/11/20	5/16/94/115	-
21	CLA	8	622	-	1/1/11/20	5/15/93/115	-
21	CLA	9	601	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	841	7	1/1/15/20	12/37/115/115	-
29	PTY	7	322	-	-	6/28/28/53	-
25	BCR	G	202	-	-	5/29/63/63	0/2/2/2
21	CLA	A	829	7	1/1/15/20	14/37/115/115	-
21	CLA	B	833	-	1/1/15/20	12/37/115/115	-
28	LHG	a	301	-	-	10/25/25/53	-
35	PQN	A	844	-	-	0/23/43/43	0/2/2/2
24	XAT	9	614	-	-	0/31/93/93	0/4/4/4
22	CHL	8	601	-	1/1/17/26	8/21/119/137	-
25	BCR	a	317	-	-	5/29/63/63	0/2/2/2
28	LHG	F	5001	-	-	12/35/35/53	-
21	CLA	8	603	5	1/1/12/20	7/19/97/115	-
21	CLA	b	315	5	1/1/11/20	5/15/93/115	-
33	LMK	8	621	-	-	6/41/41/60	-
29	PTY	2	620	-	-	8/35/35/53	-
21	CLA	T	604	-	1/1/11/20	9/16/94/115	-
21	CLA	H	204	-	1/1/11/20	3/15/93/115	-
21	CLA	a	305	-	1/1/11/20	3/13/91/115	-
21	CLA	B	828	-	1/1/15/20	8/37/115/115	-
21	CLA	a	302	1	1/1/15/20	12/37/115/115	-
21	CLA	J	5002	15	1/1/11/20	5/13/91/115	-
31	3PH	F	5002	-	-	1/27/27/49	-
21	CLA	F	5005	-	1/1/15/20	15/37/115/115	-
25	BCR	3	418	-	-	4/29/63/63	0/2/2/2
21	CLA	3	409	28	1/1/14/20	11/31/109/115	-
28	LHG	b	303	-	-	8/26/26/53	-
21	CLA	1	310	1	1/1/11/20	6/15/93/115	-
21	CLA	T	603	20	1/1/13/20	10/27/105/115	-
21	CLA	8	612	5	1/1/12/20	7/19/97/115	-
31	3PH	2	619	-	-	13/44/44/49	-
21	CLA	9	604	6	1/1/12/20	5/19/97/115	-
25	BCR	A	846	-	-	6/29/63/63	0/2/2/2
24	XAT	T	616	-	-	3/31/93/93	0/4/4/4
23	LUT	b	317	-	3/3/12/27	2/29/67/67	0/2/2/2
21	CLA	B	841	-	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHL	2	601	2	2/2/20/26	18/39/137/137	-
21	CLA	7	314	4	1/1/15/20	8/37/115/115	-
21	CLA	b	311	5	1/1/14/20	8/31/109/115	-
21	CLA	B	821	8	1/1/15/20	16/37/115/115	-
21	CLA	A	807	7	1/1/15/20	12/37/115/115	-
21	CLA	7	313	-	1/1/12/20	6/22/100/115	-
23	LUT	1	314	-	3/3/12/27	10/29/67/67	0/2/2/2
24	XAT	b	318	-	-	1/31/93/93	0/4/4/4
24	XAT	c	616	-	-	3/31/93/93	0/4/4/4
21	CLA	L	304	16	1/1/15/20	8/37/115/115	-
21	CLA	O	2001	17	1/1/9/20	1/4/78/115	-
21	CLA	B	816	8	1/1/15/20	11/37/115/115	-
21	CLA	B	809	8	1/1/15/20	17/37/115/115	-
25	BCR	c	617	-	-	4/29/63/63	0/2/2/2
21	CLA	1	312	1	1/1/11/20	5/13/91/115	-
25	BCR	F	5004	-	-	0/29/63/63	0/2/2/2
22	CHL	T	602	20	2/2/18/26	16/27/125/137	-
25	BCR	A	850	-	-	2/29/63/63	0/2/2/2
21	CLA	A	805	7	1/1/15/20	11/37/115/115	-
28	LHG	1	323	-	-	12/50/50/53	-
21	CLA	A	835	-	1/1/15/20	17/37/115/115	-
21	CLA	B	830	-	1/1/14/20	13/31/109/115	-
21	CLA	G	204	13	1/1/11/20	7/15/93/115	-
21	CLA	3	410	3	1/1/12/20	6/22/100/115	-
21	CLA	7	305	4	1/1/13/20	11/25/103/115	-
21	CLA	B	813	8	1/1/15/20	6/37/115/115	-
23	LUT	7	317	-	3/3/12/27	2/29/67/67	0/2/2/2
26	LMG	3	421	-	-	11/35/55/70	0/1/1/1
21	CLA	A	806	7	1/1/14/20	9/31/109/115	-
21	CLA	9	609	28	1/1/11/20	7/15/93/115	-
29	PTY	c	619	-	-	10/34/34/53	-
21	CLA	B	826	8	1/1/13/20	10/25/103/115	-
23	LUT	c	615	-	3/3/12/27	2/29/67/67	0/2/2/2
28	LHG	a	318	21	-	3/26/26/53	-
21	CLA	a	313	1	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	844	-	1/1/15/20	13/37/115/115	-
25	BCR	J	5003	-	-	4/29/63/63	0/2/2/2
21	CLA	A	818	-	1/1/13/20	11/25/103/115	-
21	CLA	1	313	1	1/1/11/20	7/13/91/115	-
23	LUT	3	415	-	3/3/12/27	5/29/67/67	0/2/2/2
21	CLA	A	815	7	-	16/37/115/115	-
21	CLA	c	609	4	1/1/11/20	5/15/93/115	-
25	BCR	A	851	-	-	4/29/63/63	0/2/2/2
21	CLA	1	306	-	1/1/12/20	8/19/97/115	-
32	DGD	7	301	-	-	10/28/68/95	0/2/2/2
21	CLA	A	823	-	1/1/15/20	11/37/115/115	-
21	CLA	B	819	-	1/1/15/20	12/37/115/115	-
21	CLA	A	834	7	1/1/15/20	4/37/115/115	-
21	CLA	1	308	1	1/1/14/20	10/31/109/115	-
21	CLA	8	613	5	1/1/12/20	7/22/100/115	-
32	DGD	8	602	-	-	10/36/76/95	0/2/2/2
21	CLA	T	605	-	1/1/11/20	6/15/93/115	-
26	LMG	G	207	-	-	5/37/57/70	0/1/1/1
21	CLA	1	303	-	1/1/12/20	7/19/97/115	-
28	LHG	2	617	21	-	3/23/23/53	-
21	CLA	A	843	-	1/1/15/20	12/37/115/115	-
23	LUT	B	801	-	3/3/12/27	5/29/67/67	0/2/2/2
25	BCR	B	805	-	-	5/29/63/63	0/2/2/2
21	CLA	a	314	1	1/1/12/20	5/19/97/115	-
25	BCR	B	849	-	-	1/29/63/63	0/2/2/2
21	CLA	A	810	7	1/1/15/20	13/37/115/115	-
21	CLA	2	603	2	1/1/14/20	10/31/109/115	-
21	CLA	A	811	7	1/1/15/20	12/37/115/115	-
21	CLA	1	302	1	1/1/14/20	14/31/109/115	-
21	CLA	A	832	7	1/1/15/20	9/37/115/115	-
21	CLA	1	321	28	1/1/15/20	9/37/115/115	-
21	CLA	A	836	-	1/1/14/20	9/31/109/115	-
29	PTY	I	201	-	-	11/39/39/53	-
22	CHL	b	302	-	2/2/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	821	7	1/1/15/20	11/37/115/115	-
21	CLA	2	610	2	1/1/11/20	5/15/93/115	-
32	DGD	A	802	-	-	12/55/95/95	0/2/2/2
25	BCR	b	319	-	-	2/29/63/63	0/2/2/2
23	LUT	2	616	-	3/3/12/27	4/29/67/67	0/2/2/2
21	CLA	B	812	8	1/1/15/20	8/37/115/115	-
25	BCR	A	847	-	-	7/29/63/63	0/2/2/2
23	LUT	8	616	-	3/3/12/27	1/29/67/67	0/2/2/2
22	CHL	3	401	3	2/2/20/26	17/39/137/137	-
21	CLA	2	613	-	1/1/15/20	14/37/115/115	-
21	CLA	A	826	7	1/1/14/20	8/31/109/115	-
21	CLA	A	814	7	1/1/14/20	12/34/112/115	-
21	CLA	L	305	-	1/1/12/20	0/19/97/115	-
21	CLA	b	312	-	1/1/11/20	5/15/93/115	-
21	CLA	3	412	3	1/1/13/20	8/25/103/115	-
21	CLA	B	806	-	1/1/15/20	18/37/115/115	-
25	BCR	I	202	-	-	4/29/63/63	0/2/2/2
21	CLA	B	822	8	1/1/15/20	15/37/115/115	-
21	CLA	2	608	2	1/1/11/20	3/13/91/115	-
22	CHL	T	601	4	2/2/16/26	5/18/116/137	-
21	CLA	B	811	8	1/1/13/20	7/25/103/115	-
22	CHL	c	605	-	1/1/16/26	7/15/113/137	-
21	CLA	B	832	8	1/1/15/20	16/37/115/115	-
21	CLA	B	842	-	1/1/15/20	9/37/115/115	-
21	CLA	K	202	-	1/1/13/20	7/25/103/115	-
28	LHG	B	802	-	-	7/36/36/53	-
29	PTY	H	201	-	-	16/45/45/53	-
29	PTY	8	619	-	-	4/23/23/53	-
25	BCR	T	617	-	-	4/29/63/63	0/2/2/2
26	LMG	F	5009	-	-	6/34/54/70	0/1/1/1
21	CLA	B	825	8	1/1/14/20	11/31/109/115	-
21	CLA	B	817	8	1/1/15/20	19/37/115/115	-
21	CLA	b	305	5	1/1/15/20	15/31/109/115	-
28	LHG	1	319	21	-	2/29/29/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	407	3	1/1/15/20	12/37/115/115	-
21	CLA	B	808	8	1/1/11/20	6/17/95/115	-
25	BCR	G	206	-	-	6/29/63/63	0/2/2/2
21	CLA	8	604	5	1/1/12/20	9/21/99/115	-
29	PTY	B	803	-	-	9/30/30/53	-
22	CHL	a	306	-	2/2/16/26	4/17/115/137	-
21	CLA	A	856	7	1/1/14/20	9/33/111/115	-
21	CLA	B	837	-	1/1/14/20	11/31/109/115	-
25	BCR	B	847	-	-	4/29/63/63	0/2/2/2
21	CLA	c	614	4	1/1/11/20	4/13/91/115	-
21	CLA	B	843	8	1/1/15/20	12/37/115/115	-
21	CLA	K	203	19	1/1/11/20	6/13/91/115	-
21	CLA	A	804	-	1/1/15/20	10/37/115/115	-
29	PTY	B	851	-	-	7/25/27/53	-
32	DGD	B	850	-	-	8/50/90/95	0/2/2/2
21	CLA	8	609	5	1/1/11/20	5/15/93/115	-
21	CLA	a	304	-	1/1/12/20	7/19/97/115	-
21	CLA	8	605	-	1/1/11/20	6/15/93/115	-
28	LHG	A	852	21	-	8/33/33/53	-
24	XAT	1	315	-	-	2/31/93/93	0/4/4/4
21	CLA	2	607	-	1/1/11/20	9/15/93/115	-
25	BCR	K	205	-	-	11/29/63/63	0/2/2/2
28	LHG	H	202	-	-	6/53/53/53	-
21	CLA	b	316	5	1/1/11/20	6/13/91/115	-
25	BCR	B	852	-	-	8/29/63/63	0/2/2/2
21	CLA	A	831	7	1/1/15/20	10/37/115/115	-
28	LHG	b	301	-	-	7/35/35/53	-
21	CLA	A	827	-	1/1/15/20	9/37/115/115	-
21	CLA	7	311	4	1/1/15/20	12/37/115/115	-
21	CLA	c	613	4	1/1/12/20	7/19/97/115	-
28	LHG	c	618	21	-	9/33/33/53	-
21	CLA	B	838	-	1/1/12/20	8/19/97/115	-
22	CHL	2	606	-	2/2/16/26	5/17/115/137	-
23	LUT	2	615	-	3/3/12/27	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	813	7	1/1/15/20	10/37/115/115	-
21	CLA	F	5007	-	1/1/11/20	6/18/96/115	-
24	XAT	a	316	-	-	5/31/93/93	0/4/4/4
21	CLA	9	610	6	1/1/11/20	8/13/91/115	-
24	XAT	8	617	-	-	1/31/93/93	0/4/4/4
21	CLA	2	611	-	1/1/14/20	9/31/109/115	-
27	LMU	A	854	-	-	3/21/61/61	0/2/2/2
21	CLA	K	201	-	1/1/11/20	4/13/91/115	-
21	CLA	8	615	5	1/1/11/20	4/13/91/115	-
34	CL0	A	803	7	-	12/37/135/135	-
36	SF4	A	845	8,7	-	-	0/6/5/5
25	BCR	O	2004	-	-	5/29/63/63	0/2/2/2
21	CLA	B	827	-	1/1/15/20	10/37/115/115	-
21	CLA	B	829	8	1/1/15/20	3/37/115/115	-
21	CLA	9	608	6	1/1/14/20	10/31/109/115	-
21	CLA	A	820	7	1/1/14/20	11/33/111/115	-
21	CLA	T	608	20	1/1/11/20	8/13/91/115	-
21	CLA	9	612	6	1/1/11/20	7/15/93/115	-
22	CHL	8	608	-	2/2/17/26	6/21/119/137	-

All (1356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	601	CLA	MG-NA	12.48	2.35	2.06
22	8	601	CHL	MG-NA	7.94	2.25	2.06
21	9	601	CLA	CHB-C4A	7.85	1.40	1.33
22	b	302	CHL	MG-NA	7.80	2.24	2.06
22	7	303	CHL	MG-NA	7.18	2.23	2.06
22	T	601	CHL	MG-NA	7.12	2.23	2.06
22	7	307	CHL	MG-NA	7.09	2.23	2.06
22	c	605	CHL	MG-NA	7.09	2.23	2.06
22	a	306	CHL	MG-NA	7.01	2.22	2.06
22	c	607	CHL	MG-NC	6.90	2.22	2.06
21	B	807	CLA	CHB-C4A	6.80	1.39	1.33
21	A	804	CLA	CHB-C4A	6.72	1.39	1.33
21	8	622	CLA	MG-ND	-6.69	1.92	2.05
22	T	601	CHL	MG-NC	6.56	2.21	2.06
21	A	832	CLA	CHB-C4A	6.53	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	309	CHL	MG-NC	6.49	2.21	2.06
22	T	602	CHL	MG-NC	6.47	2.21	2.06
21	B	820	CLA	CHB-C4A	6.45	1.39	1.33
21	2	603	CLA	CHB-C4A	6.41	1.39	1.33
21	9	607	CLA	CHB-C4A	6.39	1.39	1.33
21	G	205	CLA	CHB-C4A	6.39	1.39	1.33
22	7	303	CHL	MG-NC	6.38	2.21	2.06
21	7	306	CLA	CHB-C4A	6.38	1.39	1.33
21	B	840	CLA	CHB-C4A	6.37	1.39	1.33
22	2	601	CHL	MG-NC	6.36	2.21	2.06
21	2	607	CLA	CHB-C4A	6.36	1.39	1.33
21	A	805	CLA	CHB-C4A	6.35	1.39	1.33
21	K	201	CLA	CHB-C4A	6.33	1.38	1.33
21	1	307	CLA	CHB-C4A	6.33	1.38	1.33
21	T	610	CLA	CHB-C4A	6.32	1.38	1.33
21	9	611	CLA	CHB-C4A	6.31	1.38	1.33
21	b	314	CLA	CHB-C4A	6.30	1.38	1.33
21	2	611	CLA	CHB-C4A	6.30	1.38	1.33
21	9	610	CLA	CHB-C4A	6.29	1.38	1.33
21	T	611	CLA	CHB-C4A	6.29	1.38	1.33
21	A	811	CLA	CHB-C4A	6.28	1.38	1.33
21	A	827	CLA	CHB-C4A	6.28	1.38	1.33
21	c	611	CLA	CHB-C4A	6.28	1.38	1.33
22	8	608	CHL	MG-NA	6.28	2.21	2.06
21	B	843	CLA	CHB-C4A	6.27	1.38	1.33
21	2	612	CLA	CHB-C4A	6.27	1.38	1.33
21	T	605	CLA	CHB-C4A	6.26	1.38	1.33
21	b	313	CLA	CHB-C4A	6.25	1.38	1.33
21	A	826	CLA	CHB-C4A	6.24	1.38	1.33
21	c	608	CLA	CHB-C4A	6.24	1.38	1.33
21	1	304	CLA	CHB-C4A	6.23	1.38	1.33
21	A	819	CLA	CHB-C4A	6.23	1.38	1.33
21	B	825	CLA	CHB-C4A	6.22	1.38	1.33
21	T	613	CLA	CHB-C4A	6.22	1.38	1.33
21	c	614	CLA	CHB-C4A	6.22	1.38	1.33
21	3	414	CLA	CHB-C4A	6.22	1.38	1.33
21	L	305	CLA	CHB-C4A	6.22	1.38	1.33
22	b	309	CHL	MG-NA	6.22	2.21	2.06
21	1	311	CLA	CHB-C4A	6.21	1.38	1.33
21	9	604	CLA	CHB-C4A	6.21	1.38	1.33
21	A	835	CLA	CHB-C4A	6.21	1.38	1.33
21	b	312	CLA	CHB-C4A	6.21	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	609	CLA	CHB-C4A	6.21	1.38	1.33
21	3	409	CLA	CHB-C4A	6.21	1.38	1.33
21	B	837	CLA	CHB-C4A	6.20	1.38	1.33
21	A	809	CLA	CHB-C4A	6.20	1.38	1.33
21	T	608	CLA	CHB-C4A	6.20	1.38	1.33
21	T	614	CLA	CHB-C4A	6.20	1.38	1.33
21	O	2001	CLA	CHB-C4A	6.20	1.38	1.33
21	c	604	CLA	CHB-C4A	6.20	1.38	1.33
21	T	606	CLA	CHB-C4A	6.19	1.38	1.33
21	A	818	CLA	CHB-C4A	6.19	1.38	1.33
21	3	411	CLA	CHB-C4A	6.19	1.38	1.33
21	7	313	CLA	CHB-C4A	6.19	1.38	1.33
21	a	310	CLA	CHB-C4A	6.18	1.38	1.33
21	8	605	CLA	CHB-C4A	6.18	1.38	1.33
21	B	829	CLA	CHB-C4A	6.17	1.38	1.33
21	A	816	CLA	CHB-C4A	6.17	1.38	1.33
21	A	834	CLA	CHB-C4A	6.17	1.38	1.33
21	G	204	CLA	CHB-C4A	6.17	1.38	1.33
21	A	820	CLA	CHB-C4A	6.17	1.38	1.33
21	B	816	CLA	CHB-C4A	6.17	1.38	1.33
21	A	841	CLA	CHB-C4A	6.16	1.38	1.33
21	B	818	CLA	CHB-C4A	6.16	1.38	1.33
21	3	413	CLA	CHB-C4A	6.16	1.38	1.33
21	7	312	CLA	CHB-C4A	6.16	1.38	1.33
21	H	203	CLA	CHB-C4A	6.16	1.38	1.33
21	J	5002	CLA	CHB-C4A	6.16	1.38	1.33
21	T	607	CLA	CHB-C4A	6.16	1.38	1.33
21	b	305	CLA	CHB-C4A	6.16	1.38	1.33
21	1	309	CLA	CHB-C4A	6.15	1.38	1.33
21	2	613	CLA	CHB-C4A	6.15	1.38	1.33
21	c	612	CLA	CHB-C4A	6.15	1.38	1.33
21	A	817	CLA	CHB-C4A	6.15	1.38	1.33
21	F	5005	CLA	CHB-C4A	6.15	1.38	1.33
21	2	610	CLA	CHB-C4A	6.15	1.38	1.33
21	A	824	CLA	CHB-C4A	6.15	1.38	1.33
21	F	5007	CLA	CHB-C4A	6.15	1.38	1.33
21	O	2002	CLA	CHB-C4A	6.15	1.38	1.33
21	2	605	CLA	CHB-C4A	6.14	1.38	1.33
21	K	204	CLA	CHB-C4A	6.14	1.38	1.33
21	b	316	CLA	CHB-C4A	6.14	1.38	1.33
21	A	807	CLA	CHB-C4A	6.14	1.38	1.33
21	B	835	CLA	CHB-C4A	6.14	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	837	CLA	CHB-C4A	6.14	1.38	1.33
21	B	811	CLA	CHB-C4A	6.14	1.38	1.33
21	K	203	CLA	CHB-C4A	6.13	1.38	1.33
21	B	809	CLA	CHB-C4A	6.13	1.38	1.33
21	B	839	CLA	CHB-C4A	6.13	1.38	1.33
21	c	613	CLA	CHB-C4A	6.12	1.38	1.33
21	8	613	CLA	CHB-C4A	6.12	1.38	1.33
21	B	815	CLA	CHB-C4A	6.12	1.38	1.33
21	a	312	CLA	CHB-C4A	6.12	1.38	1.33
21	9	609	CLA	CHB-C4A	6.11	1.38	1.33
21	c	610	CLA	CHB-C4A	6.11	1.38	1.33
21	8	612	CLA	CHB-C4A	6.11	1.38	1.33
21	1	306	CLA	CHB-C4A	6.11	1.38	1.33
21	2	602	CLA	CHB-C4A	6.11	1.38	1.33
21	A	808	CLA	CHB-C4A	6.11	1.38	1.33
21	F	5006	CLA	CHB-C4A	6.10	1.38	1.33
21	8	615	CLA	CHB-C4A	6.10	1.38	1.33
21	1	313	CLA	CHB-C4A	6.10	1.38	1.33
21	K	202	CLA	CHB-C4A	6.10	1.38	1.33
21	a	308	CLA	CHB-C4A	6.09	1.38	1.33
21	1	312	CLA	CHB-C4A	6.09	1.38	1.33
21	B	806	CLA	CHB-C4A	6.09	1.38	1.33
21	L	306	CLA	CHB-C4A	6.08	1.38	1.33
22	b	307	CHL	MG-NA	6.08	2.20	2.06
21	3	403	CLA	CHB-C4A	6.07	1.38	1.33
21	A	836	CLA	CHB-C4A	6.07	1.38	1.33
21	b	315	CLA	CHB-C4A	6.07	1.38	1.33
21	B	808	CLA	CHB-C4A	6.07	1.38	1.33
21	a	307	CLA	CHB-C4A	6.07	1.38	1.33
21	T	612	CLA	CHB-C4A	6.07	1.38	1.33
21	3	405	CLA	CHB-C4A	6.07	1.38	1.33
21	B	817	CLA	CHB-C4A	6.07	1.38	1.33
21	1	301	CLA	CHB-C4A	6.06	1.38	1.33
21	7	305	CLA	CHB-C4A	6.06	1.38	1.33
21	A	856	CLA	CHB-C4A	6.06	1.38	1.33
21	7	314	CLA	CHB-C4A	6.06	1.38	1.33
21	a	302	CLA	CHB-C4A	6.05	1.38	1.33
21	T	603	CLA	CHB-C4A	6.05	1.38	1.33
21	B	824	CLA	CHB-C4A	6.05	1.38	1.33
21	B	831	CLA	CHB-C4A	6.04	1.38	1.33
21	a	305	CLA	CHB-C4A	6.04	1.38	1.33
21	9	603	CLA	CHB-C4A	6.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	826	CLA	CHB-C4A	6.03	1.38	1.33
21	3	404	CLA	CHB-C4A	6.03	1.38	1.33
22	7	308	CHL	MG-NC	6.02	2.20	2.06
21	B	841	CLA	CHB-C4A	6.02	1.38	1.33
21	c	602	CLA	CHB-C4A	6.01	1.38	1.33
21	a	309	CLA	CHB-C4A	6.01	1.38	1.33
21	9	605	CLA	CHB-C4A	6.01	1.38	1.33
21	c	609	CLA	CHB-C4A	6.01	1.38	1.33
21	7	304	CLA	CHB-C4A	6.01	1.38	1.33
21	A	810	CLA	CHB-C4A	6.01	1.38	1.33
21	B	813	CLA	CHB-C4A	6.00	1.38	1.33
21	A	815	CLA	CHB-C4A	6.00	1.38	1.33
21	2	608	CLA	CHB-C4A	6.00	1.38	1.33
21	B	830	CLA	CHB-C4A	6.00	1.38	1.33
21	A	806	CLA	CHB-C4A	6.00	1.38	1.33
21	1	310	CLA	CHB-C4A	5.99	1.38	1.33
21	A	822	CLA	CHB-C4A	5.99	1.38	1.33
21	9	612	CLA	CHB-C4A	5.99	1.38	1.33
21	A	825	CLA	CHB-C4A	5.99	1.38	1.33
21	3	402	CLA	CHB-C4A	5.98	1.38	1.33
21	3	410	CLA	CHB-C4A	5.98	1.38	1.33
21	B	814	CLA	CHB-C4A	5.98	1.38	1.33
21	8	614	CLA	CHB-C4A	5.98	1.38	1.33
21	A	813	CLA	CHB-C4A	5.98	1.38	1.33
21	3	407	CLA	CHB-C4A	5.97	1.38	1.33
21	c	601	CLA	CHB-C4A	5.97	1.38	1.33
21	2	604	CLA	CHB-C4A	5.96	1.38	1.33
21	G	201	CLA	CHB-C4A	5.96	1.38	1.33
21	c	603	CLA	CHB-C4A	5.96	1.38	1.33
21	8	609	CLA	CHB-C4A	5.96	1.38	1.33
21	B	819	CLA	CHB-C4A	5.96	1.38	1.33
22	9	606	CHL	MG-NA	5.95	2.20	2.06
21	H	204	CLA	CHB-C4A	5.95	1.38	1.33
21	a	311	CLA	CHB-C4A	5.95	1.38	1.33
21	a	313	CLA	CHB-C4A	5.95	1.38	1.33
21	A	823	CLA	CHB-C4A	5.94	1.38	1.33
21	9	608	CLA	CHB-C4A	5.94	1.38	1.33
21	A	812	CLA	CHB-C4A	5.94	1.38	1.33
21	7	315	CLA	CHB-C4A	5.93	1.38	1.33
21	8	611	CLA	CHB-C4A	5.92	1.38	1.33
21	B	834	CLA	CHB-C4A	5.92	1.38	1.33
21	B	812	CLA	CHB-C4A	5.92	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	606	CHL	MG-NC	5.92	2.20	2.06
21	B	821	CLA	CHB-C4A	5.92	1.38	1.33
21	O	2003	CLA	CHB-C4A	5.92	1.38	1.33
21	7	316	CLA	CHB-C4A	5.91	1.38	1.33
21	7	323	CLA	CHB-C4A	5.91	1.38	1.33
21	A	840	CLA	CHB-C4A	5.91	1.38	1.33
21	a	304	CLA	CHB-C4A	5.91	1.38	1.33
21	3	412	CLA	CHB-C4A	5.91	1.38	1.33
22	9	606	CHL	MG-NC	5.91	2.20	2.06
21	1	302	CLA	CHB-C4A	5.90	1.38	1.33
21	T	604	CLA	CHB-C4A	5.90	1.38	1.33
21	7	310	CLA	CHB-C4A	5.90	1.38	1.33
21	T	609	CLA	CHB-C4A	5.90	1.38	1.33
21	A	830	CLA	CHB-C4A	5.90	1.38	1.33
21	G	203	CLA	CHB-C4A	5.89	1.38	1.33
21	B	832	CLA	CHB-C4A	5.89	1.38	1.33
21	B	838	CLA	CHB-C4A	5.88	1.38	1.33
21	b	311	CLA	CHB-C4A	5.88	1.38	1.33
21	A	838	CLA	CHB-C4A	5.88	1.38	1.33
21	3	406	CLA	CHB-C4A	5.88	1.38	1.33
21	A	842	CLA	CHB-C4A	5.88	1.38	1.33
21	8	604	CLA	CHB-C4A	5.87	1.38	1.33
21	b	310	CLA	CHB-C4A	5.86	1.38	1.33
21	a	303	CLA	CHB-C4A	5.86	1.38	1.33
21	A	833	CLA	CHB-C4A	5.85	1.38	1.33
21	B	833	CLA	CHB-C4A	5.85	1.38	1.33
21	B	844	CLA	CHB-C4A	5.85	1.38	1.33
21	3	408	CLA	CHB-C4A	5.84	1.38	1.33
21	b	304	CLA	CHB-C4A	5.84	1.38	1.33
21	L	304	CLA	CHB-C4A	5.83	1.38	1.33
21	a	314	CLA	CHB-C4A	5.83	1.38	1.33
21	L	303	CLA	CHB-C4A	5.83	1.38	1.33
22	2	606	CHL	MG-NA	5.83	2.20	2.06
21	1	321	CLA	CHB-C4A	5.82	1.38	1.33
22	8	606	CHL	MG-NA	5.82	2.20	2.06
21	A	821	CLA	CHB-C4A	5.81	1.38	1.33
21	A	831	CLA	CHB-C4A	5.81	1.38	1.33
21	1	308	CLA	CHB-C4A	5.80	1.38	1.33
21	B	823	CLA	CHB-C4A	5.80	1.38	1.33
21	A	814	CLA	CHB-C4A	5.80	1.38	1.33
21	A	829	CLA	CHB-C4A	5.79	1.38	1.33
21	9	602	CLA	CHB-C4A	5.78	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	610	CLA	CHB-C4A	5.78	1.38	1.33
21	A	828	CLA	CHB-C4A	5.77	1.38	1.33
21	L	301	CLA	CHB-C4A	5.77	1.38	1.33
21	b	306	CLA	CHB-C4A	5.75	1.38	1.33
21	8	603	CLA	CHB-C4A	5.75	1.38	1.33
21	B	828	CLA	CHB-C4A	5.75	1.38	1.33
22	7	309	CHL	MG-NA	5.73	2.19	2.06
21	B	804	CLA	CHB-C4A	5.72	1.38	1.33
21	A	839	CLA	CHB-C4A	5.69	1.38	1.33
21	B	827	CLA	CHB-C4A	5.68	1.38	1.33
21	7	311	CLA	CHB-C4A	5.65	1.38	1.33
22	3	401	CHL	MG-NC	5.65	2.19	2.06
21	B	810	CLA	CHB-C4A	5.63	1.38	1.33
21	1	303	CLA	CHB-C4A	5.60	1.38	1.33
21	A	843	CLA	CHB-C4A	5.57	1.38	1.33
22	1	305	CHL	MG-NA	5.55	2.19	2.06
21	B	836	CLA	CHB-C4A	5.55	1.38	1.33
21	B	842	CLA	CHB-C4A	5.47	1.38	1.33
21	B	822	CLA	CHB-C4A	5.35	1.38	1.33
34	A	803	CL0	MG-NA	5.29	2.18	2.06
22	c	607	CHL	MG-NA	5.29	2.18	2.06
22	8	607	CHL	MG-NA	5.21	2.18	2.06
22	b	302	CHL	MG-NC	5.20	2.18	2.06
22	b	308	CHL	MG-NA	5.14	2.18	2.06
22	T	602	CHL	MG-NA	5.13	2.18	2.06
22	3	401	CHL	MG-NA	4.97	2.18	2.06
21	8	622	CLA	CHB-C4A	4.81	1.37	1.33
22	2	601	CHL	MG-NA	4.75	2.17	2.06
21	8	622	CLA	MG-NC	4.67	2.17	2.06
21	8	622	CLA	MG-NA	4.65	2.17	2.06
22	7	308	CHL	MG-NA	4.64	2.17	2.06
21	8	622	CLA	C1D-ND	4.53	1.43	1.37
22	c	605	CHL	MG-NC	4.50	2.16	2.06
22	b	308	CHL	MG-NC	4.46	2.16	2.06
21	1	321	CLA	CHC-C1C	4.44	1.45	1.34
22	c	606	CHL	MG-NA	4.44	2.16	2.06
22	8	606	CHL	MG-NC	4.40	2.16	2.06
22	b	307	CHL	MG-NC	4.28	2.16	2.06
22	8	608	CHL	MG-NC	4.24	2.16	2.06
22	8	601	CHL	MG-NC	4.24	2.16	2.06
21	A	829	CLA	MG-NA	4.17	2.16	2.06
22	8	607	CHL	MG-NC	4.16	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	803	CL0	MG-NC	4.11	2.16	2.06
21	B	829	CLA	MG-NA	3.97	2.15	2.06
21	9	601	CLA	CHC-C1C	3.92	1.44	1.34
22	2	606	CHL	MG-NC	3.90	2.15	2.06
21	O	2002	CLA	CAB-C3B	-3.86	1.43	1.51
22	b	309	CHL	MG-NC	3.85	2.15	2.06
21	a	310	CLA	C1D-ND	3.77	1.42	1.37
21	a	303	CLA	C1D-ND	3.74	1.42	1.37
21	8	604	CLA	C1D-ND	3.73	1.42	1.37
21	9	601	CLA	MG-NC	3.73	2.15	2.06
21	8	612	CLA	C1D-ND	3.72	1.42	1.37
21	G	203	CLA	C1D-ND	3.72	1.42	1.37
21	A	818	CLA	C1D-ND	3.72	1.42	1.37
21	T	606	CLA	C1D-ND	3.71	1.42	1.37
22	7	307	CHL	MG-NC	3.70	2.15	2.06
21	A	820	CLA	C1D-ND	3.67	1.42	1.37
22	a	306	CHL	MG-NC	3.67	2.15	2.06
21	B	820	CLA	C1D-ND	3.67	1.42	1.37
21	9	610	CLA	C1D-ND	3.67	1.42	1.37
21	J	5002	CLA	C1D-ND	3.66	1.42	1.37
21	9	603	CLA	C1D-ND	3.66	1.42	1.37
21	9	605	CLA	C1D-ND	3.65	1.42	1.37
21	1	310	CLA	C1D-ND	3.65	1.42	1.37
21	a	311	CLA	C1D-ND	3.64	1.42	1.37
21	B	835	CLA	C1D-ND	3.64	1.42	1.37
21	K	203	CLA	C1D-ND	3.63	1.42	1.37
21	A	838	CLA	C1D-ND	3.62	1.42	1.37
21	O	2003	CLA	C1D-ND	3.62	1.42	1.37
21	O	2002	CLA	C1D-ND	3.62	1.42	1.37
21	7	306	CLA	C1D-ND	3.62	1.42	1.37
21	b	313	CLA	C1D-ND	3.61	1.42	1.37
21	K	201	CLA	C1D-ND	3.61	1.42	1.37
21	b	312	CLA	C1D-ND	3.61	1.42	1.37
21	2	603	CLA	C1D-ND	3.61	1.42	1.37
21	A	843	CLA	CHC-C1C	3.60	1.43	1.34
21	B	817	CLA	C1D-ND	3.60	1.42	1.37
21	2	609	CLA	C1D-ND	3.60	1.42	1.37
21	9	609	CLA	C1D-ND	3.60	1.42	1.37
21	T	611	CLA	C1D-ND	3.60	1.42	1.37
21	A	815	CLA	C1D-ND	3.60	1.42	1.37
21	B	844	CLA	C1D-ND	3.60	1.42	1.37
21	9	607	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	815	CLA	C1D-ND	3.59	1.42	1.37
21	b	316	CLA	C1D-ND	3.59	1.42	1.37
21	B	825	CLA	C1D-ND	3.59	1.42	1.37
21	B	832	CLA	C1D-ND	3.59	1.42	1.37
21	a	305	CLA	C1D-ND	3.59	1.42	1.37
21	b	305	CLA	C1D-ND	3.59	1.42	1.37
21	c	608	CLA	C1D-ND	3.59	1.42	1.37
21	A	812	CLA	C1D-ND	3.58	1.42	1.37
21	A	806	CLA	CHC-C1C	3.58	1.43	1.34
21	3	408	CLA	C1D-ND	3.58	1.42	1.37
21	A	830	CLA	C1D-ND	3.58	1.42	1.37
21	H	204	CLA	C1D-ND	3.58	1.42	1.37
21	A	822	CLA	C1D-ND	3.58	1.42	1.37
21	c	611	CLA	C1D-ND	3.57	1.42	1.37
21	A	837	CLA	C1D-ND	3.57	1.42	1.37
21	2	607	CLA	C1D-ND	3.57	1.42	1.37
21	7	323	CLA	C1D-ND	3.57	1.42	1.37
21	8	603	CLA	C1D-ND	3.57	1.42	1.37
21	A	811	CLA	C1D-ND	3.57	1.42	1.37
21	B	811	CLA	C1D-ND	3.57	1.42	1.37
21	8	613	CLA	C1D-ND	3.57	1.42	1.37
21	A	839	CLA	CHC-C1C	3.56	1.43	1.34
21	B	827	CLA	CHC-C1C	3.56	1.43	1.34
21	7	313	CLA	C1D-ND	3.56	1.42	1.37
21	2	608	CLA	CHC-C1C	3.56	1.43	1.34
21	c	601	CLA	C1D-ND	3.56	1.42	1.37
21	B	813	CLA	C1D-ND	3.56	1.42	1.37
21	7	305	CLA	C1D-ND	3.56	1.42	1.37
21	A	814	CLA	C1D-ND	3.56	1.42	1.37
21	b	306	CLA	CHC-C1C	3.56	1.43	1.34
21	a	302	CLA	C1D-ND	3.55	1.42	1.37
21	3	402	CLA	C1D-ND	3.55	1.42	1.37
21	b	314	CLA	C1D-ND	3.55	1.42	1.37
21	T	608	CLA	C1D-ND	3.55	1.42	1.37
21	1	306	CLA	C1D-ND	3.55	1.42	1.37
21	B	808	CLA	CHC-C1C	3.55	1.43	1.34
21	B	840	CLA	CHC-C1C	3.55	1.43	1.34
21	T	612	CLA	C1D-ND	3.55	1.42	1.37
21	A	821	CLA	C1D-ND	3.55	1.42	1.37
21	G	201	CLA	C1D-ND	3.55	1.42	1.37
21	A	807	CLA	CHC-C1C	3.55	1.43	1.34
21	8	610	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	307	CLA	C1D-ND	3.54	1.42	1.37
21	3	410	CLA	C1D-ND	3.54	1.42	1.37
21	B	807	CLA	CHC-C1C	3.54	1.43	1.34
21	B	823	CLA	C1D-ND	3.54	1.42	1.37
21	G	204	CLA	C1D-ND	3.54	1.42	1.37
21	A	827	CLA	C1D-ND	3.54	1.42	1.37
21	1	301	CLA	C1D-ND	3.54	1.42	1.37
22	7	309	CHL	C1D-C2D	-3.54	1.38	1.45
21	3	404	CLA	C1D-ND	3.54	1.42	1.37
21	A	840	CLA	C1D-ND	3.54	1.42	1.37
21	A	819	CLA	C1D-ND	3.54	1.42	1.37
21	B	838	CLA	C1D-ND	3.54	1.42	1.37
21	O	2001	CLA	C1D-ND	3.53	1.42	1.37
21	T	610	CLA	C1D-ND	3.53	1.42	1.37
21	a	312	CLA	C1D-ND	3.53	1.42	1.37
21	B	824	CLA	C1D-ND	3.53	1.42	1.37
21	1	304	CLA	CHC-C1C	3.53	1.43	1.34
21	2	604	CLA	CHC-C1C	3.53	1.43	1.34
21	B	834	CLA	C1D-ND	3.53	1.42	1.37
21	7	314	CLA	C1D-ND	3.53	1.42	1.37
21	T	604	CLA	C1D-ND	3.52	1.42	1.37
21	a	314	CLA	C1D-ND	3.52	1.42	1.37
21	a	308	CLA	C1D-ND	3.52	1.42	1.37
21	7	310	CLA	CHC-C1C	3.52	1.43	1.34
21	c	612	CLA	C1D-ND	3.52	1.42	1.37
21	3	409	CLA	C1D-ND	3.52	1.42	1.37
21	B	818	CLA	CHC-C1C	3.52	1.43	1.34
21	1	308	CLA	CHC-C1C	3.52	1.43	1.34
21	A	834	CLA	C1D-ND	3.52	1.42	1.37
21	A	856	CLA	C1D-ND	3.52	1.42	1.37
21	c	603	CLA	C1D-ND	3.52	1.42	1.37
21	G	204	CLA	CHC-C1C	3.52	1.43	1.34
21	1	312	CLA	C1D-ND	3.52	1.42	1.37
21	B	828	CLA	CHC-C1C	3.52	1.43	1.34
21	A	825	CLA	C1D-ND	3.51	1.42	1.37
21	7	312	CLA	C1D-ND	3.51	1.42	1.37
21	B	809	CLA	C1D-ND	3.51	1.42	1.37
21	T	614	CLA	C1D-ND	3.51	1.42	1.37
21	B	839	CLA	C1D-ND	3.51	1.42	1.37
21	1	311	CLA	C1D-ND	3.51	1.42	1.37
21	L	306	CLA	C1D-ND	3.51	1.42	1.37
21	A	823	CLA	CHC-C1C	3.51	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	202	CLA	CHC-C1C	3.51	1.43	1.34
21	3	413	CLA	C1D-ND	3.51	1.42	1.37
21	c	602	CLA	C1D-ND	3.51	1.42	1.37
21	2	605	CLA	CHC-C1C	3.51	1.43	1.34
21	3	413	CLA	CHC-C1C	3.51	1.43	1.34
21	a	309	CLA	CHC-C1C	3.50	1.43	1.34
21	2	612	CLA	CHC-C1C	3.50	1.43	1.34
21	9	602	CLA	CHC-C1C	3.50	1.43	1.34
21	B	833	CLA	CHC-C1C	3.50	1.43	1.34
22	2	601	CHL	C1D-C2D	-3.50	1.38	1.45
21	A	808	CLA	C1D-ND	3.50	1.42	1.37
21	T	605	CLA	CHC-C1C	3.50	1.43	1.34
21	c	604	CLA	C1D-ND	3.50	1.42	1.37
21	c	614	CLA	C1D-ND	3.50	1.42	1.37
21	A	828	CLA	CHC-C1C	3.50	1.43	1.34
21	2	612	CLA	C1D-ND	3.50	1.42	1.37
21	9	602	CLA	C1D-ND	3.50	1.42	1.37
21	A	805	CLA	C1D-ND	3.50	1.42	1.37
21	3	403	CLA	C1D-ND	3.50	1.42	1.37
21	B	829	CLA	C1D-ND	3.50	1.42	1.37
21	A	829	CLA	C1D-ND	3.49	1.42	1.37
21	B	810	CLA	C1D-ND	3.49	1.42	1.37
21	H	203	CLA	C1D-ND	3.49	1.42	1.37
21	B	809	CLA	CHC-C1C	3.49	1.43	1.34
21	B	826	CLA	CHC-C1C	3.49	1.43	1.34
21	L	305	CLA	C1D-ND	3.49	1.42	1.37
21	c	610	CLA	C1D-ND	3.49	1.42	1.37
21	1	303	CLA	CHC-C1C	3.49	1.43	1.34
21	2	611	CLA	CHC-C1C	3.49	1.43	1.34
21	F	5005	CLA	C1D-ND	3.49	1.42	1.37
21	3	412	CLA	CHC-C1C	3.49	1.43	1.34
21	9	611	CLA	C1D-ND	3.49	1.42	1.37
21	3	406	CLA	C1D-ND	3.49	1.42	1.37
21	8	610	CLA	CHC-C1C	3.49	1.43	1.34
21	B	834	CLA	CHC-C1C	3.49	1.43	1.34
21	a	307	CLA	CHC-C1C	3.49	1.43	1.34
21	2	613	CLA	C1D-ND	3.49	1.42	1.37
21	A	842	CLA	C1D-ND	3.49	1.42	1.37
21	1	309	CLA	C1D-ND	3.48	1.42	1.37
21	A	813	CLA	CHC-C1C	3.48	1.43	1.34
21	b	314	CLA	CHC-C1C	3.48	1.43	1.34
21	T	603	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	817	CLA	CHC-C1C	3.48	1.43	1.34
21	A	823	CLA	C1D-ND	3.48	1.42	1.37
21	K	202	CLA	C1D-ND	3.48	1.42	1.37
21	A	832	CLA	C1D-ND	3.48	1.42	1.37
21	B	831	CLA	C1D-ND	3.48	1.42	1.37
21	A	836	CLA	CHC-C1C	3.48	1.43	1.34
21	a	311	CLA	CHC-C1C	3.48	1.43	1.34
21	3	407	CLA	C1D-ND	3.48	1.42	1.37
21	9	604	CLA	CHC-C1C	3.48	1.43	1.34
21	L	306	CLA	CHC-C1C	3.48	1.43	1.34
21	8	614	CLA	CHC-C1C	3.48	1.43	1.34
21	F	5005	CLA	CHC-C1C	3.48	1.43	1.34
21	F	5006	CLA	CHC-C1C	3.47	1.43	1.34
21	3	414	CLA	C1D-ND	3.47	1.42	1.37
21	B	820	CLA	CHC-C1C	3.47	1.43	1.34
21	a	307	CLA	C1D-ND	3.47	1.42	1.37
21	A	833	CLA	CHC-C1C	3.47	1.43	1.34
21	B	842	CLA	CHC-C1C	3.47	1.43	1.34
21	a	304	CLA	CHC-C1C	3.47	1.43	1.34
21	F	5006	CLA	C1D-ND	3.47	1.42	1.37
21	a	305	CLA	CHC-C1C	3.47	1.43	1.34
21	K	204	CLA	C1D-ND	3.47	1.42	1.37
21	7	315	CLA	C1D-ND	3.47	1.42	1.37
21	9	609	CLA	CHC-C1C	3.47	1.43	1.34
21	B	810	CLA	CHC-C1C	3.47	1.43	1.34
21	H	203	CLA	CHC-C1C	3.47	1.43	1.34
21	2	604	CLA	C1D-ND	3.47	1.42	1.37
21	c	611	CLA	CHC-C1C	3.47	1.43	1.34
21	T	607	CLA	C1D-ND	3.47	1.42	1.37
21	9	612	CLA	C1D-ND	3.46	1.42	1.37
21	A	835	CLA	C1D-ND	3.46	1.42	1.37
21	c	613	CLA	CHC-C1C	3.46	1.43	1.34
21	8	611	CLA	C1D-ND	3.46	1.42	1.37
21	T	611	CLA	CHC-C1C	3.46	1.43	1.34
21	B	819	CLA	CHC-C1C	3.46	1.43	1.34
21	F	5007	CLA	C1D-ND	3.46	1.42	1.37
21	a	313	CLA	C1D-ND	3.46	1.42	1.37
21	b	305	CLA	CHC-C1C	3.46	1.43	1.34
21	1	302	CLA	C1D-ND	3.46	1.42	1.37
21	3	404	CLA	CHC-C1C	3.46	1.43	1.34
21	1	308	CLA	C1D-ND	3.46	1.42	1.37
21	T	613	CLA	CHC-C1C	3.46	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	304	CLA	CHC-C1C	3.46	1.43	1.34
21	B	837	CLA	CHC-C1C	3.46	1.43	1.34
21	B	835	CLA	CHC-C1C	3.46	1.43	1.34
21	A	810	CLA	C1D-ND	3.46	1.42	1.37
21	A	810	CLA	CHC-C1C	3.46	1.43	1.34
21	O	2003	CLA	CHC-C1C	3.46	1.43	1.34
21	2	610	CLA	CHC-C1C	3.46	1.43	1.34
21	H	204	CLA	CHC-C1C	3.45	1.43	1.34
21	T	614	CLA	CHC-C1C	3.45	1.43	1.34
21	9	608	CLA	C1D-ND	3.45	1.42	1.37
21	A	805	CLA	CHC-C1C	3.45	1.43	1.34
21	B	808	CLA	C1D-ND	3.45	1.42	1.37
21	8	609	CLA	CHC-C1C	3.45	1.43	1.34
21	B	830	CLA	CHC-C1C	3.45	1.43	1.34
21	B	837	CLA	C1D-ND	3.45	1.42	1.37
21	G	201	CLA	CHC-C1C	3.45	1.43	1.34
21	A	826	CLA	C1D-ND	3.45	1.42	1.37
21	1	312	CLA	CHC-C1C	3.45	1.43	1.34
21	K	204	CLA	CHC-C1C	3.45	1.43	1.34
21	A	819	CLA	CHC-C1C	3.45	1.43	1.34
21	b	313	CLA	CHC-C1C	3.45	1.43	1.34
21	K	201	CLA	CHC-C1C	3.45	1.43	1.34
21	1	310	CLA	CHC-C1C	3.45	1.43	1.34
21	B	828	CLA	C1D-ND	3.45	1.42	1.37
21	2	605	CLA	C1D-ND	3.45	1.42	1.37
21	B	815	CLA	CHC-C1C	3.45	1.43	1.34
21	3	403	CLA	CHC-C1C	3.45	1.43	1.34
21	A	809	CLA	CHC-C1C	3.45	1.43	1.34
21	c	603	CLA	CHC-C1C	3.45	1.43	1.34
21	a	302	CLA	CHC-C1C	3.45	1.43	1.34
21	2	602	CLA	C1D-ND	3.44	1.42	1.37
21	b	315	CLA	C1D-ND	3.44	1.42	1.37
21	c	613	CLA	C1D-ND	3.44	1.42	1.37
21	A	842	CLA	CHC-C1C	3.44	1.43	1.34
21	2	607	CLA	CHC-C1C	3.44	1.43	1.34
21	3	405	CLA	C1D-ND	3.44	1.42	1.37
21	L	303	CLA	C1D-ND	3.44	1.42	1.37
21	1	306	CLA	CHC-C1C	3.44	1.43	1.34
21	9	611	CLA	CHC-C1C	3.44	1.43	1.34
21	T	607	CLA	CHC-C1C	3.44	1.43	1.34
21	B	812	CLA	C1D-ND	3.44	1.42	1.37
21	c	602	CLA	CHC-C1C	3.44	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	313	CLA	C1D-ND	3.44	1.42	1.37
21	L	304	CLA	CHC-C1C	3.44	1.43	1.34
21	b	312	CLA	CHC-C1C	3.44	1.43	1.34
21	B	827	CLA	C1D-ND	3.44	1.42	1.37
21	a	310	CLA	CHC-C1C	3.44	1.43	1.34
21	9	601	CLA	C1D-ND	3.44	1.42	1.37
21	A	809	CLA	C1D-ND	3.44	1.42	1.37
21	B	819	CLA	C1D-ND	3.44	1.42	1.37
21	9	612	CLA	CHC-C1C	3.43	1.43	1.34
21	A	814	CLA	CHC-C1C	3.43	1.43	1.34
21	L	301	CLA	C1D-ND	3.43	1.42	1.37
21	a	313	CLA	CHC-C1C	3.43	1.43	1.34
21	T	608	CLA	CHC-C1C	3.43	1.43	1.34
21	B	821	CLA	C1D-ND	3.43	1.42	1.37
21	2	613	CLA	CHC-C1C	3.43	1.43	1.34
21	b	306	CLA	C1D-ND	3.43	1.42	1.37
21	b	304	CLA	C1D-ND	3.43	1.42	1.37
21	A	816	CLA	CHC-C1C	3.43	1.43	1.34
21	1	311	CLA	CHC-C1C	3.43	1.43	1.34
21	8	615	CLA	CHC-C1C	3.43	1.43	1.34
21	A	824	CLA	CHC-C1C	3.43	1.43	1.34
21	B	804	CLA	CHC-C1C	3.43	1.43	1.34
21	2	610	CLA	C1D-ND	3.43	1.42	1.37
21	A	813	CLA	C1D-ND	3.43	1.42	1.37
21	A	830	CLA	CHC-C1C	3.43	1.43	1.34
21	A	837	CLA	CHC-C1C	3.42	1.43	1.34
21	A	840	CLA	CHC-C1C	3.42	1.43	1.34
21	7	311	CLA	CHC-C1C	3.42	1.43	1.34
21	1	304	CLA	C1D-ND	3.42	1.42	1.37
21	T	613	CLA	C1D-ND	3.42	1.42	1.37
21	7	315	CLA	CHC-C1C	3.42	1.43	1.34
21	9	604	CLA	C1D-ND	3.42	1.42	1.37
21	B	842	CLA	C1D-ND	3.42	1.42	1.37
21	T	610	CLA	CHC-C1C	3.42	1.43	1.34
21	3	409	CLA	CHC-C1C	3.42	1.43	1.34
22	c	607	CHL	C1D-C2D	-3.42	1.38	1.45
21	a	312	CLA	CHC-C1C	3.42	1.43	1.34
21	b	315	CLA	CHC-C1C	3.42	1.43	1.34
21	A	829	CLA	CHC-C1C	3.42	1.43	1.34
21	3	411	CLA	C1D-ND	3.42	1.42	1.37
21	7	323	CLA	CHC-C1C	3.42	1.43	1.34
21	8	605	CLA	CHC-C1C	3.42	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	816	CLA	C1D-ND	3.42	1.42	1.37
21	8	613	CLA	CHC-C1C	3.42	1.43	1.34
21	8	609	CLA	C1D-ND	3.42	1.42	1.37
21	B	836	CLA	CHC-C1C	3.42	1.43	1.34
21	1	301	CLA	CHC-C1C	3.42	1.43	1.34
21	1	309	CLA	CHC-C1C	3.42	1.43	1.34
21	B	814	CLA	C1D-ND	3.42	1.42	1.37
21	7	313	CLA	CHC-C1C	3.42	1.43	1.34
21	1	313	CLA	CHC-C1C	3.41	1.43	1.34
21	7	312	CLA	CHC-C1C	3.41	1.43	1.34
21	7	310	CLA	C1D-ND	3.41	1.42	1.37
21	B	806	CLA	CHC-C1C	3.41	1.43	1.34
21	8	605	CLA	C1D-ND	3.41	1.42	1.37
21	c	609	CLA	C1D-ND	3.41	1.42	1.37
21	3	408	CLA	CHC-C1C	3.41	1.43	1.34
21	1	303	CLA	C1D-ND	3.41	1.42	1.37
21	B	816	CLA	C1D-ND	3.41	1.42	1.37
21	A	820	CLA	CHC-C1C	3.41	1.43	1.34
21	b	311	CLA	CHC-C1C	3.41	1.43	1.34
21	9	610	CLA	CHC-C1C	3.41	1.42	1.34
21	7	305	CLA	CHC-C1C	3.41	1.42	1.34
21	L	305	CLA	CHC-C1C	3.40	1.42	1.34
21	B	804	CLA	C1D-ND	3.40	1.42	1.37
21	c	612	CLA	CHC-C1C	3.40	1.42	1.34
21	T	604	CLA	CHC-C1C	3.40	1.42	1.34
21	3	405	CLA	CHC-C1C	3.40	1.42	1.34
21	3	410	CLA	CHC-C1C	3.40	1.42	1.34
21	c	604	CLA	CHC-C1C	3.40	1.42	1.34
21	7	316	CLA	CHC-C1C	3.40	1.42	1.34
21	b	311	CLA	C1D-ND	3.40	1.42	1.37
21	B	821	CLA	CHC-C1C	3.40	1.42	1.34
21	b	316	CLA	CHC-C1C	3.40	1.42	1.34
21	B	816	CLA	CHC-C1C	3.40	1.42	1.34
21	A	841	CLA	C1D-ND	3.40	1.42	1.37
21	8	612	CLA	CHC-C1C	3.39	1.42	1.34
21	T	612	CLA	CHC-C1C	3.39	1.42	1.34
21	3	406	CLA	CHC-C1C	3.39	1.42	1.34
21	c	608	CLA	CHC-C1C	3.39	1.42	1.34
21	B	843	CLA	C1D-ND	3.39	1.42	1.37
21	F	5007	CLA	CHC-C1C	3.39	1.42	1.34
21	A	841	CLA	CHC-C1C	3.39	1.42	1.34
21	A	843	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	302	CLA	CHC-C1C	3.39	1.42	1.34
21	O	2001	CLA	CHC-C1C	3.39	1.42	1.34
21	B	831	CLA	CHC-C1C	3.39	1.42	1.34
21	A	832	CLA	CHC-C1C	3.39	1.42	1.34
21	3	414	CLA	CHC-C1C	3.39	1.42	1.34
21	T	603	CLA	CHC-C1C	3.39	1.42	1.34
21	A	808	CLA	CHC-C1C	3.39	1.42	1.34
21	7	316	CLA	C1D-ND	3.39	1.42	1.37
21	A	831	CLA	C1D-ND	3.39	1.42	1.37
21	1	307	CLA	CHC-C1C	3.39	1.42	1.34
21	3	402	CLA	CHC-C1C	3.39	1.42	1.34
21	9	608	CLA	CHC-C1C	3.39	1.42	1.34
21	b	310	CLA	C1D-ND	3.39	1.42	1.37
21	B	814	CLA	CHC-C1C	3.39	1.42	1.34
21	7	311	CLA	C1D-ND	3.39	1.42	1.37
21	a	309	CLA	C1D-ND	3.39	1.42	1.37
21	J	5002	CLA	CHC-C1C	3.38	1.42	1.34
21	L	301	CLA	CHC-C1C	3.38	1.42	1.34
21	A	806	CLA	C1D-ND	3.38	1.42	1.37
21	A	824	CLA	C1D-ND	3.38	1.42	1.37
21	8	615	CLA	C1D-ND	3.38	1.42	1.37
21	B	841	CLA	CHC-C1C	3.38	1.42	1.34
21	7	306	CLA	CHC-C1C	3.38	1.42	1.34
21	B	839	CLA	CHC-C1C	3.38	1.42	1.34
21	9	605	CLA	CHC-C1C	3.38	1.42	1.34
21	c	614	CLA	CHC-C1C	3.38	1.42	1.34
21	c	610	CLA	CHC-C1C	3.38	1.42	1.34
21	A	825	CLA	CHC-C1C	3.37	1.42	1.34
21	a	304	CLA	C1D-ND	3.37	1.42	1.37
21	T	609	CLA	CHC-C1C	3.37	1.42	1.34
21	8	604	CLA	CHC-C1C	3.37	1.42	1.34
21	B	830	CLA	C1D-ND	3.37	1.42	1.37
21	B	841	CLA	C1D-ND	3.37	1.42	1.37
21	B	822	CLA	CHC-C1C	3.37	1.42	1.34
21	a	303	CLA	CHC-C1C	3.37	1.42	1.34
21	L	303	CLA	CHC-C1C	3.37	1.42	1.34
21	8	603	CLA	CHC-C1C	3.37	1.42	1.34
21	B	838	CLA	CHC-C1C	3.37	1.42	1.34
21	A	834	CLA	CHC-C1C	3.36	1.42	1.34
21	G	205	CLA	C1D-ND	3.36	1.42	1.37
21	B	829	CLA	CHC-C1C	3.36	1.42	1.34
21	9	603	CLA	CHC-C1C	3.36	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	821	CLA	CHC-C1C	3.36	1.42	1.34
21	A	833	CLA	C1D-ND	3.36	1.42	1.37
21	2	611	CLA	C1D-ND	3.36	1.42	1.37
21	B	806	CLA	C1D-ND	3.36	1.42	1.37
21	B	823	CLA	CHC-C1C	3.36	1.42	1.34
22	1	305	CHL	MG-NC	3.36	2.14	2.06
21	A	811	CLA	CHC-C1C	3.35	1.42	1.34
21	7	304	CLA	C1D-ND	3.35	1.42	1.37
21	K	203	CLA	CHC-C1C	3.35	1.42	1.34
21	3	412	CLA	C1D-ND	3.35	1.42	1.37
21	B	824	CLA	CHC-C1C	3.35	1.42	1.34
21	A	818	CLA	CHC-C1C	3.35	1.42	1.34
21	T	609	CLA	C1D-ND	3.35	1.42	1.37
21	A	835	CLA	CHC-C1C	3.35	1.42	1.34
21	B	817	CLA	CHC-C1C	3.34	1.42	1.34
21	2	608	CLA	C1D-ND	3.34	1.42	1.37
21	A	827	CLA	CHC-C1C	3.34	1.42	1.34
21	B	844	CLA	CHC-C1C	3.34	1.42	1.34
21	7	314	CLA	CHC-C1C	3.34	1.42	1.34
21	b	310	CLA	CHC-C1C	3.34	1.42	1.34
21	b	304	CLA	CHC-C1C	3.34	1.42	1.34
21	T	605	CLA	C1D-ND	3.34	1.42	1.37
21	3	411	CLA	CHC-C1C	3.34	1.42	1.34
21	c	609	CLA	CHC-C1C	3.34	1.42	1.34
21	A	856	CLA	CHC-C1C	3.34	1.42	1.34
21	O	2002	CLA	CHC-C1C	3.33	1.42	1.34
21	8	611	CLA	CHC-C1C	3.33	1.42	1.34
21	A	812	CLA	CHC-C1C	3.33	1.42	1.34
21	G	203	CLA	CHC-C1C	3.33	1.42	1.34
21	2	609	CLA	CHC-C1C	3.33	1.42	1.34
21	A	826	CLA	CHC-C1C	3.33	1.42	1.34
21	A	831	CLA	CHC-C1C	3.33	1.42	1.34
21	B	825	CLA	CHC-C1C	3.33	1.42	1.34
21	2	602	CLA	CHC-C1C	3.32	1.42	1.34
21	B	822	CLA	C1D-ND	3.32	1.42	1.37
21	2	603	CLA	CHC-C1C	3.32	1.42	1.34
21	B	811	CLA	CHC-C1C	3.32	1.42	1.34
21	G	205	CLA	CHC-C1C	3.32	1.42	1.34
21	B	833	CLA	C1D-ND	3.32	1.42	1.37
21	8	614	CLA	C1D-ND	3.31	1.42	1.37
21	8	622	CLA	CHC-C1C	3.31	1.42	1.34
21	a	311	CLA	MG-NA	3.31	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	818	CLA	C1D-ND	3.30	1.42	1.37
21	B	840	CLA	C1D-ND	3.29	1.42	1.37
21	A	817	CLA	C1D-ND	3.29	1.42	1.37
21	B	842	CLA	MG-ND	-3.29	1.99	2.05
21	a	314	CLA	CHC-C1C	3.28	1.42	1.34
21	A	804	CLA	CHC-C1C	3.28	1.42	1.34
21	B	826	CLA	C1D-ND	3.28	1.42	1.37
21	T	606	CLA	CHC-C1C	3.28	1.42	1.34
21	B	836	CLA	C1D-ND	3.28	1.42	1.37
21	A	838	CLA	CHC-C1C	3.27	1.42	1.34
21	B	812	CLA	CHC-C1C	3.27	1.42	1.34
21	A	836	CLA	C1D-ND	3.26	1.42	1.37
21	A	839	CLA	C1D-ND	3.26	1.42	1.37
21	c	612	CLA	MG-ND	-3.25	1.99	2.05
21	c	601	CLA	CHC-C1C	3.25	1.42	1.34
21	A	815	CLA	CHC-C1C	3.24	1.42	1.34
21	9	607	CLA	CHC-C1C	3.24	1.42	1.34
21	3	407	CLA	CHC-C1C	3.23	1.42	1.34
21	A	807	CLA	C1D-ND	3.23	1.42	1.37
21	7	314	CLA	MG-ND	-3.22	1.99	2.05
21	A	828	CLA	C1D-ND	3.21	1.42	1.37
21	A	822	CLA	CHC-C1C	3.20	1.42	1.34
21	B	843	CLA	CHC-C1C	3.19	1.42	1.34
21	9	605	CLA	MG-ND	-3.18	1.99	2.05
21	B	813	CLA	CHC-C1C	3.17	1.42	1.34
21	G	203	CLA	MG-NA	3.16	2.13	2.06
22	c	605	CHL	CHB-C4A	3.15	1.36	1.33
21	B	832	CLA	CHC-C1C	3.13	1.42	1.34
22	T	602	CHL	C1D-C2D	-3.11	1.39	1.45
21	B	807	CLA	MG-NA	-3.11	1.98	2.06
22	2	606	CHL	CHB-C4A	3.11	1.35	1.33
22	b	308	CHL	CHB-C4A	3.10	1.35	1.33
21	a	308	CLA	CHC-C1C	3.10	1.42	1.34
22	9	606	CHL	C1D-C2D	-3.10	1.39	1.45
21	A	804	CLA	C1D-ND	3.10	1.41	1.37
21	1	321	CLA	C1D-ND	3.09	1.41	1.37
21	L	304	CLA	C1D-ND	3.08	1.41	1.37
21	B	832	CLA	CMB-C2B	-3.04	1.45	1.51
34	A	803	CL0	C1D-C2D	-3.04	1.39	1.45
22	2	606	CHL	C1D-C2D	-3.02	1.39	1.45
22	2	601	CHL	CHB-C4A	3.02	1.35	1.33
22	b	302	CHL	CHB-C4A	3.01	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	804	CLA	CMB-C2B	-3.01	1.45	1.51
22	b	309	CHL	CHB-C4A	2.99	1.35	1.33
22	8	607	CHL	CHB-C4A	2.99	1.35	1.33
21	A	828	CLA	MG-ND	-2.99	1.99	2.05
22	8	606	CHL	CHB-C4A	2.97	1.35	1.33
22	7	308	CHL	C1D-C2D	-2.97	1.39	1.45
22	8	608	CHL	CHB-C4A	2.96	1.35	1.33
21	B	813	CLA	CMB-C2B	-2.95	1.45	1.51
22	b	307	CHL	CHB-C4A	2.93	1.35	1.33
22	b	302	CHL	C1D-C2D	-2.92	1.39	1.45
22	7	303	CHL	C1D-C2D	-2.91	1.39	1.45
22	b	309	CHL	C1D-C2D	-2.91	1.39	1.45
22	T	602	CHL	CHB-C4A	2.90	1.35	1.33
22	c	606	CHL	CHB-C4A	2.89	1.35	1.33
22	3	401	CHL	CHB-C4A	2.88	1.35	1.33
22	7	303	CHL	CHB-C4A	2.88	1.35	1.33
21	B	823	CLA	CMB-C2B	-2.87	1.45	1.51
22	T	601	CHL	CHB-C4A	2.87	1.35	1.33
21	8	612	CLA	MG-ND	-2.87	2.00	2.05
34	A	803	CL0	CHB-C4A	2.87	1.35	1.33
22	a	306	CHL	C1D-C2D	-2.86	1.39	1.45
21	B	843	CLA	CMB-C2B	-2.85	1.45	1.51
22	8	606	CHL	C1D-C2D	-2.85	1.39	1.45
22	c	606	CHL	C1D-C2D	-2.85	1.39	1.45
21	b	311	CLA	CMC-C2C	-2.84	1.44	1.50
22	a	306	CHL	CHB-C4A	2.83	1.35	1.33
22	8	601	CHL	CHB-C4A	2.83	1.35	1.33
21	3	411	CLA	MG-ND	-2.83	2.00	2.05
22	7	308	CHL	CHB-C4A	2.82	1.35	1.33
21	K	203	CLA	MG-ND	-2.81	2.00	2.05
22	8	601	CHL	C1D-C2D	-2.80	1.39	1.45
22	b	307	CHL	C1D-C2D	-2.79	1.39	1.45
22	9	606	CHL	CHB-C4A	2.79	1.35	1.33
22	1	305	CHL	C1D-C2D	-2.79	1.39	1.45
21	B	806	CLA	MG-ND	-2.78	2.00	2.05
21	a	308	CLA	MG-ND	-2.77	2.00	2.05
22	1	305	CHL	C1C-NC	-2.77	1.33	1.37
21	8	622	CLA	CMB-C2B	-2.76	1.46	1.51
21	A	856	CLA	CMB-C2B	-2.76	1.46	1.51
21	8	611	CLA	MG-NA	2.76	2.12	2.06
22	7	309	CHL	CHB-C4A	2.75	1.35	1.33
22	c	607	CHL	CHB-C4A	2.75	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	804	CLA	CMB-C2B	-2.74	1.46	1.51
22	8	607	CHL	C1D-C2D	-2.73	1.39	1.45
21	3	406	CLA	CMB-C2B	-2.73	1.46	1.51
21	B	822	CLA	CMB-C2B	-2.72	1.46	1.51
21	T	604	CLA	CMB-C2B	-2.72	1.46	1.51
21	8	622	CLA	C2A-C1A	2.72	1.58	1.52
22	8	608	CHL	C1D-C2D	-2.71	1.40	1.45
21	B	842	CLA	MG-NA	2.71	2.12	2.06
22	T	601	CHL	C1D-C2D	-2.71	1.40	1.45
21	B	844	CLA	CMB-C2B	-2.70	1.46	1.51
22	7	307	CHL	CHB-C4A	2.70	1.35	1.33
21	L	301	CLA	CMB-C2B	-2.70	1.46	1.51
21	7	305	CLA	MG-NA	2.70	2.12	2.06
21	a	308	CLA	CMB-C2B	-2.68	1.46	1.51
21	9	607	CLA	CMB-C2B	-2.68	1.46	1.51
21	B	836	CLA	CMB-C2B	-2.68	1.46	1.51
21	B	842	CLA	CMB-C2B	-2.68	1.46	1.51
22	7	307	CHL	C1D-C2D	-2.67	1.40	1.45
21	B	824	CLA	CMB-C2B	-2.67	1.46	1.51
21	3	407	CLA	MG-ND	-2.67	2.00	2.05
21	7	316	CLA	CMB-C2B	-2.67	1.46	1.51
21	B	833	CLA	CMB-C2B	-2.67	1.46	1.51
21	B	840	CLA	CMB-C2B	-2.66	1.46	1.51
21	L	303	CLA	CMB-C2B	-2.66	1.46	1.51
21	A	827	CLA	CMB-C2B	-2.65	1.46	1.51
21	A	821	CLA	CMB-C2B	-2.65	1.46	1.51
21	8	610	CLA	CMB-C2B	-2.64	1.46	1.51
21	b	306	CLA	CMB-C2B	-2.64	1.46	1.51
21	B	820	CLA	MG-NC	2.64	2.12	2.06
22	c	605	CHL	C1D-C2D	-2.63	1.40	1.45
21	A	825	CLA	CMB-C2B	-2.63	1.46	1.51
21	7	306	CLA	CMB-C2B	-2.63	1.46	1.51
21	B	829	CLA	CMB-C2B	-2.62	1.46	1.51
21	b	305	CLA	MG-NA	2.62	2.12	2.06
21	c	603	CLA	MG-NA	2.62	2.12	2.06
21	A	831	CLA	CMB-C2B	-2.62	1.46	1.51
22	1	305	CHL	CHB-C4A	2.61	1.35	1.33
21	A	834	CLA	CMB-C2B	-2.61	1.46	1.51
21	A	823	CLA	CMB-C2B	-2.61	1.46	1.51
21	B	838	CLA	CMB-C2B	-2.61	1.46	1.51
21	B	810	CLA	CMB-C2B	-2.61	1.46	1.51
21	A	842	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	602	CLA	CMB-C2B	-2.61	1.46	1.51
21	B	835	CLA	MG-NA	2.60	2.12	2.06
21	1	308	CLA	CMB-C2B	-2.60	1.46	1.51
21	9	604	CLA	CMB-C2B	-2.60	1.46	1.51
21	9	610	CLA	MG-NC	2.60	2.12	2.06
21	3	408	CLA	CMB-C2B	-2.60	1.46	1.51
21	7	310	CLA	CMB-C2B	-2.60	1.46	1.51
21	A	817	CLA	CMB-C2B	-2.59	1.46	1.51
21	7	306	CLA	MG-NA	2.59	2.12	2.06
21	H	203	CLA	CMB-C2B	-2.59	1.46	1.51
21	3	407	CLA	CMB-C2B	-2.59	1.46	1.51
21	T	614	CLA	CMB-C2B	-2.59	1.46	1.51
21	A	827	CLA	MG-ND	-2.59	2.00	2.05
21	1	313	CLA	MG-ND	-2.59	2.00	2.05
21	1	321	CLA	MG-NA	2.59	2.12	2.06
21	7	304	CLA	CMB-C2B	-2.58	1.46	1.51
21	3	410	CLA	CMB-C2B	-2.58	1.46	1.51
21	7	312	CLA	CMB-C2B	-2.58	1.46	1.51
21	A	809	CLA	CMB-C2B	-2.58	1.46	1.51
21	3	405	CLA	CMB-C2B	-2.58	1.46	1.51
21	2	603	CLA	CMB-C2B	-2.58	1.46	1.51
21	3	402	CLA	CMB-C2B	-2.58	1.46	1.51
21	B	810	CLA	MG-ND	-2.57	2.00	2.05
21	8	605	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	826	CLA	CMB-C2B	-2.57	1.46	1.51
21	T	609	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	804	CLA	CMD-C2D	-2.57	1.45	1.50
21	7	314	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	818	CLA	CMB-C2B	-2.57	1.46	1.51
21	G	205	CLA	CMB-C2B	-2.57	1.46	1.51
21	B	831	CLA	CMB-C2B	-2.57	1.46	1.51
21	G	204	CLA	CMB-C2B	-2.57	1.46	1.51
21	T	611	CLA	MG-NA	2.57	2.12	2.06
21	A	835	CLA	CMB-C2B	-2.57	1.46	1.51
21	L	305	CLA	CMB-C2B	-2.57	1.46	1.51
21	A	822	CLA	CMB-C2B	-2.57	1.46	1.51
21	2	607	CLA	CMB-C2B	-2.56	1.46	1.51
21	A	814	CLA	CMB-C2B	-2.56	1.46	1.51
21	A	816	CLA	CMB-C2B	-2.56	1.46	1.51
21	O	2002	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	837	CLA	CMB-C2B	-2.56	1.46	1.51
21	A	836	CLA	CMB-C2B	-2.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	609	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	806	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	814	CLA	CMB-C2B	-2.56	1.46	1.51
21	2	602	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	820	CLA	CMB-C2B	-2.56	1.46	1.51
21	2	605	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	812	CLA	CMB-C2B	-2.55	1.46	1.51
21	J	5002	CLA	CMB-C2B	-2.55	1.46	1.51
21	2	612	CLA	CMB-C2B	-2.55	1.46	1.51
21	A	824	CLA	CMB-C2B	-2.55	1.46	1.51
21	H	204	CLA	CMB-C2B	-2.55	1.46	1.51
21	2	604	CLA	CMB-C2B	-2.55	1.46	1.51
21	7	311	CLA	CMB-C2B	-2.55	1.46	1.51
21	B	816	CLA	CMB-C2B	-2.55	1.46	1.51
21	c	608	CLA	CMB-C2B	-2.55	1.46	1.51
21	3	411	CLA	CMB-C2B	-2.55	1.46	1.51
22	3	401	CHL	C1D-C2D	-2.55	1.40	1.45
21	B	828	CLA	CMB-C2B	-2.54	1.46	1.51
21	2	609	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	805	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	811	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	839	CLA	CMB-C2B	-2.54	1.46	1.51
21	A	840	CLA	CMB-C2B	-2.54	1.46	1.51
21	b	316	CLA	CMB-C2B	-2.54	1.46	1.51
21	a	312	CLA	CMB-C2B	-2.54	1.46	1.51
21	T	606	CLA	MG-NA	2.54	2.12	2.06
21	B	832	CLA	MG-NA	2.54	2.12	2.06
21	F	5007	CLA	CMB-C2B	-2.54	1.46	1.51
21	8	614	CLA	CMB-C2B	-2.54	1.46	1.51
21	c	603	CLA	CMB-C2B	-2.53	1.46	1.51
21	1	310	CLA	CMB-C2B	-2.53	1.46	1.51
21	9	605	CLA	CMB-C2B	-2.53	1.46	1.51
21	1	306	CLA	CMB-C2B	-2.53	1.46	1.51
21	G	201	CLA	CMB-C2B	-2.53	1.46	1.51
21	9	608	CLA	CMB-C2B	-2.53	1.46	1.51
21	A	812	CLA	CMB-C2B	-2.53	1.46	1.51
21	c	614	CLA	CMB-C2B	-2.53	1.46	1.51
21	A	837	CLA	CMB-C2B	-2.53	1.46	1.51
21	3	413	CLA	CMB-C2B	-2.53	1.46	1.51
21	T	611	CLA	CMB-C2B	-2.53	1.46	1.51
21	9	611	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	841	CLA	CMB-C2B	-2.52	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	311	CLA	CMB-C2B	-2.52	1.46	1.51
21	c	611	CLA	CMB-C2B	-2.52	1.46	1.51
21	O	2003	CLA	CMB-C2B	-2.52	1.46	1.51
21	1	302	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	828	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	806	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	810	CLA	CMB-C2B	-2.52	1.46	1.51
21	A	833	CLA	CMB-C2B	-2.52	1.46	1.51
21	B	834	CLA	CMB-C2B	-2.52	1.46	1.51
21	8	612	CLA	CMB-C2B	-2.52	1.46	1.51
21	b	315	CLA	CMB-C2B	-2.52	1.46	1.51
21	9	609	CLA	CMB-C2B	-2.52	1.46	1.51
21	a	314	CLA	CMB-C2B	-2.52	1.46	1.51
21	3	404	CLA	CMB-C2B	-2.52	1.46	1.51
21	B	825	CLA	CMB-C2B	-2.52	1.46	1.51
21	c	602	CLA	CMB-C2B	-2.52	1.46	1.51
21	8	613	CLA	MG-ND	-2.51	2.00	2.05
21	c	612	CLA	CMB-C2B	-2.51	1.46	1.51
21	c	604	CLA	CMB-C2B	-2.51	1.46	1.51
21	2	608	CLA	CMB-C2B	-2.51	1.46	1.51
21	2	611	CLA	CMB-C2B	-2.51	1.46	1.51
21	a	310	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	409	CLA	CMB-C2B	-2.51	1.46	1.51
21	T	607	CLA	CMB-C2B	-2.51	1.46	1.51
21	9	603	CLA	CMB-C2B	-2.51	1.46	1.51
21	3	403	CLA	CMB-C2B	-2.51	1.46	1.51
21	7	305	CLA	CMB-C2B	-2.51	1.46	1.51
21	8	611	CLA	CMB-C2B	-2.51	1.46	1.51
21	a	304	CLA	CMB-C2B	-2.51	1.46	1.51
21	c	613	CLA	CMB-C2B	-2.51	1.46	1.51
21	A	830	CLA	CMB-C2B	-2.51	1.46	1.51
21	2	613	CLA	CMB-C2B	-2.50	1.46	1.51
21	T	613	CLA	CMB-C2B	-2.50	1.46	1.51
21	2	610	CLA	CMB-C2B	-2.50	1.46	1.51
21	9	612	CLA	CMB-C2B	-2.50	1.46	1.51
21	T	608	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	839	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	821	CLA	CMB-C2B	-2.50	1.46	1.51
21	b	305	CLA	CMB-C2B	-2.50	1.46	1.51
21	K	203	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	843	CLA	MG-NC	2.50	2.12	2.06
21	A	838	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	601	CLA	CMB-C2B	-2.50	1.46	1.51
21	A	820	CLA	CMB-C2B	-2.50	1.46	1.51
21	a	302	CLA	CMB-C2B	-2.50	1.46	1.51
21	c	610	CLA	CMB-C2B	-2.50	1.46	1.51
21	1	313	CLA	CMB-C2B	-2.50	1.46	1.51
21	8	615	CLA	CMB-C2B	-2.50	1.46	1.51
21	7	313	CLA	CMB-C2B	-2.50	1.46	1.51
21	1	312	CLA	CMB-C2B	-2.50	1.46	1.51
21	T	603	CLA	CMB-C2B	-2.50	1.46	1.51
21	1	304	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	831	CLA	MG-ND	-2.49	2.00	2.05
21	A	815	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	842	CLA	CMD-C2D	-2.49	1.45	1.50
21	a	303	CLA	CMB-C2B	-2.49	1.46	1.51
21	T	612	CLA	CMB-C2B	-2.49	1.46	1.51
21	T	609	CLA	CMC-C2C	-2.49	1.45	1.50
21	7	323	CLA	CMB-C2B	-2.49	1.46	1.51
29	I	201	PTY	P1-O11	2.49	1.64	1.54
21	b	314	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	827	CLA	CMB-C2B	-2.49	1.46	1.51
21	B	823	CLA	MG-ND	-2.49	2.00	2.05
21	b	310	CLA	CMB-C2B	-2.49	1.46	1.51
21	8	609	CLA	MG-ND	-2.49	2.00	2.05
21	1	311	CLA	CMB-C2B	-2.49	1.46	1.51
21	A	808	CLA	CMB-C2B	-2.49	1.46	1.51
21	3	412	CLA	CMB-C2B	-2.49	1.46	1.51
21	c	609	CLA	CMB-C2B	-2.49	1.46	1.51
21	9	603	CLA	MG-ND	-2.48	2.00	2.05
21	B	811	CLA	CMB-C2B	-2.48	1.46	1.51
21	7	315	CLA	CMB-C2B	-2.48	1.46	1.51
21	F	5005	CLA	CMB-C2B	-2.48	1.46	1.51
21	1	303	CLA	CMB-C2B	-2.48	1.46	1.51
21	8	603	CLA	CMB-C2B	-2.48	1.46	1.51
21	8	604	CLA	CMB-C2B	-2.48	1.46	1.51
21	2	612	CLA	MG-NA	2.48	2.12	2.06
21	8	613	CLA	CMB-C2B	-2.48	1.46	1.51
21	O	2001	CLA	MG-ND	-2.48	2.00	2.05
21	1	308	CLA	CMC-C2C	-2.48	1.45	1.50
21	a	313	CLA	CMB-C2B	-2.48	1.46	1.51
21	O	2001	CLA	CMB-C2B	-2.48	1.46	1.51
21	B	818	CLA	CMB-C2B	-2.48	1.46	1.51
21	b	304	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	306	CLA	CMB-C2B	-2.47	1.46	1.51
21	c	601	CLA	CMB-C2B	-2.47	1.46	1.51
21	K	204	CLA	CMB-C2B	-2.47	1.46	1.51
21	1	310	CLA	MG-NC	2.47	2.12	2.06
21	A	828	CLA	CMD-C2D	-2.47	1.45	1.50
21	1	321	CLA	CMB-C2B	-2.47	1.46	1.51
21	b	312	CLA	CMB-C2B	-2.47	1.46	1.51
21	1	307	CLA	CMB-C2B	-2.46	1.46	1.51
21	T	610	CLA	CMB-C2B	-2.46	1.46	1.51
21	F	5006	CLA	CMB-C2B	-2.46	1.46	1.51
21	1	301	CLA	CMB-C2B	-2.46	1.46	1.51
21	3	414	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	815	CLA	CMB-C2B	-2.46	1.46	1.51
21	K	202	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	819	CLA	CMB-C2B	-2.46	1.46	1.51
21	a	311	CLA	CMB-C2B	-2.46	1.46	1.51
21	B	841	CLA	CMB-C2B	-2.46	1.46	1.51
21	1	309	CLA	CMB-C2B	-2.46	1.46	1.51
21	b	313	CLA	MG-NC	2.45	2.12	2.06
21	A	804	CLA	MG-ND	-2.45	2.00	2.05
23	1	314	LUT	C22-C23	-2.45	1.49	1.52
21	a	305	CLA	CMB-C2B	-2.45	1.46	1.51
21	b	313	CLA	CMB-C2B	-2.45	1.46	1.51
21	G	203	CLA	CMB-C2B	-2.45	1.46	1.51
21	K	201	CLA	CMB-C2B	-2.45	1.46	1.51
21	a	307	CLA	CMB-C2B	-2.45	1.46	1.51
21	B	817	CLA	CMB-C2B	-2.44	1.46	1.51
21	B	826	CLA	CMB-C2B	-2.44	1.46	1.51
21	8	612	CLA	MG-NA	2.43	2.12	2.06
21	A	807	CLA	CMB-C2B	-2.43	1.46	1.51
21	A	829	CLA	CMB-C2B	-2.43	1.46	1.51
21	B	834	CLA	MG-ND	-2.43	2.01	2.05
21	B	808	CLA	CMB-C2B	-2.43	1.46	1.51
21	a	309	CLA	CMB-C2B	-2.42	1.46	1.51
21	B	807	CLA	C1D-ND	2.42	1.41	1.37
21	A	832	CLA	CMB-C2B	-2.42	1.46	1.51
21	T	605	CLA	CMB-C2B	-2.42	1.46	1.51
21	B	832	CLA	CMD-C2D	-2.41	1.45	1.50
21	a	303	CLA	MG-NC	2.41	2.12	2.06
21	B	806	CLA	CMD-C2D	-2.41	1.45	1.50
21	B	830	CLA	CMB-C2B	-2.41	1.46	1.51
21	B	807	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	612	CLA	MG-NC	2.40	2.12	2.06
21	A	813	CLA	CMB-C2B	-2.39	1.46	1.51
21	L	304	CLA	CMB-C2B	-2.39	1.46	1.51
21	T	606	CLA	CMB-C2B	-2.39	1.46	1.51
21	9	610	CLA	CMB-C2B	-2.39	1.46	1.51
21	T	603	CLA	MG-NA	2.39	2.11	2.06
21	A	819	CLA	CMB-C2B	-2.38	1.46	1.51
21	A	838	CLA	MG-ND	-2.38	2.01	2.05
21	A	843	CLA	CMB-C2B	-2.37	1.46	1.51
21	8	622	CLA	C4D-CHA	2.35	1.46	1.38
21	B	835	CLA	CMB-C2B	-2.34	1.46	1.51
21	B	823	CLA	C3B-C2B	-2.33	1.37	1.40
21	A	804	CLA	CMC-C2C	-2.32	1.46	1.50
21	A	837	CLA	MG-ND	-2.32	2.01	2.05
21	B	809	CLA	CMB-C2B	-2.32	1.47	1.51
22	7	307	CHL	C1C-NC	-2.31	1.34	1.37
21	7	312	CLA	MG-ND	-2.31	2.01	2.05
21	A	840	CLA	MG-NC	2.31	2.11	2.06
21	9	612	CLA	MG-NA	2.30	2.11	2.06
21	B	806	CLA	CMC-C2C	-2.30	1.46	1.50
21	2	603	CLA	MG-NC	2.30	2.11	2.06
21	2	608	CLA	CMD-C2D	-2.29	1.46	1.50
23	B	801	LUT	C22-C23	2.29	1.55	1.52
21	b	314	CLA	MG-ND	-2.28	2.01	2.05
21	T	608	CLA	CMD-C2D	-2.28	1.46	1.50
21	L	301	CLA	MG-ND	-2.28	2.01	2.05
21	K	203	CLA	MG-NA	2.28	2.11	2.06
22	b	307	CHL	C1C-NC	-2.27	1.34	1.37
21	B	827	CLA	CMD-C2D	-2.27	1.46	1.50
21	B	818	CLA	CMD-C2D	-2.26	1.46	1.50
21	A	831	CLA	MG-NA	2.26	2.11	2.06
21	B	844	CLA	MG-ND	-2.25	2.01	2.05
21	3	414	CLA	MG-ND	-2.24	2.01	2.05
21	B	843	CLA	C3B-C2B	-2.24	1.37	1.40
21	K	201	CLA	MG-NA	2.23	2.11	2.06
21	B	811	CLA	MG-NC	2.23	2.11	2.06
21	7	323	CLA	MG-ND	-2.22	2.01	2.05
21	8	622	CLA	C3B-C2B	-2.22	1.37	1.40
21	B	836	CLA	MG-NA	2.21	2.11	2.06
21	B	823	CLA	CMD-C2D	-2.21	1.46	1.50
28	3	420	LHG	O7-C7	-2.21	1.34	1.42
21	8	612	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	306	CLA	MG-NA	2.20	2.11	2.06
21	A	807	CLA	CMC-C2C	-2.19	1.46	1.50
21	a	312	CLA	CMD-C2D	-2.18	1.46	1.50
21	A	831	CLA	MG-ND	-2.18	2.01	2.05
21	3	406	CLA	MG-ND	-2.18	2.01	2.05
21	a	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	8	608	CHL	C1C-NC	-2.18	1.34	1.37
21	1	311	CLA	CMD-C2D	-2.17	1.46	1.50
21	a	311	CLA	CMC-C2C	-2.17	1.46	1.50
21	1	309	CLA	MG-ND	-2.17	2.01	2.05
21	B	820	CLA	CMD-C2D	-2.17	1.46	1.50
21	O	2003	CLA	MG-ND	-2.17	2.01	2.05
21	O	2001	CLA	CMD-C2D	-2.17	1.46	1.50
21	B	831	CLA	CMD-C2D	-2.16	1.46	1.50
21	7	316	CLA	CMD-C2D	-2.16	1.46	1.50
21	1	302	CLA	MG-NA	2.16	2.11	2.06
21	3	414	CLA	CMD-C2D	-2.15	1.46	1.50
21	1	309	CLA	CMD-C2D	-2.15	1.46	1.50
21	B	837	CLA	CMD-C2D	-2.15	1.46	1.50
21	2	603	CLA	MG-NA	2.15	2.11	2.06
21	b	311	CLA	MG-ND	-2.15	2.01	2.05
21	B	833	CLA	CMD-C2D	-2.15	1.46	1.50
21	A	836	CLA	CMD-C2D	-2.14	1.46	1.50
21	G	203	CLA	CMD-C2D	-2.14	1.46	1.50
21	B	826	CLA	CMC-C2C	-2.14	1.46	1.50
21	B	817	CLA	MG-ND	-2.14	2.01	2.05
21	B	836	CLA	CMC-C2C	-2.14	1.46	1.50
21	A	827	CLA	CMD-C2D	-2.14	1.46	1.50
21	A	819	CLA	CMC-C2C	-2.14	1.46	1.50
21	7	316	CLA	MG-NA	2.14	2.11	2.06
21	B	822	CLA	MG-ND	-2.14	2.01	2.05
21	T	611	CLA	MG-ND	-2.14	2.01	2.05
21	3	406	CLA	CMD-C2D	-2.13	1.46	1.50
21	c	604	CLA	MG-NA	2.13	2.11	2.06
21	B	820	CLA	CMC-C2C	-2.13	1.46	1.50
21	A	805	CLA	MG-NA	2.13	2.11	2.06
21	8	605	CLA	MG-NA	2.13	2.11	2.06
21	7	314	CLA	MG-NC	2.13	2.11	2.06
21	A	840	CLA	CMD-C2D	-2.13	1.46	1.50
21	1	313	CLA	CMD-C2D	-2.12	1.46	1.50
21	7	304	CLA	CMD-C2D	-2.12	1.46	1.50
21	2	602	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	807	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	308	CHL	C1D-C2D	-2.12	1.41	1.45
21	B	840	CLA	MG-ND	-2.12	2.01	2.05
21	B	824	CLA	MG-ND	-2.11	2.01	2.05
21	a	309	CLA	CMC-C2C	-2.11	1.46	1.50
21	B	841	CLA	CMD-C2D	-2.11	1.46	1.50
21	2	603	CLA	CMD-C2D	-2.11	1.46	1.50
21	9	611	CLA	CMD-C2D	-2.11	1.46	1.50
21	2	607	CLA	CMD-C2D	-2.11	1.46	1.50
21	B	834	CLA	CMD-C2D	-2.11	1.46	1.50
21	a	303	CLA	CMD-C2D	-2.11	1.46	1.50
22	7	309	CHL	C1C-NC	-2.11	1.34	1.37
21	B	816	CLA	CMD-C2D	-2.11	1.46	1.50
21	K	202	CLA	CMD-C2D	-2.11	1.46	1.50
21	G	204	CLA	MG-ND	-2.11	2.01	2.05
21	T	606	CLA	MG-NC	2.11	2.11	2.06
21	7	312	CLA	CMD-C2D	-2.11	1.46	1.50
21	B	844	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	309	CHL	C1C-NC	-2.11	1.34	1.37
21	b	315	CLA	CMD-C2D	-2.10	1.46	1.50
21	H	203	CLA	CMC-C2C	-2.10	1.46	1.50
21	a	304	CLA	CMD-C2D	-2.10	1.46	1.50
21	3	407	CLA	CMD-C2D	-2.10	1.46	1.50
21	A	841	CLA	CMD-C2D	-2.10	1.46	1.50
21	c	603	CLA	CMD-C2D	-2.10	1.46	1.50
21	1	310	CLA	CMD-C2D	-2.10	1.46	1.50
21	A	830	CLA	CMC-C2C	-2.09	1.46	1.50
21	8	609	CLA	CMD-C2D	-2.09	1.46	1.50
21	8	615	CLA	CMD-C2D	-2.09	1.46	1.50
21	A	856	CLA	CMD-C2D	-2.09	1.46	1.50
21	c	613	CLA	CMD-C2D	-2.09	1.46	1.50
21	A	811	CLA	CMC-C2C	-2.09	1.46	1.50
21	F	5005	CLA	CMD-C2D	-2.09	1.46	1.50
21	8	611	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	410	CLA	MG-ND	-2.09	2.01	2.05
21	7	304	CLA	CMC-C2C	-2.09	1.46	1.50
21	O	2002	CLA	CMD-C2D	-2.09	1.46	1.50
21	1	306	CLA	CMD-C2D	-2.09	1.46	1.50
21	T	608	CLA	MG-ND	-2.09	2.01	2.05
21	b	313	CLA	CMD-C2D	-2.09	1.46	1.50
21	c	609	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	404	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	820	CLA	MG-ND	-2.09	2.01	2.05
21	A	835	CLA	CMC-C2C	-2.09	1.46	1.50
21	A	835	CLA	CMD-C2D	-2.09	1.46	1.50
21	A	815	CLA	CMD-C2D	-2.08	1.46	1.50
21	K	203	CLA	CMD-C2D	-2.08	1.46	1.50
22	7	308	CHL	C1C-NC	-2.08	1.34	1.37
21	A	830	CLA	CMD-C2D	-2.08	1.46	1.50
21	L	303	CLA	CMD-C2D	-2.08	1.46	1.50
21	a	310	CLA	MG-ND	-2.08	2.01	2.05
21	a	308	CLA	CMD-C2D	-2.08	1.46	1.50
21	B	813	CLA	MG-ND	-2.08	2.01	2.05
21	7	305	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	811	CLA	MG-ND	-2.08	2.01	2.05
21	B	813	CLA	CMC-C2C	-2.08	1.46	1.50
21	B	818	CLA	CMC-C2C	-2.08	1.46	1.50
21	7	313	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	839	CLA	CMC-C2C	-2.08	1.46	1.50
21	B	840	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	820	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	843	CLA	CMD-C2D	-2.08	1.46	1.50
21	B	828	CLA	CMD-C2D	-2.08	1.46	1.50
21	B	821	CLA	CMD-C2D	-2.08	1.46	1.50
21	A	813	CLA	CMD-C2D	-2.07	1.46	1.50
21	1	302	CLA	CMD-C2D	-2.07	1.46	1.50
21	7	315	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	829	CLA	CMC-C2C	-2.07	1.46	1.50
21	A	818	CLA	MG-NA	2.07	2.11	2.06
21	B	814	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
21	A	804	CLA	C3B-C2B	-2.07	1.37	1.40
21	B	812	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	804	CLA	C3B-C2B	-2.07	1.37	1.40
22	8	606	CHL	C1C-NC	-2.07	1.34	1.37
21	2	605	CLA	CMD-C2D	-2.07	1.46	1.50
21	B	807	CLA	CMD-C2D	-2.07	1.46	1.50
21	L	306	CLA	CMD-C2D	-2.07	1.46	1.50
21	c	602	CLA	MG-ND	-2.07	2.01	2.05
21	a	305	CLA	CMD-C2D	-2.07	1.46	1.50
21	a	309	CLA	CMD-C2D	-2.07	1.46	1.50
22	c	605	CHL	C1C-NC	-2.07	1.34	1.37
21	L	304	CLA	CMD-C2D	-2.07	1.46	1.50
22	a	306	CHL	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	203	CLA	CMC-C2C	-2.07	1.46	1.50
21	B	819	CLA	CMD-C2D	-2.06	1.46	1.50
21	9	603	CLA	CMD-C2D	-2.06	1.46	1.50
21	T	607	CLA	CMD-C2D	-2.06	1.46	1.50
21	9	607	CLA	CMD-C2D	-2.06	1.46	1.50
21	8	604	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	812	CLA	CMD-C2D	-2.06	1.46	1.50
21	3	410	CLA	MG-NA	2.06	2.11	2.06
21	3	402	CLA	CMD-C2D	-2.06	1.46	1.50
21	b	312	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	812	CLA	MG-ND	-2.06	2.01	2.05
21	7	314	CLA	CMD-C2D	-2.06	1.46	1.50
21	9	610	CLA	CMD-C2D	-2.06	1.46	1.50
21	T	604	CLA	CMD-C2D	-2.06	1.46	1.50
21	a	311	CLA	CMD-C2D	-2.06	1.46	1.50
21	b	310	CLA	CMD-C2D	-2.06	1.46	1.50
21	c	601	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	830	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
21	b	311	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	808	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	815	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	819	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	825	CLA	CMD-C2D	-2.06	1.46	1.50
21	b	316	CLA	CMD-C2D	-2.06	1.46	1.50
21	9	602	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	826	CLA	CMD-C2D	-2.06	1.46	1.50
21	T	610	CLA	CMD-C2D	-2.06	1.46	1.50
21	7	312	CLA	CMC-C2C	-2.06	1.46	1.50
21	9	608	CLA	CMD-C2D	-2.06	1.46	1.50
21	c	602	CLA	CMD-C2D	-2.06	1.46	1.50
21	B	804	CLA	CMD-C2D	-2.06	1.46	1.50
21	A	826	CLA	MG-ND	-2.06	2.01	2.05
21	A	833	CLA	CMC-C2C	-2.05	1.46	1.50
21	B	829	CLA	CMC-C2C	-2.05	1.46	1.50
21	1	310	CLA	CMC-C2C	-2.05	1.46	1.50
21	B	809	CLA	CMD-C2D	-2.05	1.46	1.50
21	K	204	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	811	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	809	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	811	CLA	CMD-C2D	-2.05	1.46	1.50
21	G	203	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	305	CLA	CMD-C2D	-2.05	1.46	1.50
21	T	613	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	805	CLA	CMD-C2D	-2.05	1.46	1.50
21	L	301	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	839	CLA	CMD-C2D	-2.05	1.46	1.50
21	7	323	CLA	CMD-C2D	-2.05	1.46	1.50
21	A	810	CLA	CMD-C2D	-2.05	1.46	1.50
21	1	308	CLA	CMD-C2D	-2.05	1.46	1.50
21	c	611	CLA	CMD-C2D	-2.05	1.46	1.50
21	7	304	CLA	MG-ND	-2.05	2.01	2.05
21	A	821	CLA	CMD-C2D	-2.05	1.46	1.50
21	B	814	CLA	CMC-C2C	-2.04	1.46	1.50
22	2	606	CHL	C1C-NC	-2.04	1.34	1.37
21	2	612	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	842	CLA	CMC-C2C	-2.04	1.46	1.50
21	B	824	CLA	CMD-C2D	-2.04	1.46	1.50
21	9	612	CLA	CMD-C2D	-2.04	1.46	1.50
21	T	609	CLA	CMD-C2D	-2.04	1.46	1.50
21	F	5006	CLA	CMD-C2D	-2.04	1.46	1.50
21	1	307	CLA	CMD-C2D	-2.04	1.46	1.50
21	c	602	CLA	CMC-C2C	-2.04	1.46	1.50
21	c	610	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	610	CLA	CMD-C2D	-2.04	1.46	1.50
21	B	819	CLA	CMC-C2C	-2.04	1.46	1.50
21	A	856	CLA	MG-NC	2.04	2.11	2.06
21	2	602	CLA	CMC-C2C	-2.04	1.46	1.50
21	1	303	CLA	CMD-C2D	-2.04	1.46	1.50
21	3	405	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	613	CLA	CMD-C2D	-2.04	1.46	1.50
21	9	605	CLA	MG-NA	2.04	2.11	2.06
21	A	813	CLA	CMC-C2C	-2.04	1.46	1.50
21	O	2003	CLA	CMD-C2D	-2.04	1.46	1.50
21	A	812	CLA	MG-NC	2.04	2.11	2.06
21	A	834	CLA	MG-NC	2.04	2.11	2.06
21	a	314	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	602	CLA	MG-ND	-2.04	2.01	2.05
21	A	820	CLA	CMC-C2C	-2.03	1.46	1.50
21	F	5007	CLA	CMD-C2D	-2.03	1.46	1.50
21	3	410	CLA	CMD-C2D	-2.03	1.46	1.50
21	T	606	CLA	CMC-C2C	-2.03	1.46	1.50
21	2	610	CLA	MG-NA	2.03	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	411	CLA	CMC-C2C	-2.03	1.46	1.50
21	8	610	CLA	CMD-C2D	-2.03	1.46	1.50
21	B	807	CLA	CMC-C2C	-2.03	1.46	1.50
21	c	612	CLA	CMD-C2D	-2.03	1.46	1.50
21	A	833	CLA	CMD-C2D	-2.03	1.46	1.50
21	2	610	CLA	CMC-C2C	-2.03	1.46	1.50
21	B	836	CLA	CMD-C2D	-2.03	1.46	1.50
21	3	408	CLA	CMD-C2D	-2.03	1.46	1.50
21	b	314	CLA	CMC-C2C	-2.03	1.46	1.50
21	1	312	CLA	CMD-C2D	-2.03	1.46	1.50
21	2	611	CLA	CMC-C2C	-2.03	1.46	1.50
21	8	609	CLA	MG-NC	2.03	2.11	2.06
21	7	310	CLA	CMD-C2D	-2.03	1.46	1.50
21	B	810	CLA	CMD-C2D	-2.03	1.46	1.50
21	A	809	CLA	MG-NA	2.03	2.11	2.06
21	A	817	CLA	CMD-C2D	-2.03	1.46	1.50
21	T	606	CLA	CMD-C2D	-2.03	1.46	1.50
21	A	814	CLA	MG-NA	2.03	2.11	2.06
21	A	838	CLA	CMC-C2C	-2.03	1.46	1.50
21	A	842	CLA	CMD-C2D	-2.03	1.46	1.50
21	T	612	CLA	CMD-C2D	-2.03	1.46	1.50
21	8	604	CLA	MG-NC	2.03	2.11	2.06
21	9	605	CLA	CMD-C2D	-2.03	1.46	1.50
21	A	818	CLA	CMD-C2D	-2.02	1.46	1.50
21	1	304	CLA	CMD-C2D	-2.02	1.46	1.50
21	T	611	CLA	CMD-C2D	-2.02	1.46	1.50
21	8	603	CLA	CMD-C2D	-2.02	1.46	1.50
21	B	823	CLA	CMC-C2C	-2.02	1.46	1.50
21	B	843	CLA	CMD-C2D	-2.02	1.46	1.50
21	3	402	CLA	MG-NA	2.02	2.11	2.06
21	A	823	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	832	CLA	CMD-C2D	-2.02	1.46	1.50
21	1	321	CLA	CMD-C2D	-2.02	1.46	1.50
21	7	311	CLA	CMD-C2D	-2.02	1.46	1.50
21	T	605	CLA	CMD-C2D	-2.02	1.46	1.50
21	b	313	CLA	MG-NA	2.02	2.11	2.06
21	T	605	CLA	CMC-C2C	-2.02	1.46	1.50
21	L	305	CLA	CMC-C2C	-2.02	1.46	1.50
21	c	604	CLA	CMD-C2D	-2.02	1.46	1.50
21	a	307	CLA	MG-NC	2.02	2.11	2.06
21	c	612	CLA	MG-NC	2.02	2.11	2.06
21	1	301	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	826	CLA	CMD-C2D	-2.02	1.46	1.50
21	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
21	G	204	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	821	CLA	MG-ND	-2.02	2.01	2.05
21	3	411	CLA	CMD-C2D	-2.02	1.46	1.50
21	9	604	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	806	CLA	CMD-C2D	-2.02	1.46	1.50
21	A	812	CLA	MG-ND	-2.02	2.01	2.05
21	1	304	CLA	CMC-C2C	-2.02	1.46	1.50
21	3	413	CLA	CMD-C2D	-2.02	1.46	1.50
21	8	613	CLA	CMD-C2D	-2.01	1.46	1.50
21	3	412	CLA	C3B-C2B	-2.01	1.37	1.40
21	8	614	CLA	CMD-C2D	-2.01	1.46	1.50
21	B	827	CLA	CMC-C2C	-2.01	1.46	1.50
21	K	201	CLA	CMD-C2D	-2.01	1.46	1.50
21	A	832	CLA	CMC-C2C	-2.01	1.46	1.50
21	a	313	CLA	CMD-C2D	-2.01	1.46	1.50
21	A	824	CLA	CMD-C2D	-2.01	1.46	1.50
21	b	305	CLA	CMD-C2D	-2.01	1.46	1.50
21	B	832	CLA	C3B-C2B	-2.01	1.37	1.40
21	A	816	CLA	CMD-C2D	-2.01	1.46	1.50
21	2	611	CLA	CMD-C2D	-2.01	1.46	1.50
21	B	807	CLA	MG-ND	2.01	2.09	2.05
21	8	610	CLA	CMC-C2C	-2.00	1.46	1.50
21	B	808	CLA	CMC-C2C	-2.00	1.46	1.50
21	J	5002	CLA	CMD-C2D	-2.00	1.46	1.50
21	A	822	CLA	CMD-C2D	-2.00	1.46	1.50
21	A	839	CLA	C3B-C2B	-2.00	1.37	1.40
21	B	838	CLA	CMD-C2D	-2.00	1.46	1.50
21	T	603	CLA	CMD-C2D	-2.00	1.46	1.50
21	3	412	CLA	CMD-C2D	-2.00	1.46	1.50
21	8	605	CLA	CMD-C2D	-2.00	1.46	1.50
21	B	835	CLA	CMD-C2D	-2.00	1.46	1.50
21	9	601	CLA	CMD-C2D	-2.00	1.46	1.50
21	B	813	CLA	CMD-C2D	-2.00	1.46	1.50
21	9	610	CLA	MG-NA	2.00	2.11	2.06
21	3	409	CLA	CMD-C2D	-2.00	1.46	1.50
21	A	814	CLA	CMD-C2D	-2.00	1.46	1.50
21	A	829	CLA	CMD-C2D	-2.00	1.46	1.50

All (1864) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	601	CLA	C4A-NA-C1A	-16.26	99.26	106.68
22	7	303	CHL	C4A-NA-C1A	14.84	113.45	106.68
22	8	608	CHL	C4A-NA-C1A	14.79	113.42	106.68
22	c	605	CHL	C4A-NA-C1A	14.79	113.42	106.68
22	b	309	CHL	C4A-NA-C1A	14.73	113.40	106.68
22	c	607	CHL	C4A-NA-C1A	14.36	113.23	106.68
22	T	601	CHL	C4A-NA-C1A	14.31	113.21	106.68
22	b	307	CHL	C4A-NA-C1A	13.96	113.05	106.68
22	b	308	CHL	C4A-NA-C1A	13.89	113.02	106.68
22	8	606	CHL	C4A-NA-C1A	13.60	112.88	106.68
22	9	606	CHL	C4A-NA-C1A	13.57	112.87	106.68
22	7	308	CHL	C4A-NA-C1A	13.55	112.86	106.68
22	8	607	CHL	C4A-NA-C1A	13.51	112.84	106.68
22	2	601	CHL	C4A-NA-C1A	13.41	112.80	106.68
22	2	606	CHL	C4A-NA-C1A	13.32	112.75	106.68
22	7	307	CHL	C4A-NA-C1A	13.17	112.69	106.68
34	A	803	CL0	C4A-NA-C1A	12.72	112.48	106.68
22	3	401	CHL	C4A-NA-C1A	12.37	112.32	106.68
22	7	309	CHL	C4A-NA-C1A	11.75	112.04	106.68
22	c	606	CHL	C4A-NA-C1A	10.87	111.64	106.68
22	T	602	CHL	C4A-NA-C1A	10.64	111.53	106.68
22	a	306	CHL	C4A-NA-C1A	10.42	111.43	106.68
22	b	302	CHL	C4A-NA-C1A	10.40	111.43	106.68
22	8	601	CHL	C4A-NA-C1A	9.85	111.17	106.68
21	8	622	CLA	C4A-NA-C1A	9.34	110.94	106.68
22	1	305	CHL	C4A-NA-C1A	9.25	110.90	106.68
21	T	606	CLA	C4A-NA-C1A	7.70	110.19	106.68
21	A	811	CLA	C4A-NA-C1A	7.41	110.06	106.68
21	A	827	CLA	C4A-NA-C1A	7.39	110.05	106.68
21	B	835	CLA	C4A-NA-C1A	7.32	110.02	106.68
21	J	5002	CLA	C4A-NA-C1A	7.23	109.98	106.68
21	B	820	CLA	C4A-NA-C1A	7.17	109.95	106.68
21	B	809	CLA	C4A-NA-C1A	7.08	109.91	106.68
21	T	603	CLA	C4A-NA-C1A	7.03	109.88	106.68
21	T	608	CLA	C4A-NA-C1A	6.88	109.82	106.68
21	K	203	CLA	C4A-NA-C1A	6.87	109.81	106.68
21	2	603	CLA	C4A-NA-C1A	6.83	109.80	106.68
21	T	611	CLA	C4A-NA-C1A	6.81	109.79	106.68
21	A	834	CLA	C4A-NA-C1A	6.79	109.78	106.68
21	b	305	CLA	C4A-NA-C1A	6.78	109.77	106.68
21	7	313	CLA	C4A-NA-C1A	6.77	109.77	106.68
21	9	603	CLA	C4A-NA-C1A	6.74	109.75	106.68
21	L	305	CLA	C4A-NA-C1A	6.73	109.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	610	CLA	C4A-NA-C1A	6.72	109.75	106.68
21	B	839	CLA	C4A-NA-C1A	6.65	109.71	106.68
21	8	605	CLA	C4A-NA-C1A	6.64	109.71	106.68
21	A	816	CLA	C4A-NA-C1A	6.62	109.70	106.68
21	7	306	CLA	C4A-NA-C1A	6.57	109.68	106.68
21	2	611	CLA	C4A-NA-C1A	6.57	109.68	106.68
21	3	410	CLA	C4A-NA-C1A	6.55	109.67	106.68
21	8	612	CLA	C4A-NA-C1A	6.55	109.67	106.68
21	A	805	CLA	C4A-NA-C1A	6.53	109.66	106.68
21	9	605	CLA	C4A-NA-C1A	6.52	109.66	106.68
21	A	815	CLA	C4A-NA-C1A	6.50	109.64	106.68
21	c	611	CLA	C4A-NA-C1A	6.48	109.64	106.68
21	A	818	CLA	C4A-NA-C1A	6.48	109.63	106.68
21	a	311	CLA	C4A-NA-C1A	6.45	109.62	106.68
21	1	321	CLA	C4A-NA-C1A	6.45	109.62	106.68
21	9	611	CLA	C4A-NA-C1A	6.44	109.62	106.68
21	B	827	CLA	C4A-NA-C1A	6.44	109.62	106.68
21	K	201	CLA	C4A-NA-C1A	6.42	109.61	106.68
21	3	406	CLA	C4A-NA-C1A	6.41	109.61	106.68
21	A	838	CLA	C4A-NA-C1A	6.37	109.58	106.68
21	7	305	CLA	C4A-NA-C1A	6.36	109.58	106.68
21	b	313	CLA	C4A-NA-C1A	6.35	109.58	106.68
21	7	323	CLA	C4A-NA-C1A	6.33	109.57	106.68
21	B	844	CLA	C4A-NA-C1A	6.30	109.55	106.68
21	c	604	CLA	C4A-NA-C1A	6.30	109.55	106.68
21	B	834	CLA	C4A-NA-C1A	6.28	109.54	106.68
21	O	2001	CLA	C4A-NA-C1A	6.18	109.50	106.68
21	B	806	CLA	C4A-NA-C1A	6.16	109.49	106.68
21	A	830	CLA	C4A-NA-C1A	6.16	109.49	106.68
21	B	814	CLA	C4A-NA-C1A	6.15	109.48	106.68
21	L	306	CLA	C4A-NA-C1A	6.15	109.48	106.68
21	1	310	CLA	C4A-NA-C1A	6.14	109.48	106.68
21	A	820	CLA	C4A-NA-C1A	6.14	109.48	106.68
21	A	822	CLA	C4A-NA-C1A	6.13	109.48	106.68
21	B	817	CLA	C4A-NA-C1A	6.13	109.48	106.68
21	3	405	CLA	C4A-NA-C1A	6.12	109.47	106.68
21	A	808	CLA	C4A-NA-C1A	6.12	109.47	106.68
21	F	5007	CLA	C4A-NA-C1A	6.12	109.47	106.68
21	a	314	CLA	C4A-NA-C1A	6.10	109.46	106.68
21	7	312	CLA	C4A-NA-C1A	6.09	109.46	106.68
21	B	829	CLA	C4A-NA-C1A	6.08	109.45	106.68
21	7	314	CLA	C4A-NA-C1A	6.05	109.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	306	CLA	C4A-NA-C1A	6.02	109.42	106.68
21	8	604	CLA	C4A-NA-C1A	5.99	109.41	106.68
21	B	841	CLA	C4A-NA-C1A	5.99	109.41	106.68
21	1	306	CLA	C4A-NA-C1A	5.99	109.41	106.68
21	c	601	CLA	C4A-NA-C1A	5.97	109.40	106.68
21	A	837	CLA	C4A-NA-C1A	5.96	109.40	106.68
21	7	316	CLA	C4A-NA-C1A	5.95	109.39	106.68
21	3	403	CLA	C4A-NA-C1A	5.94	109.39	106.68
21	9	610	CLA	C4A-NA-C1A	5.94	109.39	106.68
21	A	856	CLA	C4A-NA-C1A	5.94	109.39	106.68
21	B	837	CLA	C4A-NA-C1A	5.94	109.39	106.68
21	1	302	CLA	C4A-NA-C1A	5.93	109.39	106.68
21	A	829	CLA	C4A-NA-C1A	5.92	109.38	106.68
21	a	303	CLA	C4A-NA-C1A	5.92	109.38	106.68
21	3	409	CLA	C4A-NA-C1A	5.89	109.37	106.68
21	8	613	CLA	C4A-NA-C1A	5.87	109.36	106.68
21	G	203	CLA	C4A-NA-C1A	5.86	109.35	106.68
21	H	203	CLA	C4A-NA-C1A	5.86	109.35	106.68
21	A	831	CLA	C4A-NA-C1A	5.85	109.35	106.68
21	c	613	CLA	C4A-NA-C1A	5.81	109.33	106.68
21	B	833	CLA	C4A-NA-C1A	5.80	109.33	106.68
21	3	402	CLA	C4A-NA-C1A	5.79	109.32	106.68
21	8	622	CLA	C2A-C1A-CHA	5.78	133.89	123.87
21	T	610	CLA	C4A-NA-C1A	5.78	109.31	106.68
21	T	607	CLA	C4A-NA-C1A	5.77	109.31	106.68
21	1	301	CLA	C4A-NA-C1A	5.77	109.31	106.68
21	3	414	CLA	C4A-NA-C1A	5.74	109.30	106.68
21	c	612	CLA	C4A-NA-C1A	5.72	109.29	106.68
21	9	601	CLA	C2A-C3A-C4A	-5.71	92.64	101.87
21	A	832	CLA	C4A-NA-C1A	5.68	109.27	106.68
21	c	610	CLA	C4A-NA-C1A	5.68	109.27	106.68
21	2	613	CLA	C4A-NA-C1A	5.67	109.27	106.68
21	b	314	CLA	C4A-NA-C1A	5.66	109.26	106.68
21	a	305	CLA	C4A-NA-C1A	5.66	109.26	106.68
21	B	823	CLA	C4A-NA-C1A	5.64	109.25	106.68
21	a	310	CLA	C4A-NA-C1A	5.64	109.25	106.68
21	c	603	CLA	C4A-NA-C1A	5.62	109.24	106.68
21	1	312	CLA	C4A-NA-C1A	5.60	109.23	106.68
21	A	828	CLA	C4A-NA-C1A	5.57	109.22	106.68
21	1	304	CLA	C4A-NA-C1A	5.57	109.22	106.68
21	1	307	CLA	C4A-NA-C1A	5.57	109.22	106.68
21	B	824	CLA	C4A-NA-C1A	5.55	109.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	838	CLA	C4A-NA-C1A	5.55	109.21	106.68
21	1	313	CLA	C4A-NA-C1A	5.53	109.20	106.68
21	7	315	CLA	C4A-NA-C1A	5.52	109.20	106.68
21	B	811	CLA	C4A-NA-C1A	5.46	109.17	106.68
21	G	204	CLA	C4A-NA-C1A	5.45	109.17	106.68
21	L	303	CLA	C4A-NA-C1A	5.44	109.16	106.68
21	3	411	CLA	C4A-NA-C1A	5.41	109.14	106.68
21	b	312	CLA	C4A-NA-C1A	5.40	109.14	106.68
21	2	602	CLA	C4A-NA-C1A	5.35	109.12	106.68
21	3	407	CLA	C4A-NA-C1A	5.34	109.11	106.68
21	2	612	CLA	C4A-NA-C1A	5.32	109.10	106.68
21	a	309	CLA	C4A-NA-C1A	5.31	109.10	106.68
29	I	201	PTY	O11-P1-O14	-5.28	92.91	106.67
21	T	612	CLA	C4A-NA-C1A	5.26	109.08	106.68
21	L	301	CLA	C4A-NA-C1A	5.24	109.07	106.68
21	B	825	CLA	C4A-NA-C1A	5.22	109.06	106.68
21	9	612	CLA	C4A-NA-C1A	5.20	109.05	106.68
21	2	609	CLA	C4A-NA-C1A	5.18	109.04	106.68
21	a	307	CLA	C4A-NA-C1A	5.16	109.03	106.68
21	a	313	CLA	C4A-NA-C1A	5.14	109.03	106.68
21	A	833	CLA	C4A-NA-C1A	5.14	109.02	106.68
21	B	842	CLA	C4A-NA-C1A	5.10	109.01	106.68
21	B	809	CLA	CMB-C2B-C1B	-5.05	121.06	128.46
21	K	204	CLA	C4A-NA-C1A	5.04	108.98	106.68
21	F	5006	CLA	C4A-NA-C1A	5.03	108.98	106.68
21	2	607	CLA	C4A-NA-C1A	5.02	108.97	106.68
21	A	841	CLA	C4A-NA-C1A	5.00	108.96	106.68
21	8	622	CLA	CMB-C2B-C1B	-5.00	121.13	128.46
21	A	836	CLA	C4A-NA-C1A	4.98	108.95	106.68
21	B	813	CLA	C4A-NA-C1A	4.98	108.95	106.68
21	b	316	CLA	C4A-NA-C1A	4.98	108.95	106.68
21	1	311	CLA	C4A-NA-C1A	4.95	108.94	106.68
21	A	804	CLA	C4A-NA-C1A	4.95	108.94	106.68
21	9	609	CLA	C4A-NA-C1A	4.94	108.93	106.68
21	1	308	CLA	C4A-NA-C1A	4.94	108.93	106.68
21	c	602	CLA	C4A-NA-C1A	4.94	108.93	106.68
21	T	605	CLA	C4A-NA-C1A	4.91	108.92	106.68
21	9	601	CLA	CMA-C3A-C4A	4.90	124.95	111.77
21	A	826	CLA	C4A-NA-C1A	4.88	108.91	106.68
21	O	2003	CLA	C4A-NA-C1A	4.88	108.91	106.68
21	7	304	CLA	C4A-NA-C1A	4.88	108.90	106.68
21	a	302	CLA	C4A-NA-C1A	4.86	108.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	815	CLA	C4A-NA-C1A	4.85	108.89	106.68
21	B	821	CLA	C4A-NA-C1A	4.85	108.89	106.68
23	a	315	LUT	C35-C15-C14	4.85	133.44	123.52
21	A	835	CLA	C4A-NA-C1A	4.84	108.89	106.68
21	O	2002	CLA	C4A-NA-C1A	4.83	108.88	106.68
21	B	835	CLA	CMB-C2B-C1B	-4.82	121.39	128.46
21	B	831	CLA	C4A-NA-C1A	4.79	108.87	106.68
21	B	810	CLA	C4A-NA-C1A	4.78	108.86	106.68
21	A	824	CLA	C4A-NA-C1A	4.77	108.86	106.68
21	A	843	CLA	CMB-C2B-C1B	-4.77	121.47	128.46
21	B	840	CLA	C4A-NA-C1A	4.76	108.85	106.68
21	F	5005	CLA	C4A-NA-C1A	4.74	108.84	106.68
21	T	609	CLA	C4A-NA-C1A	4.69	108.82	106.68
21	A	839	CLA	C4A-NA-C1A	4.66	108.81	106.68
21	L	304	CLA	C4A-NA-C1A	4.66	108.81	106.68
21	G	205	CLA	C4A-NA-C1A	4.65	108.80	106.68
21	7	310	CLA	C4A-NA-C1A	4.62	108.79	106.68
21	A	842	CLA	C4A-NA-C1A	4.62	108.78	106.68
21	3	408	CLA	C4A-NA-C1A	4.61	108.78	106.68
21	A	810	CLA	C4A-NA-C1A	4.60	108.78	106.68
21	8	622	CLA	CAA-C2A-C1A	4.57	126.97	111.97
21	B	830	CLA	C4A-NA-C1A	4.57	108.76	106.68
21	9	601	CLA	CHB-C4A-NA	4.55	130.97	124.40
21	c	608	CLA	C4A-NA-C1A	4.54	108.75	106.68
21	A	812	CLA	C4A-NA-C1A	4.51	108.74	106.68
21	O	2002	CLA	CAB-C3B-C4B	-4.51	121.86	128.46
21	1	309	CLA	C4A-NA-C1A	4.50	108.73	106.68
25	B	852	BCR	C16-C15-C14	-4.49	114.34	123.52
21	2	605	CLA	C4A-NA-C1A	4.48	108.72	106.68
21	B	832	CLA	C4A-NA-C1A	4.46	108.72	106.68
21	A	817	CLA	C4A-NA-C1A	4.46	108.71	106.68
21	c	614	CLA	C4A-NA-C1A	4.46	108.71	106.68
21	a	312	CLA	C4A-NA-C1A	4.44	108.70	106.68
21	B	822	CLA	CMB-C2B-C1B	-4.43	121.96	128.46
21	3	404	CLA	C4A-NA-C1A	4.43	108.70	106.68
21	H	204	CLA	C4A-NA-C1A	4.41	108.69	106.68
21	8	614	CLA	C4A-NA-C1A	4.40	108.69	106.68
21	A	828	CLA	CMB-C2B-C1B	-4.40	122.02	128.46
21	A	821	CLA	C4A-NA-C1A	4.39	108.68	106.68
21	9	604	CLA	C4A-NA-C1A	4.38	108.68	106.68
23	1	314	LUT	C35-C15-C14	4.38	132.48	123.52
21	1	308	CLA	CMB-C2B-C1B	-4.37	122.05	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	315	LUT	C15-C35-C34	-4.36	114.61	123.52
21	L	304	CLA	CMB-C2B-C1B	-4.31	122.14	128.46
21	B	807	CLA	CMB-C2B-C1B	-4.31	122.14	128.46
21	9	605	CLA	CMB-C2B-C1B	-4.30	122.16	128.46
21	a	304	CLA	C4A-NA-C1A	4.29	108.64	106.68
21	B	842	CLA	CMB-C2B-C1B	-4.29	122.17	128.46
21	A	842	CLA	CMB-C2B-C1B	-4.27	122.21	128.46
24	1	315	XAT	C27-C28-C29	4.26	132.15	125.53
21	B	808	CLA	C4A-NA-C1A	4.25	108.62	106.68
21	8	622	CLA	CHA-C1A-NA	-4.22	116.84	126.39
21	9	607	CLA	O2D-CGD-O1D	-4.21	115.66	123.85
21	8	611	CLA	C4A-NA-C1A	4.20	108.60	106.68
21	b	310	CLA	C4A-NA-C1A	4.20	108.60	106.68
21	3	406	CLA	CMB-C2B-C1B	-4.20	122.30	128.46
22	8	608	CHL	C1-C2-C3	-4.17	120.01	126.76
21	T	613	CLA	C4A-NA-C1A	4.17	108.58	106.68
21	A	819	CLA	CMB-C2B-C1B	-4.16	122.36	128.46
21	1	321	CLA	CMB-C2B-C1B	-4.15	122.38	128.46
25	B	852	BCR	C15-C16-C17	4.15	132.01	123.52
25	A	846	BCR	C16-C15-C14	4.14	131.99	123.52
34	A	803	CL0	CHD-C4C-C3C	4.14	130.81	124.77
22	8	601	CHL	C1-C2-C3	-4.13	120.08	126.76
24	a	316	XAT	O4-C5-C4	-4.10	109.65	113.49
22	b	309	CHL	C1-C2-C3	-4.10	120.13	126.76
21	B	836	CLA	CMB-C2B-C1B	-4.09	122.46	128.46
22	3	401	CHL	C1-C2-C3	-4.07	119.53	126.20
21	B	831	CLA	CMB-C2B-C1B	-4.07	122.50	128.46
21	B	808	CLA	CMB-C2B-C1B	-4.05	122.52	128.46
21	A	819	CLA	C4A-NA-C1A	4.04	108.52	106.68
21	A	809	CLA	C4A-NA-C1A	4.03	108.52	106.68
21	9	602	CLA	CMB-C2B-C1B	-4.00	122.59	128.46
21	T	605	CLA	CMB-C2B-C1B	-3.98	122.62	128.46
21	B	818	CLA	C4A-NA-C1A	3.98	108.49	106.68
22	7	309	CHL	CHD-C4C-C3C	3.96	130.54	124.77
21	8	610	CLA	CMB-C2B-C1B	-3.95	122.66	128.46
25	A	846	BCR	C8-C7-C6	3.95	137.55	127.00
22	b	307	CHL	CHD-C4C-C3C	3.94	130.52	124.77
24	T	616	XAT	C7-C8-C9	3.94	131.65	125.53
21	A	807	CLA	CMB-C2B-C1B	-3.94	122.68	128.46
21	A	815	CLA	CMB-C2B-C1B	-3.94	122.68	128.46
21	B	830	CLA	CMB-C2B-C1B	-3.93	122.69	128.46
21	B	819	CLA	CMB-C2B-C1B	-3.93	122.70	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	308	CHL	CHD-C4C-C3C	3.93	130.50	124.77
22	c	605	CHL	CHD-C4C-C3C	3.93	130.50	124.77
25	A	847	BCR	C7-C8-C9	3.92	132.04	126.23
21	B	838	CLA	CMB-C2B-C1B	-3.92	122.72	128.46
21	B	810	CLA	CMB-C2B-C1B	-3.92	122.72	128.46
21	K	201	CLA	CMB-C2B-C1B	-3.91	122.73	128.46
21	b	311	CLA	CMB-C2B-C1B	-3.90	122.74	128.46
21	B	827	CLA	CMB-C2B-C1B	-3.90	122.74	128.46
21	B	841	CLA	CMB-C2B-C1B	-3.90	122.75	128.46
21	a	309	CLA	CMB-C2B-C1B	-3.89	122.75	128.46
21	A	821	CLA	CMB-C2B-C1B	-3.89	122.76	128.46
24	3	416	XAT	O24-C25-C24	-3.89	109.85	113.49
21	9	604	CLA	CMB-C2B-C1B	-3.88	122.77	128.46
21	7	316	CLA	CMB-C2B-C1B	-3.87	122.78	128.46
21	B	817	CLA	CMB-C2B-C1B	-3.87	122.78	128.46
21	B	809	CLA	CMB-C2B-C3B	3.86	132.40	124.68
21	A	814	CLA	CMB-C2B-C1B	-3.86	122.80	128.46
21	B	840	CLA	CMB-C2B-C1B	-3.85	122.81	128.46
21	B	828	CLA	CMB-C2B-C1B	-3.85	122.81	128.46
22	b	302	CHL	CHD-C4C-C3C	3.85	130.39	124.77
21	8	605	CLA	CMB-C2B-C1B	-3.85	122.82	128.46
21	B	832	CLA	CMB-C2B-C1B	-3.85	122.82	128.46
21	c	609	CLA	C4A-NA-C1A	3.84	108.43	106.68
21	G	203	CLA	CMB-C2B-C1B	-3.84	122.83	128.46
21	8	611	CLA	CMB-C2B-C1B	-3.83	122.84	128.46
21	B	818	CLA	CMB-C2B-C1B	-3.83	122.84	128.46
21	A	829	CLA	CMB-C2B-C1B	-3.83	122.84	128.46
22	7	307	CHL	CHD-C4C-C3C	3.83	130.35	124.77
25	A	846	BCR	C7-C8-C9	-3.82	120.58	126.23
34	A	803	CL0	C1-C2-C3	-3.82	119.94	126.20
21	L	301	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
24	a	316	XAT	C27-C28-C29	3.82	131.46	125.53
22	7	309	CHL	C1D-CHD-C4C	-3.82	117.90	126.02
25	A	847	BCR	C8-C7-C6	3.82	137.20	127.00
21	b	315	CLA	C4A-NA-C1A	3.81	108.42	106.68
21	A	856	CLA	CMB-C2B-C1B	-3.81	122.88	128.46
21	9	607	CLA	C4A-NA-C1A	3.81	108.42	106.68
22	8	607	CHL	CHD-C4C-C3C	3.79	130.30	124.77
21	A	823	CLA	CMB-C2B-C1B	-3.78	122.91	128.46
22	c	607	CHL	CHD-C4C-C3C	3.78	130.28	124.77
21	L	303	CLA	CMB-C2B-C1B	-3.77	122.93	128.46
22	b	302	CHL	C1-C2-C3	-3.77	120.02	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	404	CLA	CMB-C2B-C1B	-3.77	122.94	128.46
21	B	813	CLA	CMB-C2B-C1B	-3.77	122.94	128.46
21	G	201	CLA	C4A-NA-C1A	3.77	108.40	106.68
22	7	303	CHL	C1-C2-C3	-3.76	120.03	126.20
22	T	602	CHL	C1-C2-C3	-3.76	120.03	126.20
21	2	605	CLA	CMB-C2B-C1B	-3.76	122.95	128.46
21	9	608	CLA	C4A-NA-C1A	3.75	108.39	106.68
21	a	314	CLA	CMB-C2B-C1B	-3.74	122.97	128.46
21	a	308	CLA	CHB-C4A-NA	3.74	129.80	124.40
22	1	305	CHL	CHD-C4C-C3C	3.74	130.23	124.77
21	1	301	CLA	CMB-C2B-C1B	-3.74	122.98	128.46
22	2	601	CHL	C1-C2-C3	-3.74	120.07	126.20
21	8	622	CLA	CAA-C2A-C3A	-3.74	102.90	113.00
21	8	609	CLA	C4A-NA-C1A	3.74	108.38	106.68
21	A	806	CLA	CMB-C2B-C1B	-3.74	122.98	128.46
21	3	408	CLA	CMB-C2B-C1B	-3.74	122.98	128.46
21	A	827	CLA	CMB-C2B-C1B	-3.73	123.00	128.46
21	A	839	CLA	CMB-C2B-C1B	-3.73	123.00	128.46
23	B	801	LUT	C22-C23-C24	3.72	116.72	111.18
21	A	823	CLA	C4A-NA-C1A	3.72	108.38	106.68
22	8	601	CHL	CHD-C4C-C3C	3.72	130.20	124.77
21	a	308	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
21	9	601	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
21	A	841	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
21	B	839	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
22	2	606	CHL	CHD-C4C-C3C	3.71	130.19	124.77
21	9	610	CLA	CMB-C2B-C1B	-3.71	123.01	128.46
21	9	608	CLA	CMB-C2B-C1B	-3.71	123.02	128.46
22	8	606	CHL	CHD-C4C-C3C	3.70	130.17	124.77
21	T	604	CLA	CMB-C2B-C1B	-3.70	123.04	128.46
22	7	309	CHL	C2D-C1D-ND	-3.70	106.47	110.13
22	c	606	CHL	CHD-C4C-C3C	3.69	130.15	124.77
21	B	835	CLA	CMB-C2B-C3B	3.68	132.04	124.68
21	F	5005	CLA	CMB-C2B-C1B	-3.67	123.07	128.46
21	2	608	CLA	CMB-C2B-C1B	-3.67	123.08	128.46
21	B	829	CLA	CMB-C2B-C1B	-3.67	123.08	128.46
21	A	817	CLA	CMB-C2B-C1B	-3.67	123.08	128.46
21	A	830	CLA	CMB-C2B-C1B	-3.67	123.08	128.46
22	a	306	CHL	CHD-C4C-C3C	3.67	130.12	124.77
21	A	843	CLA	C4A-NA-C1A	3.66	108.35	106.68
22	9	606	CHL	CHD-C4C-C3C	3.66	130.11	124.77
21	1	304	CLA	CMB-C2B-C1B	-3.66	123.10	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	843	CLA	CMB-C2B-C3B	3.65	131.98	124.68
21	B	815	CLA	CMB-C2B-C1B	-3.65	123.11	128.46
21	2	610	CLA	CMB-C2B-C1B	-3.64	123.13	128.46
21	7	312	CLA	CMB-C2B-C1B	-3.63	123.14	128.46
21	A	813	CLA	CMB-C2B-C1B	-3.63	123.14	128.46
21	c	608	CLA	CMB-C2B-C1B	-3.63	123.14	128.46
21	F	5007	CLA	CMB-C2B-C1B	-3.63	123.14	128.46
21	a	307	CLA	CMB-C2B-C1B	-3.62	123.15	128.46
21	K	203	CLA	CMB-C2B-C1B	-3.62	123.15	128.46
21	1	303	CLA	CMB-C2B-C1B	-3.62	123.16	128.46
21	9	607	CLA	O2D-CGD-CBD	3.62	117.55	111.23
21	L	305	CLA	CMB-C2B-C1B	-3.61	123.16	128.46
21	B	833	CLA	CMB-C2B-C1B	-3.61	123.16	128.46
21	A	837	CLA	CMB-C2B-C1B	-3.61	123.17	128.46
21	T	609	CLA	CMB-C2B-C1B	-3.61	123.17	128.46
21	A	810	CLA	CMB-C2B-C1B	-3.60	123.17	128.46
21	B	837	CLA	CMB-C2B-C1B	-3.60	123.17	128.46
21	c	609	CLA	CMB-C2B-C1B	-3.60	123.18	128.46
21	b	306	CLA	CMB-C2B-C1B	-3.60	123.18	128.46
21	2	609	CLA	CMB-C2B-C1B	-3.60	123.18	128.46
21	8	609	CLA	CMB-C2B-C1B	-3.59	123.19	128.46
21	B	821	CLA	CMB-C2B-C1B	-3.59	123.19	128.46
21	8	622	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
21	B	807	CLA	CMB-C2B-C3B	3.59	131.87	124.68
21	c	604	CLA	CMB-C2B-C1B	-3.59	123.19	128.46
21	A	836	CLA	CMB-C2B-C1B	-3.59	123.20	128.46
21	7	311	CLA	CMB-C2B-C1B	-3.58	123.20	128.46
21	9	612	CLA	CMB-C2B-C1B	-3.58	123.20	128.46
21	B	834	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
22	2	601	CHL	CHD-C4C-C3C	3.58	130.00	124.77
21	b	304	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
21	2	611	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
21	1	302	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
21	7	315	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
21	c	611	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
21	3	403	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
21	9	603	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
21	8	615	CLA	CMB-C2B-C1B	-3.57	123.22	128.46
22	c	607	CHL	C2D-C1D-ND	-3.57	106.59	110.13
21	O	2002	CLA	CMB-C2B-C1B	-3.57	123.22	128.46
25	A	848	BCR	C24-C23-C22	3.57	131.51	126.23
21	3	409	CLA	CMB-C2B-C1B	-3.56	123.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	840	CLA	CMB-C2B-C1B	-3.56	123.24	128.46
21	G	204	CLA	CMB-C2B-C1B	-3.56	123.24	128.46
23	1	314	LUT	C15-C35-C34	-3.56	116.24	123.52
21	8	613	CLA	CMB-C2B-C1B	-3.56	123.25	128.46
21	1	309	CLA	CMB-C2B-C1B	-3.55	123.25	128.46
21	B	820	CLA	CMB-C2B-C1B	-3.55	123.26	128.46
21	L	306	CLA	CMB-C2B-C1B	-3.55	123.26	128.46
21	T	611	CLA	CMB-C2B-C1B	-3.54	123.26	128.46
21	1	307	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
21	1	306	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
21	a	308	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
21	9	609	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
21	B	826	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
21	a	310	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
21	a	303	CLA	CMB-C2B-C1B	-3.54	123.28	128.46
21	c	610	CLA	CMB-C2B-C1B	-3.53	123.28	128.46
21	K	202	CLA	CMB-C2B-C1B	-3.53	123.28	128.46
21	8	622	CLA	CHB-C4A-NA	3.53	129.50	124.40
21	A	806	CLA	C4A-NA-C1A	3.53	108.29	106.68
21	A	809	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	c	613	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	8	614	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	a	313	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	c	601	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	T	603	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
21	b	305	CLA	CMB-C2B-C1B	-3.52	123.29	128.46
21	2	612	CLA	CMB-C2B-C1B	-3.52	123.29	128.46
21	T	608	CLA	CMB-C2B-C1B	-3.52	123.29	128.46
24	3	416	XAT	C7-C8-C9	3.52	131.00	125.53
21	2	613	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
21	H	204	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
21	7	305	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
21	3	410	CLA	CMB-C2B-C1B	-3.52	123.31	128.46
21	1	312	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	F	5006	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	8	604	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	B	816	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	b	312	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	2	604	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	A	808	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	O	2001	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
21	T	609	CLA	CHB-C4A-NA	3.51	129.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	313	CLA	CMB-C2B-C1B	-3.51	123.32	128.46
21	T	613	CLA	CMB-C2B-C1B	-3.51	123.32	128.46
21	O	2003	CLA	CMB-C2B-C1B	-3.50	123.32	128.46
21	a	302	CLA	CMB-C2B-C1B	-3.50	123.32	128.46
21	T	610	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
21	J	5002	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
21	T	614	CLA	C4A-NA-C1A	3.50	108.28	106.68
21	A	820	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
21	1	311	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
21	B	811	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
21	T	607	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
21	3	402	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
21	b	310	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
21	7	313	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
21	b	314	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
21	B	843	CLA	C4A-NA-C1A	3.49	108.27	106.68
21	2	608	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
21	c	614	CLA	CMB-C2B-C1B	-3.49	123.35	128.46
21	A	825	CLA	CMB-C2B-C1B	-3.48	123.35	128.46
25	A	848	BCR	C23-C24-C25	3.48	136.30	127.00
21	b	315	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
21	3	412	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
21	8	615	CLA	C4A-NA-C1A	3.48	108.27	106.68
21	B	804	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
21	9	611	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
21	a	304	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
21	T	612	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
21	A	805	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
21	B	824	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
21	8	612	CLA	CMB-C2B-C1B	-3.46	123.38	128.46
21	1	310	CLA	CMB-C2B-C1B	-3.46	123.38	128.46
22	b	309	CHL	CHD-C4C-C3C	3.46	129.82	124.77
21	a	312	CLA	CMB-C2B-C1B	-3.46	123.39	128.46
21	c	602	CLA	CMB-C2B-C1B	-3.46	123.39	128.46
21	A	804	CLA	CMB-C2B-C1B	-3.45	123.40	128.46
21	3	414	CLA	CMB-C2B-C1B	-3.45	123.40	128.46
21	K	204	CLA	CMB-C2B-C1B	-3.45	123.40	128.46
21	c	603	CLA	CMB-C2B-C1B	-3.45	123.40	128.46
21	B	804	CLA	C4A-NA-C1A	3.45	108.25	106.68
21	7	323	CLA	CMB-C2B-C1B	-3.45	123.40	128.46
21	1	307	CLA	CMB-C2B-C1B	-3.44	123.42	128.46
21	7	304	CLA	CMB-C2B-C1B	-3.44	123.42	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	311	CLA	CMB-C2B-C1B	-3.44	123.42	128.46
21	3	411	CLA	CMB-C2B-C1B	-3.44	123.42	128.46
21	b	316	CLA	CMB-C2B-C1B	-3.43	123.43	128.46
21	A	833	CLA	CMB-C2B-C1B	-3.43	123.43	128.46
22	T	602	CHL	C2A-C1A-CHA	3.43	129.81	123.87
21	A	838	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	A	821	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
22	1	305	CHL	C3D-C2D-C1D	3.42	110.50	105.83
21	A	805	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	A	812	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	B	806	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	b	313	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	7	314	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	7	310	CLA	CMB-C2B-C1B	-3.42	123.44	128.46
21	3	413	CLA	CMB-C2B-C1B	-3.42	123.45	128.46
21	8	622	CLA	CMB-C2B-C3B	3.42	131.51	124.68
21	A	831	CLA	CMB-C2B-C1B	-3.42	123.45	128.46
21	9	607	CLA	CMB-C2B-C1B	-3.42	123.45	128.46
21	2	608	CLA	CHB-C4A-NA	3.41	129.32	124.40
21	2	607	CLA	CMB-C2B-C1B	-3.41	123.47	128.46
21	T	614	CLA	CMB-C2B-C1B	-3.41	123.47	128.46
21	B	825	CLA	CMB-C2B-C1B	-3.40	123.47	128.46
21	G	201	CLA	CMB-C2B-C1B	-3.40	123.48	128.46
21	B	827	CLA	CHB-C4A-NA	3.40	129.30	124.40
21	B	823	CLA	CMB-C2B-C1B	-3.40	123.48	128.46
21	2	602	CLA	CMB-C2B-C1B	-3.39	123.49	128.46
21	8	603	CLA	CMB-C2B-C1B	-3.38	123.50	128.46
21	2	603	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
21	A	816	CLA	CMB-C2B-C1B	-3.38	123.50	128.46
21	A	824	CLA	CMB-C2B-C1B	-3.38	123.50	128.46
21	B	812	CLA	C4A-NA-C1A	3.37	108.22	106.68
25	B	805	BCR	C16-C15-C14	3.37	130.42	123.52
22	3	401	CHL	C3D-C2D-C1D	3.37	110.43	105.83
21	c	612	CLA	CMB-C2B-C1B	-3.36	123.53	128.46
21	3	405	CLA	CMB-C2B-C1B	-3.36	123.53	128.46
22	3	401	CHL	C2A-C1A-CHA	3.35	129.69	123.87
21	A	815	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
21	H	203	CLA	CMB-C2B-C1B	-3.35	123.55	128.46
21	B	844	CLA	CMB-C2B-C1B	-3.34	123.56	128.46
22	2	606	CHL	C2D-C1D-ND	-3.34	106.82	110.13
21	L	304	CLA	CMB-C2B-C3B	3.34	131.36	124.68
21	K	202	CLA	C4A-NA-C1A	3.34	108.20	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	818	CLA	CMB-C2B-C1B	-3.34	123.57	128.46
21	3	407	CLA	CMB-C2B-C1B	-3.33	123.57	128.46
22	2	601	CHL	C2D-C1D-ND	-3.32	106.84	110.13
25	B	805	BCR	C15-C16-C17	-3.31	116.75	123.52
21	2	608	CLA	C1B-CHB-C4A	-3.31	123.73	130.04
21	L	306	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
22	1	305	CHL	C2A-C1A-CHA	3.30	129.60	123.87
22	7	308	CHL	C1C-C2C-C3C	-3.29	104.26	107.28
21	B	814	CLA	CMB-C2B-C1B	-3.29	123.64	128.46
21	a	308	CLA	C4A-NA-C1A	3.28	108.18	106.68
21	B	820	CLA	CHB-C4A-NA	3.28	129.14	124.40
21	9	601	CLA	C4D-CHA-C1A	-3.28	117.33	121.24
22	c	607	CHL	C1D-CHD-C4C	-3.28	119.06	126.02
21	A	825	CLA	C4A-NA-C1A	3.27	108.17	106.68
21	B	822	CLA	CMB-C2B-C3B	3.27	131.22	124.68
21	1	303	CLA	CHB-C4A-NA	3.27	129.12	124.40
21	7	306	CLA	CMB-C2B-C1B	-3.26	123.67	128.46
21	a	305	CLA	CMB-C2B-C1B	-3.26	123.68	128.46
22	9	606	CHL	C2D-C1D-ND	-3.25	106.91	110.13
21	a	304	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
21	9	607	CLA	CHB-C4A-NA	3.24	129.08	124.40
21	B	812	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
22	b	307	CHL	C2D-C1D-ND	-3.23	106.93	110.13
21	B	809	CLA	CHB-C4A-NA	3.23	129.06	124.40
21	a	304	CLA	CHB-C4A-NA	3.22	129.05	124.40
21	3	412	CLA	C1B-CHB-C4A	-3.22	123.89	130.04
21	B	804	CLA	C1B-CHB-C4A	-3.22	123.89	130.04
24	1	315	XAT	O24-C25-C24	-3.22	110.47	113.49
21	a	303	CLA	C1B-CHB-C4A	-3.21	123.91	130.04
21	8	612	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
21	A	814	CLA	C4A-NA-C1A	3.20	108.14	106.68
21	B	836	CLA	C4A-NA-C1A	3.20	108.14	106.68
21	A	811	CLA	CMB-C2B-C1B	-3.20	123.77	128.46
22	8	608	CHL	CHD-C4C-C3C	3.19	129.43	124.77
21	A	834	CLA	CMB-C2B-C1B	-3.19	123.78	128.46
25	A	846	BCR	C10-C11-C12	-3.19	113.96	123.20
21	A	828	CLA	CMB-C2B-C3B	3.19	131.05	124.68
21	1	308	CLA	CMB-C2B-C3B	3.18	131.04	124.68
22	7	303	CHL	C2D-C1D-ND	-3.18	106.98	110.13
21	B	842	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
21	B	838	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
24	T	616	XAT	C27-C28-C29	3.17	130.45	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	845	PQN	C11-C3-C4	-3.17	115.24	118.58
21	a	308	CLA	O2D-CGD-CBD	3.17	116.76	111.23
21	B	827	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
21	8	611	CLA	C1-C2-C3	-3.16	121.01	126.20
21	B	809	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
22	a	306	CHL	C1D-CHD-C4C	-3.16	119.31	126.02
22	b	302	CHL	C2A-C1A-CHA	3.15	129.32	123.87
22	7	307	CHL	C3D-C2D-C1D	3.14	110.12	105.83
22	7	308	CHL	C1D-CHD-C4C	-3.14	119.34	126.02
21	B	807	CLA	C1B-CHB-C4A	-3.14	124.06	130.04
21	B	843	CLA	CMB-C2B-C1B	-3.13	123.88	128.46
21	A	804	CLA	C1B-CHB-C4A	-3.12	124.08	130.04
21	9	605	CLA	CMB-C2B-C3B	3.12	130.92	124.68
22	a	306	CHL	C2D-C1D-ND	-3.12	107.04	110.13
21	8	603	CLA	C4A-NA-C1A	3.11	108.10	106.68
21	A	808	CLA	CHB-C4A-NA	3.11	128.89	124.40
21	B	842	CLA	CMB-C2B-C3B	3.11	130.89	124.68
21	b	304	CLA	CHB-C4A-NA	3.11	128.88	124.40
35	A	844	PQN	C11-C3-C4	-3.10	115.31	118.58
21	G	205	CLA	CMB-C2B-C1B	-3.09	123.92	128.46
21	B	812	CLA	CMB-C2B-C1B	-3.09	123.93	128.46
21	T	603	CLA	CHB-C4A-NA	3.08	128.84	124.40
21	A	834	CLA	CHB-C4A-NA	3.08	128.84	124.40
21	A	819	CLA	CMB-C2B-C3B	3.07	130.82	124.68
24	c	616	XAT	C38-C25-C24	-3.07	110.79	114.24
22	b	308	CHL	CHD-C4C-C3C	3.07	129.25	124.77
21	1	321	CLA	CMC-C2C-C1C	3.07	129.83	125.03
21	A	822	CLA	CMB-C2B-C1B	-3.07	123.97	128.46
22	T	602	CHL	CHD-C4C-C3C	3.06	129.24	124.77
21	a	314	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
22	b	302	CHL	C2D-C1D-ND	-3.06	107.10	110.13
22	a	306	CHL	C2A-C1A-CHA	3.05	129.16	123.87
21	A	835	CLA	CMB-C2B-C1B	-3.05	123.99	128.46
21	A	830	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
21	A	815	CLA	CMB-C2B-C3B	3.05	130.78	124.68
21	A	842	CLA	CMB-C2B-C3B	3.05	130.78	124.68
21	B	840	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
23	a	315	LUT	C30-C31-C32	3.04	132.02	123.20
21	B	819	CLA	CHB-C4A-NA	3.04	128.79	124.40
21	B	827	CLA	CMB-C2B-C3B	3.04	130.76	124.68
21	A	806	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
21	b	311	CLA	CHB-C4A-NA	3.04	128.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	311	CLA	C4A-NA-C1A	3.03	108.06	106.68
21	c	608	CLA	CHB-C4A-NA	3.03	128.77	124.40
21	b	313	CLA	CHB-C4A-NA	3.03	128.77	124.40
21	B	807	CLA	CHB-C4A-NA	3.02	128.76	124.40
21	2	604	CLA	C4A-NA-C1A	3.02	108.06	106.68
21	T	611	CLA	CHB-C4A-NA	3.02	128.76	124.40
21	2	603	CLA	CMB-C2B-C1B	-3.02	124.03	128.46
21	1	310	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
21	B	818	CLA	CHB-C4A-NA	3.01	128.74	124.40
22	8	608	CHL	C3D-C2D-C1D	3.01	109.93	105.83
21	T	604	CLA	CHB-C4A-NA	3.01	128.74	124.40
21	a	311	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
21	L	304	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
21	2	605	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
21	T	606	CLA	CMB-C2B-C1B	-3.00	124.06	128.46
22	c	606	CHL	C2D-C1D-ND	-3.00	107.16	110.13
21	1	304	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
21	A	809	CLA	CHB-C4A-NA	2.99	128.72	124.40
21	A	840	CLA	C1B-CHB-C4A	-2.99	124.33	130.04
21	3	411	CLA	CHB-C4A-NA	2.99	128.72	124.40
21	9	610	CLA	CHB-C4A-NA	2.99	128.72	124.40
21	A	840	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
21	A	829	CLA	CMB-C2B-C3B	2.99	130.66	124.68
21	A	835	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
21	7	311	CLA	C4A-NA-C1A	2.99	108.04	106.68
21	T	608	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
21	B	808	CLA	CMB-C2B-C3B	2.99	130.66	124.68
22	T	601	CHL	C2D-C1D-ND	-2.99	107.17	110.13
21	A	836	CLA	CHB-C4A-NA	2.99	128.71	124.40
21	8	603	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
21	A	805	CLA	CHB-C4A-NA	2.99	128.71	124.40
21	B	841	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
21	A	832	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	7	303	CHL	C1D-ND-C4D	2.97	108.40	106.31
21	B	824	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	T	601	CHL	CHD-C4C-C3C	2.97	129.11	124.77
21	b	310	CLA	C1B-CHB-C4A	-2.97	124.37	130.04
24	9	614	XAT	C7-C8-C9	2.97	130.14	125.53
22	1	305	CHL	C1C-C2C-C3C	-2.97	104.55	107.28
21	B	830	CLA	CMB-C2B-C3B	2.97	130.62	124.68
21	9	602	CLA	C4A-NA-C1A	2.97	108.03	106.68
21	1	303	CLA	O2D-CGD-O1D	-2.97	118.07	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	5002	CLA	CHB-C4A-NA	2.97	128.68	124.40
21	A	840	CLA	CHB-C4A-NA	2.97	128.68	124.40
21	A	838	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
21	B	836	CLA	CMB-C2B-C3B	2.96	130.61	124.68
21	A	831	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
21	B	811	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
21	A	809	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
21	T	612	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
21	1	309	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
21	B	831	CLA	CMB-C2B-C3B	2.96	130.59	124.68
21	7	311	CLA	C1-C2-C3	-2.96	121.35	126.20
21	B	814	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
21	A	835	CLA	CHB-C4A-NA	2.95	128.66	124.40
21	B	828	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	2	604	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	A	832	CLA	CMB-C2B-C1B	-2.95	124.13	128.46
21	B	819	CLA	CMB-C2B-C3B	2.95	130.58	124.68
21	c	614	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	B	841	CLA	CMB-C2B-C3B	2.95	130.58	124.68
21	B	817	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
21	8	609	CLA	C1B-CHB-C4A	-2.95	124.42	130.04
21	B	822	CLA	C4A-NA-C1A	2.95	108.02	106.68
21	G	205	CLA	CHB-C4A-NA	2.94	128.65	124.40
21	2	611	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
21	1	311	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
21	b	311	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
34	A	803	CL0	C2D-C1D-ND	-2.94	107.22	110.13
21	A	834	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	7	310	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	L	301	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	A	841	CLA	CHB-C4A-NA	2.93	128.63	124.40
21	B	820	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	A	807	CLA	CMB-C2B-C3B	2.93	130.54	124.68
21	3	413	CLA	C4A-NA-C1A	2.93	108.02	106.68
21	b	306	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	A	814	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	a	305	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	A	826	CLA	CMB-C2B-C1B	-2.93	124.17	128.46
21	H	204	CLA	CHB-C4A-NA	2.93	128.62	124.40
21	T	605	CLA	CMB-C2B-C3B	2.92	130.53	124.68
22	7	303	CHL	CHD-C4C-C3C	2.92	129.04	124.77
21	1	321	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	812	CLA	CHB-C4A-NA	2.92	128.62	124.40
21	a	312	CLA	CHB-C4A-NA	2.92	128.62	124.40
21	O	2003	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	8	612	CLA	CHB-C4A-NA	2.92	128.62	124.40
21	A	826	CLA	CHB-C4A-NA	2.92	128.61	124.40
21	1	313	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	O	2002	CLA	CAB-C3B-C2B	2.92	130.80	124.69
21	A	843	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	B	817	CLA	CMB-C2B-C3B	2.92	130.51	124.68
21	A	830	CLA	CHB-C4A-NA	2.92	128.61	124.40
21	G	205	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	A	824	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
21	B	808	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
21	9	602	CLA	CMB-C2B-C3B	2.91	130.51	124.68
21	B	822	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
21	a	302	CLA	CHB-C4A-NA	2.91	128.60	124.40
21	8	610	CLA	CHB-C4A-NA	2.91	128.60	124.40
21	K	201	CLA	CMB-C2B-C3B	2.91	130.50	124.68
21	9	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
21	3	406	CLA	CMB-C2B-C3B	2.91	130.49	124.68
21	3	409	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
21	A	826	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
21	B	836	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
21	B	812	CLA	CHB-C4A-NA	2.90	128.59	124.40
21	G	203	CLA	CMB-C2B-C3B	2.90	130.49	124.68
21	9	608	CLA	CHB-C4A-NA	2.90	128.59	124.40
21	A	823	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	K	204	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	2	602	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	a	309	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	a	311	CLA	C1B-CHB-C4A	-2.90	124.51	130.04
21	3	407	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	A	833	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	B	834	CLA	CHB-C4A-NA	2.90	128.59	124.40
21	B	825	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	9	609	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
21	b	316	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
21	c	613	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
21	1	307	CLA	CHB-C4A-NA	2.89	128.58	124.40
21	K	202	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
21	O	2003	CLA	C1B-CHB-C4A	-2.89	124.52	130.04
21	3	413	CLA	O2D-CGD-O1D	-2.89	118.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	610	CLA	CMB-C2B-C3B	2.89	130.46	124.68
21	2	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	K	203	CLA	CHB-C4A-NA	2.89	128.57	124.40
21	A	856	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	K	201	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	3	411	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	F	5007	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	b	304	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	T	603	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	T	604	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	1	301	CLA	CHB-C4A-NA	2.88	128.56	124.40
21	7	314	CLA	CHB-C4A-NA	2.88	128.56	124.40
21	B	821	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	A	837	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	a	309	CLA	CMB-C2B-C3B	2.88	130.44	124.68
21	B	804	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	2	601	CHL	C1D-CHD-C4C	-2.88	119.90	126.02
21	B	810	CLA	CMB-C2B-C3B	2.88	130.44	124.68
21	B	823	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	a	307	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	9	612	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	A	822	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
21	a	313	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	A	846	BCR	C15-C16-C17	-2.88	117.63	123.52
22	9	606	CHL	C1D-CHD-C4C	-2.88	119.90	126.02
22	b	309	CHL	C2D-C1D-ND	-2.88	107.28	110.13
21	A	819	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
21	2	604	CLA	C1B-CHB-C4A	-2.88	124.55	130.04
22	8	601	CHL	C1D-ND-C4D	2.88	108.33	106.31
21	9	605	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
21	7	312	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
21	b	315	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
21	B	816	CLA	CHB-C4A-NA	2.87	128.55	124.40
21	B	810	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
21	A	813	CLA	C4A-NA-C1A	2.87	107.99	106.68
21	7	305	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
21	T	607	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
21	A	810	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	B	815	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	a	310	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	b	314	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	9	604	CLA	O2D-CGD-O1D	-2.87	118.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	202	CLA	CHB-C4A-NA	2.87	128.54	124.40
21	B	839	CLA	CMB-C2B-C3B	2.87	130.42	124.68
21	G	203	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
24	7	318	XAT	O4-C5-C4	-2.87	110.80	113.49
21	8	609	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
21	b	311	CLA	CMB-C2B-C3B	2.87	130.41	124.68
22	7	309	CHL	CHD-C1D-C2D	2.87	131.45	125.49
21	9	605	CLA	CHB-C4A-NA	2.87	128.53	124.40
21	2	611	CLA	CHB-C4A-NA	2.86	128.53	124.40
21	A	828	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
21	a	312	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
21	1	321	CLA	CMB-C2B-C3B	2.86	130.41	124.68
21	7	306	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	A	808	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	2	610	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	T	609	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	B	816	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	c	604	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	B	828	CLA	CHB-C4A-NA	2.86	128.53	124.40
21	B	818	CLA	CMB-C2B-C3B	2.86	130.40	124.68
21	A	822	CLA	CHB-C4A-NA	2.86	128.53	124.40
22	c	606	CHL	C1C-C2C-C3C	-2.86	104.65	107.28
21	8	614	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	B	826	CLA	CHB-C4A-NA	2.86	128.53	124.40
21	c	609	CLA	CHB-C4A-NA	2.86	128.52	124.40
21	2	613	CLA	CHB-C4A-NA	2.86	128.52	124.40
21	B	835	CLA	CHB-C4A-NA	2.86	128.52	124.40
21	1	307	CLA	O2D-CGD-CBD	2.85	116.22	111.23
21	T	609	CLA	C1B-CHB-C4A	-2.85	124.60	130.04
21	A	816	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
21	B	829	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
21	A	804	CLA	CHB-C4A-NA	2.85	128.52	124.40
21	A	817	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
21	9	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
21	A	818	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
21	b	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	8	607	CHL	C2D-C1D-ND	-2.85	107.31	110.13
21	8	605	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
21	J	5002	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
21	B	814	CLA	CHB-C4A-NA	2.85	128.51	124.40
21	A	825	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
21	B	832	CLA	O2D-CGD-O1D	-2.85	118.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	836	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
21	1	310	CLA	CHB-C4A-NA	2.85	128.51	124.40
21	1	303	CLA	CMB-C2B-C3B	2.84	130.37	124.68
21	G	201	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
21	9	603	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
21	8	611	CLA	CMB-C2B-C3B	2.84	130.37	124.68
22	8	601	CHL	C2D-C1D-ND	-2.84	107.31	110.13
21	T	614	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
21	3	410	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
21	T	610	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	b	308	CHL	C3D-C2D-C1D	2.84	109.71	105.83
21	A	811	CLA	CHB-C4A-NA	2.84	128.50	124.40
21	B	830	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
21	3	414	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
21	B	828	CLA	CMB-C2B-C3B	2.84	130.35	124.68
22	8	606	CHL	C2D-C1D-ND	-2.84	107.32	110.13
21	7	304	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
21	A	815	CLA	CHB-C4A-NA	2.83	128.49	124.40
21	A	832	CLA	CHB-C4A-NA	2.83	128.49	124.40
21	A	821	CLA	O2D-CGD-CBD	2.83	116.18	111.23
21	A	827	CLA	CHB-C4A-NA	2.83	128.49	124.40
21	T	613	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
21	3	405	CLA	CHB-C4A-NA	2.83	128.49	124.40
21	H	203	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
21	7	315	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
21	c	611	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
21	F	5005	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
21	2	609	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
21	A	842	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
21	1	301	CLA	CMB-C2B-C3B	2.83	130.33	124.68
21	L	304	CLA	CHB-C4A-NA	2.83	128.48	124.40
21	c	602	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
21	3	403	CLA	CHB-C4A-NA	2.82	128.48	124.40
21	B	833	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
21	T	611	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
21	3	410	CLA	CHB-C4A-NA	2.82	128.47	124.40
21	A	810	CLA	CHB-C4A-NA	2.82	128.47	124.40
21	2	608	CLA	O2D-CGD-CBD	2.82	116.16	111.23
21	A	807	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
21	B	818	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
21	1	310	CLA	C1B-CHB-C4A	-2.82	124.67	130.04
21	T	606	CLA	O2D-CGD-O1D	-2.82	118.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	830	CLA	CMB-C2B-C3B	2.81	130.31	124.68
21	7	310	CLA	CHB-C4A-NA	2.81	128.46	124.40
21	T	604	CLA	C4A-NA-C1A	2.81	107.96	106.68
21	b	312	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
21	T	605	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
21	B	810	CLA	CHB-C4A-NA	2.81	128.46	124.40
21	9	610	CLA	C2A-C1A-CHA	2.81	128.75	123.87
21	A	817	CLA	CHB-C4A-NA	2.81	128.46	124.40
21	B	826	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
21	7	311	CLA	CHB-C4A-NA	2.81	128.45	124.40
21	A	813	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
21	B	843	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	b	318	XAT	C7-C8-C9	2.81	129.88	125.53
21	1	303	CLA	C1B-CHB-C4A	-2.81	124.69	130.04
21	B	819	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
21	7	315	CLA	CHB-C4A-NA	2.80	128.45	124.40
21	A	843	CLA	C1B-CHB-C4A	-2.80	124.69	130.04
21	B	807	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
21	B	821	CLA	CHB-C4A-NA	2.80	128.45	124.40
21	1	302	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
21	B	839	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
21	7	313	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	8	601	CHL	C3D-C2D-C1D	2.80	109.66	105.83
21	B	836	CLA	C1B-CHB-C4A	-2.80	124.70	130.04
21	c	609	CLA	C1B-CHB-C4A	-2.80	124.70	130.04
21	2	602	CLA	C1B-CHB-C4A	-2.80	124.70	130.04
21	3	408	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	a	307	CLA	C1B-CHB-C4A	-2.80	124.70	130.04
23	a	315	LUT	C26-C27-C28	2.80	128.94	124.58
21	a	302	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	A	812	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	K	203	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	A	827	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	A	819	CLA	CHB-C4A-NA	2.80	128.44	124.40
21	L	301	CLA	CMB-C2B-C3B	2.80	130.27	124.68
21	c	612	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
21	8	610	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
21	9	601	CLA	C1B-CHB-C4A	2.80	135.38	130.04
21	c	601	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
21	B	834	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
21	1	306	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	8	601	CHL	C2A-C1A-CHA	2.79	128.71	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	412	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	8	606	CHL	C3D-C2D-C1D	2.79	109.64	105.83
21	c	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
21	B	840	CLA	CHB-C4A-NA	2.79	128.42	124.40
21	9	610	CLA	CMB-C2B-C3B	2.79	130.25	124.68
21	c	612	CLA	CHB-C4A-NA	2.79	128.42	124.40
21	2	604	CLA	CHB-C4A-NA	2.79	128.42	124.40
21	L	303	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	c	607	CHL	CHD-C1D-C2D	2.79	131.28	125.49
21	3	404	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
21	A	821	CLA	CMB-C2B-C3B	2.78	130.25	124.68
21	B	838	CLA	CMB-C2B-C3B	2.78	130.24	124.68
21	c	610	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
21	9	608	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
21	A	839	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
21	1	301	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
21	B	831	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
21	A	806	CLA	CMB-C2B-C3B	2.78	130.24	124.68
21	A	837	CLA	CHB-C4A-NA	2.78	128.41	124.40
21	9	604	CLA	CMB-C2B-C3B	2.78	130.23	124.68
21	7	316	CLA	CMB-C2B-C3B	2.78	130.23	124.68
21	9	601	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
22	c	606	CHL	C1D-CHD-C4C	-2.77	120.12	126.02
21	T	610	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	a	314	CLA	CMB-C2B-C3B	2.77	130.23	124.68
21	A	806	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	2	607	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
21	b	313	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
21	F	5007	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	A	813	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	b	315	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	T	607	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	3	406	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
21	8	604	CLA	CHB-C4A-NA	2.77	128.40	124.40
21	c	608	CLA	C1B-CHB-C4A	-2.77	124.76	130.04
21	9	608	CLA	CMB-C2B-C3B	2.77	130.21	124.68
21	1	312	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
21	A	811	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
21	L	303	CLA	CHB-C4A-NA	2.76	128.39	124.40
21	3	405	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
21	3	404	CLA	CMB-C2B-C3B	2.76	130.21	124.68
21	B	837	CLA	CHB-C4A-NA	2.76	128.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	839	CLA	CMB-C2B-C3B	2.76	130.20	124.68
21	A	841	CLA	CMB-C2B-C3B	2.76	130.20	124.68
21	2	607	CLA	CHB-C4A-NA	2.76	128.38	124.40
21	1	306	CLA	CHB-C4A-NA	2.76	128.38	124.40
21	A	807	CLA	C4A-NA-C1A	2.76	107.94	106.68
21	b	304	CLA	C1B-CHB-C4A	-2.76	124.78	130.04
21	1	302	CLA	CHB-C4A-NA	2.76	128.38	124.40
21	K	204	CLA	CHB-C4A-NA	2.76	128.38	124.40
21	c	608	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
21	8	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	9	606	CHL	CHD-C1D-C2D	2.76	131.22	125.49
21	8	605	CLA	CMB-C2B-C3B	2.76	130.19	124.68
21	B	825	CLA	C1B-CHB-C4A	-2.75	124.79	130.04
22	8	607	CHL	C3D-C2D-C1D	2.75	109.59	105.83
22	T	602	CHL	C2D-C1D-ND	-2.75	107.40	110.13
21	B	839	CLA	CHB-C4A-NA	2.75	128.37	124.40
22	T	602	CHL	C1C-C2C-C3C	-2.75	104.75	107.28
21	8	615	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
21	3	403	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	7	316	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	8	613	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	7	311	CLA	C1B-CHB-C4A	-2.75	124.80	130.04
21	A	823	CLA	CMB-C2B-C3B	2.75	130.17	124.68
21	B	813	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
21	3	408	CLA	CMB-C2B-C3B	2.75	130.17	124.68
21	A	820	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
21	7	314	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	B	843	CLA	C1B-CHB-C4A	-2.74	124.81	130.04
21	B	844	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	A	829	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	B	825	CLA	CHB-C4A-NA	2.74	128.36	124.40
21	9	611	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
21	G	204	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
21	b	305	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
24	8	617	XAT	C7-C8-C9	2.74	129.78	125.53
21	8	613	CLA	CHB-C4A-NA	2.74	128.35	124.40
21	9	603	CLA	CHB-C4A-NA	2.74	128.35	124.40
21	B	808	CLA	CHB-C4A-NA	2.74	128.35	124.40
21	G	201	CLA	CHB-C4A-NA	2.74	128.35	124.40
21	2	610	CLA	CMB-C2B-C3B	2.73	130.15	124.68
21	8	611	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
21	B	813	CLA	C1B-CHB-C4A	-2.73	124.83	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	835	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
21	3	413	CLA	CHB-C4A-NA	2.73	128.34	124.40
21	8	609	CLA	CMB-C2B-C3B	2.73	130.14	124.68
21	T	614	CLA	CHB-C4A-NA	2.73	128.34	124.40
21	3	402	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	a	315	LUT	C35-C34-C33	2.73	131.11	127.28
21	L	305	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	7	303	CHL	CHD-C1D-C2D	2.73	131.16	125.49
21	2	608	CLA	CMB-C2B-C3B	2.73	130.14	124.68
21	A	810	CLA	CMB-C2B-C3B	2.73	130.13	124.68
21	b	314	CLA	CHB-C4A-NA	2.73	128.34	124.40
21	B	834	CLA	CMB-C2B-C3B	2.73	130.13	124.68
21	O	2002	CLA	C1B-CHB-C4A	-2.73	124.84	130.04
21	A	804	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
21	T	609	CLA	CMB-C2B-C3B	2.72	130.13	124.68
21	2	612	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
21	B	812	CLA	C1B-CHB-C4A	-2.72	124.85	130.04
21	A	813	CLA	CMB-C2B-C3B	2.72	130.12	124.68
21	B	837	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	7	318	XAT	C38-C25-C24	-2.72	111.19	114.24
21	F	5006	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
21	a	303	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
21	1	304	CLA	CHB-C4A-NA	2.72	128.32	124.40
21	7	313	CLA	CHB-C4A-NA	2.72	128.32	124.40
21	L	306	CLA	CHB-C4A-NA	2.72	128.32	124.40
21	8	615	CLA	CHB-C4A-NA	2.71	128.32	124.40
21	c	610	CLA	CHB-C4A-NA	2.71	128.32	124.40
21	A	841	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
22	8	608	CHL	C2D-C1D-ND	-2.71	107.44	110.13
21	8	612	CLA	O2D-CGD-CBD	2.71	115.97	111.23
21	9	604	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	A	829	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	c	601	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	c	614	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	b	304	CLA	CMB-C2B-C3B	2.71	130.10	124.68
21	L	303	CLA	CMB-C2B-C3B	2.71	130.10	124.68
21	B	816	CLA	C1B-CHB-C4A	-2.71	124.87	130.04
22	2	601	CHL	C2A-C1A-CHA	2.71	128.57	123.87
21	B	815	CLA	CMB-C2B-C3B	2.71	130.09	124.68
21	9	609	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	A	807	CLA	CHB-C4A-NA	2.71	128.31	124.40
22	2	601	CHL	CHD-C1D-C2D	2.71	131.12	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	815	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	b	316	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	c	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
21	A	825	CLA	CHB-C4A-NA	2.71	128.31	124.40
21	A	840	CLA	CMB-C2B-C3B	2.71	130.09	124.68
21	A	825	CLA	C1B-CHB-C4A	-2.70	124.88	130.04
22	7	308	CHL	C2D-C1D-ND	-2.70	107.45	110.13
21	8	611	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
21	F	5005	CLA	CMB-C2B-C3B	2.70	130.09	124.68
21	A	838	CLA	CMB-C2B-C3B	2.70	130.08	124.68
21	1	304	CLA	CMB-C2B-C3B	2.70	130.08	124.68
21	3	410	CLA	CMB-C2B-C3B	2.70	130.08	124.68
21	1	302	CLA	CMB-C2B-C3B	2.70	130.08	124.68
21	9	602	CLA	C1B-CHB-C4A	-2.70	124.89	130.04
21	a	304	CLA	CMB-C2B-C3B	2.70	130.07	124.68
21	A	843	CLA	C1-C2-C3	-2.70	121.78	126.20
21	L	301	CLA	C1B-CHB-C4A	-2.69	124.90	130.04
21	B	821	CLA	CMB-C2B-C3B	2.69	130.07	124.68
21	B	822	CLA	C1B-CHB-C4A	-2.69	124.90	130.04
21	A	837	CLA	CMB-C2B-C3B	2.69	130.06	124.68
21	O	2002	CLA	CMB-C2B-C3B	2.69	130.33	124.69
21	8	610	CLA	C1B-CHB-C4A	-2.69	124.91	130.04
21	B	811	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	2	605	CLA	CMB-C2B-C3B	2.69	130.06	124.68
21	a	307	CLA	CMB-C2B-C3B	2.69	130.06	124.68
21	J	5002	CLA	CMB-C2B-C3B	2.69	130.06	124.68
21	8	603	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	2	609	CLA	C1B-CHB-C4A	-2.69	124.91	130.04
21	H	204	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
21	B	843	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	B	844	CLA	CHB-C4A-NA	2.69	128.28	124.40
22	c	605	CHL	C3D-C2D-C1D	2.69	109.50	105.83
21	b	311	CLA	CHC-C1C-NC	2.69	128.36	124.31
21	a	303	CLA	CMB-C2B-C3B	2.69	130.06	124.68
21	7	304	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	2	611	CLA	CMB-C2B-C3B	2.69	130.05	124.68
21	K	203	CLA	CMB-C2B-C3B	2.69	130.05	124.68
21	8	614	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	T	605	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	A	823	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	T	613	CLA	CHB-C4A-NA	2.68	128.27	124.40
21	1	310	CLA	CMB-C2B-C3B	2.68	130.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	607	CLA	C1B-CHB-C4A	-2.68	124.92	130.04
21	7	311	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
21	c	611	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	c	605	CHL	C2D-C1D-ND	-2.68	107.47	110.13
21	A	805	CLA	O2D-CGD-CBD	2.68	115.92	111.23
21	1	321	CLA	CHD-C4C-NC	2.68	128.38	124.23
22	a	306	CHL	CHD-C1D-C2D	2.68	131.06	125.49
21	B	830	CLA	CHB-C4A-NA	2.68	128.26	124.40
21	9	603	CLA	CMB-C2B-C3B	2.68	130.03	124.68
22	9	606	CHL	C1C-C2C-C3C	-2.68	104.82	107.28
22	b	308	CHL	C1D-ND-C4D	2.68	108.19	106.31
21	B	807	CLA	CHD-C1D-ND	-2.67	121.04	124.80
21	B	828	CLA	C4A-NA-C1A	2.67	107.90	106.68
21	B	829	CLA	CHB-C4A-NA	2.67	128.26	124.40
21	2	604	CLA	CMB-C2B-C3B	2.67	130.02	124.68
21	A	820	CLA	CHB-C4A-NA	2.67	128.26	124.40
22	a	306	CHL	C1C-C2C-C3C	-2.67	104.82	107.28
21	A	827	CLA	CMB-C2B-C3B	2.67	130.02	124.68
21	c	601	CLA	CMB-C2B-C3B	2.67	130.02	124.68
21	7	311	CLA	CMB-C2B-C3B	2.67	130.02	124.68
21	1	311	CLA	CHB-C4A-NA	2.67	128.25	124.40
21	B	833	CLA	CHB-C4A-NA	2.67	128.25	124.40
21	7	315	CLA	CMB-C2B-C3B	2.67	130.01	124.68
21	9	608	CLA	C1B-CHB-C4A	-2.67	124.95	130.04
22	b	309	CHL	C3D-C2D-C1D	2.67	109.47	105.83
21	9	611	CLA	CHB-C4A-NA	2.67	128.25	124.40
21	B	840	CLA	CMB-C2B-C3B	2.67	130.01	124.68
21	9	612	CLA	CMB-C2B-C3B	2.67	130.01	124.68
21	2	603	CLA	CHB-C4A-NA	2.66	128.25	124.40
21	8	604	CLA	CMB-C2B-C3B	2.66	130.01	124.68
21	F	5005	CLA	CHB-C4A-NA	2.66	128.24	124.40
21	3	403	CLA	CMB-C2B-C3B	2.66	130.00	124.68
21	3	402	CLA	CHB-C4A-NA	2.66	128.24	124.40
21	T	612	CLA	CHB-C4A-NA	2.66	128.24	124.40
21	A	836	CLA	CMB-C2B-C3B	2.66	130.00	124.68
21	c	609	CLA	CMB-C2B-C3B	2.66	130.00	124.68
22	3	401	CHL	CHD-C4C-C3C	2.66	128.65	124.77
21	T	612	CLA	C1B-CHB-C4A	-2.66	124.97	130.04
21	F	5006	CLA	CHB-C4A-NA	2.66	128.23	124.40
21	9	609	CLA	CMB-C2B-C3B	2.66	129.99	124.68
21	B	820	CLA	CMB-C2B-C3B	2.66	129.99	124.68
23	B	801	LUT	C21-C26-C27	2.65	115.88	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	2001	CLA	C3A-C2A-C1A	-2.65	103.58	106.30
21	B	831	CLA	CHB-C4A-NA	2.65	128.23	124.40
21	A	820	CLA	CMB-C2B-C3B	2.65	129.99	124.68
21	A	821	CLA	C1B-CHB-C4A	-2.65	124.98	130.04
21	7	323	CLA	CHB-C4A-NA	2.65	128.23	124.40
21	B	817	CLA	CHB-C4A-NA	2.65	128.23	124.40
21	B	830	CLA	C1B-CHB-C4A	-2.65	124.98	130.04
21	c	608	CLA	CMB-C2B-C3B	2.65	129.98	124.68
21	2	612	CLA	CMB-C2B-C3B	2.65	129.98	124.68
21	T	603	CLA	CMB-C2B-C3B	2.65	129.98	124.68
21	A	814	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	O	2003	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	b	306	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	c	611	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	T	611	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	a	302	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	7	312	CLA	CMB-C2B-C3B	2.65	129.97	124.68
21	3	408	CLA	C1B-CHB-C4A	-2.65	125.00	130.04
21	T	608	CLA	CHB-C4A-NA	2.64	128.22	124.40
21	b	305	CLA	CMB-C2B-C3B	2.64	129.97	124.68
21	T	604	CLA	C1B-CHB-C4A	-2.64	125.00	130.04
21	G	204	CLA	CMB-C2B-C3B	2.64	129.97	124.68
21	2	605	CLA	CHB-C4A-NA	2.64	128.22	124.40
21	8	603	CLA	C1B-CHB-C4A	-2.64	125.00	130.04
21	a	308	CLA	C2A-C1A-CHA	2.64	128.45	123.87
21	8	622	CLA	O1D-CGD-CBD	2.64	129.73	124.52
21	7	304	CLA	CMB-C2B-C3B	2.64	129.96	124.68
21	H	204	CLA	CMB-C2B-C3B	2.64	129.96	124.68
21	7	305	CLA	CMB-C2B-C3B	2.64	129.96	124.68
21	3	402	CLA	CMB-C2B-C3B	2.64	129.95	124.68
21	A	834	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
21	1	313	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
21	F	5007	CLA	CMB-C2B-C3B	2.63	129.95	124.68
21	2	610	CLA	CHB-C4A-NA	2.63	128.20	124.40
21	3	404	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
21	B	833	CLA	CMB-C2B-C3B	2.63	129.94	124.68
21	8	603	CLA	CMB-C2B-C3B	2.63	129.94	124.68
21	B	826	CLA	CMB-C2B-C3B	2.63	129.94	124.68
21	7	323	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
21	A	830	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
21	A	839	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
21	1	312	CLA	CMB-C2B-C3B	2.63	129.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	323	CLA	CMB-C2B-C3B	2.63	129.94	124.68
21	A	808	CLA	CMB-C2B-C3B	2.63	129.93	124.68
21	T	612	CLA	CMB-C2B-C3B	2.63	129.93	124.68
21	1	313	CLA	CMB-C2B-C3B	2.62	129.93	124.68
21	2	602	CLA	CMB-C2B-C3B	2.62	129.93	124.68
21	B	806	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
21	A	812	CLA	CMB-C2B-C3B	2.62	129.92	124.68
21	1	310	CLA	C2A-C1A-CHA	2.62	128.42	123.87
21	3	409	CLA	CHB-C4A-NA	2.62	128.18	124.40
21	a	309	CLA	CHB-C4A-NA	2.62	128.18	124.40
21	3	409	CLA	CMB-C2B-C3B	2.62	129.92	124.68
21	G	203	CLA	C1B-CHB-C4A	-2.62	125.04	130.04
21	A	833	CLA	CMB-C2B-C3B	2.62	129.92	124.68
21	9	611	CLA	CMB-C2B-C3B	2.62	129.92	124.68
21	L	306	CLA	CMB-C2B-C3B	2.62	129.92	124.68
21	3	412	CLA	CMB-C2B-C3B	2.62	129.91	124.68
21	T	613	CLA	CMB-C2B-C3B	2.62	129.91	124.68
22	8	601	CHL	C1D-CHD-C4C	-2.62	120.46	126.02
21	c	602	CLA	CHB-C4A-NA	2.62	128.18	124.40
21	1	309	CLA	CMB-C2B-C3B	2.62	129.91	124.68
21	c	613	CLA	CMB-C2B-C3B	2.62	129.91	124.68
21	B	811	CLA	CMB-C2B-C3B	2.61	129.91	124.68
21	A	816	CLA	CHB-C4A-NA	2.61	128.17	124.40
21	2	613	CLA	CMB-C2B-C3B	2.61	129.91	124.68
21	a	313	CLA	CMB-C2B-C3B	2.61	129.91	124.68
21	K	202	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	b	315	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	O	2001	CLA	O2D-CGD-O1D	-2.61	118.16	124.08
21	A	809	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	8	614	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	b	312	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	3	414	CLA	CHB-C4A-NA	2.61	128.16	124.40
21	8	613	CLA	CMB-C2B-C3B	2.61	129.90	124.68
21	b	312	CLA	CHB-C4A-NA	2.61	128.16	124.40
21	b	310	CLA	CMB-C2B-C3B	2.61	129.89	124.68
21	L	301	CLA	CHB-C4A-NA	2.61	128.16	124.40
21	T	606	CLA	C1B-CHB-C4A	-2.61	125.07	130.04
21	G	201	CLA	CMB-C2B-C3B	2.60	129.89	124.68
21	8	615	CLA	CMB-C2B-C3B	2.60	129.89	124.68
21	a	310	CLA	CMB-C2B-C3B	2.60	129.89	124.68
21	1	308	CLA	CHB-C4A-NA	2.60	128.16	124.40
21	A	840	CLA	C4A-NA-C1A	2.60	107.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	602	CLA	CHB-C4A-NA	2.60	128.16	124.40
21	c	610	CLA	CMB-C2B-C3B	2.60	129.88	124.68
21	c	604	CLA	CMB-C2B-C3B	2.60	129.88	124.68
21	L	305	CLA	CMB-C2B-C3B	2.60	129.88	124.68
21	b	306	CLA	CHB-C4A-NA	2.60	128.15	124.40
21	T	604	CLA	CMB-C2B-C3B	2.60	129.88	124.68
21	B	837	CLA	CMB-C2B-C3B	2.60	129.88	124.68
21	B	819	CLA	C1B-CHB-C4A	-2.60	125.08	130.04
21	c	603	CLA	C1B-CHB-C4A	-2.60	125.09	130.04
21	8	605	CLA	CHB-C4A-NA	2.60	128.15	124.40
21	a	303	CLA	CHB-C4A-NA	2.60	128.15	124.40
21	1	302	CLA	C1B-CHB-C4A	-2.60	125.09	130.04
22	T	601	CHL	C1D-ND-C4D	2.60	108.13	106.31
21	B	826	CLA	C1B-CHB-C4A	-2.59	125.09	130.04
21	T	608	CLA	CMB-C2B-C3B	2.59	129.87	124.68
21	1	309	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	9	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	7	312	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	c	602	CLA	CMB-C2B-C3B	2.59	129.86	124.68
21	1	306	CLA	CMB-C2B-C3B	2.59	129.86	124.68
21	A	817	CLA	CMB-C2B-C3B	2.59	129.86	124.68
21	B	829	CLA	CMB-C2B-C3B	2.59	129.86	124.68
21	1	311	CLA	CMB-C2B-C3B	2.59	129.85	124.68
21	T	607	CLA	CMB-C2B-C3B	2.59	129.85	124.68
21	B	832	CLA	C1B-CHB-C4A	-2.59	125.11	130.04
21	c	603	CLA	CMB-C2B-C3B	2.58	129.85	124.68
21	c	613	CLA	CHB-C4A-NA	2.58	128.13	124.40
21	3	402	CLA	C1B-CHB-C4A	-2.58	125.11	130.04
21	1	303	CLA	C4A-NA-C1A	2.58	107.86	106.68
21	K	204	CLA	CMB-C2B-C3B	2.58	129.85	124.68
21	1	313	CLA	CHB-C4A-NA	2.58	128.13	124.40
21	F	5006	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	8	612	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	B	821	CLA	C1B-CHB-C4A	-2.58	125.11	130.04
21	1	307	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	B	806	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	3	408	CLA	CHB-C4A-NA	2.58	128.12	124.40
21	8	612	CLA	C1-C2-C3	-2.58	122.59	126.76
21	A	805	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	a	311	CLA	CMB-C2B-C3B	2.58	129.84	124.68
21	H	203	CLA	C1B-CHB-C4A	-2.58	125.12	130.04
25	A	848	BCR	C21-C20-C19	2.58	130.67	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	609	CLA	CMB-C2B-C3B	2.58	129.83	124.68
21	A	831	CLA	CMB-C2B-C3B	2.58	129.83	124.68
21	A	838	CLA	CHB-C4A-NA	2.57	128.12	124.40
21	1	321	CLA	CHB-C4A-NA	2.57	128.12	124.40
21	H	204	CLA	C1B-CHB-C4A	-2.57	125.13	130.04
21	B	827	CLA	O2D-CGD-CBD	2.57	115.73	111.23
25	O	2004	BCR	C16-C15-C14	2.57	128.78	123.52
21	A	833	CLA	C1B-CHB-C4A	-2.57	125.13	130.04
21	B	838	CLA	CHB-C4A-NA	2.57	128.11	124.40
21	A	812	CLA	C1B-CHB-C4A	-2.57	125.14	130.04
21	A	856	CLA	CMB-C2B-C3B	2.57	129.82	124.68
21	A	815	CLA	C1B-CHB-C4A	-2.57	125.14	130.04
21	a	311	CLA	CHB-C4A-NA	2.57	128.10	124.40
21	b	314	CLA	CMB-C2B-C3B	2.57	129.81	124.68
21	T	610	CLA	CMB-C2B-C3B	2.56	129.81	124.68
21	A	842	CLA	CHB-C4A-NA	2.56	128.10	124.40
21	B	824	CLA	CHB-C4A-NA	2.56	128.10	124.40
21	H	203	CLA	CHB-C4A-NA	2.56	128.10	124.40
25	B	805	BCR	C21-C20-C19	2.56	130.63	123.20
21	2	609	CLA	CHB-C4A-NA	2.56	128.10	124.40
21	B	841	CLA	CHB-C4A-NA	2.56	128.10	124.40
21	b	313	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	c	614	CLA	CMB-C2B-C3B	2.56	129.80	124.68
21	a	312	CLA	CMB-C2B-C3B	2.56	129.80	124.68
21	K	202	CLA	C1B-CHB-C4A	-2.56	125.16	130.04
21	T	611	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	b	313	CLA	CMB-C2B-C3B	2.56	129.79	124.68
21	G	201	CLA	C4-C3-C5	2.56	119.66	115.23
21	A	838	CLA	C1B-CHB-C4A	-2.56	125.17	130.04
21	a	305	CLA	C1B-CHB-C4A	-2.56	125.17	130.04
21	B	842	CLA	C1B-CHB-C4A	-2.55	125.17	130.04
21	O	2001	CLA	CMB-C2B-C3B	2.55	129.78	124.68
21	A	835	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
21	B	817	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
22	9	606	CHL	C2A-C1A-CHA	2.55	128.29	123.87
21	7	310	CLA	CMB-C2B-C3B	2.55	129.77	124.68
21	A	816	CLA	CMB-C2B-C3B	2.55	129.77	124.68
21	7	305	CLA	C1B-CHB-C4A	-2.55	125.19	130.04
21	A	826	CLA	C1B-CHB-C4A	-2.55	125.19	130.04
22	T	601	CHL	CHD-C1D-C2D	2.55	130.78	125.49
21	A	814	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
21	T	613	CLA	C1B-CHB-C4A	-2.54	125.19	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	201	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
21	3	411	CLA	CMB-C2B-C3B	2.54	129.77	124.68
21	b	305	CLA	CHB-C4A-NA	2.54	128.07	124.40
21	B	822	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	2	606	CHL	CHD-C1D-C2D	2.54	130.77	125.49
21	1	312	CLA	CHB-C4A-NA	2.54	128.06	124.40
21	3	414	CLA	CMB-C2B-C3B	2.54	129.75	124.68
21	b	311	CLA	C1B-CHB-C4A	-2.54	125.20	130.04
21	B	806	CLA	CHB-C4A-NA	2.54	128.06	124.40
21	1	311	CLA	O2A-CGA-O1A	-2.54	117.29	123.63
21	8	614	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
22	7	307	CHL	C2D-C1D-ND	-2.53	107.62	110.13
21	A	839	CLA	CHB-C4A-NA	2.53	128.05	124.40
21	8	611	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
21	B	838	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
21	3	406	CLA	CHB-C4A-NA	2.53	128.05	124.40
21	2	610	CLA	C1B-CHB-C4A	-2.52	125.23	130.04
21	a	305	CLA	CHB-C4A-NA	2.52	128.04	124.40
21	a	313	CLA	C1B-CHB-C4A	-2.52	125.23	130.04
21	A	833	CLA	CHB-C4A-NA	2.52	128.04	124.40
21	b	315	CLA	C1B-CHB-C4A	-2.52	125.23	130.04
21	B	816	CLA	CMB-C2B-C3B	2.52	129.72	124.68
21	7	316	CLA	C1B-CHB-C4A	-2.52	125.24	130.04
21	B	804	CLA	CMB-C2B-C3B	2.52	129.71	124.68
21	A	824	CLA	CHB-C4A-NA	2.52	128.03	124.40
21	8	611	CLA	CHB-C4A-NA	2.51	128.03	124.40
21	A	828	CLA	CHB-C4A-NA	2.51	128.03	124.40
21	a	304	CLA	C1B-CHB-C4A	-2.51	125.25	130.04
21	B	825	CLA	CMB-C2B-C3B	2.51	129.70	124.68
21	B	841	CLA	C1B-CHB-C4A	-2.51	125.25	130.04
21	3	407	CLA	C1B-CHB-C4A	-2.51	125.26	130.04
22	7	303	CHL	C2A-C1A-CHA	2.51	128.22	123.87
21	1	309	CLA	C1B-CHB-C4A	-2.51	125.26	130.04
21	a	308	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
25	A	846	BCR	C12-C13-C14	2.51	122.95	119.01
21	7	313	CLA	CMB-C2B-C3B	2.50	129.69	124.68
21	T	614	CLA	C1B-CHB-C4A	-2.50	125.27	130.04
21	a	308	CLA	CMB-C2B-C3B	2.50	129.68	124.68
22	T	601	CHL	C2A-C1A-CHA	2.50	128.21	123.87
21	a	313	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	B	818	CLA	C1B-CHB-C4A	-2.50	125.27	130.04
21	A	810	CLA	C1B-CHB-C4A	-2.50	125.28	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	820	CLA	C1B-CHB-C4A	-2.50	125.28	130.04
22	7	308	CHL	CHD-C1D-C2D	2.50	130.68	125.49
21	B	824	CLA	CMB-C2B-C3B	2.50	129.67	124.68
21	3	413	CLA	CMB-C2B-C3B	2.50	129.67	124.68
21	7	310	CLA	C1B-CHB-C4A	-2.49	125.28	130.04
21	A	824	CLA	CMB-C2B-C3B	2.49	129.67	124.68
22	7	308	CHL	C3D-C2D-C1D	2.49	109.23	105.83
21	B	813	CLA	CMB-C2B-C3B	2.49	129.67	124.68
21	A	825	CLA	CMB-C2B-C3B	2.49	129.66	124.68
22	7	307	CHL	C2A-C1A-CHA	2.49	128.19	123.87
21	A	813	CLA	C1B-CHB-C4A	-2.49	125.29	130.04
21	A	814	CLA	CHB-C4A-NA	2.49	127.99	124.40
21	7	314	CLA	CMB-C2B-C3B	2.49	129.65	124.68
21	H	203	CLA	CMB-C2B-C3B	2.48	129.65	124.68
21	a	308	CLA	C1B-CHB-C4A	-2.48	125.31	130.04
25	B	852	BCR	C15-C14-C13	2.48	130.76	127.28
21	9	612	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	1	308	CLA	C1B-CHB-C4A	-2.48	125.31	130.04
21	b	310	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	7	306	CLA	C1-C2-C3	-2.48	122.75	126.76
25	A	846	BCR	C11-C12-C13	2.48	133.16	126.36
25	K	205	BCR	C10-C11-C12	2.48	130.38	123.20
21	A	809	CLA	C1B-CHB-C4A	-2.48	125.32	130.04
21	b	305	CLA	C1B-CHB-C4A	-2.48	125.32	130.04
21	L	305	CLA	CHB-C4A-NA	2.48	127.97	124.40
21	3	407	CLA	CHB-C4A-NA	2.48	127.97	124.40
21	B	832	CLA	CMB-C2B-C3B	2.48	129.63	124.68
21	3	407	CLA	CMB-C2B-C3B	2.47	129.63	124.68
21	7	305	CLA	CHB-C4A-NA	2.47	127.97	124.40
21	B	813	CLA	CHB-C4A-NA	2.47	127.97	124.40
21	2	612	CLA	CHB-C4A-NA	2.47	127.97	124.40
21	A	821	CLA	CHB-C4A-NA	2.47	127.97	124.40
21	2	613	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
21	B	810	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
21	A	823	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
21	c	601	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
22	1	305	CHL	C2D-C1D-ND	-2.47	107.68	110.13
22	c	606	CHL	CHD-C1D-C2D	2.47	130.62	125.49
22	8	607	CHL	CHD-C1D-C2D	2.46	130.61	125.49
33	8	621	LMK	O2-C4-C3	2.46	117.58	111.88
21	8	603	CLA	C1-C2-C3	-2.46	122.78	126.76
21	3	404	CLA	CHB-C4A-NA	2.46	127.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	307	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
21	a	302	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
22	b	308	CHL	C2A-C1A-CHA	2.46	128.13	123.87
21	A	807	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
21	B	828	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
21	3	411	CLA	C1B-CHB-C4A	-2.46	125.36	130.04
21	B	813	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
21	a	314	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
21	a	304	CLA	C1-C2-C3	-2.45	122.80	126.76
21	A	824	CLA	C1B-CHB-C4A	-2.45	125.37	130.04
21	3	405	CLA	CMB-C2B-C3B	2.45	129.58	124.68
22	b	307	CHL	C3D-C2D-C1D	2.45	109.17	105.83
21	L	303	CLA	C1B-CHB-C4A	-2.45	125.37	130.04
21	2	607	CLA	CMB-C2B-C3B	2.45	129.57	124.68
21	c	614	CLA	C1B-CHB-C4A	-2.45	125.37	130.04
21	B	831	CLA	C1B-CHB-C4A	-2.45	125.37	130.04
22	T	602	CHL	C3D-C2D-C1D	2.44	109.17	105.83
21	8	609	CLA	CHB-C4A-NA	2.44	127.93	124.40
21	T	607	CLA	C1-C2-C3	-2.44	122.81	126.76
23	c	615	LUT	C21-C26-C27	2.44	115.63	112.83
21	B	814	CLA	CMB-C2B-C3B	2.44	129.56	124.68
21	G	204	CLA	CHB-C4A-NA	2.44	127.92	124.40
21	7	315	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
21	B	837	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
21	a	309	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
21	c	612	CLA	CMB-C2B-C3B	2.44	129.56	124.68
21	A	818	CLA	CHB-C4A-NA	2.44	127.92	124.40
21	B	836	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	3	416	XAT	C27-C28-C29	2.44	129.31	125.53
21	b	316	CLA	CMB-C2B-C3B	2.43	129.55	124.68
21	a	307	CLA	CHB-C4A-NA	2.43	127.91	124.40
21	G	203	CLA	CHB-C4A-NA	2.43	127.91	124.40
21	A	841	CLA	C1-C2-C3	-2.43	122.22	126.20
21	c	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
21	T	614	CLA	CMB-C2B-C3B	2.43	129.54	124.68
21	A	841	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
21	9	609	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
21	A	856	CLA	CHB-C4A-NA	2.43	127.90	124.40
21	B	806	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
21	3	403	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
21	7	311	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
21	9	607	CLA	CMB-C2B-C3B	2.42	129.53	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	812	CLA	CMB-C2B-C3B	2.42	129.53	124.68
23	a	315	LUT	C32-C33-C34	2.42	122.82	119.01
21	G	204	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
21	1	312	CLA	C1B-CHB-C4A	-2.42	125.43	130.04
21	O	2002	CLA	O2D-CGD-O1D	-2.42	118.60	124.08
21	7	316	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	c	606	CHL	C2A-C1A-CHA	2.41	128.05	123.87
21	A	837	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
28	2	617	LHG	O3-P-O6	-2.41	100.38	106.67
21	9	601	CLA	C3A-C2A-C1A	2.41	104.95	101.34
21	G	201	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
21	A	822	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
21	B	823	CLA	CHB-C4A-NA	2.41	127.88	124.40
21	8	615	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
21	B	811	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
21	b	312	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
21	L	304	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
21	A	829	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
21	a	305	CLA	CMB-C2B-C3B	2.41	129.49	124.68
21	7	306	CLA	CHB-C4A-NA	2.40	127.87	124.40
21	c	602	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
21	T	606	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	7	323	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
21	a	314	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	a	311	CLA	C2A-C1A-CHA	2.40	128.03	123.87
23	1	314	LUT	C22-C23-C24	-2.40	107.62	111.18
21	F	5005	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
21	A	806	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
21	3	413	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
21	B	823	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
21	B	824	CLA	C1B-CHB-C4A	-2.39	125.47	130.04
21	B	819	CLA	C4A-NA-C1A	2.39	107.77	106.68
21	K	201	CLA	CHB-C4A-NA	2.39	127.85	124.40
21	B	844	CLA	CMB-C2B-C3B	2.39	129.47	124.68
21	9	604	CLA	C1B-CHB-C4A	-2.39	125.48	130.04
21	A	815	CLA	O2D-CGD-CBD	2.39	115.41	111.23
21	A	832	CLA	C1B-CHB-C4A	-2.39	125.48	130.04
21	2	605	CLA	C1B-CHB-C4A	-2.39	125.49	130.04
21	9	603	CLA	C1B-CHB-C4A	-2.39	125.49	130.04
22	b	308	CHL	C2D-C1D-ND	-2.39	107.76	110.13
21	1	308	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
21	1	301	CLA	C1B-CHB-C4A	-2.38	125.50	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	610	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
21	K	204	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
21	B	842	CLA	CHB-C4A-NA	2.38	127.83	124.40
21	B	834	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
21	7	314	CLA	C1B-CHB-C4A	-2.38	125.50	130.04
22	c	605	CHL	C1D-CHD-C4C	-2.38	120.97	126.02
21	8	604	CLA	C2A-C1A-CHA	2.38	127.99	123.87
22	b	302	CHL	C1D-ND-C4D	2.37	107.97	106.31
21	B	815	CLA	C1B-CHB-C4A	-2.37	125.52	130.04
21	A	836	CLA	C1B-CHB-C4A	-2.37	125.53	130.04
21	B	820	CLA	O2D-CGD-CBD	2.37	115.37	111.23
22	7	303	CHL	C1D-CHD-C4C	-2.37	120.99	126.02
21	A	816	CLA	C1-C2-C3	-2.37	122.32	126.20
21	b	304	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
21	B	826	CLA	C4A-NA-C1A	2.36	107.76	106.68
25	B	805	BCR	C23-C24-C25	2.36	133.31	127.00
21	7	304	CLA	C1B-CHB-C4A	-2.36	125.54	130.04
22	c	605	CHL	CHC-C1C-NC	-2.36	120.75	124.31
21	B	809	CLA	O2D-CGD-CBD	2.36	115.36	111.23
21	8	613	CLA	C1B-CHB-C4A	-2.35	125.55	130.04
21	L	301	CLA	C1-C2-C3	-2.35	122.95	126.76
21	A	834	CLA	C1-C2-C3	-2.35	122.34	126.20
21	7	306	CLA	CMB-C2B-C3B	2.35	129.38	124.68
22	3	401	CHL	C2D-C1D-ND	-2.35	107.80	110.13
22	1	305	CHL	CHC-C1C-NC	-2.35	120.77	124.31
21	a	310	CLA	CHB-C4A-NA	2.35	127.79	124.40
21	3	412	CLA	CHB-C4A-NA	2.35	127.79	124.40
21	9	607	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
21	T	607	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
22	c	607	CHL	CHC-C1C-NC	-2.35	120.78	124.31
21	F	5007	CLA	C1B-CHB-C4A	-2.35	125.57	130.04
22	7	307	CHL	CHC-C1C-NC	-2.35	120.78	124.31
21	T	609	CLA	CHC-C1C-NC	2.34	127.84	124.31
21	O	2002	CLA	CHB-C4A-NA	2.34	127.78	124.40
21	A	816	CLA	C1B-CHB-C4A	-2.34	125.57	130.04
21	A	856	CLA	C1B-CHB-C4A	-2.34	125.57	130.04
34	A	803	CL0	C3D-C2D-C1D	2.34	109.03	105.83
21	T	606	CLA	C2A-C1A-CHA	2.34	127.93	123.87
21	L	305	CLA	C1B-CHB-C4A	-2.34	125.58	130.04
21	A	818	CLA	CMB-C2B-C3B	2.34	129.36	124.68
21	b	316	CLA	C1B-CHB-C4A	-2.34	125.58	130.04
25	B	852	BCR	C21-C20-C19	2.34	129.97	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	2001	CLA	C1B-CHB-C4A	-2.34	125.58	130.04
22	1	305	CHL	C1D-CHD-C4C	-2.34	121.05	126.02
21	1	321	CLA	C3B-C4B-NB	-2.34	106.19	109.21
21	B	840	CLA	C1B-CHB-C4A	-2.33	125.59	130.04
21	A	809	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
21	A	843	CLA	CHB-C4A-NA	2.33	127.77	124.40
21	A	834	CLA	CMB-C2B-C3B	2.33	129.34	124.68
21	2	612	CLA	C1B-CHB-C4A	-2.33	125.59	130.04
21	A	818	CLA	C1B-CHB-C4A	-2.33	125.59	130.04
21	B	839	CLA	C1B-CHB-C4A	-2.33	125.59	130.04
21	G	205	CLA	C1B-CHB-C4A	-2.33	125.60	130.04
25	B	852	BCR	C10-C11-C12	2.33	129.94	123.20
25	K	205	BCR	C11-C12-C13	2.33	132.74	126.36
21	L	306	CLA	C1B-CHB-C4A	-2.33	125.61	130.04
21	3	414	CLA	C1B-CHB-C4A	-2.32	125.61	130.04
21	O	2001	CLA	CHB-C4A-NA	2.32	127.75	124.40
21	B	841	CLA	C1-C2-C3	-2.32	123.00	126.76
22	c	606	CHL	C3D-C2D-C1D	2.32	109.00	105.83
21	A	811	CLA	C2A-C1A-CHA	2.32	127.89	123.87
21	1	304	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
21	7	315	CLA	C1-C2-C3	-2.32	123.01	126.76
21	A	817	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
21	B	827	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
21	A	842	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
23	O	2005	LUT	C26-C27-C28	2.31	128.17	124.58
21	1	303	CLA	C1-C2-C3	-2.31	123.03	126.76
22	2	606	CHL	C2A-C1A-CHA	2.31	127.87	123.87
21	c	610	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
21	A	811	CLA	CMB-C2B-C3B	2.31	129.29	124.68
21	F	5006	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
21	b	314	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
25	O	2004	BCR	C15-C14-C13	2.31	130.51	127.28
21	9	612	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
21	A	811	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
21	B	808	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
22	b	302	CHL	CHD-C1D-C2D	2.30	130.28	125.49
22	2	606	CHL	C1D-CHD-C4C	-2.30	121.12	126.02
21	A	835	CLA	CMB-C2B-C3B	2.30	129.29	124.68
21	1	306	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
21	c	603	CLA	CHB-C4A-NA	2.30	127.72	124.40
21	9	601	CLA	CMB-C2B-C3B	2.30	129.28	124.68
21	3	405	CLA	C1B-CHB-C4A	-2.30	125.65	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	819	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
21	A	831	CLA	C1B-CHB-C4A	-2.30	125.65	130.04
22	b	302	CHL	C1D-CHD-C4C	-2.30	121.13	126.02
21	L	304	CLA	O2D-CGD-CBD	2.30	115.25	111.23
22	8	601	CHL	CHD-C1D-C2D	2.30	130.27	125.49
25	A	846	BCR	C11-C10-C9	2.30	130.50	127.28
21	1	311	CLA	C1B-CHB-C4A	-2.30	125.66	130.04
21	B	819	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
21	1	306	CLA	C1-C2-C3	-2.29	123.05	126.76
21	8	622	CLA	CHA-C4D-ND	2.29	137.28	132.55
21	G	205	CLA	CMB-C2B-C3B	2.29	129.26	124.68
21	9	611	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
21	a	312	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
21	3	406	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
22	8	607	CHL	C2A-C1A-CHA	2.29	127.84	123.87
21	b	305	CLA	C2A-C1A-CHA	2.29	127.84	123.87
22	7	309	CHL	CHC-C1C-NC	-2.29	120.87	124.31
24	1	315	XAT	C7-C8-C9	2.29	129.08	125.53
21	c	613	CLA	C1-C2-C3	-2.29	123.06	126.76
21	3	403	CLA	C1-C2-C3	-2.28	123.07	126.76
21	B	835	CLA	CAA-CBA-CGA	-2.28	106.72	113.21
21	B	814	CLA	C1B-CHB-C4A	-2.28	125.69	130.04
21	3	406	CLA	C1-C2-C3	-2.28	122.46	126.20
21	A	808	CLA	C1-C2-C3	-2.28	122.46	126.20
21	A	840	CLA	C1-C2-C3	-2.28	122.46	126.20
21	T	612	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
21	A	809	CLA	C2A-C1A-CHA	2.28	127.82	123.87
21	a	309	CLA	C1-C2-C3	-2.27	122.47	126.20
22	b	309	CHL	CHC-C1C-NC	-2.27	120.89	124.31
21	A	827	CLA	C2A-C1A-CHA	2.27	127.81	123.87
22	8	608	CHL	C2A-C1A-CHA	2.27	127.81	123.87
21	c	613	CLA	C1B-CHB-C4A	-2.27	125.70	130.04
34	A	803	CL0	CHD-C1D-C2D	2.27	130.21	125.49
21	B	807	CLA	CBA-CAA-C2A	-2.27	107.03	113.79
22	T	601	CHL	C3D-C2D-C1D	2.27	108.93	105.83
21	B	823	CLA	CMB-C2B-C3B	2.27	129.22	124.68
22	8	607	CHL	C1D-CHD-C4C	-2.27	121.19	126.02
21	T	605	CLA	C1B-CHB-C4A	-2.27	125.71	130.04
21	B	812	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
21	A	831	CLA	CHB-C4A-NA	2.27	127.67	124.40
21	2	603	CLA	C1B-CHB-C4A	-2.26	125.73	130.04
21	A	830	CLA	O2A-CGA-O1A	-2.26	117.98	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	409	CLA	C1B-CHB-C4A	-2.26	125.73	130.04
21	c	612	CLA	C1B-CHB-C4A	-2.26	125.74	130.04
21	2	609	CLA	CAA-C2A-C3A	-2.26	111.06	116.23
22	2	606	CHL	CHC-C1C-NC	-2.25	120.92	124.31
21	B	833	CLA	C1B-CHB-C4A	-2.25	125.74	130.04
21	A	820	CLA	CAC-C3C-C4C	2.25	127.72	124.79
21	B	822	CLA	C1-C2-C3	-2.25	122.51	126.20
23	7	317	LUT	C21-C26-C27	2.25	115.41	112.83
22	8	608	CHL	CHC-C1C-NC	-2.25	120.92	124.31
21	T	603	CLA	C1B-CHB-C4A	-2.25	125.75	130.04
22	7	303	CHL	CHC-C1C-NC	-2.25	120.93	124.31
21	a	314	CLA	C1-C2-C3	-2.25	123.13	126.76
21	7	312	CLA	C1B-CHB-C4A	-2.25	125.76	130.04
21	a	308	CLA	CHA-C1A-NA	-2.25	121.31	126.39
21	B	812	CLA	C1-C2-C3	-2.24	122.52	126.20
21	1	310	CLA	CAA-C2A-C3A	-2.24	106.93	113.00
23	a	315	LUT	C22-C23-C24	2.24	114.52	111.18
22	b	307	CHL	CHD-C1D-C2D	2.24	130.15	125.49
22	8	606	CHL	CHC-C1C-NC	-2.24	120.94	124.31
21	c	604	CLA	C1-C2-C3	-2.24	123.14	126.76
21	B	822	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
21	B	840	CLA	O2D-CGD-CBD	2.23	115.13	111.23
22	a	306	CHL	C1D-ND-C4D	2.23	107.88	106.31
24	7	318	XAT	C36-C21-C26	2.23	116.07	110.05
21	a	310	CLA	C1B-CHB-C4A	-2.23	125.79	130.04
21	A	808	CLA	C1B-CHB-C4A	-2.23	125.79	130.04
21	B	832	CLA	CHB-C4A-NA	2.23	127.61	124.40
21	A	826	CLA	CMB-C2B-C3B	2.22	129.12	124.68
21	B	833	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
21	B	808	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	b	307	CHL	CHC-C1C-NC	-2.22	120.97	124.31
21	3	410	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	B	837	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	B	816	CLA	C4A-NA-C1A	2.22	107.69	106.68
23	a	315	LUT	C21-C26-C27	2.22	115.38	112.83
21	B	824	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	7	313	CLA	C1B-CHB-C4A	-2.22	125.81	130.04
21	b	311	CLA	CMC-C2C-C1C	-2.22	121.57	125.03
21	O	2002	CLA	CAA-C2A-C3A	-2.22	111.15	116.23
21	3	411	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	A	848	BCR	C20-C19-C18	2.21	132.43	126.36
21	1	310	CLA	CHA-C1A-NA	-2.21	121.38	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	617	LHG	O4-P-O5	2.21	119.44	110.83
21	B	828	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
21	T	611	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
21	2	603	CLA	CMB-C2B-C3B	2.20	129.08	124.68
34	A	803	CL0	CHD-C4C-NC	-2.20	120.82	124.23
21	T	610	CLA	C1B-CHB-C4A	-2.20	125.84	130.04
21	B	809	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	c	616	XAT	C36-C21-C26	2.20	115.98	110.05
21	9	601	CLA	CHD-C4C-NC	2.20	127.64	124.23
21	8	604	CLA	C1B-CHB-C4A	-2.20	125.85	130.04
21	B	838	CLA	C1-C2-C3	-2.20	123.21	126.76
21	B	835	CLA	C1B-CHB-C4A	-2.20	125.85	130.04
21	B	844	CLA	C1B-CHB-C4A	-2.20	125.85	130.04
29	I	201	PTY	O12-P1-O13	2.20	119.40	110.83
21	B	833	CLA	C1-C2-C3	-2.20	122.60	126.20
24	a	316	XAT	C16-C1-C6	2.20	115.97	110.05
21	9	601	CLA	CMA-C3A-C2A	2.19	122.47	113.98
21	A	832	CLA	CMB-C2B-C3B	2.19	129.07	124.68
25	B	805	BCR	C16-C17-C18	2.19	130.35	127.28
22	b	302	CHL	C3D-C2D-C1D	2.19	108.82	105.83
21	b	306	CLA	C1B-CHB-C4A	-2.19	125.86	130.04
23	O	2005	LUT	C27-C28-C29	2.19	131.03	126.32
21	9	601	CLA	C2D-C1D-ND	-2.19	107.96	110.13
21	b	314	CLA	C1-C2-C3	-2.19	123.22	126.76
21	A	839	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
21	A	816	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
22	b	309	CHL	C2A-C1A-CHA	2.19	127.66	123.87
21	O	2003	CLA	CHB-C4A-NA	2.18	127.55	124.40
21	8	603	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
21	b	305	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
21	7	304	CLA	C1-C2-C3	-2.18	122.62	126.20
22	2	601	CHL	CHC-C1C-NC	-2.18	121.02	124.31
21	9	603	CLA	C2A-C1A-CHA	2.18	127.66	123.87
21	b	304	CLA	C1-C2-C3	-2.18	122.62	126.20
21	3	410	CLA	C1B-CHB-C4A	-2.18	125.88	130.04
21	B	818	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
21	b	313	CLA	C1-C2-C3	-2.18	123.24	126.76
22	b	308	CHL	CHD-C1D-C2D	2.18	130.01	125.49
21	9	605	CLA	C2A-C1A-CHA	2.18	127.64	123.87
21	T	611	CLA	CHA-C1A-NA	-2.17	121.47	126.39
21	K	203	CLA	C2A-C1A-CHA	2.17	127.64	123.87
21	B	810	CLA	C1-C2-C3	-2.17	122.64	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	832	CLA	C2D-C1D-ND	-2.17	107.98	110.13
21	9	610	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	A	841	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
34	A	803	CL0	C1D-CHD-C4C	-2.17	121.41	126.02
30	2	618	SQD	C45-O47-C7	2.17	122.98	117.80
22	b	307	CHL	CHD-C4C-NC	-2.16	120.88	124.23
21	A	822	CLA	CMB-C2B-C3B	2.16	129.01	124.68
21	A	828	CLA	C1-C2-C3	-2.16	122.65	126.20
22	T	601	CHL	C1D-CHD-C4C	-2.16	121.42	126.02
21	B	830	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
21	A	813	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
21	T	608	CLA	C1B-CHB-C4A	-2.16	125.92	130.04
21	3	410	CLA	C1-C2-C3	-2.16	122.66	126.20
22	8	606	CHL	CHD-C1D-C2D	2.16	129.98	125.49
21	T	606	CLA	CMB-C2B-C3B	2.16	129.00	124.68
21	c	611	CLA	C1B-CHB-C4A	-2.16	125.93	130.04
21	B	804	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
23	1	314	LUT	C26-C27-C28	2.15	127.93	124.58
21	A	821	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	c	606	CHL	CHC-C1C-NC	-2.15	121.07	124.31
21	A	842	CLA	C1-C2-C3	-2.15	122.67	126.20
22	7	307	CHL	C1D-CHD-C4C	-2.15	121.45	126.02
21	B	842	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
21	B	827	CLA	C2A-C1A-CHA	2.15	127.60	123.87
21	2	611	CLA	C1B-CHB-C4A	-2.15	125.94	130.04
21	A	805	CLA	C1B-CHB-C4A	-2.15	125.94	130.04
22	c	607	CHL	C1C-C2C-C3C	-2.15	105.31	107.28
21	1	321	CLA	C2A-C1A-CHA	2.15	127.59	123.87
21	b	314	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
21	B	823	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
21	3	405	CLA	C1-C2-C3	-2.14	123.29	126.76
21	B	841	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
21	a	311	CLA	CHA-C1A-NA	-2.14	121.54	126.39
22	c	605	CHL	CHD-C1D-C2D	2.14	129.93	125.49
22	1	305	CHL	CHA-C1A-NA	-2.14	121.55	126.39
21	c	604	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	A	826	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	B	834	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
21	A	828	CLA	C1B-CHB-C4A	-2.13	125.97	130.04
22	b	309	CHL	CHD-C1D-C2D	2.13	129.93	125.49
21	A	831	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
23	1	314	LUT	C35-C34-C33	2.13	130.27	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	308	CHL	CHC-C1C-NC	-2.13	121.10	124.31
21	c	604	CLA	C1B-CHB-C4A	-2.13	125.97	130.04
21	3	406	CLA	C1B-CHB-C4A	-2.13	125.97	130.04
21	B	836	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
21	3	412	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
21	A	818	CLA	C1-C2-C3	-2.12	122.72	126.20
25	B	852	BCR	C12-C13-C14	2.12	122.35	119.01
21	L	306	CLA	C1-C2-C3	-2.12	123.33	126.76
22	7	309	CHL	C1C-C2C-C3C	-2.12	105.33	107.28
21	7	304	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
21	8	613	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
21	A	829	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
21	K	203	CLA	C1B-CHB-C4A	-2.12	126.00	130.04
21	A	821	CLA	C1-C2-C3	-2.12	122.72	126.20
28	7	324	LHG	C5-O7-C7	2.12	122.86	117.80
21	A	809	CLA	CHA-C1A-NA	-2.12	121.60	126.39
21	F	5007	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
21	B	829	CLA	C1B-CHB-C4A	-2.11	126.01	130.04
21	1	302	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
21	A	805	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
22	a	306	CHL	CHC-C1C-NC	-2.11	121.13	124.31
21	B	806	CLA	C1-C2-C3	-2.11	122.73	126.20
22	b	309	CHL	C1C-C2C-C3C	-2.11	105.34	107.28
21	B	804	CLA	CHB-C4A-NA	2.11	127.44	124.40
21	T	609	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	b	307	CHL	C1D-CHD-C4C	-2.11	121.54	126.02
21	T	607	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
21	a	314	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
21	3	409	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
21	T	603	CLA	C2A-C1A-CHA	2.11	127.52	123.87
22	3	401	CHL	C4D-CHA-C1A	-2.11	118.73	121.24
24	a	316	XAT	O24-C25-C24	-2.10	111.52	113.49
22	c	605	CHL	CHD-C4C-NC	-2.10	120.97	124.23
22	7	308	CHL	CHD-C4C-NC	-2.10	120.97	124.23
22	T	602	CHL	CHC-C1C-NC	-2.10	121.15	124.31
21	A	823	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	b	308	CHL	CHC-C1C-NC	-2.10	121.15	124.31
21	T	603	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
21	1	321	CLA	C2C-C1C-NC	-2.10	107.78	109.98
21	B	835	CLA	C2A-C1A-CHA	2.10	127.51	123.87
21	B	820	CLA	C1B-CHB-C4A	-2.10	126.04	130.04
21	B	835	CLA	O2A-CGA-O1A	-2.10	118.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	612	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
21	A	832	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
21	A	806	CLA	O2D-CGD-CBD	2.10	114.89	111.23
22	8	607	CHL	CHC-C1C-NC	-2.10	121.15	124.31
22	7	303	CHL	CHD-C1D-ND	-2.10	121.85	124.80
21	A	830	CLA	CHD-C1D-ND	-2.10	121.85	124.80
21	7	305	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
21	A	842	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	a	316	XAT	O4-C6-C7	-2.09	110.88	116.88
21	B	828	CLA	C1-C2-C3	-2.09	122.77	126.20
21	b	313	CLA	CHA-C1A-NA	-2.09	121.65	126.39
21	B	838	CLA	O2D-CGD-CBD	2.09	114.89	111.23
21	8	604	CLA	CHA-C1A-NA	-2.09	121.66	126.39
21	2	603	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	1	305	CHL	C2A-C3A-C4A	-2.09	98.50	101.87
21	8	605	CLA	C1B-CHB-C4A	-2.09	126.06	130.04
21	1	306	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
22	T	601	CHL	CHC-C1C-NC	-2.09	121.17	124.31
21	A	815	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
21	9	602	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
21	T	611	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
22	7	308	CHL	CHD-C1D-ND	-2.08	121.87	124.80
21	8	612	CLA	C2A-C1A-CHA	2.08	127.48	123.87
22	7	308	CHL	C2A-C1A-CHA	2.08	127.48	123.87
21	B	809	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
21	B	817	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
21	1	303	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
21	J	5002	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
22	b	302	CHL	CHC-C1C-NC	-2.08	121.18	124.31
21	b	313	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
21	K	202	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
21	B	827	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
22	9	606	CHL	CHD-C1D-ND	-2.08	121.88	124.80
21	A	804	CLA	CMB-C2B-C3B	2.08	128.84	124.68
21	B	810	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
21	a	302	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
21	G	203	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
21	A	810	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
21	3	409	CLA	C1-C2-C3	-2.08	122.79	126.20
21	G	205	CLA	CHD-C1D-ND	-2.08	121.88	124.80
21	B	843	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
22	7	309	CHL	CHD-C4C-NC	-2.08	121.01	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	803	CL0	CHC-C1C-NC	-2.07	121.19	124.31
21	A	814	CLA	C1-C2-C3	-2.07	122.80	126.20
21	7	314	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
21	c	602	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
24	9	615	XAT	C35-C15-C14	2.07	127.76	123.52
21	a	305	CLA	CAC-C3C-C4C	2.07	127.48	124.79
22	8	601	CHL	CHC-C1C-NC	-2.07	121.19	124.31
21	A	814	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	c	603	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	A	843	CLA	CHD-C1D-ND	-2.07	121.89	124.80
21	9	607	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	A	819	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	7	315	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	A	856	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	7	313	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
22	8	606	CHL	C1D-CHD-C4C	-2.06	121.63	126.02
21	2	604	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
21	A	828	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
21	A	836	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
21	c	613	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
21	A	835	CLA	CHD-C1D-ND	-2.06	121.90	124.80
21	a	312	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	8	607	CHL	CHD-C4C-NC	-2.06	121.03	124.23
21	8	612	CLA	C1B-CHB-C4A	-2.06	126.11	130.04
21	T	606	CLA	CHA-C1A-NA	-2.06	121.72	126.39
22	a	306	CHL	CHD-C1D-ND	-2.06	121.90	124.80
21	G	201	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	7	306	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	A	835	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	B	836	CLA	C1-C2-C3	-2.06	122.82	126.20
21	B	840	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	9	605	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	T	604	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	B	824	CLA	C1-C2-C3	-2.06	122.83	126.20
21	J	5002	CLA	C2A-C1A-CHA	2.05	127.43	123.87
21	A	818	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	2	606	CHL	CHD-C4C-NC	-2.05	121.05	124.23
21	9	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
21	8	622	CLA	CBA-CAA-C2A	2.05	119.89	113.79
21	B	823	CLA	C1-C2-C3	-2.05	122.84	126.20
21	B	832	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
21	B	820	CLA	C1-C2-C3	-2.05	122.84	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	307	CLA	C1-C2-C3	-2.05	123.45	126.76
21	9	603	CLA	CHA-C1A-NA	-2.05	121.76	126.39
21	3	407	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
21	2	604	CLA	C1-C2-C3	-2.04	123.46	126.76
21	A	807	CLA	CHD-C1D-ND	-2.04	121.93	124.80
22	8	601	CHL	CHD-C4C-NC	-2.04	121.06	124.23
21	A	808	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
21	A	829	CLA	C1-C2-C3	-2.04	122.85	126.20
21	1	321	CLA	CHA-C1A-NA	-2.04	121.77	126.39
21	7	306	CLA	C1B-CHB-C4A	-2.04	126.15	130.04
21	2	613	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	9	615	XAT	C7-C8-C9	2.04	128.69	125.53
34	A	803	CL0	C2A-C1A-CHA	2.04	127.40	123.87
21	K	202	CLA	C1-C2-C3	-2.03	122.86	126.20
21	B	825	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
21	A	834	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	B	805	BCR	C19-C18-C17	2.03	122.20	119.01
21	a	304	CLA	O2D-CGD-CBD	2.03	114.78	111.23
21	b	305	CLA	CHA-C1A-NA	-2.03	121.80	126.39
22	8	606	CHL	C1D-ND-C4D	2.03	107.73	106.31
25	A	846	BCR	C15-C14-C13	-2.03	124.44	127.28
24	a	316	XAT	C18-C5-C4	2.03	116.52	114.24
21	9	604	CLA	C1-C2-C3	-2.03	123.48	126.76
21	A	806	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	A	811	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
21	B	829	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	A	825	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	B	806	CLA	O2D-CGD-CBD	2.02	114.77	111.23
21	F	5006	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	A	822	CLA	C1-C2-C3	-2.02	122.89	126.20
21	a	312	CLA	C1-C2-C3	-2.02	122.89	126.20
22	c	607	CHL	C2A-C1A-CHA	2.02	127.37	123.87
21	F	5005	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
21	A	810	CLA	C1-C2-C3	-2.01	122.90	126.20
21	K	204	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	7	307	CHL	CHD-C4C-NC	-2.01	121.11	124.23
24	9	615	XAT	C38-C25-C24	-2.01	111.98	114.24
22	1	305	CHL	CHD-C4C-NC	-2.01	121.11	124.23
21	A	830	CLA	O2D-CGD-CBD	2.01	114.75	111.23
21	8	610	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
21	T	609	CLA	C1-C2-C3	-2.01	122.91	126.20
21	a	303	CLA	CHA-C1A-NA	-2.01	121.84	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	316	CLA	C1-C2-C3	-2.01	122.91	126.20
21	B	843	CLA	CMB-C2B-C3B	2.01	128.69	124.68
25	B	805	BCR	C24-C23-C22	-2.00	123.27	126.23
21	A	833	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
21	K	203	CLA	CHA-C1A-NA	-2.00	121.85	126.39
21	A	827	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	3	408	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
21	A	839	CLA	CHD-C1D-ND	-2.00	121.98	124.80
21	B	827	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	1	301	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
21	3	402	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	T	601	CHL	C1C-C2C-C3C	-2.00	105.44	107.28
21	B	840	CLA	CHD-C1D-ND	-2.00	121.99	124.80
21	8	612	CLA	CHA-C1A-NA	-2.00	121.86	126.39
21	b	313	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (295) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	301	CLA	ND
21	1	302	CLA	ND
21	1	303	CLA	ND
21	1	304	CLA	ND
21	1	306	CLA	ND
21	1	307	CLA	ND
21	1	308	CLA	ND
21	1	309	CLA	ND
21	1	310	CLA	ND
21	1	311	CLA	ND
21	1	312	CLA	ND
21	1	313	CLA	ND
21	1	321	CLA	ND
21	2	602	CLA	ND
21	2	603	CLA	ND
21	2	604	CLA	ND
21	2	605	CLA	ND
21	2	607	CLA	ND
21	2	608	CLA	ND
21	2	609	CLA	ND
21	2	610	CLA	ND
21	2	611	CLA	ND
21	2	612	CLA	ND

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Mol	Chain	Res	Type	Atom
21	2	613	CLA	ND
21	3	402	CLA	ND
21	3	403	CLA	ND
21	3	404	CLA	ND
21	3	405	CLA	ND
21	3	406	CLA	ND
21	3	407	CLA	ND
21	3	408	CLA	ND
21	3	409	CLA	ND
21	3	410	CLA	ND
21	3	411	CLA	ND
21	3	412	CLA	ND
21	3	413	CLA	ND
21	3	414	CLA	ND
21	7	304	CLA	ND
21	7	305	CLA	ND
21	7	306	CLA	ND
21	7	310	CLA	ND
21	7	311	CLA	ND
21	7	312	CLA	ND
21	7	313	CLA	ND
21	7	314	CLA	ND
21	7	315	CLA	ND
21	7	316	CLA	ND
21	7	323	CLA	ND
21	8	603	CLA	ND
21	8	604	CLA	ND
21	8	605	CLA	ND
21	8	609	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	612	CLA	ND
21	8	613	CLA	ND
21	8	614	CLA	ND
21	8	615	CLA	ND
21	8	622	CLA	ND
21	9	601	CLA	ND
21	9	602	CLA	ND
21	9	603	CLA	ND
21	9	604	CLA	ND
21	9	605	CLA	ND
21	9	607	CLA	ND

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Mol	Chain	Res	Type	Atom
21	9	608	CLA	ND
21	9	609	CLA	ND
21	9	610	CLA	ND
21	9	611	CLA	ND
21	9	612	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND
21	A	807	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	810	CLA	ND
21	A	811	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND
21	A	814	CLA	ND
21	A	816	CLA	ND
21	A	817	CLA	ND
21	A	818	CLA	ND
21	A	819	CLA	ND
21	A	820	CLA	ND
21	A	821	CLA	ND
21	A	822	CLA	ND
21	A	823	CLA	ND
21	A	824	CLA	ND
21	A	825	CLA	ND
21	A	826	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND
21	A	831	CLA	ND
21	A	832	CLA	ND
21	A	833	CLA	ND
21	A	834	CLA	ND
21	A	835	CLA	ND
21	A	836	CLA	ND
21	A	837	CLA	ND
21	A	838	CLA	ND
21	A	839	CLA	ND
21	A	840	CLA	ND
21	A	841	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	842	CLA	ND
21	A	843	CLA	ND
21	A	856	CLA	ND
21	B	804	CLA	ND
21	B	806	CLA	ND
21	B	807	CLA	ND
21	B	808	CLA	ND
21	B	809	CLA	ND
21	B	810	CLA	ND
21	B	811	CLA	ND
21	B	812	CLA	ND
21	B	813	CLA	ND
21	B	814	CLA	ND
21	B	815	CLA	ND
21	B	816	CLA	ND
21	B	817	CLA	ND
21	B	818	CLA	ND
21	B	819	CLA	ND
21	B	820	CLA	ND
21	B	821	CLA	ND
21	B	822	CLA	ND
21	B	823	CLA	ND
21	B	824	CLA	ND
21	B	825	CLA	ND
21	B	826	CLA	ND
21	B	827	CLA	ND
21	B	828	CLA	ND
21	B	829	CLA	ND
21	B	830	CLA	ND
21	B	831	CLA	ND
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	834	CLA	ND
21	B	835	CLA	ND
21	B	836	CLA	ND
21	B	837	CLA	ND
21	B	838	CLA	ND
21	B	839	CLA	ND
21	B	840	CLA	ND
21	B	841	CLA	ND
21	B	842	CLA	ND
21	B	843	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	844	CLA	ND
21	F	5005	CLA	ND
21	F	5006	CLA	ND
21	F	5007	CLA	ND
21	G	201	CLA	ND
21	G	203	CLA	ND
21	G	204	CLA	ND
21	G	205	CLA	ND
21	H	203	CLA	ND
21	H	204	CLA	ND
21	J	5002	CLA	ND
21	L	301	CLA	ND
21	L	303	CLA	ND
21	L	304	CLA	ND
21	L	305	CLA	ND
21	L	306	CLA	ND
21	O	2001	CLA	ND
21	O	2002	CLA	ND
21	O	2003	CLA	ND
21	a	302	CLA	ND
21	a	303	CLA	ND
21	a	304	CLA	ND
21	a	305	CLA	ND
21	a	307	CLA	ND
21	a	308	CLA	ND
21	a	309	CLA	ND
21	a	310	CLA	ND
21	a	311	CLA	ND
21	a	312	CLA	ND
21	a	313	CLA	ND
21	a	314	CLA	ND
21	b	304	CLA	ND
21	b	305	CLA	ND
21	b	306	CLA	ND
21	b	310	CLA	ND
21	b	311	CLA	ND
21	b	312	CLA	ND
21	b	313	CLA	ND
21	b	314	CLA	ND
21	b	315	CLA	ND
21	b	316	CLA	ND
21	c	601	CLA	ND

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Mol	Chain	Res	Type	Atom
21	c	602	CLA	ND
21	c	603	CLA	ND
21	c	604	CLA	ND
21	c	608	CLA	ND
21	c	609	CLA	ND
21	c	610	CLA	ND
21	c	611	CLA	ND
21	c	612	CLA	ND
21	c	613	CLA	ND
21	c	614	CLA	ND
21	K	201	CLA	ND
21	K	202	CLA	ND
21	K	203	CLA	ND
21	K	204	CLA	ND
21	T	603	CLA	ND
21	T	604	CLA	ND
21	T	605	CLA	ND
21	T	607	CLA	ND
21	T	608	CLA	ND
21	T	609	CLA	ND
21	T	610	CLA	ND
21	T	611	CLA	ND
21	T	612	CLA	ND
21	T	613	CLA	ND
21	T	614	CLA	ND
22	1	305	CHL	NA
22	1	305	CHL	ND
22	2	601	CHL	NC
22	2	601	CHL	C8
22	2	606	CHL	NC
22	2	606	CHL	C3A
22	3	401	CHL	C8
22	3	401	CHL	NC
22	7	303	CHL	C8
22	7	303	CHL	NA
22	7	303	CHL	ND
22	7	307	CHL	NC
22	7	308	CHL	NC
22	7	309	CHL	NA
22	7	309	CHL	ND
22	8	601	CHL	ND
22	8	606	CHL	NC

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Mol	Chain	Res	Type	Atom
22	8	607	CHL	NC
22	8	608	CHL	NA
22	8	608	CHL	ND
22	9	606	CHL	NC
22	a	306	CHL	NA
22	a	306	CHL	ND
22	b	302	CHL	C8
22	b	302	CHL	ND
22	b	307	CHL	NC
22	b	308	CHL	NC
22	b	309	CHL	NA
22	b	309	CHL	ND
22	c	605	CHL	NC
22	c	606	CHL	NC
22	c	607	CHL	NA
22	c	607	CHL	ND
22	T	601	CHL	NA
22	T	601	CHL	ND
22	T	602	CHL	NC
22	T	602	CHL	C8
23	1	314	LUT	C3
23	1	314	LUT	C23
23	1	314	LUT	C26
23	2	614	LUT	C3
23	2	614	LUT	C23
23	2	614	LUT	C26
23	2	615	LUT	C3
23	2	615	LUT	C23
23	2	615	LUT	C26
23	2	616	LUT	C3
23	2	616	LUT	C23
23	2	616	LUT	C26
23	3	415	LUT	C3
23	3	415	LUT	C23
23	3	415	LUT	C26
23	7	317	LUT	C3
23	7	317	LUT	C23
23	7	317	LUT	C26
23	8	616	LUT	C3
23	8	616	LUT	C23
23	8	616	LUT	C26
23	9	613	LUT	C3

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Mol	Chain	Res	Type	Atom
23	9	613	LUT	C23
23	9	613	LUT	C26
23	B	801	LUT	C3
23	B	801	LUT	C23
23	B	801	LUT	C26
23	O	2005	LUT	C3
23	O	2005	LUT	C23
23	O	2005	LUT	C26
23	a	315	LUT	C3
23	a	315	LUT	C23
23	a	315	LUT	C26
23	b	317	LUT	C3
23	b	317	LUT	C23
23	b	317	LUT	C26
23	c	615	LUT	C3
23	c	615	LUT	C23
23	c	615	LUT	C26
23	T	615	LUT	C3
23	T	615	LUT	C23
23	T	615	LUT	C26

All (2724) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	303	CLA	CAD-CBD-CGD-O1D
21	1	303	CLA	CAD-CBD-CGD-O2D
21	1	303	CLA	CBD-CGD-O2D-CED
21	1	304	CLA	CBD-CGD-O2D-CED
21	1	306	CLA	C1A-C2A-CAA-CBA
21	1	306	CLA	C3A-C2A-CAA-CBA
21	1	307	CLA	CHA-CBD-CGD-O2D
21	1	307	CLA	CBD-CGD-O2D-CED
21	1	310	CLA	C1A-C2A-CAA-CBA
21	1	310	CLA	CBA-CGA-O2A-C1
21	1	310	CLA	O1A-CGA-O2A-C1
21	1	311	CLA	CBA-CGA-O2A-C1
21	1	311	CLA	O1A-CGA-O2A-C1
21	1	311	CLA	CBD-CGD-O2D-CED
21	1	313	CLA	CBD-CGD-O2D-CED
21	2	603	CLA	CAD-CBD-CGD-O1D
21	2	603	CLA	CAD-CBD-CGD-O2D
21	2	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	604	CLA	C1A-C2A-CAA-CBA
21	2	604	CLA	CBD-CGD-O2D-CED
21	2	604	CLA	O1D-CGD-O2D-CED
21	2	605	CLA	C1A-C2A-CAA-CBA
21	2	605	CLA	C3A-C2A-CAA-CBA
21	2	608	CLA	C1A-C2A-CAA-CBA
21	2	608	CLA	C3A-C2A-CAA-CBA
21	2	611	CLA	C1A-C2A-CAA-CBA
21	2	611	CLA	CBD-CGD-O2D-CED
21	2	613	CLA	C1A-C2A-CAA-CBA
21	2	613	CLA	C3A-C2A-CAA-CBA
21	3	402	CLA	CBD-CGD-O2D-CED
21	3	404	CLA	CBA-CGA-O2A-C1
21	3	404	CLA	O1A-CGA-O2A-C1
21	3	407	CLA	C3A-C2A-CAA-CBA
21	3	407	CLA	CHA-CBD-CGD-O1D
21	3	407	CLA	CHA-CBD-CGD-O2D
21	3	411	CLA	O1A-CGA-O2A-C1
21	3	413	CLA	C1A-C2A-CAA-CBA
21	3	413	CLA	CBD-CGD-O2D-CED
21	7	304	CLA	C1A-C2A-CAA-CBA
21	7	304	CLA	C3A-C2A-CAA-CBA
21	7	304	CLA	CBD-CGD-O2D-CED
21	7	310	CLA	C1A-C2A-CAA-CBA
21	7	310	CLA	C3A-C2A-CAA-CBA
21	7	311	CLA	C3A-C2A-CAA-CBA
21	7	313	CLA	C3-C5-C6-C7
21	7	315	CLA	CBD-CGD-O2D-CED
21	7	323	CLA	C1A-C2A-CAA-CBA
21	7	323	CLA	C3A-C2A-CAA-CBA
21	8	603	CLA	C1A-C2A-CAA-CBA
21	8	604	CLA	CHA-CBD-CGD-O1D
21	8	604	CLA	CHA-CBD-CGD-O2D
21	8	604	CLA	C2-C3-C5-C6
21	8	604	CLA	C4-C3-C5-C6
21	8	609	CLA	C3A-C2A-CAA-CBA
21	8	609	CLA	CBA-CGA-O2A-C1
21	8	610	CLA	C1A-C2A-CAA-CBA
21	8	612	CLA	CHA-CBD-CGD-O1D
21	8	612	CLA	CHA-CBD-CGD-O2D
21	8	613	CLA	CBD-CGD-O2D-CED
21	8	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	8	615	CLA	C1A-C2A-CAA-CBA
21	8	615	CLA	C3A-C2A-CAA-CBA
21	9	601	CLA	C1A-C2A-CAA-CBA
21	9	601	CLA	CBA-CGA-O2A-C1
21	9	602	CLA	C1A-C2A-CAA-CBA
21	9	602	CLA	C3A-C2A-CAA-CBA
21	9	602	CLA	CBD-CGD-O2D-CED
21	9	603	CLA	CBD-CGD-O2D-CED
21	9	605	CLA	CBD-CGD-O2D-CED
21	9	607	CLA	CHA-CBD-CGD-O1D
21	9	607	CLA	CHA-CBD-CGD-O2D
21	9	608	CLA	C1A-C2A-CAA-CBA
21	9	608	CLA	C3A-C2A-CAA-CBA
21	9	609	CLA	CBA-CGA-O2A-C1
21	9	609	CLA	O1A-CGA-O2A-C1
21	9	610	CLA	CHA-CBD-CGD-O1D
21	9	610	CLA	CHA-CBD-CGD-O2D
21	9	612	CLA	C1A-C2A-CAA-CBA
21	9	612	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	CBD-CGD-O2D-CED
21	A	805	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	810	CLA	C3A-C2A-CAA-CBA
21	A	810	CLA	CHA-CBD-CGD-O1D
21	A	810	CLA	CHA-CBD-CGD-O2D
21	A	812	CLA	C1A-C2A-CAA-CBA
21	A	812	CLA	C3A-C2A-CAA-CBA
21	A	813	CLA	C1A-C2A-CAA-CBA
21	A	814	CLA	C1A-C2A-CAA-CBA
21	A	815	CLA	CBD-CGD-O2D-CED
21	A	816	CLA	CBD-CGD-O2D-CED
21	A	817	CLA	C1A-C2A-CAA-CBA
21	A	817	CLA	C3A-C2A-CAA-CBA
21	A	818	CLA	CBD-CGD-O2D-CED
21	A	819	CLA	CHA-CBD-CGD-O2D
21	A	821	CLA	CHA-CBD-CGD-O1D
21	A	821	CLA	CHA-CBD-CGD-O2D
21	A	822	CLA	CBD-CGD-O2D-CED
21	A	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	825	CLA	C1A-C2A-CAA-CBA
21	A	828	CLA	CHA-CBD-CGD-O1D
21	A	828	CLA	CHA-CBD-CGD-O2D
21	A	828	CLA	CBD-CGD-O2D-CED
21	A	830	CLA	C1A-C2A-CAA-CBA
21	A	832	CLA	CHA-CBD-CGD-O1D
21	A	832	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	C1A-C2A-CAA-CBA
21	A	838	CLA	CHA-CBD-CGD-O1D
21	A	838	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	C1A-C2A-CAA-CBA
21	A	841	CLA	C1A-C2A-CAA-CBA
21	A	841	CLA	C3A-C2A-CAA-CBA
21	A	842	CLA	CAD-CBD-CGD-O2D
21	B	806	CLA	C1A-C2A-CAA-CBA
21	B	806	CLA	CBD-CGD-O2D-CED
21	B	807	CLA	CBD-CGD-O2D-CED
21	B	808	CLA	CHA-CBD-CGD-O1D
21	B	808	CLA	CHA-CBD-CGD-O2D
21	B	809	CLA	C1A-C2A-CAA-CBA
21	B	809	CLA	C3A-C2A-CAA-CBA
21	B	809	CLA	CHA-CBD-CGD-O1D
21	B	809	CLA	CHA-CBD-CGD-O2D
21	B	809	CLA	C6-C7-C8-C9
21	B	810	CLA	CBD-CGD-O2D-CED
21	B	810	CLA	O1D-CGD-O2D-CED
21	B	811	CLA	CBD-CGD-O2D-CED
21	B	815	CLA	CBD-CGD-O2D-CED
21	B	817	CLA	CBD-CGD-O2D-CED
21	B	819	CLA	C1A-C2A-CAA-CBA
21	B	820	CLA	C1A-C2A-CAA-CBA
21	B	820	CLA	C3A-C2A-CAA-CBA
21	B	821	CLA	C1A-C2A-CAA-CBA
21	B	821	CLA	C3A-C2A-CAA-CBA
21	B	822	CLA	C1A-C2A-CAA-CBA
21	B	822	CLA	C3A-C2A-CAA-CBA
21	B	824	CLA	C1A-C2A-CAA-CBA
21	B	824	CLA	C3A-C2A-CAA-CBA
21	B	826	CLA	C1A-C2A-CAA-CBA
21	B	826	CLA	C3A-C2A-CAA-CBA
21	B	828	CLA	CHA-CBD-CGD-O1D
21	B	828	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	829	CLA	C1A-C2A-CAA-CBA
21	B	830	CLA	C1A-C2A-CAA-CBA
21	B	830	CLA	C3A-C2A-CAA-CBA
21	B	830	CLA	CBD-CGD-O2D-CED
21	B	831	CLA	C1A-C2A-CAA-CBA
21	B	831	CLA	C3A-C2A-CAA-CBA
21	B	836	CLA	C3A-C2A-CAA-CBA
21	B	837	CLA	C1A-C2A-CAA-CBA
21	B	837	CLA	C3A-C2A-CAA-CBA
21	B	838	CLA	CAD-CBD-CGD-O1D
21	B	838	CLA	CAD-CBD-CGD-O2D
21	B	838	CLA	CBD-CGD-O2D-CED
21	B	843	CLA	C3A-C2A-CAA-CBA
21	F	5005	CLA	CBD-CGD-O2D-CED
21	G	205	CLA	C1A-C2A-CAA-CBA
21	G	205	CLA	C3A-C2A-CAA-CBA
21	L	301	CLA	CBD-CGD-O2D-CED
21	L	303	CLA	C1A-C2A-CAA-CBA
21	L	303	CLA	C3A-C2A-CAA-CBA
21	L	306	CLA	C1A-C2A-CAA-CBA
21	L	306	CLA	C3A-C2A-CAA-CBA
21	L	306	CLA	CAD-CBD-CGD-O1D
21	L	306	CLA	CAD-CBD-CGD-O2D
21	L	306	CLA	CBD-CGD-O2D-CED
21	O	2003	CLA	CHA-CBD-CGD-O1D
21	O	2003	CLA	CHA-CBD-CGD-O2D
21	a	303	CLA	CBD-CGD-O2D-CED
21	a	304	CLA	CAD-CBD-CGD-O1D
21	a	304	CLA	CAD-CBD-CGD-O2D
21	a	305	CLA	CBD-CGD-O2D-CED
21	a	308	CLA	O1A-CGA-O2A-C1
21	a	308	CLA	CHA-CBD-CGD-O1D
21	a	308	CLA	CHA-CBD-CGD-O2D
21	a	309	CLA	CBD-CGD-O2D-CED
21	a	311	CLA	C1A-C2A-CAA-CBA
21	a	311	CLA	C3A-C2A-CAA-CBA
21	a	311	CLA	CBA-CGA-O2A-C1
21	a	312	CLA	C1A-C2A-CAA-CBA
21	a	312	CLA	O1A-CGA-O2A-C1
21	a	312	CLA	CBD-CGD-O2D-CED
21	a	313	CLA	CBA-CGA-O2A-C1
21	a	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	b	304	CLA	C3A-C2A-CAA-CBA
21	b	305	CLA	CBD-CGD-O2D-CED
21	b	310	CLA	C3A-C2A-CAA-CBA
21	b	312	CLA	CBA-CGA-O2A-C1
21	b	312	CLA	O1A-CGA-O2A-C1
21	b	313	CLA	CHA-CBD-CGD-O1D
21	b	313	CLA	CHA-CBD-CGD-O2D
21	b	314	CLA	CBD-CGD-O2D-CED
21	b	315	CLA	CBD-CGD-O2D-CED
21	c	601	CLA	C3A-C2A-CAA-CBA
21	c	601	CLA	CBA-CGA-O2A-C1
21	c	602	CLA	C1A-C2A-CAA-CBA
21	c	602	CLA	C3A-C2A-CAA-CBA
21	c	602	CLA	CBD-CGD-O2D-CED
21	c	608	CLA	C1A-C2A-CAA-CBA
21	c	608	CLA	C3A-C2A-CAA-CBA
21	c	609	CLA	C3A-C2A-CAA-CBA
21	c	611	CLA	CBD-CGD-O2D-CED
21	c	613	CLA	CBD-CGD-O2D-CED
21	c	613	CLA	O1D-CGD-O2D-CED
21	K	201	CLA	CBD-CGD-O2D-CED
21	K	203	CLA	C1A-C2A-CAA-CBA
21	K	203	CLA	C3A-C2A-CAA-CBA
21	K	204	CLA	C1A-C2A-CAA-CBA
21	K	204	CLA	C3A-C2A-CAA-CBA
21	T	603	CLA	CBD-CGD-O2D-CED
21	T	604	CLA	C1A-C2A-CAA-CBA
21	T	605	CLA	CBA-CGA-O2A-C1
21	T	605	CLA	O1A-CGA-O2A-C1
21	T	607	CLA	C1A-C2A-CAA-CBA
21	T	607	CLA	C3A-C2A-CAA-CBA
21	T	608	CLA	C1A-C2A-CAA-CBA
21	T	608	CLA	C3A-C2A-CAA-CBA
21	T	608	CLA	CHA-CBD-CGD-O1D
21	T	608	CLA	CHA-CBD-CGD-O2D
21	T	614	CLA	C1A-C2A-CAA-CBA
21	T	614	CLA	C3A-C2A-CAA-CBA
22	1	305	CHL	C1C-C2C-CMC-OMC
22	1	305	CHL	C3C-C2C-CMC-OMC
22	1	305	CHL	CBD-CGD-O2D-CED
22	2	606	CHL	C3A-C2A-CAA-CBA
22	2	606	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
22	3	401	CHL	C1C-C2C-CMC-OMC
22	3	401	CHL	C3C-C2C-CMC-OMC
22	7	307	CHL	C1C-C2C-CMC-OMC
22	7	307	CHL	C3C-C2C-CMC-OMC
22	7	308	CHL	C1C-C2C-CMC-OMC
22	7	308	CHL	C3C-C2C-CMC-OMC
22	7	309	CHL	C1A-C2A-CAA-CBA
22	7	309	CHL	C3A-C2A-CAA-CBA
22	7	309	CHL	C3C-C2C-CMC-OMC
22	8	601	CHL	C3A-C2A-CAA-CBA
22	8	601	CHL	CHA-CBD-CGD-O1D
22	8	601	CHL	CHA-CBD-CGD-O2D
22	8	606	CHL	C1C-C2C-CMC-OMC
22	8	606	CHL	CHA-CBD-CGD-O1D
22	8	606	CHL	CHA-CBD-CGD-O2D
22	8	608	CHL	C1C-C2C-CMC-OMC
22	8	608	CHL	C1-C2-C3-C4
22	8	608	CHL	C1-C2-C3-C5
22	9	606	CHL	C1A-C2A-CAA-CBA
22	9	606	CHL	C1C-C2C-CMC-OMC
22	9	606	CHL	C3C-C2C-CMC-OMC
22	a	306	CHL	C3C-C2C-CMC-OMC
22	a	306	CHL	CBD-CGD-O2D-CED
22	b	302	CHL	C3A-C2A-CAA-CBA
22	b	302	CHL	C3C-C2C-CMC-OMC
22	b	302	CHL	CHA-CBD-CGD-O1D
22	b	302	CHL	CHA-CBD-CGD-O2D
22	b	302	CHL	CBD-CGD-O2D-CED
22	b	307	CHL	C1C-C2C-CMC-OMC
22	b	307	CHL	CHA-CBD-CGD-O1D
22	b	307	CHL	CHA-CBD-CGD-O2D
22	b	309	CHL	C3C-C2C-CMC-OMC
22	b	309	CHL	C1-C2-C3-C4
22	b	309	CHL	C1-C2-C3-C5
22	c	605	CHL	C1C-C2C-CMC-OMC
22	c	607	CHL	C1C-C2C-CMC-OMC
22	T	602	CHL	C1A-C2A-CAA-CBA
22	T	602	CHL	C3A-C2A-CAA-CBA
22	T	602	CHL	C1C-C2C-CMC-OMC
22	T	602	CHL	C3C-C2C-CMC-OMC
23	1	314	LUT	C13-C14-C15-C35
23	2	615	LUT	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	3	415	LUT	C25-C26-C27-C28
23	7	317	LUT	C21-C26-C27-C28
23	7	317	LUT	C25-C26-C27-C28
23	B	801	LUT	C21-C26-C27-C28
23	B	801	LUT	C25-C26-C27-C28
23	B	801	LUT	C29-C30-C31-C32
23	O	2005	LUT	C26-C27-C28-C29
23	a	315	LUT	C21-C26-C27-C28
23	a	315	LUT	C25-C26-C27-C28
23	c	615	LUT	C21-C26-C27-C28
23	c	615	LUT	C25-C26-C27-C28
23	T	615	LUT	C25-C26-C27-C28
24	1	315	XAT	O4-C6-C7-C8
24	1	315	XAT	C6-C7-C8-C9
24	8	617	XAT	C6-C7-C8-C9
24	9	615	XAT	C6-C7-C8-C9
24	9	615	XAT	C26-C27-C28-C29
24	a	316	XAT	C1-C6-C7-C8
24	a	316	XAT	C7-C8-C9-C10
24	a	316	XAT	C26-C27-C28-C29
24	b	318	XAT	C6-C7-C8-C9
24	T	616	XAT	C6-C7-C8-C9
25	3	418	BCR	C23-C24-C25-C26
25	A	847	BCR	C7-C8-C9-C10
25	A	847	BCR	C9-C10-C11-C12
25	A	848	BCR	C17-C18-C19-C20
25	A	848	BCR	C36-C18-C19-C20
25	A	849	BCR	C19-C20-C21-C22
25	A	850	BCR	C13-C14-C15-C16
25	B	852	BCR	C7-C8-C9-C34
25	B	852	BCR	C17-C18-C19-C20
25	G	202	BCR	C1-C6-C7-C8
25	G	202	BCR	C5-C6-C7-C8
25	G	202	BCR	C19-C20-C21-C22
25	L	302	BCR	C11-C12-C13-C14
25	L	302	BCR	C11-C12-C13-C35
25	L	302	BCR	C36-C18-C19-C20
25	a	317	BCR	C13-C14-C15-C16
25	I	202	BCR	C21-C22-C23-C24
25	I	202	BCR	C23-C24-C25-C26
25	I	202	BCR	C23-C24-C25-C30
25	K	205	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	K	205	BCR	C5-C6-C7-C8
25	K	205	BCR	C7-C8-C9-C10
25	K	205	BCR	C11-C12-C13-C14
25	K	205	BCR	C11-C12-C13-C35
26	1	317	LMG	O9-C10-O7-C8
26	1	317	LMG	C11-C10-O7-C8
26	1	317	LMG	O10-C28-O8-C9
26	1	317	LMG	C29-C28-O8-C9
26	3	421	LMG	C2-C1-O1-C7
26	3	421	LMG	O6-C1-O1-C7
26	7	320	LMG	O9-C10-O7-C8
26	7	320	LMG	C11-C10-O7-C8
26	A	801	LMG	O9-C10-O7-C8
26	A	801	LMG	C11-C10-O7-C8
27	1	318	LMU	O5'-C1'-O1'-C1
27	9	616	LMU	C2'-C1'-O1'-C1
27	9	616	LMU	O5'-C1'-O1'-C1
28	1	322	LHG	C3-O3-P-O4
28	1	322	LHG	C4-O6-P-O3
28	1	322	LHG	C4-O6-P-O5
28	1	322	LHG	O7-C5-C6-O8
28	1	323	LHG	C3-O3-P-O6
28	1	323	LHG	O6-C4-C5-O7
28	1	323	LHG	O9-C7-O7-C5
28	1	323	LHG	C8-C7-O7-C5
28	3	420	LHG	C3-O3-P-O4
28	3	420	LHG	C3-O3-P-O5
28	3	420	LHG	C3-O3-P-O6
28	3	420	LHG	C4-O6-P-O3
28	3	420	LHG	C4-O6-P-O4
28	3	420	LHG	O7-C5-C6-O8
28	3	424	LHG	C3-O3-P-O5
28	3	424	LHG	C4-O6-P-O4
28	7	321	LHG	C3-O3-P-O4
28	7	321	LHG	C3-O3-P-O5
28	7	321	LHG	C3-O3-P-O6
28	7	321	LHG	C4-O6-P-O3
28	7	321	LHG	C4-O6-P-O4
28	7	321	LHG	C4-O6-P-O5
28	7	324	LHG	C3-O3-P-O5
28	7	324	LHG	C3-O3-P-O6
28	7	324	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
28	7	324	LHG	C4-O6-P-O4
28	7	324	LHG	O9-C7-O7-C5
28	7	324	LHG	C8-C7-O7-C5
28	7	324	LHG	O10-C23-O8-C6
28	7	324	LHG	C24-C23-O8-C6
28	8	620	LHG	C3-O3-P-O4
28	8	620	LHG	C3-O3-P-O6
28	8	620	LHG	C4-O6-P-O3
28	8	620	LHG	C4-O6-P-O4
28	9	617	LHG	C2-C3-O3-P
28	9	617	LHG	C3-O3-P-O4
28	9	617	LHG	C3-O3-P-O6
28	9	617	LHG	C4-O6-P-O4
28	9	617	LHG	O9-C7-O7-C5
28	9	617	LHG	C8-C7-O7-C5
28	A	852	LHG	C3-O3-P-O4
28	A	852	LHG	C3-O3-P-O5
28	A	852	LHG	C3-O3-P-O6
28	A	852	LHG	C4-O6-P-O3
28	A	852	LHG	C4-O6-P-O5
28	A	853	LHG	O7-C5-C6-O8
28	B	802	LHG	C4-O6-P-O5
28	F	5001	LHG	C3-O3-P-O4
28	F	5001	LHG	C4-O6-P-O3
28	F	5001	LHG	C4-O6-P-O4
28	F	5001	LHG	C4-O6-P-O5
28	F	5003	LHG	C3-O3-P-O4
28	F	5003	LHG	C3-O3-P-O6
28	F	5003	LHG	O10-C23-O8-C6
28	F	5003	LHG	C24-C23-O8-C6
28	H	202	LHG	C3-O3-P-O4
28	H	202	LHG	C3-O3-P-O5
28	H	202	LHG	C3-O3-P-O6
28	H	202	LHG	C4-O6-P-O5
28	a	301	LHG	O9-C7-O7-C5
28	a	301	LHG	C8-C7-O7-C5
28	b	301	LHG	C4-O6-P-O3
28	b	303	LHG	C3-O3-P-O5
28	b	303	LHG	C4-O6-P-O3
28	b	303	LHG	C4-O6-P-O5
28	b	303	LHG	O9-C7-O7-C5
28	b	303	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
28	c	618	LHG	C3-O3-P-O4
28	c	618	LHG	C3-O3-P-O6
28	c	618	LHG	C4-O6-P-O3
28	c	618	LHG	C4-O6-P-O4
29	2	620	PTY	C5-O14-P1-O11
29	2	620	PTY	C5-O14-P1-O12
29	2	620	PTY	C5-O14-P1-O13
29	7	302	PTY	N1-C2-C3-O11
29	7	302	PTY	C3-O11-P1-O14
29	7	302	PTY	C5-O14-P1-O11
29	7	302	PTY	C5-O14-P1-O13
29	7	322	PTY	O4-C1-C6-O7
29	7	322	PTY	C3-O11-P1-O13
29	8	619	PTY	C3-O11-P1-O12
29	8	619	PTY	C3-O11-P1-O14
29	B	803	PTY	C3-O11-P1-O12
29	B	803	PTY	C3-O11-P1-O13
29	B	803	PTY	C3-O11-P1-O14
29	B	803	PTY	C5-O14-P1-O11
29	H	201	PTY	O4-C1-C6-O7
29	H	201	PTY	O30-C30-O4-C1
29	J	5001	PTY	N1-C2-C3-O11
29	J	5001	PTY	C6-C5-O14-P1
29	J	5001	PTY	C3-O11-P1-O14
29	J	5001	PTY	C5-O14-P1-O11
29	L	308	PTY	O10-C8-O7-C6
29	L	308	PTY	C11-C8-O7-C6
29	L	308	PTY	C3-O11-P1-O12
29	L	308	PTY	C3-O11-P1-O14
29	L	308	PTY	C5-O14-P1-O11
29	L	308	PTY	C5-O14-P1-O12
29	L	308	PTY	C5-O14-P1-O13
29	a	319	PTY	N1-C2-C3-O11
29	a	319	PTY	C3-O11-P1-O13
29	a	319	PTY	C5-O14-P1-O11
29	a	319	PTY	C5-O14-P1-O12
29	a	319	PTY	C5-O14-P1-O13
29	c	619	PTY	N1-C2-C3-O11
29	c	619	PTY	C3-O11-P1-O14
29	c	619	PTY	C5-O14-P1-O11
29	c	619	PTY	C5-O14-P1-O12
29	c	619	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
29	c	620	PTY	O10-C8-O7-C6
29	c	620	PTY	C11-C8-O7-C6
29	c	620	PTY	C3-O11-P1-O13
29	c	620	PTY	C5-O14-P1-O11
29	c	620	PTY	C5-O14-P1-O12
29	c	620	PTY	C5-O14-P1-O13
29	I	201	PTY	O10-C8-O7-C6
30	2	618	SQD	O49-C7-O47-C45
30	2	618	SQD	C8-C7-O47-C45
30	2	618	SQD	O10-C23-O48-C46
30	2	618	SQD	C24-C23-O48-C46
30	2	618	SQD	O5-C5-C6-S
30	3	422	SQD	O49-C7-O47-C45
30	3	422	SQD	C8-C7-O47-C45
30	3	422	SQD	O10-C23-O48-C46
30	3	422	SQD	C24-C23-O48-C46
30	3	422	SQD	O5-C5-C6-S
31	2	619	3PH	O32-C31-O31-C3
31	2	619	3PH	C32-C31-O31-C3
32	7	301	DGD	C2A-C1A-O1G-C1G
32	7	301	DGD	O1A-C1A-O1G-C1G
32	7	301	DGD	C2B-C1B-O2G-C2G
32	7	301	DGD	O1B-C1B-O2G-C2G
32	7	301	DGD	C2D-C1D-O3G-C3G
32	7	301	DGD	O6D-C1D-O3G-C3G
32	8	602	DGD	C2A-C1A-O1G-C1G
32	8	602	DGD	O1A-C1A-O1G-C1G
32	8	602	DGD	C2E-C1E-O5D-C6D
32	8	602	DGD	O6E-C1E-O5D-C6D
32	B	850	DGD	C2B-C1B-O2G-C2G
32	B	850	DGD	O1B-C1B-O2G-C2G
33	8	621	LMK	O10-C28-C29-C30
21	3	402	CLA	O1D-CGD-O2D-CED
21	7	306	CLA	O1D-CGD-O2D-CED
21	8	613	CLA	O1D-CGD-O2D-CED
21	9	609	CLA	O1D-CGD-O2D-CED
21	A	834	CLA	O1D-CGD-O2D-CED
21	B	817	CLA	O1D-CGD-O2D-CED
21	F	5005	CLA	O1D-CGD-O2D-CED
21	a	307	CLA	O1D-CGD-O2D-CED
21	a	313	CLA	O1D-CGD-O2D-CED
21	T	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	305	CHL	O1D-CGD-O2D-CED
22	7	309	CHL	O1D-CGD-O2D-CED
21	2	611	CLA	O1D-CGD-O2D-CED
21	B	806	CLA	O1D-CGD-O2D-CED
21	B	807	CLA	O1D-CGD-O2D-CED
21	a	309	CLA	O1D-CGD-O2D-CED
21	a	312	CLA	O1D-CGD-O2D-CED
21	b	306	CLA	O1D-CGD-O2D-CED
21	b	314	CLA	O1D-CGD-O2D-CED
22	c	607	CHL	O1D-CGD-O2D-CED
21	1	302	CLA	CBD-CGD-O2D-CED
21	1	309	CLA	CBD-CGD-O2D-CED
21	2	610	CLA	CBD-CGD-O2D-CED
21	3	407	CLA	CBD-CGD-O2D-CED
21	3	408	CLA	CBD-CGD-O2D-CED
21	3	409	CLA	CBD-CGD-O2D-CED
21	7	306	CLA	CBD-CGD-O2D-CED
21	7	313	CLA	CBD-CGD-O2D-CED
21	8	605	CLA	CBD-CGD-O2D-CED
21	8	614	CLA	CBD-CGD-O2D-CED
21	9	607	CLA	CBD-CGD-O2D-CED
21	9	608	CLA	CBD-CGD-O2D-CED
21	9	609	CLA	CBD-CGD-O2D-CED
21	A	808	CLA	CBD-CGD-O2D-CED
21	A	831	CLA	CBD-CGD-O2D-CED
21	A	834	CLA	CBD-CGD-O2D-CED
21	A	842	CLA	CBD-CGD-O2D-CED
21	A	856	CLA	CBD-CGD-O2D-CED
21	B	812	CLA	CBD-CGD-O2D-CED
21	B	818	CLA	CBD-CGD-O2D-CED
21	B	832	CLA	CBD-CGD-O2D-CED
21	B	836	CLA	CBD-CGD-O2D-CED
21	B	839	CLA	CBD-CGD-O2D-CED
21	B	840	CLA	CBD-CGD-O2D-CED
21	F	5007	CLA	CBD-CGD-O2D-CED
21	G	201	CLA	CBD-CGD-O2D-CED
21	G	204	CLA	CBD-CGD-O2D-CED
21	G	205	CLA	CBD-CGD-O2D-CED
21	O	2003	CLA	CBD-CGD-O2D-CED
21	a	307	CLA	CBD-CGD-O2D-CED
21	a	308	CLA	CBD-CGD-O2D-CED
21	a	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	b	306	CLA	CBD-CGD-O2D-CED
21	b	316	CLA	CBD-CGD-O2D-CED
21	K	204	CLA	CBD-CGD-O2D-CED
21	T	607	CLA	CBD-CGD-O2D-CED
21	T	609	CLA	CBD-CGD-O2D-CED
21	T	612	CLA	CBD-CGD-O2D-CED
21	T	614	CLA	CBD-CGD-O2D-CED
22	7	307	CHL	CBD-CGD-O2D-CED
22	7	309	CHL	CBD-CGD-O2D-CED
22	8	601	CHL	CBD-CGD-O2D-CED
22	c	607	CHL	CBD-CGD-O2D-CED
21	2	613	CLA	O1A-CGA-O2A-C1
21	3	406	CLA	O1A-CGA-O2A-C1
21	8	611	CLA	O1A-CGA-O2A-C1
21	9	607	CLA	O1A-CGA-O2A-C1
21	A	805	CLA	O1A-CGA-O2A-C1
21	A	835	CLA	O1A-CGA-O2A-C1
21	B	813	CLA	O1A-CGA-O2A-C1
21	B	821	CLA	O1A-CGA-O2A-C1
21	F	5006	CLA	O1A-CGA-O2A-C1
21	G	201	CLA	O1A-CGA-O2A-C1
21	L	303	CLA	O1A-CGA-O2A-C1
21	T	612	CLA	O1A-CGA-O2A-C1
21	a	311	CLA	O1A-CGA-O2A-C1
21	a	313	CLA	O1A-CGA-O2A-C1
21	b	310	CLA	O1A-CGA-O2A-C1
22	1	305	CHL	O1A-CGA-O2A-C1
21	G	204	CLA	O1D-CGD-O2D-CED
21	7	323	CLA	CBA-CGA-O2A-C1
21	8	622	CLA	CBA-CGA-O2A-C1
21	a	310	CLA	CBA-CGA-O2A-C1
21	b	310	CLA	CBA-CGA-O2A-C1
22	1	305	CHL	CBA-CGA-O2A-C1
21	1	302	CLA	O1D-CGD-O2D-CED
21	3	408	CLA	O1D-CGD-O2D-CED
21	8	605	CLA	O1D-CGD-O2D-CED
21	B	815	CLA	O1D-CGD-O2D-CED
21	B	832	CLA	O1D-CGD-O2D-CED
21	B	839	CLA	O1D-CGD-O2D-CED
21	O	2003	CLA	O1D-CGD-O2D-CED
21	3	406	CLA	CBA-CGA-O2A-C1
21	B	813	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	821	CLA	CBA-CGA-O2A-C1
21	G	201	CLA	CBA-CGA-O2A-C1
21	L	303	CLA	CBA-CGA-O2A-C1
21	a	309	CLA	CBA-CGA-O2A-C1
29	a	319	PTY	C11-C8-O7-C6
21	B	814	CLA	CBD-CGD-O2D-CED
21	T	608	CLA	CBD-CGD-O2D-CED
21	1	308	CLA	O1A-CGA-O2A-C1
21	1	321	CLA	O1A-CGA-O2A-C1
21	2	603	CLA	O1A-CGA-O2A-C1
21	3	407	CLA	O1A-CGA-O2A-C1
21	3	409	CLA	O1A-CGA-O2A-C1
21	3	410	CLA	O1A-CGA-O2A-C1
21	8	603	CLA	O1A-CGA-O2A-C1
21	8	613	CLA	O1A-CGA-O2A-C1
21	A	804	CLA	O1A-CGA-O2A-C1
21	A	808	CLA	O1A-CGA-O2A-C1
21	A	816	CLA	O1A-CGA-O2A-C1
21	A	830	CLA	O1A-CGA-O2A-C1
21	B	807	CLA	O1A-CGA-O2A-C1
21	B	818	CLA	O1A-CGA-O2A-C1
21	B	824	CLA	O1A-CGA-O2A-C1
21	B	825	CLA	O1A-CGA-O2A-C1
21	B	827	CLA	O1A-CGA-O2A-C1
21	B	828	CLA	O1A-CGA-O2A-C1
21	B	833	CLA	O1A-CGA-O2A-C1
21	B	835	CLA	O1A-CGA-O2A-C1
21	B	836	CLA	O1A-CGA-O2A-C1
21	G	203	CLA	O1A-CGA-O2A-C1
21	a	309	CLA	O1A-CGA-O2A-C1
21	b	304	CLA	O1A-CGA-O2A-C1
21	b	305	CLA	O1A-CGA-O2A-C1
21	b	306	CLA	O1A-CGA-O2A-C1
21	b	314	CLA	O1A-CGA-O2A-C1
21	K	202	CLA	O1A-CGA-O2A-C1
21	T	607	CLA	O1A-CGA-O2A-C1
21	T	611	CLA	O1A-CGA-O2A-C1
29	7	322	PTY	O30-C30-O4-C1
29	B	851	PTY	O30-C30-O4-C1
21	7	323	CLA	O1A-CGA-O2A-C1
21	8	609	CLA	O1A-CGA-O2A-C1
21	9	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	c	601	CLA	O1A-CGA-O2A-C1
21	1	304	CLA	O1D-CGD-O2D-CED
21	1	311	CLA	O1D-CGD-O2D-CED
21	1	313	CLA	O1D-CGD-O2D-CED
21	9	612	CLA	O1D-CGD-O2D-CED
21	A	804	CLA	O1D-CGD-O2D-CED
21	A	815	CLA	O1D-CGD-O2D-CED
21	A	816	CLA	O1D-CGD-O2D-CED
21	A	824	CLA	O1D-CGD-O2D-CED
21	B	838	CLA	O1D-CGD-O2D-CED
21	a	303	CLA	O1D-CGD-O2D-CED
21	b	316	CLA	O1D-CGD-O2D-CED
21	c	611	CLA	O1D-CGD-O2D-CED
21	T	607	CLA	O1D-CGD-O2D-CED
22	b	302	CHL	O1D-CGD-O2D-CED
21	2	603	CLA	O1D-CGD-O2D-CED
21	3	413	CLA	O1D-CGD-O2D-CED
21	9	605	CLA	O1D-CGD-O2D-CED
21	A	822	CLA	O1D-CGD-O2D-CED
21	A	828	CLA	O1D-CGD-O2D-CED
21	B	830	CLA	O1D-CGD-O2D-CED
21	L	301	CLA	O1D-CGD-O2D-CED
21	L	306	CLA	O1D-CGD-O2D-CED
21	a	305	CLA	O1D-CGD-O2D-CED
21	b	305	CLA	O1D-CGD-O2D-CED
21	A	815	CLA	O1A-CGA-O2A-C1
21	c	602	CLA	O1A-CGA-O2A-C1
21	9	612	CLA	CBA-CGA-O2A-C1
21	b	315	CLA	CBA-CGA-O2A-C1
21	2	607	CLA	O1A-CGA-O2A-C1
21	8	605	CLA	O1A-CGA-O2A-C1
21	9	612	CLA	O1A-CGA-O2A-C1
21	G	204	CLA	O1A-CGA-O2A-C1
21	T	610	CLA	O1A-CGA-O2A-C1
21	1	302	CLA	C3-C5-C6-C7
21	2	603	CLA	C3-C5-C6-C7
21	2	611	CLA	C3-C5-C6-C7
21	9	607	CLA	C3-C5-C6-C7
21	9	608	CLA	C3-C5-C6-C7
21	A	810	CLA	C3-C5-C6-C7
21	A	814	CLA	C3-C5-C6-C7
21	A	822	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	832	CLA	C3-C5-C6-C7
21	A	836	CLA	C3-C5-C6-C7
21	B	813	CLA	C3-C5-C6-C7
21	B	815	CLA	C3-C5-C6-C7
21	B	826	CLA	C3-C5-C6-C7
21	B	827	CLA	C3-C5-C6-C7
21	a	303	CLA	C3-C5-C6-C7
21	T	603	CLA	C3-C5-C6-C7
34	A	803	CL0	C3-C5-C6-C7
21	9	603	CLA	O1D-CGD-O2D-CED
21	1	308	CLA	CBA-CGA-O2A-C1
21	2	603	CLA	CBA-CGA-O2A-C1
21	2	613	CLA	CBA-CGA-O2A-C1
21	3	408	CLA	CBA-CGA-O2A-C1
21	3	410	CLA	CBA-CGA-O2A-C1
21	3	411	CLA	CBA-CGA-O2A-C1
21	7	305	CLA	CBA-CGA-O2A-C1
21	8	611	CLA	CBA-CGA-O2A-C1
21	8	612	CLA	CBA-CGA-O2A-C1
21	8	613	CLA	CBA-CGA-O2A-C1
21	9	607	CLA	CBA-CGA-O2A-C1
21	A	805	CLA	CBA-CGA-O2A-C1
21	A	808	CLA	CBA-CGA-O2A-C1
21	A	812	CLA	CBA-CGA-O2A-C1
21	A	835	CLA	CBA-CGA-O2A-C1
21	A	842	CLA	CBA-CGA-O2A-C1
21	B	818	CLA	CBA-CGA-O2A-C1
21	B	824	CLA	CBA-CGA-O2A-C1
21	B	825	CLA	CBA-CGA-O2A-C1
21	B	827	CLA	CBA-CGA-O2A-C1
21	B	828	CLA	CBA-CGA-O2A-C1
21	B	833	CLA	CBA-CGA-O2A-C1
21	F	5006	CLA	CBA-CGA-O2A-C1
21	F	5007	CLA	CBA-CGA-O2A-C1
21	G	203	CLA	CBA-CGA-O2A-C1
21	a	308	CLA	CBA-CGA-O2A-C1
21	a	312	CLA	CBA-CGA-O2A-C1
21	b	314	CLA	CBA-CGA-O2A-C1
21	T	607	CLA	CBA-CGA-O2A-C1
21	T	611	CLA	CBA-CGA-O2A-C1
21	T	612	CLA	CBA-CGA-O2A-C1
29	7	322	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
29	B	851	PTY	C31-C30-O4-C1
29	H	201	PTY	C31-C30-O4-C1
21	1	310	CLA	CBD-CGD-O2D-CED
21	1	321	CLA	CBD-CGD-O2D-CED
21	2	613	CLA	CBD-CGD-O2D-CED
21	3	411	CLA	CBD-CGD-O2D-CED
21	3	412	CLA	CBD-CGD-O2D-CED
21	8	622	CLA	CBD-CGD-O2D-CED
21	9	604	CLA	CBD-CGD-O2D-CED
21	9	610	CLA	CBD-CGD-O2D-CED
21	A	809	CLA	CBD-CGD-O2D-CED
21	A	810	CLA	CBD-CGD-O2D-CED
21	A	811	CLA	CBD-CGD-O2D-CED
21	A	813	CLA	CBD-CGD-O2D-CED
21	A	819	CLA	CBD-CGD-O2D-CED
21	A	821	CLA	CBD-CGD-O2D-CED
21	A	835	CLA	CBD-CGD-O2D-CED
21	B	804	CLA	CBD-CGD-O2D-CED
21	B	831	CLA	CBD-CGD-O2D-CED
21	B	841	CLA	CBD-CGD-O2D-CED
21	B	842	CLA	CBD-CGD-O2D-CED
21	B	843	CLA	CBD-CGD-O2D-CED
21	H	203	CLA	CBD-CGD-O2D-CED
21	J	5002	CLA	CBD-CGD-O2D-CED
21	a	302	CLA	CBD-CGD-O2D-CED
21	a	304	CLA	CBD-CGD-O2D-CED
21	a	310	CLA	CBD-CGD-O2D-CED
21	c	604	CLA	CBD-CGD-O2D-CED
21	c	612	CLA	CBD-CGD-O2D-CED
21	K	203	CLA	CBD-CGD-O2D-CED
21	T	604	CLA	CBD-CGD-O2D-CED
22	2	601	CHL	CBD-CGD-O2D-CED
22	T	602	CHL	CBD-CGD-O2D-CED
29	I	201	PTY	C11-C8-O7-C6
21	1	303	CLA	O1D-CGD-O2D-CED
21	1	307	CLA	O1D-CGD-O2D-CED
21	7	304	CLA	O1D-CGD-O2D-CED
21	9	602	CLA	O1D-CGD-O2D-CED
21	A	818	CLA	O1D-CGD-O2D-CED
21	B	811	CLA	O1D-CGD-O2D-CED
21	b	315	CLA	O1D-CGD-O2D-CED
21	c	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	K	201	CLA	O1D-CGD-O2D-CED
22	a	306	CHL	O1D-CGD-O2D-CED
21	T	613	CLA	O1A-CGA-O2A-C1
21	7	315	CLA	O1D-CGD-O2D-CED
21	1	308	CLA	C4-C3-C5-C6
21	9	608	CLA	C4-C3-C5-C6
21	A	819	CLA	C4-C3-C5-C6
21	A	820	CLA	C4-C3-C5-C6
21	B	825	CLA	C4-C3-C5-C6
21	B	836	CLA	C4-C3-C5-C6
21	F	5005	CLA	C4-C3-C5-C6
21	A	820	CLA	C2-C3-C5-C6
21	B	836	CLA	C2-C3-C5-C6
21	F	5005	CLA	C2-C3-C5-C6
21	1	309	CLA	CBA-CGA-O2A-C1
21	8	605	CLA	CBA-CGA-O2A-C1
21	G	204	CLA	CBA-CGA-O2A-C1
21	T	610	CLA	CBA-CGA-O2A-C1
21	T	613	CLA	CBA-CGA-O2A-C1
22	9	606	CHL	CBD-CGD-O2D-CED
21	1	309	CLA	O1D-CGD-O2D-CED
21	3	409	CLA	O1D-CGD-O2D-CED
21	F	5007	CLA	O1D-CGD-O2D-CED
21	G	201	CLA	O1D-CGD-O2D-CED
21	G	205	CLA	O1D-CGD-O2D-CED
21	a	311	CLA	O1D-CGD-O2D-CED
21	T	609	CLA	O1D-CGD-O2D-CED
21	O	2003	CLA	C2A-CAA-CBA-CGA
21	7	311	CLA	C3-C5-C6-C7
21	A	809	CLA	C3-C5-C6-C7
21	A	817	CLA	C3-C5-C6-C7
21	A	819	CLA	C3-C5-C6-C7
21	A	843	CLA	C3-C5-C6-C7
21	B	812	CLA	C3-C5-C6-C7
21	B	830	CLA	C3-C5-C6-C7
21	B	834	CLA	C3-C5-C6-C7
21	B	844	CLA	C3-C5-C6-C7
21	G	201	CLA	C3-C5-C6-C7
21	K	202	CLA	C3-C5-C6-C7
21	1	303	CLA	CBA-CGA-O2A-C1
21	1	321	CLA	CBA-CGA-O2A-C1
21	3	403	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	3	407	CLA	CBA-CGA-O2A-C1
21	3	409	CLA	CBA-CGA-O2A-C1
21	8	603	CLA	CBA-CGA-O2A-C1
21	9	602	CLA	CBA-CGA-O2A-C1
21	A	804	CLA	CBA-CGA-O2A-C1
21	A	815	CLA	CBA-CGA-O2A-C1
21	A	816	CLA	CBA-CGA-O2A-C1
21	A	817	CLA	CBA-CGA-O2A-C1
21	A	820	CLA	CBA-CGA-O2A-C1
21	A	822	CLA	CBA-CGA-O2A-C1
21	A	830	CLA	CBA-CGA-O2A-C1
21	B	807	CLA	CBA-CGA-O2A-C1
21	B	835	CLA	CBA-CGA-O2A-C1
21	B	836	CLA	CBA-CGA-O2A-C1
21	B	837	CLA	CBA-CGA-O2A-C1
21	L	306	CLA	CBA-CGA-O2A-C1
21	b	304	CLA	CBA-CGA-O2A-C1
21	b	305	CLA	CBA-CGA-O2A-C1
21	b	306	CLA	CBA-CGA-O2A-C1
21	b	311	CLA	CBA-CGA-O2A-C1
21	b	313	CLA	CBA-CGA-O2A-C1
21	c	602	CLA	CBA-CGA-O2A-C1
21	c	603	CLA	CBA-CGA-O2A-C1
21	K	202	CLA	CBA-CGA-O2A-C1
21	T	609	CLA	CBA-CGA-O2A-C1
24	9	615	XAT	C13-C14-C15-C35
25	A	849	BCR	C15-C16-C17-C18
21	1	303	CLA	O1A-CGA-O2A-C1
21	3	408	CLA	O1A-CGA-O2A-C1
21	7	305	CLA	O1A-CGA-O2A-C1
21	8	612	CLA	O1A-CGA-O2A-C1
21	9	602	CLA	O1A-CGA-O2A-C1
21	A	822	CLA	O1A-CGA-O2A-C1
21	A	826	CLA	O1A-CGA-O2A-C1
21	A	842	CLA	O1A-CGA-O2A-C1
21	F	5007	CLA	O1A-CGA-O2A-C1
21	b	313	CLA	O1A-CGA-O2A-C1
21	2	607	CLA	CBA-CGA-O2A-C1
22	b	307	CHL	CBA-CGA-O2A-C1
29	1	320	PTY	O30-C30-O4-C1
21	8	622	CLA	O1A-CGA-O2A-C1
21	a	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	b	315	CLA	O1A-CGA-O2A-C1
21	8	614	CLA	O1D-CGD-O2D-CED
21	9	608	CLA	O1D-CGD-O2D-CED
21	T	612	CLA	O1D-CGD-O2D-CED
21	T	614	CLA	O1D-CGD-O2D-CED
21	3	402	CLA	C3-C5-C6-C7
21	3	409	CLA	C3-C5-C6-C7
21	A	829	CLA	C3-C5-C6-C7
21	A	830	CLA	C3-C5-C6-C7
21	B	817	CLA	C3-C5-C6-C7
21	B	835	CLA	C3-C5-C6-C7
21	B	839	CLA	C3-C5-C6-C7
21	A	817	CLA	CBD-CGD-O2D-CED
21	A	838	CLA	CBD-CGD-O2D-CED
28	F	5003	LHG	O2-C2-C3-O3
21	2	610	CLA	O1D-CGD-O2D-CED
21	3	407	CLA	O1D-CGD-O2D-CED
21	9	607	CLA	O1D-CGD-O2D-CED
21	B	818	CLA	O1D-CGD-O2D-CED
21	7	304	CLA	CBA-CGA-O2A-C1
21	A	813	CLA	CBA-CGA-O2A-C1
21	A	826	CLA	CBA-CGA-O2A-C1
21	B	838	CLA	CBA-CGA-O2A-C1
21	7	304	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	O1A-CGA-O2A-C1
21	a	304	CLA	O1A-CGA-O2A-C1
21	T	609	CLA	O1A-CGA-O2A-C1
21	B	840	CLA	O1D-CGD-O2D-CED
21	A	806	CLA	CBD-CGD-O2D-CED
21	B	826	CLA	CBD-CGD-O2D-CED
21	b	312	CLA	CBD-CGD-O2D-CED
21	3	414	CLA	CBA-CGA-O2A-C1
21	9	611	CLA	CBA-CGA-O2A-C1
21	A	817	CLA	O1A-CGA-O2A-C1
21	B	837	CLA	O1A-CGA-O2A-C1
21	B	838	CLA	O1A-CGA-O2A-C1
29	1	320	PTY	C31-C30-O4-C1
21	A	808	CLA	O1D-CGD-O2D-CED
21	A	842	CLA	O1D-CGD-O2D-CED
21	K	204	CLA	O1D-CGD-O2D-CED
22	7	307	CHL	O1D-CGD-O2D-CED
21	2	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	825	CLA	C3-C5-C6-C7
21	2	605	CLA	CBD-CGD-O2D-CED
21	2	609	CLA	CBD-CGD-O2D-CED
21	A	823	CLA	CBD-CGD-O2D-CED
21	c	603	CLA	CBD-CGD-O2D-CED
21	T	611	CLA	CBD-CGD-O2D-CED
21	7	313	CLA	O1D-CGD-O2D-CED
21	A	831	CLA	O1D-CGD-O2D-CED
21	A	856	CLA	O1D-CGD-O2D-CED
21	B	836	CLA	O1D-CGD-O2D-CED
22	8	601	CHL	O1D-CGD-O2D-CED
21	a	304	CLA	CBA-CGA-O2A-C1
21	B	844	CLA	C4-C3-C5-C6
21	T	603	CLA	C4-C3-C5-C6
22	3	401	CHL	C4-C3-C5-C6
21	9	608	CLA	C2-C3-C5-C6
21	A	856	CLA	C2-C3-C5-C6
21	B	825	CLA	C2-C3-C5-C6
22	3	401	CHL	C2-C3-C5-C6
21	3	403	CLA	O1A-CGA-O2A-C1
21	A	813	CLA	O1A-CGA-O2A-C1
21	A	820	CLA	O1A-CGA-O2A-C1
21	L	306	CLA	O1A-CGA-O2A-C1
21	b	311	CLA	O1A-CGA-O2A-C1
21	c	603	CLA	O1A-CGA-O2A-C1
21	a	308	CLA	O1D-CGD-O2D-CED
21	3	410	CLA	CBD-CGD-O2D-CED
21	A	837	CLA	CBD-CGD-O2D-CED
21	T	613	CLA	CBD-CGD-O2D-CED
22	T	601	CHL	CBD-CGD-O2D-CED
21	1	309	CLA	O1A-CGA-O2A-C1
21	B	812	CLA	O1D-CGD-O2D-CED
29	a	319	PTY	C6-C5-O14-P1
21	A	831	CLA	C2A-CAA-CBA-CGA
27	9	616	LMU	O5B-C1B-O1B-C4'
21	T	608	CLA	O1D-CGD-O2D-CED
26	F	5009	LMG	O6-C1-O1-C7
26	G	207	LMG	O6-C1-O1-C7
30	3	422	SQD	O5-C1-O6-C44
21	3	405	CLA	CBA-CGA-O2A-C1
21	A	810	CLA	CBA-CGA-O2A-C1
21	B	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	1	301	CLA	CBD-CGD-O2D-CED
21	8	603	CLA	CBD-CGD-O2D-CED
21	A	826	CLA	CBD-CGD-O2D-CED
21	A	840	CLA	CBD-CGD-O2D-CED
21	B	821	CLA	CBD-CGD-O2D-CED
21	B	825	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	CBD-CGD-O2D-CED
21	c	601	CLA	CBD-CGD-O2D-CED
21	c	614	CLA	CBD-CGD-O2D-CED
22	3	401	CHL	CBD-CGD-O2D-CED
21	9	611	CLA	O1A-CGA-O2A-C1
22	b	307	CHL	O1A-CGA-O2A-C1
22	8	607	CHL	CBA-CGA-O2A-C1
21	3	405	CLA	O1A-CGA-O2A-C1
21	A	810	CLA	O1A-CGA-O2A-C1
21	B	814	CLA	O1D-CGD-O2D-CED
21	2	607	CLA	CBD-CGD-O2D-CED
21	7	323	CLA	CBD-CGD-O2D-CED
21	B	837	CLA	CBD-CGD-O2D-CED
21	B	817	CLA	O1A-CGA-O2A-C1
21	2	604	CLA	CBA-CGA-O2A-C1
21	7	311	CLA	CBA-CGA-O2A-C1
21	8	610	CLA	CBA-CGA-O2A-C1
21	A	807	CLA	CBA-CGA-O2A-C1
21	A	811	CLA	CBA-CGA-O2A-C1
21	A	819	CLA	CBA-CGA-O2A-C1
21	B	811	CLA	CBA-CGA-O2A-C1
21	B	814	CLA	CBA-CGA-O2A-C1
21	B	822	CLA	CBA-CGA-O2A-C1
21	B	826	CLA	CBA-CGA-O2A-C1
21	F	5005	CLA	CBA-CGA-O2A-C1
21	A	810	CLA	O1D-CGD-O2D-CED
21	J	5002	CLA	O1D-CGD-O2D-CED
27	9	616	LMU	C2B-C1B-O1B-C4'
21	A	811	CLA	O1A-CGA-O2A-C1
21	A	815	CLA	C4-C3-C5-C6
21	A	856	CLA	C4-C3-C5-C6
21	1	308	CLA	C2-C3-C5-C6
21	A	819	CLA	C2-C3-C5-C6
22	7	303	CHL	CBD-CGD-O2D-CED
21	1	311	CLA	C6-C7-C8-C9
21	A	830	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	835	CLA	C14-C13-C15-C16
21	A	836	CLA	C6-C7-C8-C9
21	A	841	CLA	C6-C7-C8-C9
22	2	601	CHL	C11-C12-C13-C14
22	3	401	CHL	C11-C12-C13-C14
22	7	303	CHL	C11-C10-C8-C9
22	7	303	CHL	C11-C12-C13-C14
35	B	845	PQN	C16-C17-C18-C19
35	B	845	PQN	C21-C22-C23-C24
21	3	412	CLA	O1D-CGD-O2D-CED
21	A	835	CLA	O1D-CGD-O2D-CED
21	B	841	CLA	O1D-CGD-O2D-CED
21	B	842	CLA	O1D-CGD-O2D-CED
21	a	302	CLA	O1D-CGD-O2D-CED
21	a	304	CLA	O1D-CGD-O2D-CED
21	c	604	CLA	O1D-CGD-O2D-CED
21	c	612	CLA	O1D-CGD-O2D-CED
21	K	203	CLA	O1D-CGD-O2D-CED
26	F	5009	LMG	C2-C1-O1-C7
26	G	207	LMG	C2-C1-O1-C7
27	1	318	LMU	C2'-C1'-O1'-C1
30	3	422	SQD	C2-C1-O6-C44
21	1	310	CLA	O1D-CGD-O2D-CED
21	A	813	CLA	O1D-CGD-O2D-CED
21	A	807	CLA	O1A-CGA-O2A-C1
21	F	5005	CLA	O1A-CGA-O2A-C1
21	7	305	CLA	CBD-CGD-O2D-CED
21	9	604	CLA	O1D-CGD-O2D-CED
21	A	821	CLA	O1D-CGD-O2D-CED
23	2	616	LUT	C7-C8-C9-C19
24	3	416	XAT	C27-C28-C29-C39
24	T	616	XAT	C27-C28-C29-C39
25	A	846	BCR	C11-C12-C13-C35
25	A	847	BCR	C7-C8-C9-C34
25	A	847	BCR	C37-C22-C23-C24
25	B	847	BCR	C7-C8-C9-C34
25	B	847	BCR	C37-C22-C23-C24
25	J	5004	BCR	C37-C22-C23-C24
25	a	317	BCR	C37-C22-C23-C24
25	I	202	BCR	C37-C22-C23-C24
25	K	205	BCR	C7-C8-C9-C34
29	a	319	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
23	2	616	LUT	C7-C8-C9-C10
24	3	416	XAT	C27-C28-C29-C30
24	T	616	XAT	C27-C28-C29-C30
25	A	846	BCR	C11-C12-C13-C14
25	A	847	BCR	C21-C22-C23-C24
25	B	847	BCR	C7-C8-C9-C10
25	B	847	BCR	C21-C22-C23-C24
25	B	852	BCR	C7-C8-C9-C10
25	J	5004	BCR	C21-C22-C23-C24
25	L	302	BCR	C17-C18-C19-C20
25	a	317	BCR	C21-C22-C23-C24
21	7	311	CLA	C2A-CAA-CBA-CGA
21	8	610	CLA	C2A-CAA-CBA-CGA
21	A	837	CLA	C2A-CAA-CBA-CGA
21	B	822	CLA	C2A-CAA-CBA-CGA
21	B	826	CLA	C2A-CAA-CBA-CGA
21	B	831	CLA	C2A-CAA-CBA-CGA
21	B	834	CLA	C2A-CAA-CBA-CGA
21	L	303	CLA	C3-C5-C6-C7
21	a	308	CLA	C2A-CAA-CBA-CGA
21	B	811	CLA	O1A-CGA-O2A-C1
21	B	814	CLA	C3-C5-C6-C7
21	A	826	CLA	C10-C11-C12-C13
21	c	609	CLA	CBA-CGA-O2A-C1
32	B	850	DGD	O2G-C2G-C3G-O3G
21	7	306	CLA	CBA-CGA-O2A-C1
21	B	806	CLA	CBA-CGA-O2A-C1
21	A	811	CLA	C8-C10-C11-C12
21	8	611	CLA	C2-C1-O2A-CGA
21	B	835	CLA	C2-C1-O2A-CGA
21	2	604	CLA	O1A-CGA-O2A-C1
21	H	203	CLA	O1D-CGD-O2D-CED
21	A	825	CLA	CBD-CGD-O2D-CED
21	A	810	CLA	C5-C6-C7-C8
21	A	829	CLA	C10-C11-C12-C13
21	A	835	CLA	C8-C10-C11-C12
21	B	818	CLA	C15-C16-C17-C18
21	B	825	CLA	C10-C11-C12-C13
21	B	843	CLA	C5-C6-C7-C8
21	7	314	CLA	C3-C5-C6-C7
21	8	610	CLA	C3-C5-C6-C7
21	B	804	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	a	310	CLA	O1D-CGD-O2D-CED
22	T	602	CHL	O1D-CGD-O2D-CED
21	7	311	CLA	O1A-CGA-O2A-C1
21	8	611	CLA	C5-C6-C7-C8
21	1	306	CLA	CBD-CGD-O2D-CED
21	7	312	CLA	CBD-CGD-O2D-CED
21	b	304	CLA	CBD-CGD-O2D-CED
22	8	606	CHL	CBD-CGD-O2D-CED
22	c	605	CHL	CBD-CGD-O2D-CED
21	A	823	CLA	C12-C13-C15-C16
21	A	829	CLA	C11-C10-C8-C7
22	2	601	CHL	C11-C10-C8-C7
34	A	803	CL0	C11-C12-C13-C15
35	B	845	PQN	C22-C23-C25-C26
21	A	825	CLA	CBA-CGA-O2A-C1
21	A	817	CLA	C4-C3-C5-C6
21	B	831	CLA	C4-C3-C5-C6
21	a	303	CLA	C4-C3-C5-C6
21	A	841	CLA	C13-C15-C16-C17
37	A	857	4RF	C22-C24-C25-C26
23	a	315	LUT	C13-C14-C15-C35
21	2	602	CLA	C3-C5-C6-C7
21	A	811	CLA	C10-C11-C12-C13
21	A	819	CLA	C10-C11-C12-C13
21	B	807	CLA	C10-C11-C12-C13
21	B	827	CLA	C13-C15-C16-C17
21	F	5005	CLA	C15-C16-C17-C18
22	2	601	CHL	C10-C11-C12-C13
22	2	601	CHL	C13-C15-C16-C17
29	B	803	PTY	C8-C11-C12-C13
21	8	610	CLA	O1A-CGA-O2A-C1
21	A	819	CLA	O1A-CGA-O2A-C1
21	B	806	CLA	O1A-CGA-O2A-C1
21	K	202	CLA	CBD-CGD-O2D-CED
21	8	622	CLA	O1D-CGD-O2D-CED
21	A	811	CLA	O1D-CGD-O2D-CED
21	T	604	CLA	O1D-CGD-O2D-CED
21	3	409	CLA	C5-C6-C7-C8
21	A	815	CLA	C15-C16-C17-C18
21	A	827	CLA	C8-C10-C11-C12
21	A	839	CLA	C13-C15-C16-C17
21	B	814	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	B	819	CLA	C10-C11-C12-C13
21	B	828	CLA	C8-C10-C11-C12
32	7	301	DGD	O6D-C5D-C6D-O5D
21	2	610	CLA	C2A-CAA-CBA-CGA
21	3	405	CLA	C2A-CAA-CBA-CGA
21	A	815	CLA	C2A-CAA-CBA-CGA
21	A	838	CLA	C2A-CAA-CBA-CGA
21	B	818	CLA	C2A-CAA-CBA-CGA
21	B	830	CLA	C2A-CAA-CBA-CGA
21	B	838	CLA	C2A-CAA-CBA-CGA
21	B	844	CLA	C2A-CAA-CBA-CGA
21	J	5002	CLA	C2A-CAA-CBA-CGA
21	L	306	CLA	C2A-CAA-CBA-CGA
21	c	609	CLA	C2A-CAA-CBA-CGA
22	1	305	CHL	C2A-CAA-CBA-CGA
22	2	606	CHL	C2A-CAA-CBA-CGA
22	7	307	CHL	C2A-CAA-CBA-CGA
22	T	602	CHL	C2A-CAA-CBA-CGA
21	A	807	CLA	C5-C6-C7-C8
21	A	821	CLA	C8-C10-C11-C12
21	A	822	CLA	C5-C6-C7-C8
21	A	822	CLA	C8-C10-C11-C12
21	A	829	CLA	C8-C10-C11-C12
21	A	834	CLA	C5-C6-C7-C8
21	A	835	CLA	C5-C6-C7-C8
21	B	817	CLA	C5-C6-C7-C8
22	2	601	CHL	C8-C10-C11-C12
22	2	601	CHL	C15-C16-C17-C18
21	1	321	CLA	O1D-CGD-O2D-CED
21	A	809	CLA	O1D-CGD-O2D-CED
21	B	814	CLA	O1A-CGA-O2A-C1
21	B	822	CLA	O1A-CGA-O2A-C1
21	B	826	CLA	O1A-CGA-O2A-C1
32	8	602	DGD	O6D-C1D-O3G-C3G
21	3	411	CLA	O1D-CGD-O2D-CED
21	9	610	CLA	O1D-CGD-O2D-CED
22	2	601	CHL	O1D-CGD-O2D-CED
21	3	402	CLA	C10-C11-C12-C13
21	A	814	CLA	C8-C10-C11-C12
21	A	817	CLA	C13-C15-C16-C17
21	A	823	CLA	C8-C10-C11-C12
21	A	843	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	810	CLA	C8-C10-C11-C12
21	B	831	CLA	C8-C10-C11-C12
21	B	831	CLA	C15-C16-C17-C18
21	a	302	CLA	C15-C16-C17-C18
21	a	309	CLA	C10-C11-C12-C13
32	A	802	DGD	O6D-C5D-C6D-O5D
21	2	613	CLA	O1D-CGD-O2D-CED
32	7	301	DGD	C4D-C5D-C6D-O5D
29	c	619	PTY	C8-C11-C12-C13
21	2	613	CLA	C5-C6-C7-C8
21	3	407	CLA	C5-C6-C7-C8
21	7	316	CLA	C15-C16-C17-C18
21	A	821	CLA	C15-C16-C17-C18
21	A	825	CLA	C5-C6-C7-C8
21	A	819	CLA	O1D-CGD-O2D-CED
21	B	843	CLA	O1D-CGD-O2D-CED
22	9	606	CHL	O1D-CGD-O2D-CED
21	7	305	CLA	C5-C6-C7-C8
21	A	807	CLA	C8-C10-C11-C12
21	F	5005	CLA	C10-C11-C12-C13
21	L	304	CLA	C8-C10-C11-C12
21	A	838	CLA	O1D-CGD-O2D-CED
21	B	831	CLA	O1D-CGD-O2D-CED
21	3	414	CLA	O1A-CGA-O2A-C1
32	A	802	DGD	C4D-C5D-C6D-O5D
21	2	602	CLA	C5-C6-C7-C8
21	A	823	CLA	C15-C16-C17-C18
21	B	804	CLA	C8-C10-C11-C12
21	B	827	CLA	C15-C16-C17-C18
21	B	832	CLA	C10-C11-C12-C13
21	B	837	CLA	C5-C6-C7-C8
21	2	602	CLA	CBA-CGA-O2A-C1
21	A	814	CLA	CBA-CGA-O2A-C1
21	B	816	CLA	CBA-CGA-O2A-C1
21	T	604	CLA	CBA-CGA-O2A-C1
21	8	610	CLA	CBD-CGD-O2D-CED
21	7	306	CLA	O1A-CGA-O2A-C1
21	c	611	CLA	CBA-CGA-O2A-C1
21	T	606	CLA	CBA-CGA-O2A-C1
21	B	833	CLA	C15-C16-C17-C18
21	9	603	CLA	C3-C5-C6-C7
21	B	821	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	824	CLA	C2A-CAA-CBA-CGA
21	B	842	CLA	C2A-CAA-CBA-CGA
21	F	5006	CLA	C2A-CAA-CBA-CGA
21	H	203	CLA	C2A-CAA-CBA-CGA
21	T	612	CLA	C2A-CAA-CBA-CGA
21	3	412	CLA	CBA-CGA-O2A-C1
21	B	844	CLA	CBA-CGA-O2A-C1
21	c	604	CLA	CBA-CGA-O2A-C1
21	2	602	CLA	C8-C10-C11-C12
21	2	603	CLA	C5-C6-C7-C8
21	A	811	CLA	C15-C16-C17-C18
21	A	816	CLA	C8-C10-C11-C12
21	A	817	CLA	C8-C10-C11-C12
21	A	820	CLA	C8-C10-C11-C12
21	A	823	CLA	C10-C11-C12-C13
21	A	843	CLA	C13-C15-C16-C17
21	B	812	CLA	C5-C6-C7-C8
21	B	817	CLA	C8-C10-C11-C12
21	B	823	CLA	C8-C10-C11-C12
21	B	844	CLA	C13-C15-C16-C17
21	A	817	CLA	O1D-CGD-O2D-CED
21	A	806	CLA	O1D-CGD-O2D-CED
21	b	312	CLA	O1D-CGD-O2D-CED
21	B	826	CLA	C5-C6-C7-C8
21	B	832	CLA	C15-C16-C17-C18
21	B	833	CLA	C13-C15-C16-C17
21	G	201	CLA	C8-C10-C11-C12
21	b	304	CLA	C5-C6-C7-C8
21	T	612	CLA	C13-C15-C16-C17
21	9	607	CLA	C5-C6-C7-C8
21	A	840	CLA	C10-C11-C12-C13
21	A	843	CLA	C8-C10-C11-C12
21	B	810	CLA	C10-C11-C12-C13
21	G	201	CLA	C10-C11-C12-C13
21	7	314	CLA	CBA-CGA-O2A-C1
21	7	315	CLA	CBA-CGA-O2A-C1
21	B	826	CLA	O1D-CGD-O2D-CED
21	A	815	CLA	C10-C11-C12-C13
21	T	611	CLA	O1D-CGD-O2D-CED
21	B	808	CLA	O2A-C1-C2-C3
32	8	602	DGD	C2D-C1D-O3G-C3G
21	1	302	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	7	316	CLA	CBA-CGA-O2A-C1
21	A	806	CLA	CBA-CGA-O2A-C1
21	A	818	CLA	C6-C7-C8-C10
21	B	837	CLA	C11-C12-C13-C14
21	B	843	CLA	C16-C17-C18-C19
28	a	301	LHG	C24-C23-O8-C6
21	A	818	CLA	C5-C6-C7-C8
23	1	314	LUT	C27-C28-C29-C39
24	a	316	XAT	C7-C8-C9-C19
25	B	852	BCR	C36-C18-C19-C20
29	I	201	PTY	C13-C14-C15-C16
21	3	412	CLA	O1A-CGA-O2A-C1
21	A	825	CLA	O1A-CGA-O2A-C1
21	c	604	CLA	O1A-CGA-O2A-C1
21	T	604	CLA	O1A-CGA-O2A-C1
21	1	313	CLA	C2A-CAA-CBA-CGA
21	2	602	CLA	C2A-CAA-CBA-CGA
21	3	403	CLA	C2A-CAA-CBA-CGA
21	3	406	CLA	C2A-CAA-CBA-CGA
21	8	603	CLA	C2A-CAA-CBA-CGA
21	9	602	CLA	C2A-CAA-CBA-CGA
21	A	820	CLA	C2A-CAA-CBA-CGA
21	A	822	CLA	C2A-CAA-CBA-CGA
21	A	841	CLA	C2A-CAA-CBA-CGA
21	a	314	CLA	C2A-CAA-CBA-CGA
21	c	613	CLA	C2A-CAA-CBA-CGA
21	T	607	CLA	C2A-CAA-CBA-CGA
21	A	813	CLA	C15-C16-C17-C18
21	A	830	CLA	C13-C15-C16-C17
22	b	302	CHL	C5-C6-C7-C8
21	A	823	CLA	O1D-CGD-O2D-CED
21	c	603	CLA	O1D-CGD-O2D-CED
21	8	610	CLA	C11-C12-C13-C14
21	9	608	CLA	C11-C12-C13-C15
21	A	816	CLA	C16-C17-C18-C19
21	A	817	CLA	C16-C17-C18-C19
21	A	817	CLA	C16-C17-C18-C20
21	B	827	CLA	C16-C17-C18-C20
21	B	839	CLA	C6-C7-C8-C10
21	B	842	CLA	C16-C17-C18-C20
21	G	201	CLA	C16-C17-C18-C20
21	b	311	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	T	609	CLA	C6-C7-C8-C9
21	2	605	CLA	O1D-CGD-O2D-CED
21	2	602	CLA	O1A-CGA-O2A-C1
23	1	314	LUT	C12-C13-C14-C15
23	a	315	LUT	C12-C13-C14-C15
21	A	815	CLA	C2-C3-C5-C6
21	B	831	CLA	C2-C3-C5-C6
21	B	844	CLA	C2-C3-C5-C6
21	T	603	CLA	C2-C3-C5-C6
21	2	609	CLA	O1D-CGD-O2D-CED
21	3	410	CLA	O1D-CGD-O2D-CED
21	A	837	CLA	O1D-CGD-O2D-CED
21	T	613	CLA	O1D-CGD-O2D-CED
22	T	601	CHL	O1D-CGD-O2D-CED
21	8	604	CLA	CBA-CGA-O2A-C1
21	A	831	CLA	C15-C16-C17-C18
21	7	316	CLA	C2-C1-O2A-CGA
21	A	804	CLA	C2-C1-O2A-CGA
21	B	833	CLA	C2-C1-O2A-CGA
21	1	311	CLA	C11-C12-C13-C15
21	9	607	CLA	C16-C17-C18-C19
21	9	608	CLA	C11-C12-C13-C14
21	A	812	CLA	C6-C7-C8-C9
21	A	815	CLA	C16-C17-C18-C19
21	B	827	CLA	C16-C17-C18-C19
21	B	837	CLA	C11-C12-C13-C15
21	B	843	CLA	C16-C17-C18-C20
21	H	203	CLA	C11-C12-C13-C14
21	b	305	CLA	C11-C10-C8-C7
21	T	609	CLA	C6-C7-C8-C10
22	T	602	CHL	C6-C7-C8-C10
34	A	803	CL0	C16-C17-C18-C19
21	A	832	CLA	C13-C15-C16-C17
27	1	318	LMU	C3-C4-C5-C6
28	1	323	LHG	C7-C8-C9-C10
21	A	856	CLA	C10-C11-C12-C13
21	A	814	CLA	O1A-CGA-O2A-C1
21	B	830	CLA	CBA-CGA-O2A-C1
33	8	621	LMK	O9-C10-C11-C12
37	A	857	4RF	C10-C11-C12-C13
37	A	857	4RF	C44-C45-C46-C47
21	L	304	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	8	614	CLA	CBA-CGA-O2A-C1
21	A	815	CLA	C16-C17-C18-C20
21	A	816	CLA	C16-C17-C18-C20
21	G	201	CLA	C16-C17-C18-C19
21	b	305	CLA	C11-C10-C8-C9
21	b	311	CLA	C11-C12-C13-C15
34	A	803	CL0	C16-C17-C18-C20
21	A	826	CLA	O1D-CGD-O2D-CED
21	B	828	CLA	O1D-CGD-O2D-CED
22	8	607	CHL	O1A-CGA-O2A-C1
21	B	816	CLA	O1A-CGA-O2A-C1
21	A	804	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	C2A-CAA-CBA-CGA
22	3	401	CHL	C2A-CAA-CBA-CGA
21	1	308	CLA	C10-C11-C12-C13
21	B	825	CLA	O1D-CGD-O2D-CED
21	A	830	CLA	C11-C10-C8-C7
21	A	841	CLA	C6-C7-C8-C10
29	H	201	PTY	C8-C11-C12-C13
21	A	831	CLA	C5-C6-C7-C8
29	H	201	PTY	C20-C21-C22-C23
21	8	604	CLA	O1A-CGA-O2A-C1
21	B	809	CLA	C3-C5-C6-C7
21	F	5005	CLA	C3-C5-C6-C7
27	1	318	LMU	C3'-C4'-O1B-C1B
21	1	310	CLA	C3A-C2A-CAA-CBA
21	1	313	CLA	C3A-C2A-CAA-CBA
21	2	604	CLA	C3A-C2A-CAA-CBA
21	2	607	CLA	C3A-C2A-CAA-CBA
21	2	610	CLA	C3A-C2A-CAA-CBA
21	3	404	CLA	C3A-C2A-CAA-CBA
21	8	603	CLA	C3A-C2A-CAA-CBA
21	8	604	CLA	C3A-C2A-CAA-CBA
21	8	610	CLA	C3A-C2A-CAA-CBA
21	9	601	CLA	C3A-C2A-CAA-CBA
21	9	610	CLA	C3A-C2A-CAA-CBA
21	9	612	CLA	C3A-C2A-CAA-CBA
21	A	807	CLA	C3A-C2A-CAA-CBA
21	A	808	CLA	C3A-C2A-CAA-CBA
21	A	813	CLA	C3A-C2A-CAA-CBA
21	A	825	CLA	C3A-C2A-CAA-CBA
21	A	829	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	838	CLA	C3A-C2A-CAA-CBA
21	B	804	CLA	C3A-C2A-CAA-CBA
21	B	806	CLA	C3A-C2A-CAA-CBA
21	B	814	CLA	C3A-C2A-CAA-CBA
21	B	829	CLA	C3A-C2A-CAA-CBA
21	B	839	CLA	C3A-C2A-CAA-CBA
21	G	201	CLA	C3A-C2A-CAA-CBA
21	G	204	CLA	C3A-C2A-CAA-CBA
21	H	203	CLA	C3A-C2A-CAA-CBA
21	O	2003	CLA	C3A-C2A-CAA-CBA
21	a	314	CLA	C3A-C2A-CAA-CBA
21	b	305	CLA	C3A-C2A-CAA-CBA
21	c	614	CLA	C3A-C2A-CAA-CBA
21	T	603	CLA	C3A-C2A-CAA-CBA
21	T	605	CLA	C3A-C2A-CAA-CBA
22	9	606	CHL	C3A-C2A-CAA-CBA
21	A	840	CLA	O1D-CGD-O2D-CED
21	B	821	CLA	O1D-CGD-O2D-CED
21	c	614	CLA	O1D-CGD-O2D-CED
22	3	401	CHL	O1D-CGD-O2D-CED
21	A	817	CLA	C2-C3-C5-C6
21	a	303	CLA	C2-C3-C5-C6
21	1	308	CLA	C5-C6-C7-C8
21	8	610	CLA	C11-C12-C13-C15
21	9	607	CLA	C16-C17-C18-C20
21	A	812	CLA	C6-C7-C8-C10
21	A	825	CLA	C11-C12-C13-C15
21	B	840	CLA	C11-C12-C13-C15
21	B	842	CLA	C16-C17-C18-C19
21	7	314	CLA	O1A-CGA-O2A-C1
21	7	315	CLA	O1A-CGA-O2A-C1
21	B	844	CLA	O1A-CGA-O2A-C1
21	1	301	CLA	CBA-CGA-O2A-C1
21	A	818	CLA	CBA-CGA-O2A-C1
21	B	834	CLA	CBA-CGA-O2A-C1
21	B	842	CLA	CBA-CGA-O2A-C1
21	a	303	CLA	CBA-CGA-O2A-C1
22	b	302	CHL	CBA-CGA-O2A-C1
29	7	302	PTY	O4-C1-C6-C5
26	3	421	LMG	C11-C12-C13-C14
21	A	807	CLA	C3-C5-C6-C7
21	7	311	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	B	829	CLA	C13-C15-C16-C17
28	8	620	LHG	C16-C17-C18-C19
21	7	316	CLA	O1A-CGA-O2A-C1
28	8	620	LHG	C12-C13-C14-C15
21	1	301	CLA	O1D-CGD-O2D-CED
21	8	603	CLA	O1D-CGD-O2D-CED
21	1	311	CLA	C11-C12-C13-C14
21	1	302	CLA	O1A-CGA-O2A-C1
21	A	806	CLA	O1A-CGA-O2A-C1
23	1	314	LUT	C1-C6-C7-C8
23	1	314	LUT	C5-C6-C7-C8
23	2	614	LUT	C1-C6-C7-C8
23	2	616	LUT	C1-C6-C7-C8
23	2	616	LUT	C5-C6-C7-C8
23	O	2005	LUT	C1-C6-C7-C8
25	3	417	BCR	C1-C6-C7-C8
25	3	417	BCR	C5-C6-C7-C8
25	3	417	BCR	C23-C24-C25-C26
25	3	417	BCR	C23-C24-C25-C30
25	3	418	BCR	C23-C24-C25-C30
25	7	319	BCR	C23-C24-C25-C30
25	8	618	BCR	C1-C6-C7-C8
25	8	618	BCR	C5-C6-C7-C8
25	8	618	BCR	C23-C24-C25-C26
25	8	618	BCR	C23-C24-C25-C30
25	A	849	BCR	C23-C24-C25-C26
25	A	849	BCR	C23-C24-C25-C30
25	B	848	BCR	C23-C24-C25-C26
25	B	848	BCR	C23-C24-C25-C30
25	J	5003	BCR	C1-C6-C7-C8
25	J	5003	BCR	C5-C6-C7-C8
25	J	5003	BCR	C23-C24-C25-C26
25	J	5003	BCR	C23-C24-C25-C30
25	L	302	BCR	C1-C6-C7-C8
25	L	302	BCR	C5-C6-C7-C8
25	O	2004	BCR	C23-C24-C25-C30
25	b	319	BCR	C23-C24-C25-C26
25	b	319	BCR	C23-C24-C25-C30
25	c	617	BCR	C1-C6-C7-C8
25	c	617	BCR	C5-C6-C7-C8
25	I	203	BCR	C1-C6-C7-C8
25	I	203	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	T	617	BCR	C1-C6-C7-C8
25	T	617	BCR	C5-C6-C7-C8
21	A	830	CLA	CBD-CGD-O2D-CED
21	B	841	CLA	CBA-CGA-O2A-C1
21	c	613	CLA	CBA-CGA-O2A-C1
21	A	813	CLA	C13-C15-C16-C17
26	3	421	LMG	C18-C19-C20-C21
28	7	321	LHG	C9-C10-C11-C12
27	1	318	LMU	C5'-C4'-O1B-C1B
29	I	201	PTY	C32-C33-C34-C35
21	2	613	CLA	C2A-CAA-CBA-CGA
21	3	408	CLA	C2A-CAA-CBA-CGA
21	3	411	CLA	C2A-CAA-CBA-CGA
21	A	843	CLA	C2A-CAA-CBA-CGA
29	H	201	PTY	C30-C31-C32-C33
28	F	5003	LHG	C17-C18-C19-C20
29	I	201	PTY	C35-C36-C37-C38
21	B	830	CLA	O1A-CGA-O2A-C1
21	a	303	CLA	O1A-CGA-O2A-C1
21	c	601	CLA	O1D-CGD-O2D-CED
21	B	823	CLA	CBA-CGA-O2A-C1
21	B	834	CLA	O1A-CGA-O2A-C1
21	A	835	CLA	C11-C10-C8-C9
21	B	837	CLA	O1D-CGD-O2D-CED
21	B	831	CLA	C5-C6-C7-C8
21	A	818	CLA	C6-C7-C8-C9
21	H	203	CLA	C11-C12-C13-C15
21	A	826	CLA	C5-C6-C7-C8
21	A	856	CLA	C5-C6-C7-C8
21	c	609	CLA	O1A-CGA-O2A-C1
29	H	201	PTY	C16-C17-C18-C19
21	B	842	CLA	O1A-CGA-O2A-C1
21	A	830	CLA	C8-C10-C11-C12
37	A	857	4RF	C04-C05-C06-C07
21	a	309	CLA	C2A-CAA-CBA-CGA
21	B	824	CLA	C6-C7-C8-C9
21	B	824	CLA	C6-C7-C8-C10
21	B	839	CLA	C6-C7-C8-C9
21	B	840	CLA	C11-C12-C13-C14
21	B	835	CLA	C4-C3-C5-C6
21	b	304	CLA	C4-C3-C5-C6
21	2	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	a	301	LHG	O10-C23-O8-C6
21	1	301	CLA	O1A-CGA-O2A-C1
22	b	302	CHL	O1A-CGA-O2A-C1
21	B	810	CLA	C3-C5-C6-C7
27	A	855	LMU	O5B-C5B-C6B-O6B
21	2	613	CLA	C15-C16-C17-C18
21	A	839	CLA	C15-C16-C17-C18
21	A	841	CLA	C5-C6-C7-C8
21	B	832	CLA	C5-C6-C7-C8
22	2	601	CHL	C5-C6-C7-C8
21	A	825	CLA	C11-C12-C13-C14
22	T	602	CHL	C6-C7-C8-C9
21	c	613	CLA	O1A-CGA-O2A-C1
27	A	854	LMU	O5B-C5B-C6B-O6B
32	A	802	DGD	O6E-C5E-C6E-O5E
21	8	611	CLA	C3-C5-C6-C7
28	7	321	LHG	O7-C5-C6-O8
29	7	302	PTY	O4-C1-C6-O7
32	A	802	DGD	CAB-CBB-CCB-CDB
21	7	323	CLA	O1D-CGD-O2D-CED
21	7	313	CLA	CBA-CGA-O2A-C1
21	A	823	CLA	CBA-CGA-O2A-C1
21	A	818	CLA	O1A-CGA-O2A-C1
21	A	820	CLA	C10-C11-C12-C13
26	A	801	LMG	O6-C5-C6-O5
21	9	607	CLA	C2-C1-O2A-CGA
21	B	813	CLA	C2-C1-O2A-CGA
21	B	844	CLA	C2-C1-O2A-CGA
28	F	5003	LHG	C1-C2-C3-O3
21	7	314	CLA	C2A-CAA-CBA-CGA
21	8	613	CLA	C2A-CAA-CBA-CGA
21	A	808	CLA	C2A-CAA-CBA-CGA
21	a	312	CLA	C2A-CAA-CBA-CGA
21	b	314	CLA	C2A-CAA-CBA-CGA
21	K	204	CLA	C2A-CAA-CBA-CGA
21	T	606	CLA	CBD-CGD-O2D-CED
21	A	829	CLA	CBA-CGA-O2A-C1
22	T	602	CHL	CBA-CGA-O2A-C1
26	3	421	LMG	O6-C5-C6-O5
22	7	303	CHL	O1D-CGD-O2D-CED
21	B	806	CLA	C10-C11-C12-C13
28	1	322	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	F	5001	LHG	C7-C8-C9-C10
27	A	855	LMU	O5'-C5'-C6'-O6'
21	B	841	CLA	O1A-CGA-O2A-C1
21	1	303	CLA	C1A-C2A-CAA-CBA
21	1	309	CLA	C1A-C2A-CAA-CBA
21	1	311	CLA	C1A-C2A-CAA-CBA
21	1	313	CLA	C1A-C2A-CAA-CBA
21	2	607	CLA	C1A-C2A-CAA-CBA
21	2	610	CLA	C1A-C2A-CAA-CBA
21	3	403	CLA	C1A-C2A-CAA-CBA
21	3	404	CLA	C1A-C2A-CAA-CBA
21	3	406	CLA	C1A-C2A-CAA-CBA
21	3	407	CLA	C1A-C2A-CAA-CBA
21	3	408	CLA	C1A-C2A-CAA-CBA
21	3	409	CLA	C1A-C2A-CAA-CBA
21	3	414	CLA	C1A-C2A-CAA-CBA
21	7	311	CLA	C1A-C2A-CAA-CBA
21	8	604	CLA	C1A-C2A-CAA-CBA
21	8	609	CLA	C1A-C2A-CAA-CBA
21	8	611	CLA	C1A-C2A-CAA-CBA
21	8	614	CLA	C1A-C2A-CAA-CBA
21	9	604	CLA	C1A-C2A-CAA-CBA
21	9	609	CLA	C1A-C2A-CAA-CBA
21	9	610	CLA	C1A-C2A-CAA-CBA
21	A	806	CLA	C1A-C2A-CAA-CBA
21	A	807	CLA	C1A-C2A-CAA-CBA
21	A	808	CLA	C1A-C2A-CAA-CBA
21	A	810	CLA	C1A-C2A-CAA-CBA
21	A	829	CLA	C1A-C2A-CAA-CBA
21	A	832	CLA	C1A-C2A-CAA-CBA
21	A	835	CLA	C1A-C2A-CAA-CBA
21	A	836	CLA	C1A-C2A-CAA-CBA
21	A	838	CLA	C1A-C2A-CAA-CBA
21	B	804	CLA	C1A-C2A-CAA-CBA
21	B	808	CLA	C1A-C2A-CAA-CBA
21	B	814	CLA	C1A-C2A-CAA-CBA
21	B	816	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	C1A-C2A-CAA-CBA
21	B	825	CLA	C1A-C2A-CAA-CBA
21	B	832	CLA	C1A-C2A-CAA-CBA
21	B	835	CLA	C1A-C2A-CAA-CBA
21	B	836	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	839	CLA	C1A-C2A-CAA-CBA
21	B	843	CLA	C1A-C2A-CAA-CBA
21	G	204	CLA	C1A-C2A-CAA-CBA
21	H	203	CLA	C1A-C2A-CAA-CBA
21	L	304	CLA	C1A-C2A-CAA-CBA
21	O	2003	CLA	C1A-C2A-CAA-CBA
21	a	309	CLA	C1A-C2A-CAA-CBA
21	a	313	CLA	C1A-C2A-CAA-CBA
21	a	314	CLA	C1A-C2A-CAA-CBA
21	b	304	CLA	C1A-C2A-CAA-CBA
21	b	305	CLA	C1A-C2A-CAA-CBA
21	b	306	CLA	C1A-C2A-CAA-CBA
21	b	310	CLA	C1A-C2A-CAA-CBA
21	b	311	CLA	C1A-C2A-CAA-CBA
21	b	315	CLA	C1A-C2A-CAA-CBA
21	c	601	CLA	C1A-C2A-CAA-CBA
21	c	609	CLA	C1A-C2A-CAA-CBA
21	c	610	CLA	C1A-C2A-CAA-CBA
21	c	614	CLA	C1A-C2A-CAA-CBA
21	T	603	CLA	C1A-C2A-CAA-CBA
21	T	605	CLA	C1A-C2A-CAA-CBA
21	T	610	CLA	C1A-C2A-CAA-CBA
21	T	612	CLA	C1A-C2A-CAA-CBA
22	2	601	CHL	C1A-C2A-CAA-CBA
22	2	606	CHL	C1A-C2A-CAA-CBA
22	7	308	CHL	C1A-C2A-CAA-CBA
22	8	601	CHL	C1A-C2A-CAA-CBA
22	8	608	CHL	C1A-C2A-CAA-CBA
22	b	302	CHL	C1A-C2A-CAA-CBA
22	b	309	CHL	C1A-C2A-CAA-CBA
21	B	821	CLA	C10-C11-C12-C13
29	1	320	PTY	O14-C5-C6-C1
29	B	851	PTY	O14-C5-C6-C1
29	H	201	PTY	O14-C5-C6-C1
32	8	602	DGD	O6E-C5E-C6E-O5E
21	A	816	CLA	C3-C5-C6-C7
21	2	611	CLA	C6-C7-C8-C10
21	3	408	CLA	C6-C7-C8-C10
21	7	316	CLA	C6-C7-C8-C10
21	A	805	CLA	C11-C10-C8-C7
21	A	808	CLA	C12-C13-C15-C16
21	A	814	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	816	CLA	C6-C7-C8-C10
21	A	829	CLA	C6-C7-C8-C10
21	A	831	CLA	C12-C13-C15-C16
21	A	843	CLA	C11-C10-C8-C7
21	B	806	CLA	C6-C7-C8-C10
21	B	812	CLA	C11-C12-C13-C15
21	B	816	CLA	C6-C7-C8-C10
21	B	819	CLA	C6-C7-C8-C10
21	B	820	CLA	C11-C10-C8-C7
21	B	822	CLA	C6-C7-C8-C10
21	B	831	CLA	C11-C10-C8-C7
21	F	5005	CLA	C12-C13-C15-C16
21	T	612	CLA	C6-C7-C8-C10
22	2	601	CHL	C11-C12-C13-C15
22	3	401	CHL	C11-C12-C13-C15
35	B	845	PQN	C17-C18-C20-C21
21	B	807	CLA	C16-C17-C18-C20
21	A	805	CLA	C10-C11-C12-C13
21	3	413	CLA	C3A-C2A-CAA-CBA
21	1	302	CLA	C10-C11-C12-C13
21	2	613	CLA	C8-C10-C11-C12
21	A	829	CLA	C2-C3-C5-C6
21	B	816	CLA	C2-C3-C5-C6
21	B	816	CLA	C13-C15-C16-C17
21	a	309	CLA	C5-C6-C7-C8
34	A	803	CL0	C10-C11-C12-C13
22	8	601	CHL	C1-C2-C3-C5
21	7	305	CLA	C2A-CAA-CBA-CGA
21	8	615	CLA	C2A-CAA-CBA-CGA
21	B	820	CLA	C2A-CAA-CBA-CGA
21	H	204	CLA	C2A-CAA-CBA-CGA
21	c	612	CLA	C2A-CAA-CBA-CGA
21	1	301	CLA	C6-C7-C8-C9
21	1	302	CLA	C11-C10-C8-C9
21	3	408	CLA	C6-C7-C8-C9
21	7	314	CLA	C6-C7-C8-C9
21	9	607	CLA	C6-C7-C8-C9
21	A	804	CLA	C6-C7-C8-C9
21	A	808	CLA	C14-C13-C15-C16
21	A	816	CLA	C6-C7-C8-C9
21	A	817	CLA	C11-C12-C13-C14
21	A	821	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	A	829	CLA	C6-C7-C8-C9
21	A	829	CLA	C11-C10-C8-C9
21	B	804	CLA	C11-C10-C8-C9
21	B	812	CLA	C11-C12-C13-C14
21	F	5005	CLA	C11-C10-C8-C9
21	a	309	CLA	C6-C7-C8-C9
21	b	311	CLA	C6-C7-C8-C9
21	T	612	CLA	C6-C7-C8-C9
30	2	618	SQD	C9-C10-C11-C12
21	A	827	CLA	C5-C6-C7-C8
21	B	823	CLA	O1A-CGA-O2A-C1
21	c	611	CLA	O1A-CGA-O2A-C1
21	7	305	CLA	O1D-CGD-O2D-CED
21	A	831	CLA	C8-C10-C11-C12
21	B	835	CLA	C13-C15-C16-C17
26	A	801	LMG	C7-C8-C9-O8
28	1	322	LHG	C4-C5-C6-O8
28	3	420	LHG	C4-C5-C6-O8
28	7	324	LHG	C4-C5-C6-O8
28	A	853	LHG	C4-C5-C6-O8
28	F	5003	LHG	C4-C5-C6-O8
28	b	301	LHG	C4-C5-C6-O8
32	B	850	DGD	C1G-C2G-C3G-O3G
21	A	825	CLA	O1D-CGD-O2D-CED
21	A	832	CLA	CBD-CGD-O2D-CED
32	A	802	DGD	C3A-C4A-C5A-C6A
21	A	828	CLA	CBA-CGA-O2A-C1
21	A	835	CLA	C13-C15-C16-C17
21	T	606	CLA	O1A-CGA-O2A-C1
31	2	619	3PH	C3F-C3G-C3H-C3I
21	7	312	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	C4B-C5B-C6B-C7B
21	B	816	CLA	C4-C3-C5-C6
21	B	835	CLA	C2-C3-C5-C6
21	3	402	CLA	C5-C6-C7-C8
28	1	319	LHG	C2-C3-O3-P
21	1	306	CLA	O1D-CGD-O2D-CED
21	7	313	CLA	O1A-CGA-O2A-C1
21	A	823	CLA	O1A-CGA-O2A-C1
21	1	301	CLA	C2A-CAA-CBA-CGA
22	b	308	CHL	CBA-CGA-O2A-C1
21	b	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	8	606	CHL	O1D-CGD-O2D-CED
21	1	306	CLA	CBA-CGA-O2A-C1
21	A	836	CLA	CBA-CGA-O2A-C1
21	L	304	CLA	CBA-CGA-O2A-C1
21	a	302	CLA	CBA-CGA-O2A-C1
21	B	813	CLA	O2A-C1-C2-C3
28	7	324	LHG	C4-C5-O7-C7
30	2	618	SQD	C44-C45-O47-C7
22	8	606	CHL	C3C-C2C-CMC-OMC
22	8	608	CHL	C3C-C2C-CMC-OMC
22	b	307	CHL	C3C-C2C-CMC-OMC
22	c	605	CHL	C3C-C2C-CMC-OMC
22	c	606	CHL	C3C-C2C-CMC-OMC
22	c	607	CHL	C3C-C2C-CMC-OMC
25	O	2004	BCR	C13-C14-C15-C16
21	B	807	CLA	C16-C17-C18-C19
21	A	829	CLA	O1A-CGA-O2A-C1
22	T	602	CHL	O1A-CGA-O2A-C1
21	G	203	CLA	C2-C1-O2A-CGA
21	K	202	CLA	O1D-CGD-O2D-CED
22	c	605	CHL	O1D-CGD-O2D-CED
21	A	833	CLA	CBD-CGD-O2D-CED
21	B	822	CLA	C2-C3-C5-C6
27	A	855	LMU	C5'-C4'-O1B-C1B
28	c	618	LHG	O7-C5-C6-O8
32	7	301	DGD	O1G-C1G-C2G-O2G
32	A	802	DGD	O2G-C2G-C3G-O3G
21	B	819	CLA	CAA-CBA-CGA-O2A
21	7	315	CLA	C2A-CAA-CBA-CGA
21	B	813	CLA	C2A-CAA-CBA-CGA
21	B	823	CLA	C10-C11-C12-C13
21	3	412	CLA	C2-C1-O2A-CGA
21	T	611	CLA	C2-C1-O2A-CGA
21	B	806	CLA	C16-C17-C18-C19
21	B	806	CLA	C16-C17-C18-C20
27	A	855	LMU	C3'-C4'-O1B-C1B
29	7	302	PTY	C12-C13-C14-C15
34	A	803	CL0	C5-C6-C7-C8
21	A	811	CLA	C3-C5-C6-C7
21	8	610	CLA	O1D-CGD-O2D-CED
21	B	804	CLA	C10-C11-C12-C13
21	b	305	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	8	611	CLA	C6-C7-C8-C9
21	B	818	CLA	C4-C3-C5-C6
21	A	825	CLA	C8-C10-C11-C12
37	A	857	4RF	C46-C47-C48-C49
27	9	616	LMU	C2-C1-O1'-C1'
27	A	855	LMU	C2-C1-O1'-C1'
21	1	321	CLA	C11-C12-C13-C14
21	2	602	CLA	C11-C12-C13-C14
21	3	402	CLA	C11-C12-C13-C14
21	3	409	CLA	C11-C10-C8-C9
21	A	805	CLA	C11-C10-C8-C9
21	A	814	CLA	C14-C13-C15-C16
21	A	823	CLA	C11-C12-C13-C14
21	A	831	CLA	C14-C13-C15-C16
21	A	843	CLA	C11-C10-C8-C9
21	A	843	CLA	C14-C13-C15-C16
21	B	817	CLA	C6-C7-C8-C9
21	B	819	CLA	C6-C7-C8-C9
21	B	820	CLA	C11-C10-C8-C9
21	B	822	CLA	C6-C7-C8-C9
21	B	830	CLA	C11-C10-C8-C9
21	B	833	CLA	C11-C10-C8-C9
21	F	5005	CLA	C14-C13-C15-C16
21	a	302	CLA	C6-C7-C8-C9
21	a	312	CLA	C6-C7-C8-C9
21	b	304	CLA	C11-C10-C8-C9
22	2	601	CHL	C11-C10-C8-C9
35	B	845	PQN	C19-C18-C20-C21
21	A	805	CLA	C15-C16-C17-C18
21	A	817	CLA	C10-C11-C12-C13
21	9	611	CLA	C2A-CAA-CBA-CGA
32	A	802	DGD	C2D-C1D-O3G-C3G
29	a	319	PTY	O14-C5-C6-C1
21	1	301	CLA	C6-C7-C8-C10
21	1	302	CLA	C11-C10-C8-C7
21	1	308	CLA	C6-C7-C8-C10
21	1	321	CLA	C11-C12-C13-C15
21	2	602	CLA	C11-C12-C13-C15
21	3	409	CLA	C11-C10-C8-C7
21	7	314	CLA	C6-C7-C8-C10
21	9	607	CLA	C6-C7-C8-C10
21	A	804	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	A	808	CLA	C11-C12-C13-C15
21	A	811	CLA	C11-C12-C13-C15
21	A	817	CLA	C11-C12-C13-C15
21	A	821	CLA	C11-C12-C13-C15
21	A	823	CLA	C11-C12-C13-C15
21	A	830	CLA	C11-C12-C13-C15
21	A	835	CLA	C11-C12-C13-C15
21	A	841	CLA	C11-C10-C8-C7
21	A	843	CLA	C12-C13-C15-C16
21	B	804	CLA	C11-C10-C8-C7
21	B	806	CLA	C11-C10-C8-C7
21	B	807	CLA	C6-C7-C8-C10
21	B	810	CLA	C6-C7-C8-C10
21	B	810	CLA	C12-C13-C15-C16
21	B	817	CLA	C6-C7-C8-C10
21	B	821	CLA	C11-C10-C8-C7
21	B	830	CLA	C11-C10-C8-C7
21	B	844	CLA	C6-C7-C8-C10
21	F	5005	CLA	C11-C10-C8-C7
21	a	302	CLA	C6-C7-C8-C10
21	b	304	CLA	C11-C10-C8-C7
21	b	311	CLA	C6-C7-C8-C10
22	7	303	CHL	C11-C10-C8-C7
21	B	809	CLA	C13-C15-C16-C17
22	7	303	CHL	C15-C16-C17-C18
21	2	611	CLA	C3A-C2A-CAA-CBA
21	A	829	CLA	C4-C3-C5-C6
21	A	830	CLA	C3A-C2A-CAA-CBA
21	A	837	CLA	C3A-C2A-CAA-CBA
21	B	816	CLA	C3A-C2A-CAA-CBA
21	B	819	CLA	C3A-C2A-CAA-CBA
22	3	401	CHL	C3A-C2A-CAA-CBA
22	7	308	CHL	C3A-C2A-CAA-CBA
28	A	853	LHG	C26-C27-C28-C29
21	1	309	CLA	CAA-CBA-CGA-O2A
21	B	818	CLA	C2-C3-C5-C6
21	A	828	CLA	O1A-CGA-O2A-C1
21	1	301	CLA	C8-C10-C11-C12
21	B	807	CLA	C13-C15-C16-C17
21	B	819	CLA	C8-C10-C11-C12
21	B	819	CLA	CBA-CGA-O2A-C1
21	B	843	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	846	BCR	C13-C14-C15-C16
21	B	822	CLA	C5-C6-C7-C8
23	1	314	LUT	C27-C28-C29-C30
21	K	204	CLA	O2A-C1-C2-C3
21	8	605	CLA	C2A-CAA-CBA-CGA
26	3	421	LMG	C7-C8-C9-O8
28	2	617	LHG	C4-C5-C6-O8
28	7	321	LHG	C4-C5-C6-O8
28	8	620	LHG	C4-C5-C6-O8
28	c	618	LHG	C4-C5-C6-O8
29	7	322	PTY	O4-C1-C6-C5
29	L	308	PTY	O4-C1-C6-C5
32	8	602	DGD	C1G-C2G-C3G-O3G
21	A	833	CLA	C3-C5-C6-C7
21	8	611	CLA	C6-C7-C8-C10
21	T	612	CLA	C16-C17-C18-C20
22	2	601	CHL	C16-C17-C18-C20
21	B	809	CLA	CBD-CGD-O2D-CED
21	B	822	CLA	C4-C3-C5-C6
21	1	306	CLA	O1A-CGA-O2A-C1
21	L	304	CLA	O1A-CGA-O2A-C1
21	B	819	CLA	C3-C5-C6-C7
21	B	836	CLA	C3-C5-C6-C7
21	7	305	CLA	C6-C7-C8-C10
21	B	831	CLA	C16-C17-C18-C20
33	8	621	LMK	C2-C1-O1-C7
23	b	317	LUT	C1-C6-C7-C8
25	1	316	BCR	C23-C24-C25-C30
25	3	418	BCR	C1-C6-C7-C8
25	A	847	BCR	C1-C6-C7-C8
25	A	849	BCR	C1-C6-C7-C8
25	B	846	BCR	C1-C6-C7-C8
25	F	5008	BCR	C23-C24-C25-C30
25	G	202	BCR	C23-C24-C25-C30
25	L	309	BCR	C1-C6-C7-C8
25	O	2004	BCR	C23-C24-C25-C26
25	c	617	BCR	C23-C24-C25-C30
25	K	205	BCR	C23-C24-C25-C26
25	K	205	BCR	C23-C24-C25-C30
25	T	617	BCR	C23-C24-C25-C30
32	B	850	DGD	CCB-CDB-CEB-CFB
21	B	843	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	F	5001	LHG	C5-C4-O6-P
21	H	204	CLA	CBA-CGA-O2A-C1
21	A	824	CLA	C10-C11-C12-C13
21	B	820	CLA	CAA-CBA-CGA-O2A
21	L	303	CLA	C2A-CAA-CBA-CGA
21	A	843	CLA	C5-C6-C7-C8
26	3	421	LMG	O7-C8-C9-O8
28	8	620	LHG	O7-C5-C6-O8
28	F	5003	LHG	O7-C5-C6-O8
28	a	301	LHG	O7-C5-C6-O8
29	2	620	PTY	O4-C1-C6-O7
30	2	618	SQD	O6-C44-C45-O47
32	A	802	DGD	O1G-C1G-C2G-O2G
21	a	302	CLA	O1A-CGA-O2A-C1
28	2	617	LHG	C7-C8-C9-C10
29	B	851	PTY	C8-C11-C12-C13
21	A	836	CLA	O1A-CGA-O2A-C1
21	A	808	CLA	C10-C11-C12-C13
21	B	840	CLA	C5-C6-C7-C8
22	T	602	CHL	C1-C2-C3-C5
34	A	803	CL0	C1-C2-C3-C5
27	A	855	LMU	C2-C3-C4-C5
29	B	803	PTY	C11-C12-C13-C14
21	A	827	CLA	CBA-CGA-O2A-C1
22	8	601	CHL	C1-C2-C3-C4
21	3	412	CLA	C3-C5-C6-C7
21	2	611	CLA	C6-C7-C8-C9
21	7	316	CLA	C6-C7-C8-C9
21	A	825	CLA	C11-C10-C8-C9
21	A	830	CLA	C11-C12-C13-C14
21	A	835	CLA	C11-C12-C13-C14
21	B	806	CLA	C6-C7-C8-C9
21	B	807	CLA	C6-C7-C8-C9
21	B	821	CLA	C11-C10-C8-C9
21	B	821	CLA	C11-C12-C13-C14
26	G	207	LMG	O7-C10-C11-C12
21	T	606	CLA	O1D-CGD-O2D-CED
21	B	831	CLA	C3-C5-C6-C7
31	2	619	3PH	C22-C23-C24-C25
21	b	306	CLA	C2A-CAA-CBA-CGA
27	A	854	LMU	C3'-C4'-O1B-C1B
21	A	820	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	7	305	CLA	C6-C7-C8-C9
21	B	831	CLA	C16-C17-C18-C19
21	T	612	CLA	C16-C17-C18-C19
22	2	601	CHL	C16-C17-C18-C19
21	7	304	CLA	C8-C10-C11-C12
21	B	809	CLA	CBA-CGA-O2A-C1
21	B	832	CLA	CBA-CGA-O2A-C1
28	1	323	LHG	O6-C4-C5-C6
28	F	5003	LHG	O6-C4-C5-C6
21	A	827	CLA	O1A-CGA-O2A-C1
21	B	814	CLA	C10-C11-C12-C13
23	O	2005	LUT	C11-C12-C13-C20
21	2	603	CLA	C6-C7-C8-C10
21	A	811	CLA	C11-C10-C8-C7
21	A	814	CLA	C11-C10-C8-C7
21	A	825	CLA	C11-C10-C8-C7
21	A	839	CLA	C6-C7-C8-C10
21	A	843	CLA	C6-C7-C8-C10
21	A	856	CLA	C11-C12-C13-C15
21	B	806	CLA	C12-C13-C15-C16
21	B	821	CLA	C11-C12-C13-C15
21	B	822	CLA	C11-C10-C8-C7
21	B	833	CLA	C11-C10-C8-C7
21	a	309	CLA	C11-C10-C8-C7
21	1	302	CLA	C5-C6-C7-C8
21	7	311	CLA	C8-C10-C11-C12
21	B	837	CLA	C10-C11-C12-C13
24	9	615	XAT	C11-C12-C13-C14
24	c	616	XAT	C27-C28-C29-C30
21	B	804	CLA	CBA-CGA-O2A-C1
21	c	612	CLA	CBA-CGA-O2A-C1
21	A	819	CLA	C2A-CAA-CBA-CGA
21	B	806	CLA	C2A-CAA-CBA-CGA
21	G	204	CLA	C2A-CAA-CBA-CGA
21	T	609	CLA	C2A-CAA-CBA-CGA
21	3	402	CLA	C4-C3-C5-C6
21	7	316	CLA	C4-C3-C5-C6
28	8	620	LHG	O8-C23-C24-C25
21	B	819	CLA	O1A-CGA-O2A-C1
21	8	614	CLA	O1A-CGA-O2A-C1
31	2	619	3PH	C3E-C3F-C3G-C3H
21	B	843	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	a	302	CLA	C10-C11-C12-C13
29	H	201	PTY	C15-C16-C17-C18
21	A	805	CLA	C8-C10-C11-C12
28	F	5003	LHG	O6-C4-C5-O7
29	B	851	PTY	O14-C5-C6-O7
29	H	201	PTY	O14-C5-C6-O7
31	2	619	3PH	O11-C1-C2-O21
21	F	5007	CLA	O2A-C1-C2-C3
28	A	853	LHG	C31-C32-C33-C34
26	F	5009	LMG	C7-C8-C9-O8
29	H	201	PTY	O4-C1-C6-C5
32	7	301	DGD	O1G-C1G-C2G-C3G
32	A	802	DGD	O1G-C1G-C2G-C3G
21	G	203	CLA	CBD-CGD-O2D-CED
21	A	830	CLA	O1D-CGD-O2D-CED
21	A	832	CLA	O1D-CGD-O2D-CED
21	b	304	CLA	C2-C3-C5-C6
29	8	619	PTY	C2-C3-O11-P1
21	B	833	CLA	C8-C10-C11-C12
26	A	801	LMG	O1-C7-C8-O7
26	F	5009	LMG	O7-C8-C9-O8
28	7	324	LHG	O7-C5-C6-O8
28	b	301	LHG	O7-C5-C6-O8
29	L	308	PTY	O4-C1-C6-O7
30	3	422	SQD	O6-C44-C45-O47
32	8	602	DGD	O2G-C2G-C3G-O3G
21	A	811	CLA	C11-C10-C8-C9
21	A	839	CLA	C6-C7-C8-C9
21	B	810	CLA	C6-C7-C8-C9
22	3	401	CHL	C6-C7-C8-C9
34	A	803	CL0	C14-C13-C15-C16
27	A	854	LMU	C5'-C4'-O1B-C1B
21	B	809	CLA	O1A-CGA-O2A-C1
23	1	314	LUT	C26-C27-C28-C29
32	A	802	DGD	C2A-C3A-C4A-C5A
29	H	201	PTY	C23-C24-C25-C26
31	2	619	3PH	C2-C1-O11-P
21	A	818	CLA	C4-C3-C5-C6
21	a	309	CLA	C4-C3-C5-C6
21	3	402	CLA	C2-C3-C5-C6
22	c	605	CHL	C2C-C3C-CAC-CBC
21	2	608	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	7	311	CLA	C16-C17-C18-C20
21	A	836	CLA	C11-C12-C13-C15
21	3	409	CLA	C8-C10-C11-C12
21	B	831	CLA	C13-C15-C16-C17
21	b	311	CLA	C3-C5-C6-C7
21	B	810	CLA	CBA-CGA-O2A-C1
22	8	607	CHL	C2C-C3C-CAC-CBC
21	A	829	CLA	C5-C6-C7-C8
21	1	308	CLA	C1A-C2A-CAA-CBA
21	1	312	CLA	C1A-C2A-CAA-CBA
21	2	612	CLA	C1A-C2A-CAA-CBA
21	9	607	CLA	C1A-C2A-CAA-CBA
21	A	823	CLA	C1A-C2A-CAA-CBA
21	G	201	CLA	C1A-C2A-CAA-CBA
21	a	304	CLA	C1A-C2A-CAA-CBA
21	b	312	CLA	C1A-C2A-CAA-CBA
22	3	401	CHL	C1A-C2A-CAA-CBA
21	A	833	CLA	O1D-CGD-O2D-CED
21	B	809	CLA	O1D-CGD-O2D-CED
21	B	840	CLA	CBA-CGA-O2A-C1
21	L	304	CLA	C4-C3-C5-C6
21	9	607	CLA	C8-C10-C11-C12
22	2	601	CHL	C3-C5-C6-C7
28	3	420	LHG	C5-C6-O8-C23
21	B	832	CLA	O1A-CGA-O2A-C1
21	c	612	CLA	O1A-CGA-O2A-C1
28	b	303	LHG	O6-C4-C5-C6
29	7	302	PTY	O14-C5-C6-C1
21	c	610	CLA	CBD-CGD-O2D-CED
30	2	618	SQD	C17-C18-C19-C20
21	7	311	CLA	C12-C13-C15-C16
21	A	805	CLA	C6-C7-C8-C10
21	A	815	CLA	C6-C7-C8-C10
21	A	824	CLA	C6-C7-C8-C10
21	B	804	CLA	C6-C7-C8-C10
21	B	807	CLA	C11-C12-C13-C15
21	B	818	CLA	C11-C10-C8-C7
21	B	821	CLA	C12-C13-C15-C16
21	B	831	CLA	C6-C7-C8-C10
21	B	832	CLA	C11-C10-C8-C7
21	B	835	CLA	C11-C10-C8-C7
21	F	5005	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	b	305	CLA	C11-C12-C13-C15
35	B	845	PQN	C16-C17-C18-C20
28	B	802	LHG	O2-C2-C3-O3
21	B	804	CLA	O1A-CGA-O2A-C1
28	1	322	LHG	C2-C3-O3-P
28	7	321	LHG	C2-C3-O3-P
28	b	301	LHG	C2-C3-O3-P
29	c	619	PTY	C6-C5-O14-P1
21	3	406	CLA	C3A-C2A-CAA-CBA
21	H	203	CLA	C4-C3-C5-C6
21	T	613	CLA	C3A-C2A-CAA-CBA
21	7	316	CLA	C2-C3-C5-C6
29	1	320	PTY	O14-C5-C6-O7
29	a	319	PTY	O14-C5-C6-O7
22	c	605	CHL	C2A-CAA-CBA-CGA
21	2	603	CLA	C6-C7-C8-C9
21	A	805	CLA	C6-C7-C8-C9
21	A	808	CLA	C11-C12-C13-C14
21	A	811	CLA	C11-C12-C13-C14
21	A	814	CLA	C11-C10-C8-C9
21	A	843	CLA	C6-C7-C8-C9
21	A	856	CLA	C11-C12-C13-C14
21	B	817	CLA	C14-C13-C15-C16
21	B	822	CLA	C11-C10-C8-C9
21	B	832	CLA	C11-C10-C8-C9
21	a	309	CLA	C11-C10-C8-C9
21	B	837	CLA	C8-C10-C11-C12
22	2	606	CHL	C1C-C2C-CMC-OMC
22	7	309	CHL	C1C-C2C-CMC-OMC
22	a	306	CHL	C1C-C2C-CMC-OMC
22	b	302	CHL	C1C-C2C-CMC-OMC
22	b	309	CHL	C1C-C2C-CMC-OMC
22	c	606	CHL	C1C-C2C-CMC-OMC
21	T	612	CLA	C3-C5-C6-C7
22	3	401	CHL	C15-C16-C17-C18
21	B	810	CLA	O1A-CGA-O2A-C1
21	B	840	CLA	O1A-CGA-O2A-C1
26	A	801	LMG	O7-C8-C9-O8
26	F	5009	LMG	O1-C7-C8-O7
28	B	802	LHG	O7-C5-C6-O8
29	H	201	PTY	C11-C12-C13-C14
26	A	801	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	F	5009	LMG	O1-C7-C8-C9
28	B	802	LHG	C4-C5-C6-O8
29	2	620	PTY	O4-C1-C6-C5
30	2	618	SQD	O6-C44-C45-C46
30	3	422	SQD	O6-C44-C45-C46
32	B	850	DGD	O1G-C1G-C2G-C3G
21	2	602	CLA	C4-C3-C5-C6
21	9	601	CLA	CAD-CBD-CGD-O2D
21	9	602	CLA	CAD-CBD-CGD-O2D
21	9	609	CLA	CAD-CBD-CGD-O2D
21	B	836	CLA	CAD-CBD-CGD-O2D
21	B	830	CLA	C8-C10-C11-C12
21	G	203	CLA	O1D-CGD-O2D-CED
21	2	611	CLA	CBA-CGA-O2A-C1
21	A	841	CLA	C15-C16-C17-C18
35	B	845	PQN	C15-C16-C17-C18
21	7	311	CLA	C16-C17-C18-C19
21	A	856	CLA	C3-C5-C6-C7
21	a	305	CLA	C2A-CAA-CBA-CGA
22	b	307	CHL	C2A-CAA-CBA-CGA
21	1	307	CLA	CHA-CBD-CGD-O1D
21	2	607	CLA	CHA-CBD-CGD-O1D
21	2	607	CLA	CHA-CBD-CGD-O2D
21	9	601	CLA	CAD-CBD-CGD-O1D
21	9	602	CLA	CAD-CBD-CGD-O1D
21	9	609	CLA	CAD-CBD-CGD-O1D
21	A	808	CLA	CHA-CBD-CGD-O1D
21	A	808	CLA	CHA-CBD-CGD-O2D
21	A	818	CLA	CHA-CBD-CGD-O1D
21	A	818	CLA	CHA-CBD-CGD-O2D
21	A	819	CLA	CHA-CBD-CGD-O1D
21	A	835	CLA	CHA-CBD-CGD-O2D
21	A	842	CLA	CAD-CBD-CGD-O1D
21	B	836	CLA	CAD-CBD-CGD-O1D
21	O	2001	CLA	CAD-CBD-CGD-O2D
21	K	204	CLA	CHA-CBD-CGD-O1D
21	K	204	CLA	CHA-CBD-CGD-O2D
21	T	612	CLA	CHA-CBD-CGD-O1D
22	T	601	CHL	CHA-CBD-CGD-O1D
22	T	601	CHL	CHA-CBD-CGD-O2D
23	1	314	LUT	C25-C26-C27-C28
28	1	319	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
28	1	322	LHG	C3-O3-P-O6
28	1	323	LHG	C3-O3-P-O5
28	1	323	LHG	C4-O6-P-O5
28	3	420	LHG	C4-O6-P-O5
28	3	424	LHG	C3-O3-P-O4
28	3	424	LHG	C3-O3-P-O6
28	3	424	LHG	C4-O6-P-O3
28	3	424	LHG	C4-O6-P-O5
28	7	324	LHG	C3-O3-P-O4
28	7	324	LHG	C4-O6-P-O5
28	8	620	LHG	C3-O3-P-O5
28	9	617	LHG	C4-O6-P-O3
28	9	617	LHG	C4-O6-P-O5
28	A	852	LHG	C4-O6-P-O4
28	B	802	LHG	C3-O3-P-O5
28	B	802	LHG	C4-O6-P-O3
28	F	5001	LHG	C3-O3-P-O6
28	F	5003	LHG	C3-O3-P-O5
28	H	202	LHG	C4-O6-P-O3
28	a	301	LHG	C4-O6-P-O5
28	b	301	LHG	C4-O6-P-O5
28	b	303	LHG	C4-O6-P-O4
28	c	618	LHG	C3-O3-P-O5
28	c	618	LHG	C4-O6-P-O5
29	1	320	PTY	C3-O11-P1-O13
29	1	320	PTY	C5-O14-P1-O11
29	1	320	PTY	C5-O14-P1-O12
29	1	320	PTY	C5-O14-P1-O13
29	7	302	PTY	C3-O11-P1-O13
29	8	619	PTY	C5-O14-P1-O13
29	B	803	PTY	N1-C2-C3-O11
29	B	803	PTY	C5-O14-P1-O13
29	J	5001	PTY	C3-O11-P1-O13
29	J	5001	PTY	C5-O14-P1-O13
29	c	619	PTY	C3-O11-P1-O13
33	8	621	LMK	C29-C30-C31-C32
21	3	411	CLA	C4-C3-C5-C6
34	A	803	CL0	C4-C3-C5-C6
23	O	2005	LUT	C5-C6-C7-C8
25	3	419	BCR	C1-C6-C7-C8
25	a	317	BCR	C23-C24-C25-C30
26	3	421	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	3	421	LMG	C17-C18-C19-C20
28	1	323	LHG	C5-C4-O6-P
28	7	324	LHG	C2-C3-O3-P
28	7	324	LHG	C5-C4-O6-P
28	A	853	LHG	C2-C3-O3-P
28	B	802	LHG	C2-C3-O3-P
29	1	320	PTY	C6-C5-O14-P1
21	A	828	CLA	C5-C6-C7-C8
28	9	617	LHG	O8-C23-C24-C25
21	2	611	CLA	O1A-CGA-O2A-C1
25	A	848	BCR	C18-C19-C20-C21
25	L	302	BCR	C10-C11-C12-C13
25	L	302	BCR	C18-C19-C20-C21
25	K	205	BCR	C10-C11-C12-C13
21	3	411	CLA	C5-C6-C7-C8
21	B	835	CLA	C5-C6-C7-C8
29	2	620	PTY	C15-C16-C17-C18
21	3	402	CLA	C8-C10-C11-C12
31	2	619	3PH	O11-C1-C2-C3
22	b	308	CHL	O1A-CGA-O2A-C1
21	A	839	CLA	CBA-CGA-O2A-C1
21	1	308	CLA	C6-C7-C8-C9
21	B	804	CLA	C6-C7-C8-C9
21	B	806	CLA	C11-C10-C8-C9
21	B	810	CLA	C14-C13-C15-C16
21	B	831	CLA	C11-C10-C8-C9
21	B	844	CLA	C6-C7-C8-C9
21	a	302	CLA	C11-C12-C13-C14
35	B	845	PQN	C24-C23-C25-C26
21	2	602	CLA	C11-C10-C8-C7
21	A	822	CLA	C11-C10-C8-C7
21	B	817	CLA	C12-C13-C15-C16
29	I	201	PTY	C8-C11-C12-C13
28	b	303	LHG	O6-C4-C5-O7
29	7	302	PTY	O14-C5-C6-O7
21	A	836	CLA	C11-C12-C13-C14
21	a	310	CLA	CAA-CBA-CGA-O2A
28	F	5001	LHG	O7-C7-C8-C9
28	b	301	LHG	O8-C23-C24-C25
21	b	305	CLA	C16-C17-C18-C20
21	1	312	CLA	CBD-CGD-O2D-CED
27	1	318	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	2	619	3PH	C3D-C3E-C3F-C3G
28	2	617	LHG	O7-C5-C6-O8
28	3	424	LHG	O7-C5-C6-O8
29	I	201	PTY	C17-C18-C19-C20
21	c	610	CLA	O1D-CGD-O2D-CED
21	a	302	CLA	C8-C10-C11-C12
21	1	308	CLA	C2A-CAA-CBA-CGA
21	B	811	CLA	C2A-CAA-CBA-CGA
21	3	410	CLA	C2-C1-O2A-CGA
21	7	313	CLA	C2-C1-O2A-CGA
22	b	302	CHL	C2-C1-O2A-CGA
21	B	825	CLA	C11-C12-C13-C15
21	H	203	CLA	CAA-CBA-CGA-O2A
32	A	802	DGD	C1G-C2G-C3G-O3G
29	I	201	PTY	C15-C16-C17-C18
21	A	807	CLA	C16-C17-C18-C20
24	7	318	XAT	C27-C28-C29-C30
21	A	839	CLA	O1A-CGA-O2A-C1
21	B	844	CLA	C15-C16-C17-C18
21	3	412	CLA	C2A-CAA-CBA-CGA
21	A	827	CLA	C2A-CAA-CBA-CGA
21	b	304	CLA	C2A-CAA-CBA-CGA
21	B	823	CLA	C11-C12-C13-C15
21	A	807	CLA	C4-C3-C5-C6
21	A	813	CLA	C4-C3-C5-C6
21	L	304	CLA	C2-C3-C5-C6
34	A	803	CL0	C2-C3-C5-C6
31	2	619	3PH	C21-C22-C23-C24
21	A	815	CLA	C6-C7-C8-C9
21	A	831	CLA	C11-C12-C13-C14
21	A	841	CLA	C11-C10-C8-C9
21	B	806	CLA	C11-C12-C13-C14
21	B	818	CLA	C11-C10-C8-C9
21	B	833	CLA	C14-C13-C15-C16
22	2	601	CHL	C14-C13-C15-C16
29	c	620	PTY	C30-C31-C32-C33
21	A	835	CLA	C10-C11-C12-C13
21	b	305	CLA	C10-C11-C12-C13
21	B	812	CLA	C4-C3-C5-C6
21	A	804	CLA	C5-C6-C7-C8
21	A	830	CLA	C12-C13-C15-C16
21	B	806	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	B	831	CLA	C12-C13-C15-C16
21	B	832	CLA	C11-C12-C13-C15
22	2	601	CHL	C12-C13-C15-C16
21	2	613	CLA	C10-C11-C12-C13
21	B	819	CLA	CAA-CBA-CGA-O1A
29	I	201	PTY	O4-C1-C6-O7
21	A	809	CLA	C3A-C2A-CAA-CBA
21	A	814	CLA	C3A-C2A-CAA-CBA
21	A	840	CLA	C3A-C2A-CAA-CBA
21	a	307	CLA	C3A-C2A-CAA-CBA
21	b	316	CLA	C3A-C2A-CAA-CBA
21	K	202	CLA	C3A-C2A-CAA-CBA
21	T	604	CLA	C3A-C2A-CAA-CBA
21	H	204	CLA	O1A-CGA-O2A-C1
27	9	616	LMU	C3-C4-C5-C6
23	1	314	LUT	C40-C33-C34-C35
23	B	801	LUT	C40-C33-C34-C35
23	a	315	LUT	C40-C33-C34-C35
25	A	846	BCR	C11-C10-C9-C34
25	A	851	BCR	C11-C10-C9-C34
25	A	851	BCR	C16-C17-C18-C36
25	B	805	BCR	C11-C10-C9-C34
25	B	805	BCR	C16-C17-C18-C36
25	B	852	BCR	C35-C13-C14-C15
25	F	5008	BCR	C16-C17-C18-C36
25	G	206	BCR	C35-C13-C14-C15
25	G	206	BCR	C16-C17-C18-C36
25	L	302	BCR	C11-C10-C9-C34
25	L	302	BCR	C20-C21-C22-C37
25	L	309	BCR	C11-C10-C9-C34
25	O	2004	BCR	C11-C10-C9-C34
25	I	203	BCR	C35-C13-C14-C15
25	K	205	BCR	C11-C10-C9-C34
26	A	801	LMG	O6-C1-O1-C7
28	a	301	LHG	C2-C3-O3-P
29	c	619	PTY	C33-C34-C35-C36
28	A	853	LHG	C24-C25-C26-C27
37	A	857	4RF	C07-C08-C09-C10
21	1	312	CLA	O1D-CGD-O2D-CED
22	7	303	CHL	C4-C3-C5-C6
37	A	857	4RF	O21-C22-C24-C25
21	2	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	H	203	CLA	C2-C3-C5-C6
37	A	857	4RF	C12-C13-C14-C15
21	A	804	CLA	C13-C15-C16-C17
28	F	5001	LHG	C4-C5-C6-O8
21	B	809	CLA	C5-C6-C7-C8
21	7	311	CLA	C14-C13-C15-C16
21	7	314	CLA	C14-C13-C15-C16
21	A	807	CLA	C11-C10-C8-C9
21	B	831	CLA	C14-C13-C15-C16
21	7	304	CLA	C11-C12-C13-C15
21	B	811	CLA	C6-C7-C8-C10
28	1	322	LHG	O7-C7-C8-C9
29	a	319	PTY	C1-C6-O7-C8
22	T	602	CHL	C1-C2-C3-C4
34	A	803	CL0	C1-C2-C3-C4
21	B	823	CLA	CBD-CGD-O2D-CED
21	A	807	CLA	C2-C3-C5-C6
21	G	201	CLA	C5-C6-C7-C8
21	B	830	CLA	CAA-CBA-CGA-O2A
21	2	602	CLA	C1A-C2A-CAA-CBA
21	7	305	CLA	C1A-C2A-CAA-CBA
21	A	824	CLA	C1A-C2A-CAA-CBA
21	A	826	CLA	C1A-C2A-CAA-CBA
21	A	827	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C1A-C2A-CAA-CBA
21	a	307	CLA	C1A-C2A-CAA-CBA
21	b	313	CLA	C1A-C2A-CAA-CBA
21	K	202	CLA	C1A-C2A-CAA-CBA
21	T	613	CLA	C1A-C2A-CAA-CBA
23	1	314	LUT	C32-C33-C34-C35
23	B	801	LUT	C32-C33-C34-C35
23	a	315	LUT	C32-C33-C34-C35
25	A	846	BCR	C11-C10-C9-C8
25	A	851	BCR	C11-C10-C9-C8
25	A	851	BCR	C16-C17-C18-C19
25	B	805	BCR	C11-C10-C9-C8
25	B	805	BCR	C16-C17-C18-C19
25	B	852	BCR	C12-C13-C14-C15
25	F	5008	BCR	C16-C17-C18-C19
25	G	206	BCR	C12-C13-C14-C15
25	G	206	BCR	C16-C17-C18-C19
25	L	302	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	L	302	BCR	C20-C21-C22-C23
25	L	309	BCR	C11-C10-C9-C8
25	O	2004	BCR	C11-C10-C9-C8
25	I	203	BCR	C12-C13-C14-C15
25	K	205	BCR	C11-C10-C9-C8
22	8	607	CHL	C4C-C3C-CAC-CBC
21	A	807	CLA	C16-C17-C18-C19
21	A	819	CLA	C11-C12-C13-C15
22	c	605	CHL	C4C-C3C-CAC-CBC
23	2	614	LUT	C5-C6-C7-C8
23	2	615	LUT	C1-C6-C7-C8
23	3	415	LUT	C1-C6-C7-C8
23	8	616	LUT	C1-C6-C7-C8
23	9	613	LUT	C1-C6-C7-C8
23	a	315	LUT	C1-C6-C7-C8
23	b	317	LUT	C5-C6-C7-C8
25	1	316	BCR	C1-C6-C7-C8
25	1	316	BCR	C23-C24-C25-C26
25	3	418	BCR	C5-C6-C7-C8
25	3	419	BCR	C5-C6-C7-C8
25	7	319	BCR	C23-C24-C25-C26
25	A	847	BCR	C5-C6-C7-C8
25	A	849	BCR	C5-C6-C7-C8
25	B	846	BCR	C5-C6-C7-C8
25	B	852	BCR	C1-C6-C7-C8
25	F	5008	BCR	C23-C24-C25-C26
25	G	202	BCR	C23-C24-C25-C26
25	L	309	BCR	C5-C6-C7-C8
25	c	617	BCR	C23-C24-C25-C26
25	T	617	BCR	C23-C24-C25-C26
21	K	201	CLA	CAA-CBA-CGA-O2A
21	A	810	CLA	C13-C15-C16-C17
21	A	817	CLA	C15-C16-C17-C18
21	B	821	CLA	C15-C16-C17-C18
28	a	318	LHG	C5-C4-O6-P
21	A	816	CLA	C5-C6-C7-C8
33	8	621	LMK	N4-C3-C4-O2
21	A	809	CLA	C4-C3-C5-C6
21	A	830	CLA	C4-C3-C5-C6
21	B	824	CLA	C4-C3-C5-C6
21	B	817	CLA	C2C-C3C-CAC-CBC
21	K	201	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	1	321	CLA	C11-C10-C8-C7
21	A	816	CLA	C11-C10-C8-C7
21	A	831	CLA	C11-C12-C13-C15
21	A	832	CLA	C6-C7-C8-C10
21	B	818	CLA	C11-C12-C13-C15
21	B	833	CLA	C12-C13-C15-C16
21	B	834	CLA	C6-C7-C8-C10
21	a	302	CLA	C11-C12-C13-C15
21	b	305	CLA	C16-C17-C18-C19
21	2	604	CLA	C2A-CAA-CBA-CGA
21	9	608	CLA	C2A-CAA-CBA-CGA
21	a	302	CLA	C2A-CAA-CBA-CGA
28	F	5001	LHG	O7-C5-C6-O8
31	F	5002	3PH	O21-C2-C3-O31
32	B	850	DGD	O1G-C1G-C2G-O2G
26	G	207	LMG	C33-C34-C35-C36
28	3	420	LHG	C4-C5-O7-C7
28	3	420	LHG	C6-C5-O7-C7
37	A	857	4RF	C41-C43-C44-C45
21	K	203	CLA	CAA-CBA-CGA-O2A
29	B	851	PTY	C14-C15-C16-C17
21	B	824	CLA	C5-C6-C7-C8
21	1	312	CLA	CAA-CBA-CGA-O2A
21	A	835	CLA	C4-C3-C5-C6
21	B	823	CLA	O1D-CGD-O2D-CED
21	B	812	CLA	C2-C3-C5-C6
22	7	303	CHL	C2-C3-C5-C6
28	H	202	LHG	C17-C18-C19-C20
21	8	613	CLA	C2-C1-O2A-CGA
21	O	2003	CLA	CAA-CBA-CGA-O2A
27	1	318	LMU	O5B-C1B-O1B-C4'
21	B	822	CLA	C11-C12-C13-C14
21	B	835	CLA	C11-C10-C8-C9
21	G	201	CLA	C11-C12-C13-C14
22	T	601	CHL	C2-C1-O2A-CGA
29	H	201	PTY	C14-C15-C16-C17
21	B	809	CLA	C4-C3-C5-C6
21	A	818	CLA	C2-C3-C5-C6
21	a	309	CLA	C2-C3-C5-C6
21	1	307	CLA	CBA-CGA-O2A-C1
21	B	819	CLA	C5-C6-C7-C8
21	1	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	821	CLA	C2A-CAA-CBA-CGA
22	7	309	CHL	C2A-CAA-CBA-CGA
30	2	618	SQD	C18-C19-C20-C21
21	J	5002	CLA	CAA-CBA-CGA-O2A
21	O	2003	CLA	CAA-CBA-CGA-O1A
28	a	318	LHG	O6-C4-C5-O7
21	3	408	CLA	C4-C3-C5-C6
21	B	826	CLA	C4-C3-C5-C6
21	2	612	CLA	CAA-CBA-CGA-O2A
21	9	605	CLA	CAA-CBA-CGA-O2A
21	1	309	CLA	CAA-CBA-CGA-O1A
21	A	841	CLA	CAA-CBA-CGA-O2A
21	F	5007	CLA	CAA-CBA-CGA-O2A
21	B	825	CLA	C11-C12-C13-C14
22	3	401	CHL	O1A-CGA-O2A-C1
21	K	203	CLA	CAA-CBA-CGA-O1A
21	2	605	CLA	CAA-CBA-CGA-O1A
21	9	610	CLA	CAA-CBA-CGA-O1A
21	9	610	CLA	CAA-CBA-CGA-O2A
21	B	823	CLA	C11-C12-C13-C14
21	a	303	CLA	C5-C6-C7-C8
28	A	853	LHG	C25-C26-C27-C28
29	L	308	PTY	O14-C5-C6-C1
28	a	318	LHG	O8-C23-C24-C25
21	A	815	CLA	C8-C10-C11-C12
21	A	820	CLA	C11-C12-C13-C15
21	A	835	CLA	C12-C13-C15-C16
21	B	833	CLA	C6-C7-C8-C10
35	B	845	PQN	C21-C22-C23-C25
21	A	815	CLA	C3-C5-C6-C7
21	9	605	CLA	CAA-CBA-CGA-O1A
21	3	402	CLA	C14-C13-C15-C16
21	8	610	CLA	C6-C7-C8-C9
21	A	828	CLA	C11-C10-C8-C9
21	A	839	CLA	C14-C13-C15-C16
21	B	807	CLA	C11-C12-C13-C14
21	B	833	CLA	C6-C7-C8-C9
21	B	842	CLA	C6-C7-C8-C9
30	2	618	SQD	C5-C6-S-O8
33	8	621	LMK	C8-C7-O1-C1
21	A	817	CLA	C2-C1-O2A-CGA
21	B	827	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	a	308	CLA	C2-C1-O2A-CGA
22	7	303	CHL	C2-C1-O2A-CGA
21	3	405	CLA	C3A-C2A-CAA-CBA
21	7	305	CLA	C3A-C2A-CAA-CBA
21	A	827	CLA	C3A-C2A-CAA-CBA
21	F	5006	CLA	C3A-C2A-CAA-CBA
22	c	606	CHL	C3A-C2A-CAA-CBA
21	3	411	CLA	C2-C3-C5-C6
21	B	843	CLA	CAA-CBA-CGA-O1A
21	1	312	CLA	CAA-CBA-CGA-O1A
22	3	401	CHL	CBA-CGA-O2A-C1
21	2	607	CLA	CAA-CBA-CGA-O2A
21	B	807	CLA	O2A-C1-C2-C3
29	a	319	PTY	C5-C6-O7-C8
21	B	818	CLA	C8-C10-C11-C12
29	c	619	PTY	O4-C30-C31-C32
21	B	808	CLA	CBA-CGA-O2A-C1
21	B	811	CLA	C6-C7-C8-C9
21	c	608	CLA	CAA-CBA-CGA-O2A
21	2	612	CLA	CAA-CBA-CGA-O1A
21	7	310	CLA	CAA-CBA-CGA-O2A
21	A	809	CLA	C2-C3-C5-C6
24	7	318	XAT	O24-C26-C27-C28
24	c	616	XAT	O24-C26-C27-C28
21	J	5002	CLA	CAA-CBA-CGA-O1A
29	L	308	PTY	O14-C5-C6-O7
21	B	808	CLA	O1A-CGA-O2A-C1
21	A	819	CLA	C5-C6-C7-C8
28	a	301	LHG	C4-C5-C6-O8
21	a	309	CLA	C8-C10-C11-C12
21	B	820	CLA	CAA-CBA-CGA-O1A
29	I	201	PTY	C31-C32-C33-C34
21	A	810	CLA	C2A-CAA-CBA-CGA
21	B	832	CLA	C2A-CAA-CBA-CGA
31	2	619	3PH	O21-C21-C22-C23
21	1	313	CLA	CAA-CBA-CGA-O1A
21	F	5006	CLA	C2-C1-O2A-CGA
26	G	207	LMG	O9-C10-C11-C12
21	c	608	CLA	CAA-CBA-CGA-O1A
28	A	853	LHG	O8-C23-C24-C25
27	1	318	LMU	O1'-C1-C2-C3
29	B	803	PTY	O4-C1-C6-O7

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Mol	Chain	Res	Type	Atoms
21	1	301	CLA	C11-C12-C13-C14
21	B	831	CLA	C6-C7-C8-C9
21	b	305	CLA	C11-C12-C13-C14
21	T	612	CLA	C11-C10-C8-C9
21	a	314	CLA	CAA-CBA-CGA-O2A
29	H	201	PTY	O4-C30-C31-C32
21	1	313	CLA	CAA-CBA-CGA-O2A
21	7	310	CLA	CAA-CBA-CGA-O1A
22	T	602	CHL	C2C-C3C-CAC-CBC
21	1	302	CLA	CAA-CBA-CGA-O2A
21	7	315	CLA	CAA-CBA-CGA-O2A
21	b	313	CLA	CAA-CBA-CGA-O2A
28	3	424	LHG	O7-C7-C8-C9
21	A	830	CLA	C2-C3-C5-C6
21	T	608	CLA	CAA-CBA-CGA-O2A
21	A	839	CLA	C2A-CAA-CBA-CGA
21	B	828	CLA	C2A-CAA-CBA-CGA
21	1	302	CLA	C6-C7-C8-C10
21	3	407	CLA	C11-C10-C8-C7
21	7	314	CLA	C12-C13-C15-C16
21	8	610	CLA	C6-C7-C8-C10
21	A	828	CLA	C11-C10-C8-C7
21	A	836	CLA	C11-C10-C8-C7
21	B	809	CLA	C12-C13-C15-C16
21	B	822	CLA	C11-C12-C13-C15
21	B	843	CLA	C6-C7-C8-C10
21	G	201	CLA	C11-C12-C13-C15
22	7	303	CHL	C11-C12-C13-C15
34	A	803	CL0	C6-C7-C8-C10
22	2	601	CHL	C2C-C3C-CAC-CBC
23	2	615	LUT	C5-C6-C7-C8
23	3	415	LUT	C5-C6-C7-C8
23	a	315	LUT	C5-C6-C7-C8
25	1	316	BCR	C5-C6-C7-C8
25	3	419	BCR	C23-C24-C25-C26
25	3	419	BCR	C23-C24-C25-C30
25	7	319	BCR	C1-C6-C7-C8
25	7	319	BCR	C5-C6-C7-C8
25	A	846	BCR	C5-C6-C7-C8
25	B	805	BCR	C23-C24-C25-C26
25	B	852	BCR	C5-C6-C7-C8
25	G	206	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	G	206	BCR	C23-C24-C25-C30
25	a	317	BCR	C23-C24-C25-C26
28	a	301	LHG	O7-C7-C8-C9
28	c	618	LHG	O8-C23-C24-C25
29	3	423	PTY	O4-C30-C31-C32
21	A	833	CLA	C2-C1-O2A-CGA
21	b	306	CLA	C2-C1-O2A-CGA
24	a	316	XAT	C6-C7-C8-C9
24	c	616	XAT	C26-C27-C28-C29
21	3	402	CLA	CAA-CBA-CGA-O2A
21	A	814	CLA	CAA-CBA-CGA-O2A
21	A	827	CLA	CAA-CBA-CGA-O2A
22	3	401	CHL	CAA-CBA-CGA-O2A
21	A	830	CLA	C10-C11-C12-C13
21	B	815	CLA	CBA-CGA-O2A-C1
21	A	819	CLA	C11-C12-C13-C14
28	1	323	LHG	O8-C23-C24-C25
28	F	5001	LHG	O8-C23-C24-C25
21	2	613	CLA	C2-C3-C5-C6
21	A	821	CLA	C2-C3-C5-C6
21	7	312	CLA	CAA-CBA-CGA-O2A
21	9	603	CLA	CAA-CBA-CGA-O2A
21	A	822	CLA	CAA-CBA-CGA-O2A
21	B	809	CLA	CAA-CBA-CGA-O2A
21	A	834	CLA	C3-C5-C6-C7
28	1	323	LHG	C9-C10-C11-C12
21	7	304	CLA	C11-C12-C13-C14
26	3	421	LMG	O10-C28-C29-C30
21	1	304	CLA	CAA-CBA-CGA-O1A
21	B	834	CLA	C5-C6-C7-C8
21	3	408	CLA	CAA-CBA-CGA-O2A
21	A	824	CLA	CAA-CBA-CGA-O2A
21	B	831	CLA	CAA-CBA-CGA-O2A
21	c	613	CLA	CAA-CBA-CGA-O2A
21	2	613	CLA	C4-C3-C5-C6
21	A	822	CLA	C4-C3-C5-C6
28	A	852	LHG	O8-C23-C24-C25
21	3	407	CLA	C2-C3-C5-C6
21	A	813	CLA	C2-C3-C5-C6
21	2	605	CLA	CAA-CBA-CGA-O2A
28	A	853	LHG	C11-C12-C13-C14
21	T	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	T	605	CLA	CAA-CBA-CGA-O2A
28	F	5003	LHG	C24-C25-C26-C27
21	1	302	CLA	C8-C10-C11-C12
21	B	839	CLA	C5-C6-C7-C8
21	c	610	CLA	CAA-CBA-CGA-O2A
21	1	302	CLA	C6-C7-C8-C9
21	A	816	CLA	C11-C10-C8-C9
21	A	824	CLA	C6-C7-C8-C9
21	A	841	CLA	C11-C12-C13-C14
21	B	816	CLA	C6-C7-C8-C9
21	B	818	CLA	C11-C12-C13-C14
21	B	821	CLA	C14-C13-C15-C16
21	1	321	CLA	C15-C16-C17-C18
29	7	322	PTY	C6-C5-O14-P1
21	B	815	CLA	O1A-CGA-O2A-C1
31	2	619	3PH	C1-C2-C3-O31
32	8	602	DGD	O1G-C1G-C2G-C3G
21	3	405	CLA	C1A-C2A-CAA-CBA
21	3	410	CLA	C1A-C2A-CAA-CBA
21	8	605	CLA	C1A-C2A-CAA-CBA
21	8	612	CLA	C1A-C2A-CAA-CBA
21	A	842	CLA	C1A-C2A-CAA-CBA
21	F	5006	CLA	C1A-C2A-CAA-CBA
21	a	310	CLA	C1A-C2A-CAA-CBA
21	b	316	CLA	C1A-C2A-CAA-CBA
21	c	603	CLA	C1A-C2A-CAA-CBA
22	c	606	CHL	C1A-C2A-CAA-CBA
21	B	816	CLA	C3-C5-C6-C7
21	3	407	CLA	C4-C3-C5-C6
21	A	821	CLA	C4-C3-C5-C6
21	A	828	CLA	C4-C3-C5-C6
21	B	830	CLA	C4-C3-C5-C6
21	1	306	CLA	CAA-CBA-CGA-O2A
21	B	807	CLA	CAA-CBA-CGA-O2A
21	a	308	CLA	CAA-CBA-CGA-O2A
29	2	620	PTY	O4-C30-C31-C32
28	9	617	LHG	O7-C5-C6-O8
25	A	850	BCR	C17-C18-C19-C20
25	B	849	BCR	C21-C22-C23-C24
21	8	604	CLA	CAA-CBA-CGA-O2A
21	8	612	CLA	CAA-CBA-CGA-O2A
21	9	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	832	CLA	CAA-CBA-CGA-O2A
21	T	606	CLA	CAA-CBA-CGA-O2A
22	T	602	CHL	CAA-CBA-CGA-O2A
21	B	804	CLA	C16-C17-C18-C19
22	8	607	CHL	CAA-CBA-CGA-O2A
30	2	618	SQD	C5-C6-S-O9
22	8	608	CHL	O1D-CGD-O2D-CED
21	B	817	CLA	C4-C3-C5-C6
21	B	821	CLA	C2-C1-O2A-CGA
21	B	832	CLA	C2-C1-O2A-CGA
21	L	304	CLA	C2-C1-O2A-CGA
26	A	801	LMG	O7-C10-C11-C12
21	1	311	CLA	C6-C7-C8-C10
21	7	304	CLA	C11-C10-C8-C7
21	A	815	CLA	C11-C10-C8-C7
21	B	809	CLA	C6-C7-C8-C10
21	B	842	CLA	C6-C7-C8-C10
21	T	608	CLA	CAA-CBA-CGA-O1A
22	T	602	CHL	C4C-C3C-CAC-CBC
21	a	303	CLA	CAA-CBA-CGA-O2A
21	T	604	CLA	CAA-CBA-CGA-O2A
28	3	424	LHG	O8-C23-C24-C25
26	3	421	LMG	C19-C20-C21-C22
21	A	809	CLA	C5-C6-C7-C8
21	B	815	CLA	C2A-CAA-CBA-CGA
21	3	406	CLA	CAA-CBA-CGA-O2A
21	B	836	CLA	CAA-CBA-CGA-O2A
21	b	313	CLA	CAA-CBA-CGA-O1A
21	B	806	CLA	C8-C10-C11-C12
21	1	304	CLA	CAA-CBA-CGA-O2A
21	8	615	CLA	CAA-CBA-CGA-O1A
21	8	622	CLA	C3A-C2A-CAA-CBA
21	B	817	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C3A-C2A-CAA-CBA
21	a	308	CLA	C3A-C2A-CAA-CBA
21	a	312	CLA	C3A-C2A-CAA-CBA
21	b	313	CLA	C3A-C2A-CAA-CBA
21	B	827	CLA	C5-C6-C7-C8
21	A	835	CLA	C2-C3-C5-C6
21	B	817	CLA	C2-C3-C5-C6
21	B	824	CLA	C2-C3-C5-C6
28	8	620	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	H	201	PTY	O30-C30-C31-C32
21	T	603	CLA	CBA-CGA-O2A-C1
29	I	201	PTY	C36-C37-C38-C39
32	A	802	DGD	C4B-C5B-C6B-C7B
21	B	827	CLA	CAA-CBA-CGA-O2A
21	9	603	CLA	CAA-CBA-CGA-O1A
21	A	822	CLA	CAA-CBA-CGA-O1A
21	A	827	CLA	CAA-CBA-CGA-O1A
21	7	312	CLA	CAA-CBA-CGA-O1A
21	1	321	CLA	C11-C10-C8-C9
21	2	602	CLA	C11-C10-C8-C9
21	A	816	CLA	C14-C13-C15-C16
21	A	820	CLA	C11-C12-C13-C14
21	A	832	CLA	C6-C7-C8-C9
21	B	834	CLA	C6-C7-C8-C9
21	F	5005	CLA	C11-C12-C13-C14
21	c	613	CLA	CAA-CBA-CGA-O1A
21	B	822	CLA	C13-C15-C16-C17
21	B	844	CLA	C8-C10-C11-C12
21	B	844	CLA	C10-C11-C12-C13
21	3	402	CLA	CAA-CBA-CGA-O1A
21	a	314	CLA	CAA-CBA-CGA-O1A
22	3	401	CHL	CAA-CBA-CGA-O1A
28	F	5001	LHG	O10-C23-C24-C25
29	2	620	PTY	O30-C30-C31-C32
21	A	810	CLA	C8-C10-C11-C12
23	3	415	LUT	C21-C26-C27-C28
21	T	603	CLA	O1A-CGA-O2A-C1
21	9	607	CLA	C15-C16-C17-C18
21	T	613	CLA	CAA-CBA-CGA-O2A
29	B	851	PTY	C12-C11-C8-O7
21	b	316	CLA	CAA-CBA-CGA-O2A
21	A	806	CLA	C8-C10-C11-C12
23	3	415	LUT	C27-C28-C29-C30
25	3	419	BCR	C21-C22-C23-C24
28	7	321	LHG	C18-C19-C20-C21
28	a	301	LHG	O9-C7-C8-C9
21	1	302	CLA	CAA-CBA-CGA-O1A
21	a	303	CLA	CAA-CBA-CGA-O1A
31	2	619	3PH	O22-C21-C22-C23
21	B	817	CLA	C4C-C3C-CAC-CBC
26	7	320	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
27	A	855	LMU	C3-C4-C5-C6
21	c	610	CLA	CAA-CBA-CGA-O1A
21	1	306	CLA	CAA-CBA-CGA-O1A
21	3	408	CLA	CAA-CBA-CGA-O1A
21	7	315	CLA	CAA-CBA-CGA-O1A
21	A	824	CLA	CAA-CBA-CGA-O1A
21	B	831	CLA	CAA-CBA-CGA-O1A
21	B	832	CLA	CAA-CBA-CGA-O1A
28	A	853	LHG	O10-C23-C24-C25
21	3	412	CLA	CAA-CBA-CGA-O2A
21	B	817	CLA	CAA-CBA-CGA-O2A
21	a	312	CLA	CAA-CBA-CGA-O2A
21	T	605	CLA	CAA-CBA-CGA-O1A
21	3	402	CLA	C15-C16-C17-C18
21	B	807	CLA	CAA-CBA-CGA-O1A
28	1	323	LHG	O10-C23-C24-C25
27	1	318	LMU	C2B-C1B-O1B-C4'
21	1	301	CLA	CAD-CBD-CGD-O2D
21	3	409	CLA	CAD-CBD-CGD-O2D
21	7	304	CLA	CAD-CBD-CGD-O2D
21	A	820	CLA	CAD-CBD-CGD-O2D
21	B	816	CLA	CAD-CBD-CGD-O2D
21	c	602	CLA	CAD-CBD-CGD-O2D
30	3	422	SQD	O48-C23-C24-C25
21	T	604	CLA	CAA-CBA-CGA-O1A
37	A	857	4RF	C13-C14-C15-C16
21	A	839	CLA	C5-C6-C7-C8
21	3	402	CLA	C2-C1-O2A-CGA
21	7	305	CLA	C2-C1-O2A-CGA
21	b	305	CLA	C2-C1-O2A-CGA
21	B	809	CLA	CAA-CBA-CGA-O1A
21	a	308	CLA	CAA-CBA-CGA-O1A
22	8	607	CHL	CAA-CBA-CGA-O1A
22	7	303	CHL	C1-C2-C3-C4
22	b	302	CHL	C1-C2-C3-C4
21	T	604	CLA	C2A-CAA-CBA-CGA
21	T	606	CLA	C2A-CAA-CBA-CGA
28	A	852	LHG	O10-C23-C24-C25
21	A	824	CLA	C5-C6-C7-C8
21	B	831	CLA	O1A-CGA-O2A-C1
21	9	612	CLA	CAA-CBA-CGA-O2A
21	A	826	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	a	313	CLA	CAA-CBA-CGA-O2A
21	T	603	CLA	CAA-CBA-CGA-O2A
28	F	5003	LHG	O7-C7-C8-C9
28	b	301	LHG	O7-C7-C8-C9
21	b	316	CLA	CAA-CBA-CGA-O1A
21	B	817	CLA	CAA-CBA-CGA-O1A
21	3	403	CLA	CAA-CBA-CGA-O2A
21	3	404	CLA	CAA-CBA-CGA-O2A
21	8	609	CLA	CAA-CBA-CGA-O2A
21	A	812	CLA	CAA-CBA-CGA-O2A
21	A	836	CLA	CAA-CBA-CGA-O2A
21	B	810	CLA	CAA-CBA-CGA-O2A
21	B	838	CLA	CAA-CBA-CGA-O2A
26	1	317	LMG	O7-C10-C11-C12
30	3	422	SQD	O47-C7-C8-C9
21	8	612	CLA	CAA-CBA-CGA-O1A
21	9	604	CLA	CAA-CBA-CGA-O1A
26	A	801	LMG	O9-C10-C11-C12

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	317	LMG	C1-C2-C3-C4-C5-O6

306 monomers are involved in 846 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	807	CLA	13	0
21	G	201	CLA	5	0
21	3	406	CLA	2	0
21	2	602	CLA	5	0
23	9	613	LUT	3	0
21	3	403	CLA	1	0
21	A	812	CLA	4	0
21	3	408	CLA	2	0
21	a	308	CLA	3	0
23	O	2005	LUT	1	0
21	c	611	CLA	1	0
21	B	831	CLA	6	0
21	3	405	CLA	2	0
24	9	615	XAT	2	0
21	A	839	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	404	CLA	1	0
21	7	306	CLA	2	0
21	c	604	CLA	2	0
22	c	607	CHL	4	0
21	A	824	CLA	7	0
22	7	303	CHL	9	0
21	b	306	CLA	1	0
27	9	616	LMU	4	0
25	B	848	BCR	1	0
21	A	838	CLA	4	0
30	3	422	SQD	4	0
21	a	303	CLA	1	0
22	8	606	CHL	7	0
21	A	809	CLA	4	0
29	c	620	PTY	2	0
25	B	846	BCR	1	0
21	7	323	CLA	3	0
22	7	308	CHL	5	0
21	3	413	CLA	2	0
21	A	828	CLA	4	0
21	B	818	CLA	3	0
22	9	606	CHL	5	0
21	3	411	CLA	4	0
21	B	815	CLA	1	0
25	7	319	BCR	4	0
36	C	101	SF4	1	0
21	G	205	CLA	4	0
21	A	830	CLA	9	0
21	a	311	CLA	1	0
21	b	314	CLA	1	0
21	9	611	CLA	1	0
21	B	834	CLA	3	0
21	L	301	CLA	4	0
26	7	320	LMG	7	0
21	B	810	CLA	5	0
21	c	601	CLA	3	0
21	b	313	CLA	1	0
21	9	607	CLA	1	0
21	1	301	CLA	4	0
21	1	304	CLA	3	0
21	B	835	CLA	3	0
21	B	836	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	816	CLA	2	0
28	8	620	LHG	3	0
21	A	840	CLA	6	0
25	L	309	BCR	3	0
21	1	307	CLA	6	0
21	H	203	CLA	1	0
21	3	414	CLA	1	0
21	B	814	CLA	3	0
28	A	853	LHG	3	0
22	b	307	CHL	7	0
22	b	309	CHL	4	0
25	A	849	BCR	4	0
25	J	5004	BCR	4	0
28	7	321	LHG	4	0
21	T	610	CLA	1	0
22	b	308	CHL	3	0
23	a	315	LUT	6	0
26	1	317	LMG	4	0
25	A	848	BCR	8	0
21	c	608	CLA	1	0
21	B	840	CLA	3	0
21	A	819	CLA	5	0
21	a	312	CLA	1	0
35	B	845	PQN	4	0
21	7	315	CLA	2	0
21	8	611	CLA	3	0
29	J	5001	PTY	2	0
21	c	602	CLA	2	0
22	7	309	CHL	10	0
25	1	316	BCR	3	0
21	F	5006	CLA	2	0
21	7	304	CLA	5	0
25	3	419	BCR	2	0
22	c	606	CHL	5	0
27	A	855	LMU	2	0
28	7	324	LHG	1	0
22	7	307	CHL	4	0
21	B	804	CLA	11	0
21	1	309	CLA	2	0
21	a	307	CLA	3	0
21	a	309	CLA	3	0
21	B	824	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	318	LMU	1	0
21	A	817	CLA	20	0
25	3	417	BCR	2	0
24	3	416	XAT	6	0
21	b	304	CLA	5	0
23	T	615	LUT	3	0
21	L	303	CLA	3	0
25	F	5008	BCR	4	0
22	8	607	CHL	2	0
28	1	322	LHG	2	0
21	7	310	CLA	3	0
21	T	612	CLA	2	0
21	A	825	CLA	3	0
21	9	603	CLA	1	0
21	A	822	CLA	3	0
21	A	808	CLA	2	0
22	1	305	CHL	3	0
37	A	857	4RF	2	0
30	2	618	SQD	4	0
29	L	308	PTY	1	0
21	B	823	CLA	1	0
26	A	801	LMG	2	0
25	I	203	BCR	4	0
21	9	605	CLA	3	0
21	T	606	CLA	4	0
21	1	311	CLA	4	0
21	T	611	CLA	1	0
23	2	614	LUT	1	0
21	O	2002	CLA	1	0
25	8	618	BCR	6	0
28	F	5003	LHG	3	0
21	B	820	CLA	2	0
21	T	609	CLA	2	0
21	A	833	CLA	5	0
21	b	310	CLA	1	0
21	B	839	CLA	2	0
24	7	318	XAT	3	0
21	3	402	CLA	2	0
21	9	602	CLA	2	0
21	c	612	CLA	1	0
21	8	622	CLA	10	0
21	9	601	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	841	CLA	5	0
25	G	202	BCR	4	0
21	A	829	CLA	8	0
21	B	833	CLA	6	0
28	a	301	LHG	1	0
35	A	844	PQN	1	0
24	9	614	XAT	5	0
22	8	601	CHL	2	0
28	F	5001	LHG	1	0
21	8	603	CLA	2	0
29	2	620	PTY	1	0
21	a	305	CLA	2	0
21	B	828	CLA	3	0
21	a	302	CLA	5	0
21	J	5002	CLA	2	0
31	F	5002	3PH	1	0
21	F	5005	CLA	2	0
25	3	418	BCR	4	0
21	3	409	CLA	2	0
28	b	303	LHG	3	0
21	1	310	CLA	3	0
21	T	603	CLA	2	0
21	8	612	CLA	1	0
31	2	619	3PH	4	0
21	9	604	CLA	2	0
25	A	846	BCR	6	0
24	T	616	XAT	4	0
23	b	317	LUT	2	0
21	B	841	CLA	1	0
22	2	601	CHL	6	0
21	7	314	CLA	4	0
21	b	311	CLA	4	0
21	B	821	CLA	3	0
21	A	807	CLA	6	0
21	7	313	CLA	1	0
23	1	314	LUT	7	0
24	b	318	XAT	3	0
24	c	616	XAT	1	0
21	L	304	CLA	5	0
21	O	2001	CLA	1	0
21	B	816	CLA	6	0
21	B	809	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	617	BCR	2	0
25	F	5004	BCR	5	0
22	T	602	CHL	10	0
25	A	850	BCR	5	0
21	A	805	CLA	2	0
28	1	323	LHG	5	0
21	A	835	CLA	5	0
21	B	830	CLA	5	0
21	3	410	CLA	3	0
21	B	813	CLA	3	0
23	7	317	LUT	1	0
26	3	421	LMG	2	0
21	A	806	CLA	1	0
29	c	619	PTY	2	0
21	B	826	CLA	7	0
23	c	615	LUT	1	0
28	a	318	LHG	1	0
21	a	313	CLA	3	0
21	B	844	CLA	7	0
25	J	5003	BCR	4	0
21	A	818	CLA	2	0
23	3	415	LUT	1	0
21	A	815	CLA	6	0
21	c	609	CLA	1	0
25	A	851	BCR	3	0
21	1	306	CLA	2	0
32	7	301	DGD	2	0
21	A	823	CLA	6	0
21	B	819	CLA	1	0
21	A	834	CLA	3	0
21	1	308	CLA	3	0
21	8	613	CLA	3	0
32	8	602	DGD	4	0
26	G	207	LMG	5	0
21	1	303	CLA	3	0
21	A	843	CLA	6	0
23	B	801	LUT	4	0
25	B	805	BCR	8	0
25	B	849	BCR	4	0
21	A	810	CLA	7	0
21	2	603	CLA	8	0
21	A	811	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	302	CLA	3	0
21	A	832	CLA	5	0
21	1	321	CLA	4	0
21	A	836	CLA	4	0
29	I	201	PTY	7	0
22	b	302	CHL	10	0
21	A	821	CLA	6	0
21	2	610	CLA	2	0
32	A	802	DGD	4	0
25	b	319	BCR	6	0
23	2	616	LUT	1	0
21	B	812	CLA	5	0
25	A	847	BCR	5	0
22	3	401	CHL	8	0
21	2	613	CLA	3	0
21	A	826	CLA	7	0
21	A	814	CLA	6	0
21	L	305	CLA	1	0
21	3	412	CLA	5	0
21	B	806	CLA	4	0
25	I	202	BCR	5	0
21	B	822	CLA	5	0
21	2	608	CLA	4	0
22	T	601	CHL	5	0
21	B	811	CLA	3	0
22	c	605	CHL	5	0
21	B	832	CLA	5	0
21	B	842	CLA	5	0
21	K	202	CLA	2	0
29	H	201	PTY	1	0
25	T	617	BCR	1	0
26	F	5009	LMG	3	0
21	B	825	CLA	4	0
21	B	817	CLA	6	0
21	b	305	CLA	2	0
28	1	319	LHG	2	0
21	3	407	CLA	8	0
21	B	808	CLA	2	0
21	8	604	CLA	9	0
22	a	306	CHL	2	0
21	A	856	CLA	2	0
21	B	837	CLA	7	0

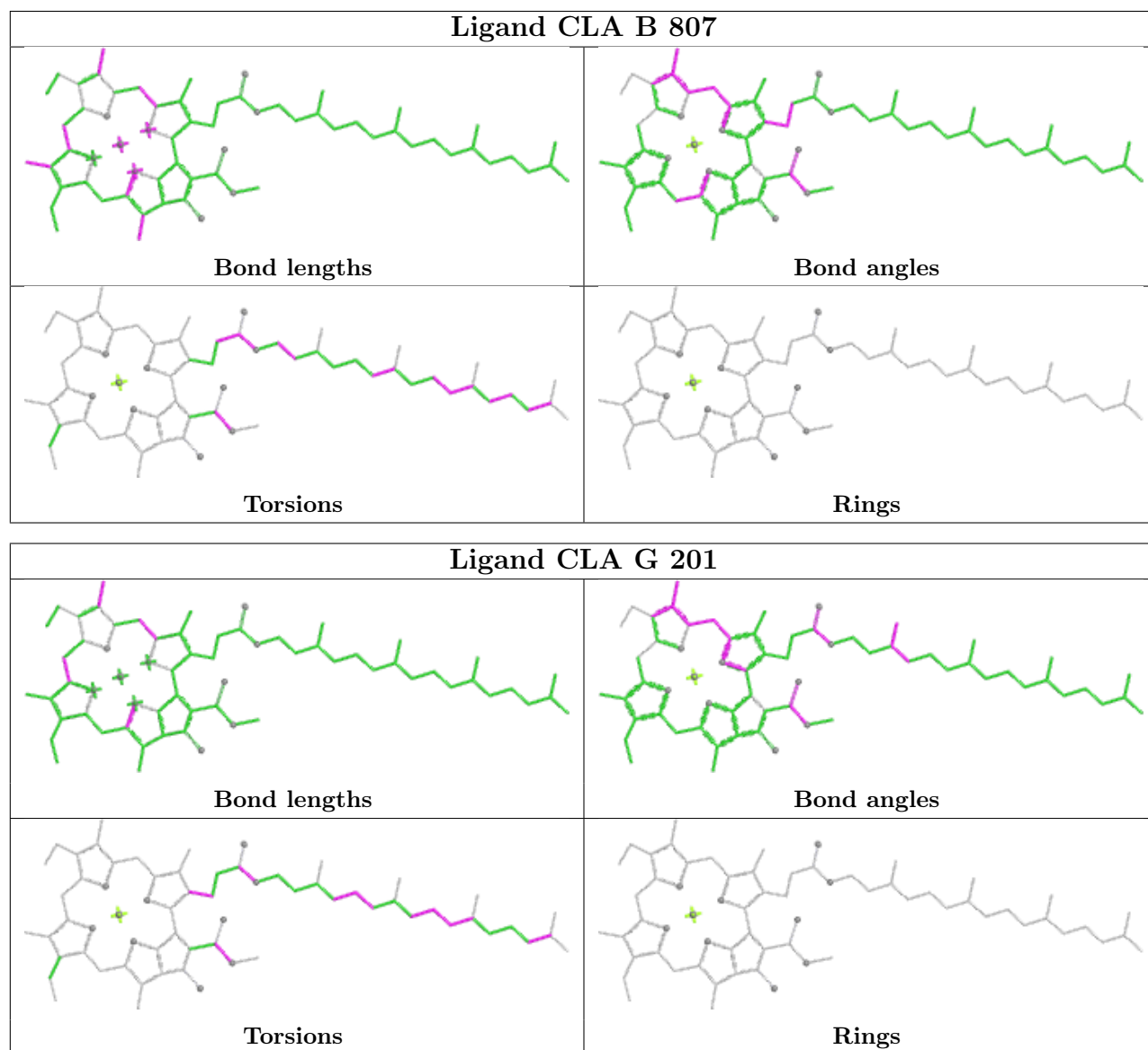
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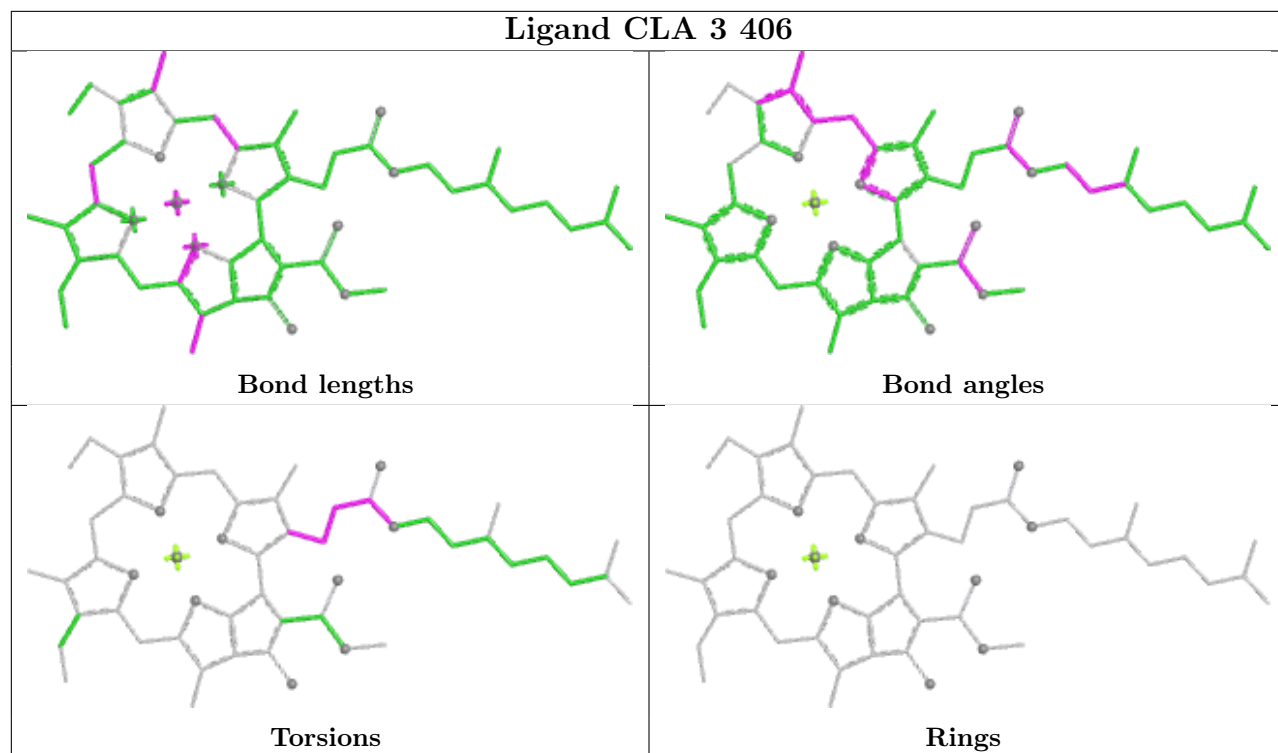
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	847	BCR	8	0
21	c	614	CLA	1	0
21	B	843	CLA	3	0
21	K	203	CLA	3	0
21	A	804	CLA	8	0
32	B	850	DGD	3	0
21	a	304	CLA	2	0
21	8	605	CLA	2	0
28	A	852	LHG	2	0
24	1	315	XAT	12	0
21	2	607	CLA	1	0
25	K	205	BCR	6	0
28	H	202	LHG	3	0
21	b	316	CLA	2	0
25	B	852	BCR	4	0
21	A	831	CLA	8	0
21	A	827	CLA	6	0
21	7	311	CLA	2	0
21	B	838	CLA	3	0
22	2	606	CHL	2	0
23	2	615	LUT	4	0
21	A	813	CLA	3	0
21	F	5007	CLA	1	0
24	a	316	XAT	5	0
21	9	610	CLA	1	0
24	8	617	XAT	3	0
21	2	611	CLA	3	0
27	A	854	LMU	2	0
21	K	201	CLA	1	0
21	8	615	CLA	1	0
34	A	803	CL0	8	0
36	A	845	SF4	4	0
25	O	2004	BCR	1	0
21	B	827	CLA	4	0
21	B	829	CLA	5	0
21	9	608	CLA	2	0
21	A	820	CLA	4	0
21	T	608	CLA	2	0
22	8	608	CHL	5	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

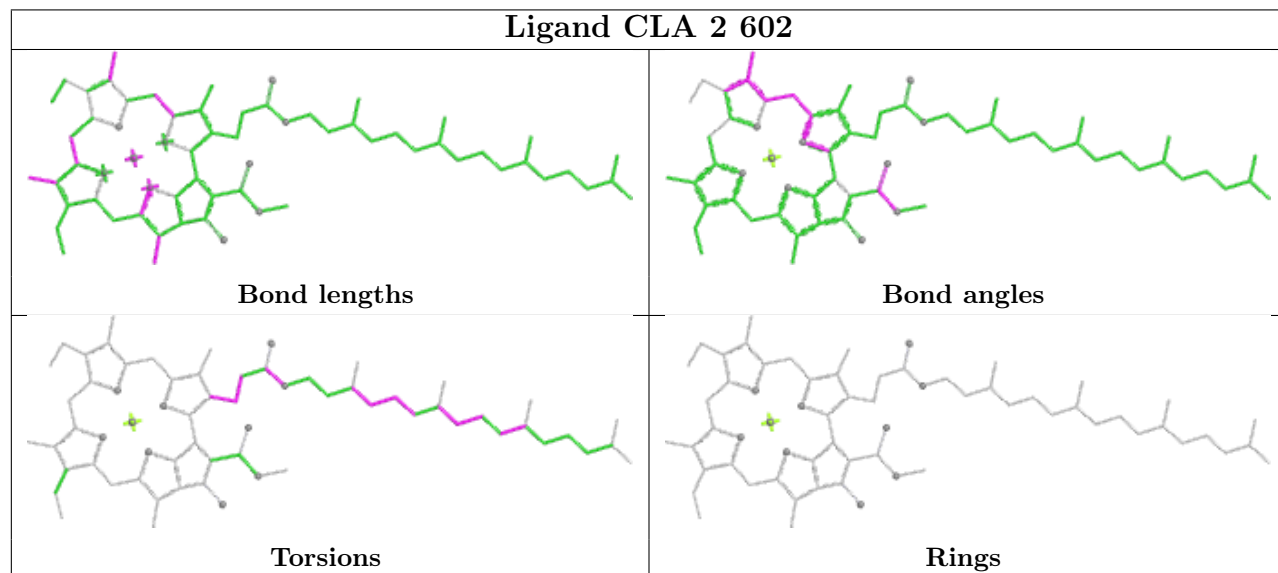
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



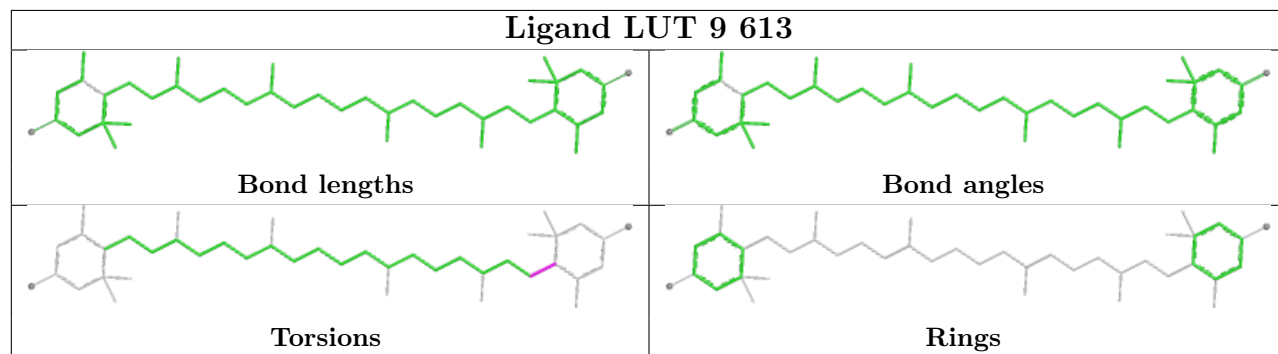
Ligand CLA 3 406



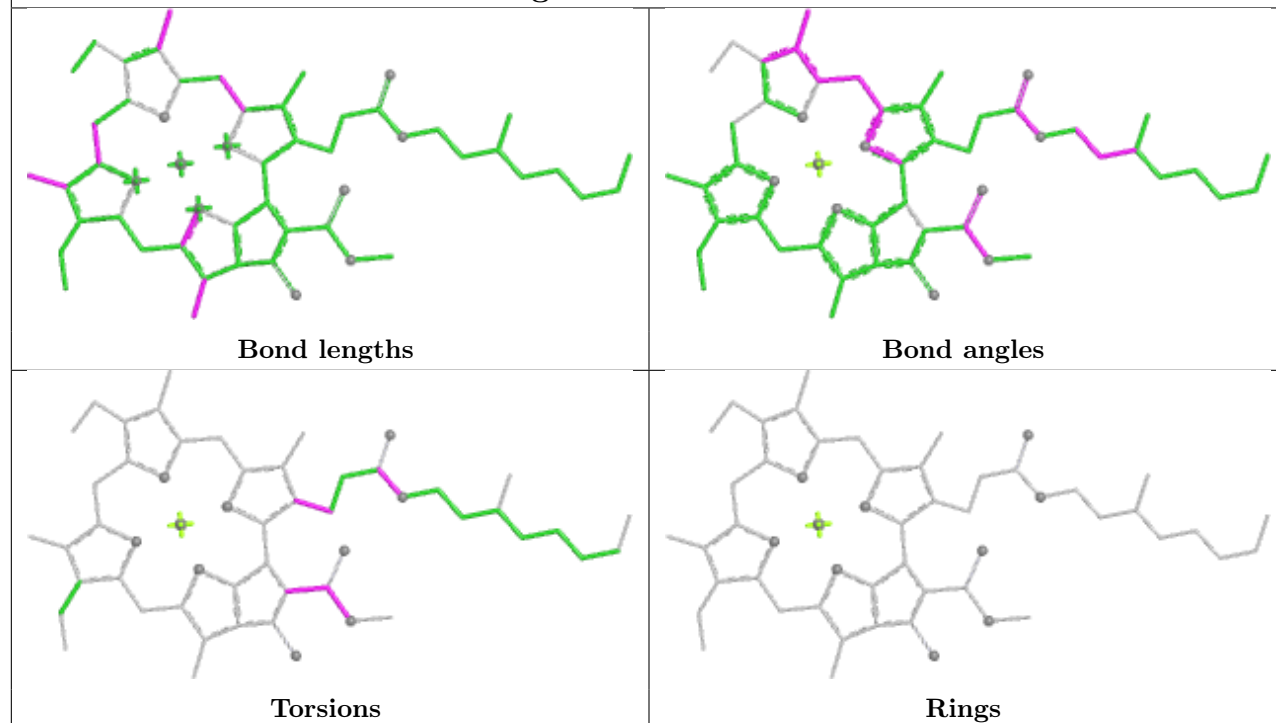
Ligand CLA 2 602



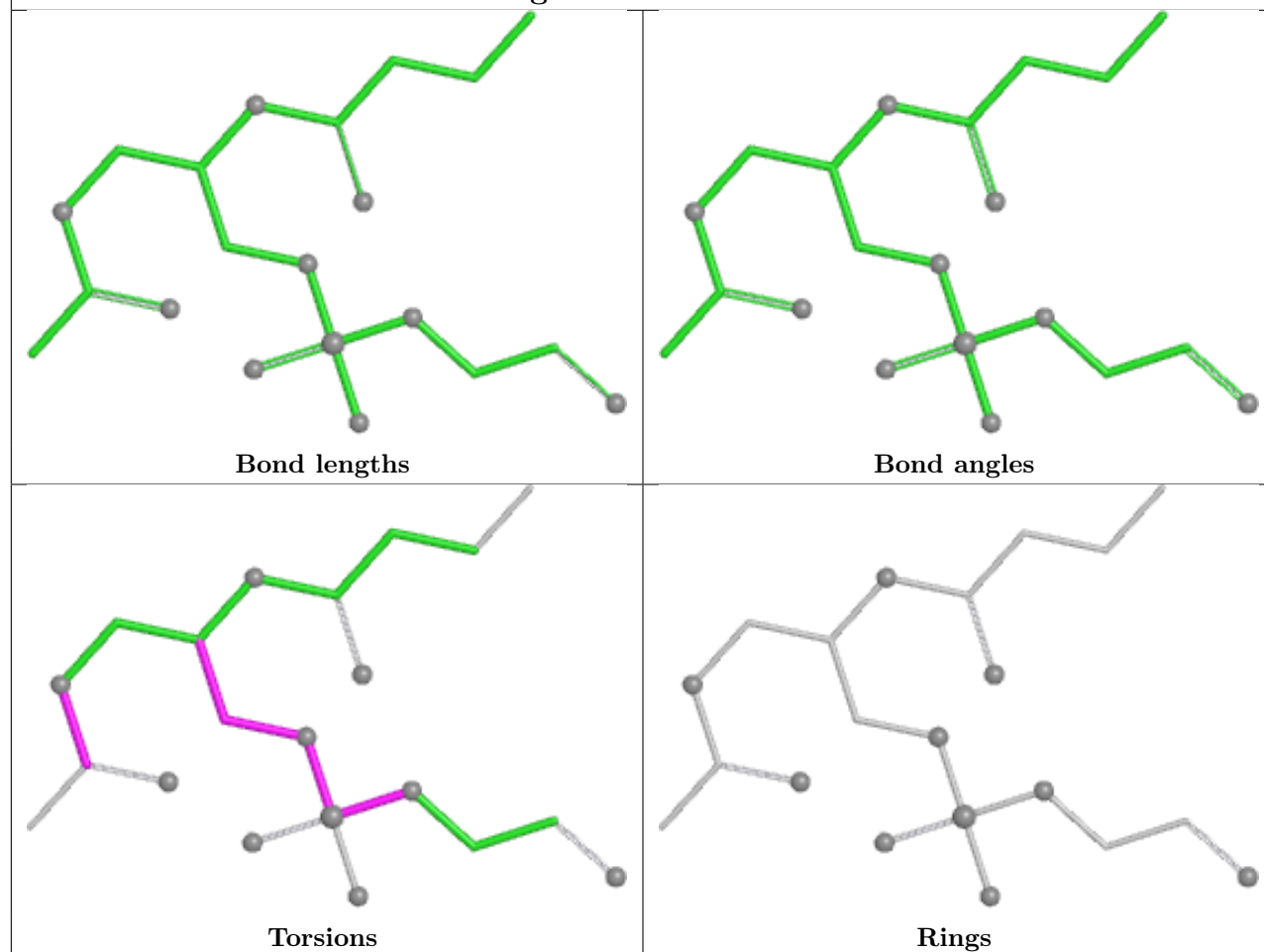
Ligand LUT 9 613



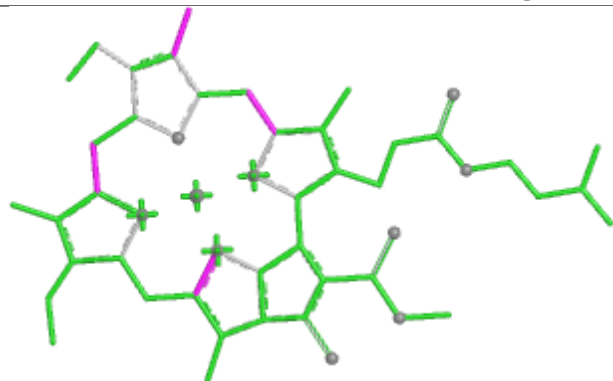
Ligand CLA A 842



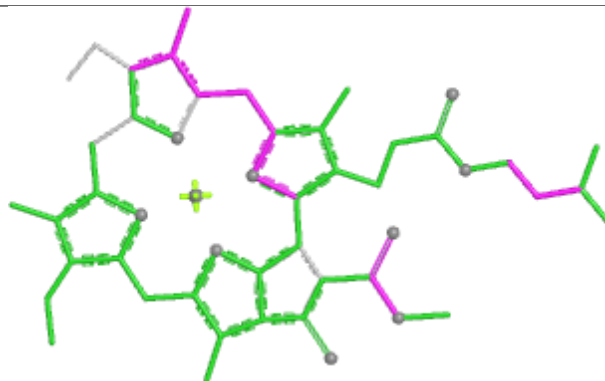
Ligand PTY 1 320



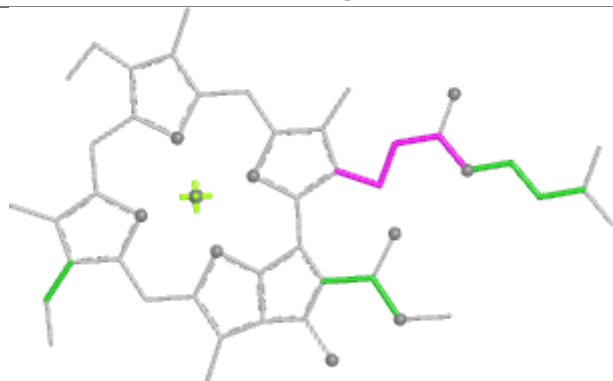
Ligand CLA 3 403



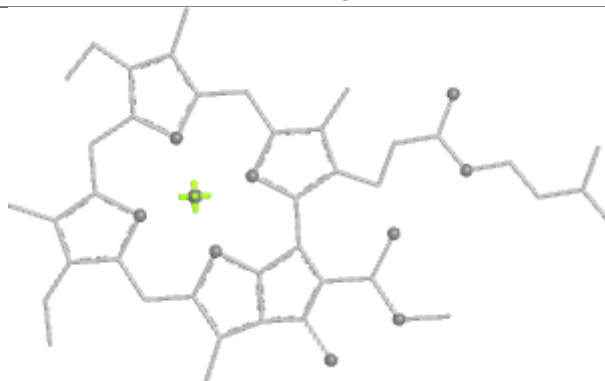
Bond lengths



Bond angles

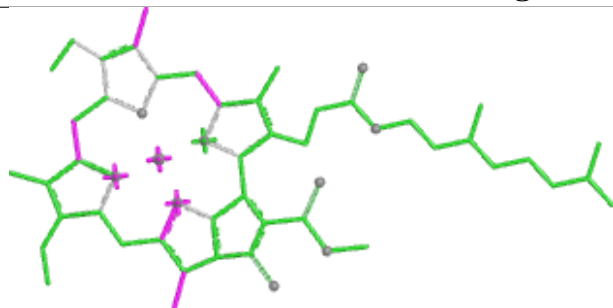


Torsions

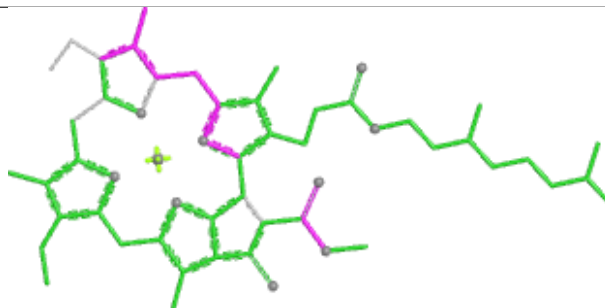


Rings

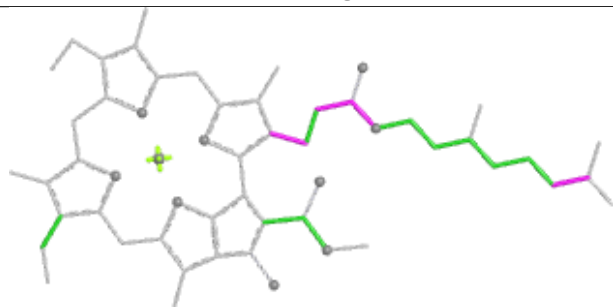
Ligand CLA A 812



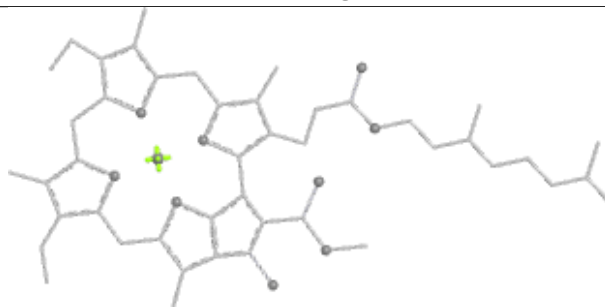
Bond lengths



Bond angles

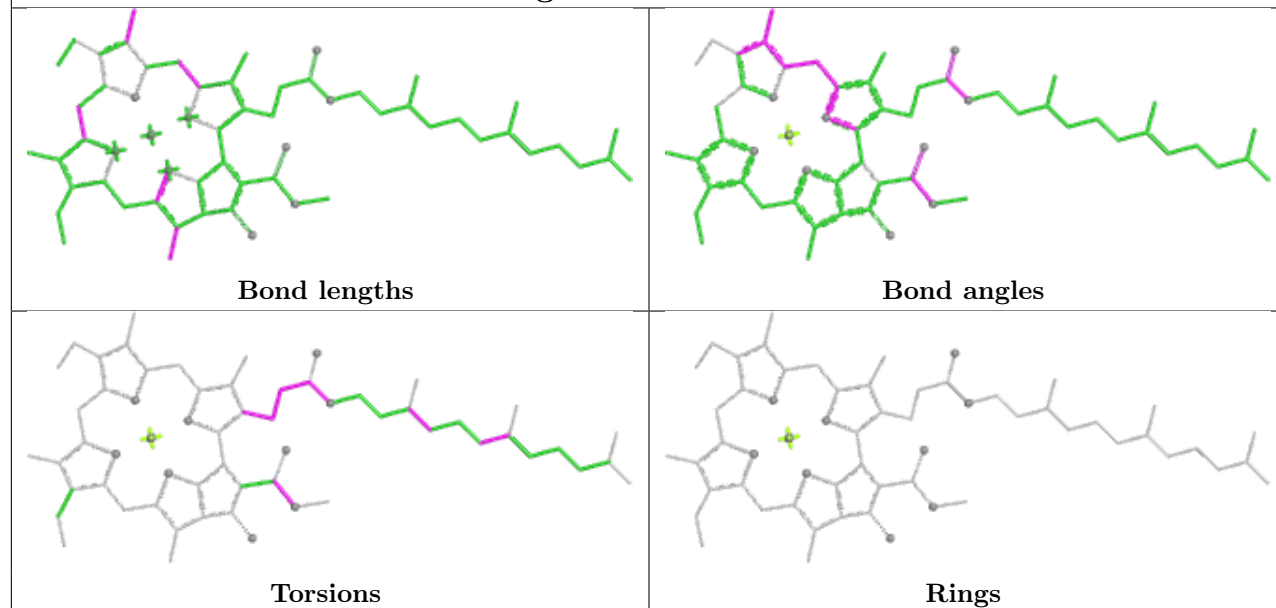


Torsions

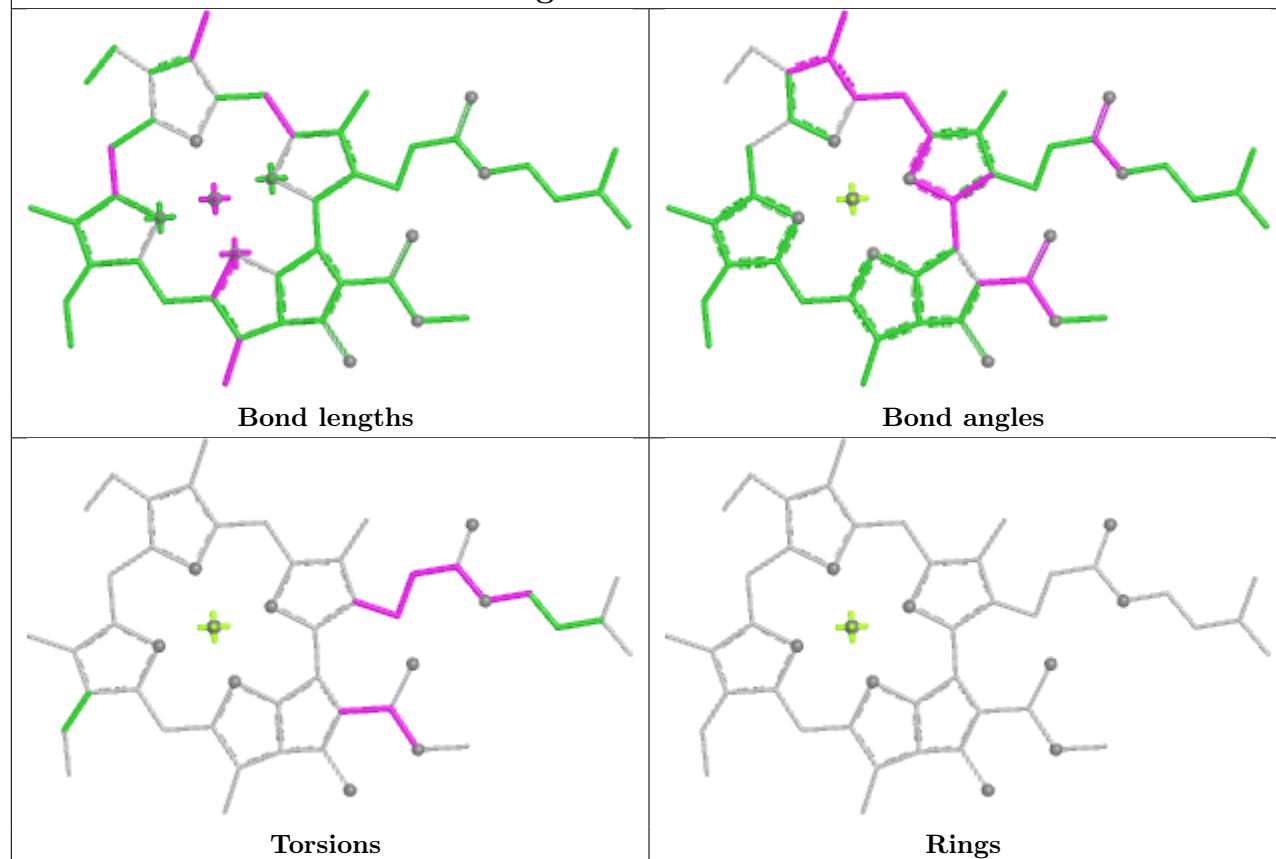


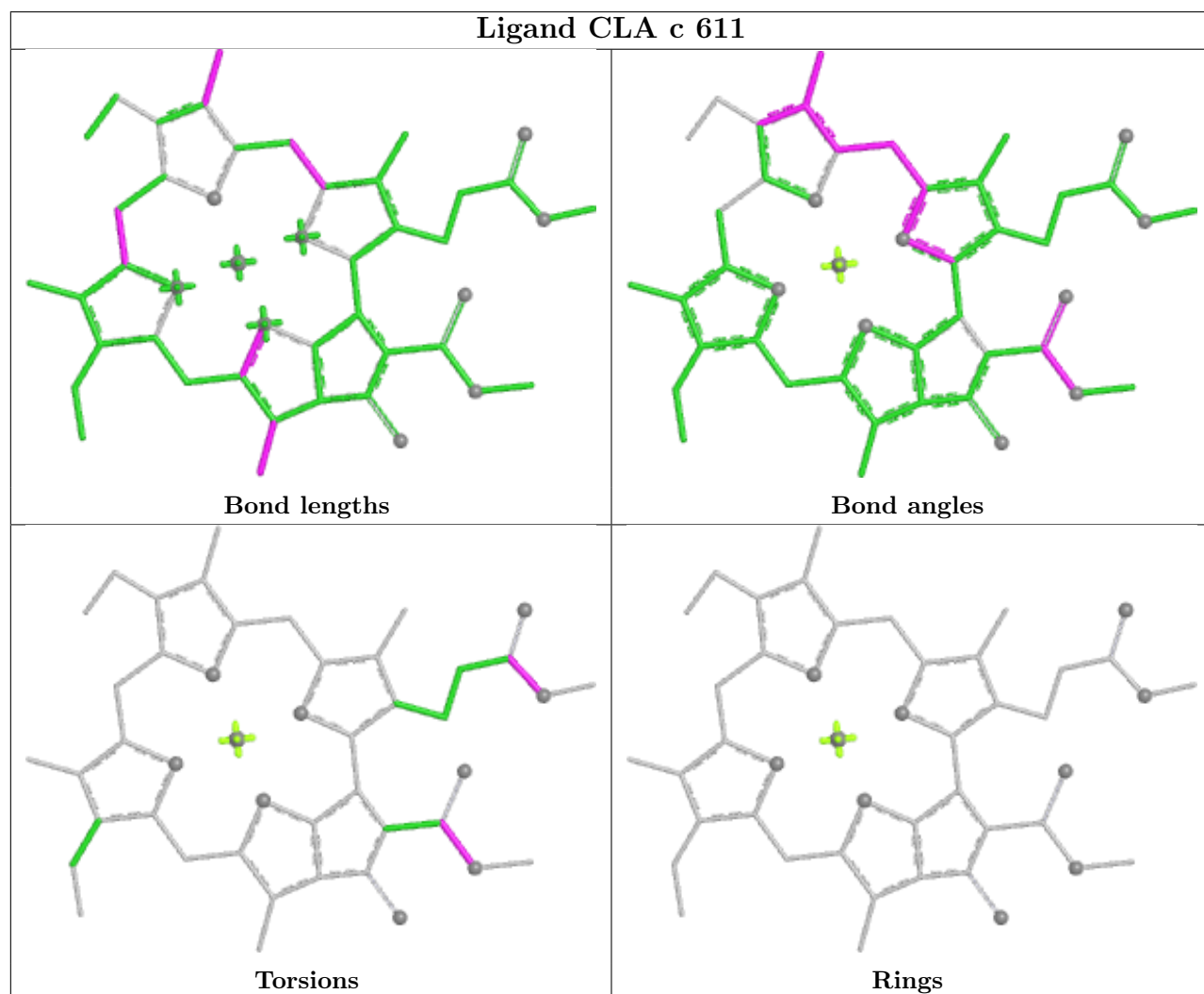
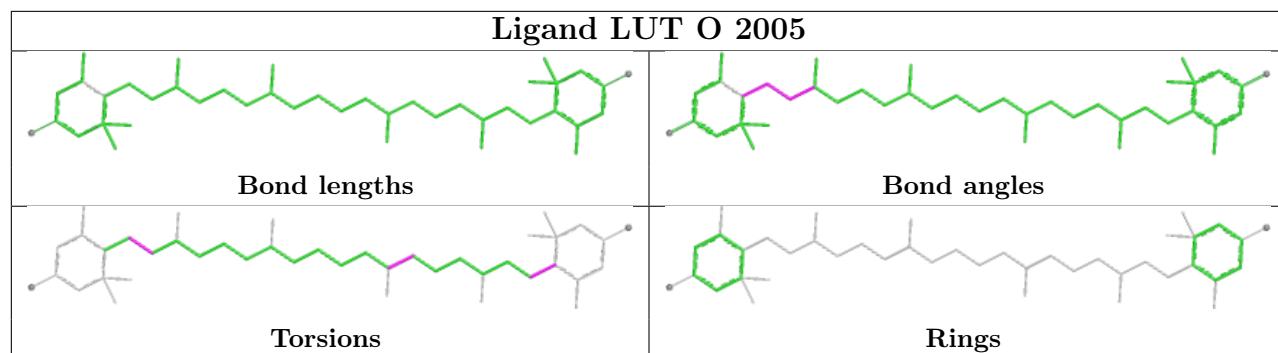
Rings

Ligand CLA 3 408

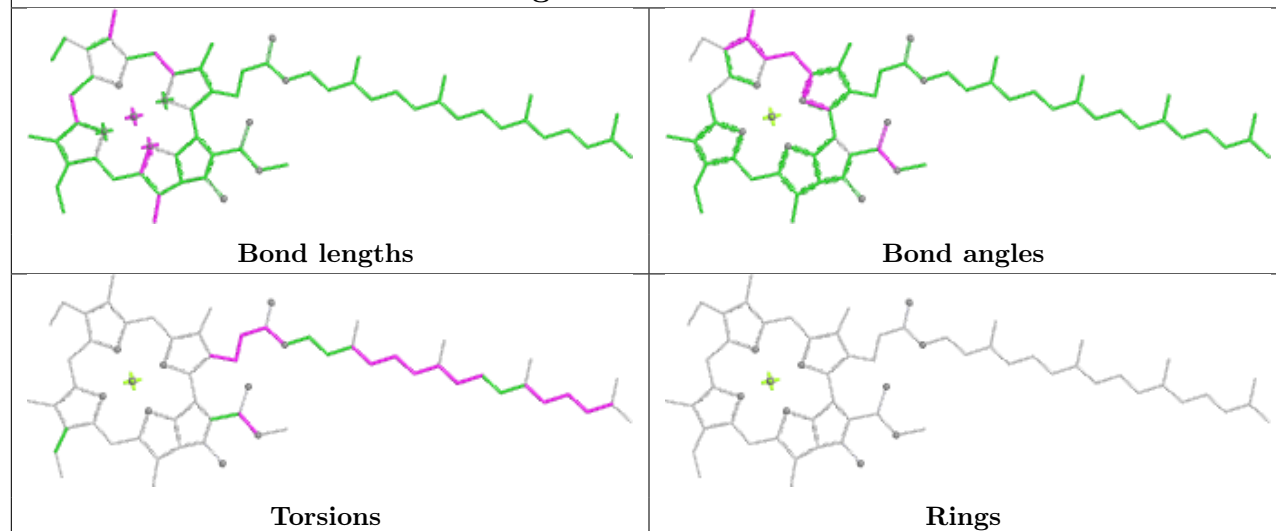


Ligand CLA a 308

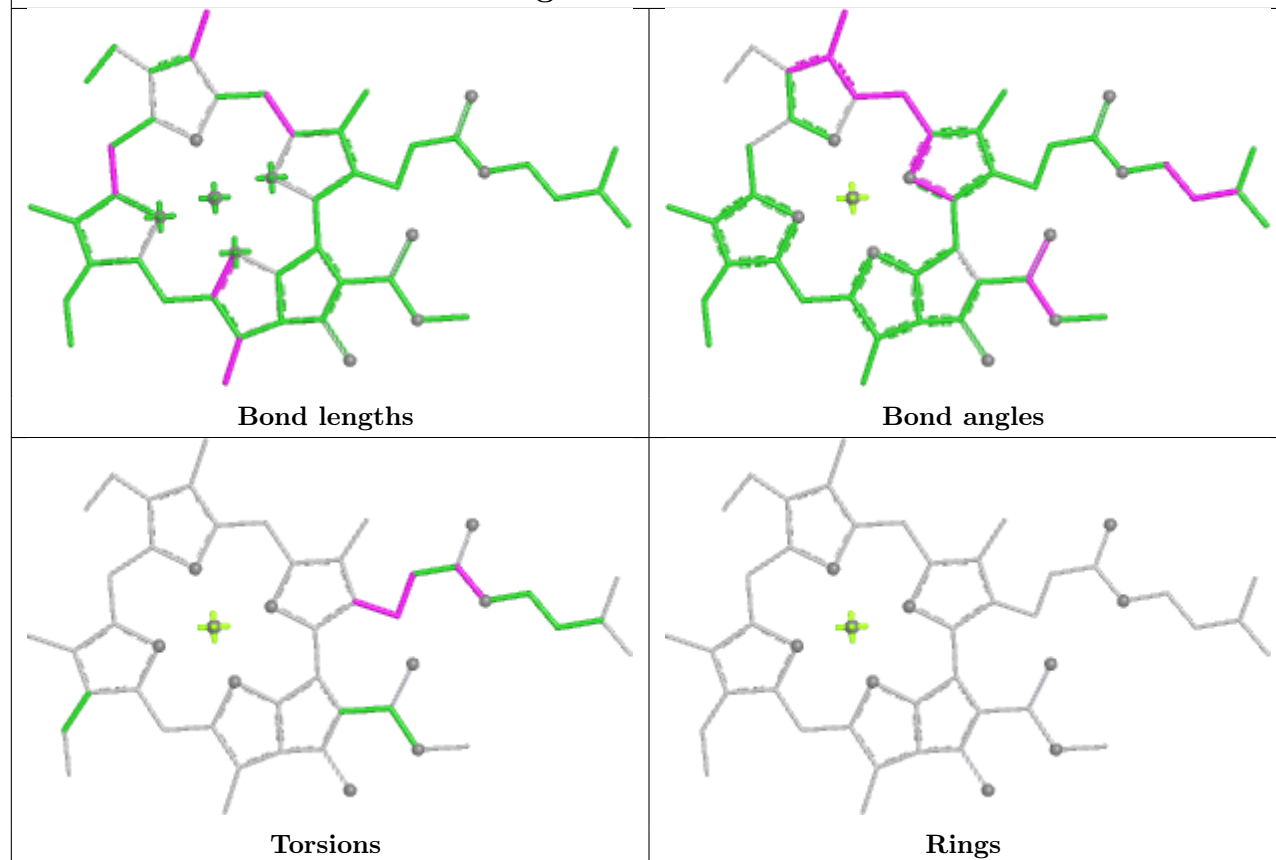


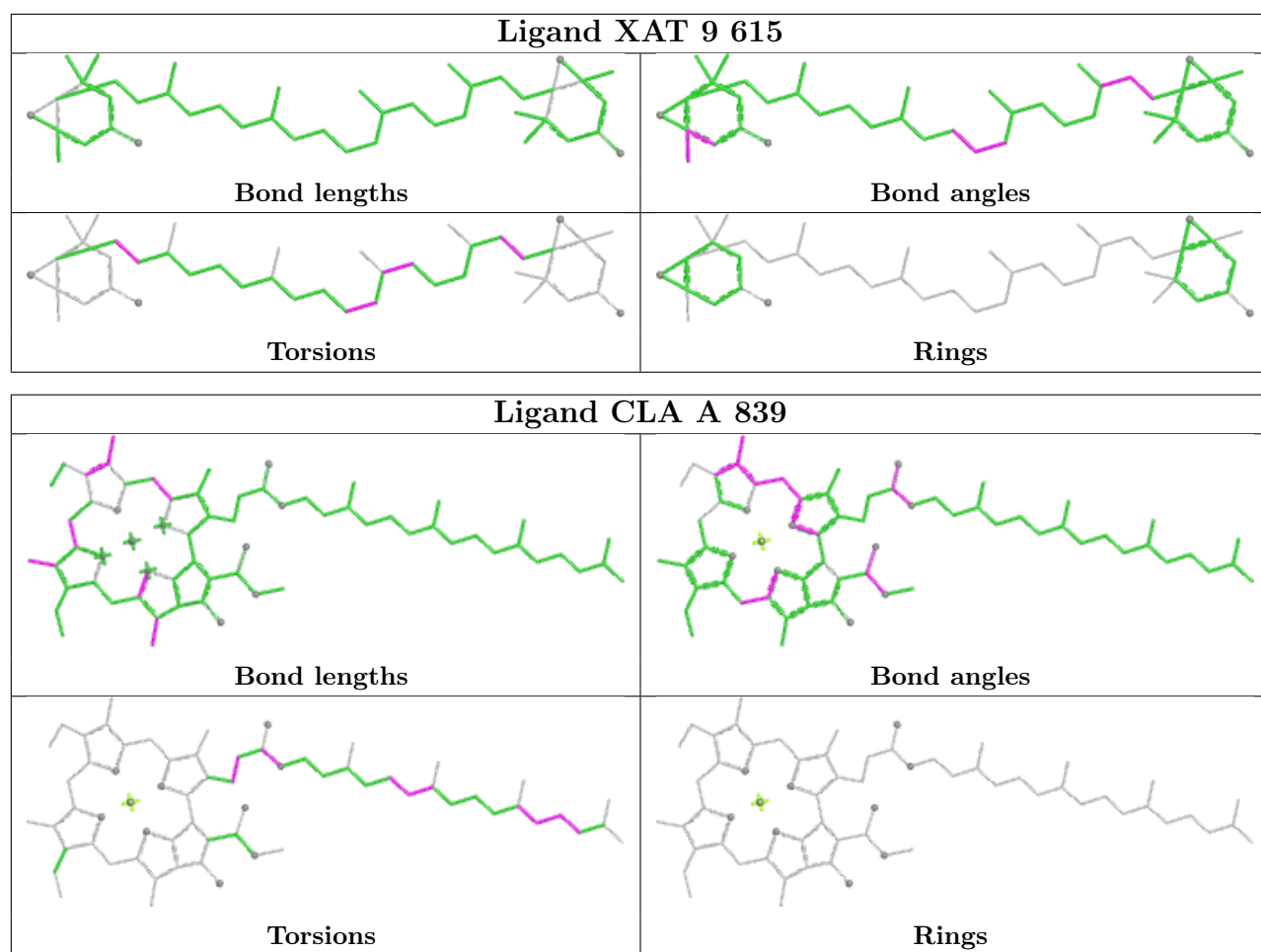


Ligand CLA B 831

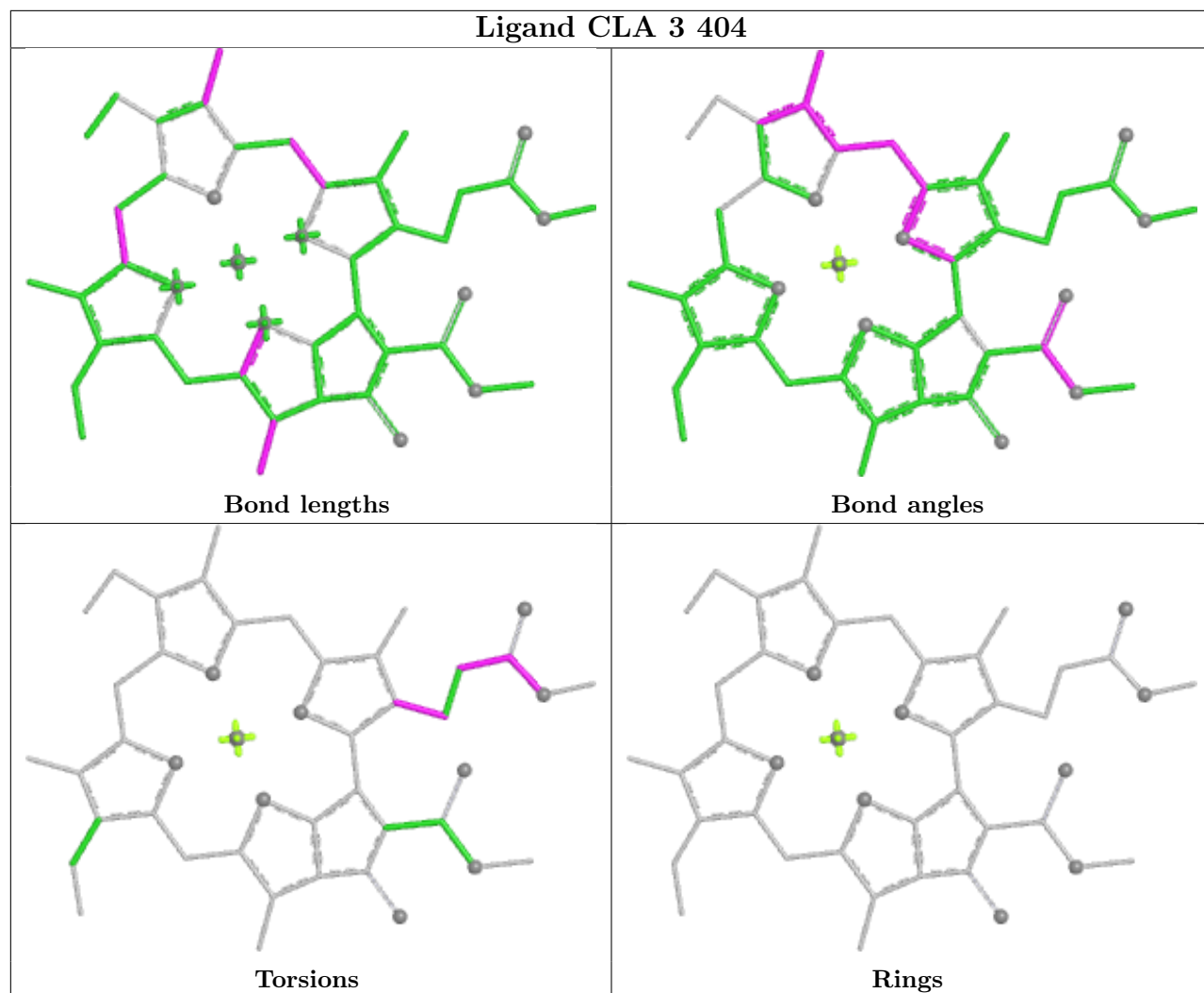


Ligand CLA 3 405

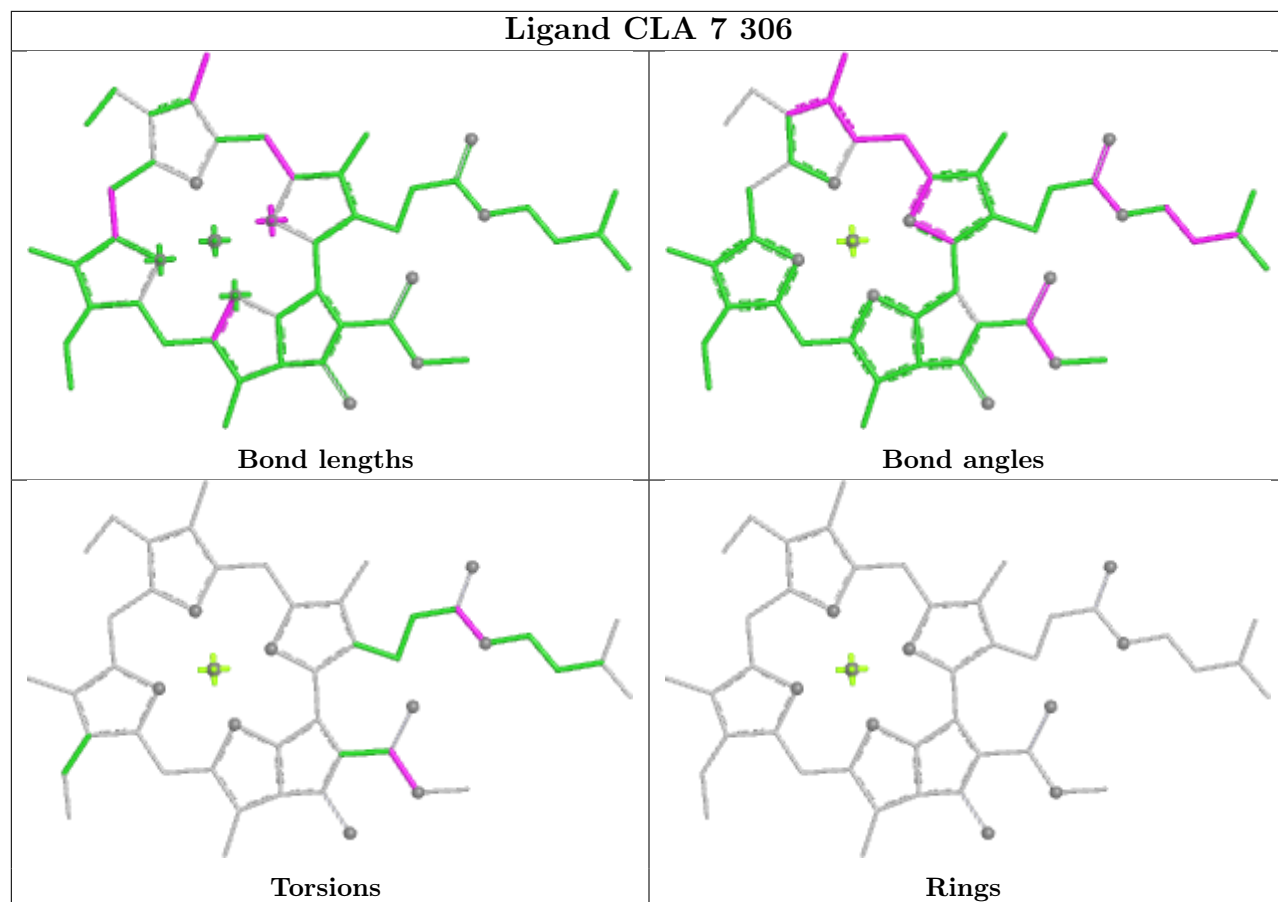




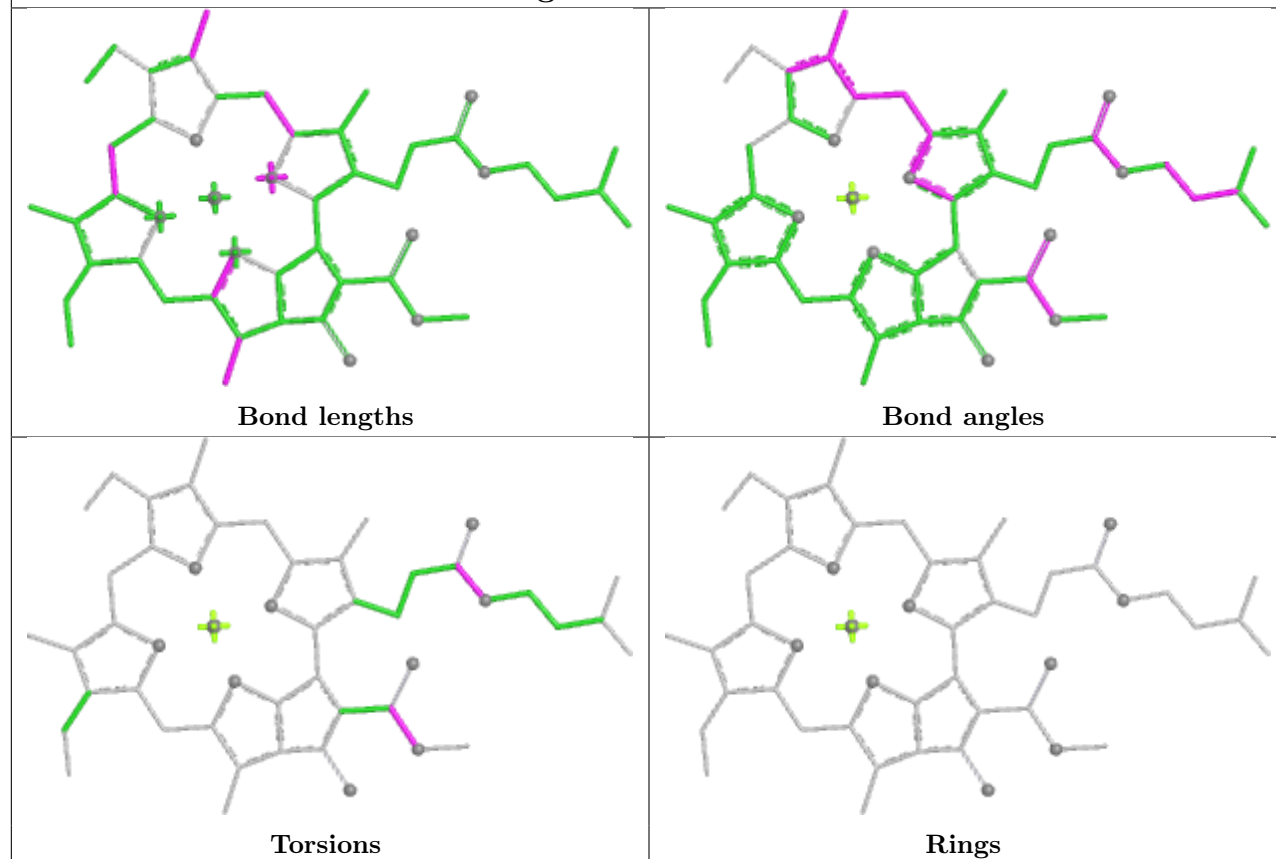
Ligand CLA 3 404



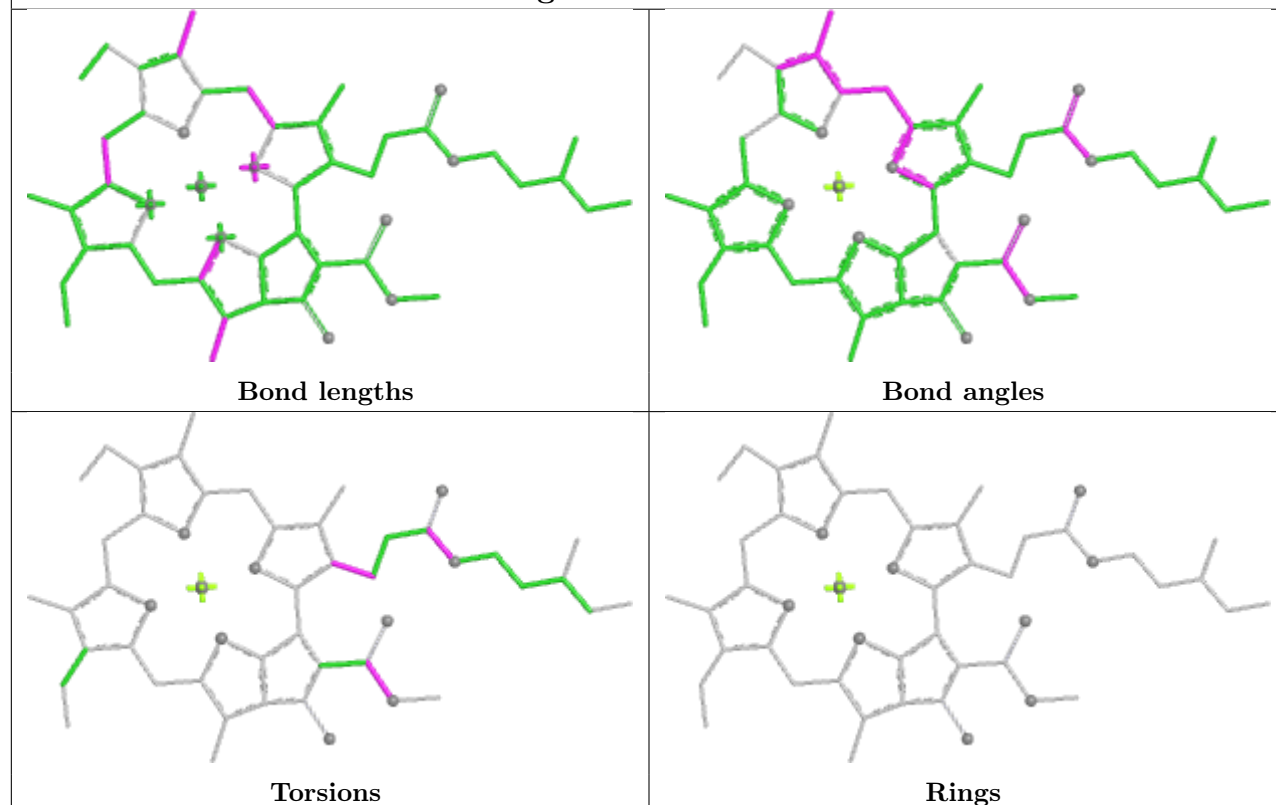
Ligand CLA 7 306



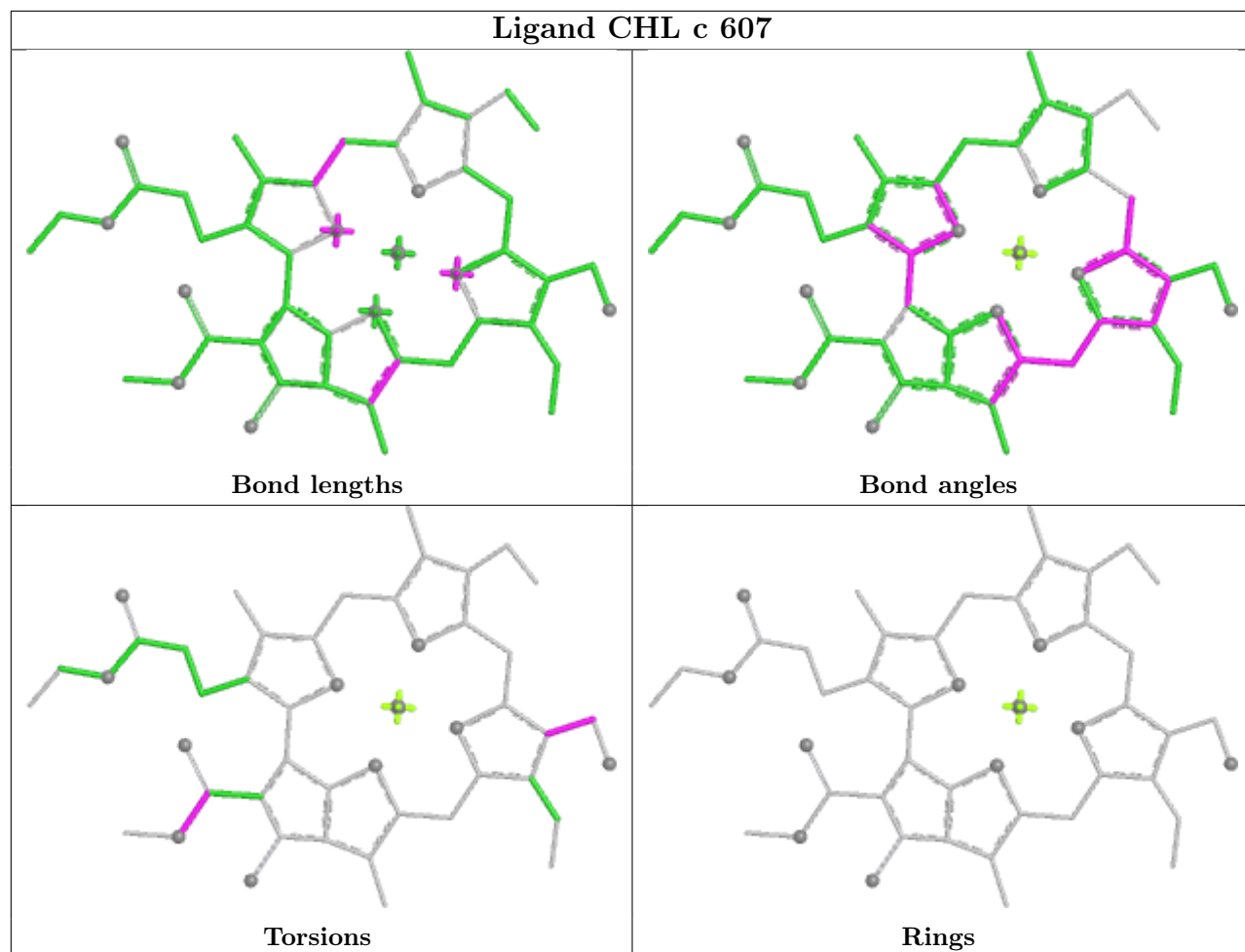
Ligand CLA c 604



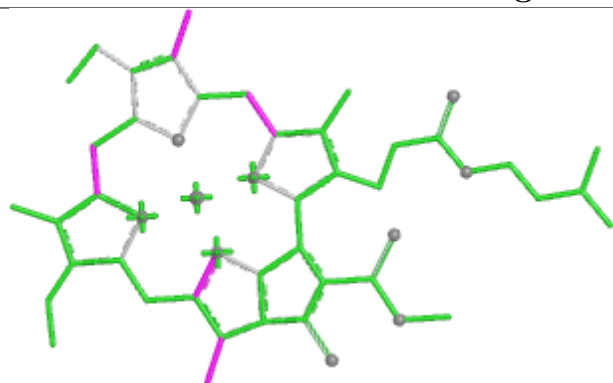
Ligand CLA c 603



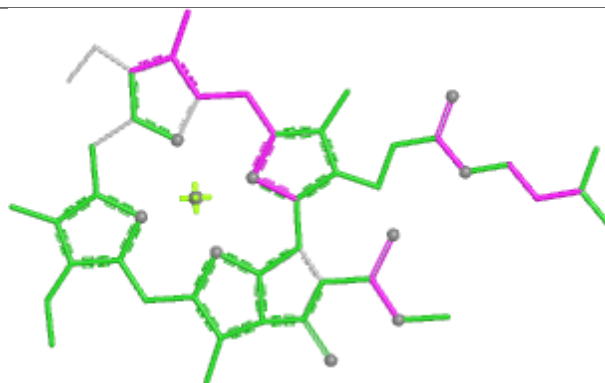
Ligand CHL c 607



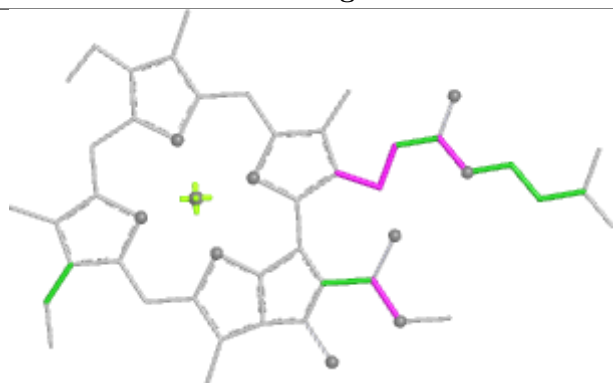
Ligand CLA T 607



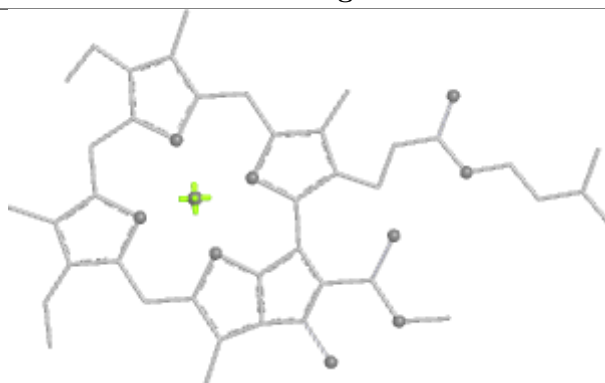
Bond lengths



Bond angles

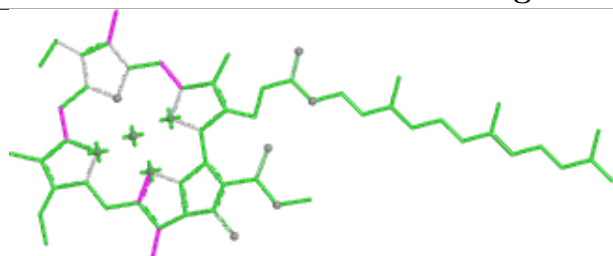


Torsions

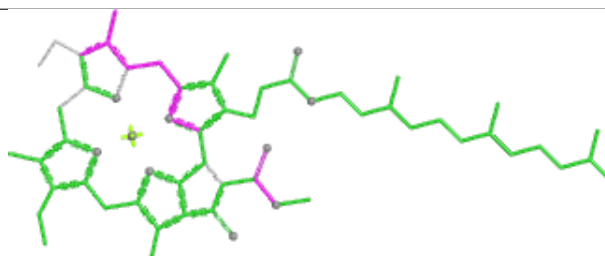


Rings

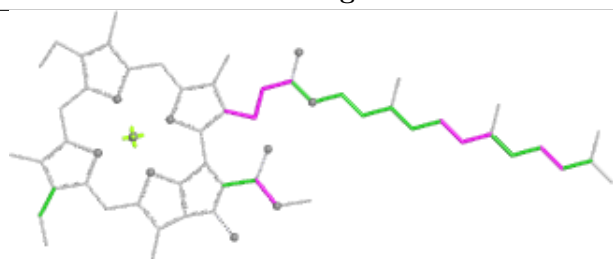
Ligand CLA A 824



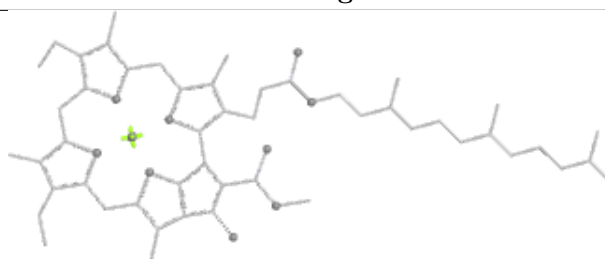
Bond lengths



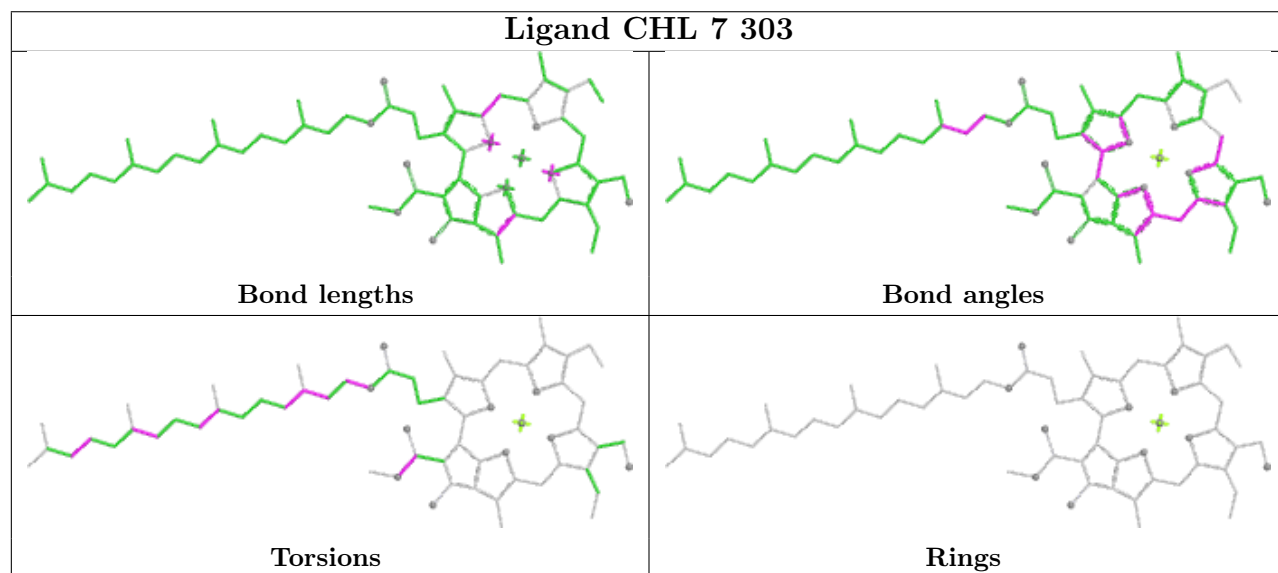
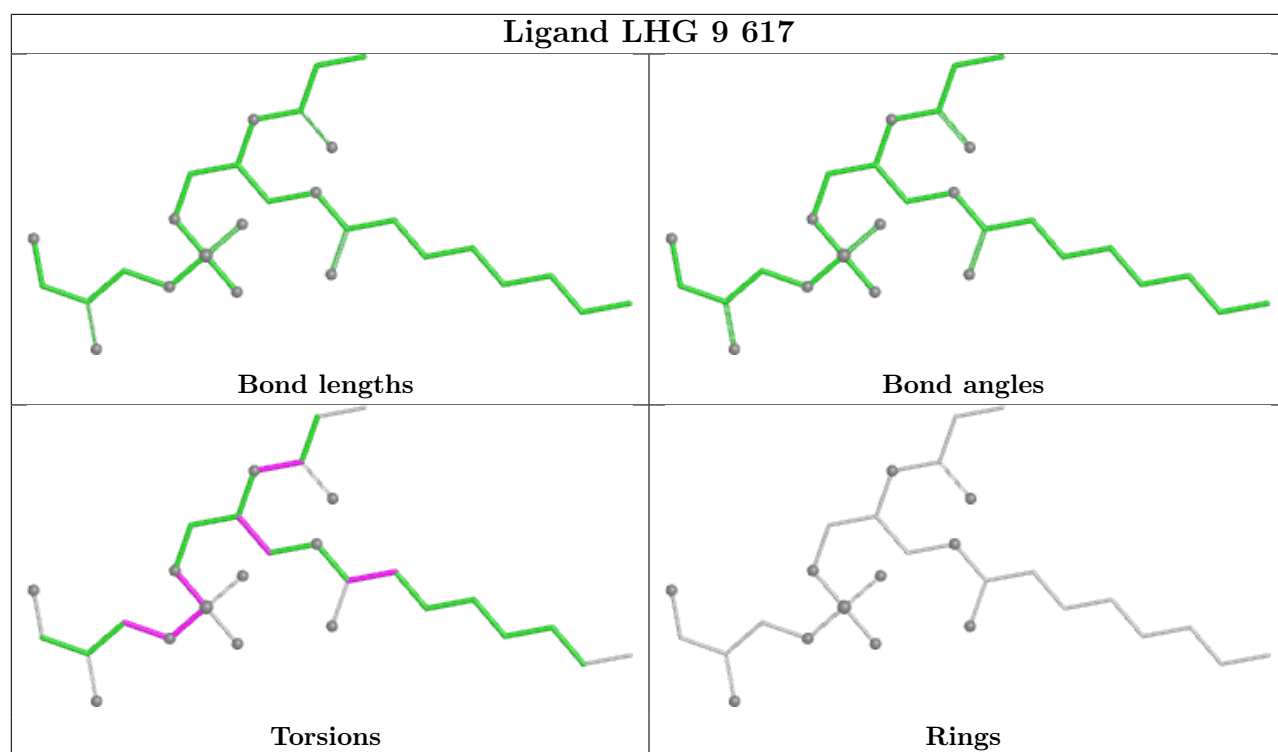
Bond angles



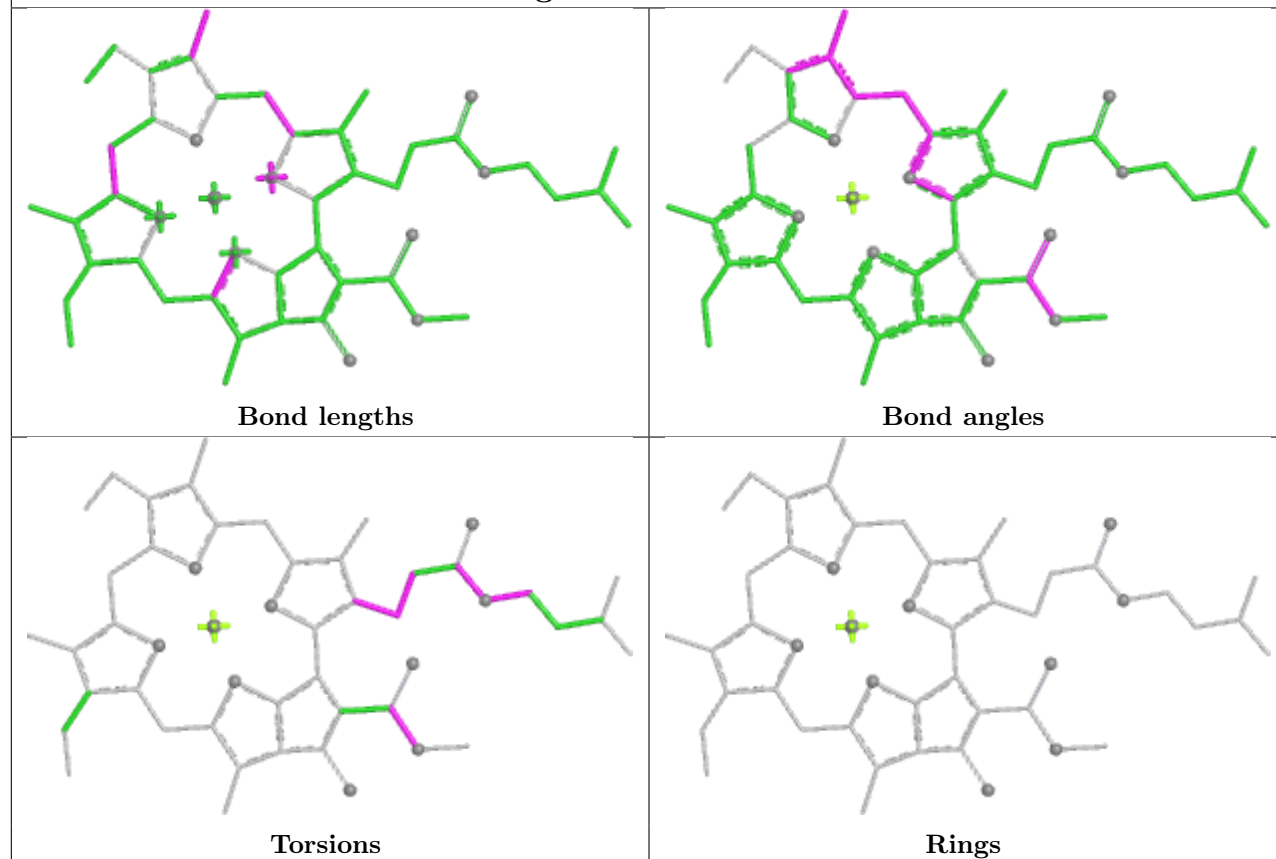
Torsions



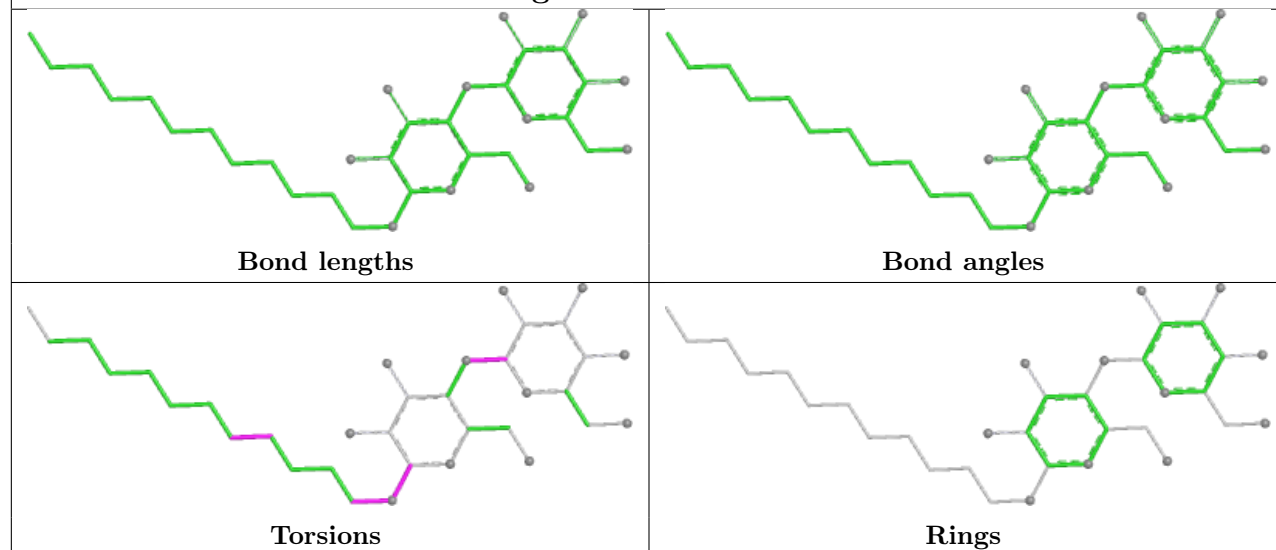
Rings

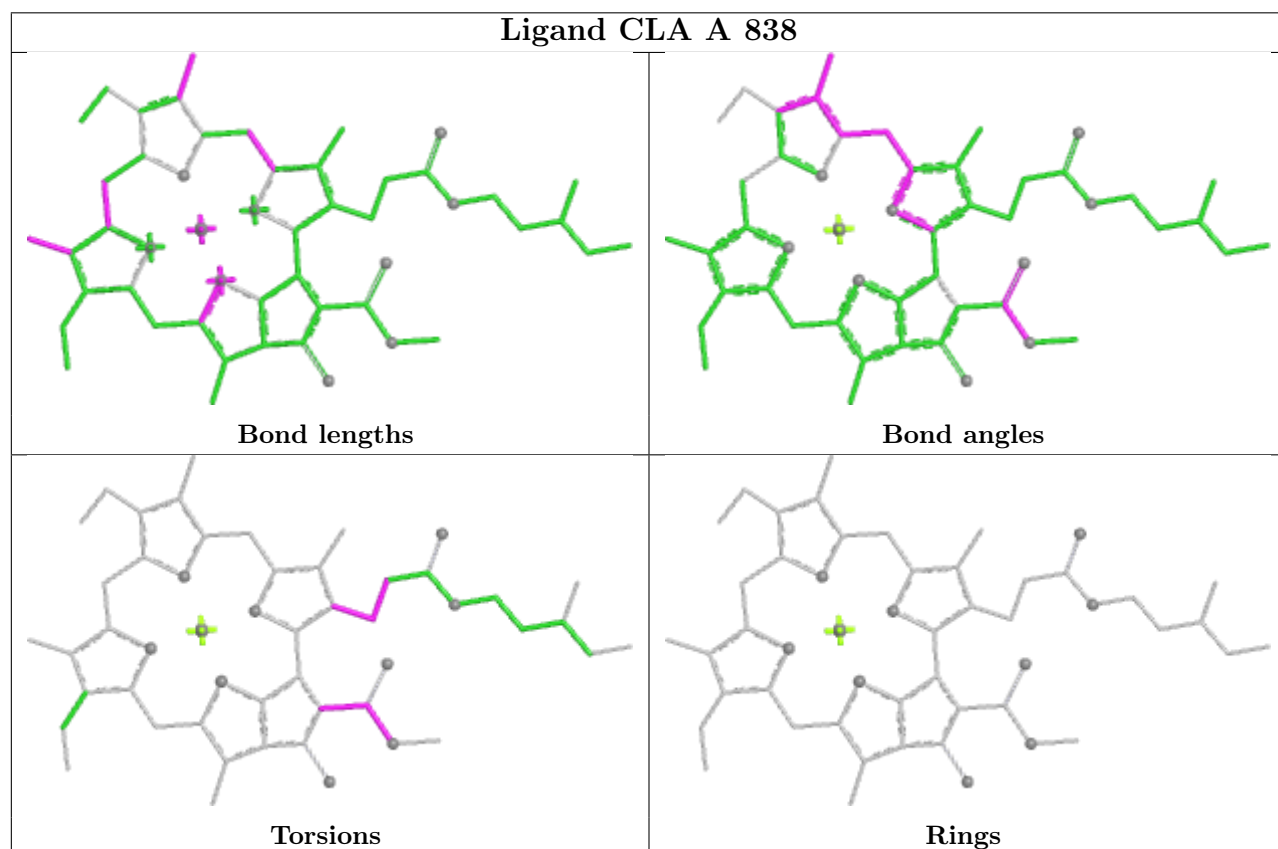
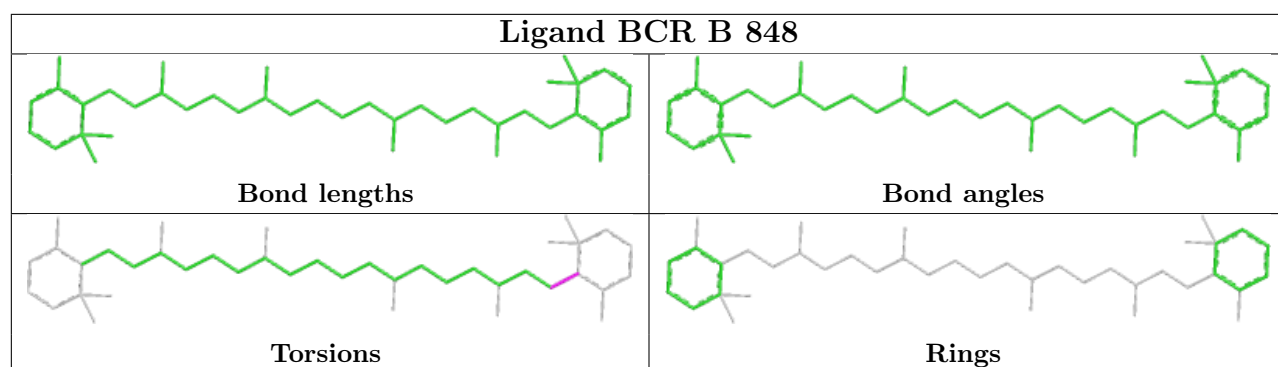


Ligand CLA b 306

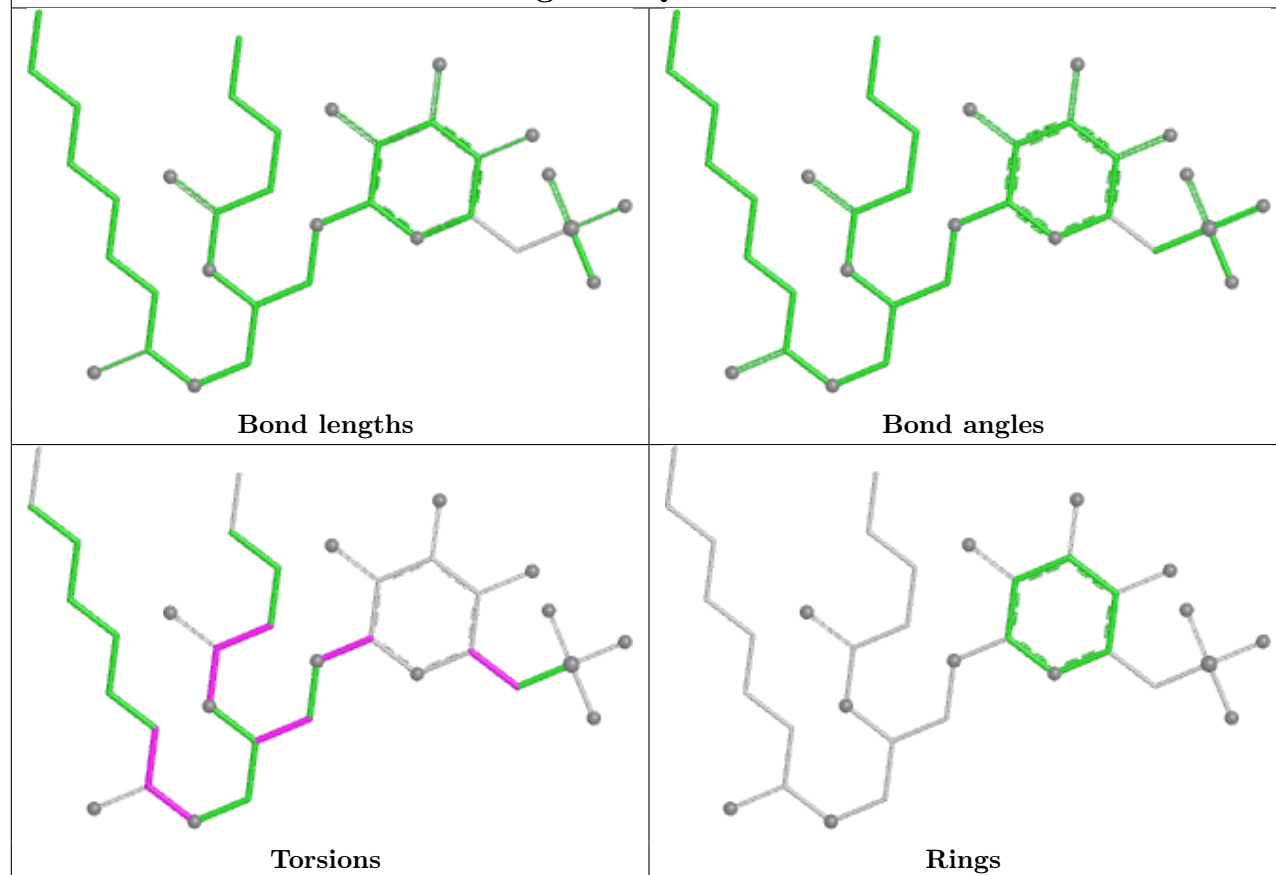


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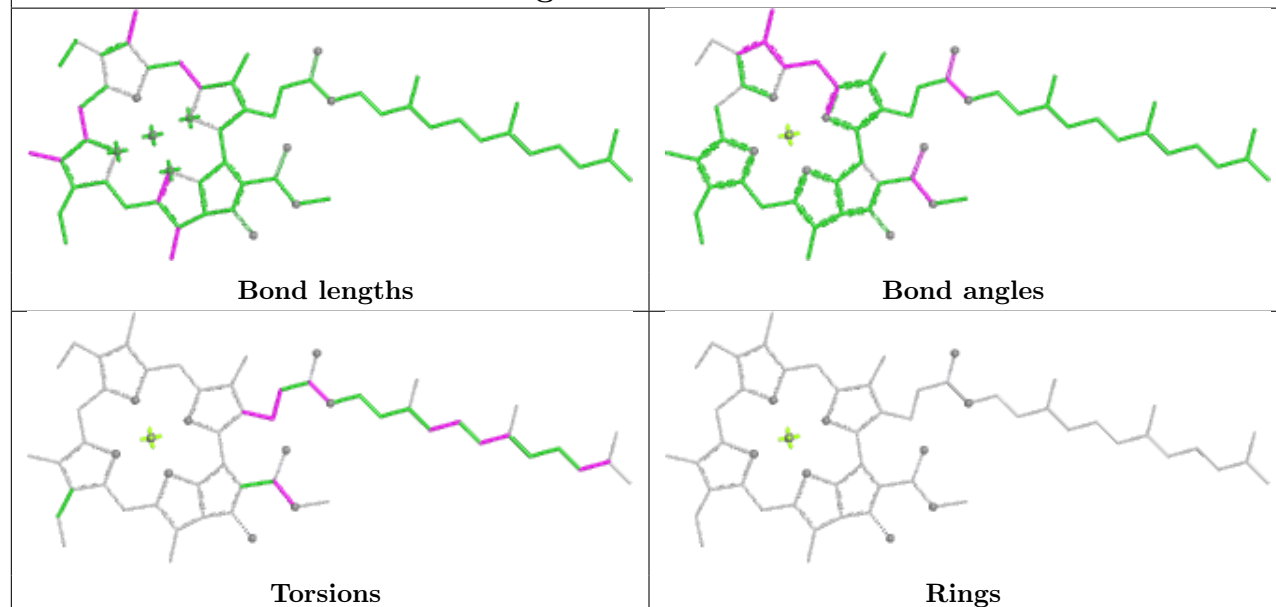




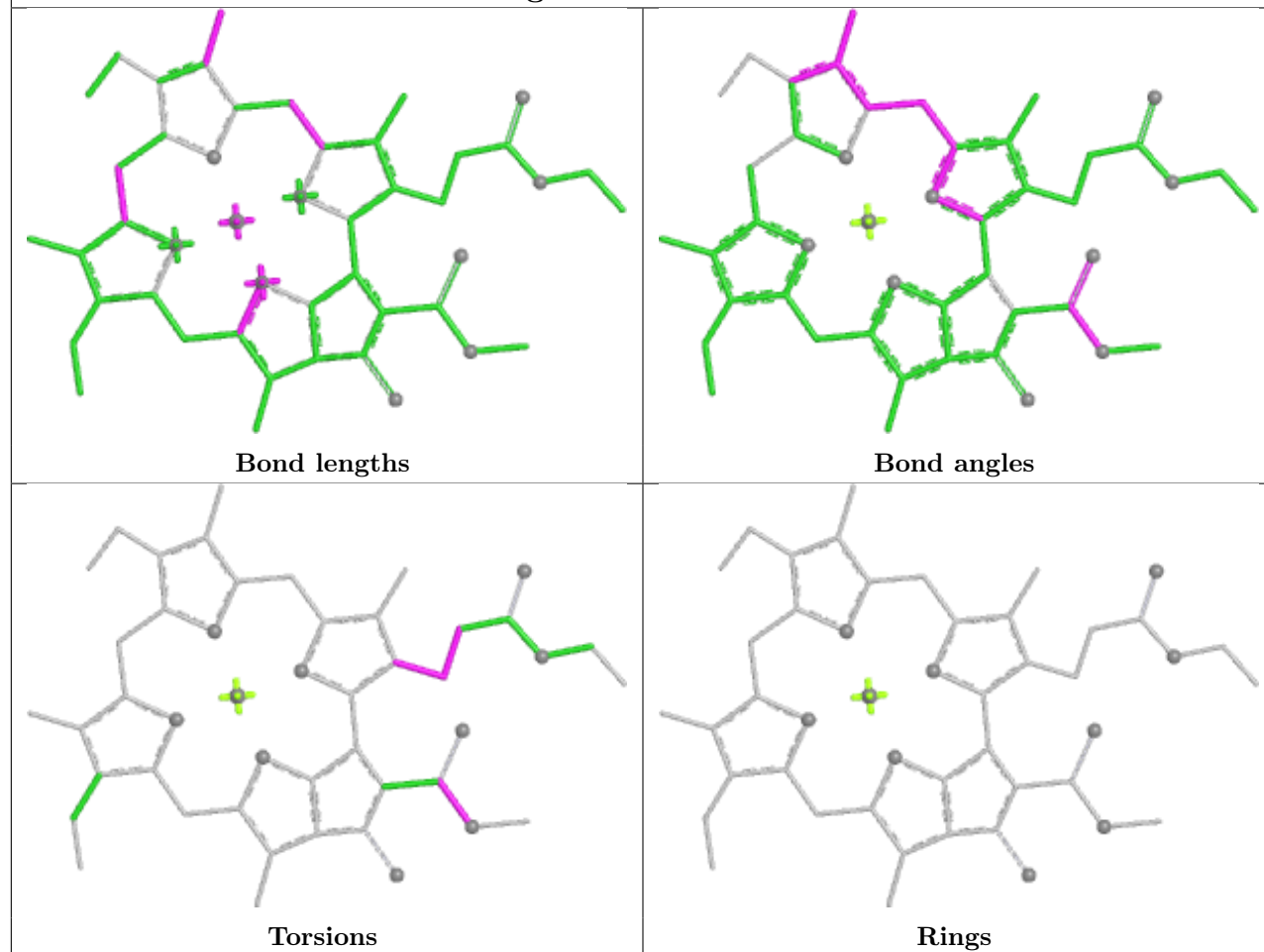
Ligand SQD 3 422



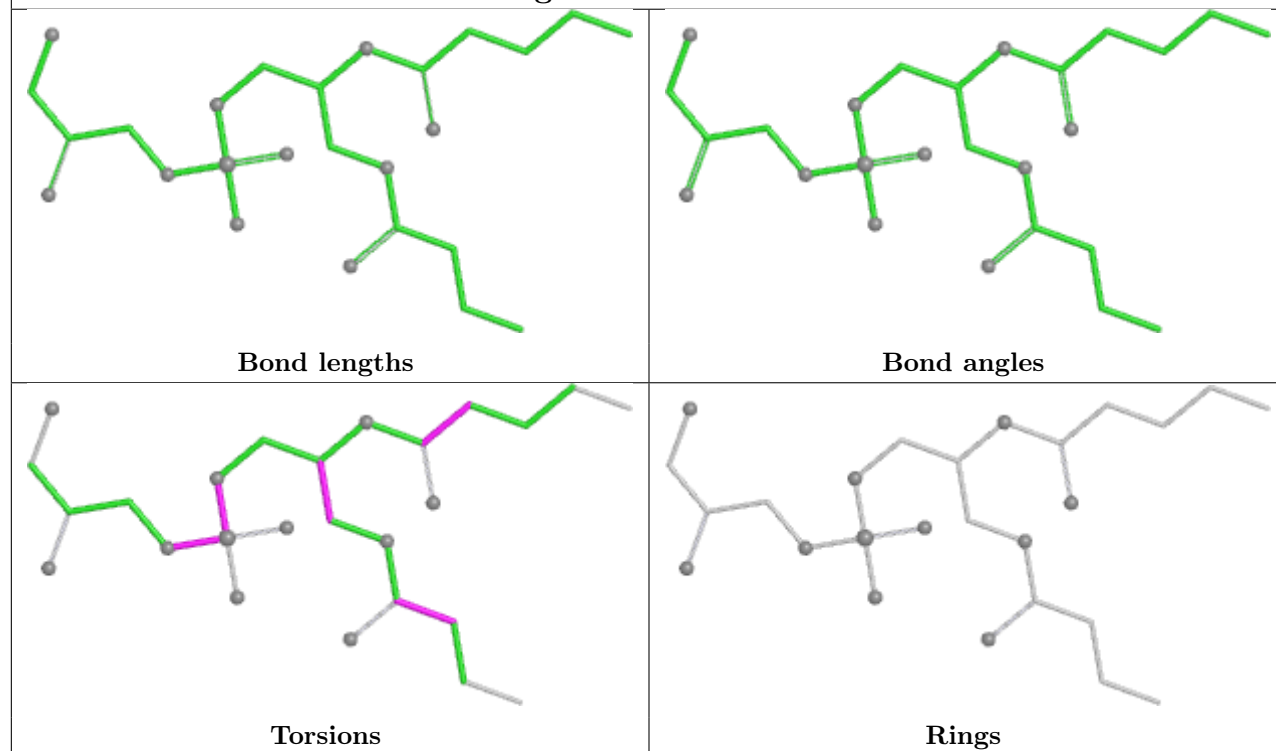
Ligand CLA 8 610

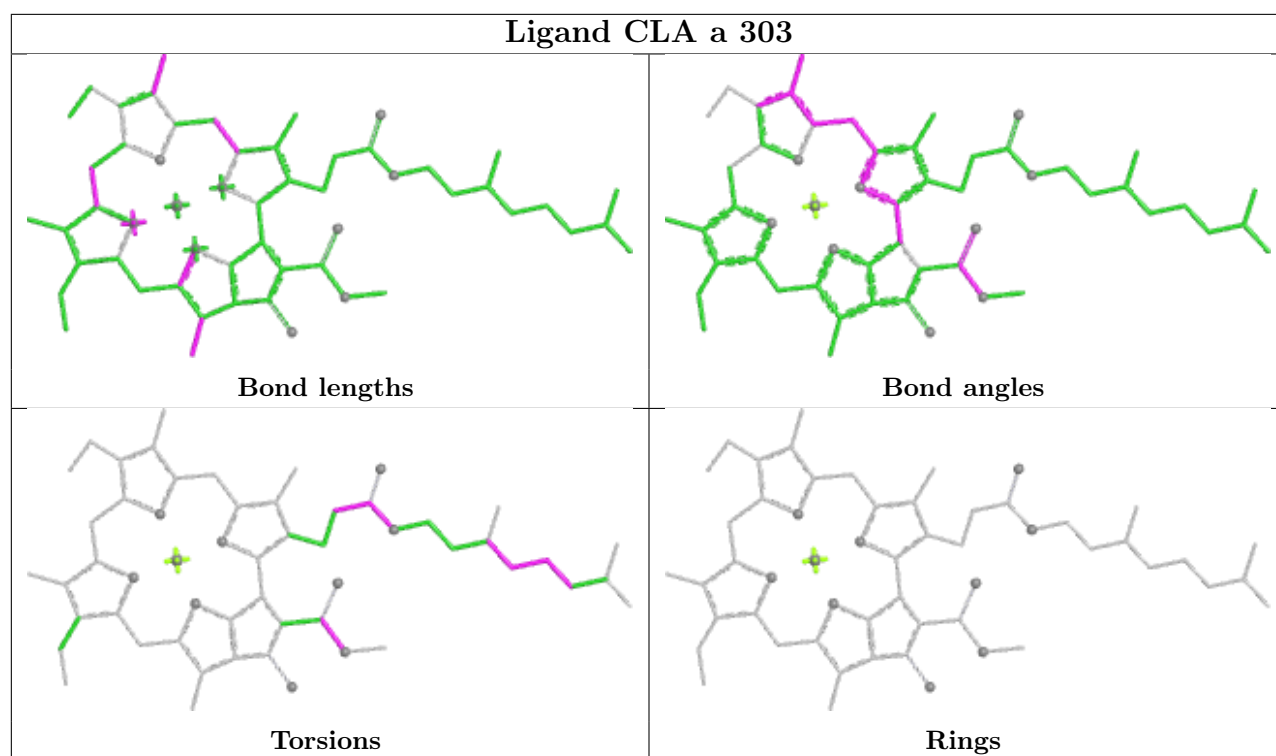


Ligand CLA A 837

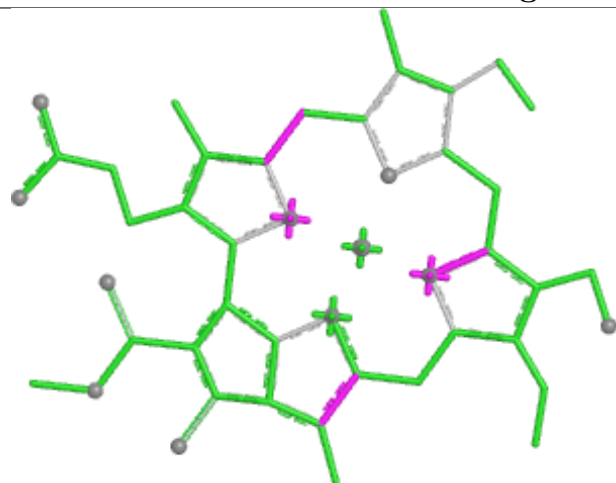


Ligand LHG 3 424

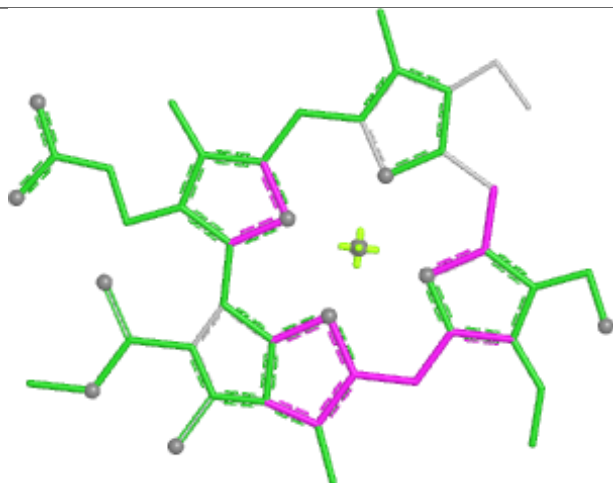




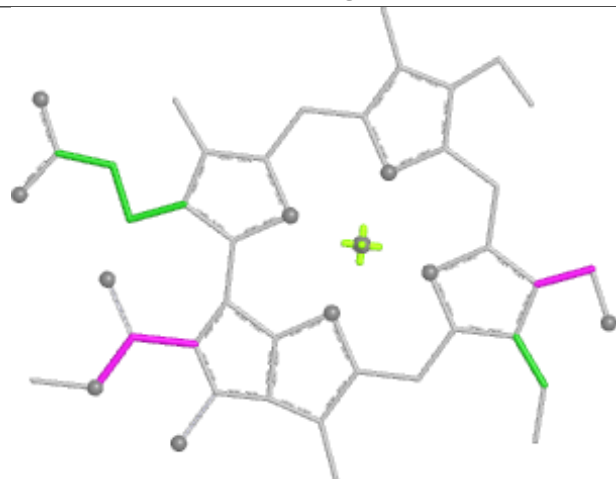
Ligand CHL 8 606



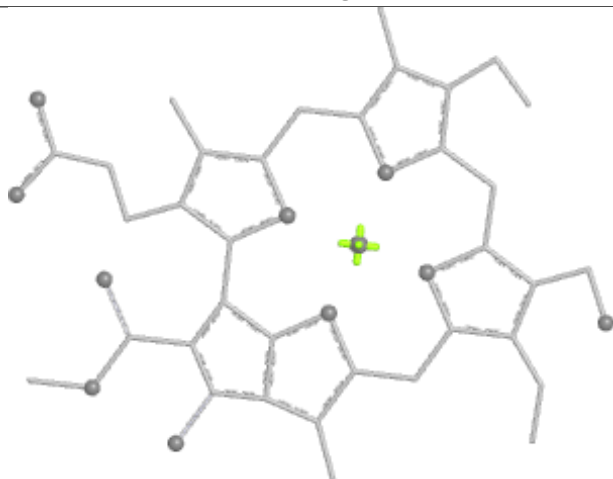
Bond lengths



Bond angles

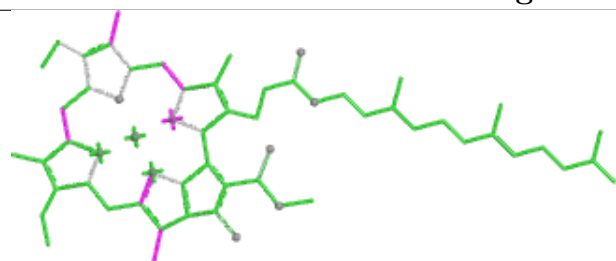


Torsions

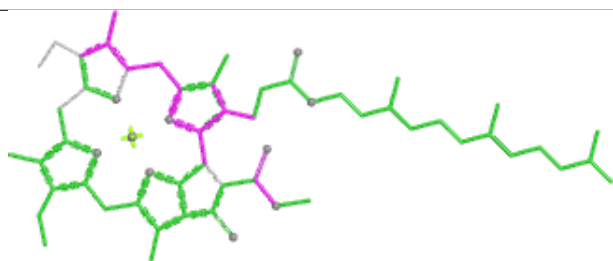


Rings

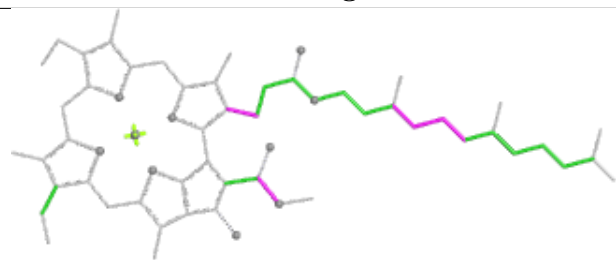
Ligand CLA A 809



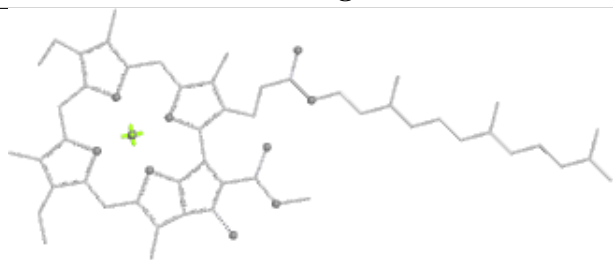
Bond lengths



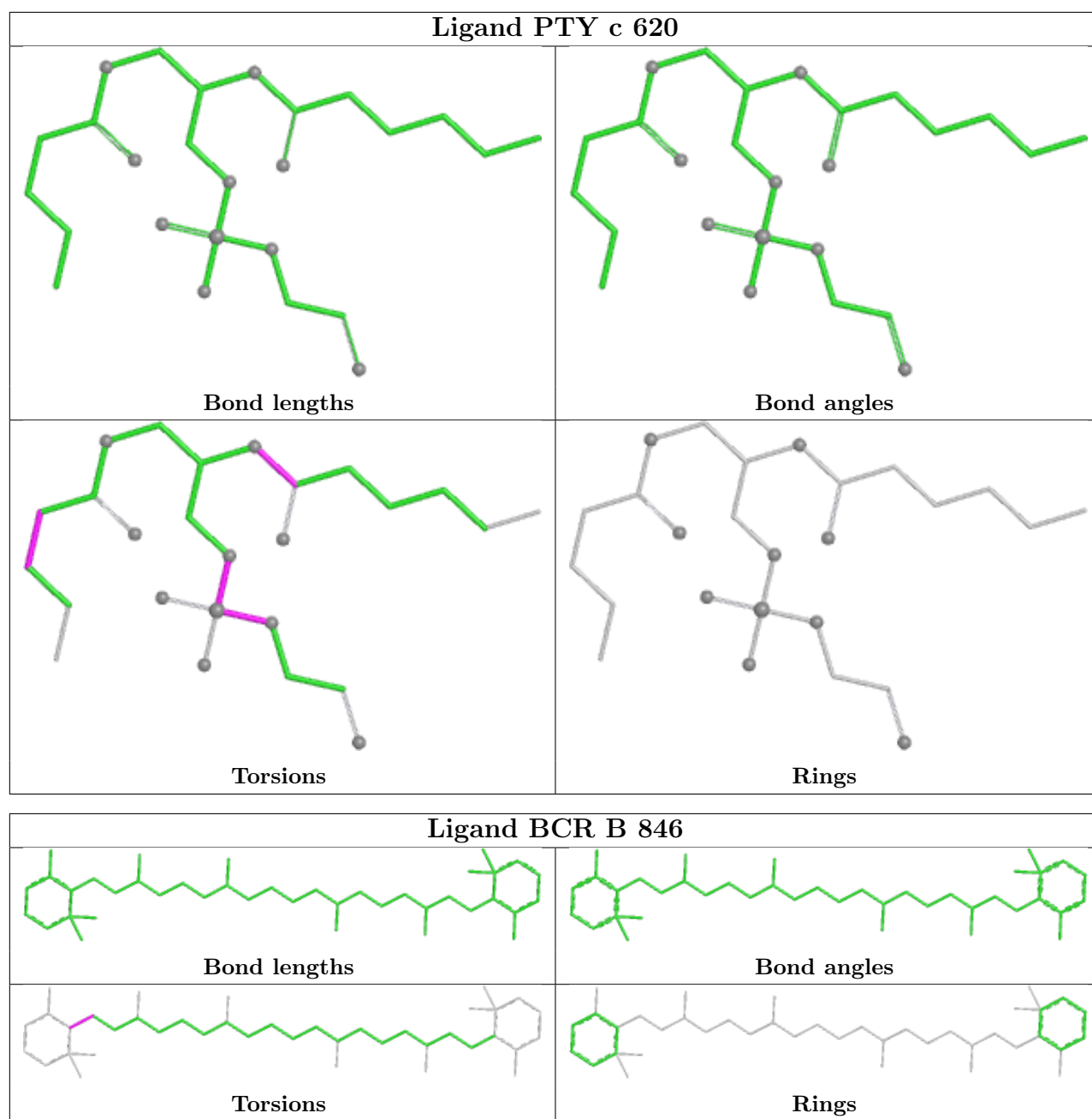
Bond angles



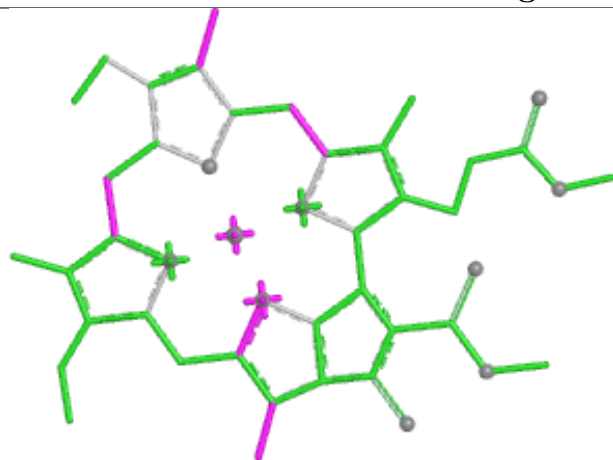
Torsions



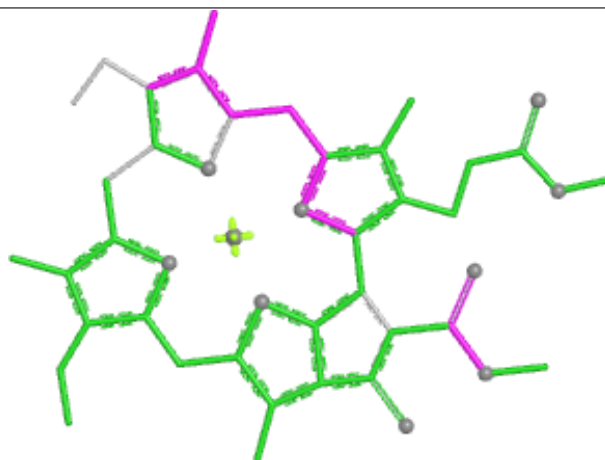
Rings



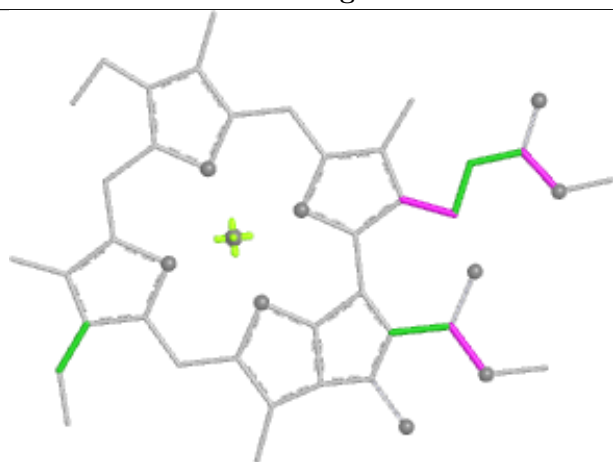
Ligand CLA 7 323



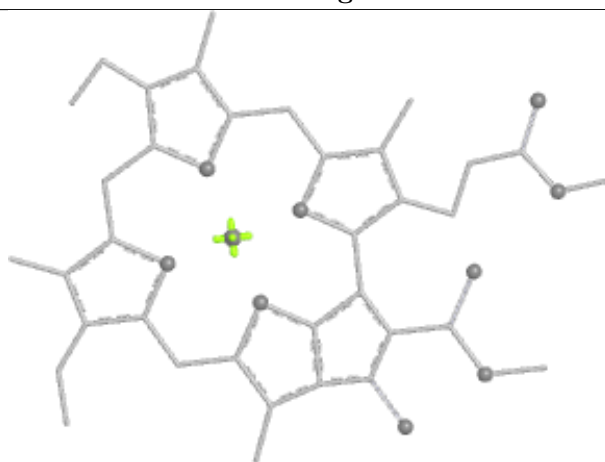
Bond lengths



Bond angles

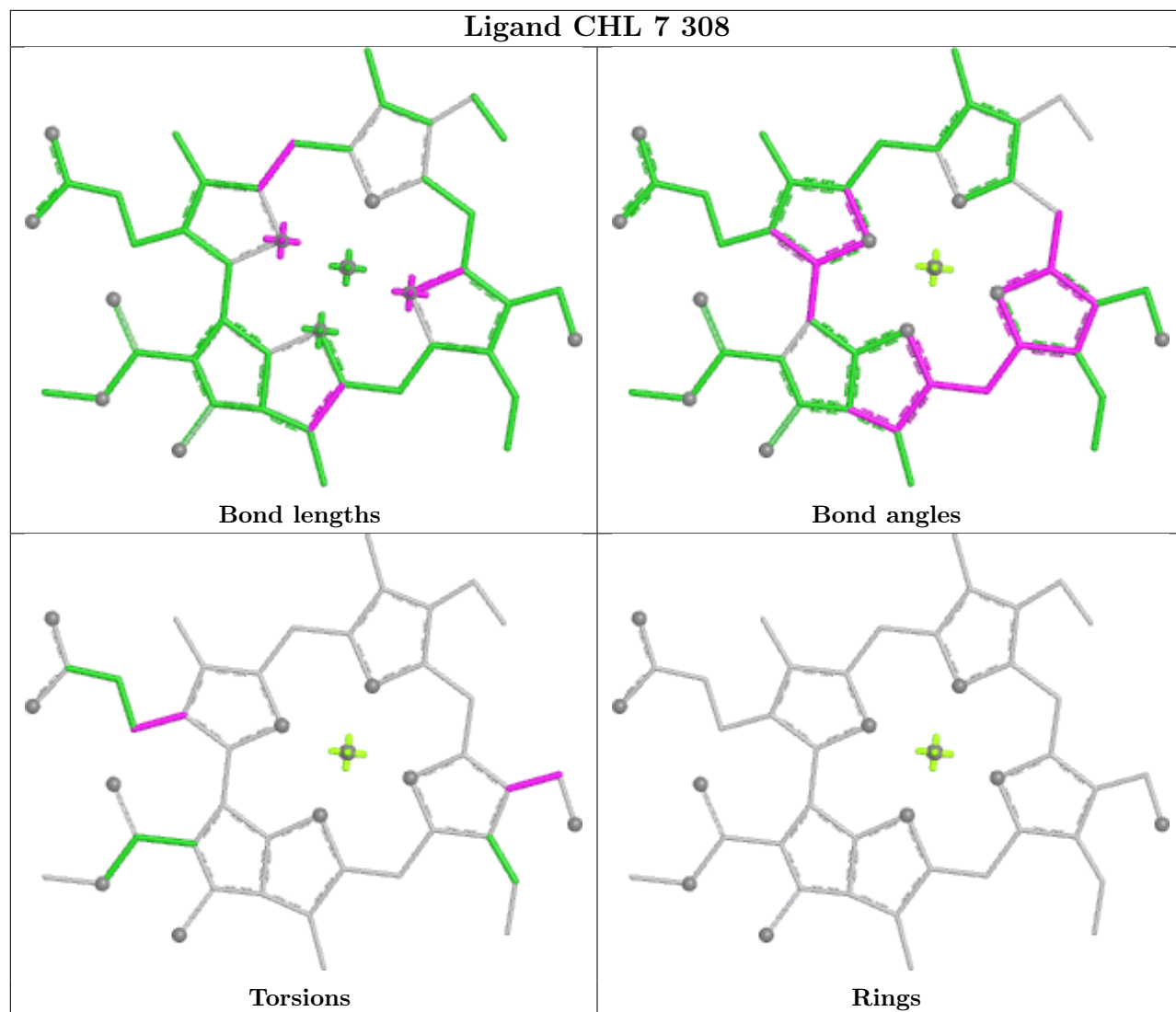


Torsions

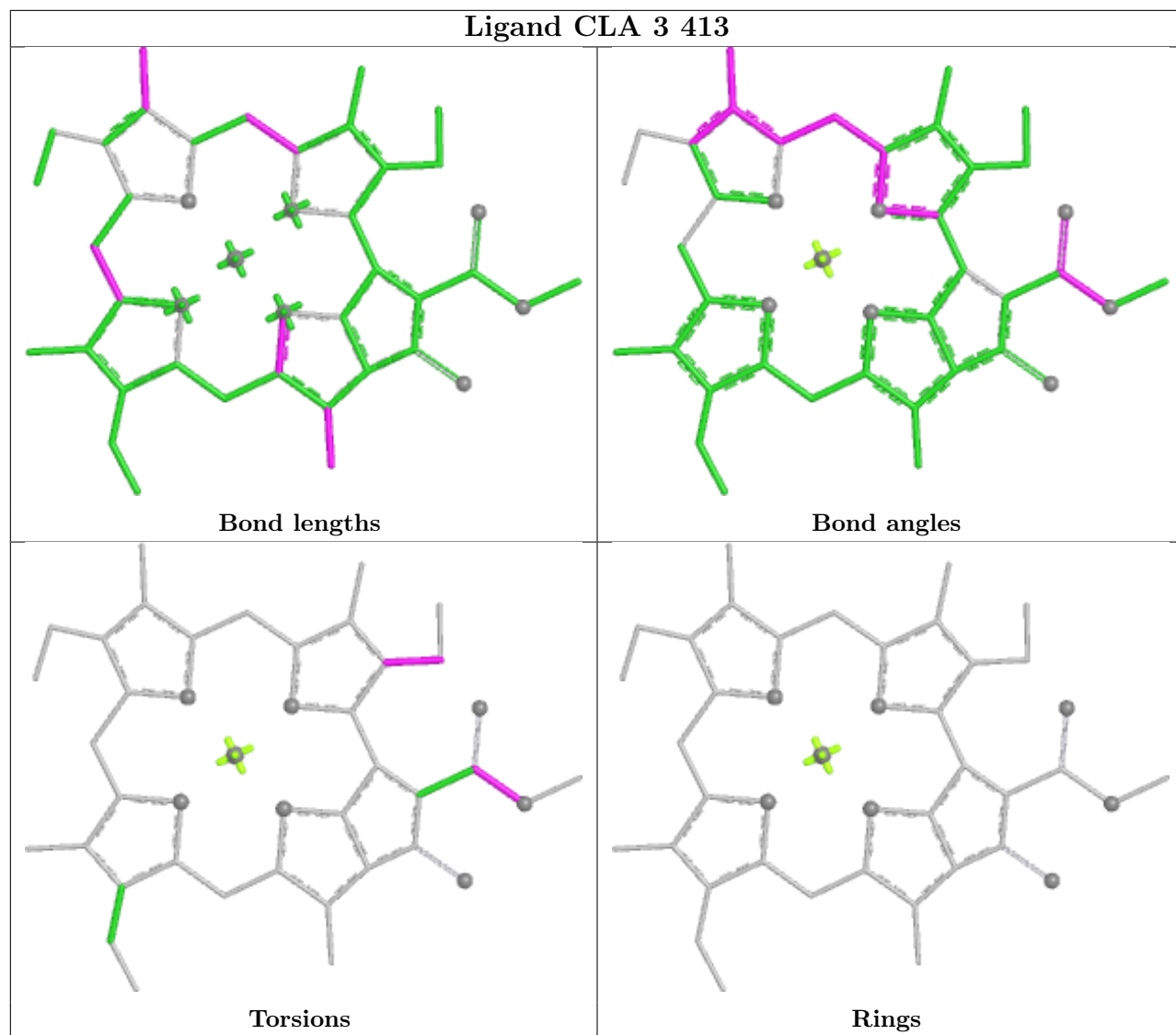


Rings

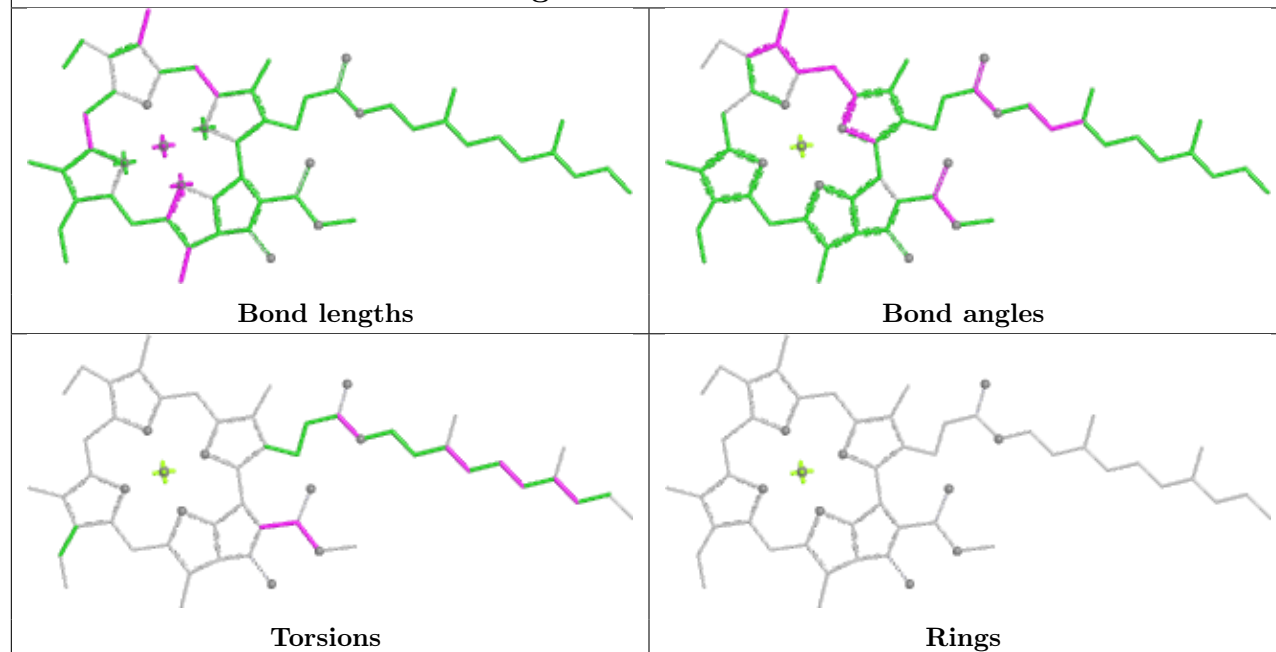
Ligand CHL 7 308



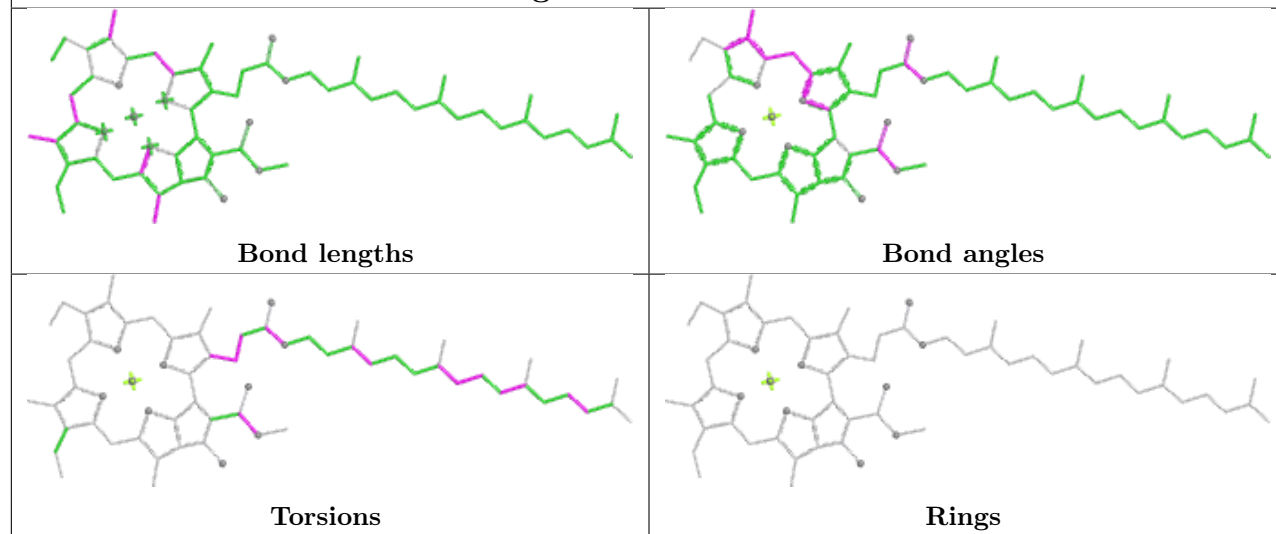
Ligand CLA 3 413



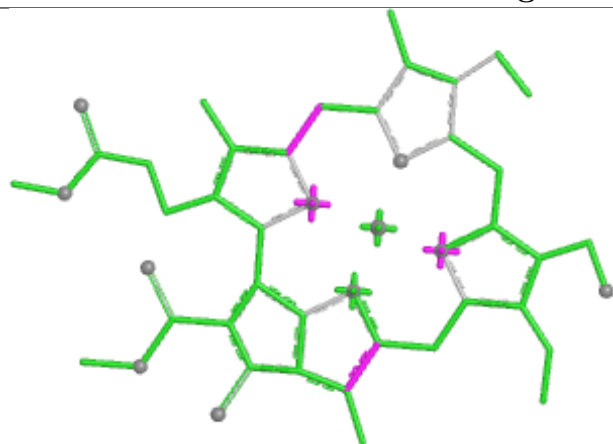
Ligand CLA A 828



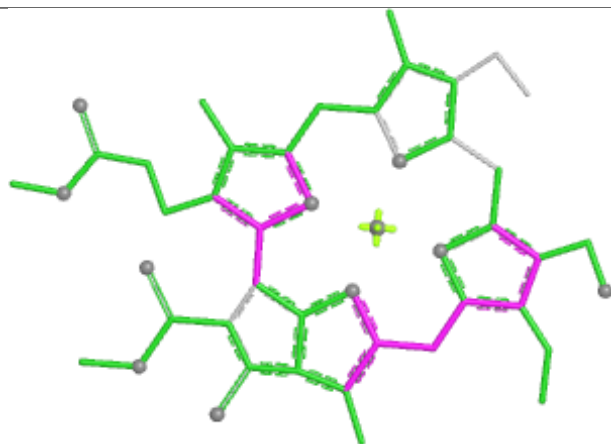
Ligand CLA B 818



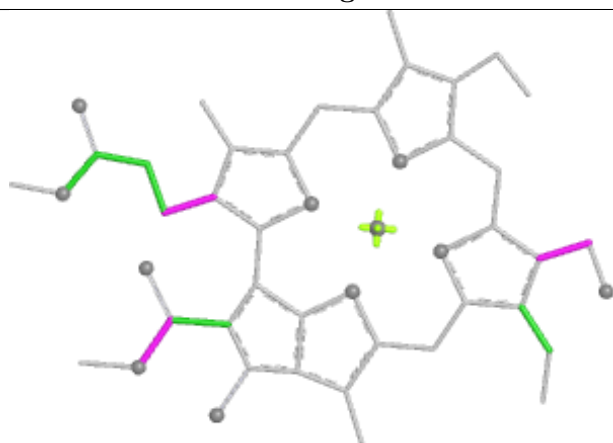
Ligand CHL 9 606



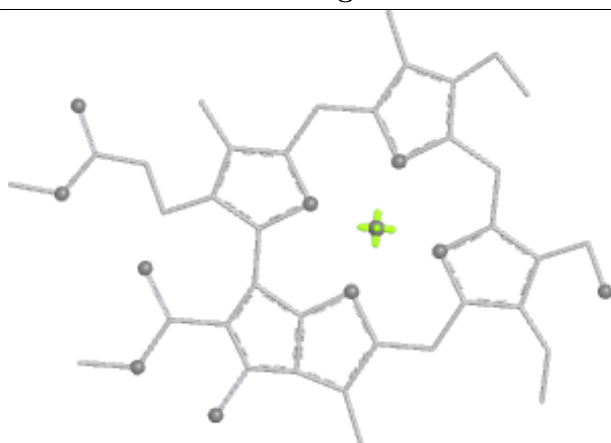
Bond lengths



Bond angles

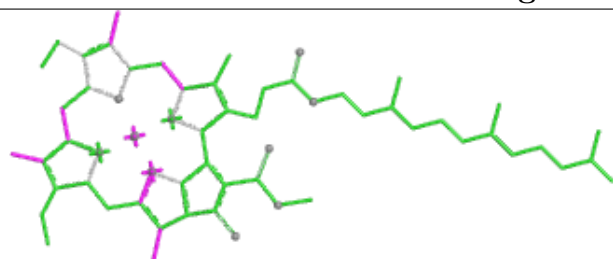


Torsions

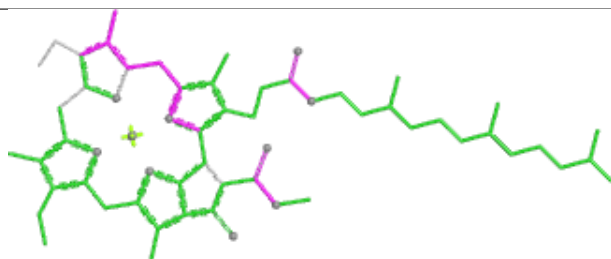


Rings

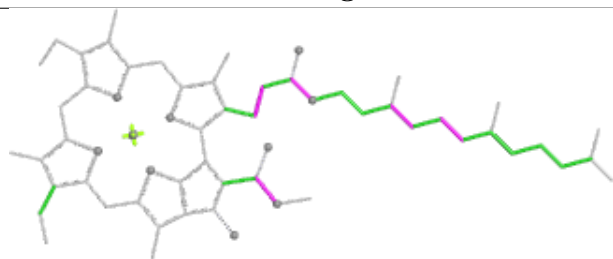
Ligand CLA 3 411



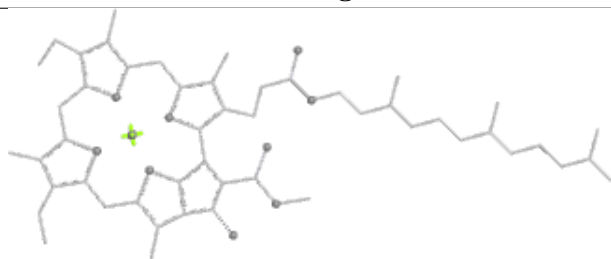
Bond lengths



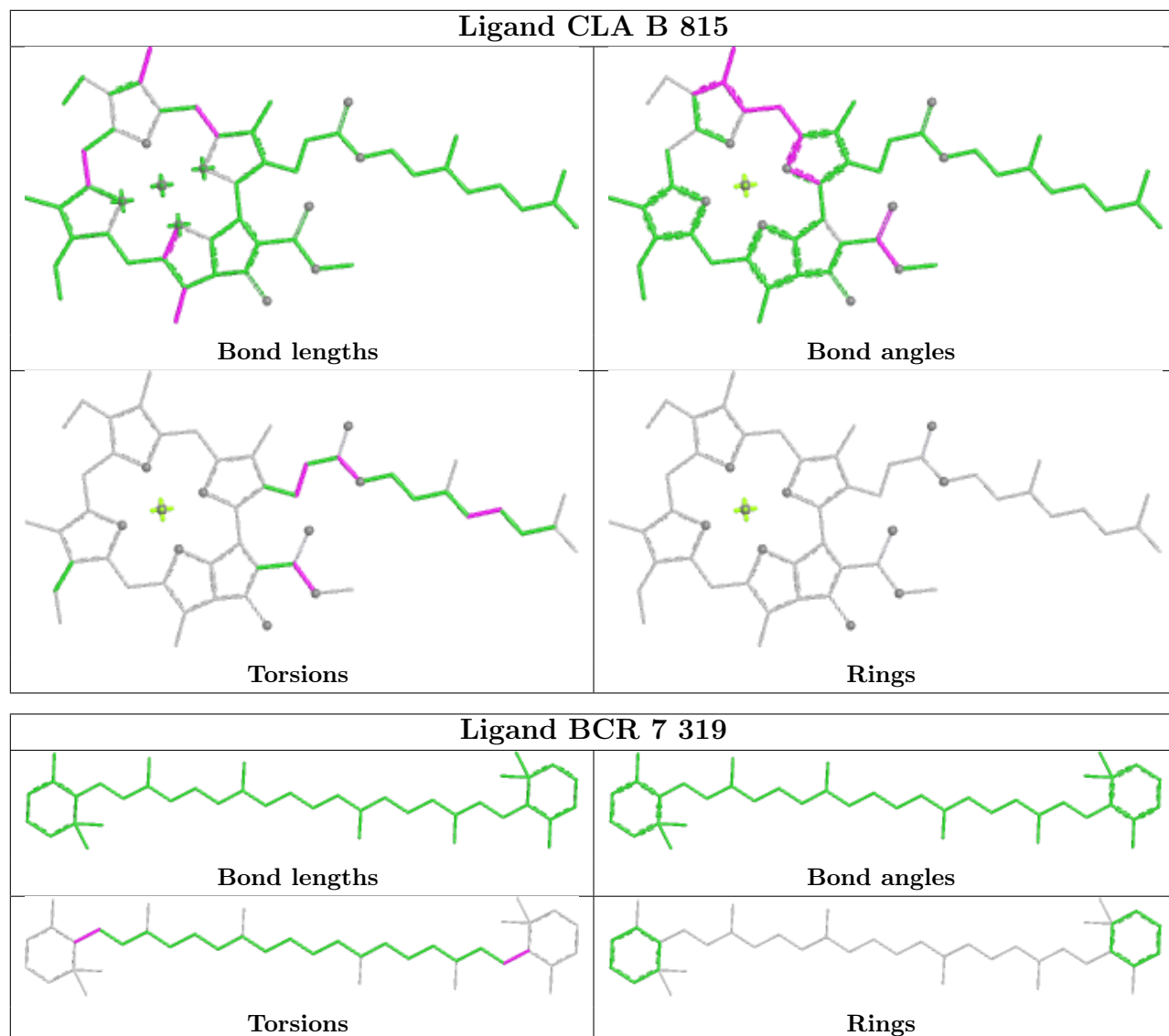
Bond angles



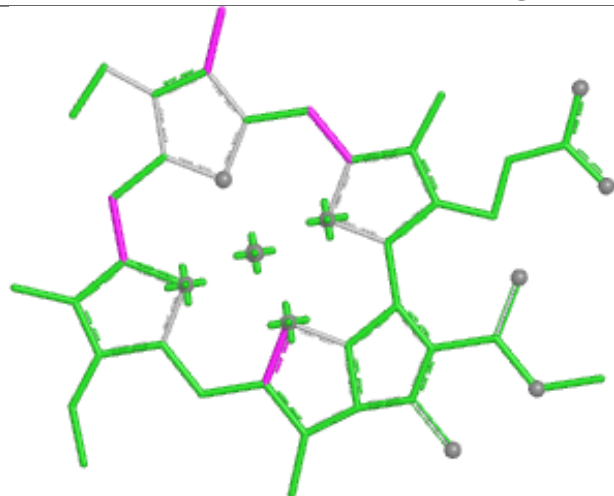
Torsions



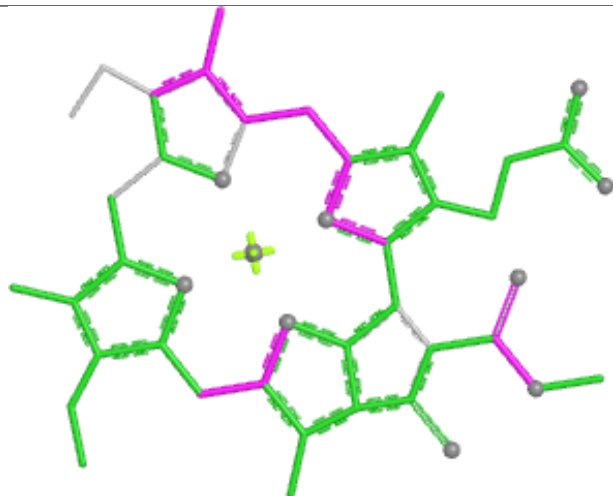
Rings



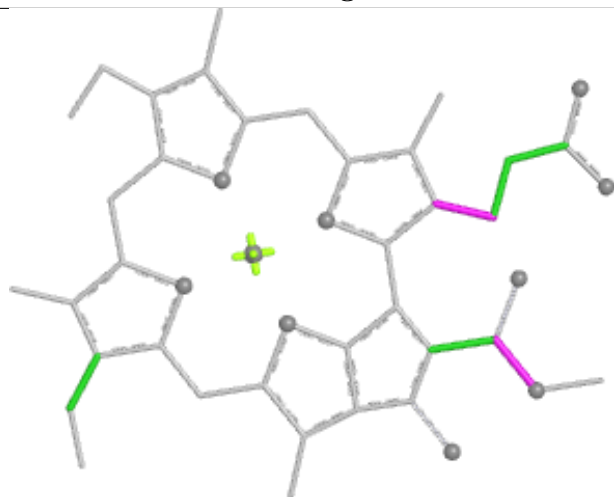
Ligand CLA G 205



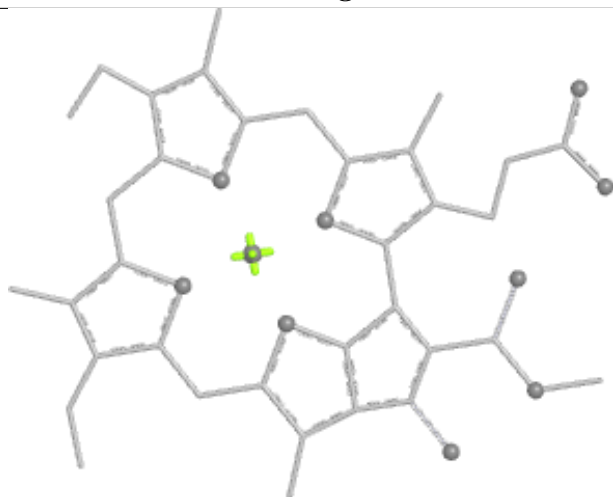
Bond lengths



Bond angles

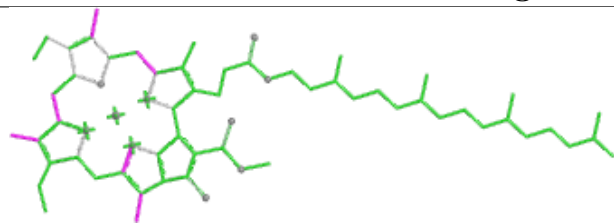


Torsions

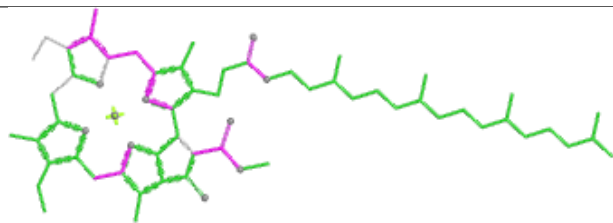


Rings

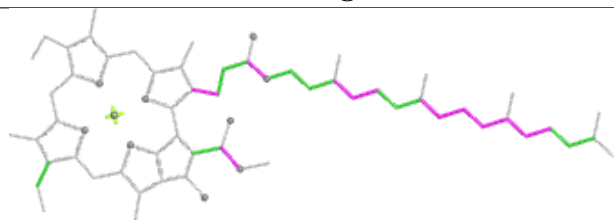
Ligand CLA A 830



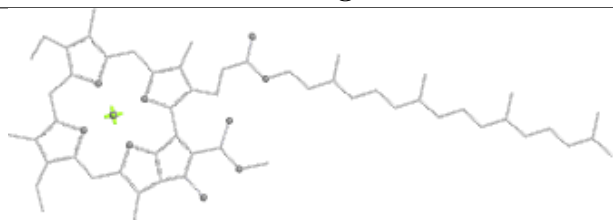
Bond lengths



Bond angles

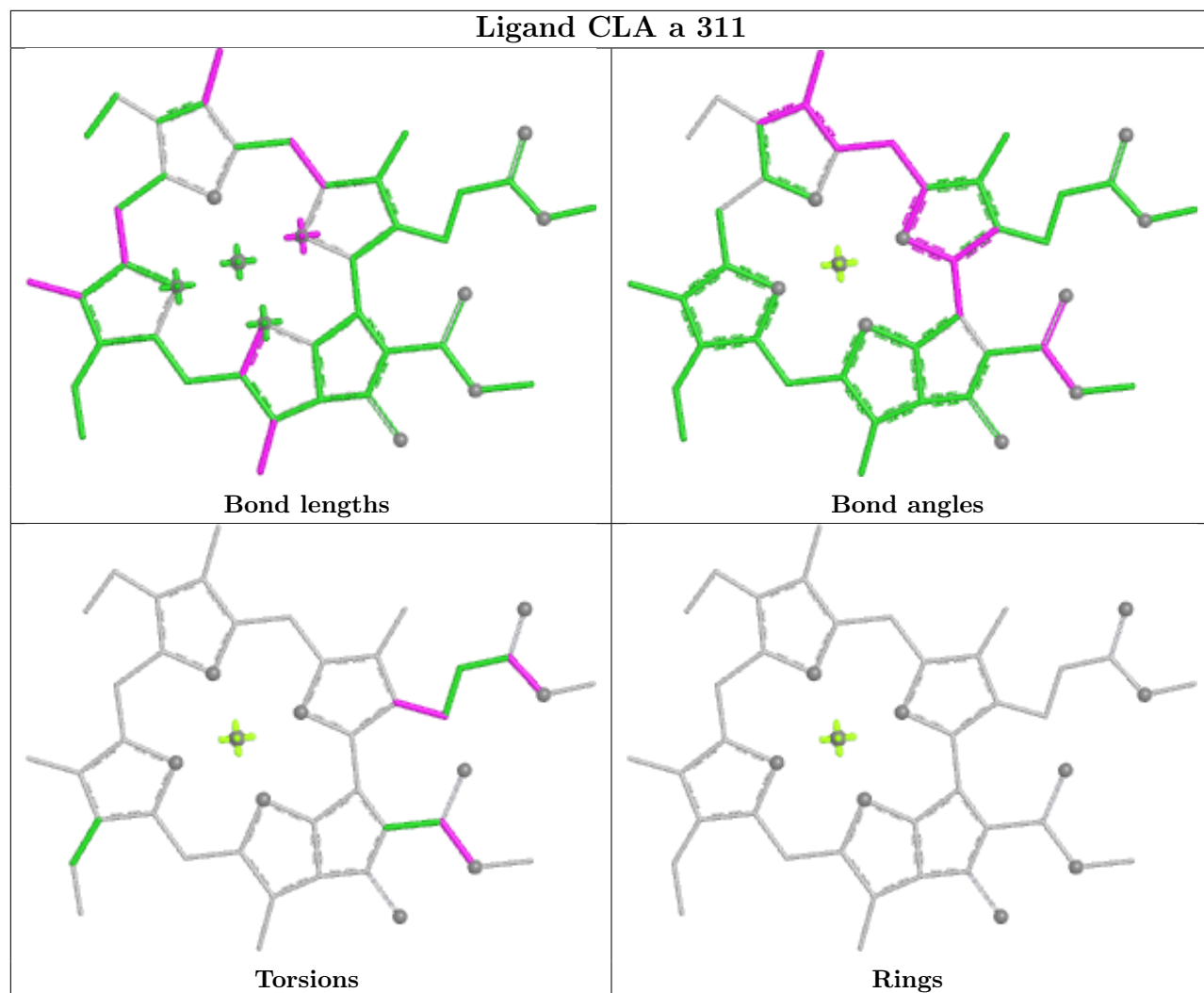


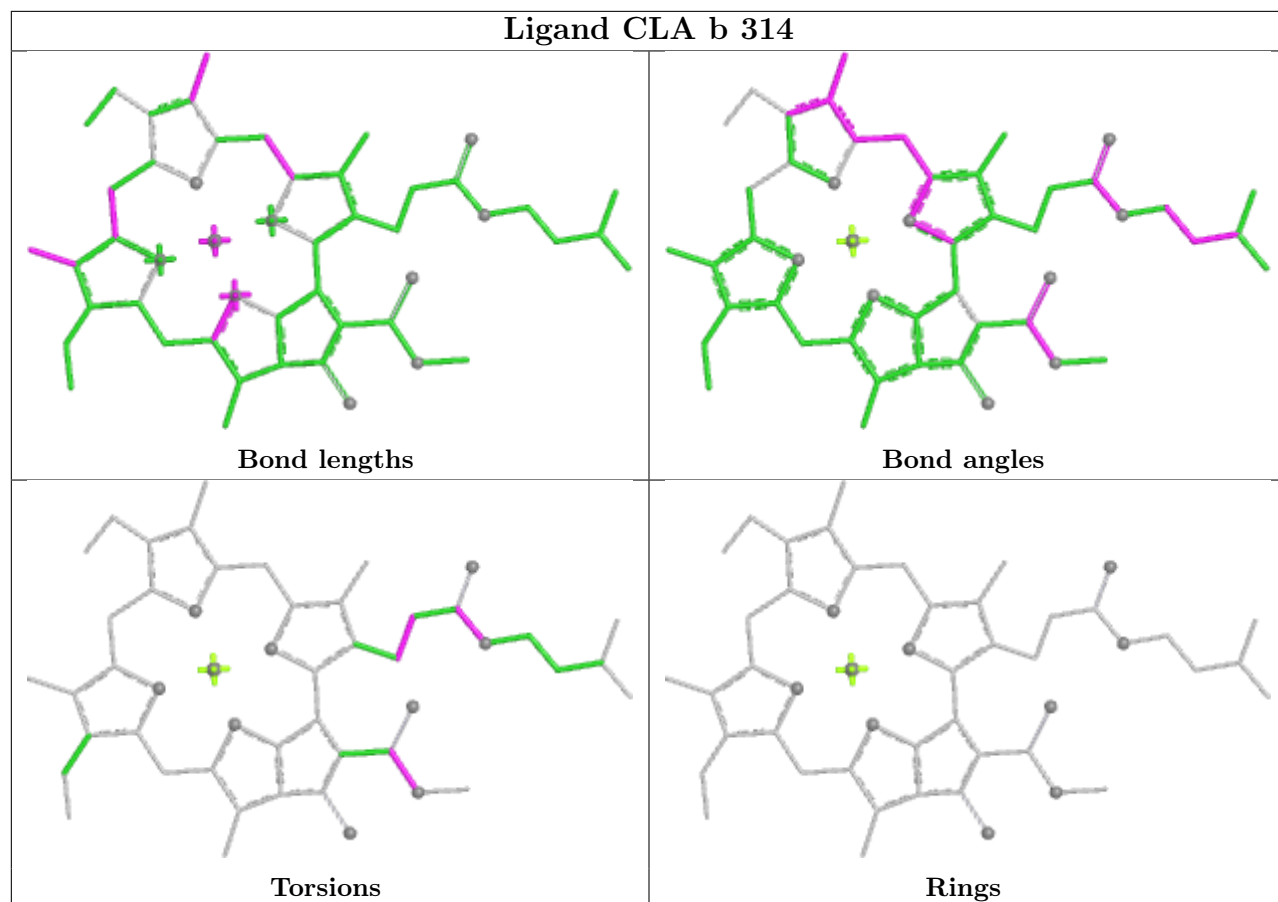
Torsions



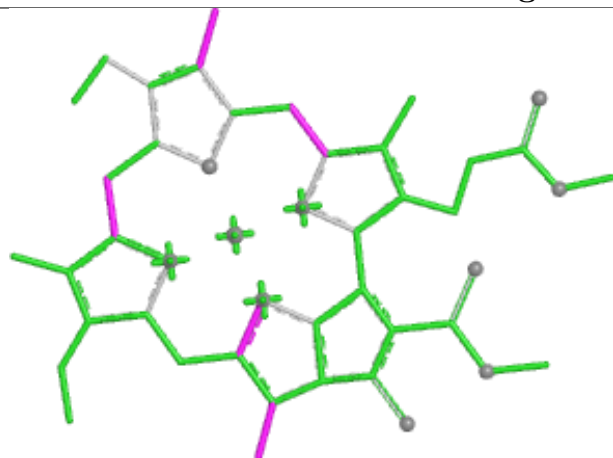
Rings

Ligand CLA a 311

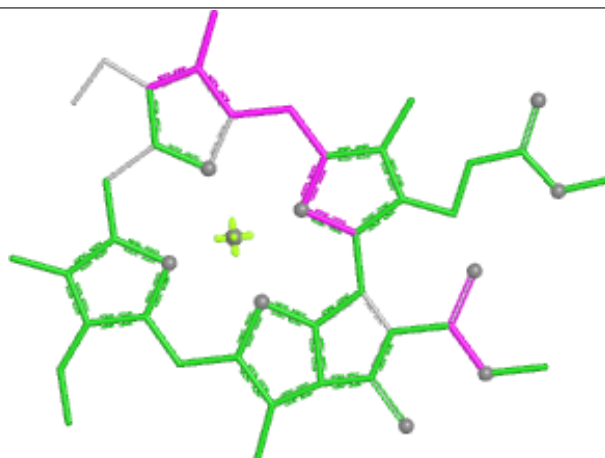




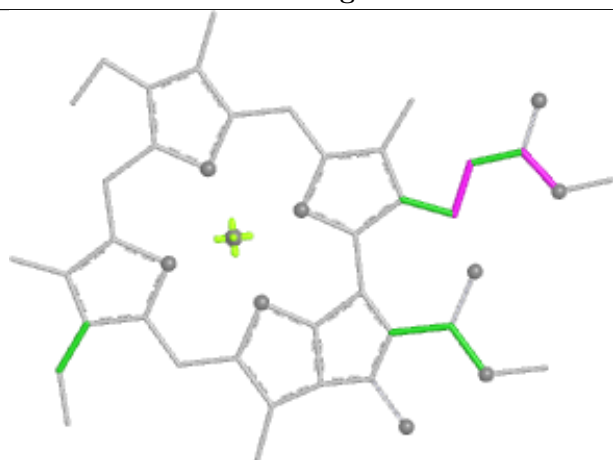
Ligand CLA 9 611



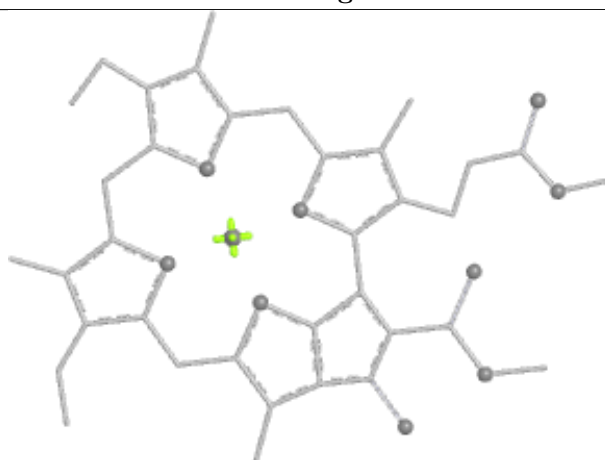
Bond lengths



Bond angles

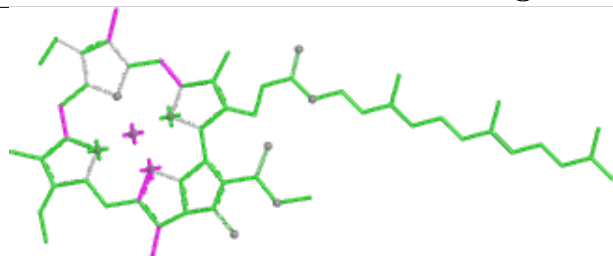


Torsions

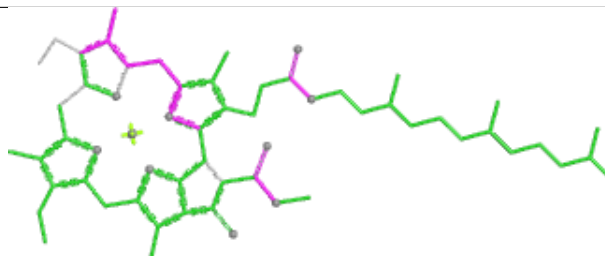


Rings

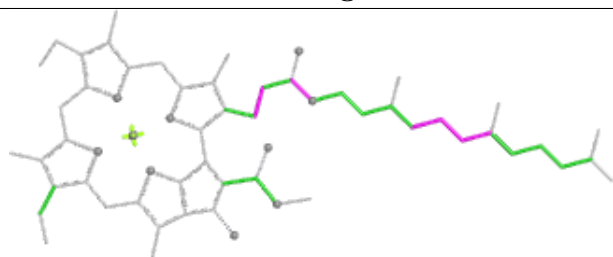
Ligand CLA B 834



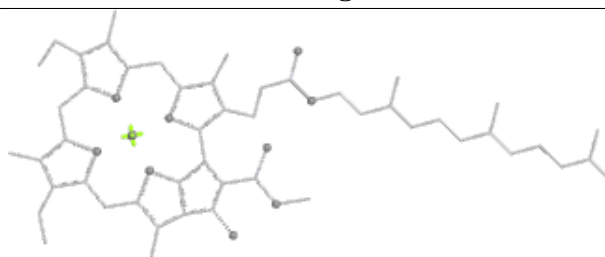
Bond lengths



Bond angles

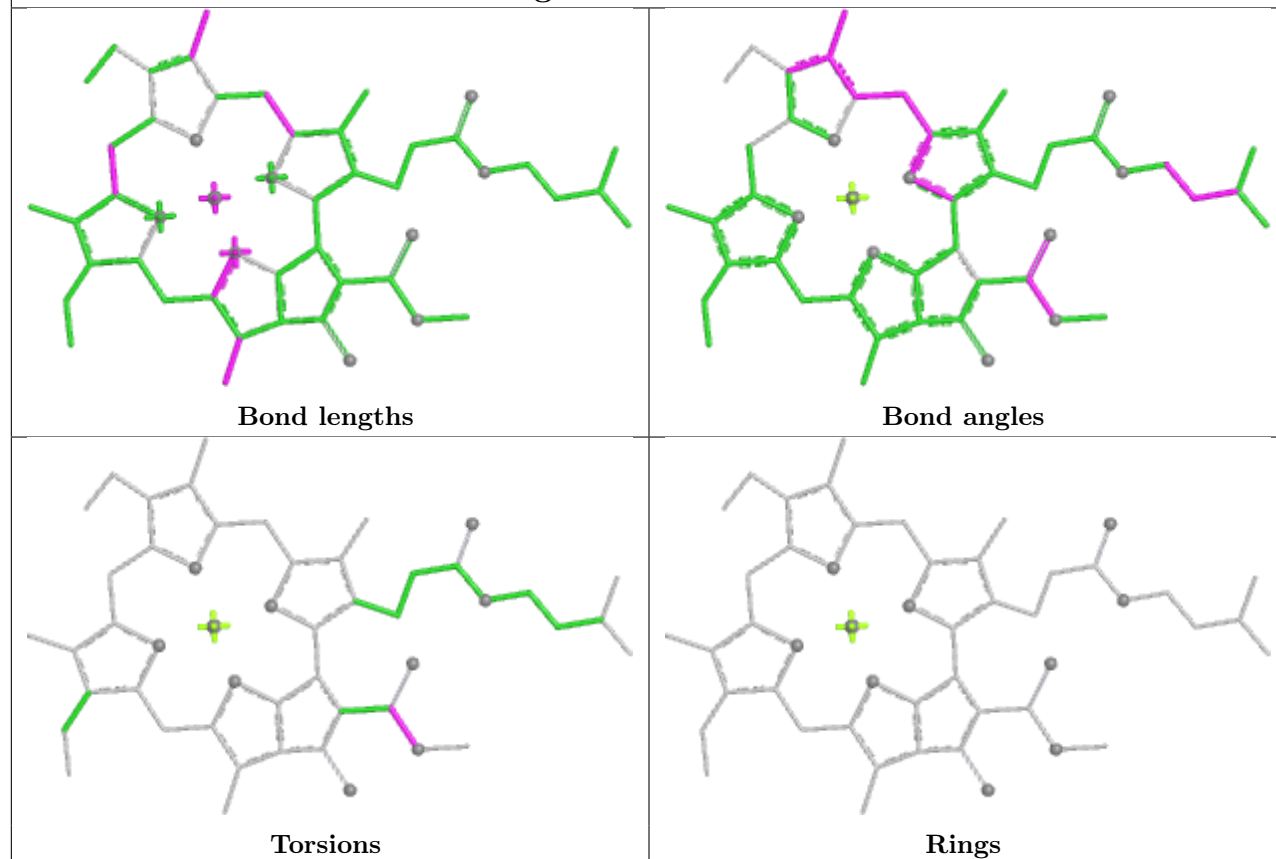


Torsions

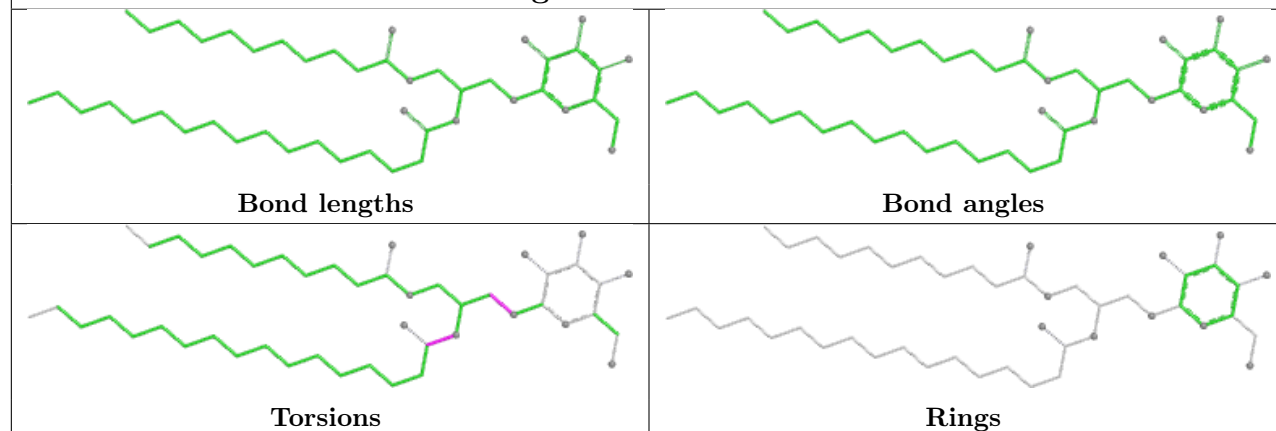


Rings

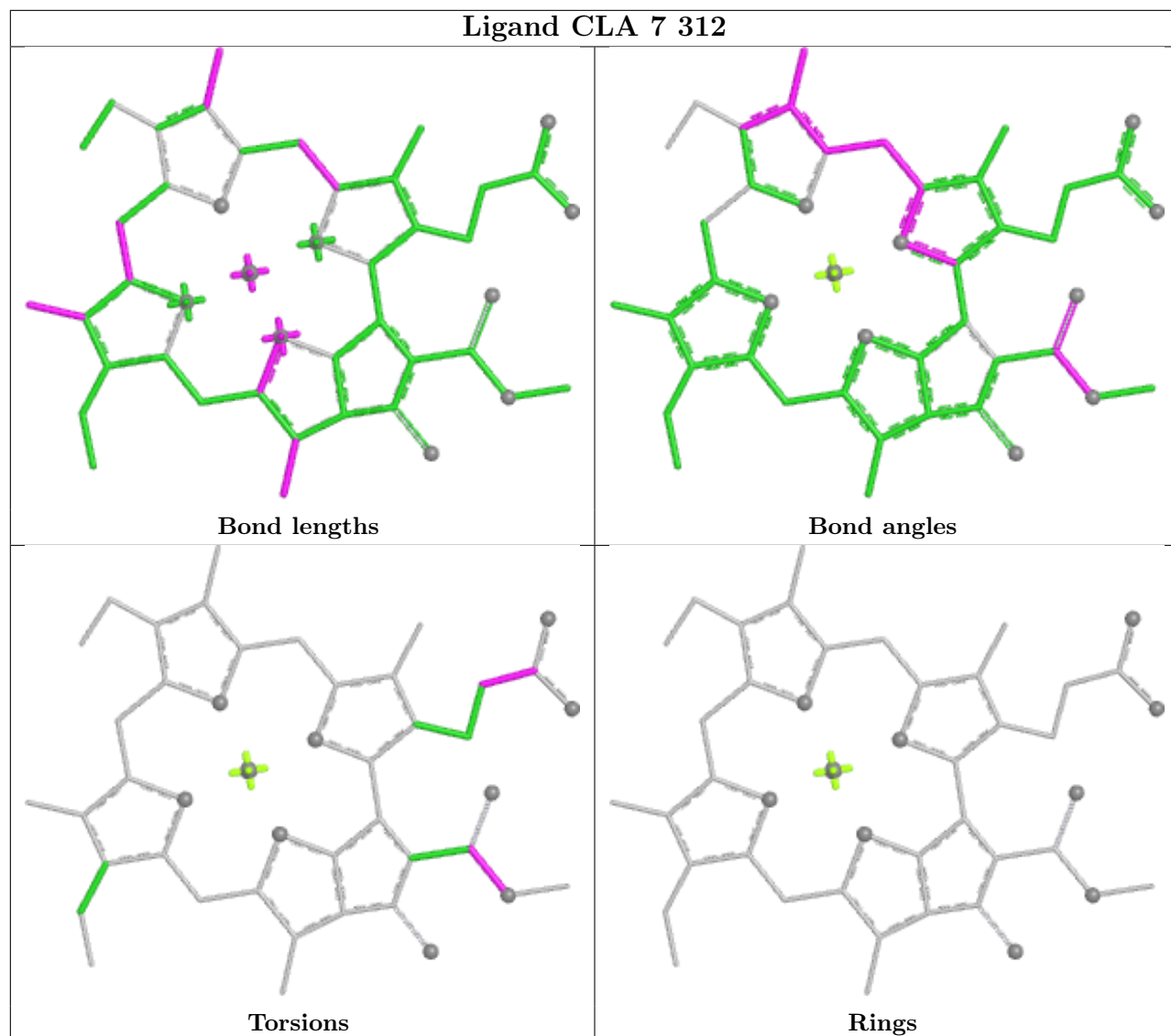
Ligand CLA L 301



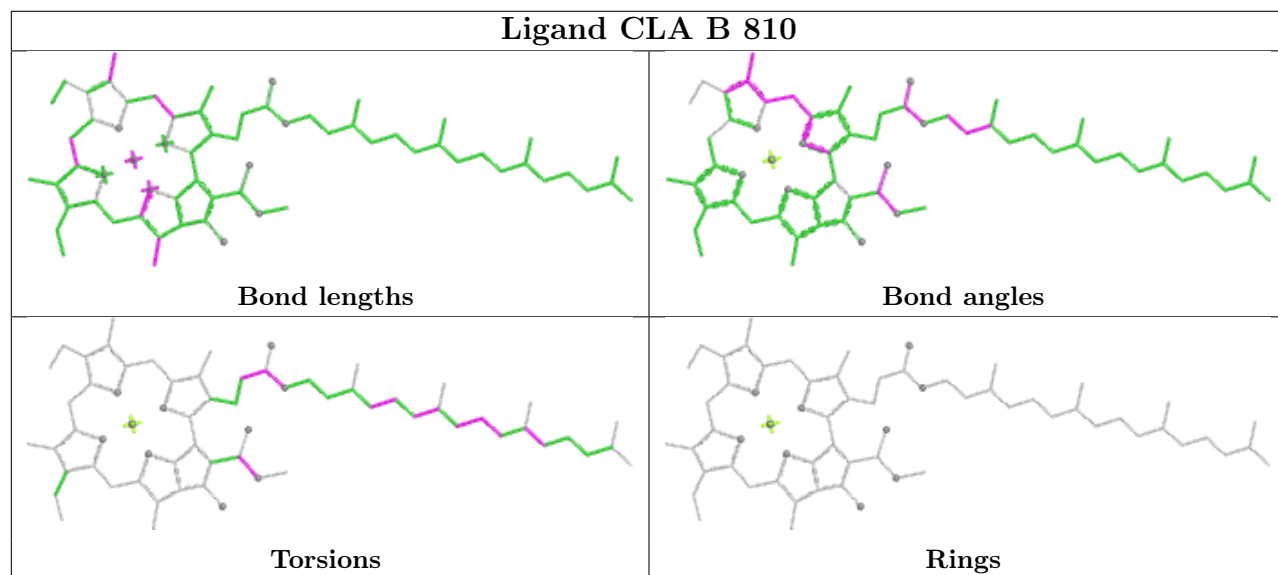
Ligand LMG 7 320

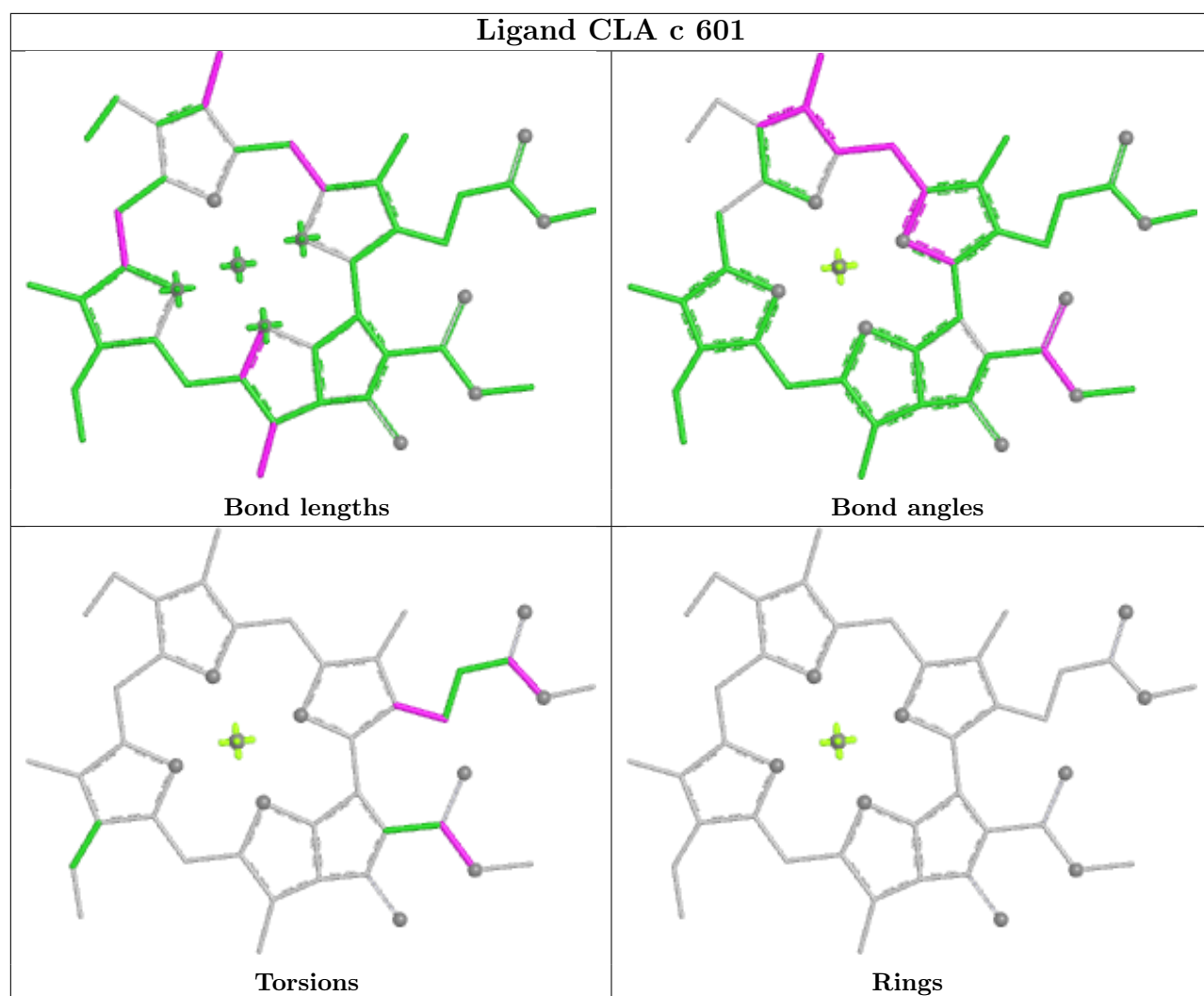


Ligand CLA 7 312

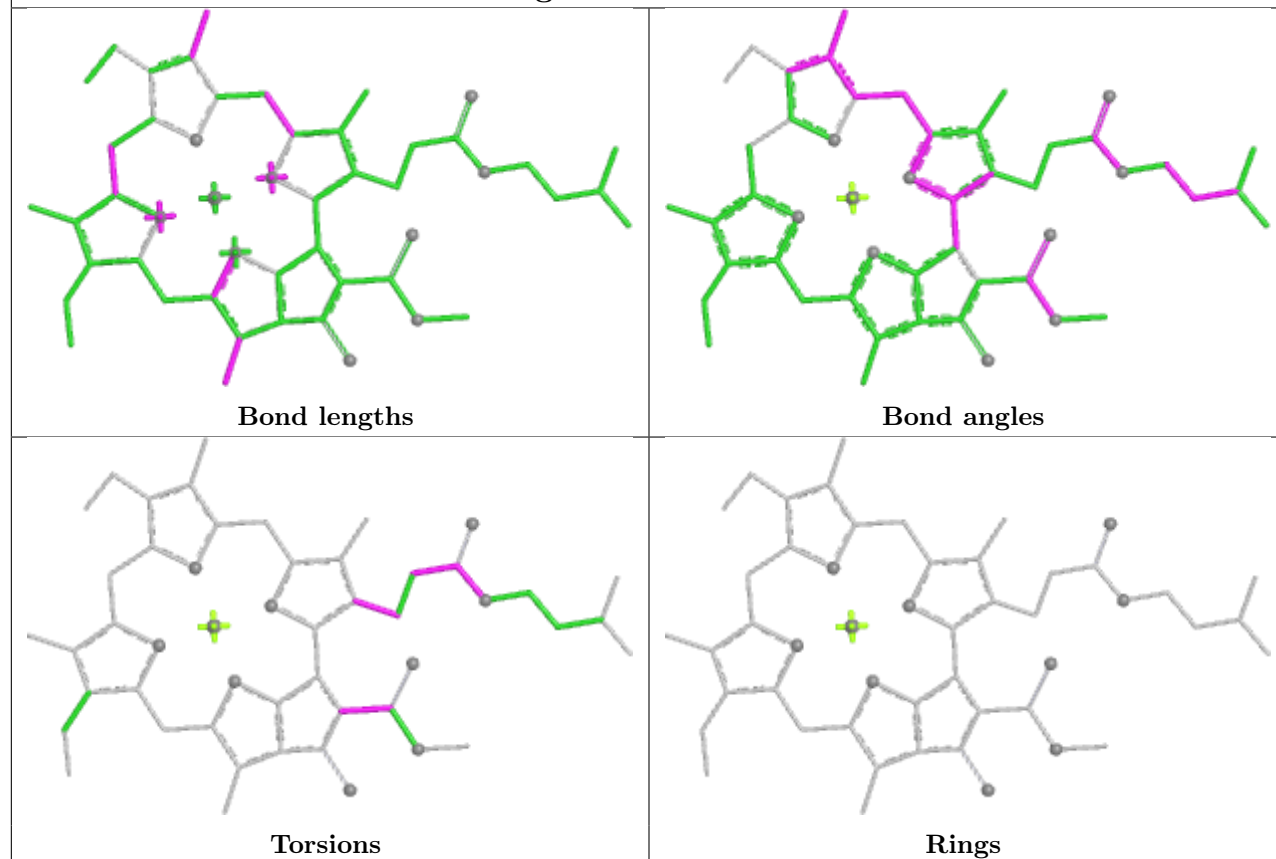


Ligand CLA B 810

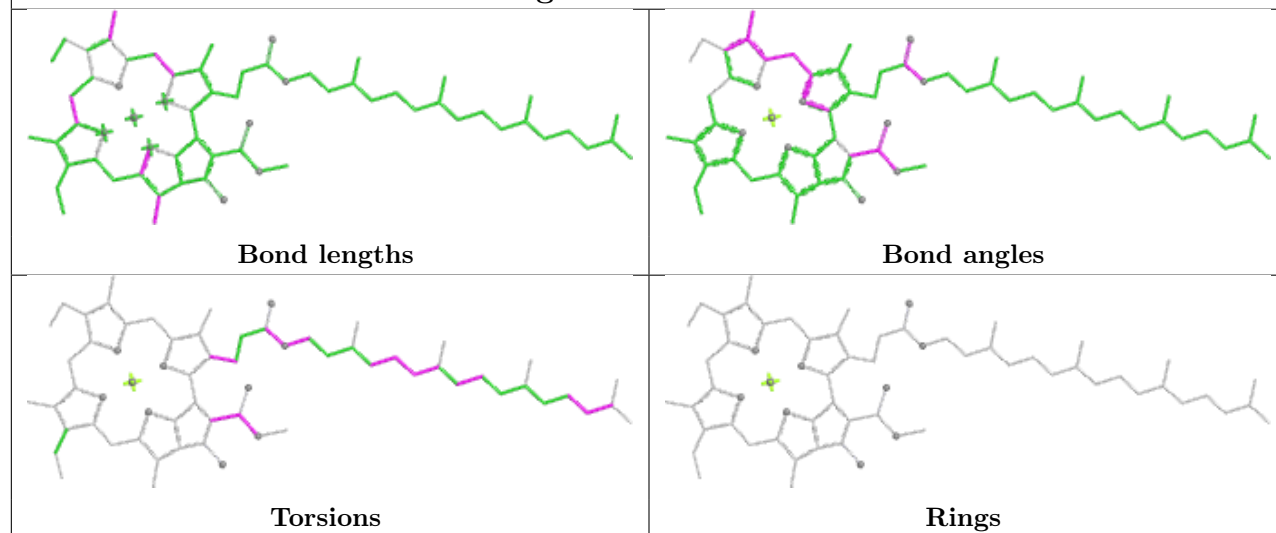




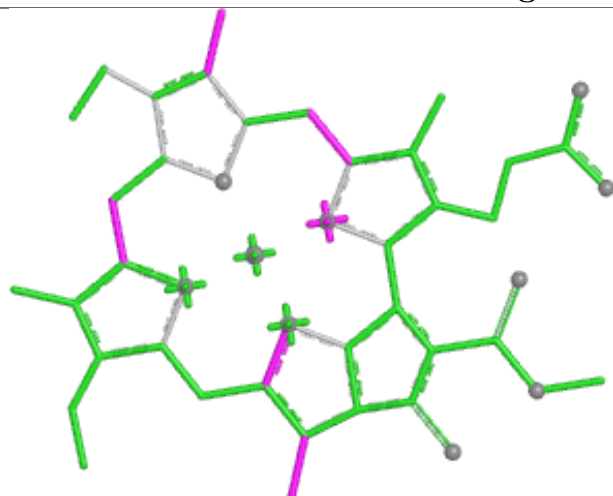
Ligand CLA b 313



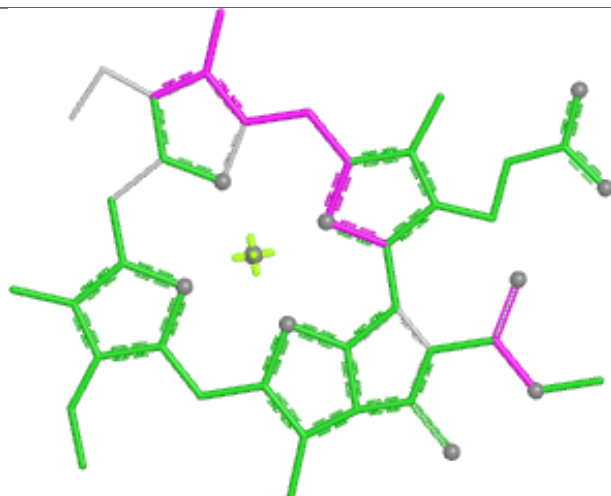
Ligand CLA 9 607



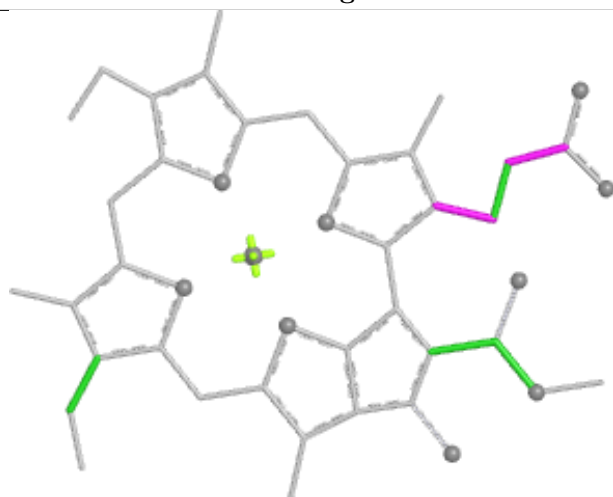
Ligand CLA 2 612



Bond lengths



Bond angles

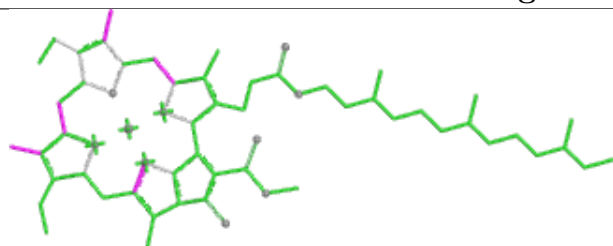


Torsions

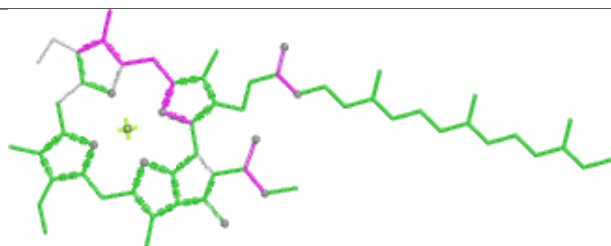


Rings

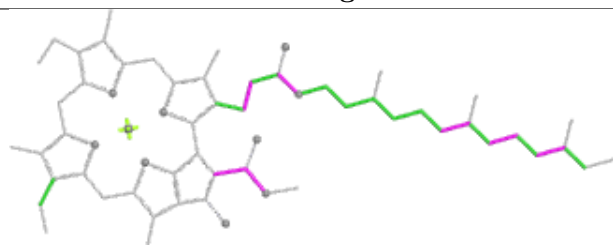
Ligand CLA 1 301



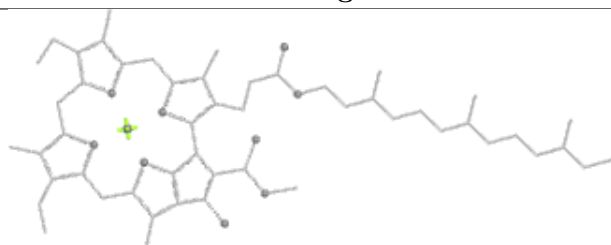
Bond lengths



Bond angles

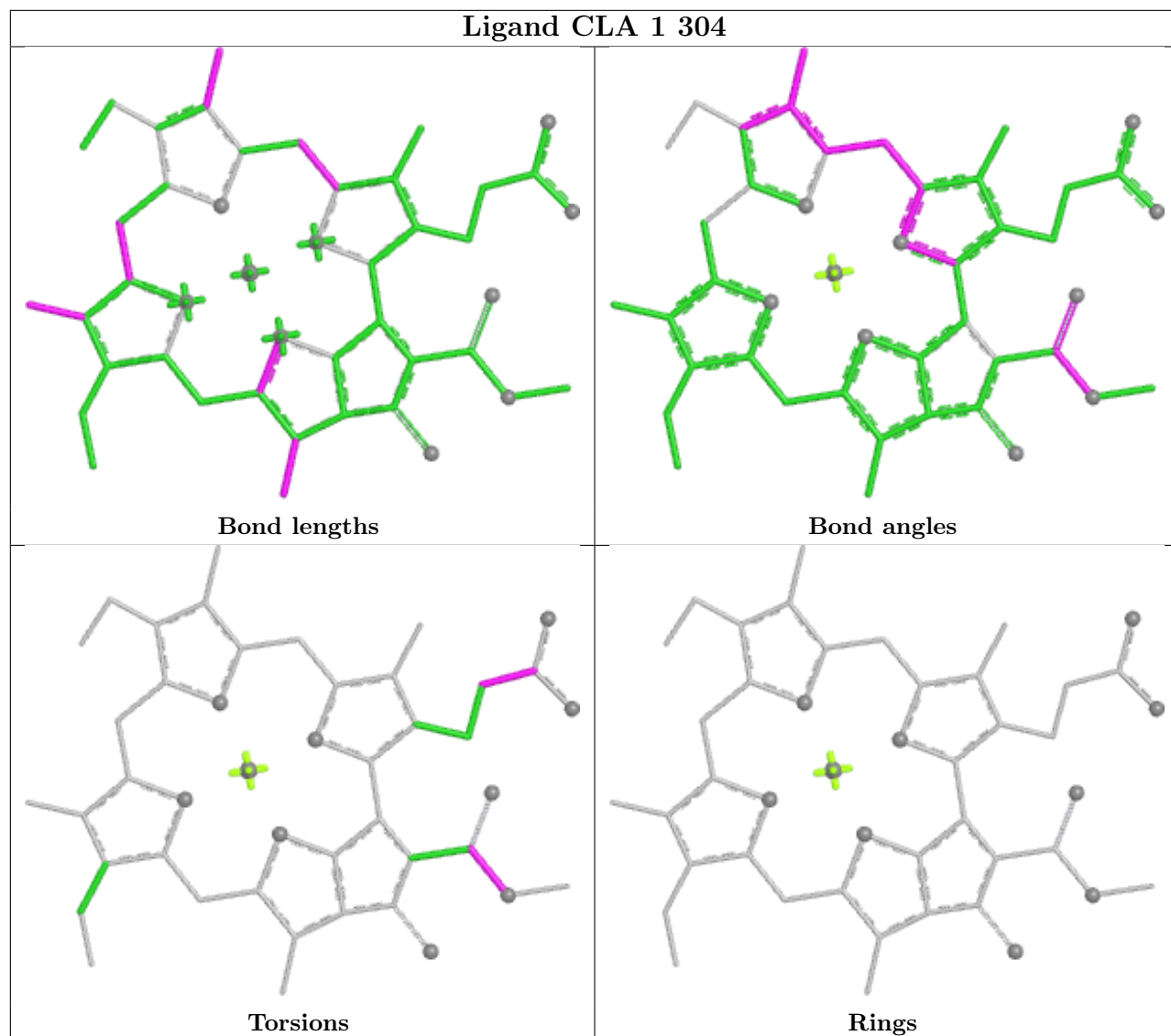


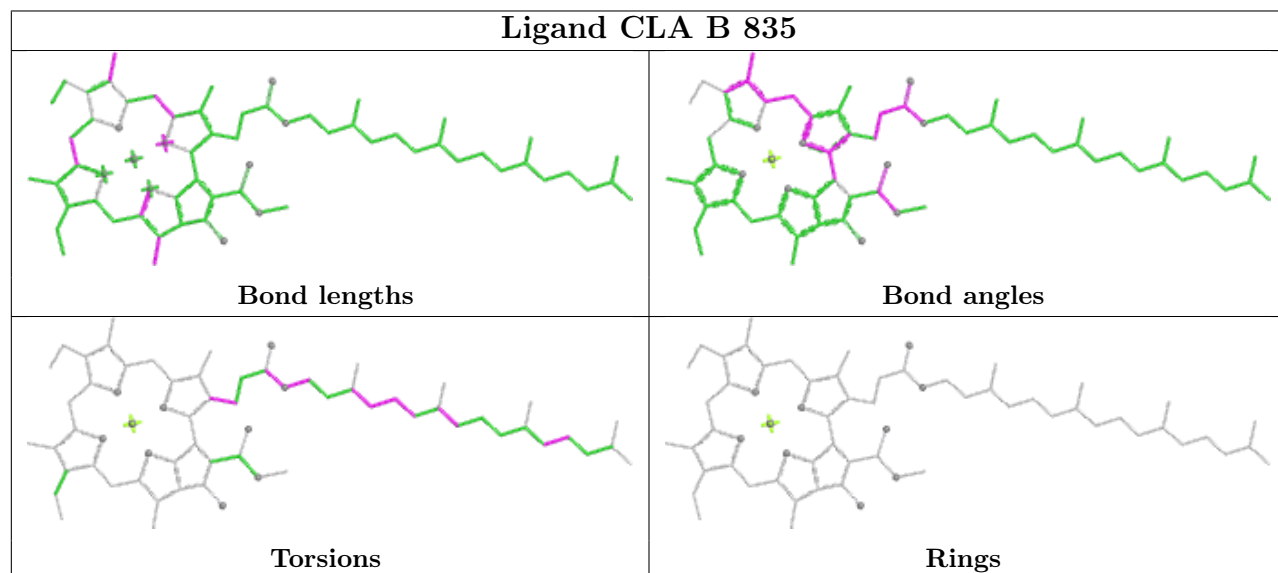
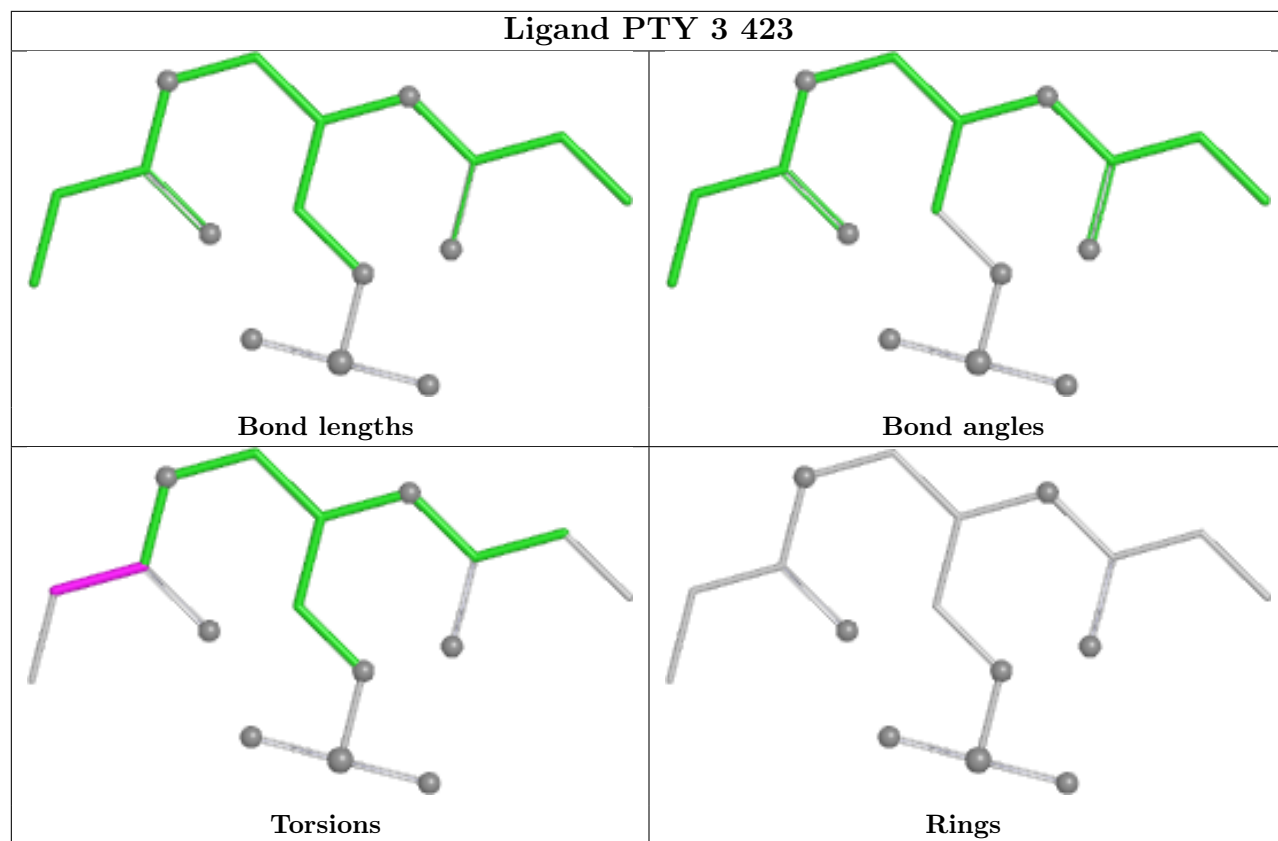
Torsions

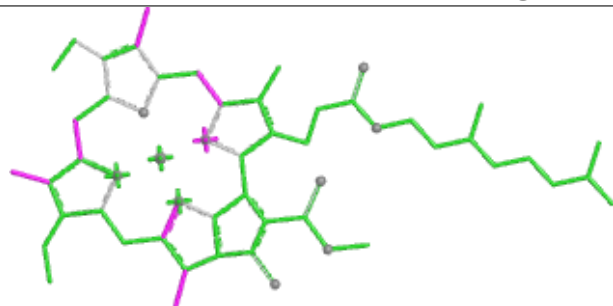


Rings

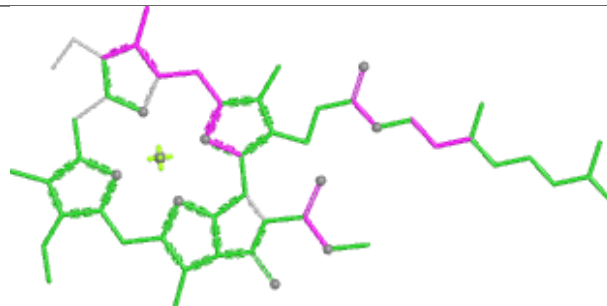
Ligand CLA 1 304



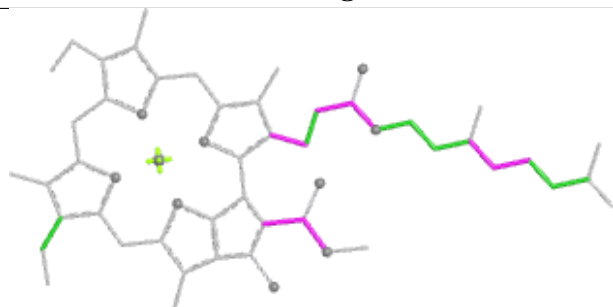


Ligand CLA B 836

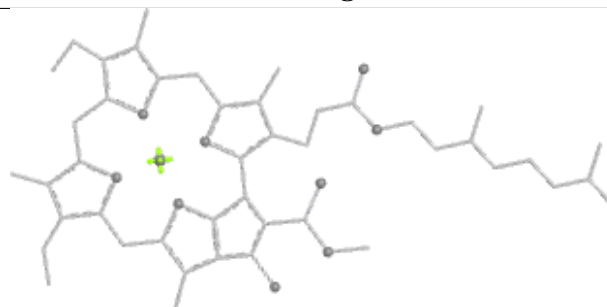
Bond lengths



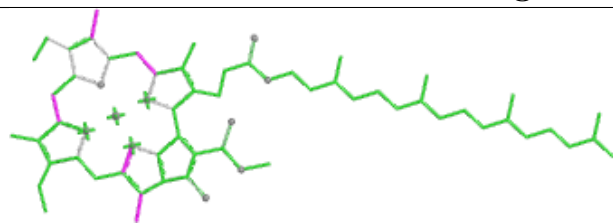
Bond angles



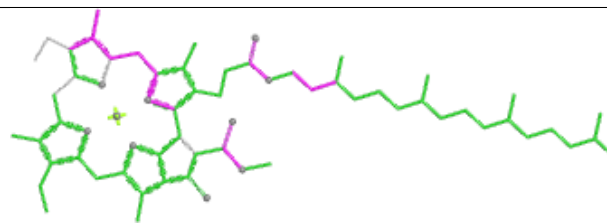
Torsions



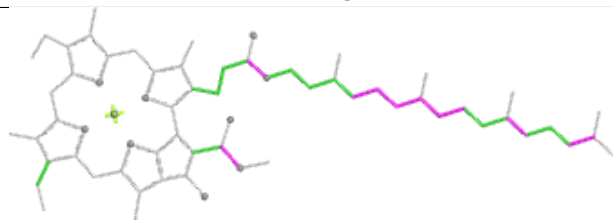
Rings

Ligand CLA A 816

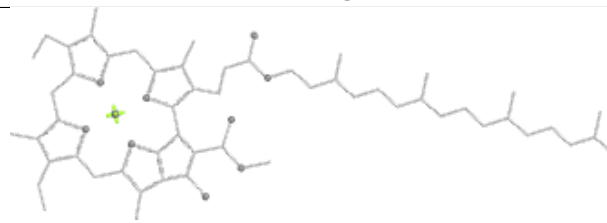
Bond lengths



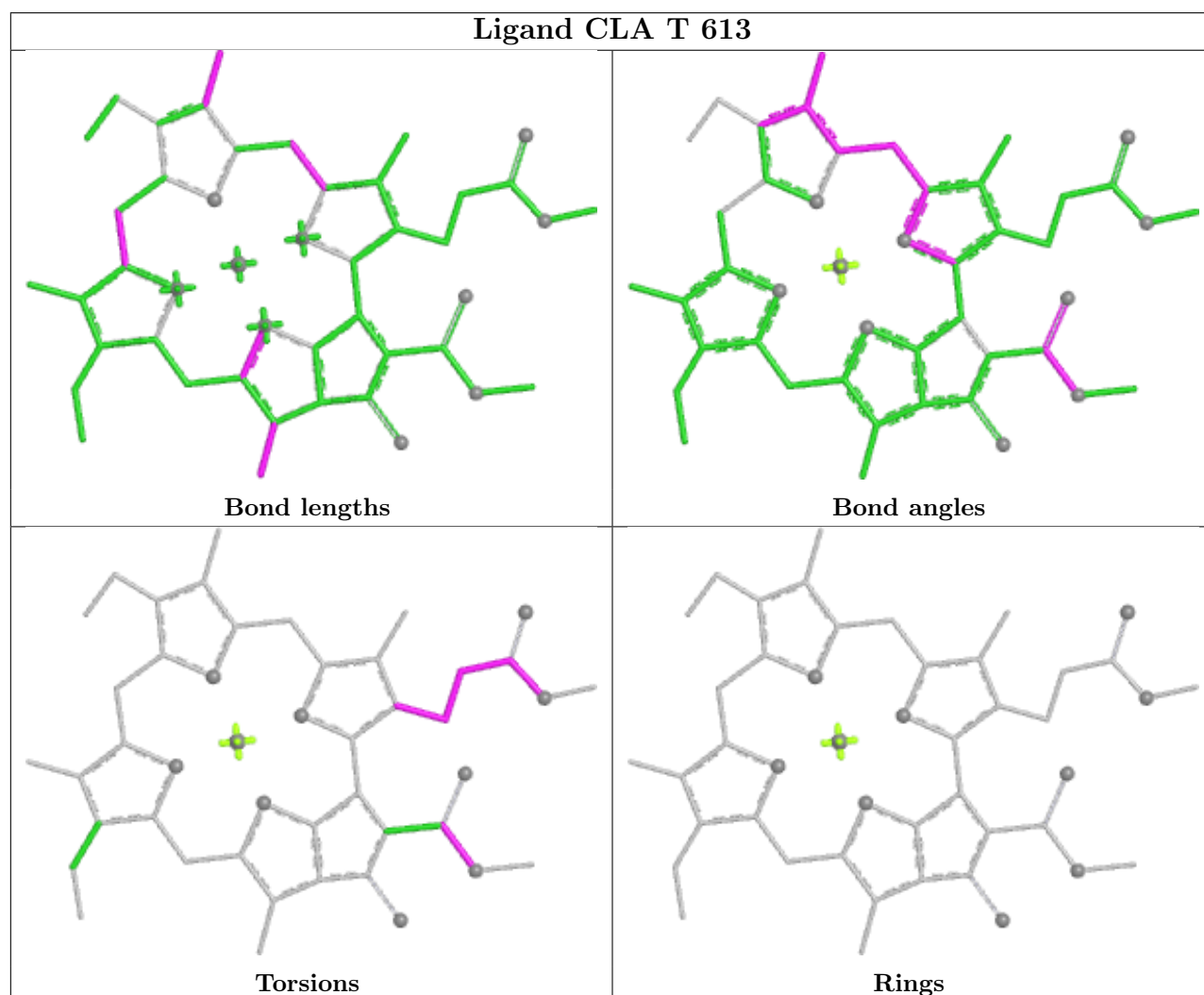
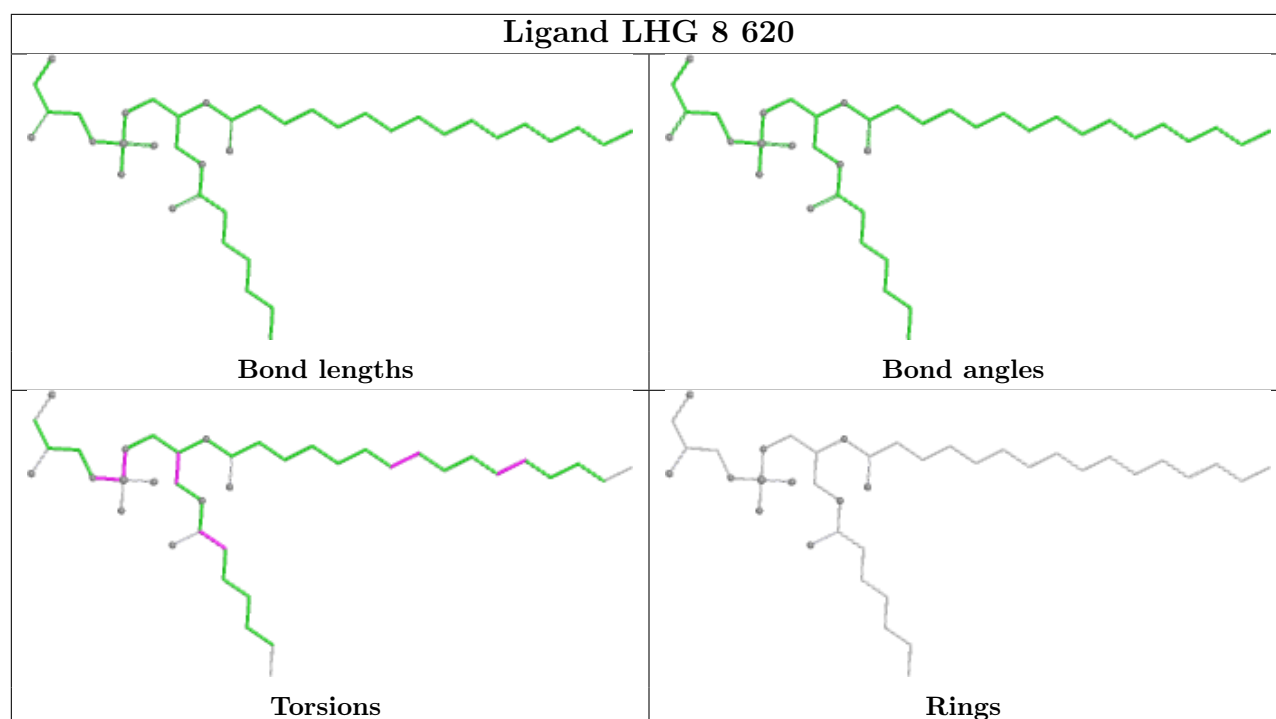
Bond angles



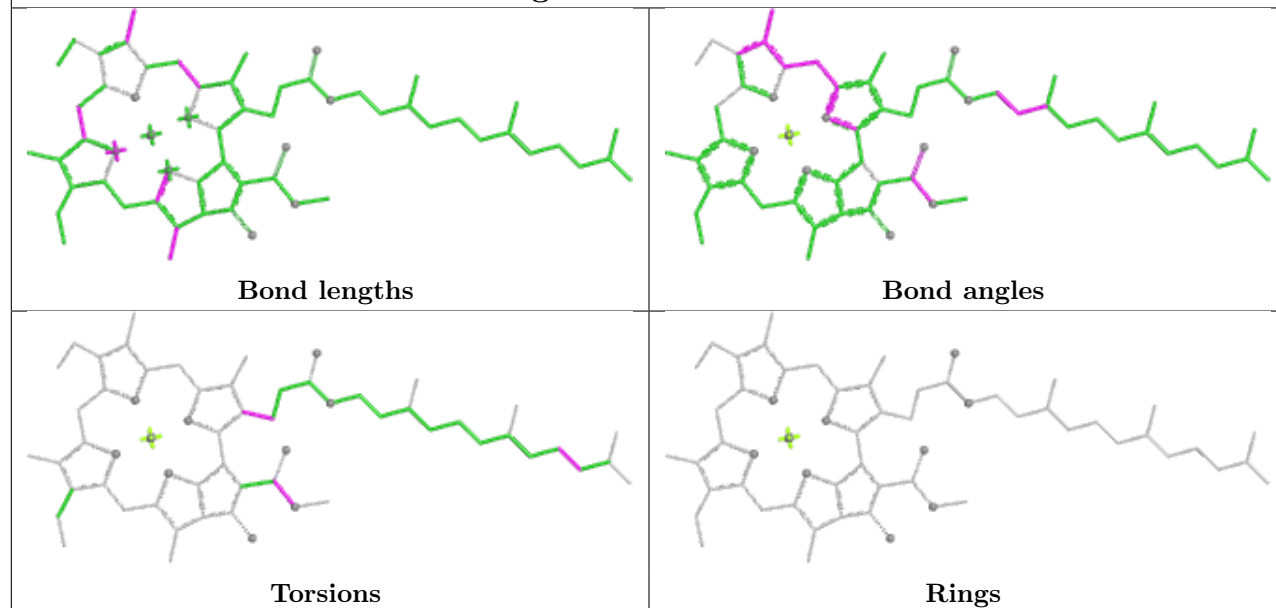
Torsions



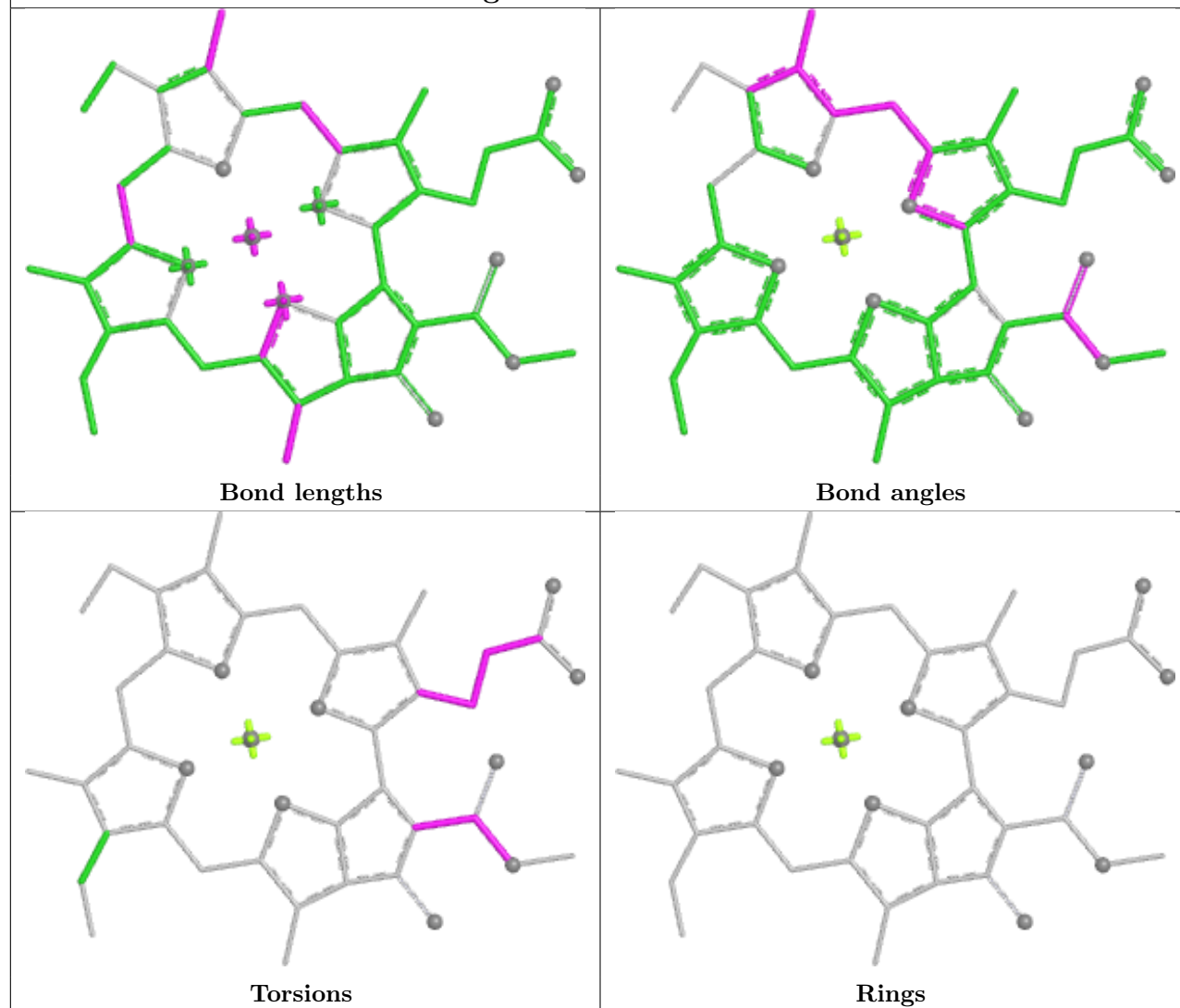
Rings

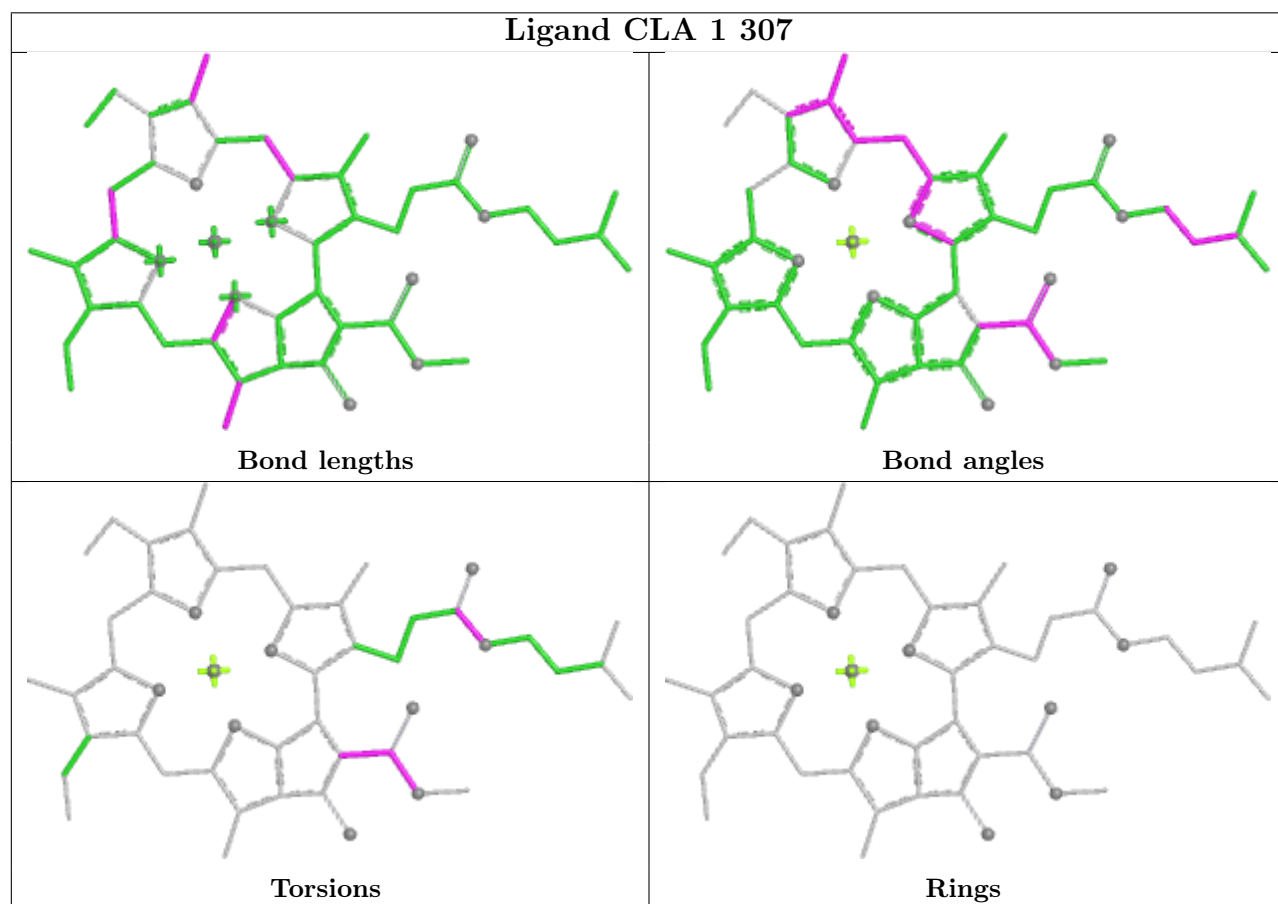
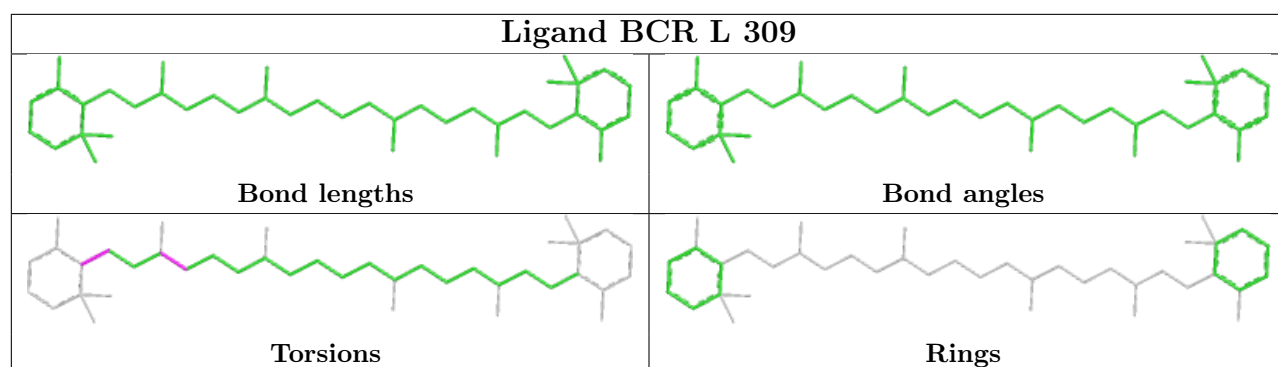


Ligand CLA A 840

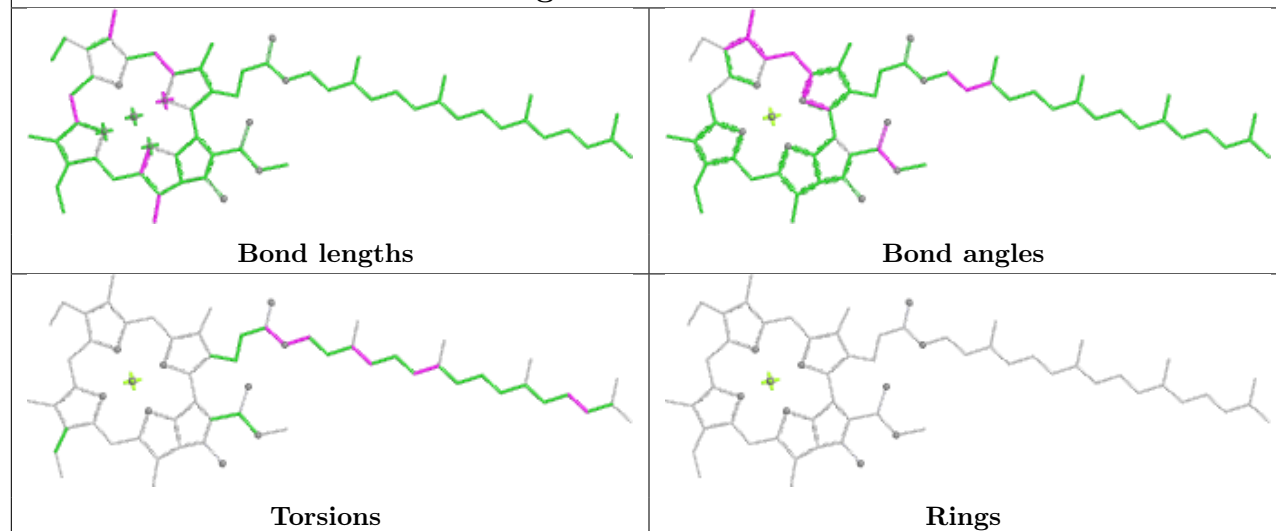


Ligand CLA O 2003

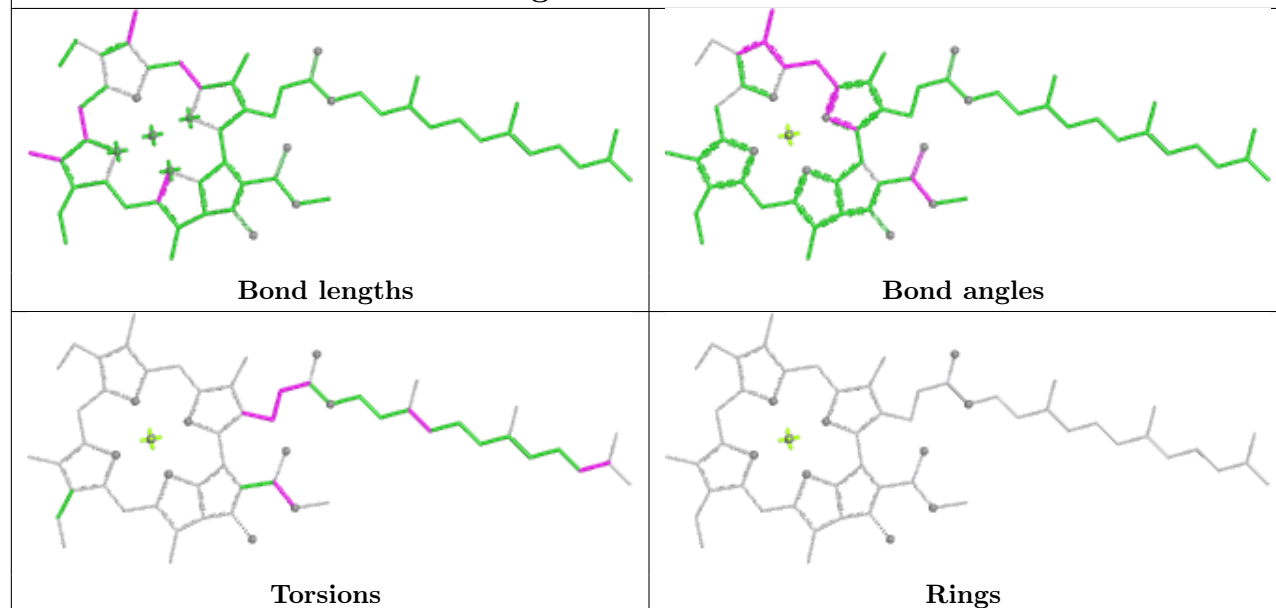




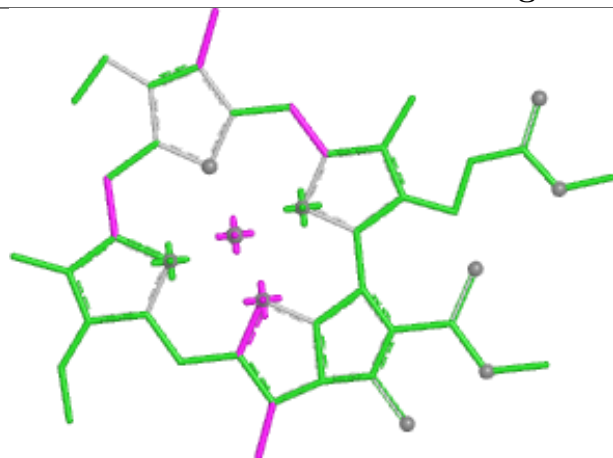
Ligand CLA 7 316



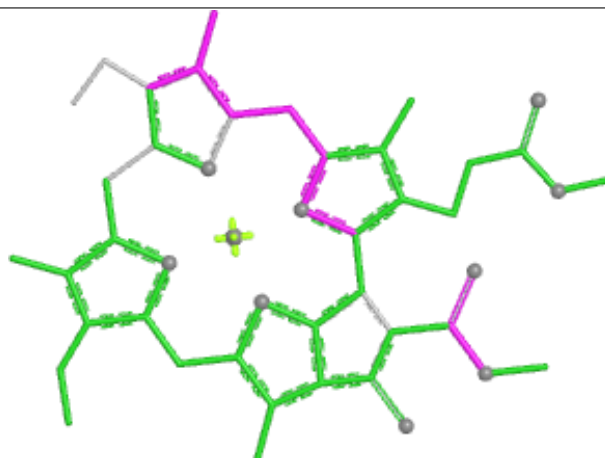
Ligand CLA H 203



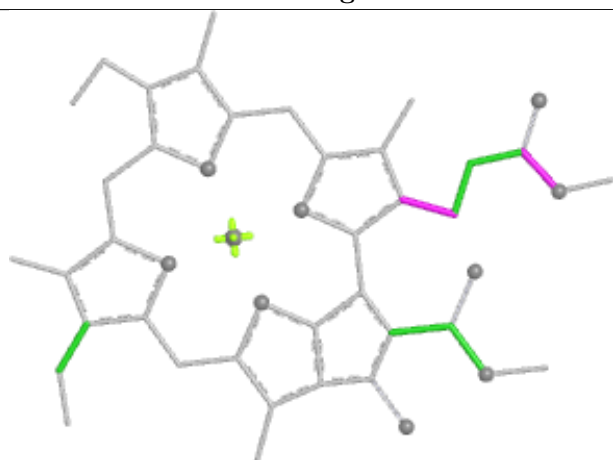
Ligand CLA 3 414



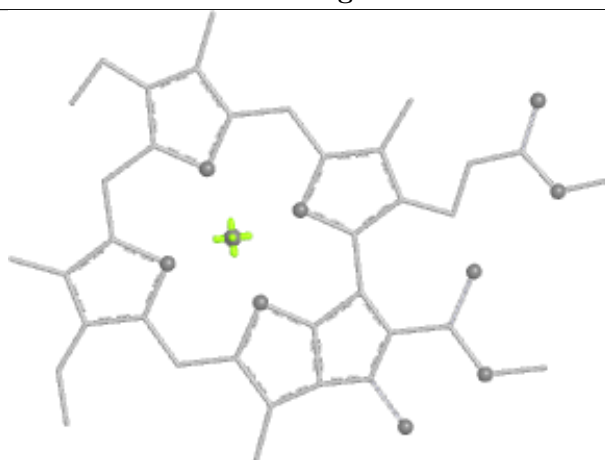
Bond lengths



Bond angles

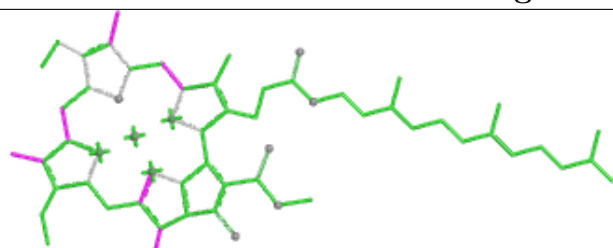


Torsions

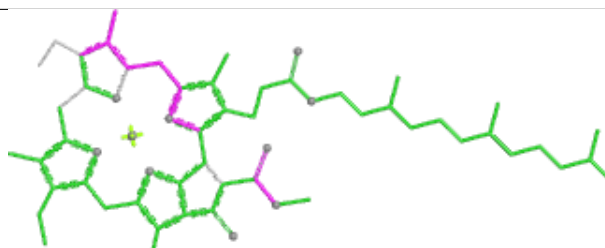


Rings

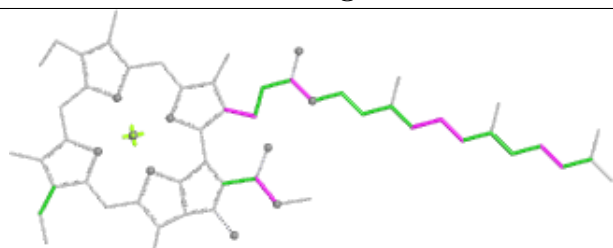
Ligand CLA B 814



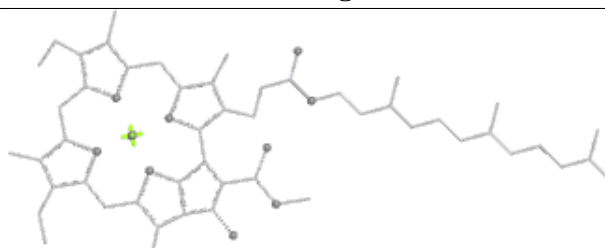
Bond lengths



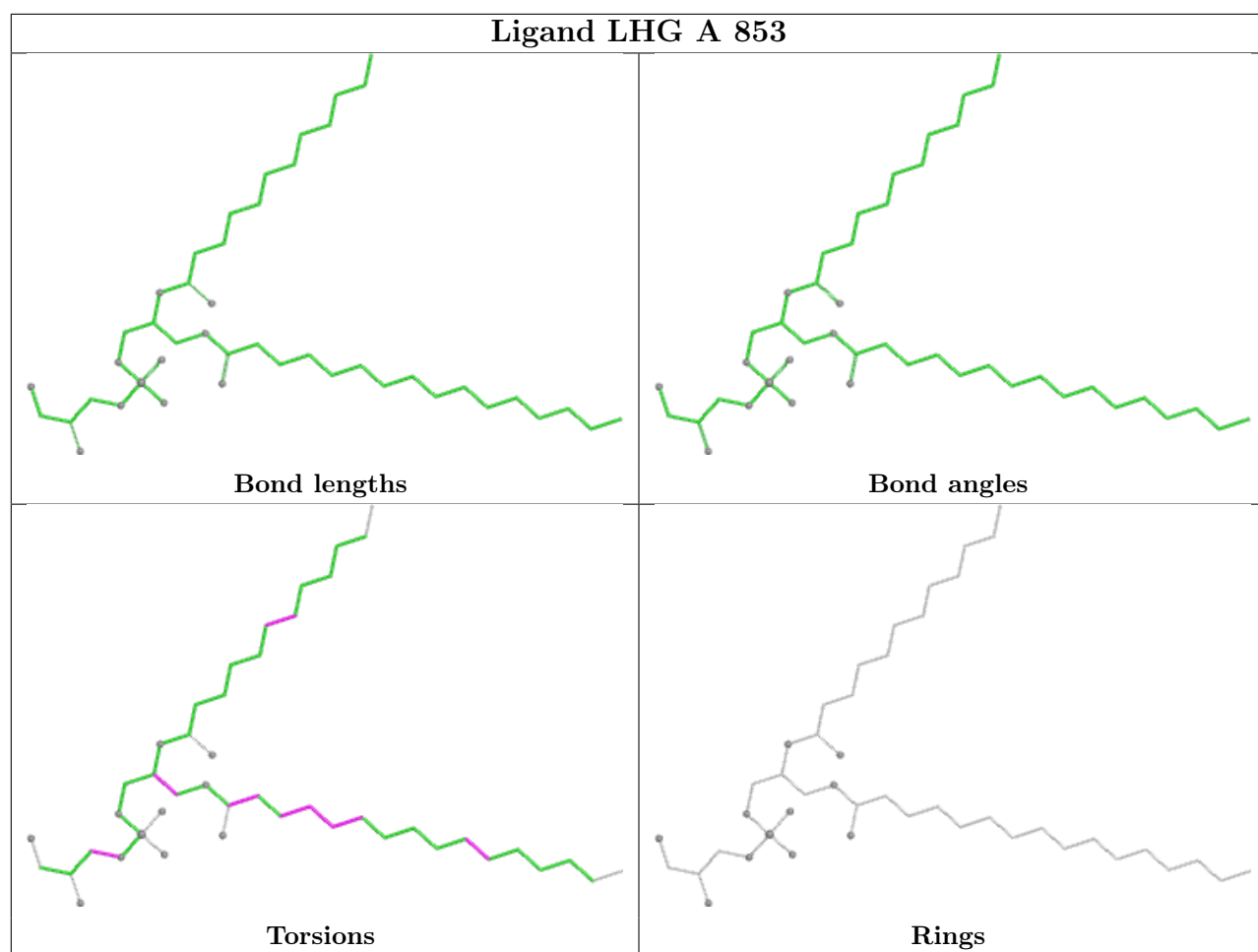
Bond angles

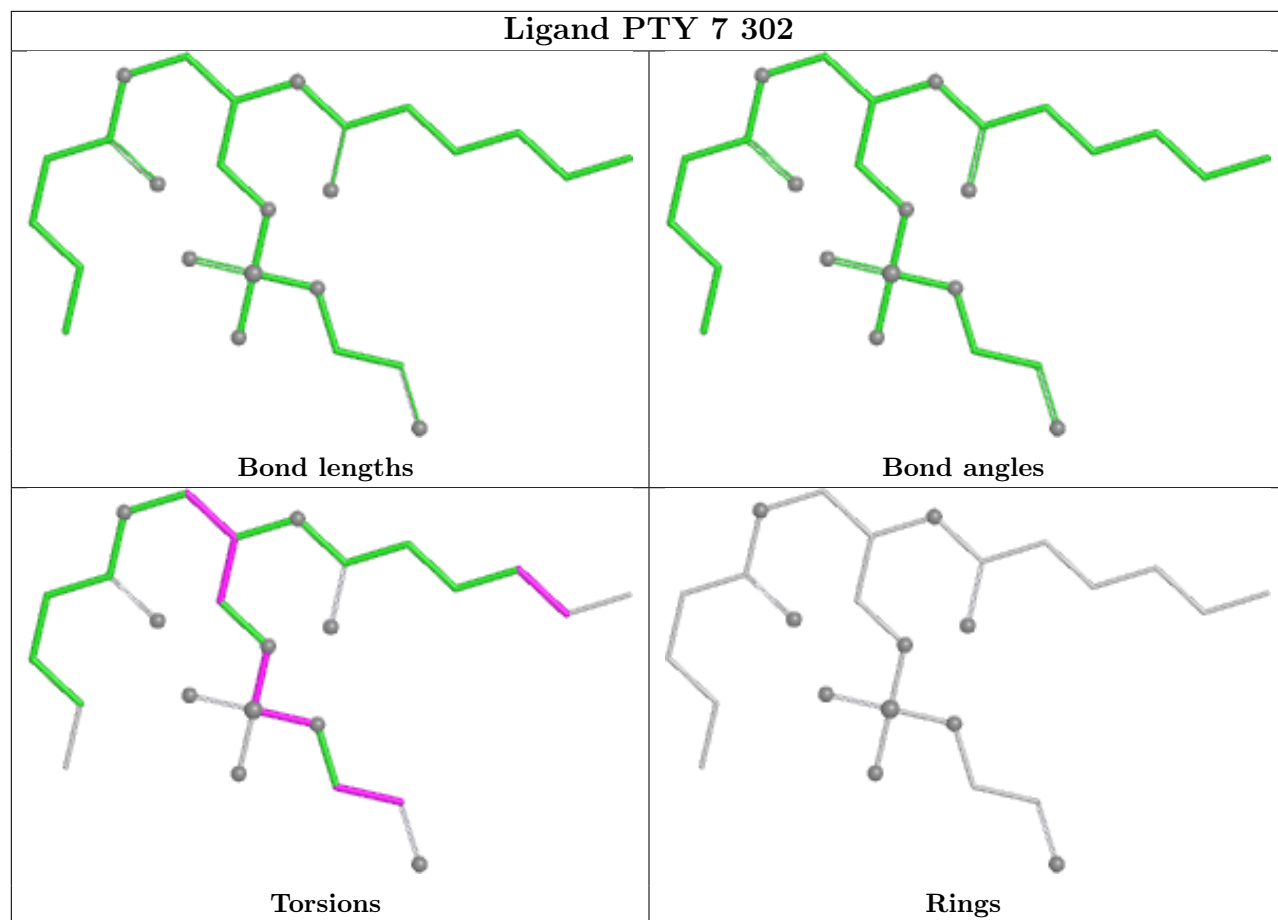


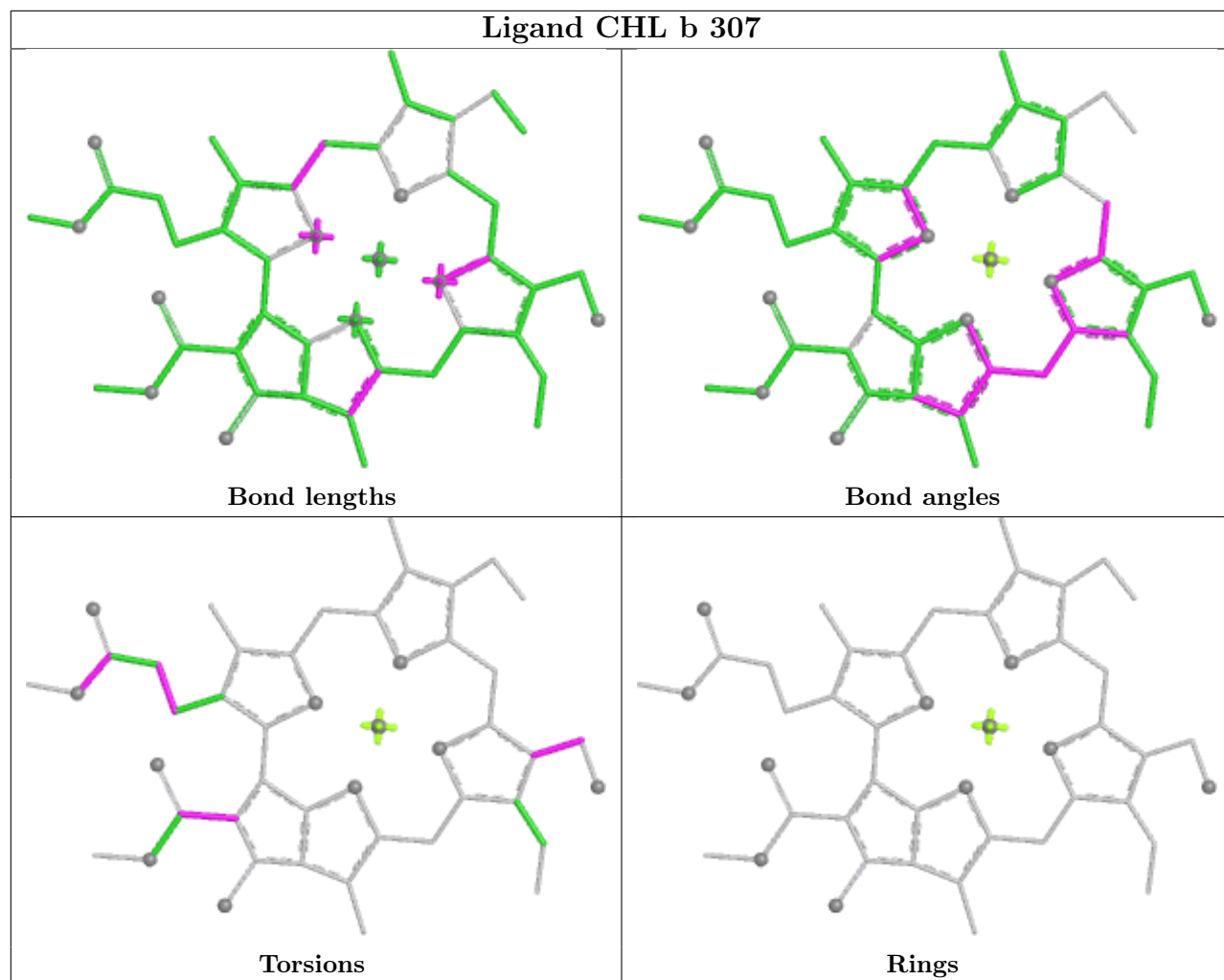
Torsions

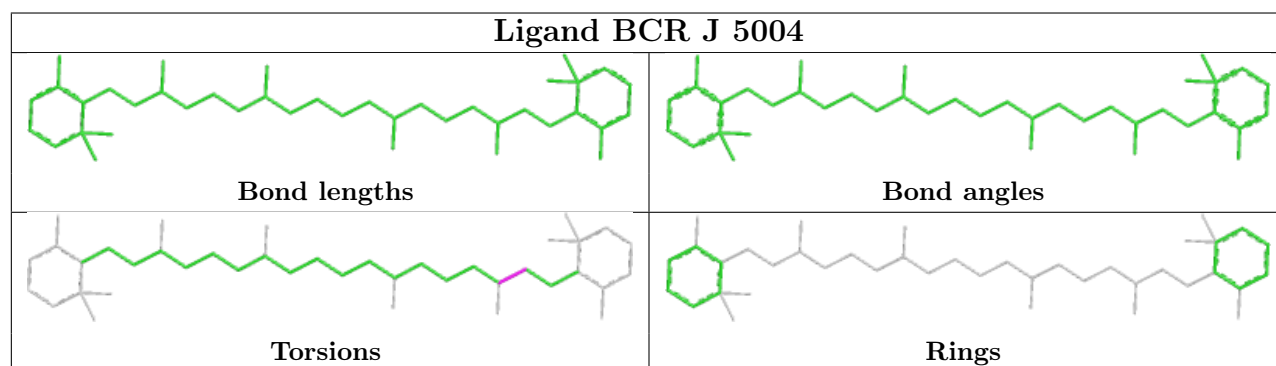
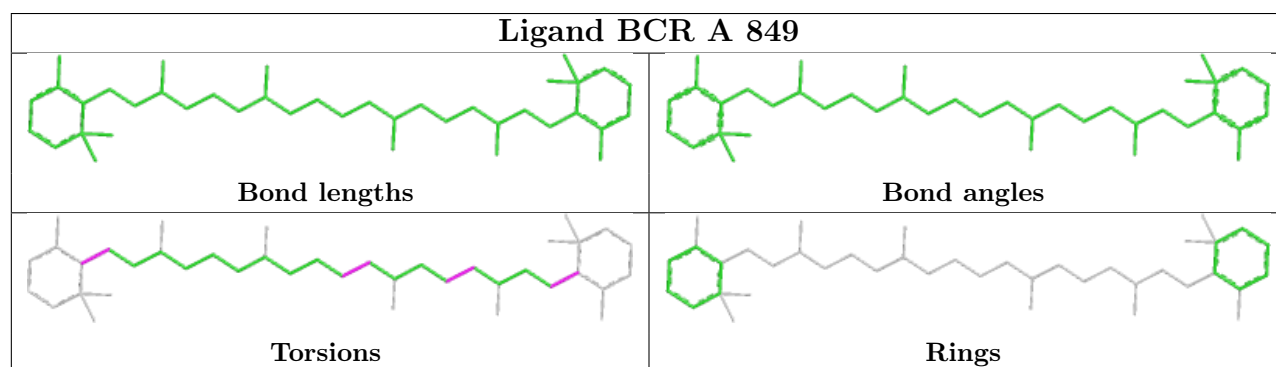
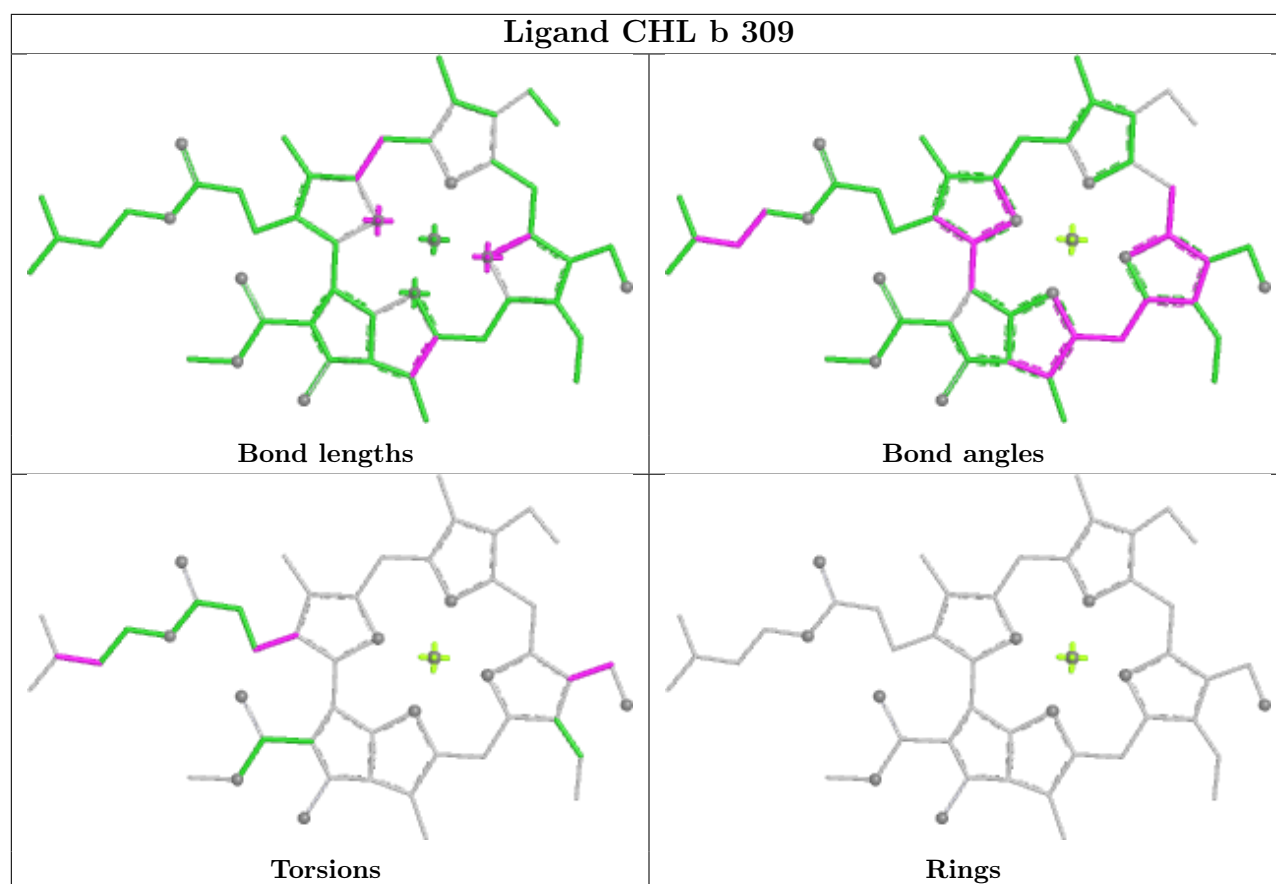


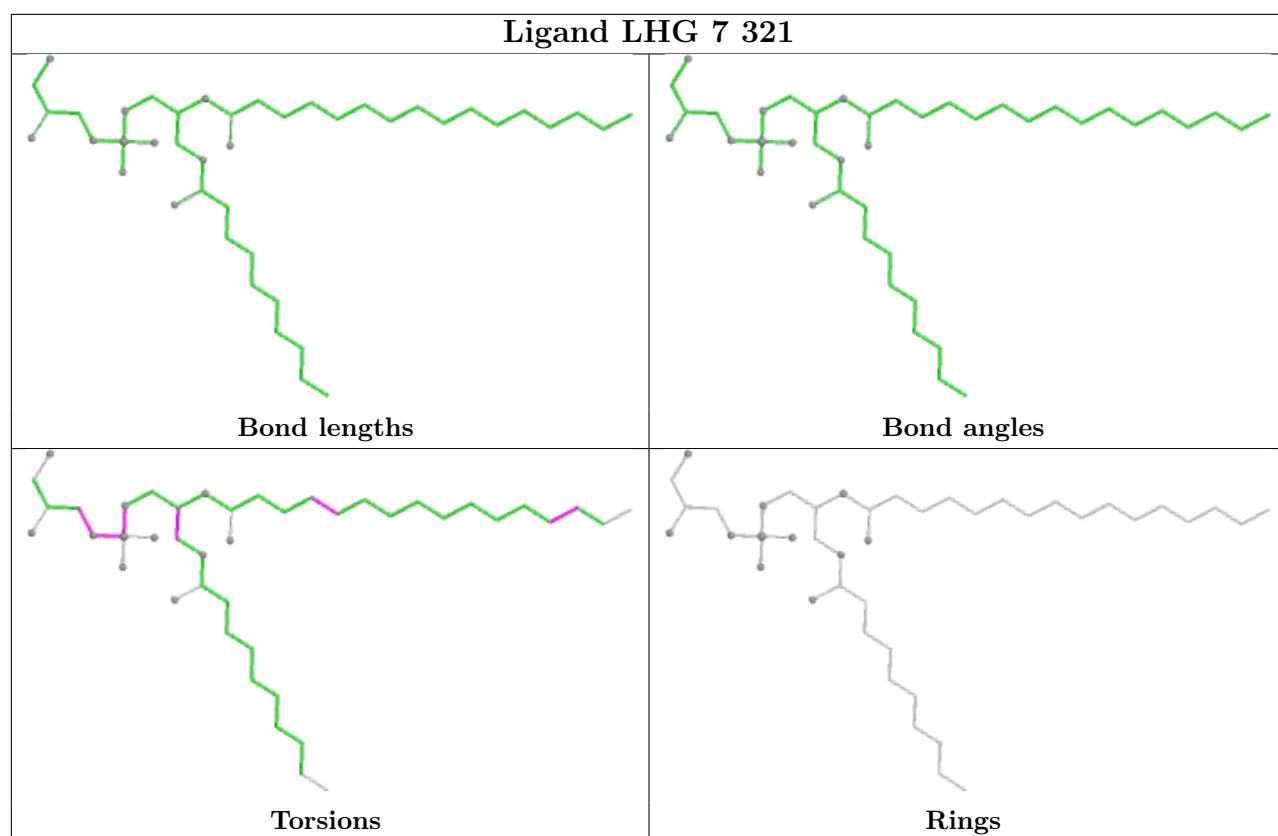
Rings



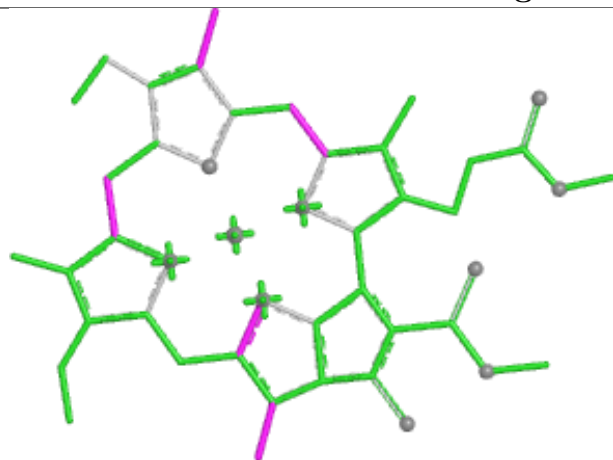




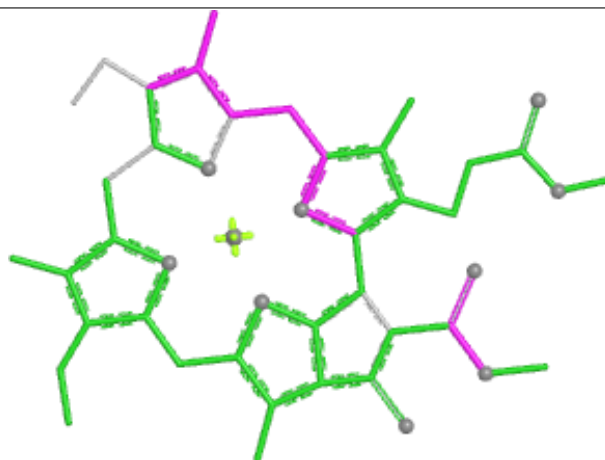




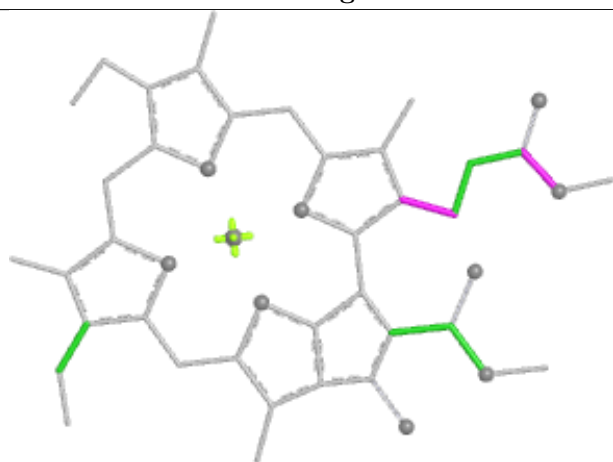
Ligand CLA T 610



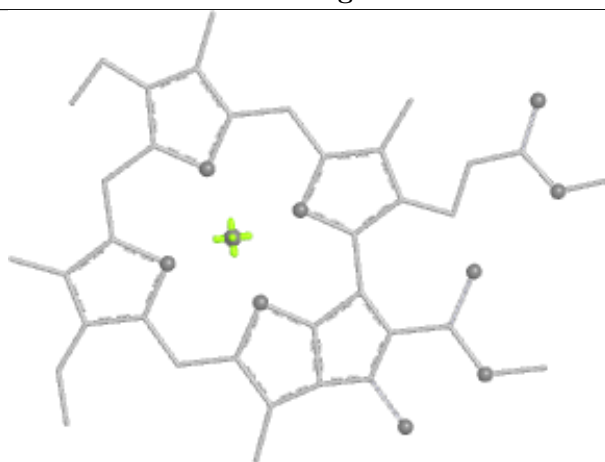
Bond lengths



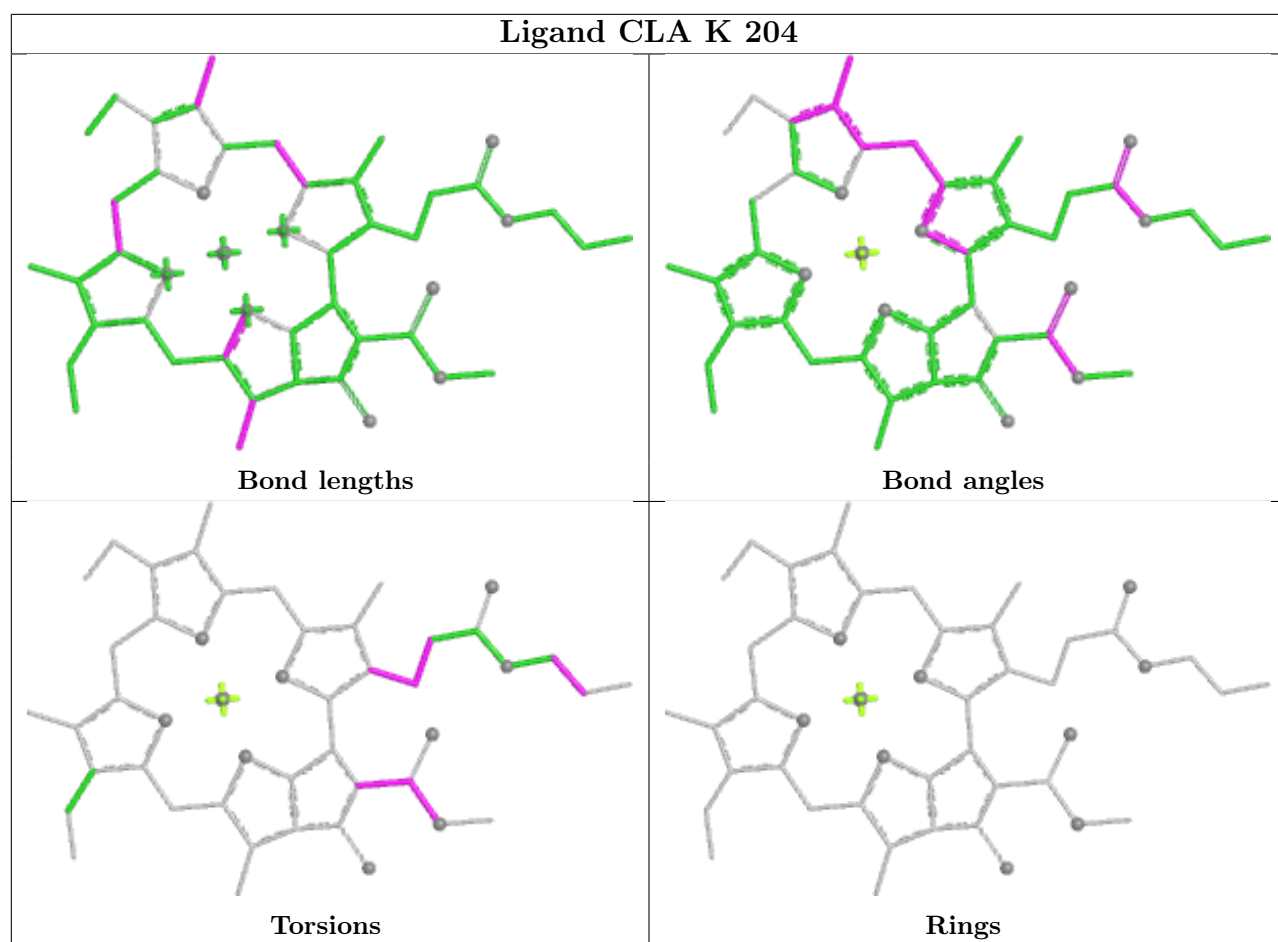
Bond angles



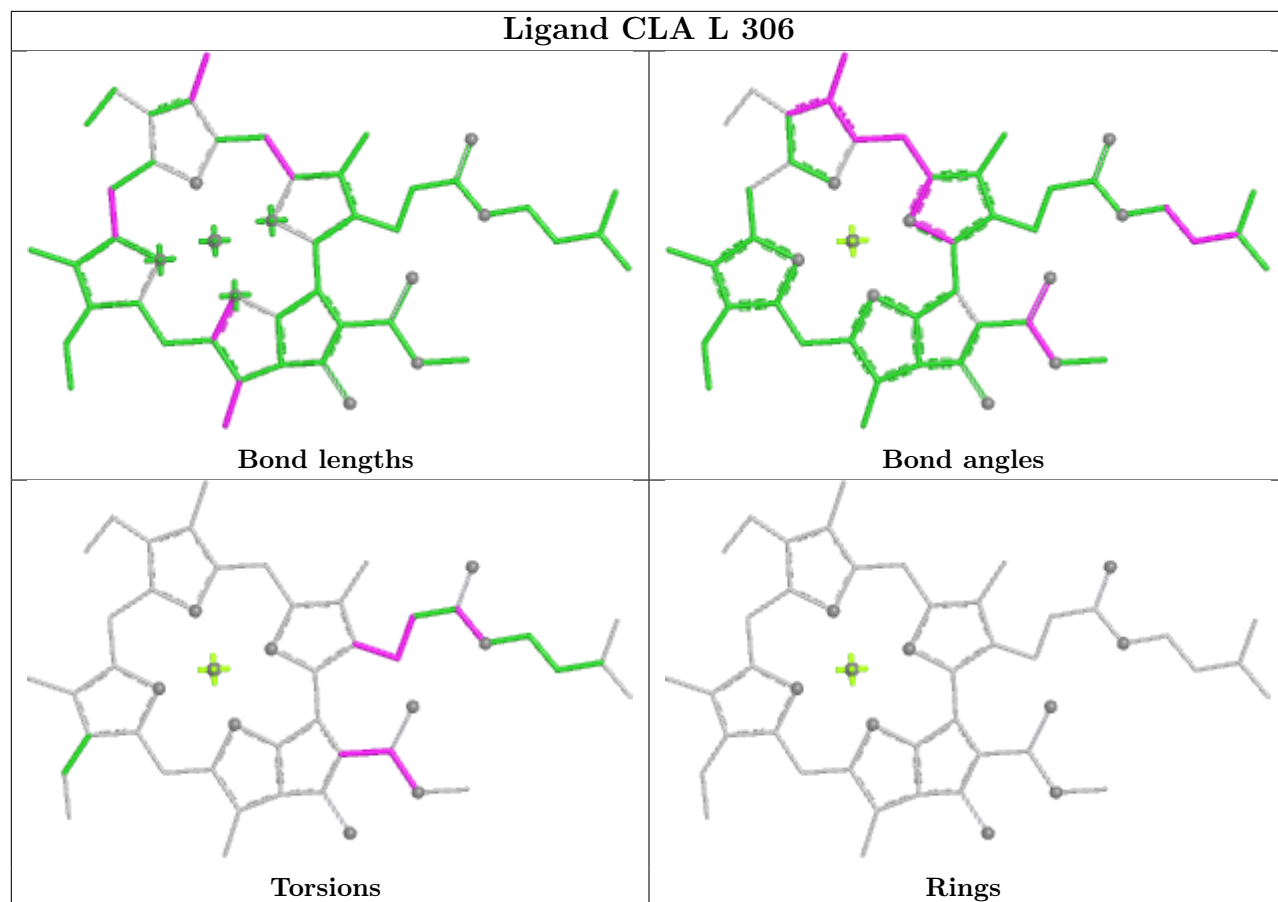
Torsions



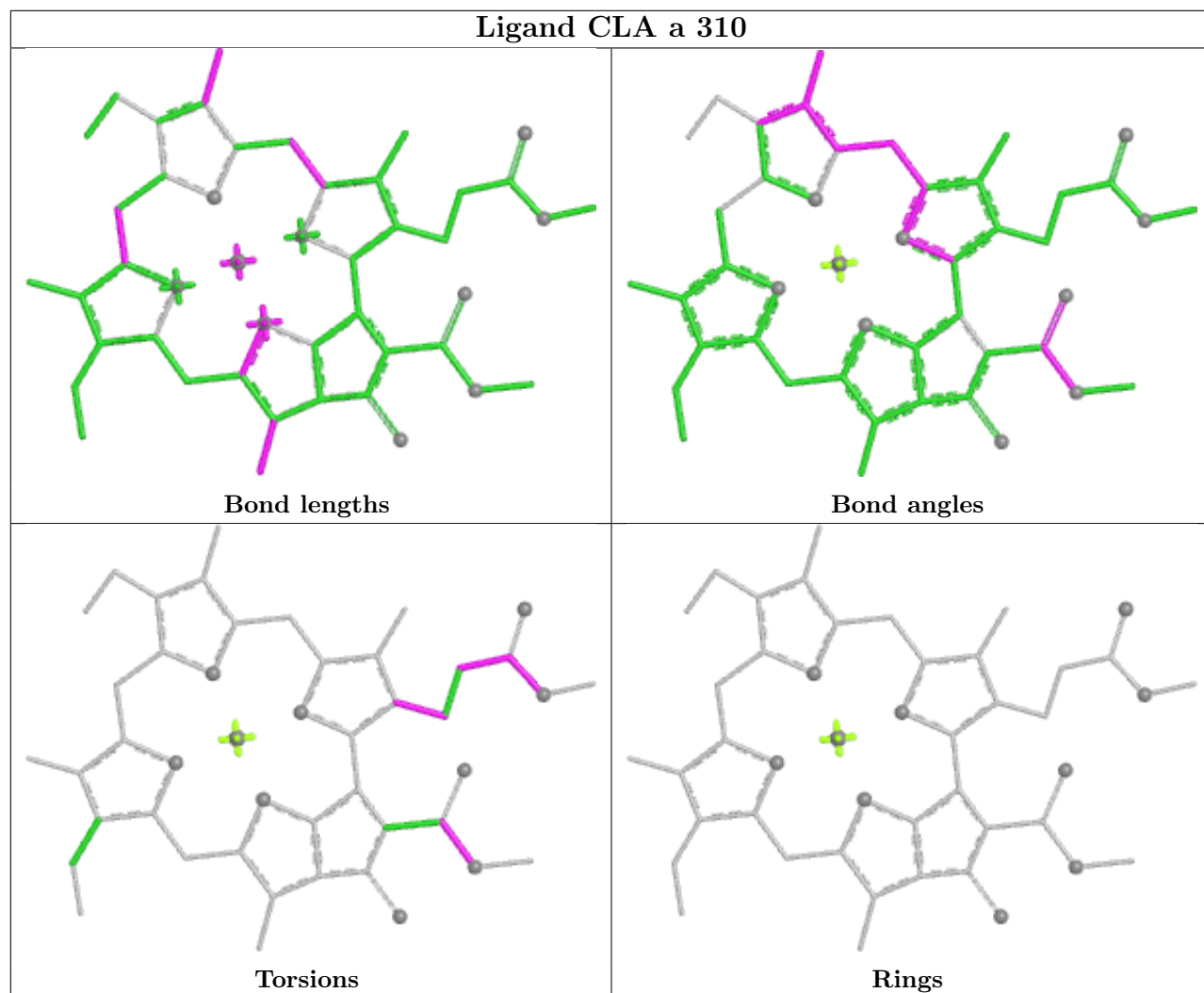
Rings

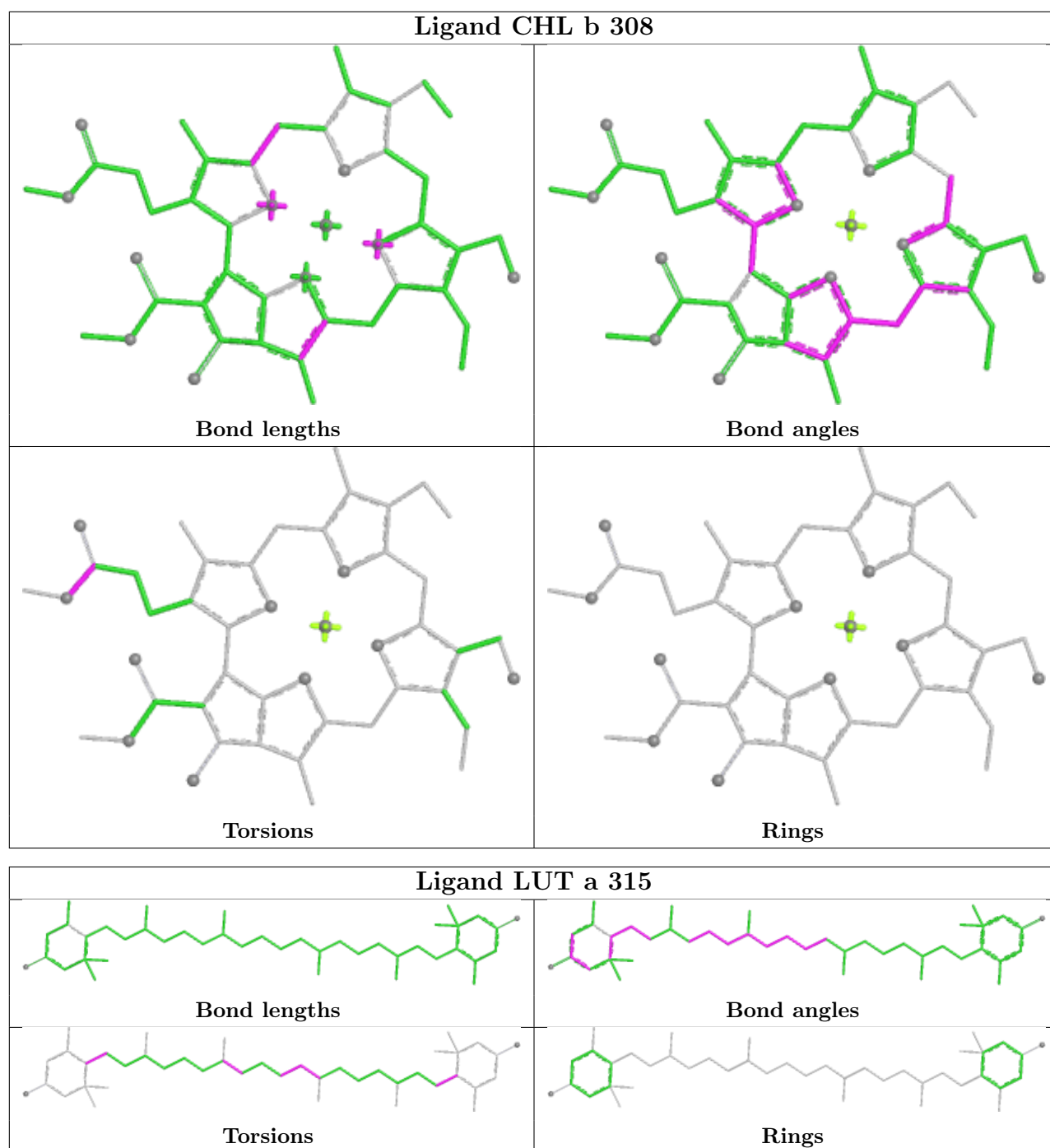


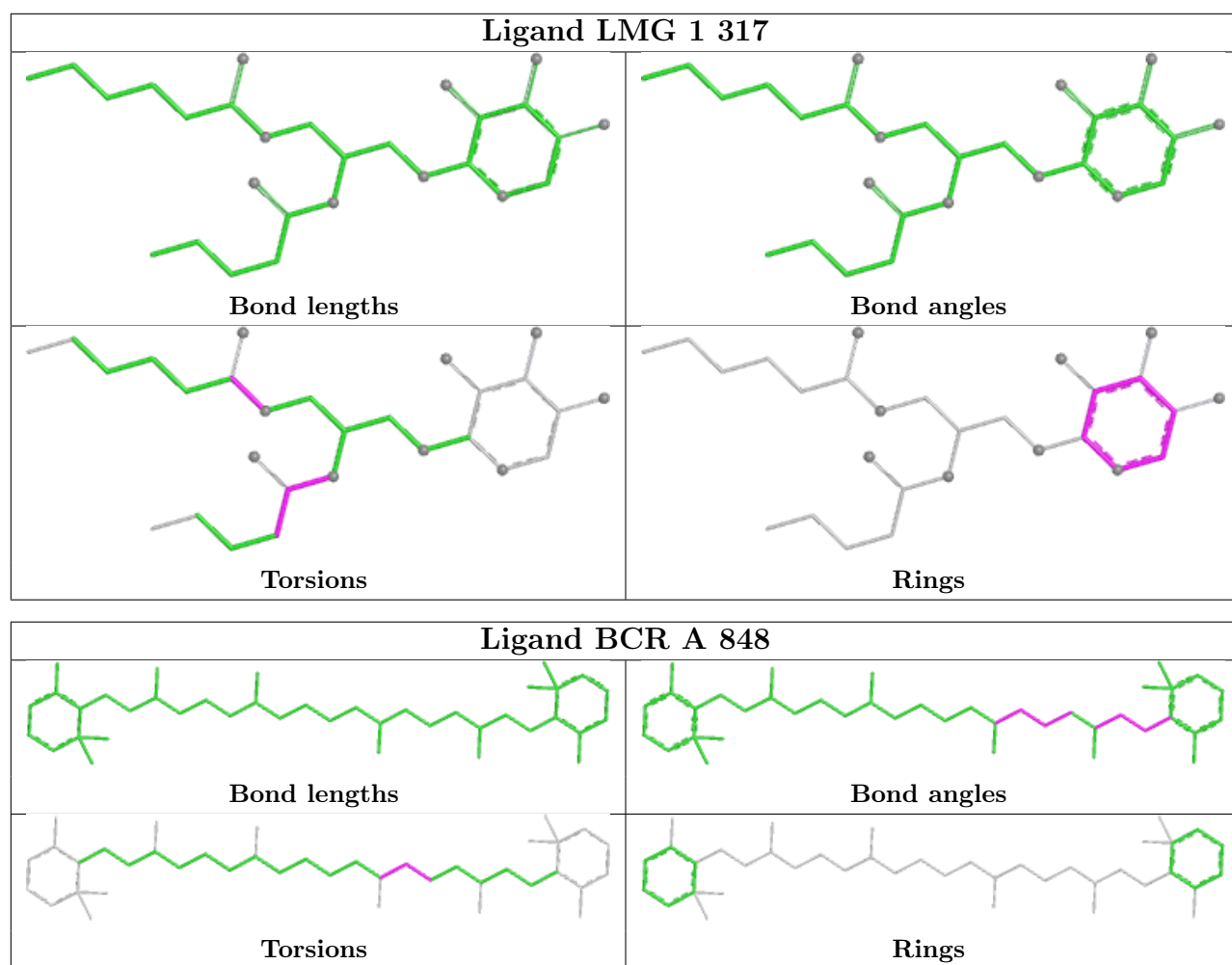
Ligand CLA L 306



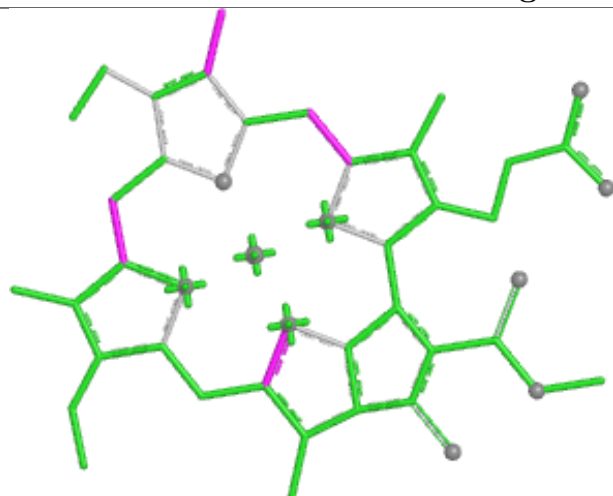
Ligand CLA a 310



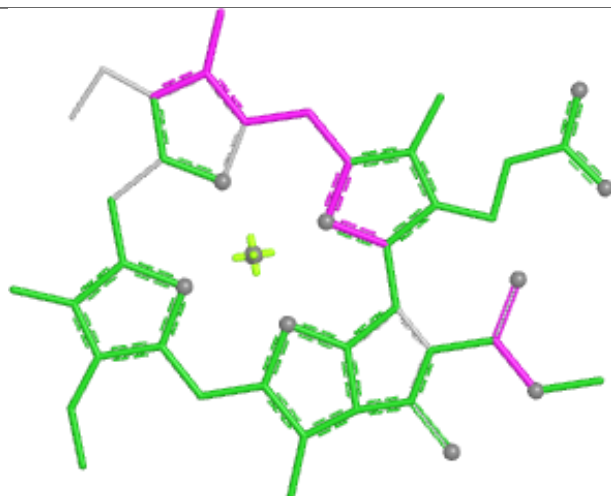




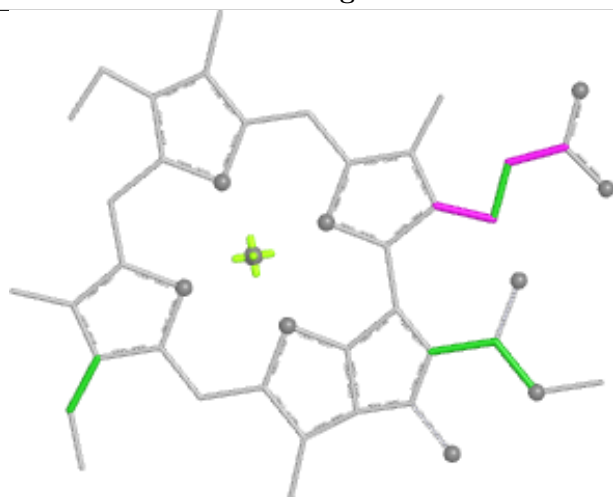
Ligand CLA c 608



Bond lengths



Bond angles

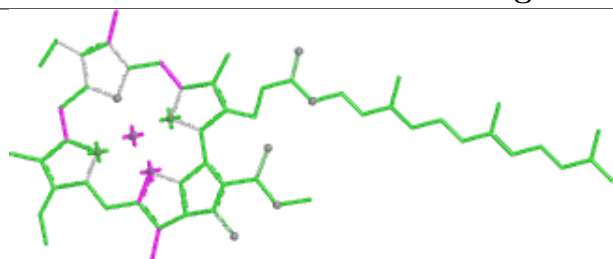


Torsions

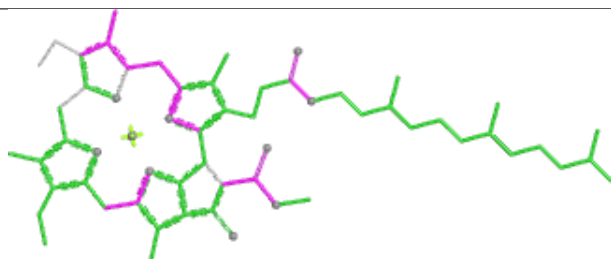


Rings

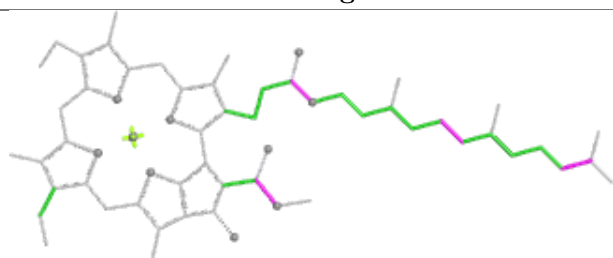
Ligand CLA B 840



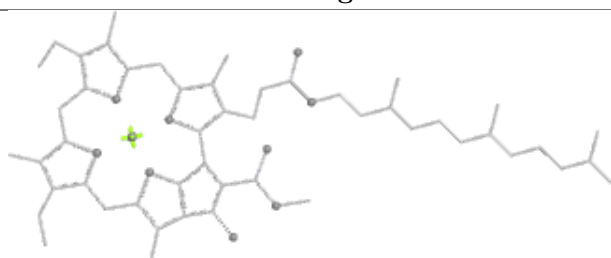
Bond lengths



Bond angles

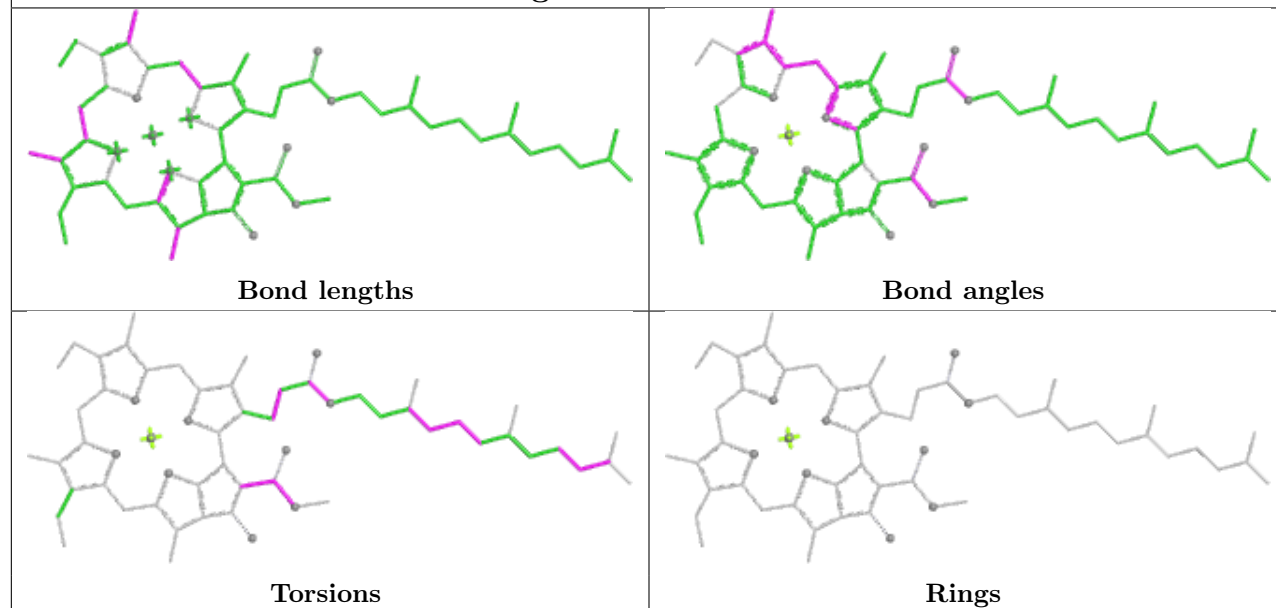


Torsions

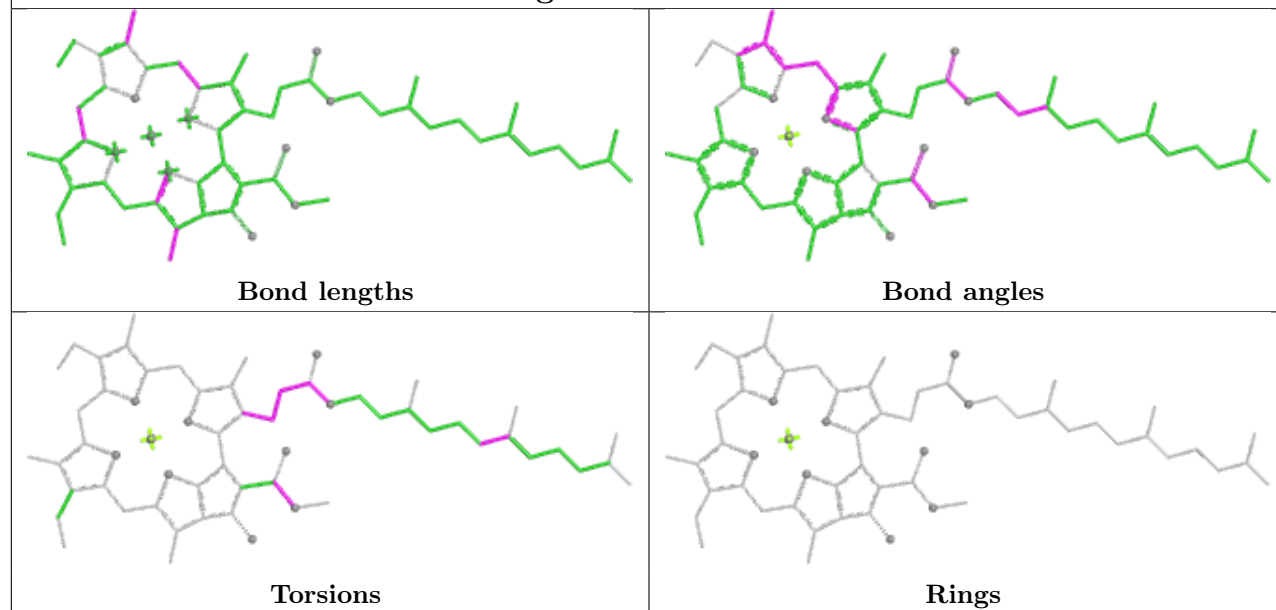


Rings

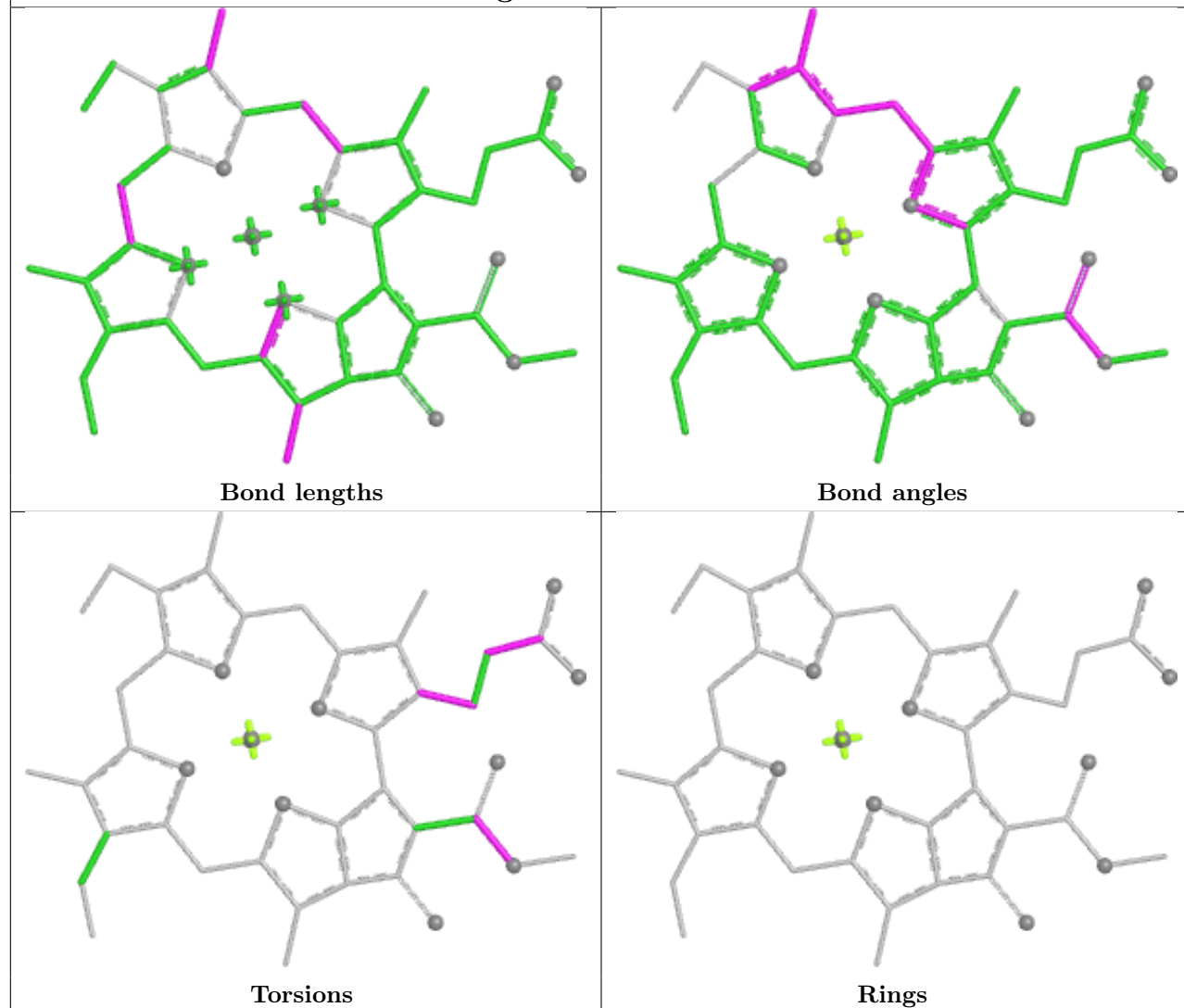
Ligand CLA A 819



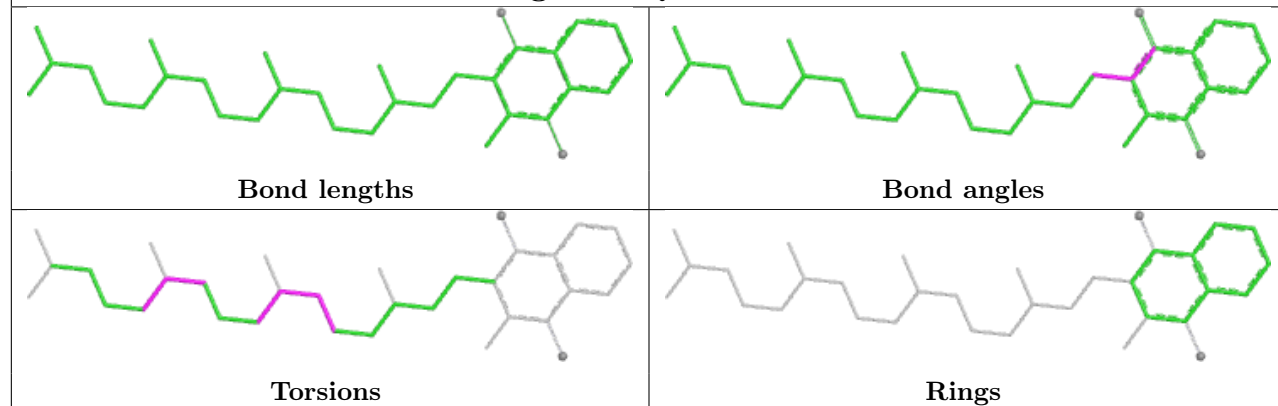
Ligand CLA a 312



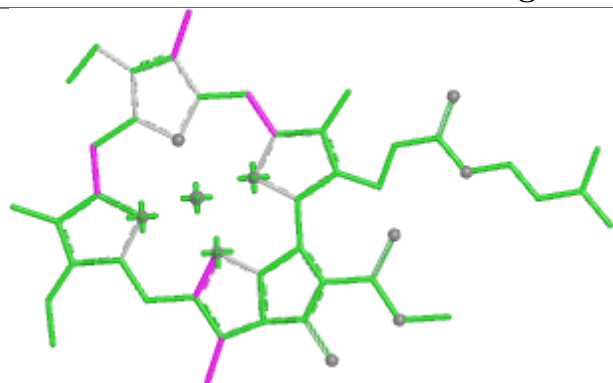
Ligand CLA 2 605



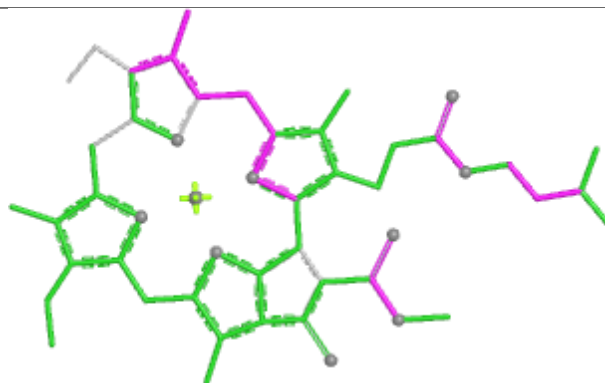
Ligand PQN B 845



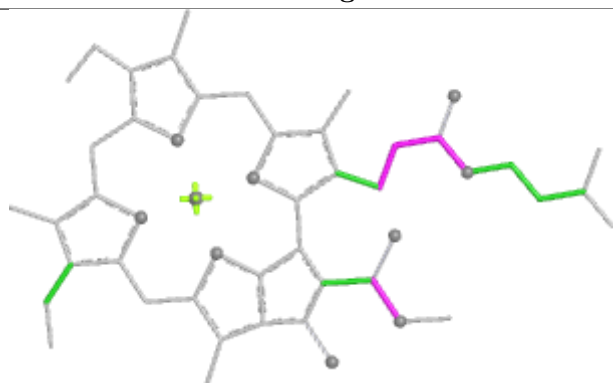
Ligand CLA 7 315



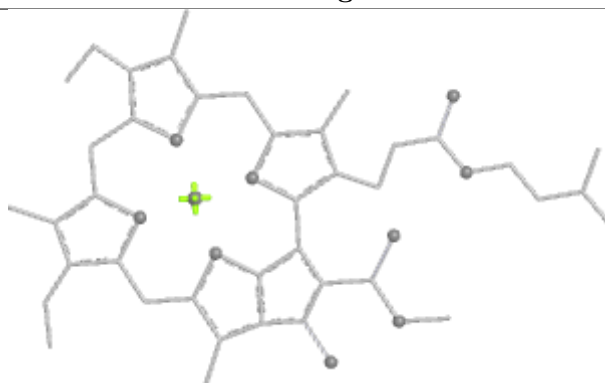
Bond lengths



Bond angles

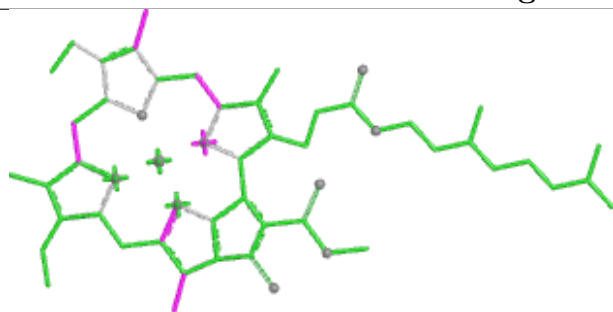


Torsions

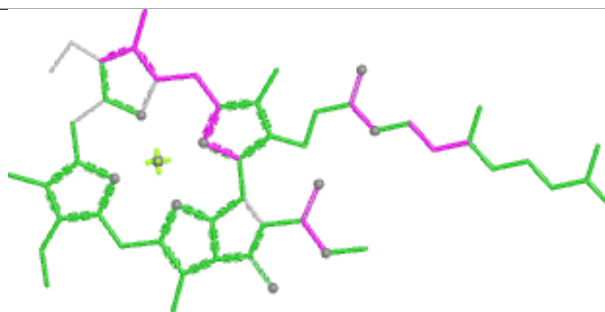


Rings

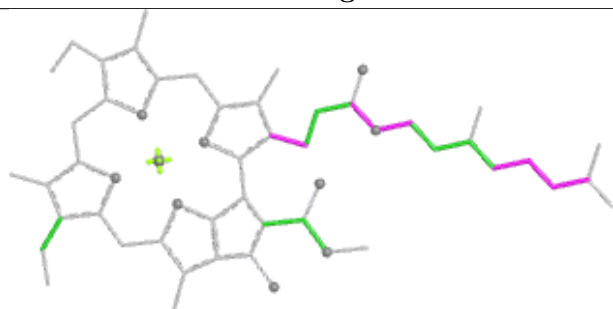
Ligand CLA 8 611



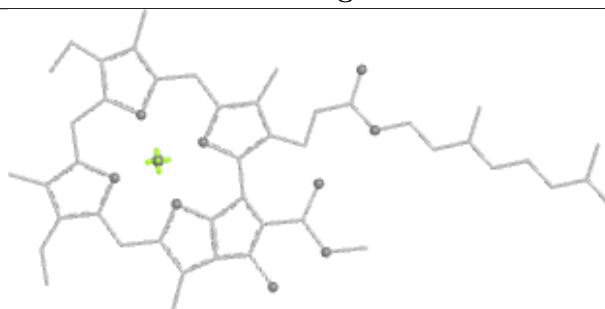
Bond lengths



Bond angles

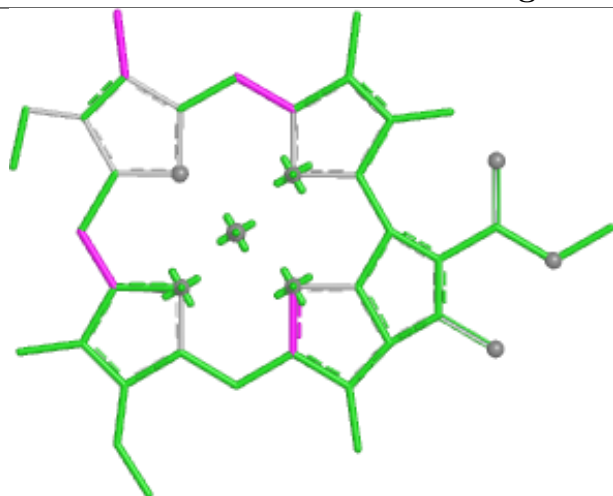


Torsions

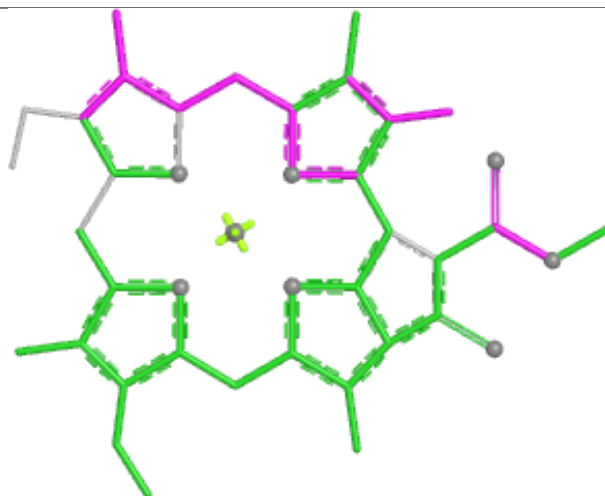


Rings

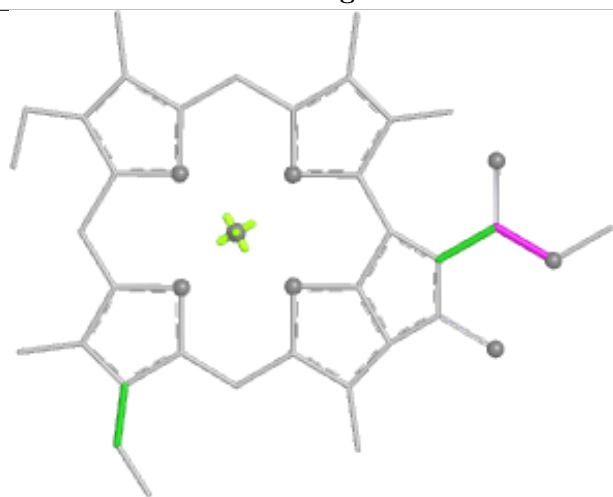
Ligand CLA 2 609



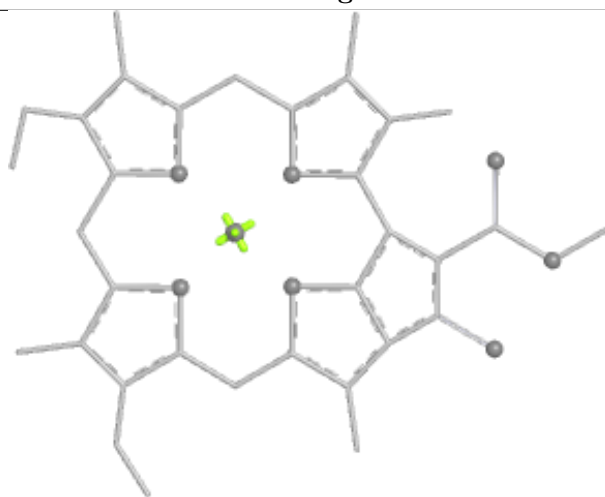
Bond lengths



Bond angles

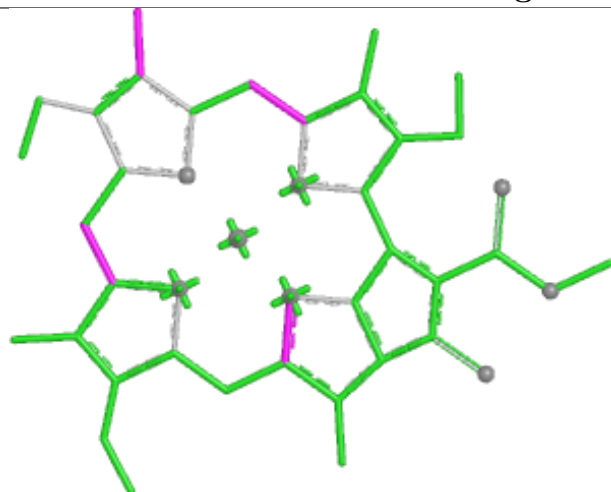


Torsions



Rings

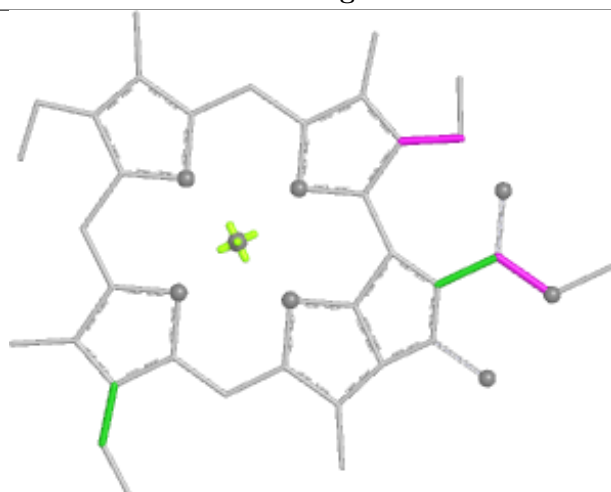
Ligand CLA T 614



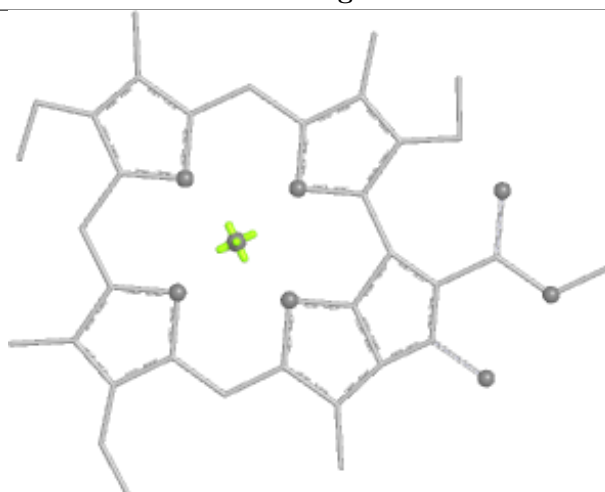
Bond lengths



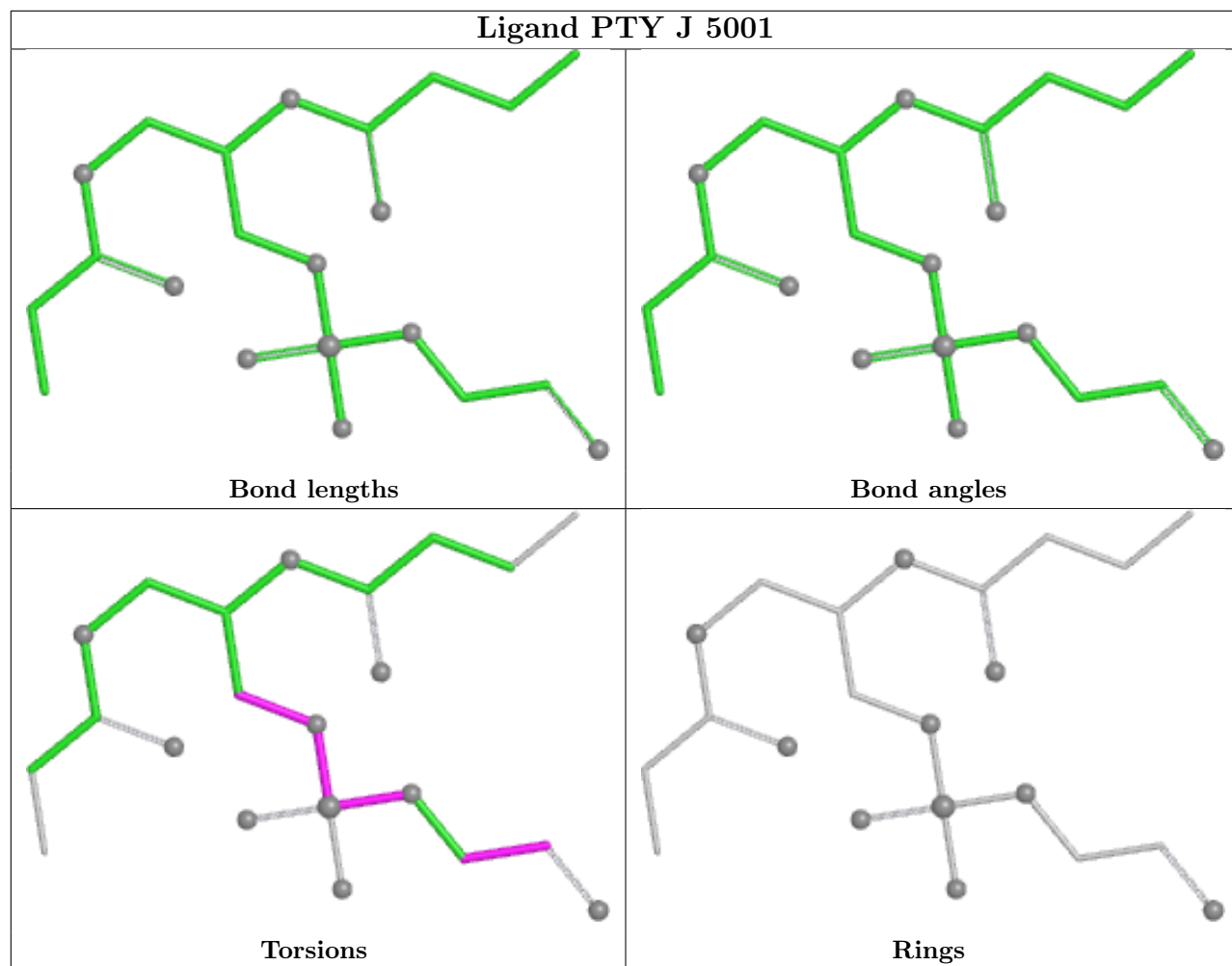
Bond angles



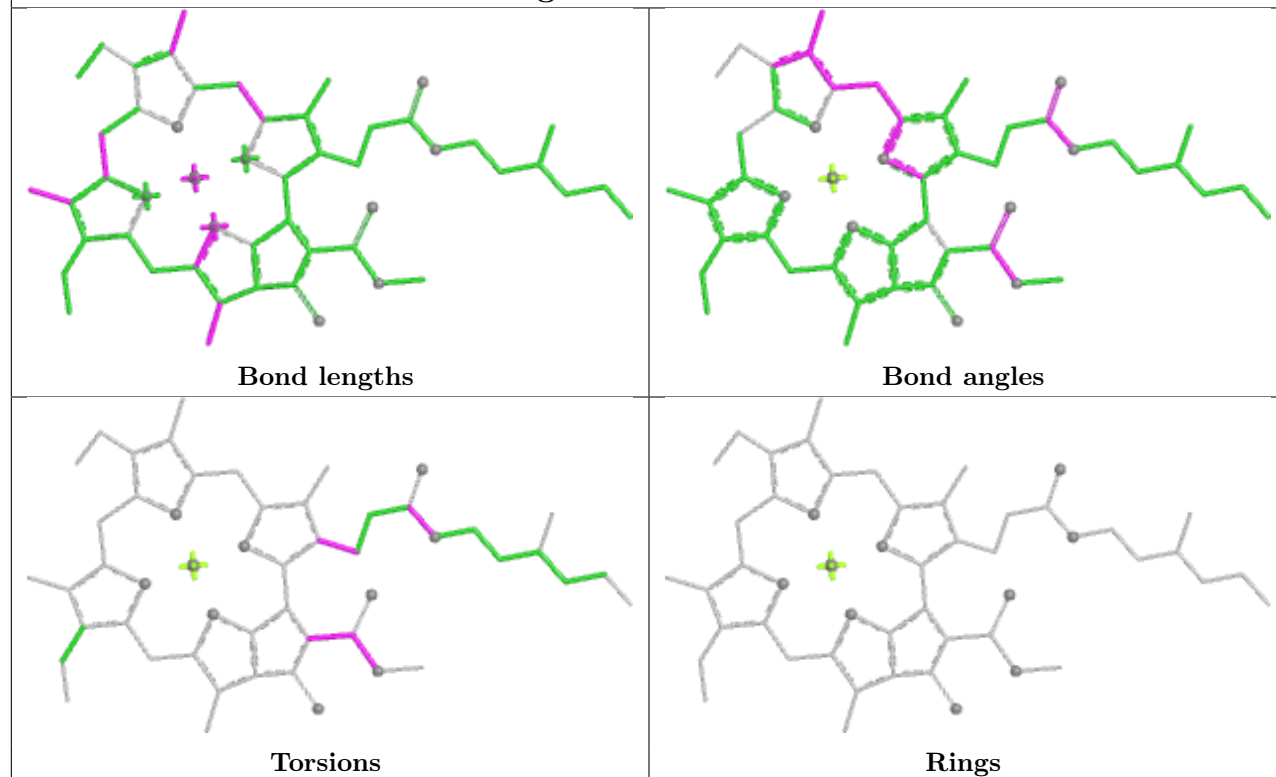
Torsions



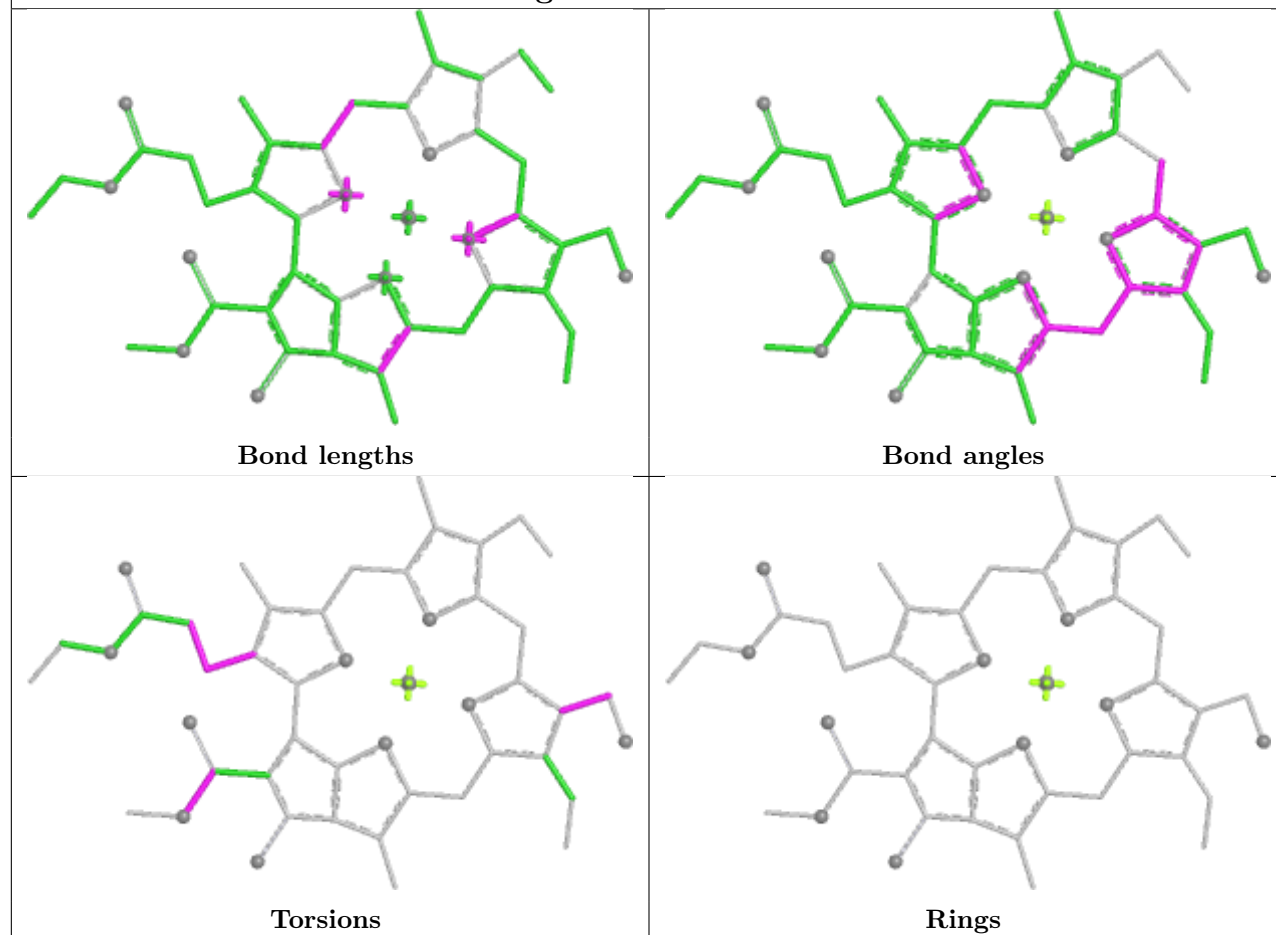
Rings

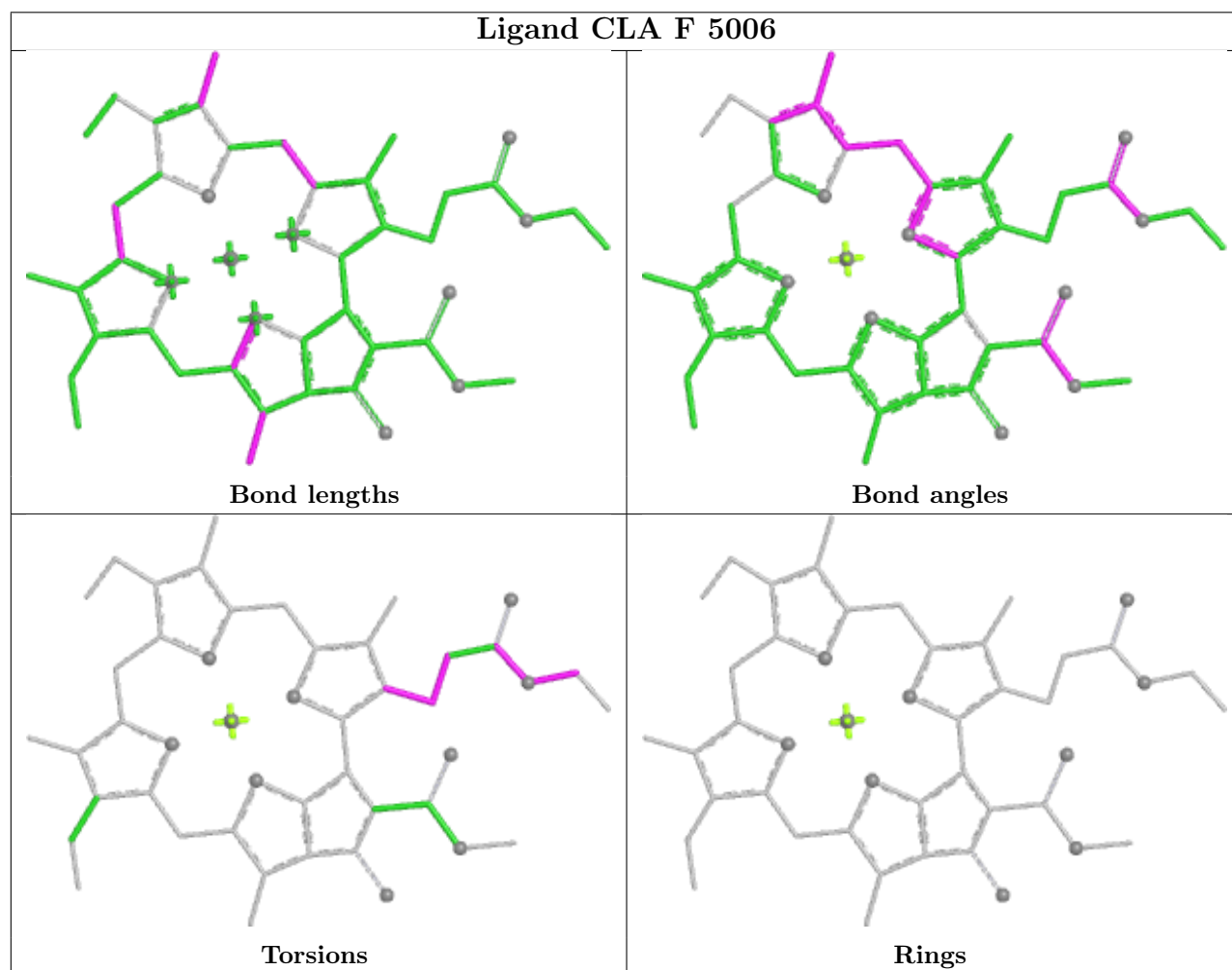
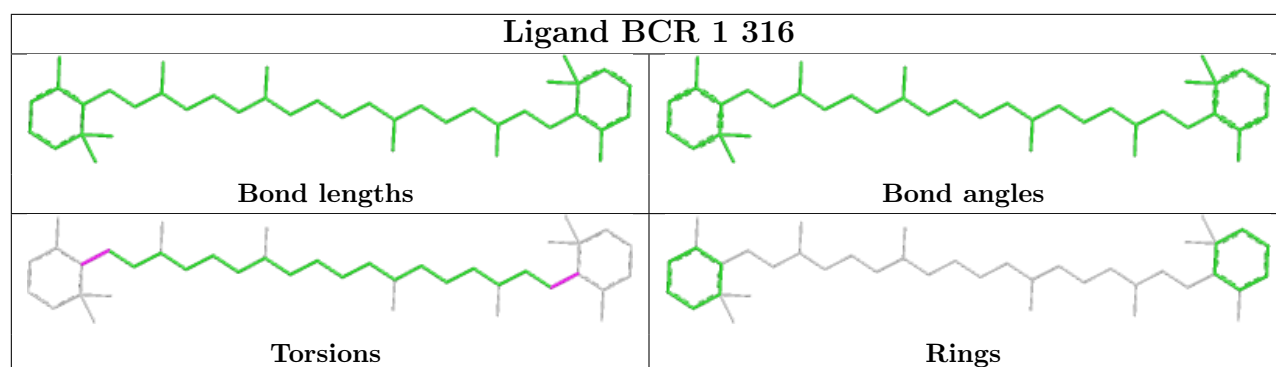


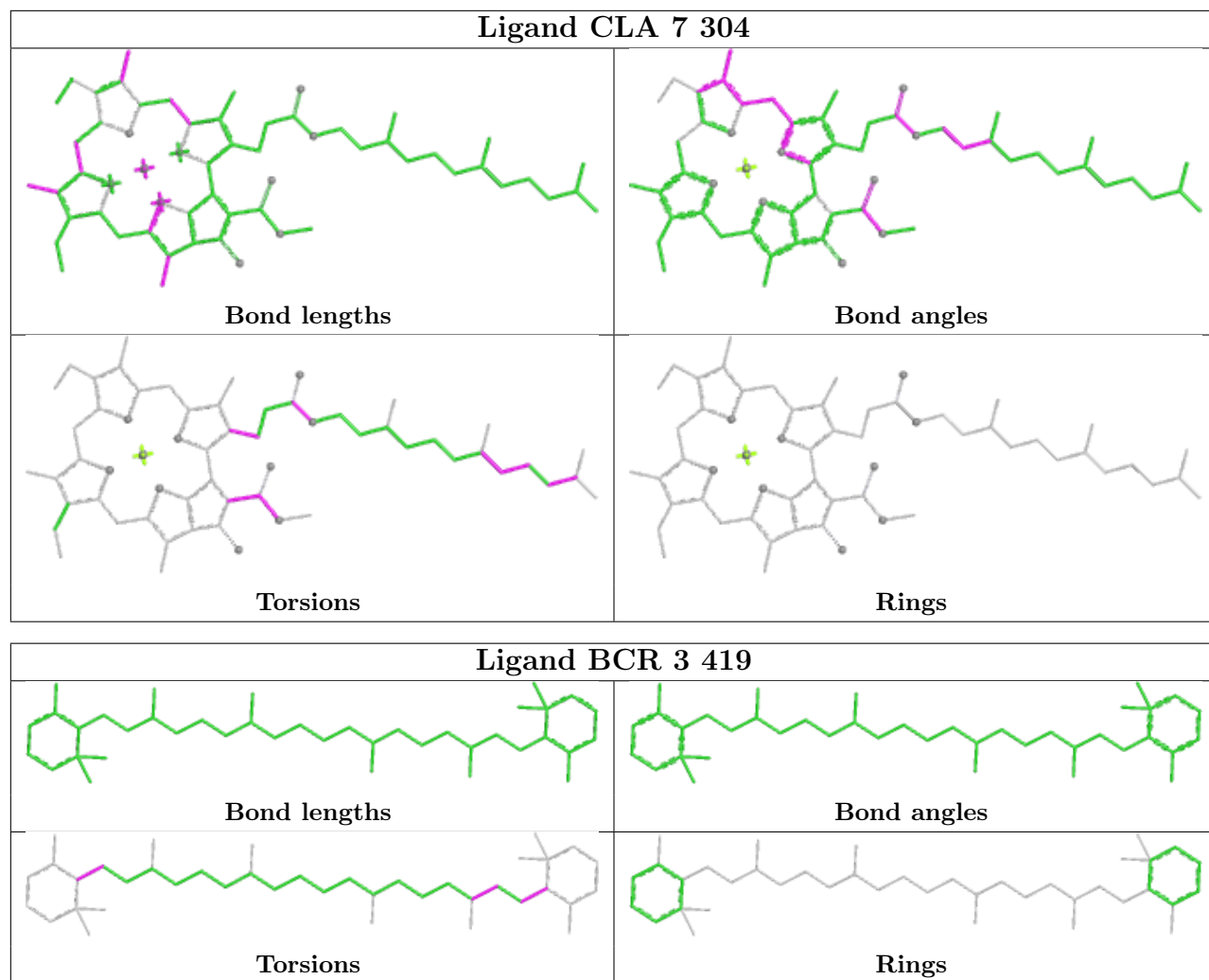
Ligand CLA c 602

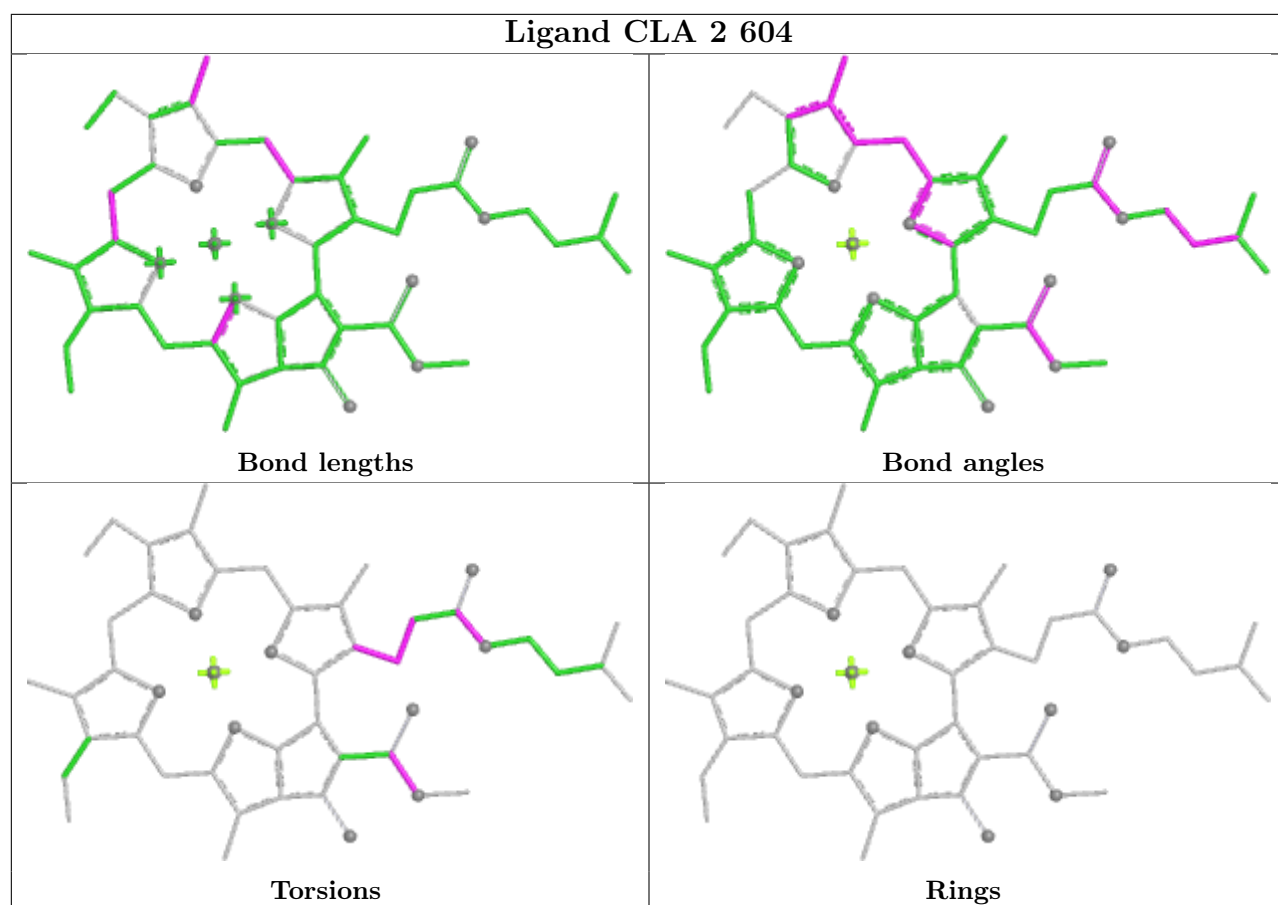


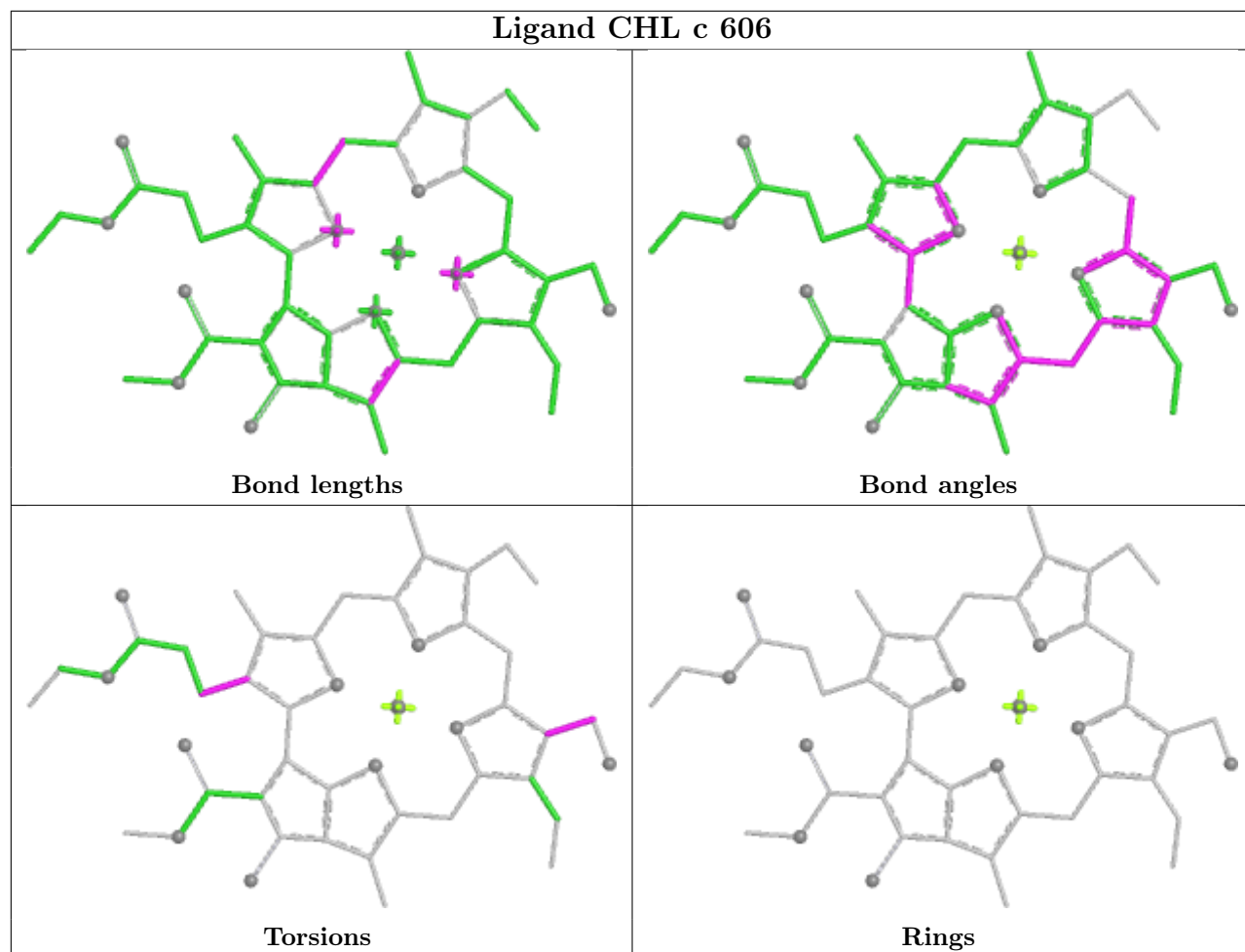
Ligand CHL 7 309



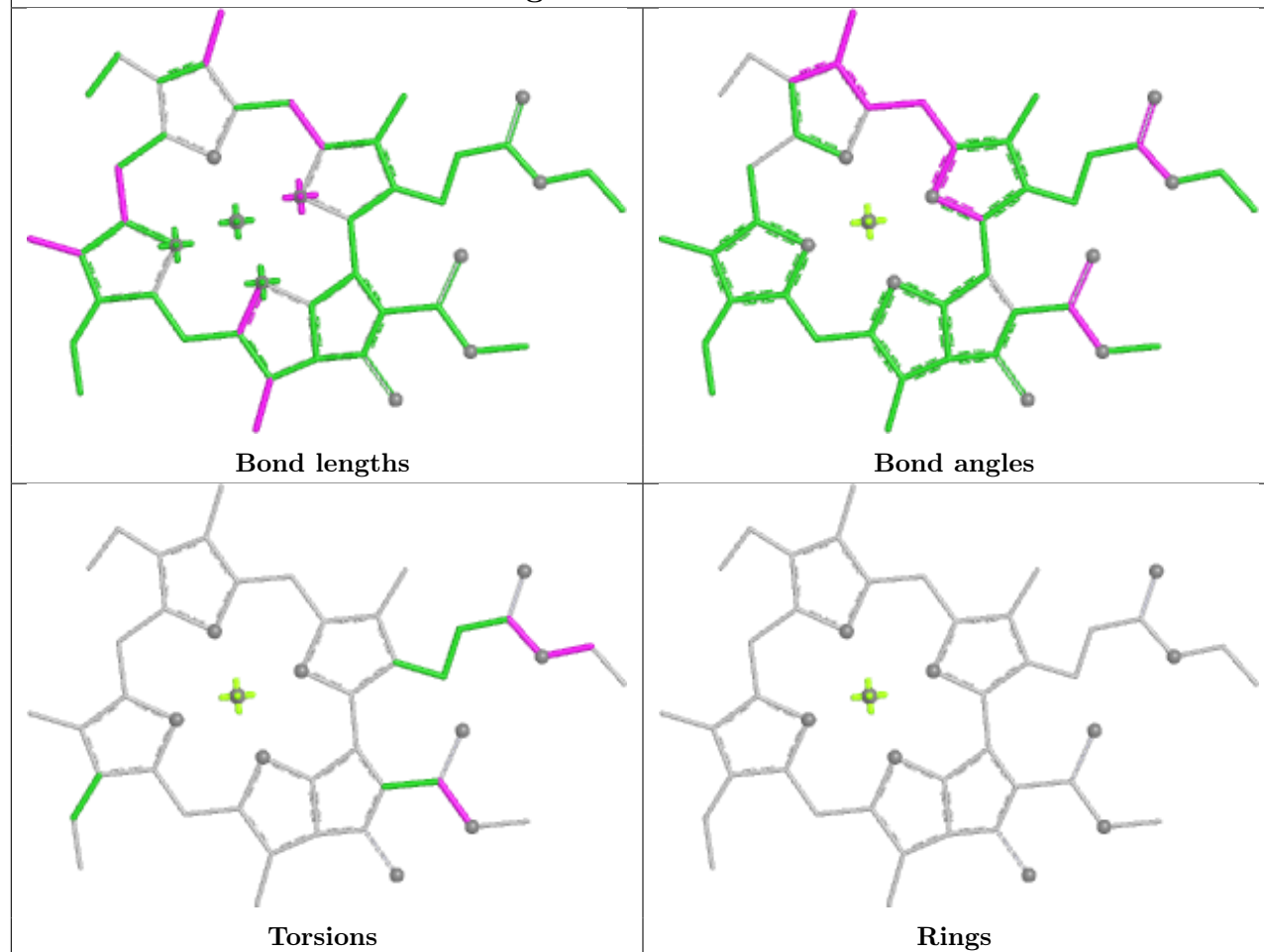




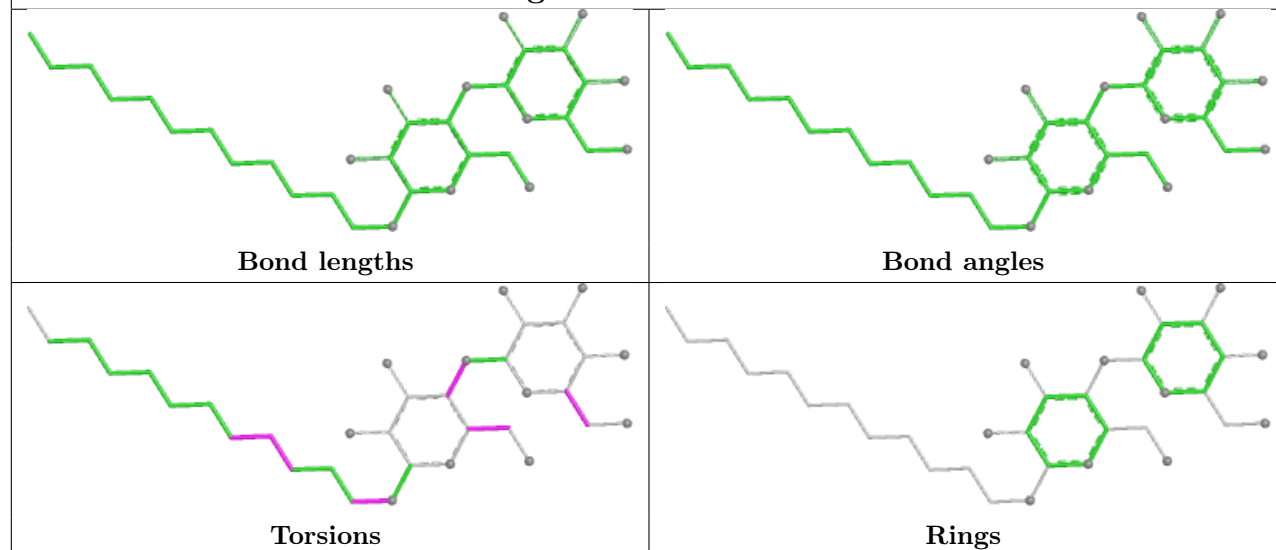


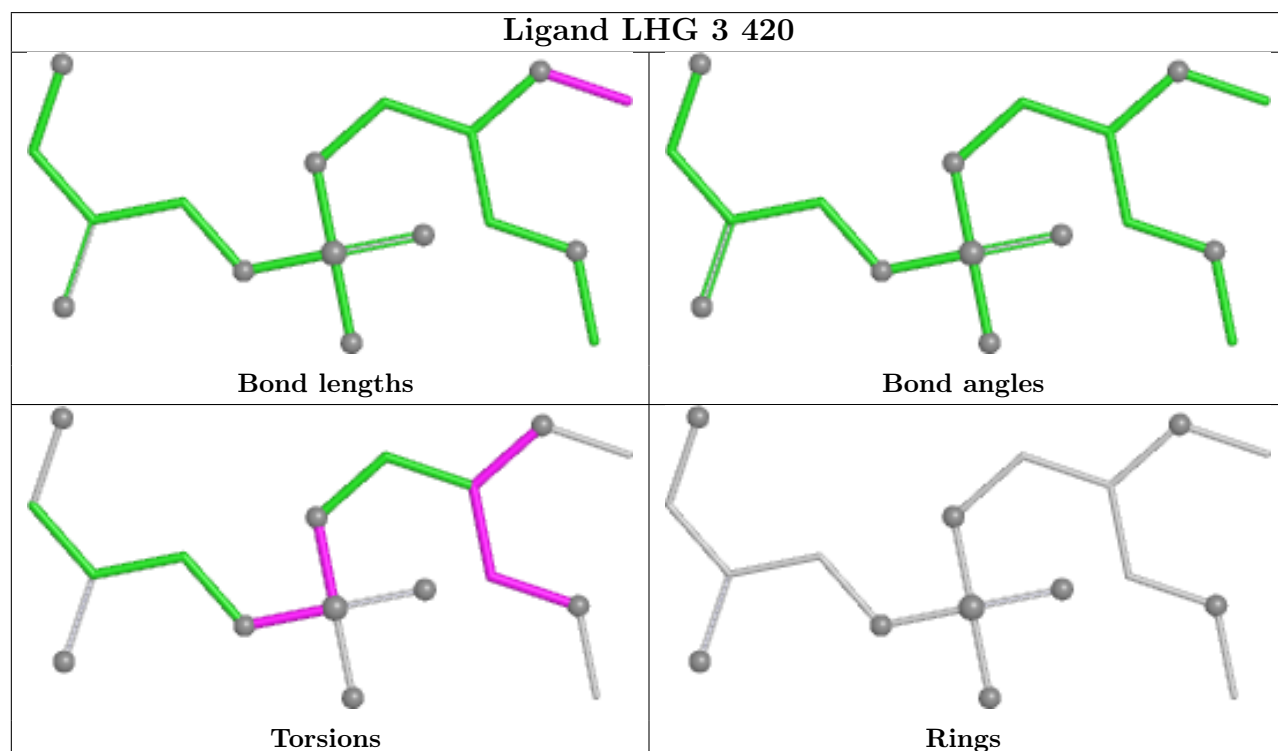
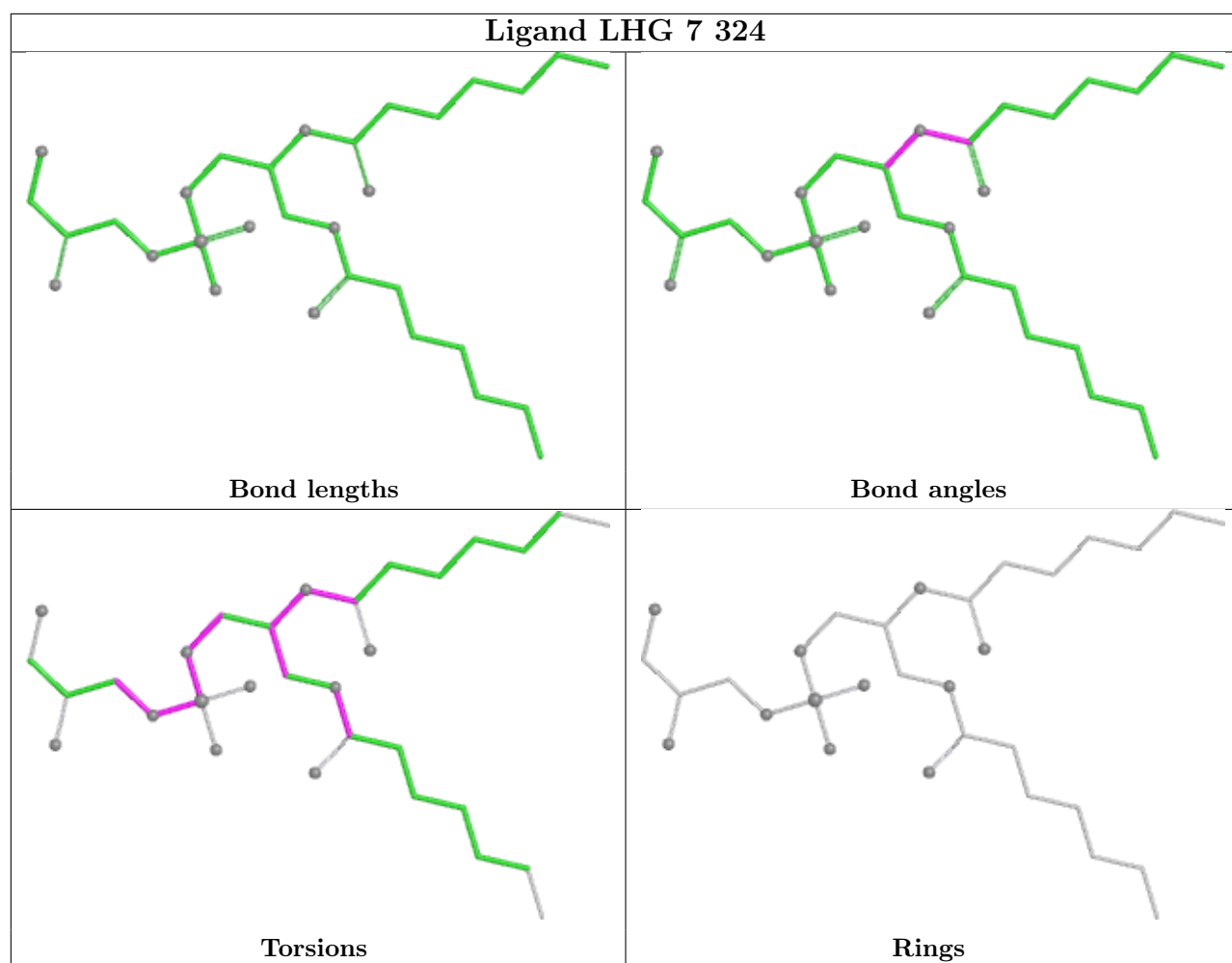


Ligand CLA G 203

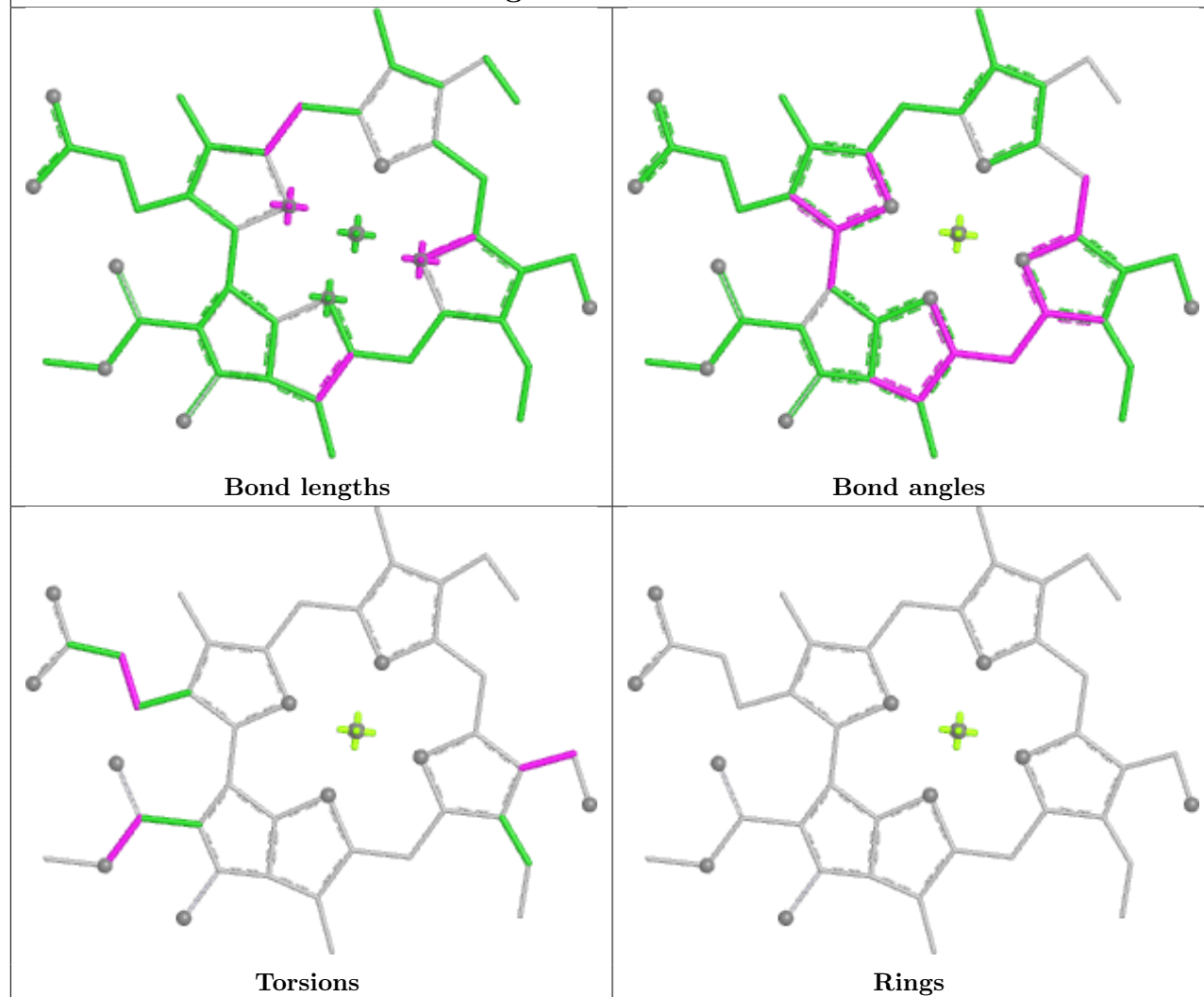


Ligand LMU A 855

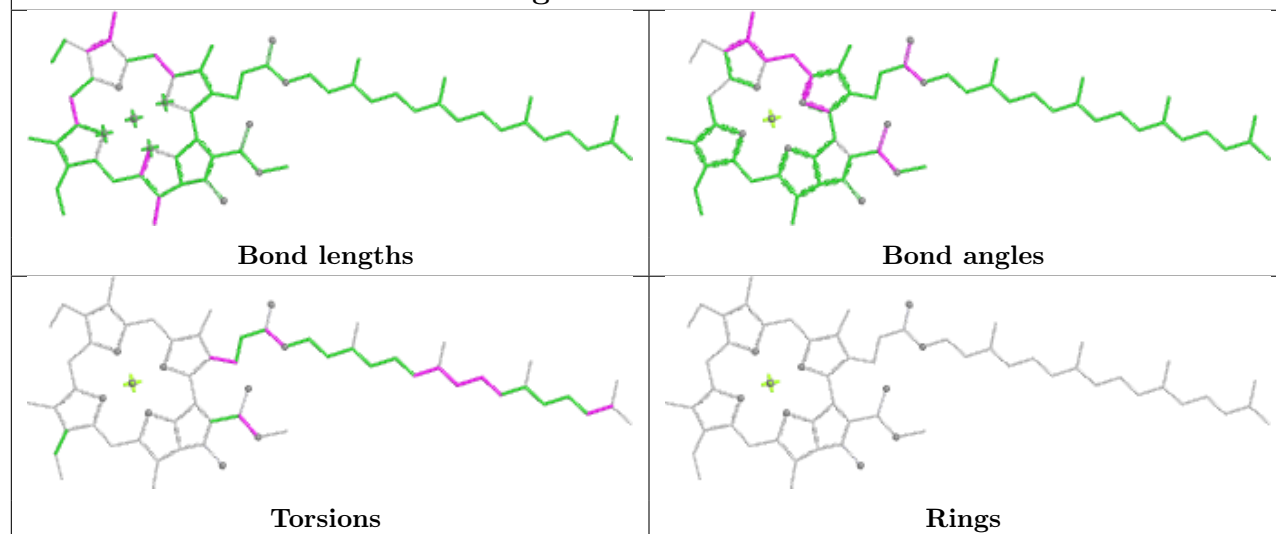




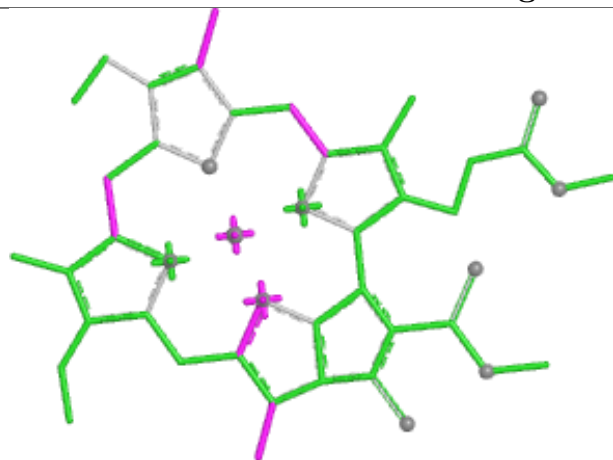
Ligand CHL 7 307



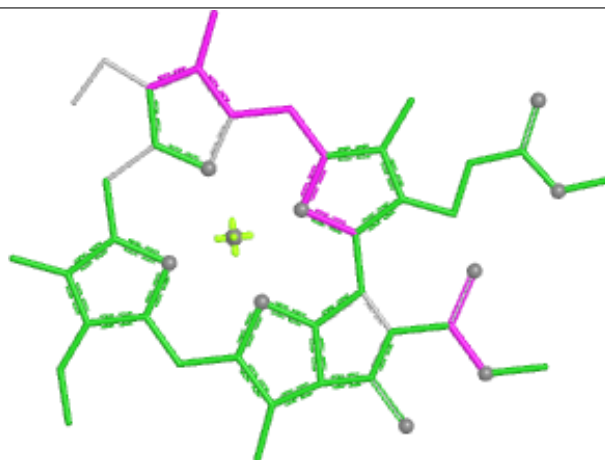
Ligand CLA B 804



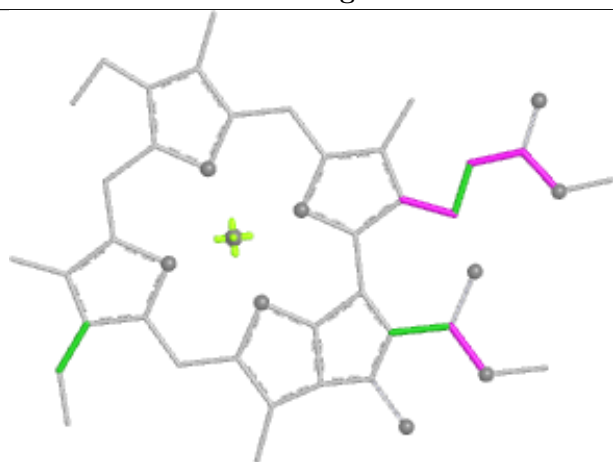
Ligand CLA 1 309



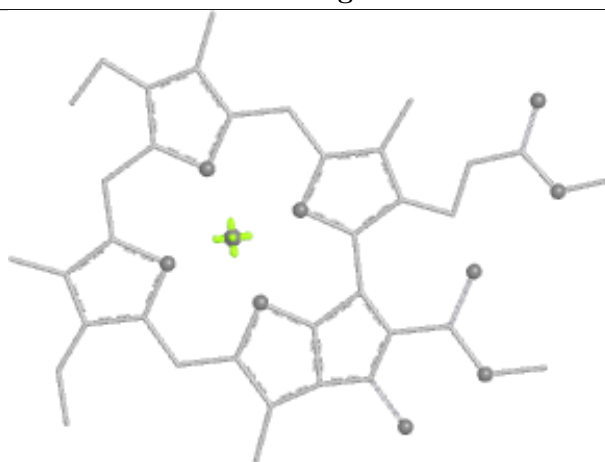
Bond lengths



Bond angles

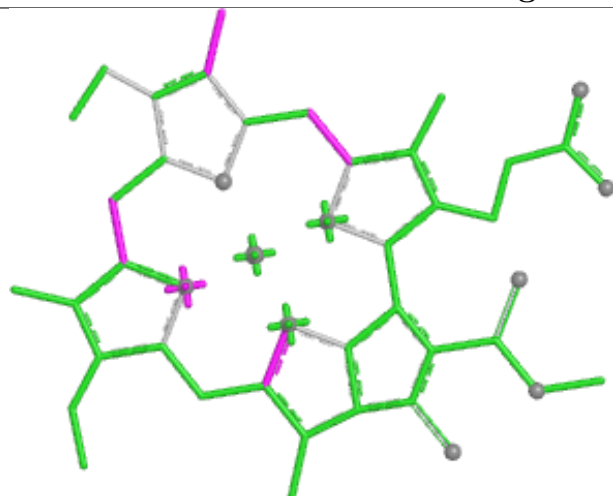


Torsions

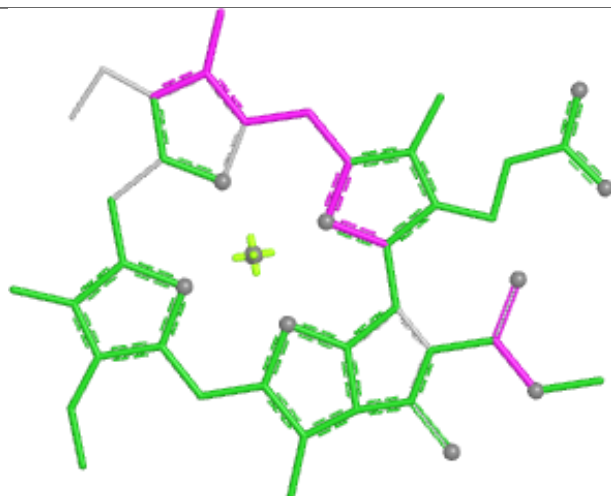


Rings

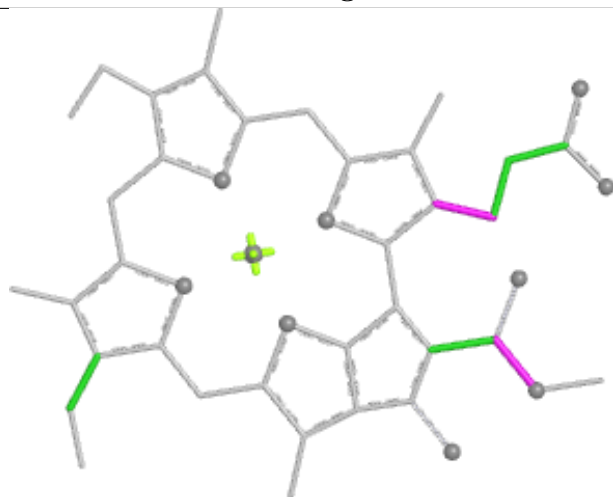
Ligand CLA a 307



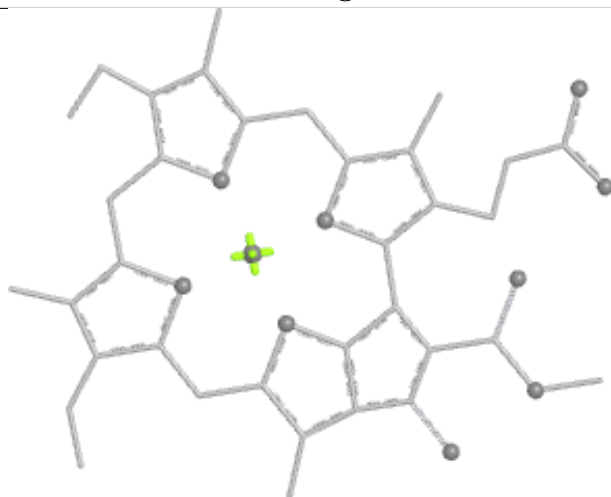
Bond lengths



Bond angles

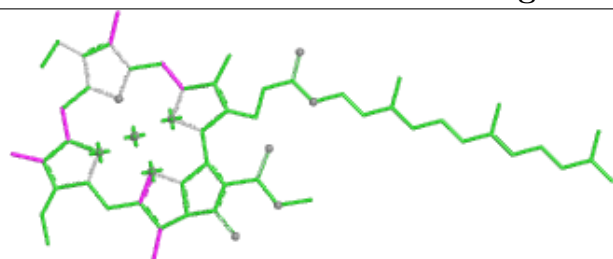


Torsions

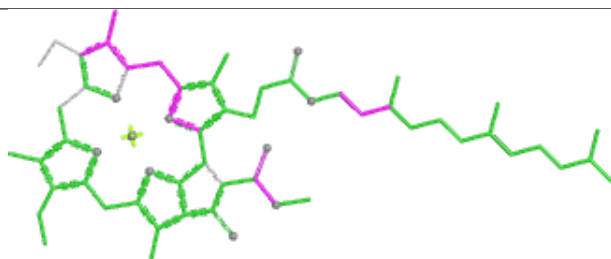


Rings

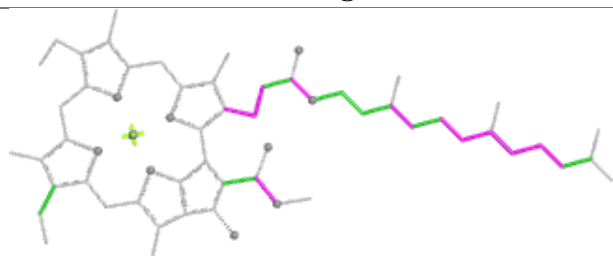
Ligand CLA a 309



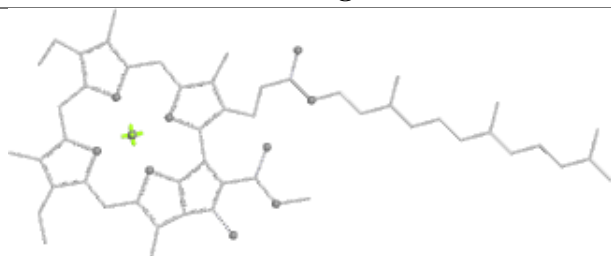
Bond lengths



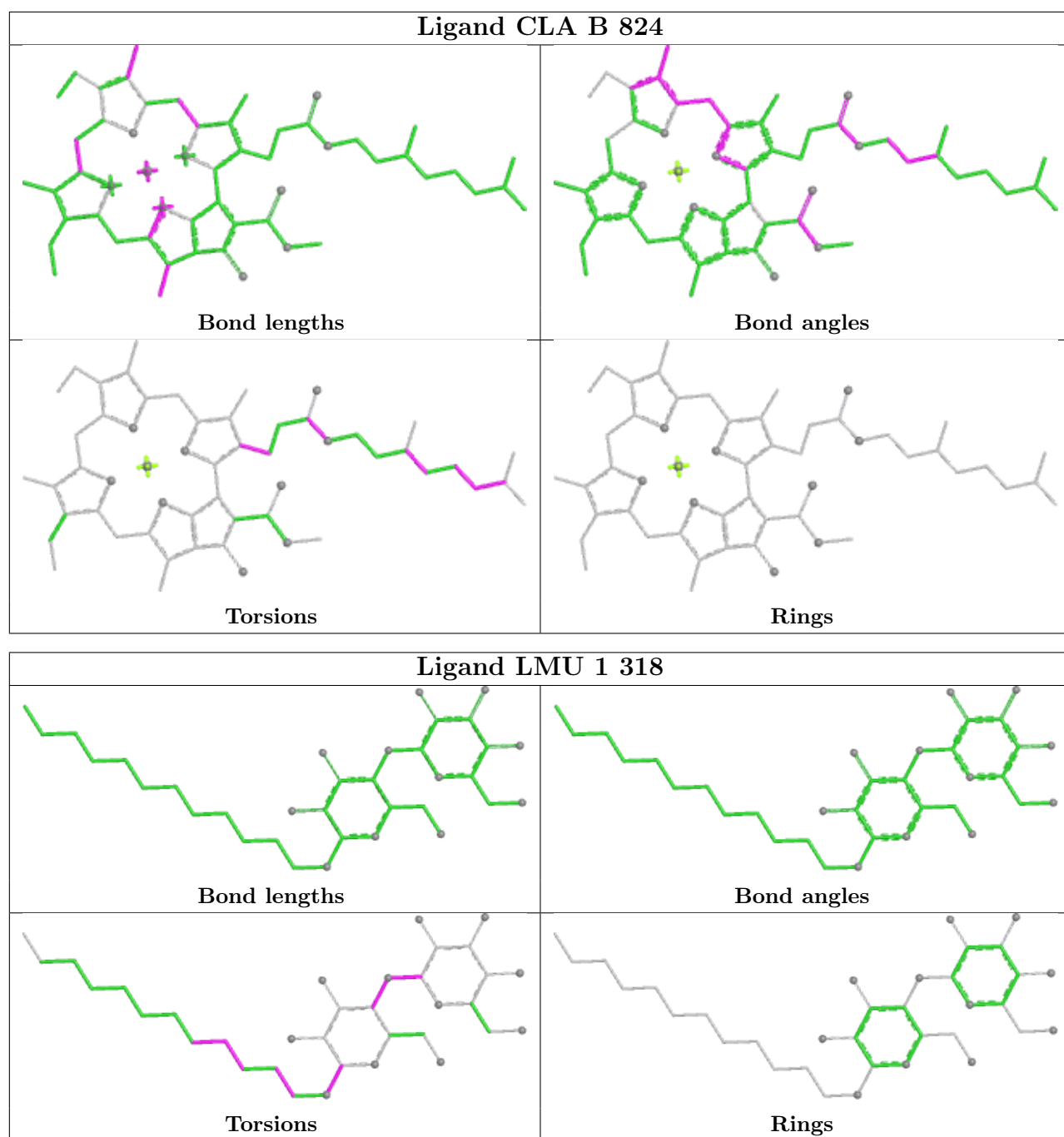
Bond angles

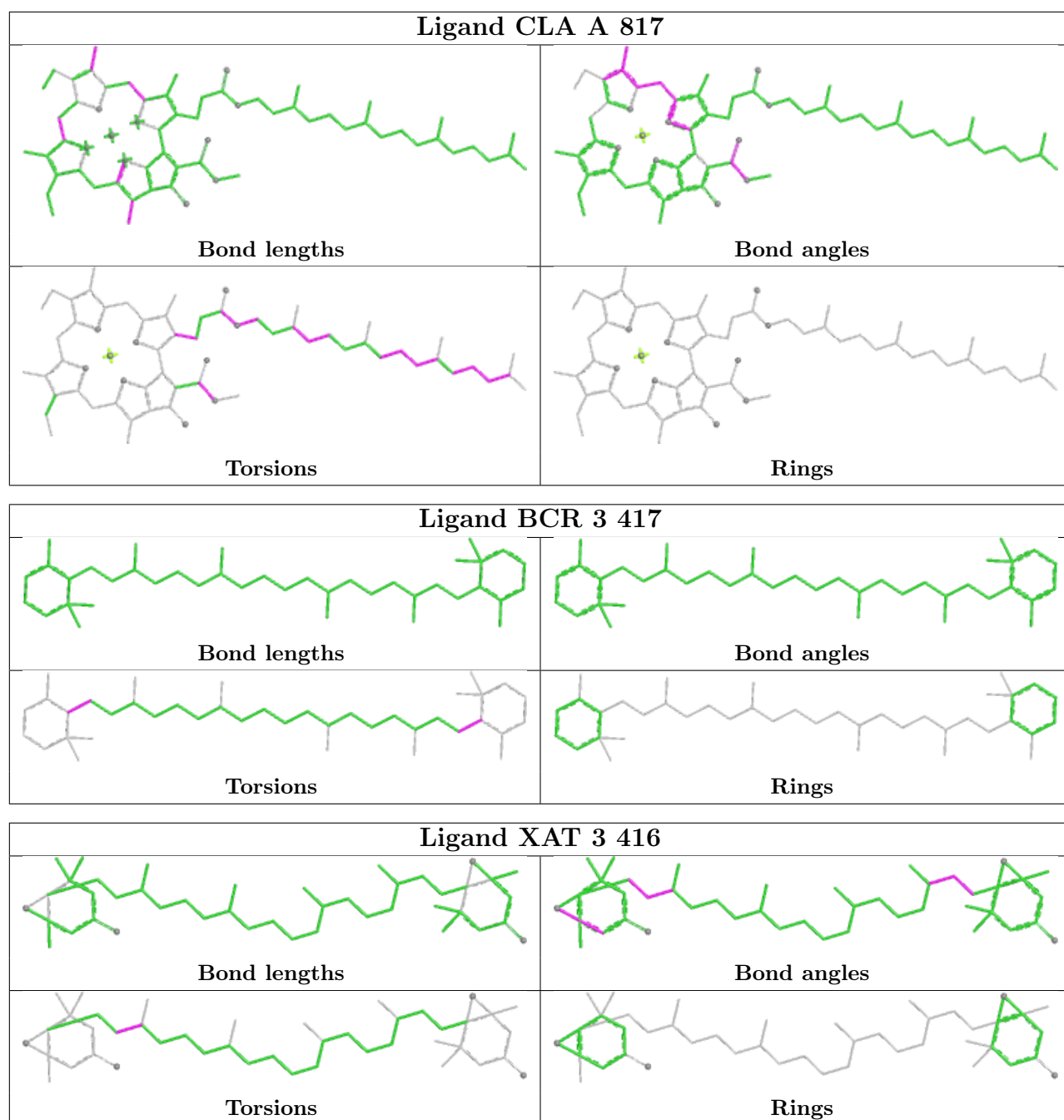


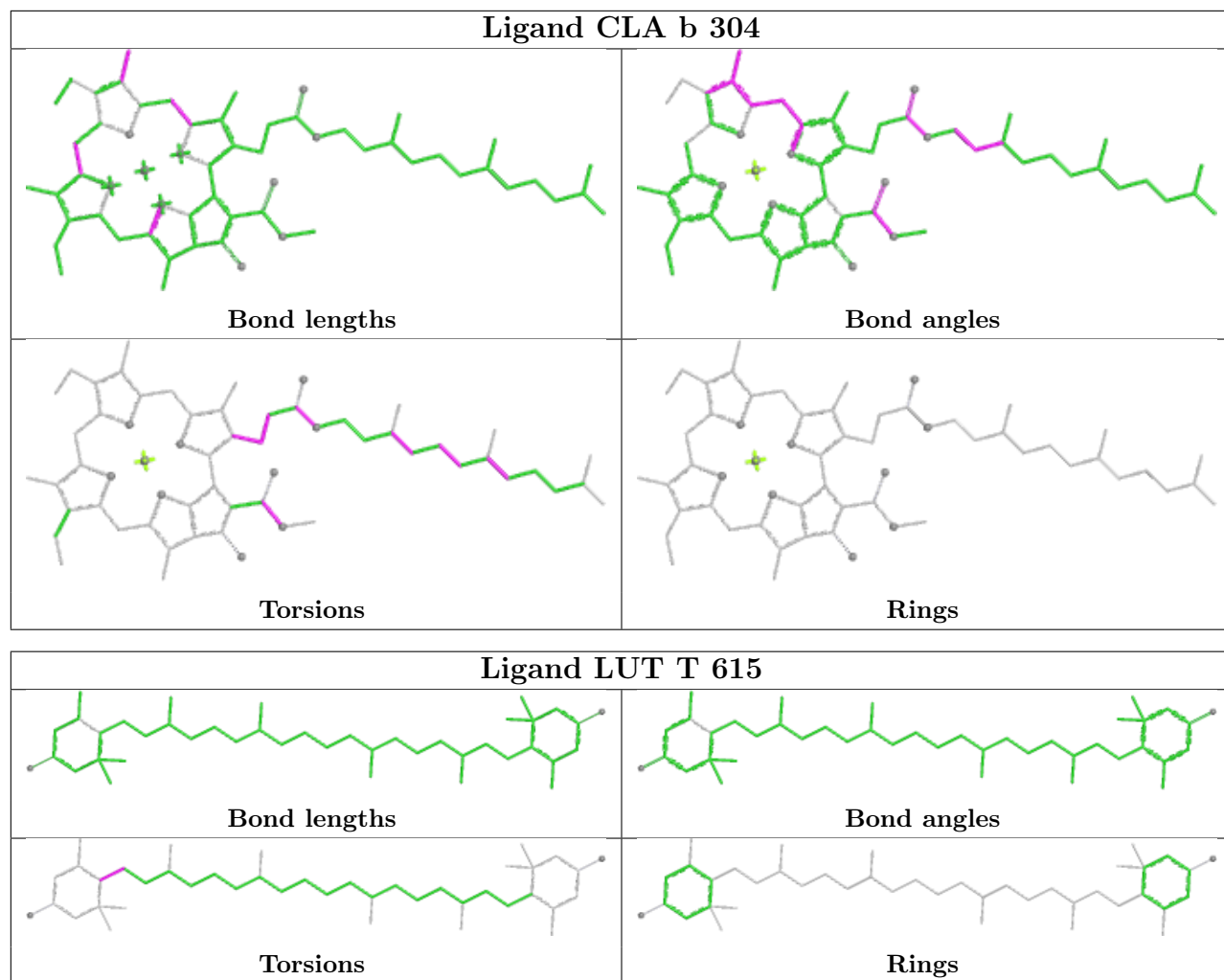
Torsions

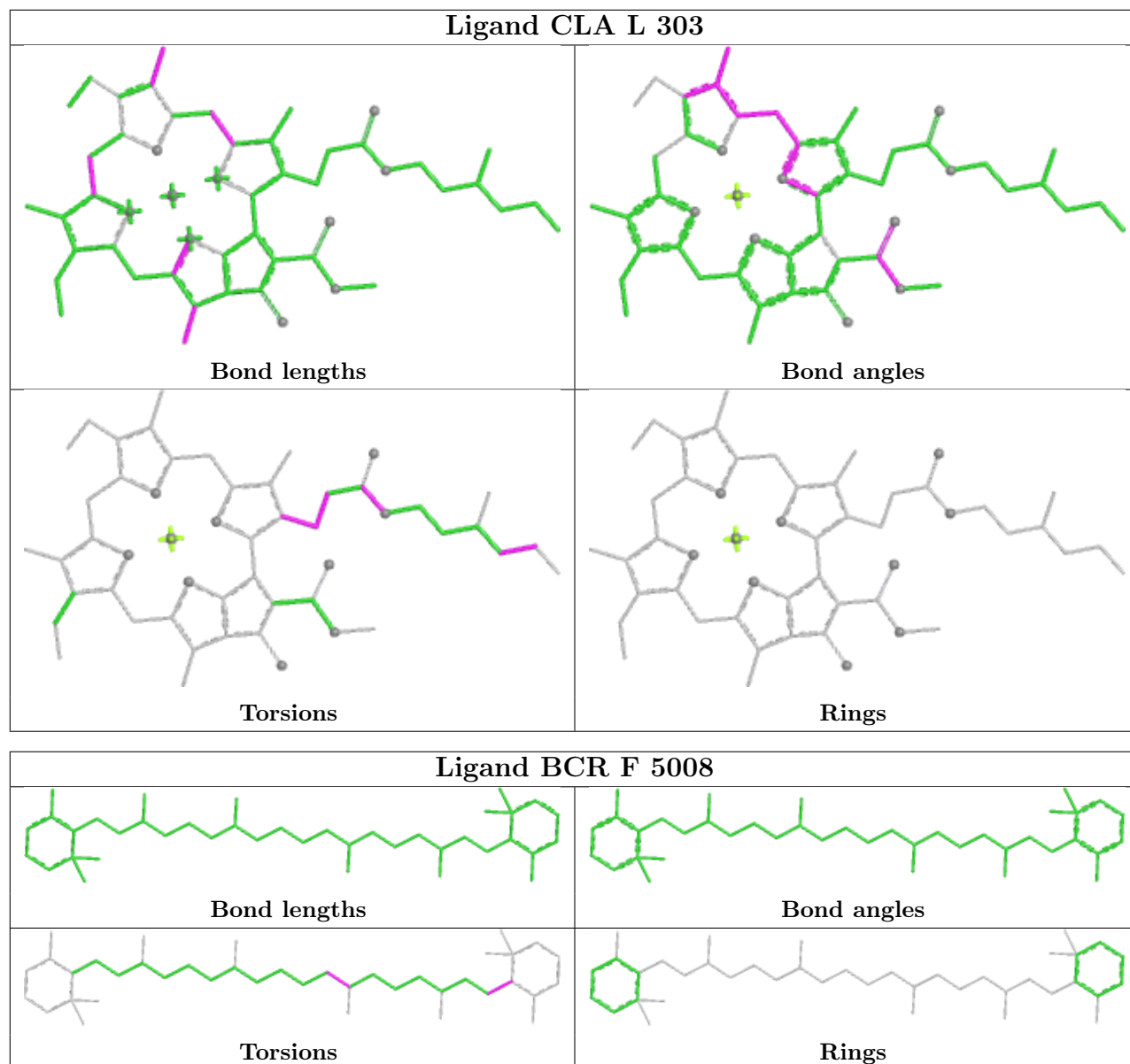


Rings

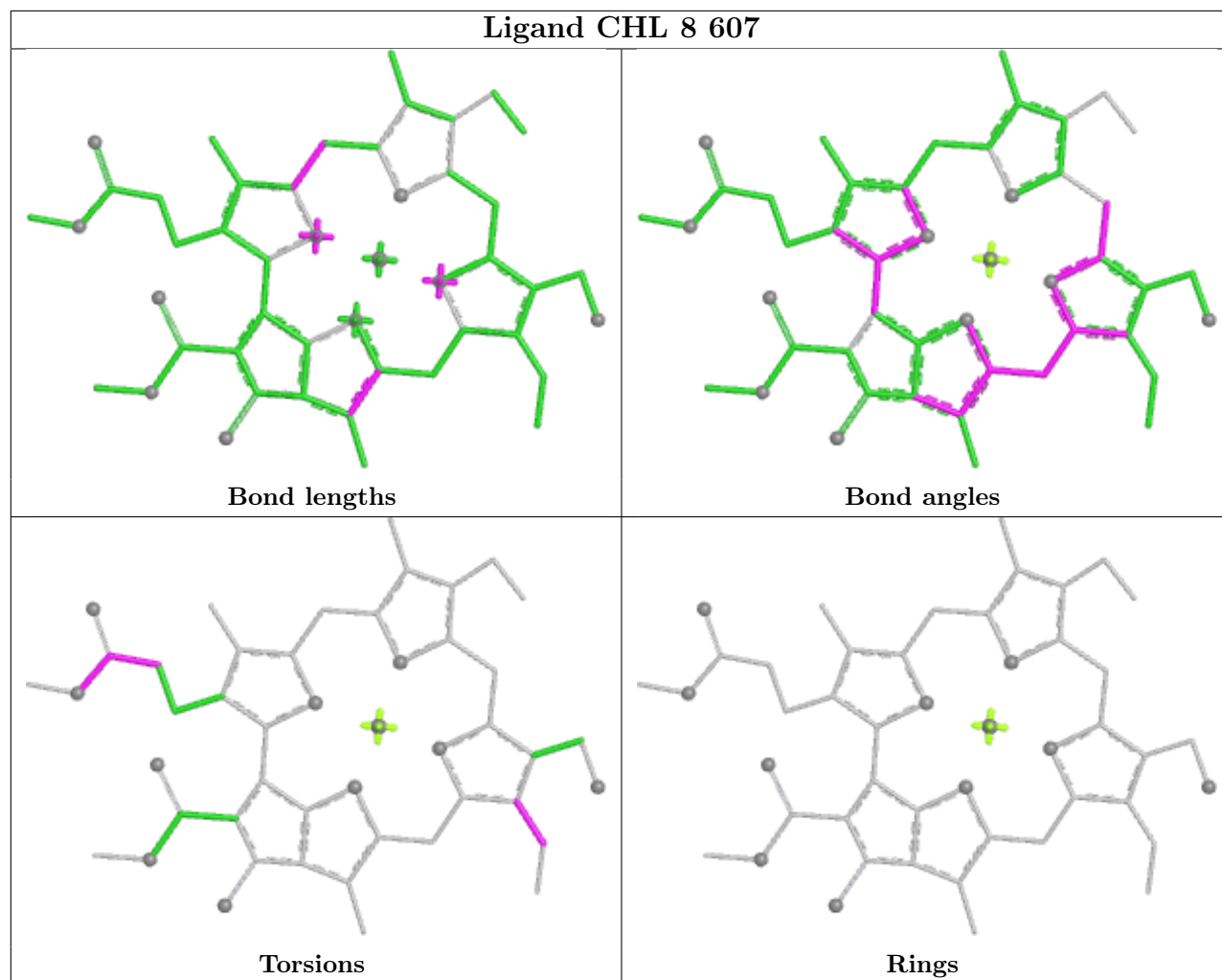


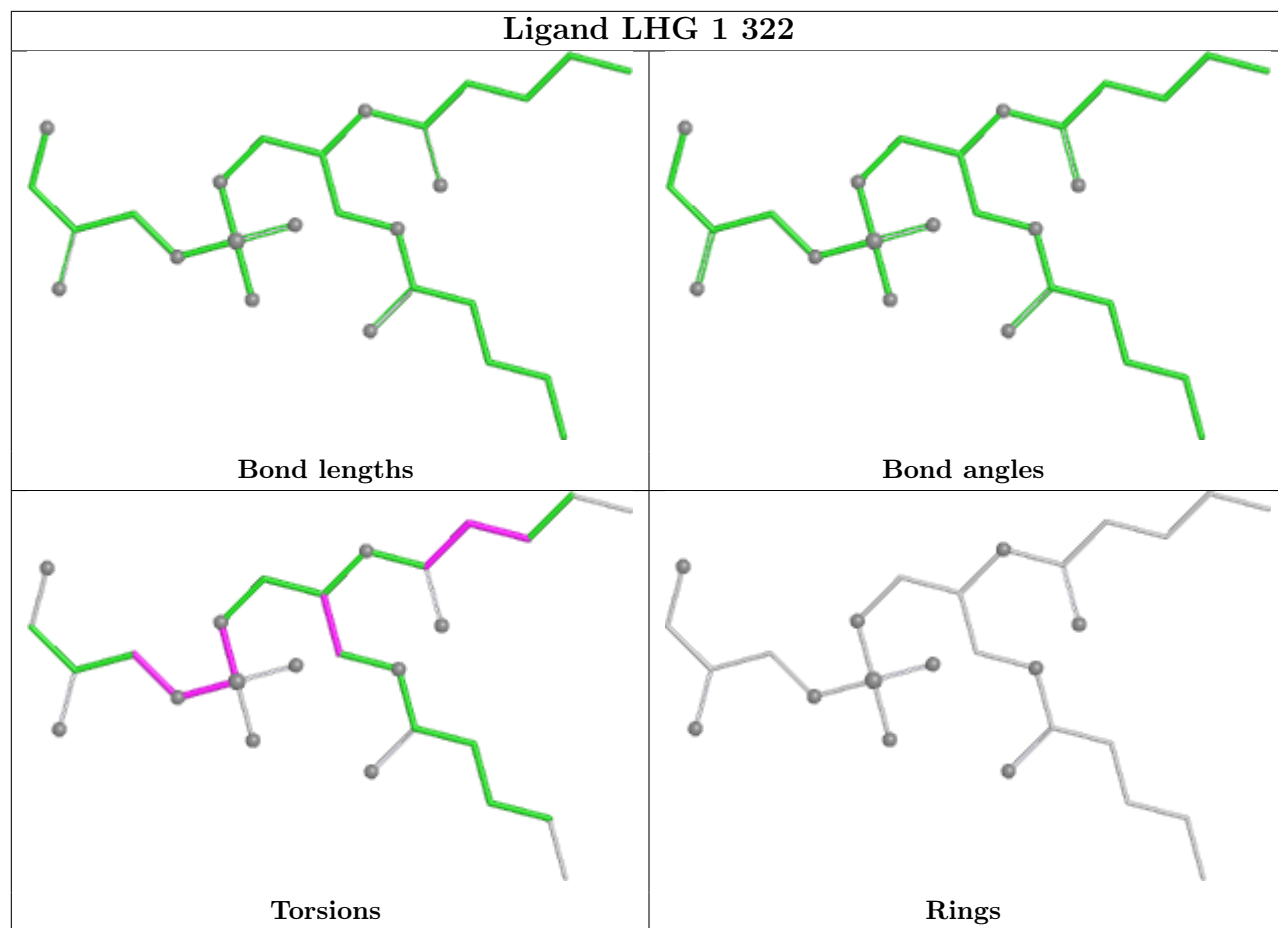




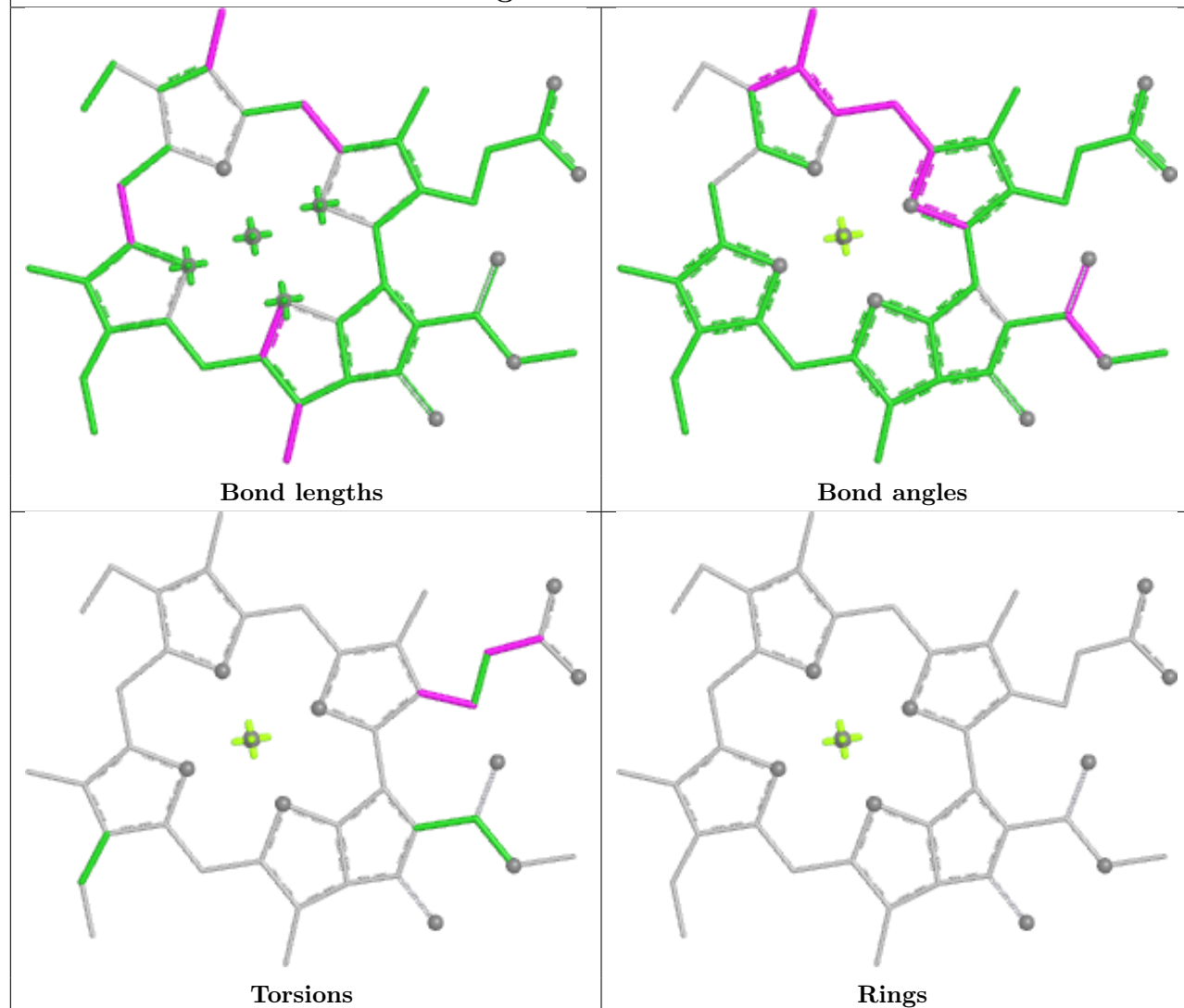


Ligand CHL 8 607

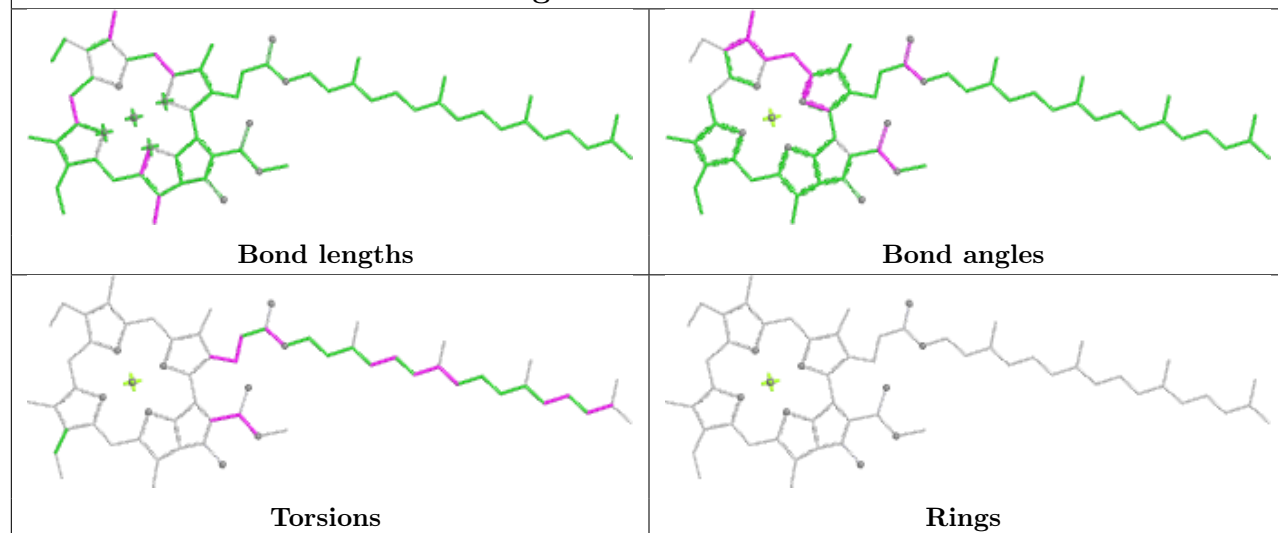




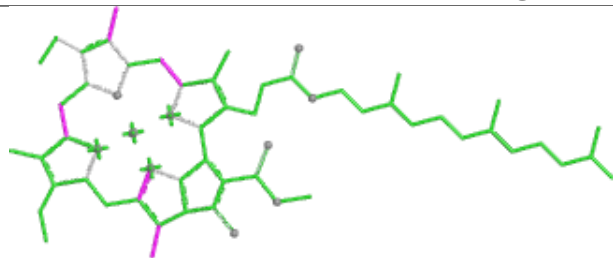
Ligand CLA 7 310



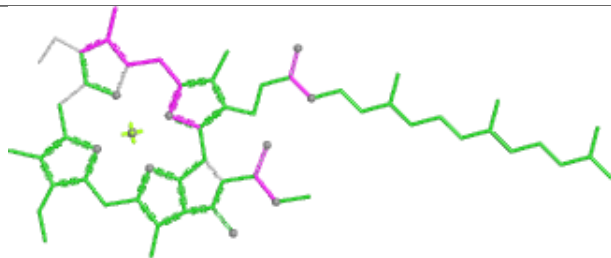
Ligand CLA T 612



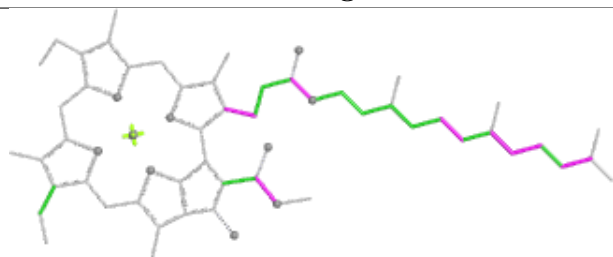
Ligand CLA A 825



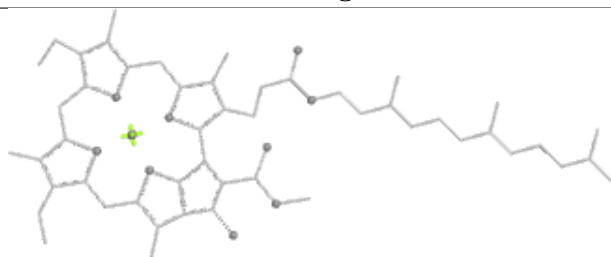
Bond lengths



Bond angles

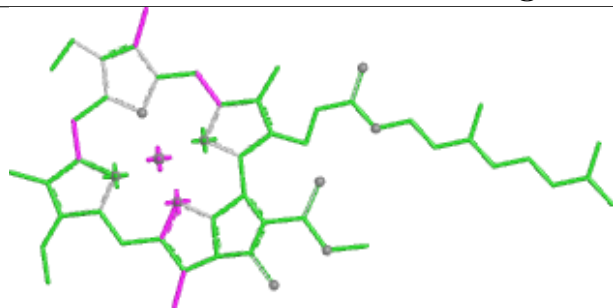


Torsions

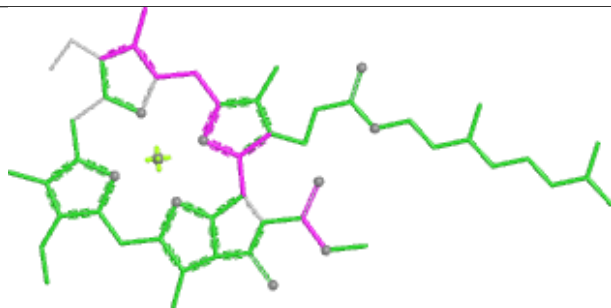


Rings

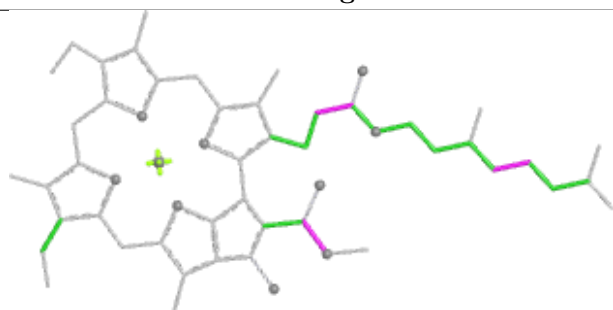
Ligand CLA 9 603



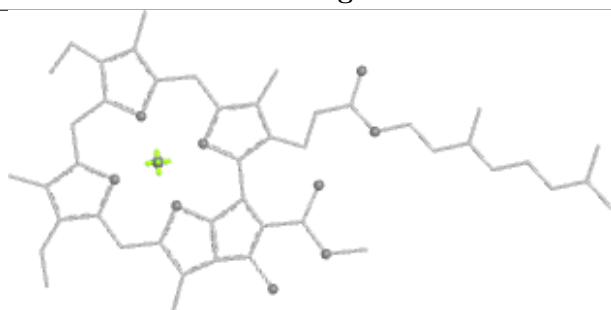
Bond lengths



Bond angles

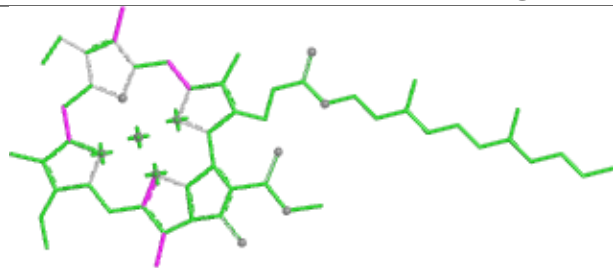


Torsions

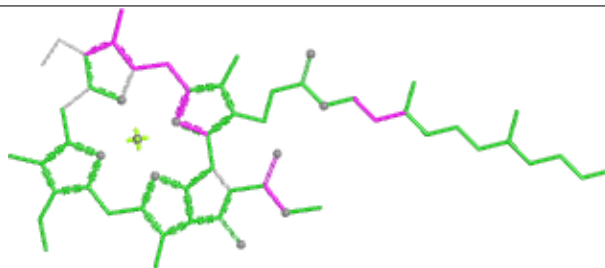


Rings

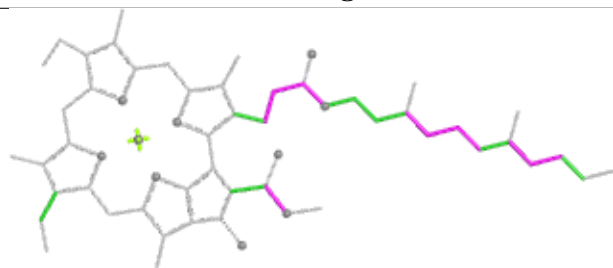
Ligand CLA A 822



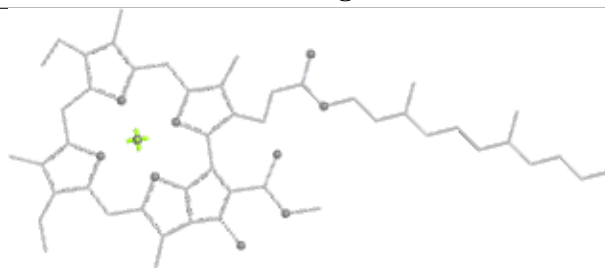
Bond lengths



Bond angles

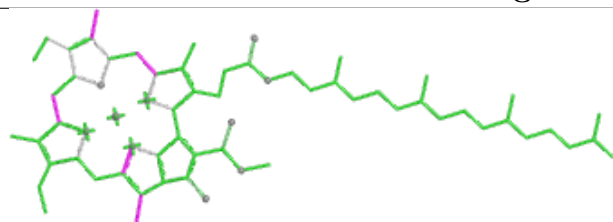


Torsions

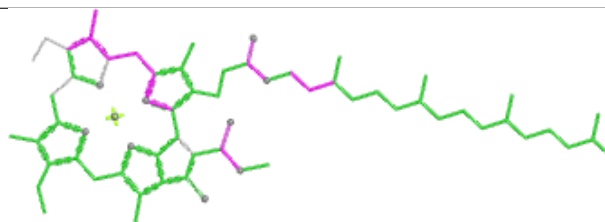


Rings

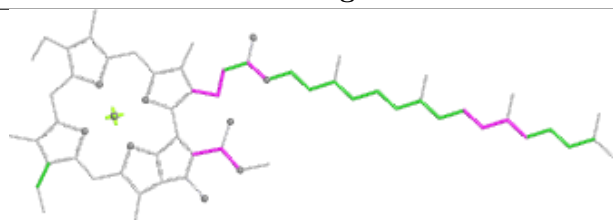
Ligand CLA A 808



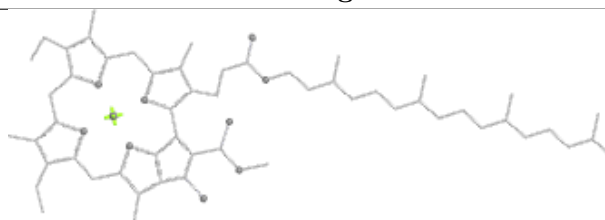
Bond lengths



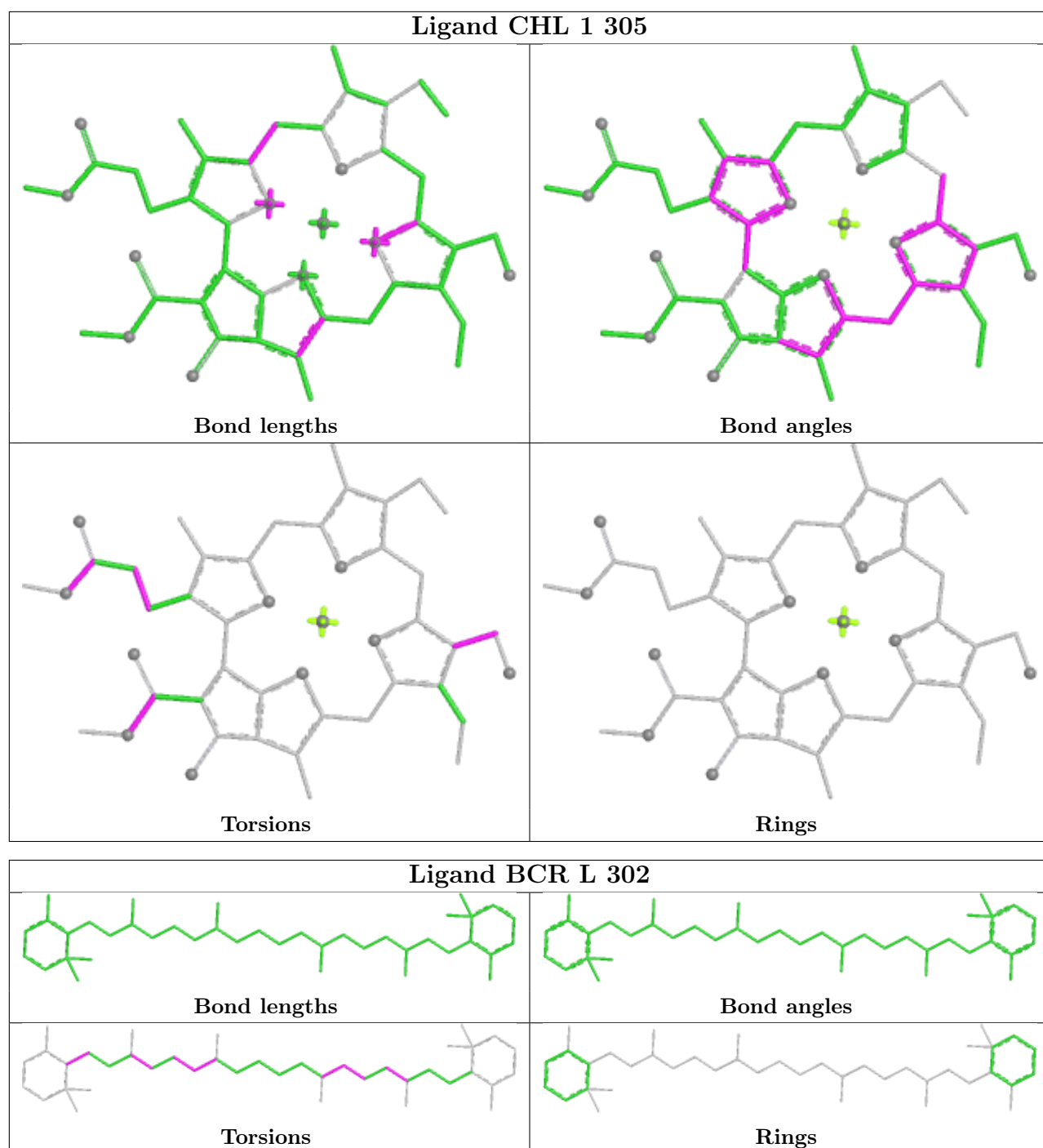
Bond angles

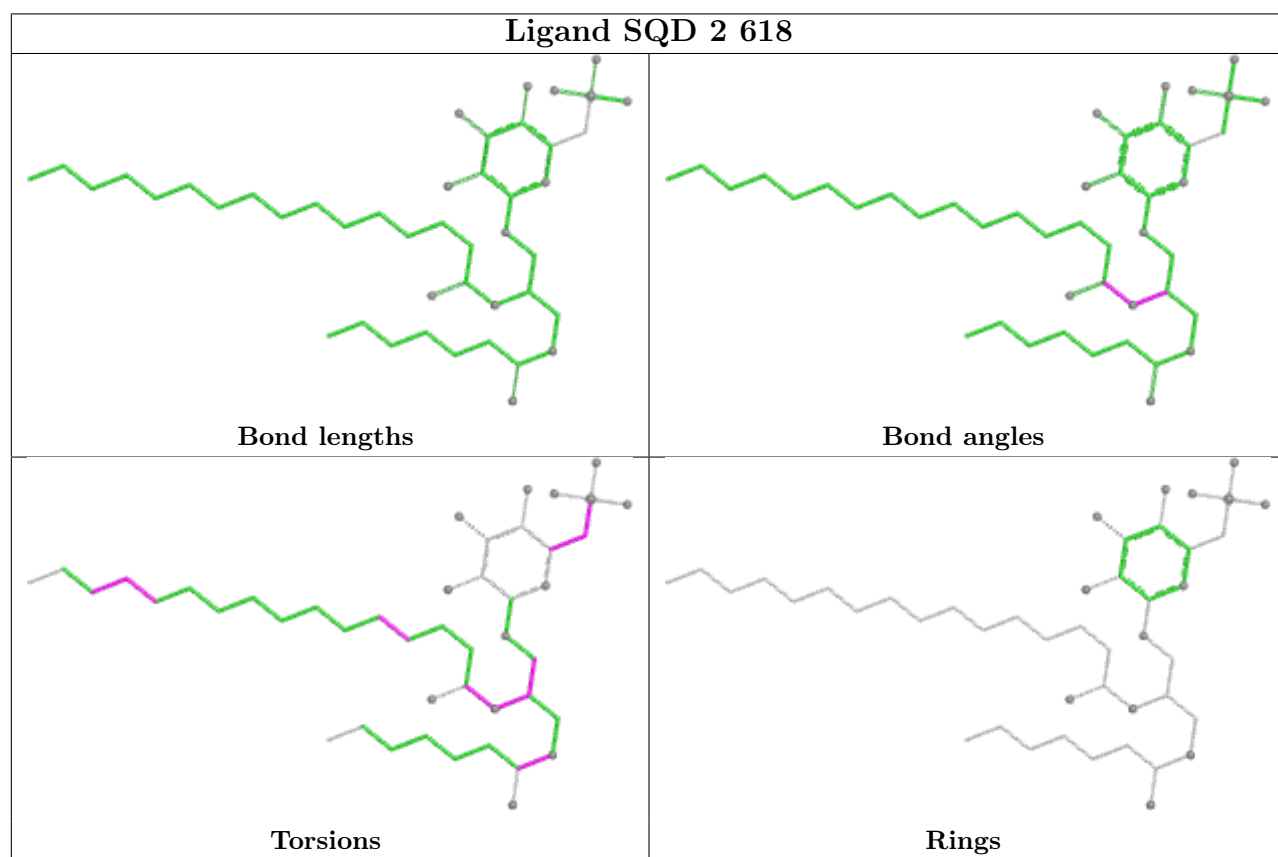
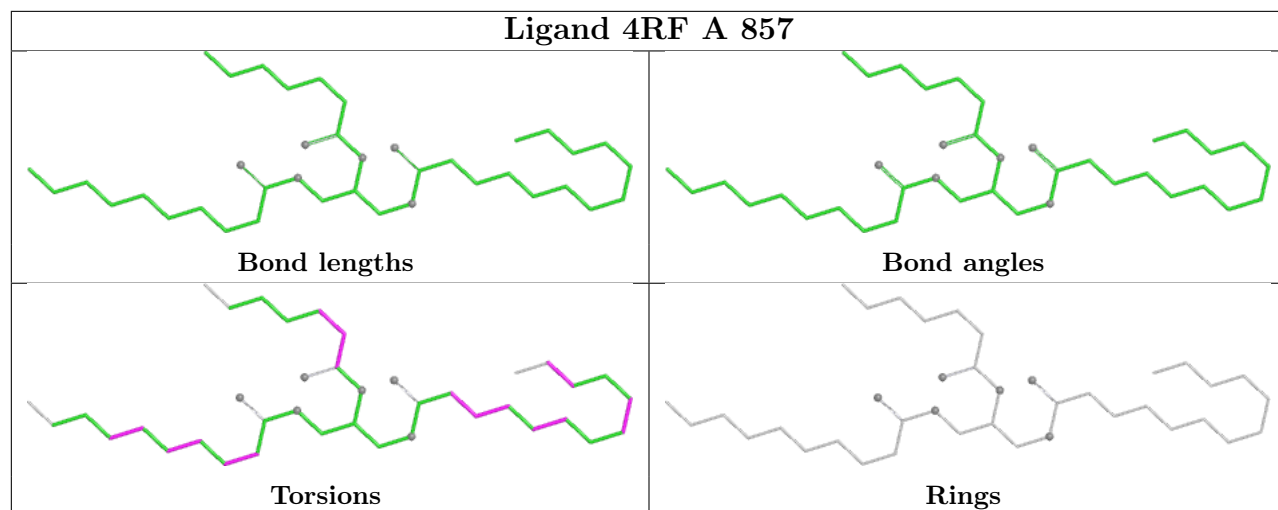


Torsions

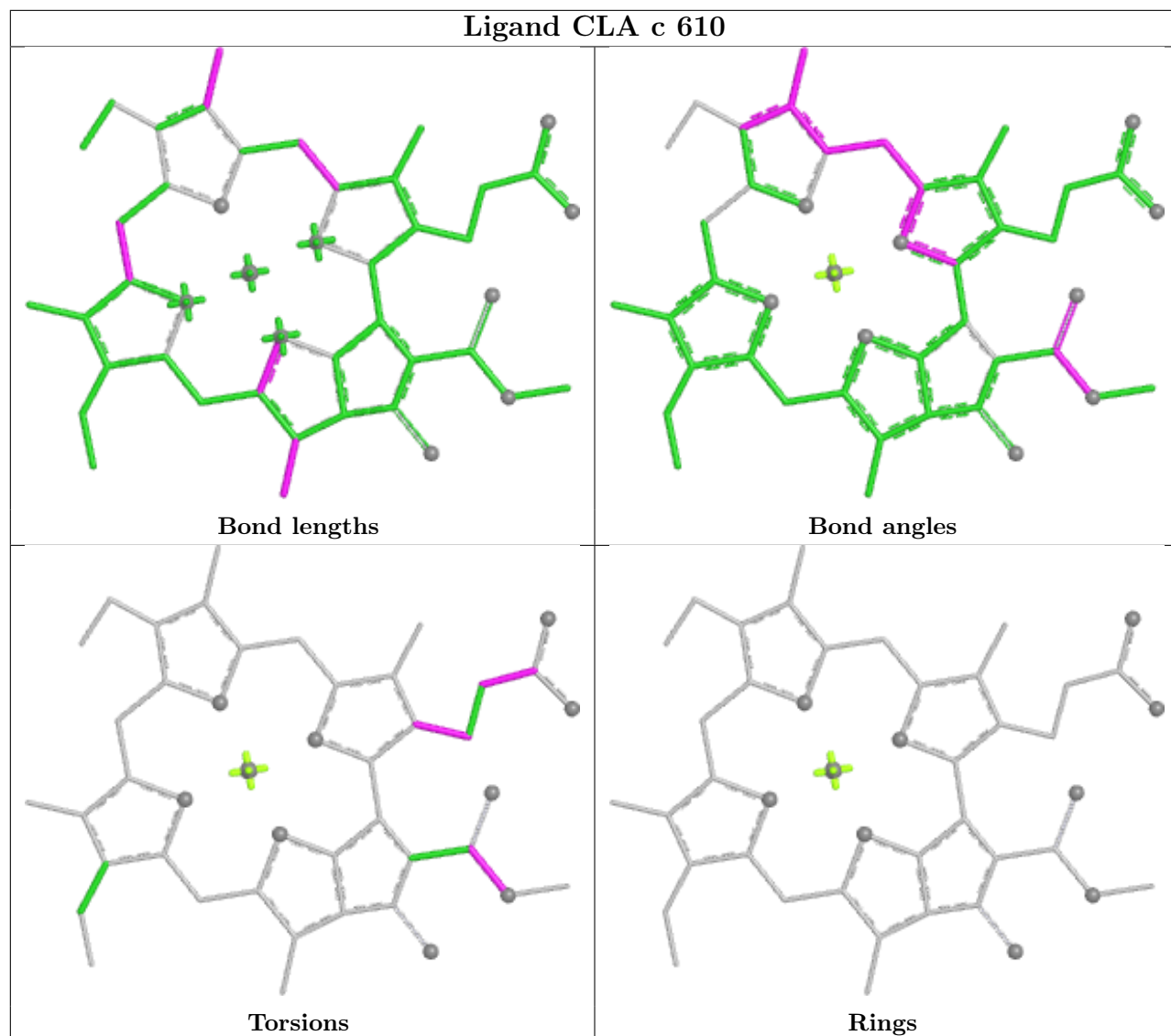


Rings

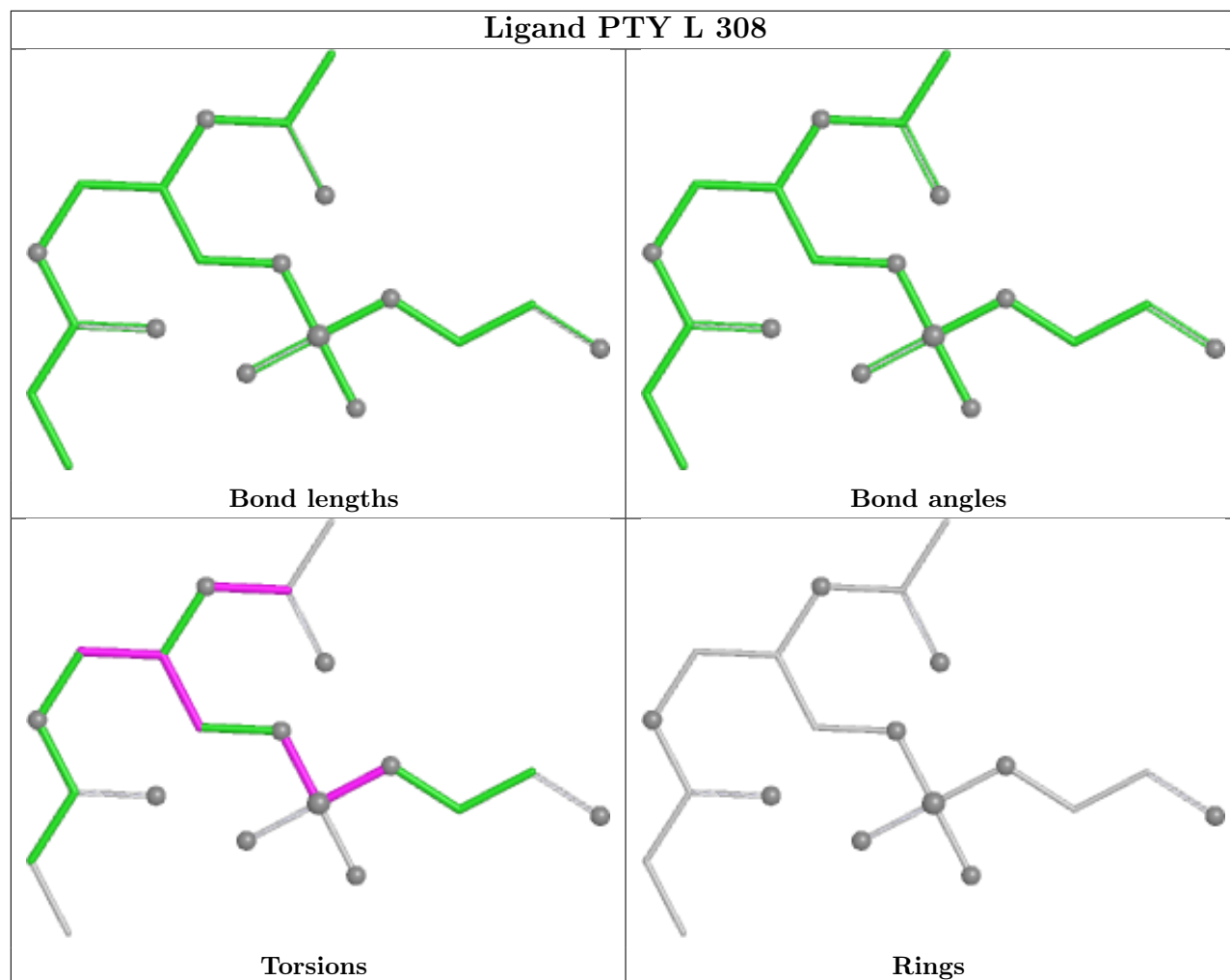




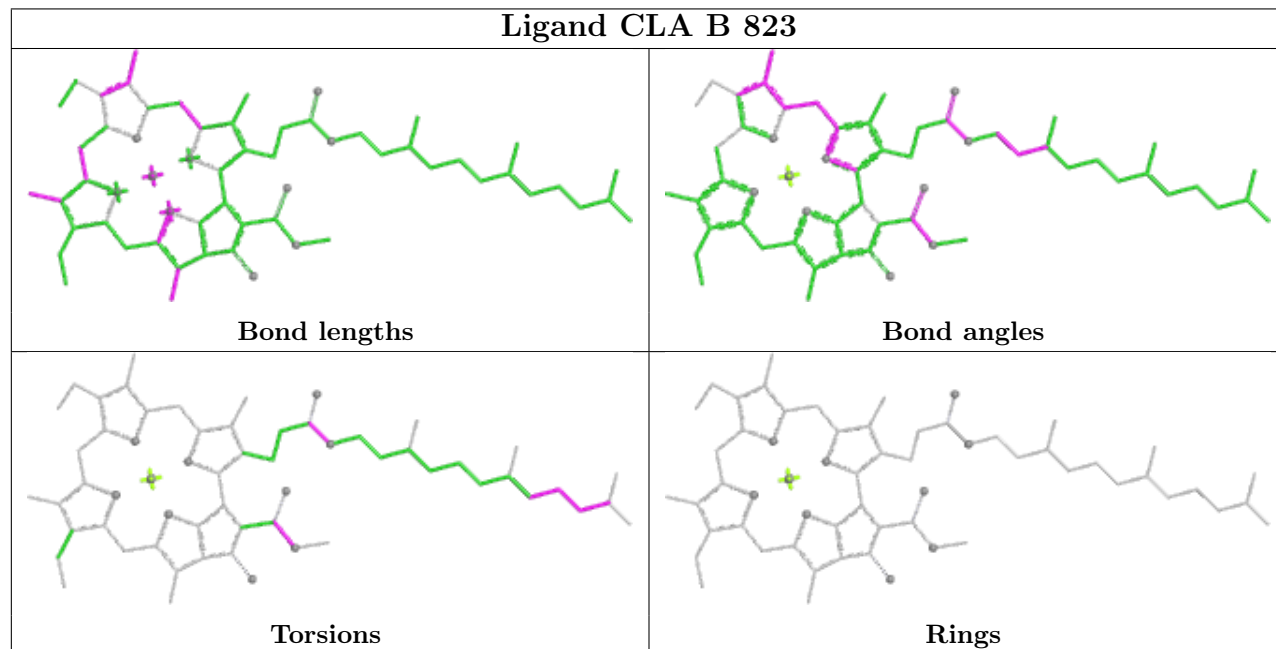
Ligand CLA c 610

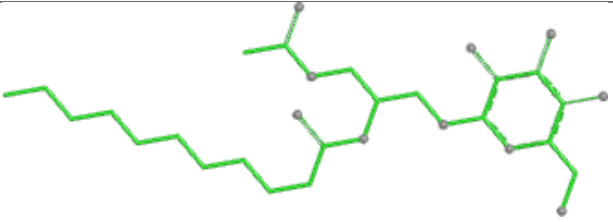
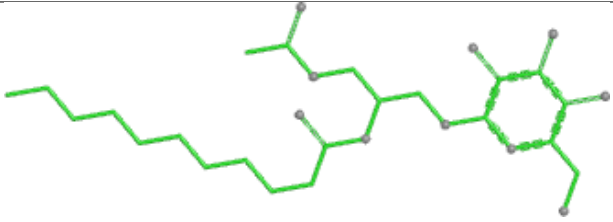
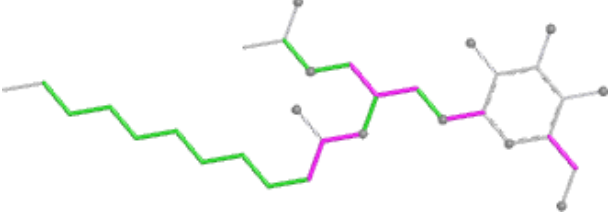
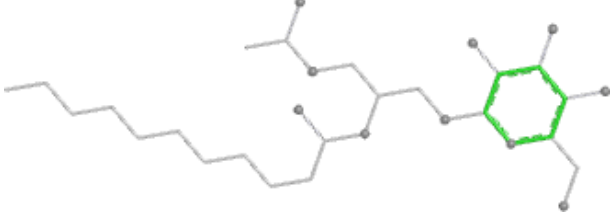


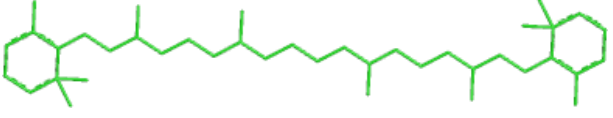
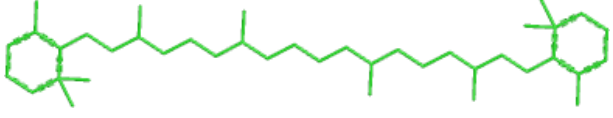
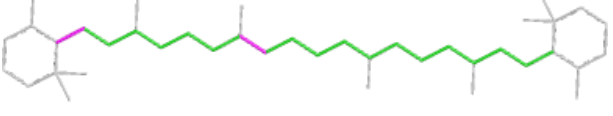
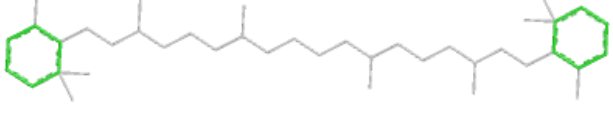
Ligand PTY L 308



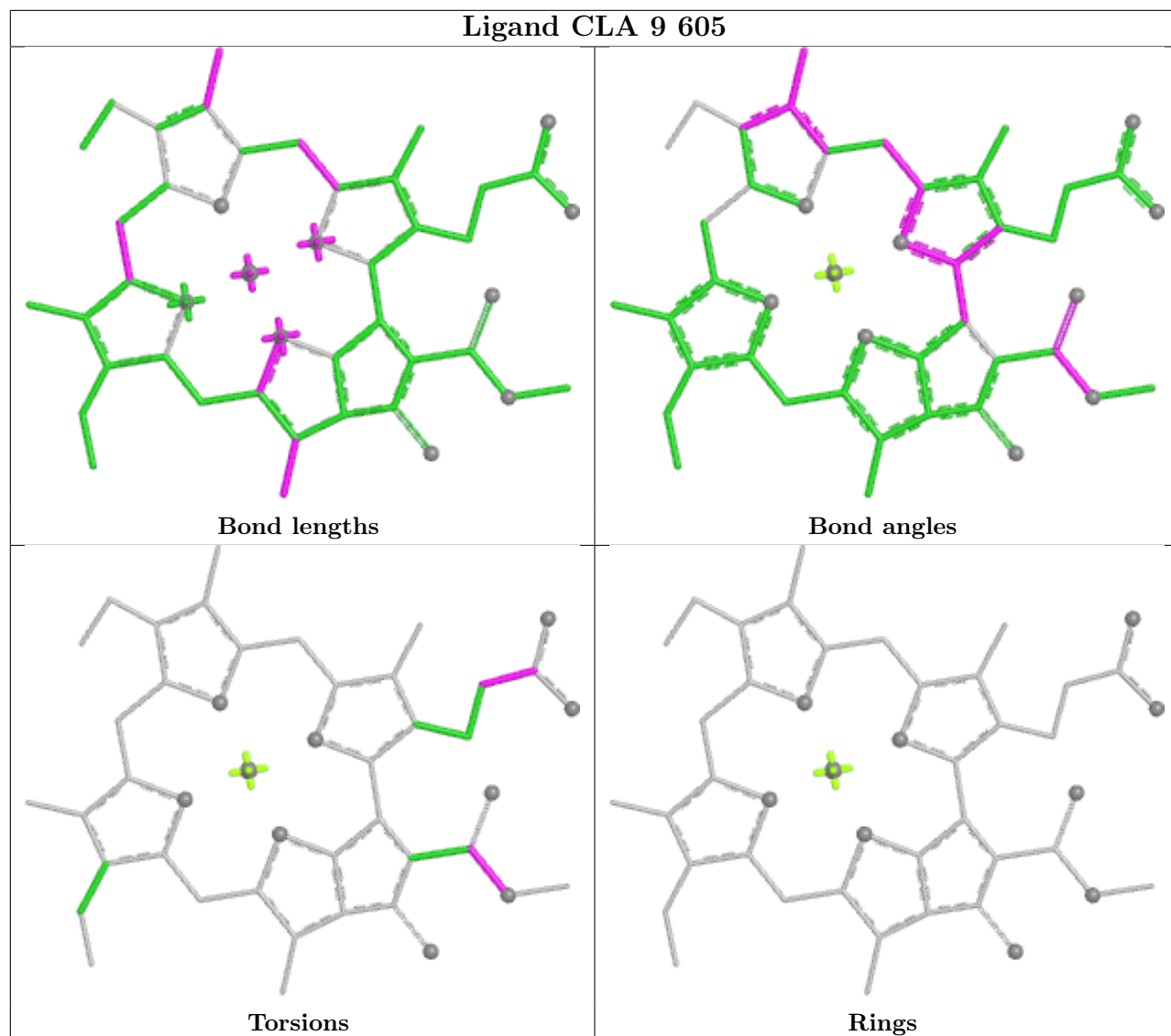
Ligand CLA B 823



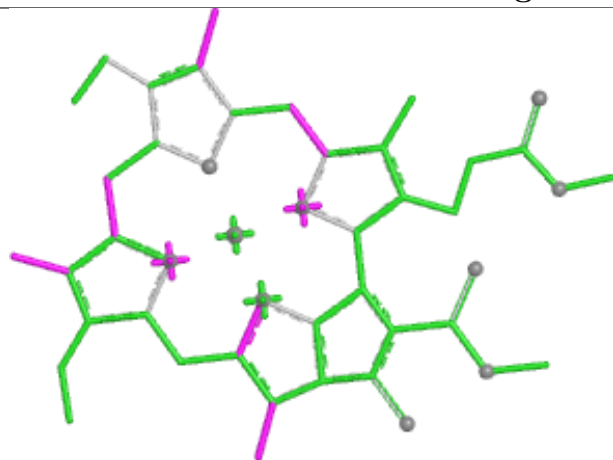
Ligand LMG A 801			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR I 203			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

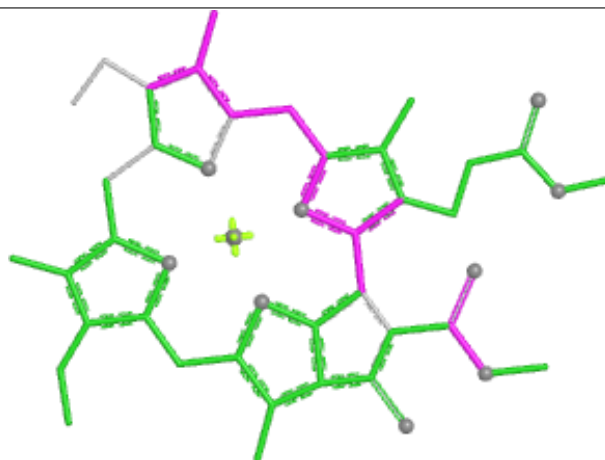
Ligand CLA 9 605



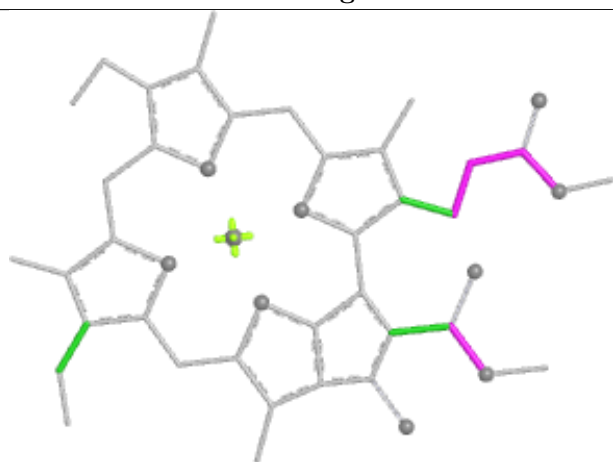
Ligand CLA T 606



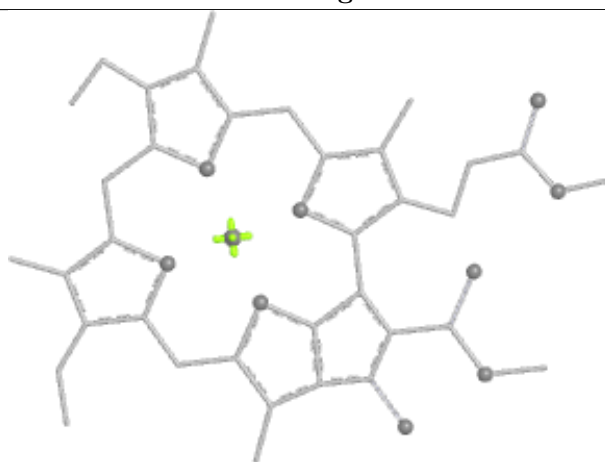
Bond lengths



Bond angles

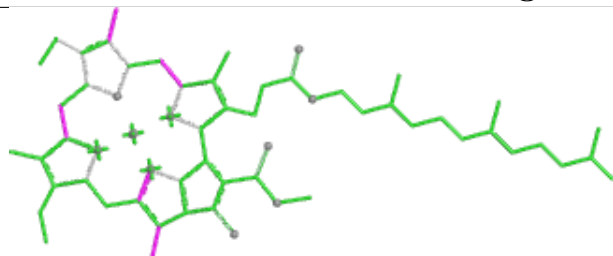


Torsions

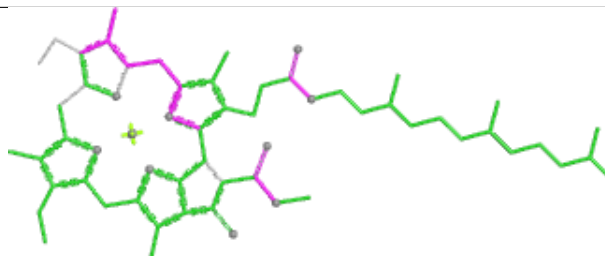


Rings

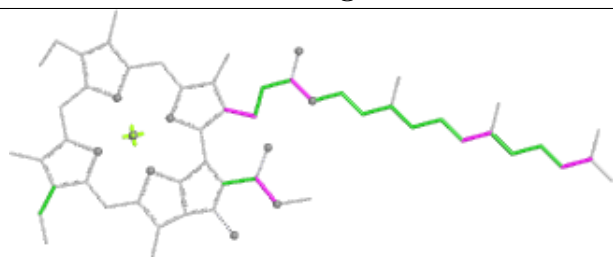
Ligand CLA 1 311



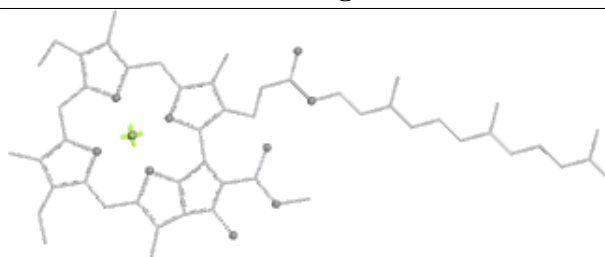
Bond lengths



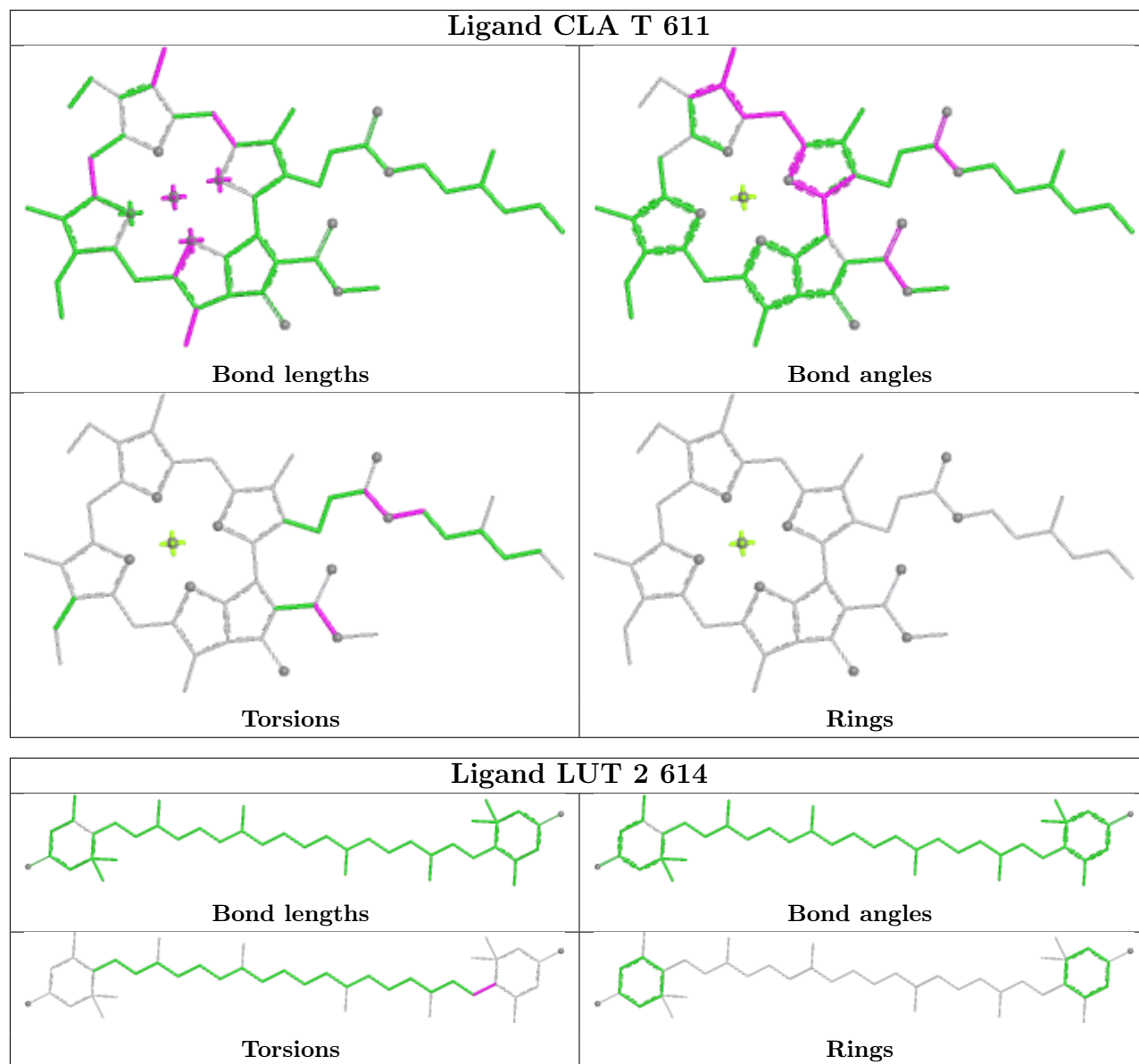
Bond angles

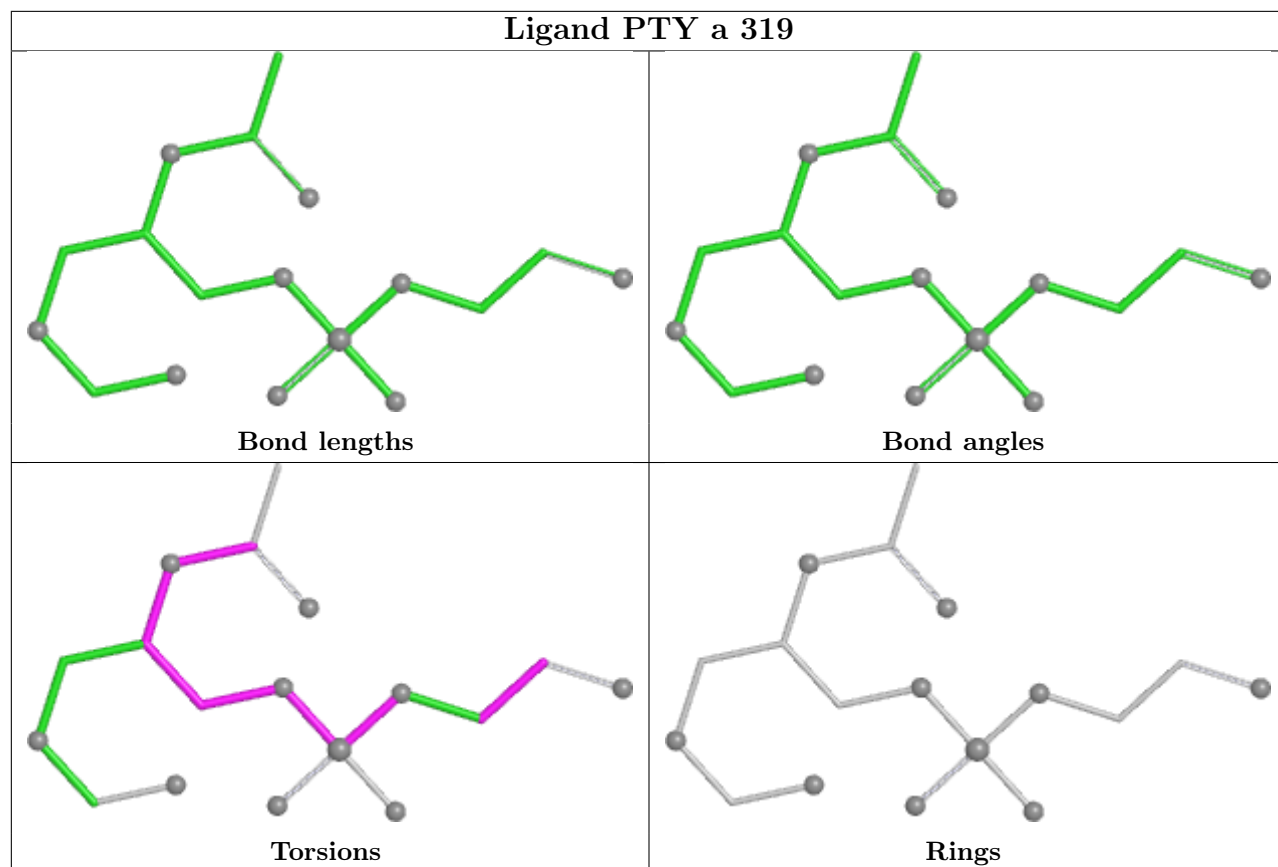


Torsions

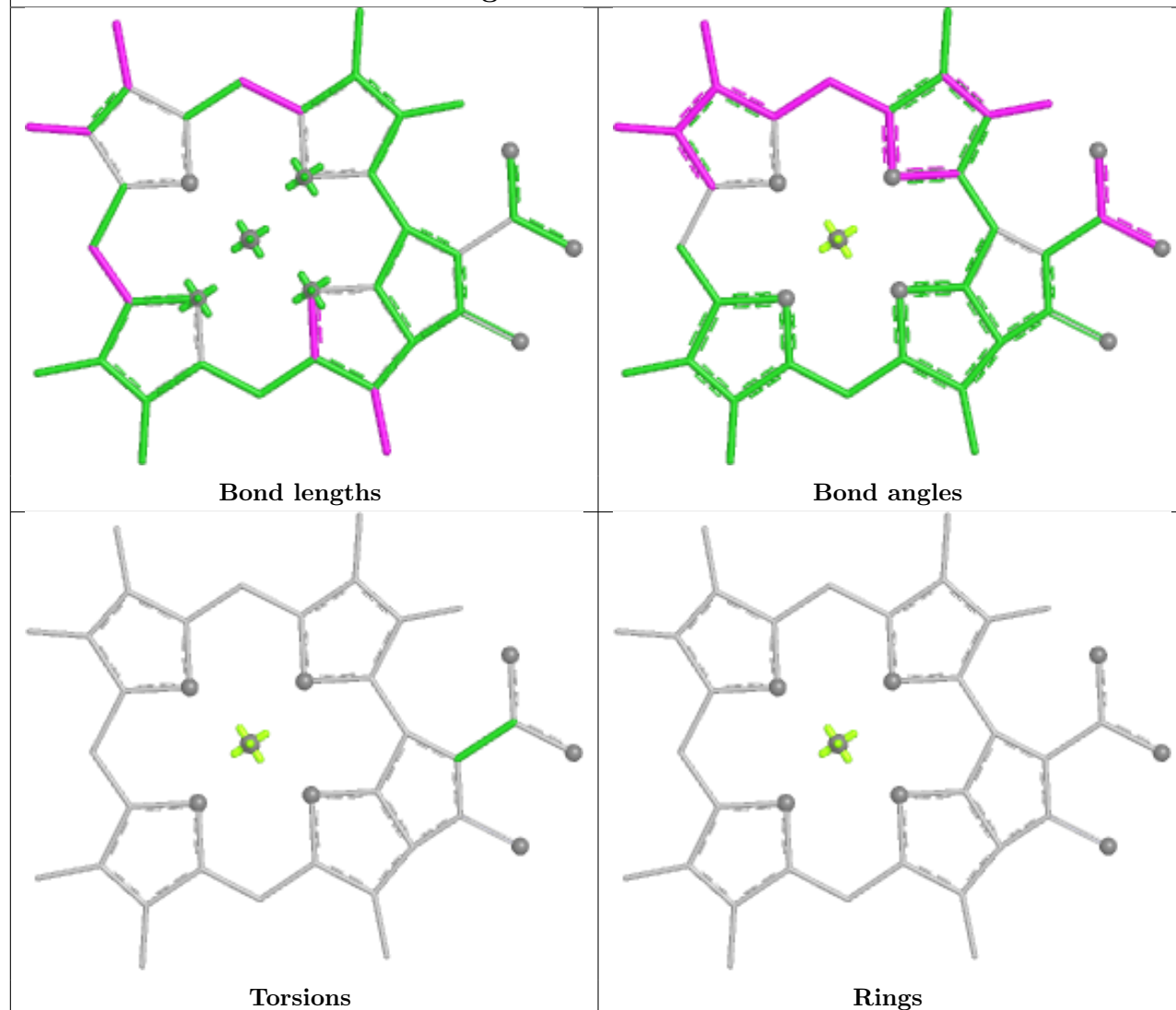


Rings

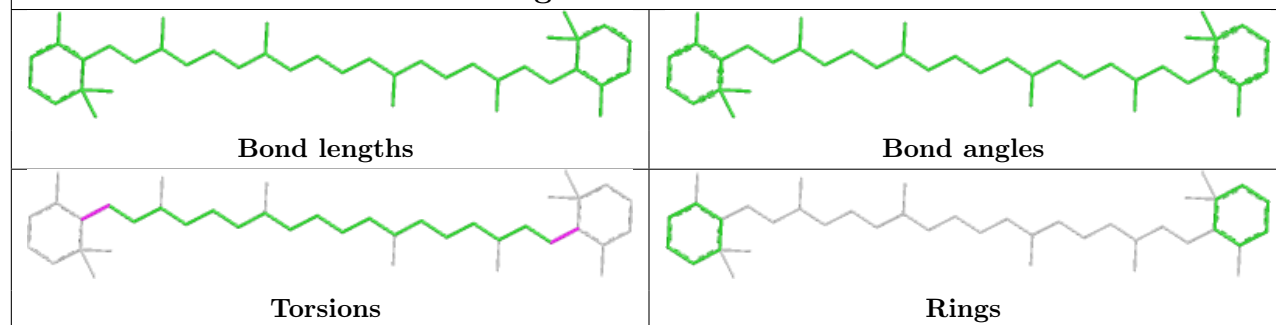


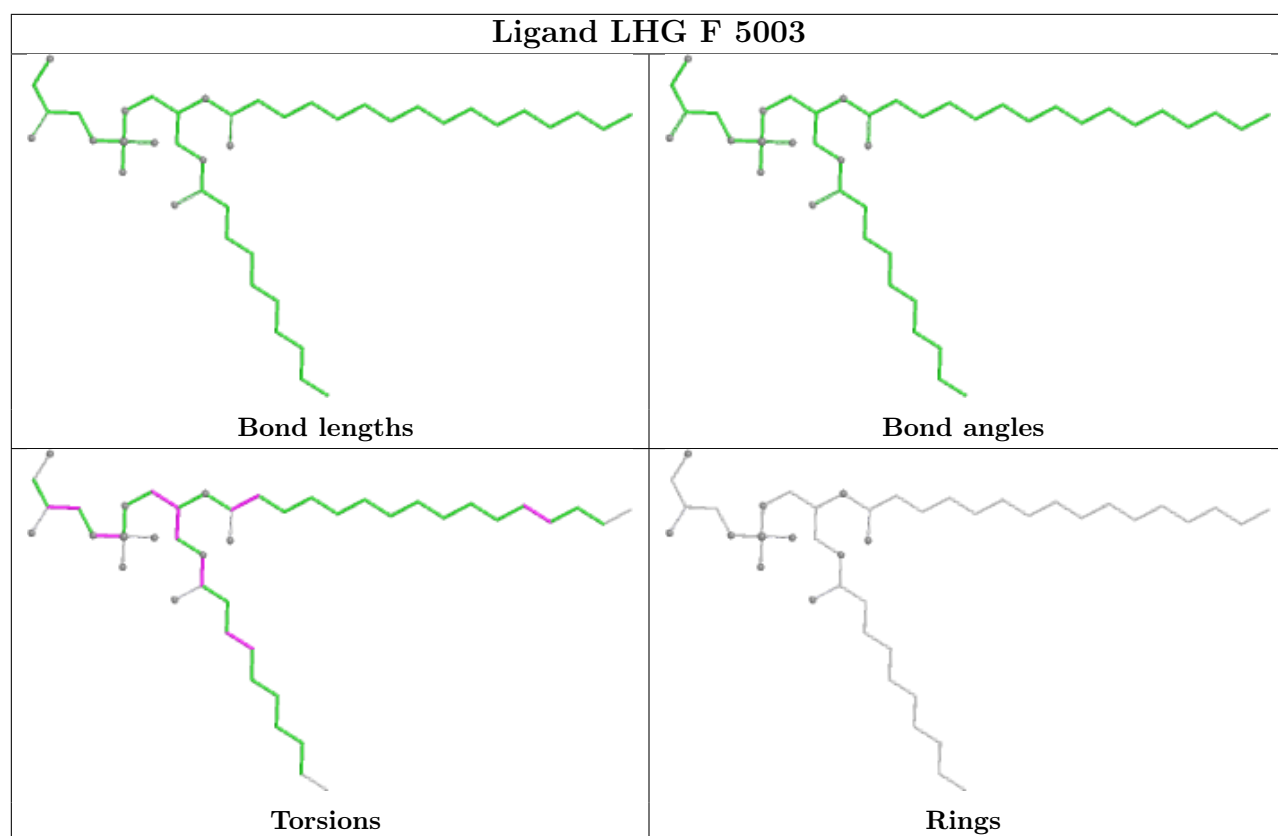


Ligand CLA O 2002

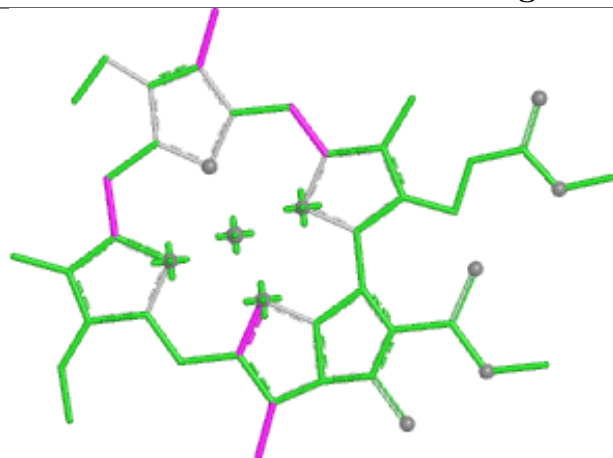


Ligand BCR 8 618

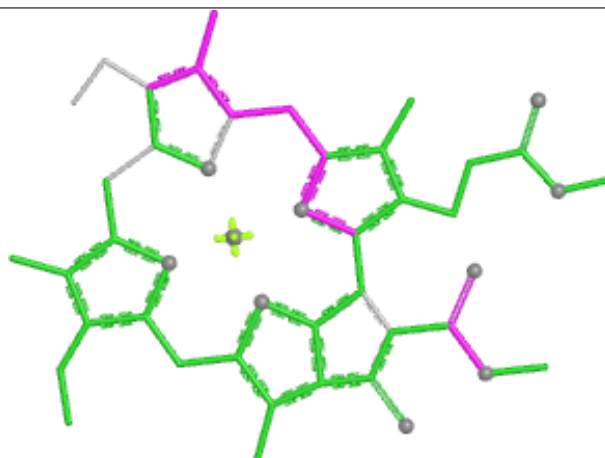




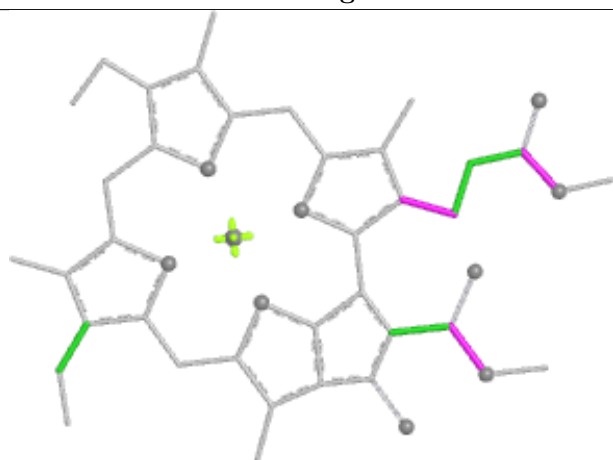
Ligand CLA 8 614



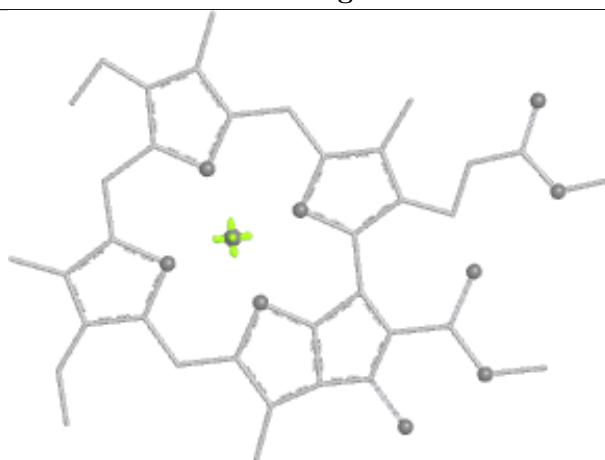
Bond lengths



Bond angles

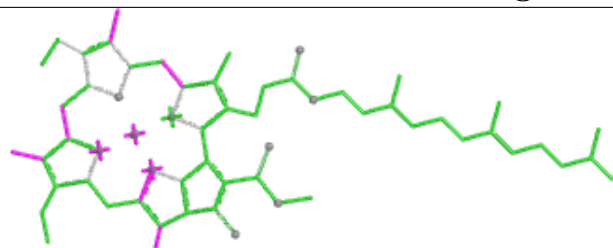


Torsions

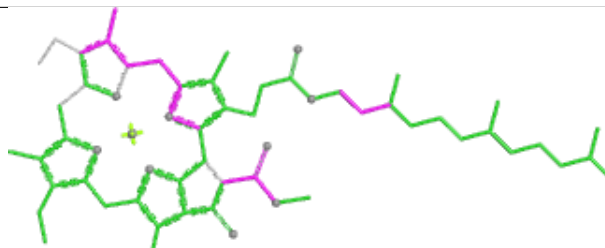


Rings

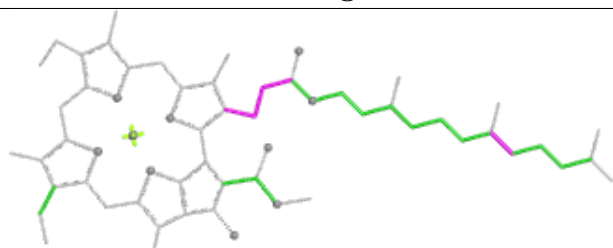
Ligand CLA B 820



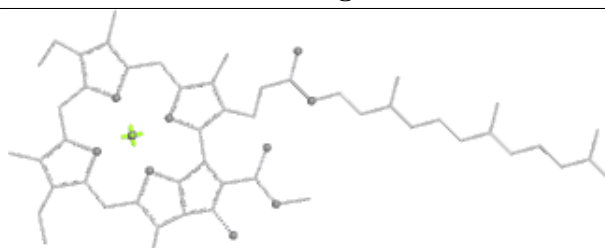
Bond lengths



Bond angles

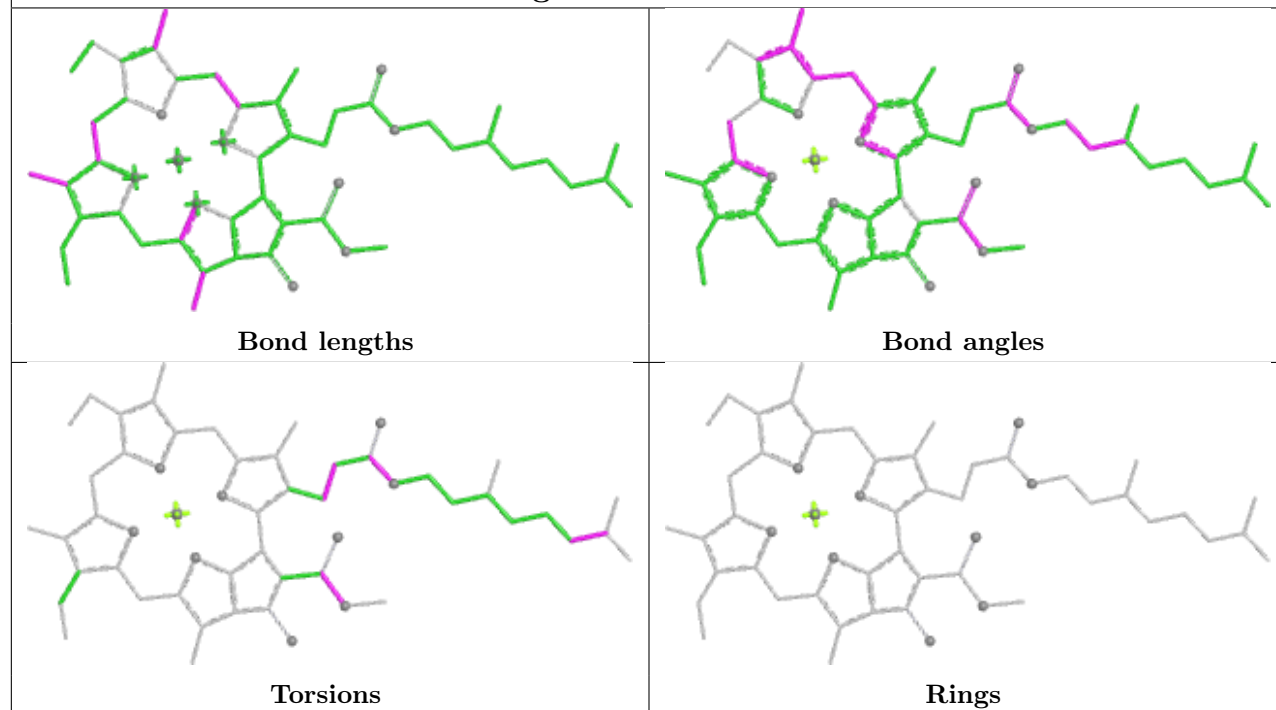


Torsions

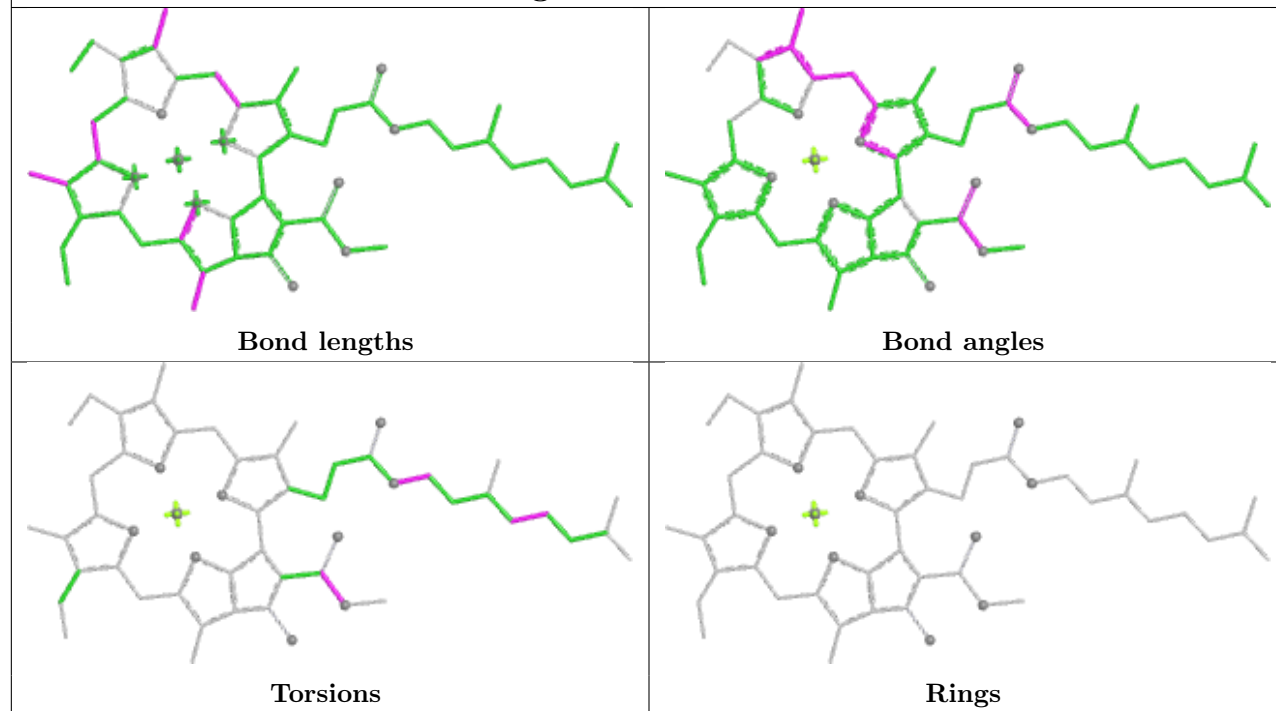


Rings

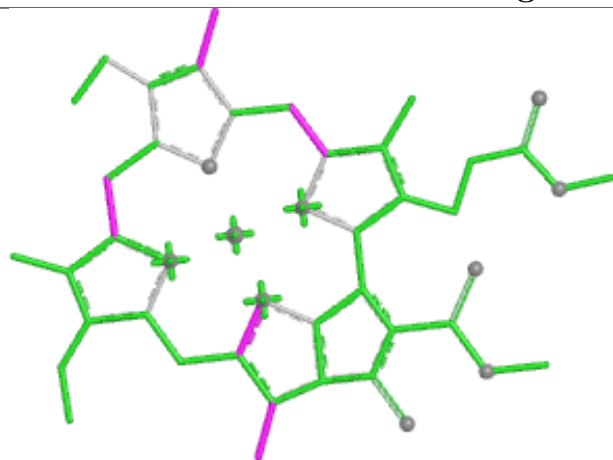
Ligand CLA T 609



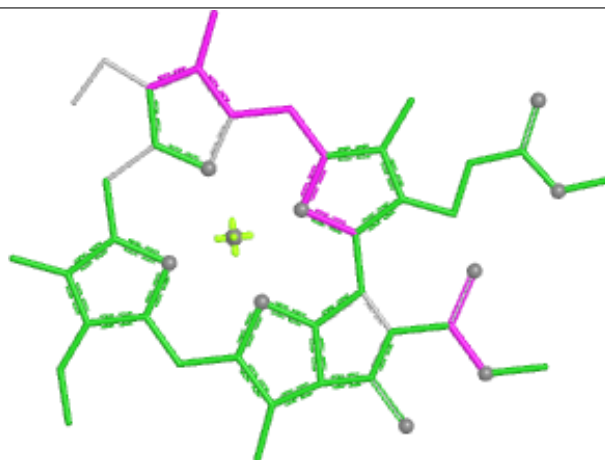
Ligand CLA A 833



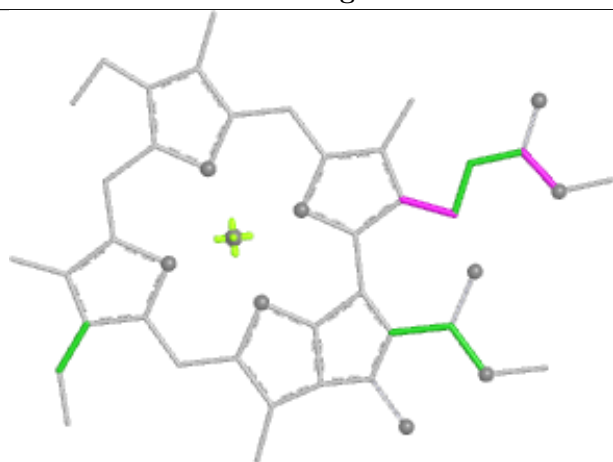
Ligand CLA b 310



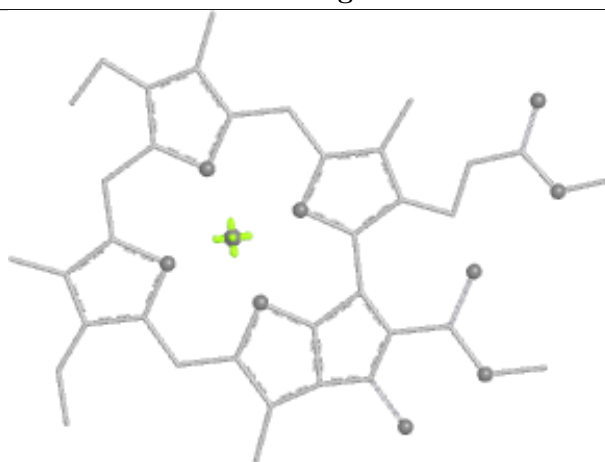
Bond lengths



Bond angles

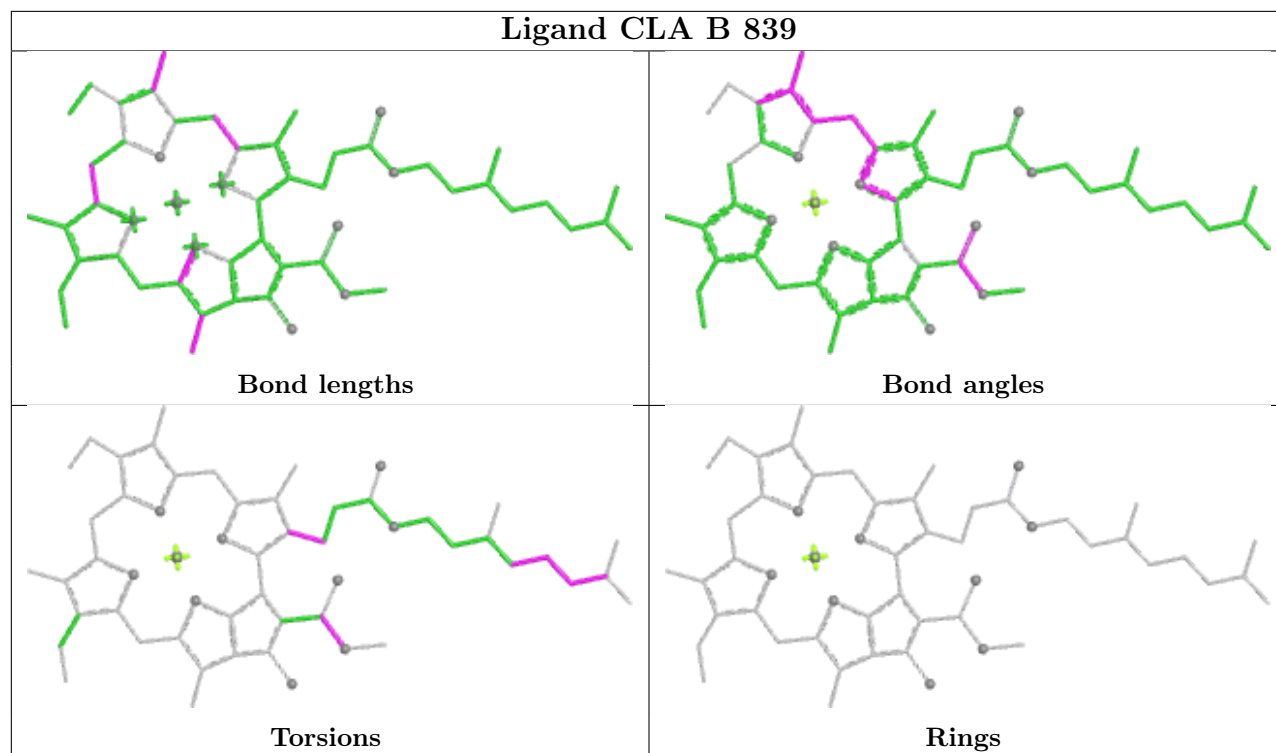


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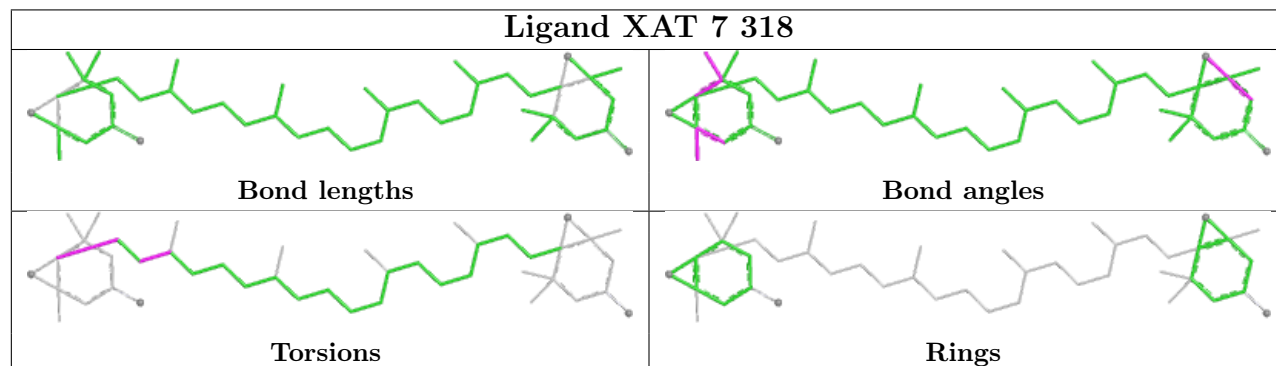


Rings

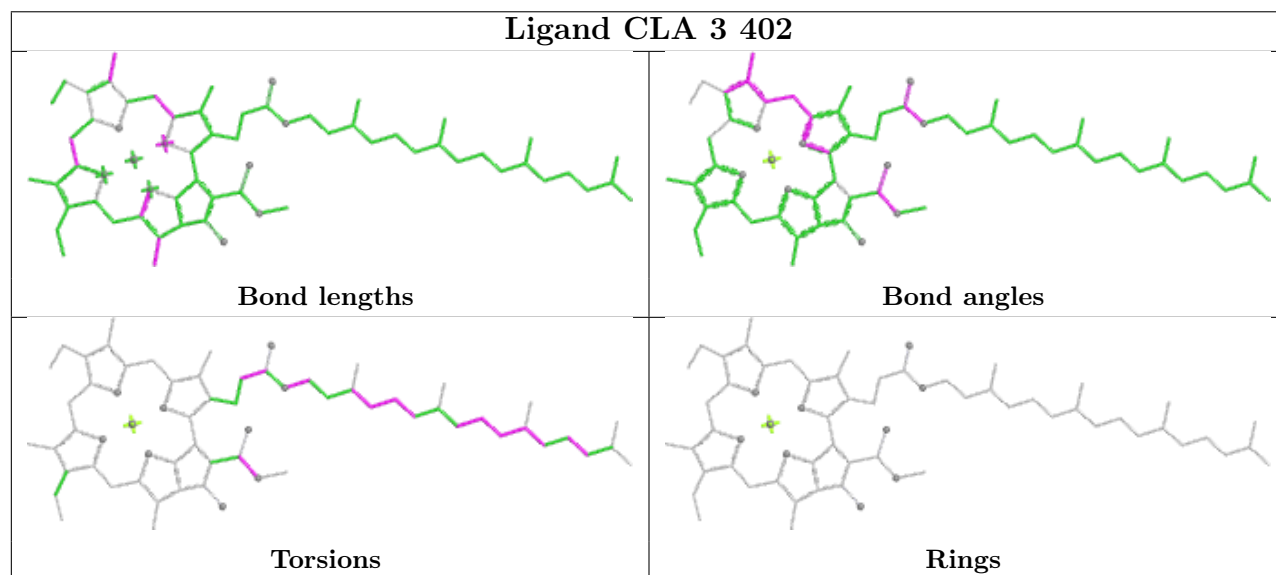
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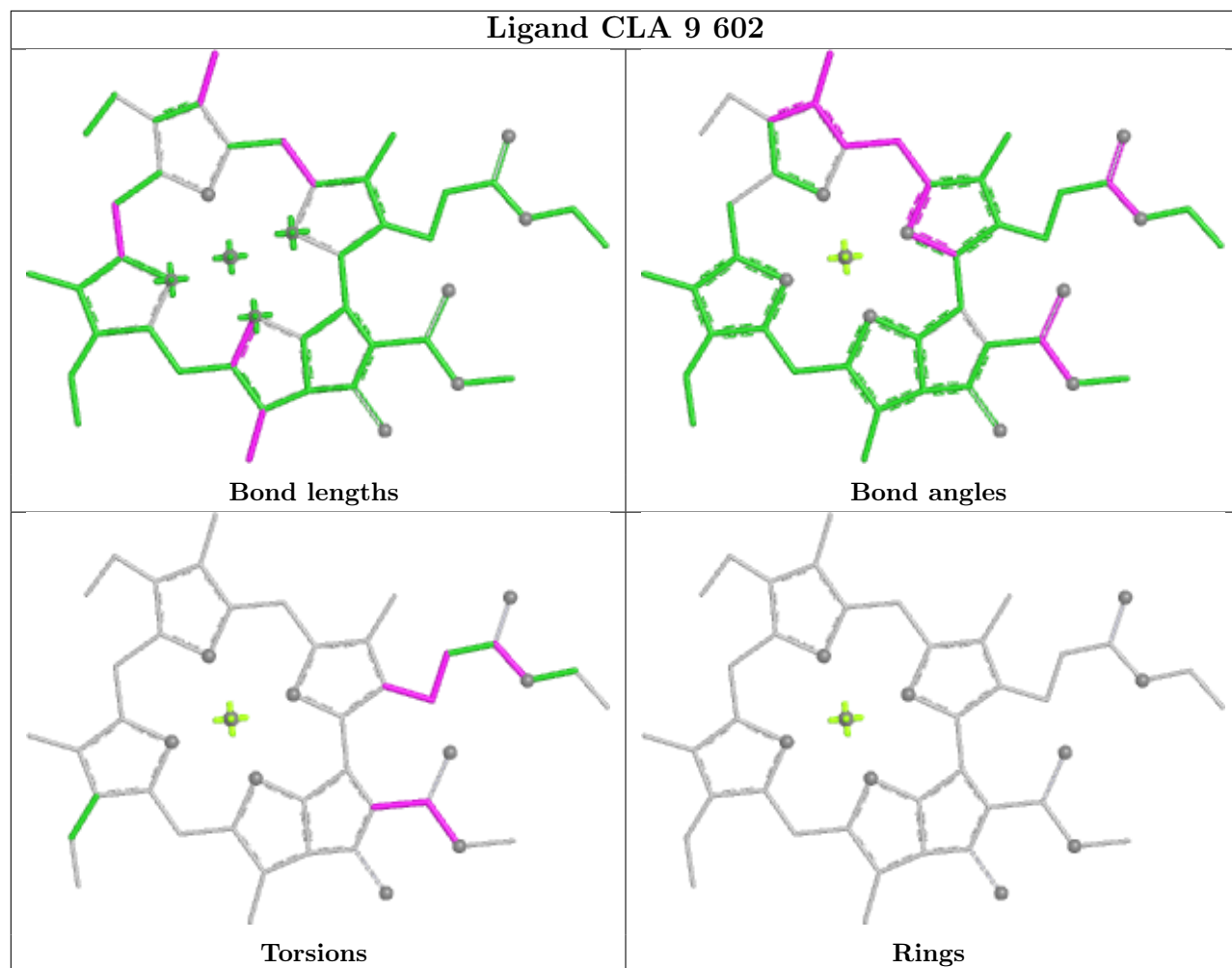
Ligand XAT 7 318



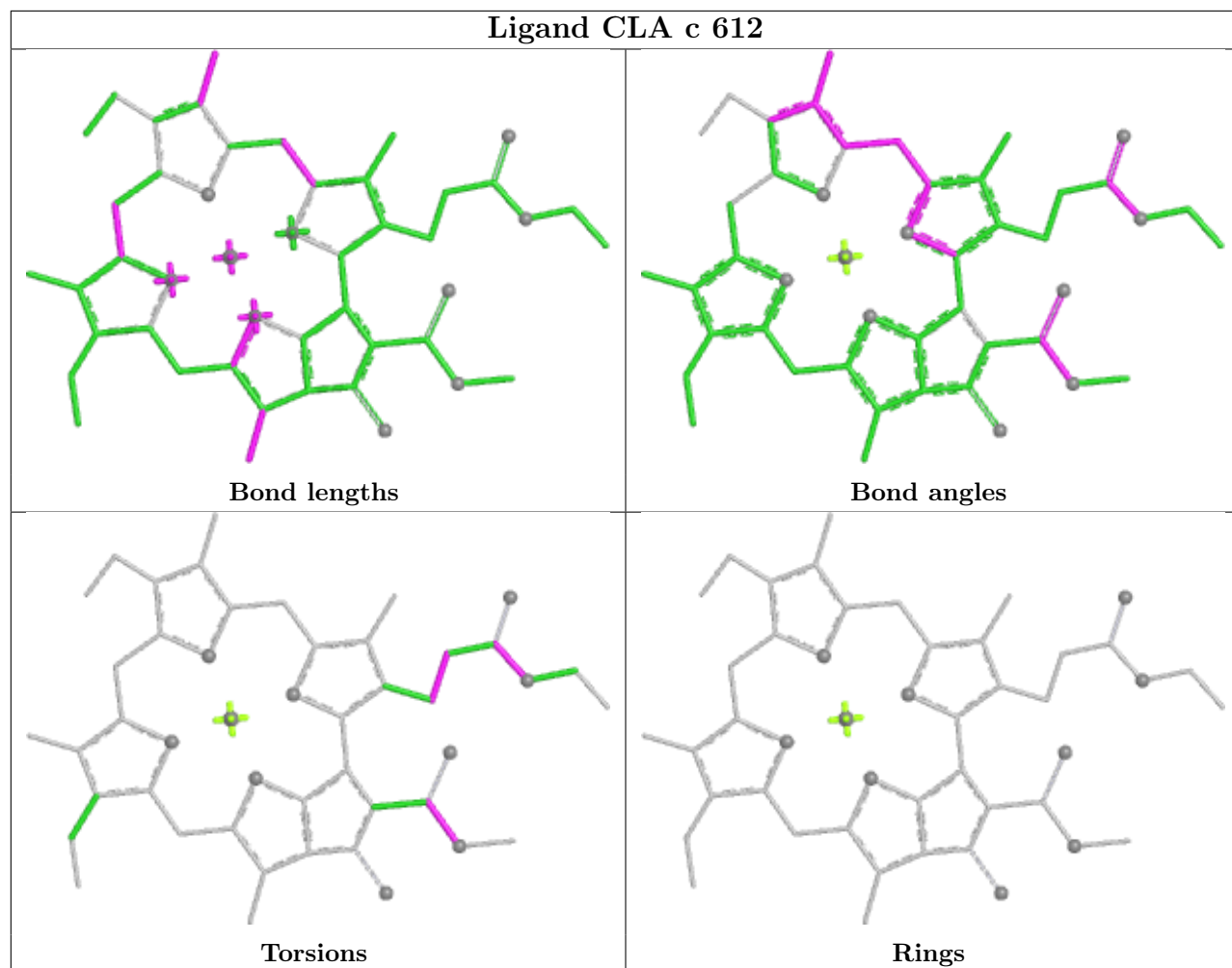
Ligand CLA 3 402



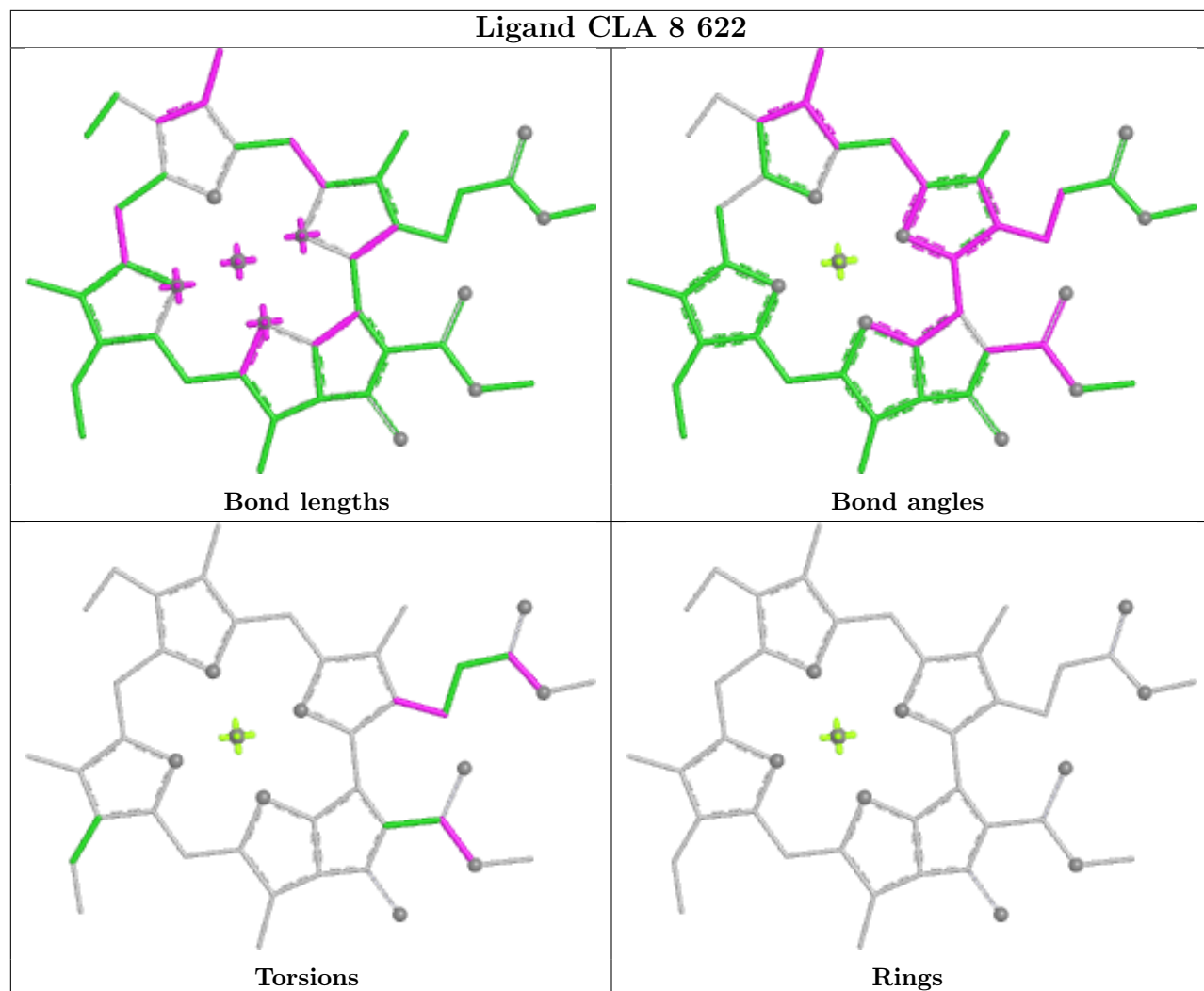
Ligand CLA 9 602



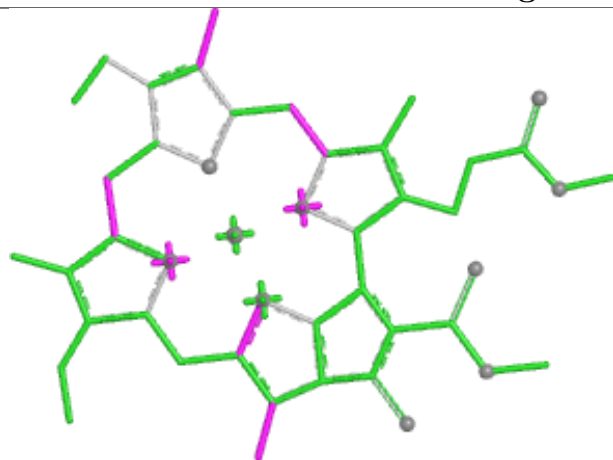
Ligand CLA c 612



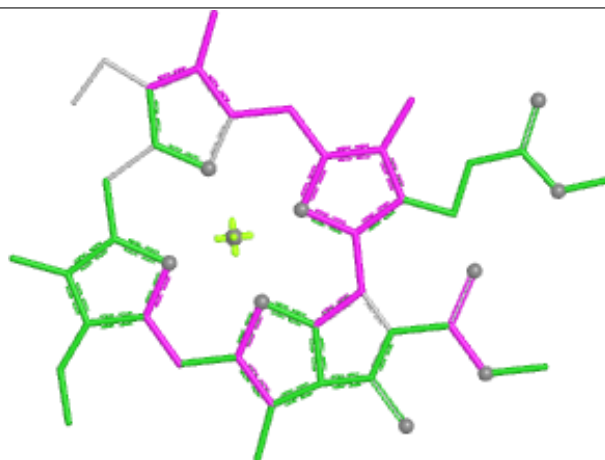
Ligand CLA 8 622



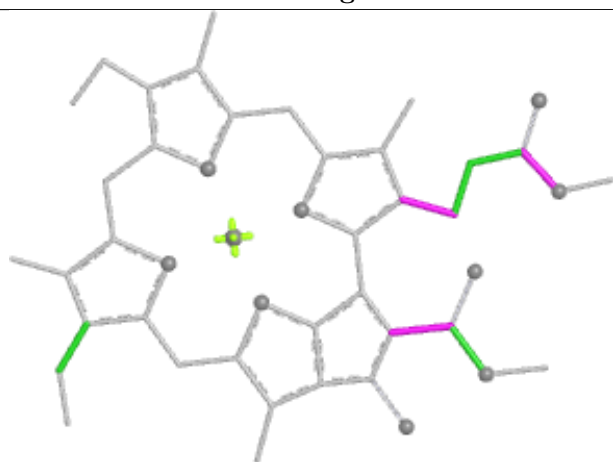
Ligand CLA 9 601



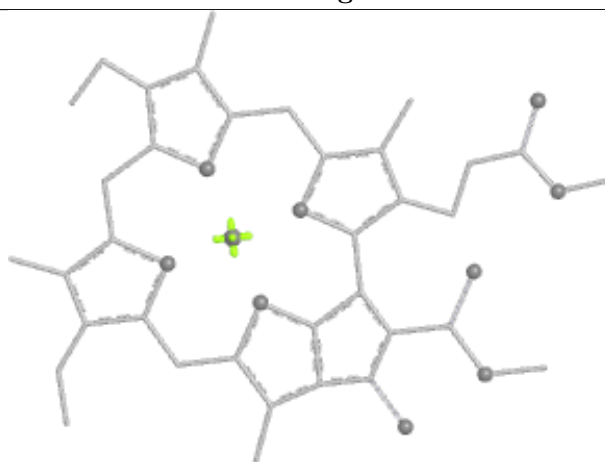
Bond lengths



Bond angles

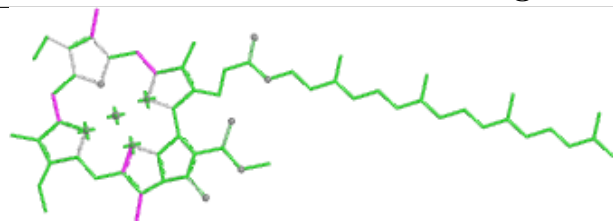


Torsions

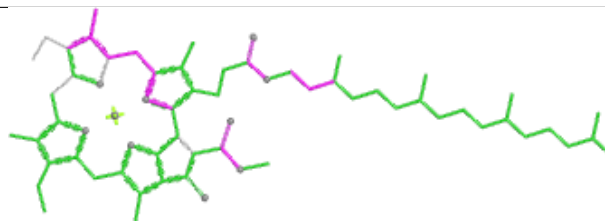


Rings

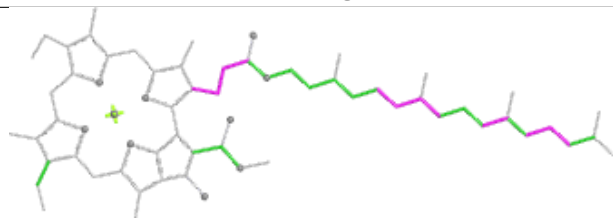
Ligand CLA A 841



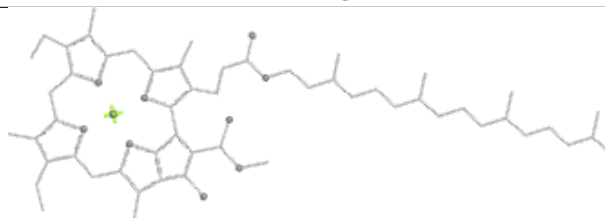
Bond lengths



Bond angles

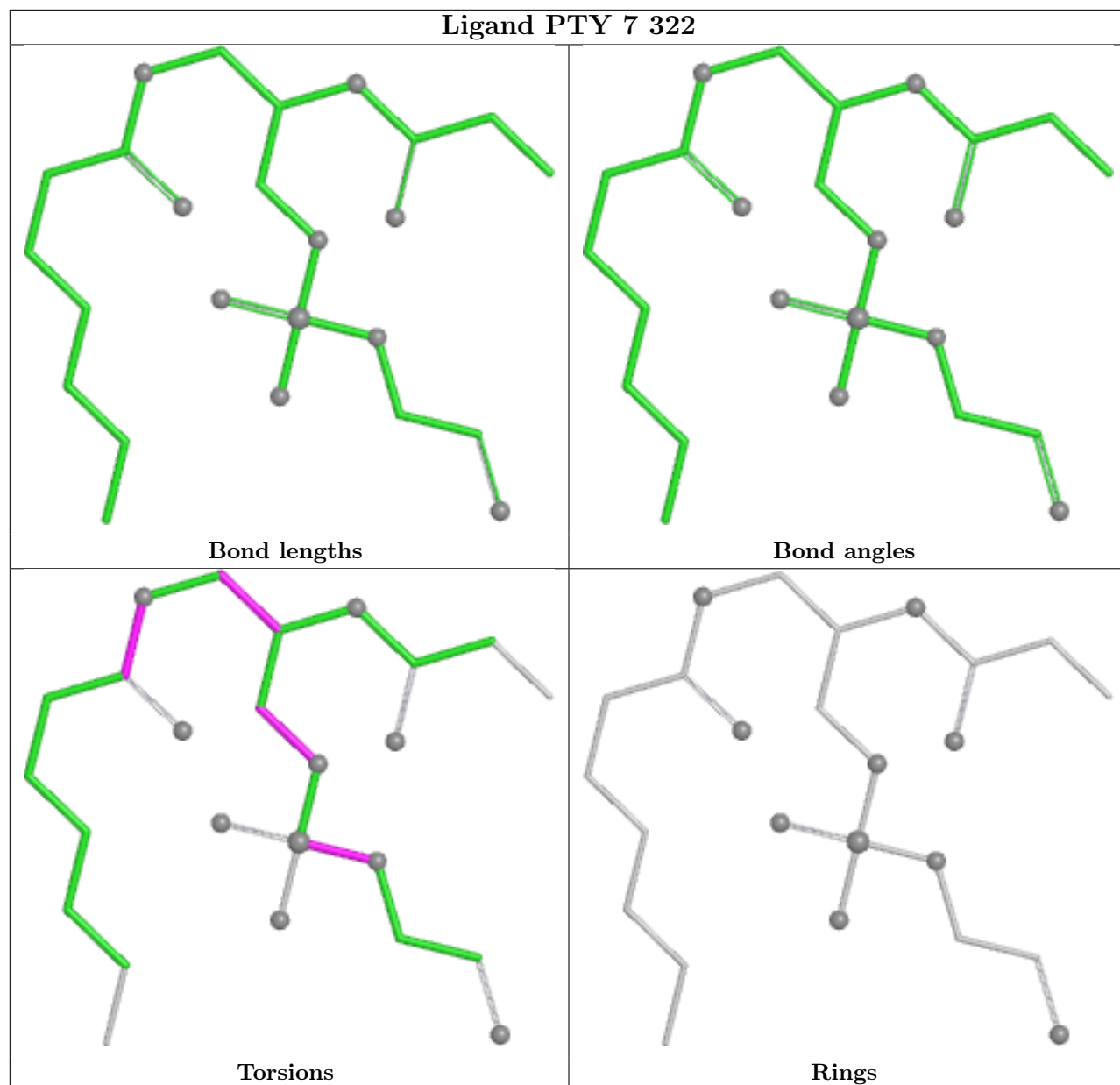


Torsions

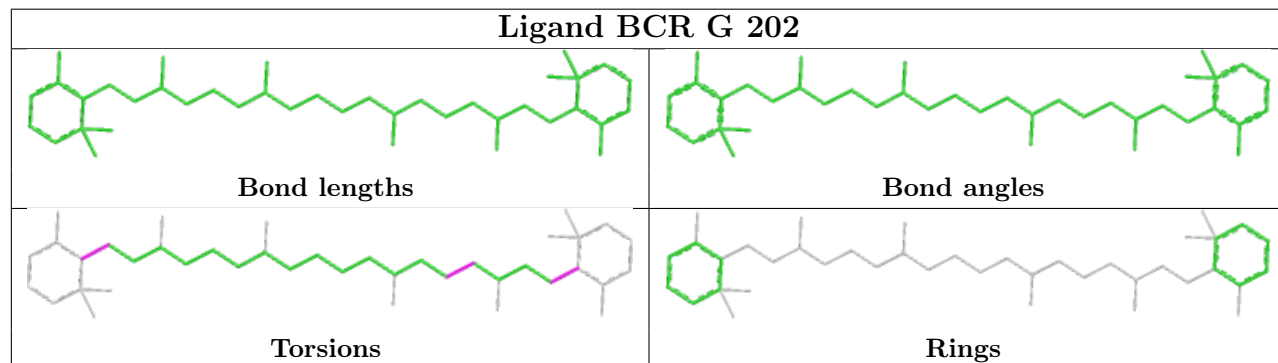


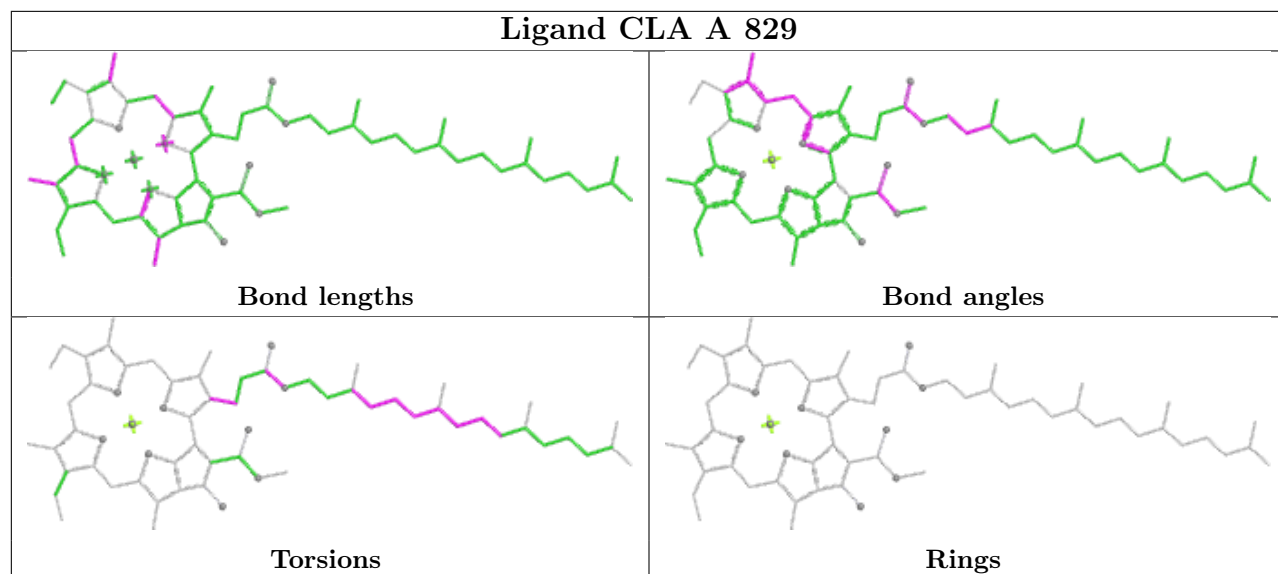
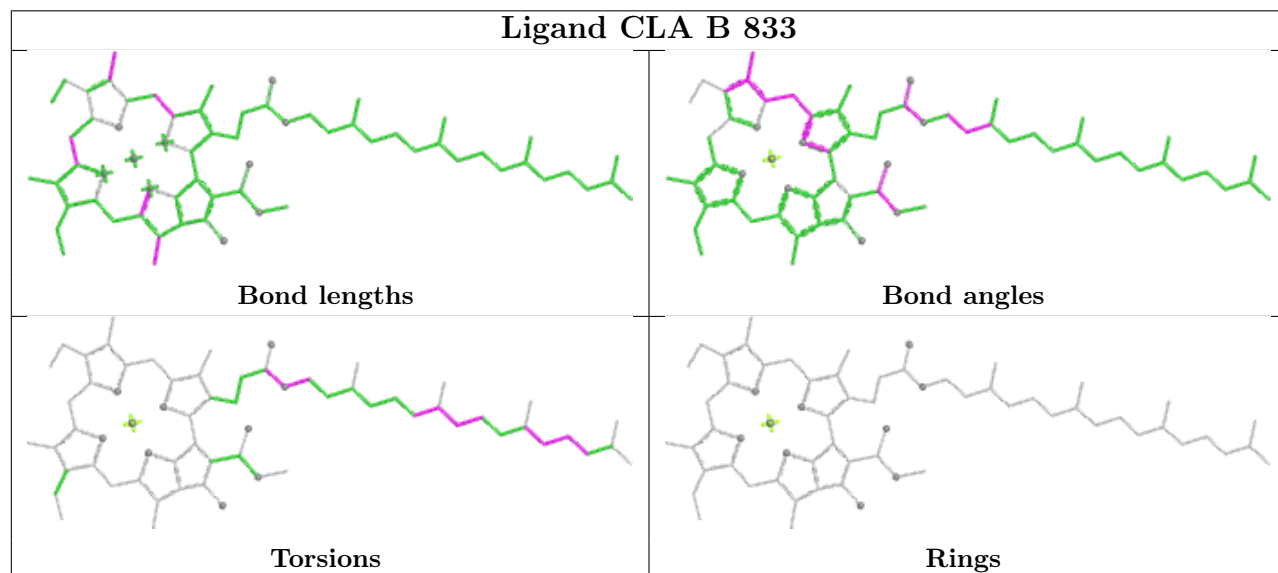
Rings

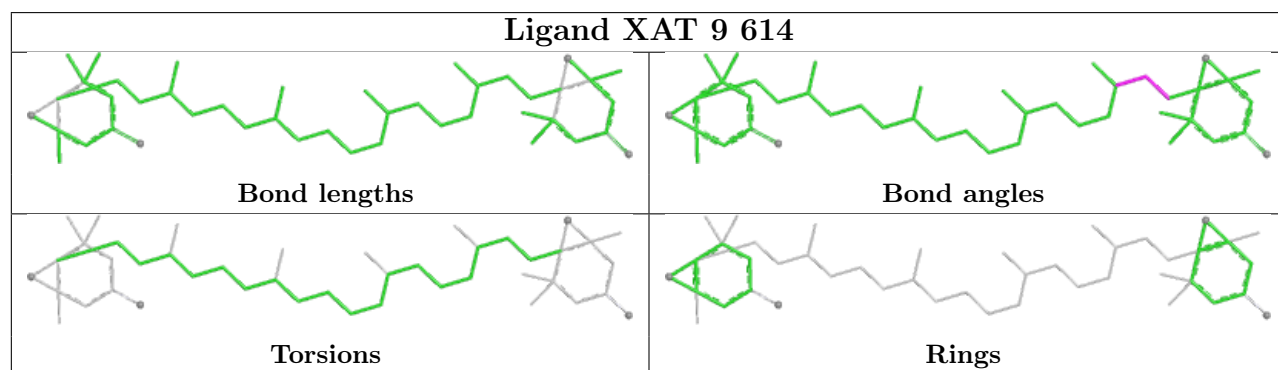
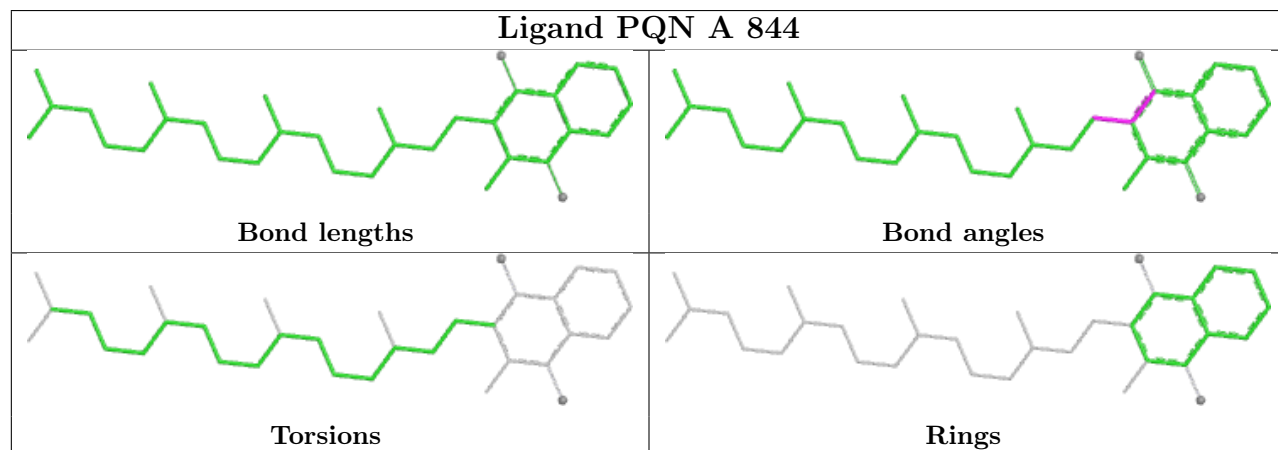
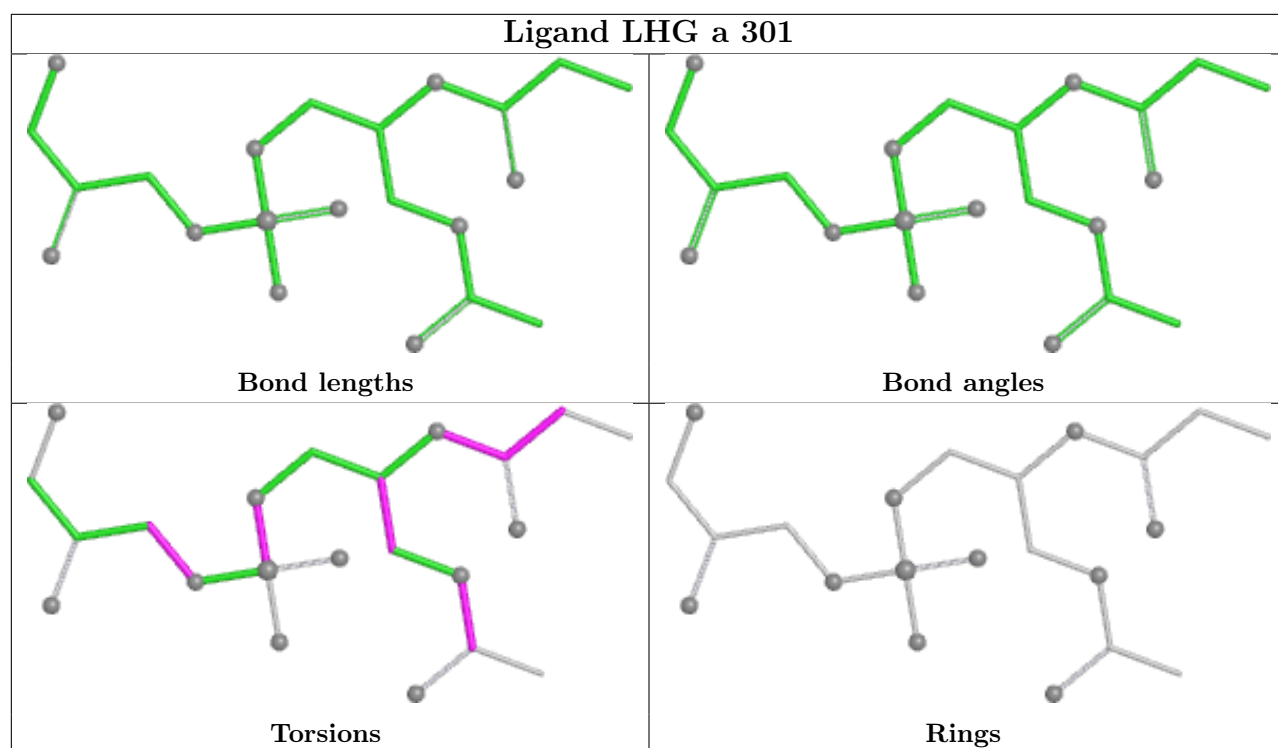
Ligand PTY 7 322



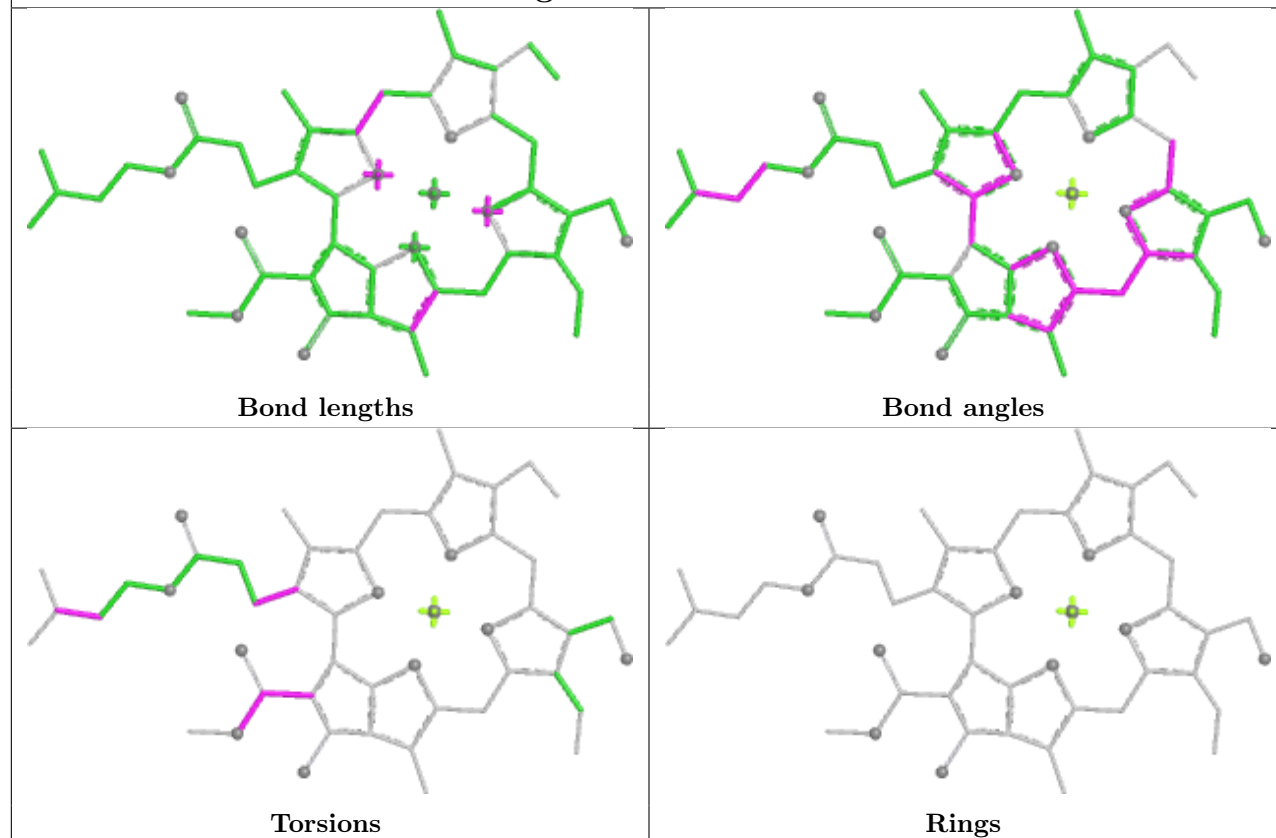
Ligand BCR G 202



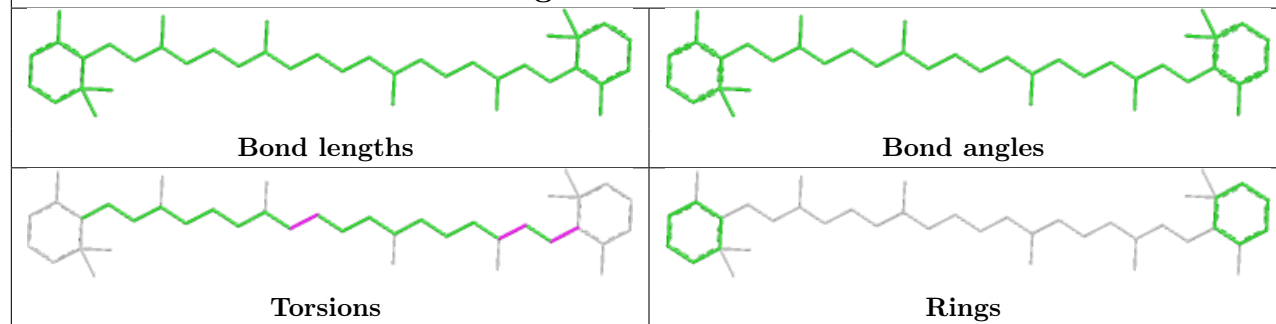
Ligand CLA A 829**Ligand CLA B 833**

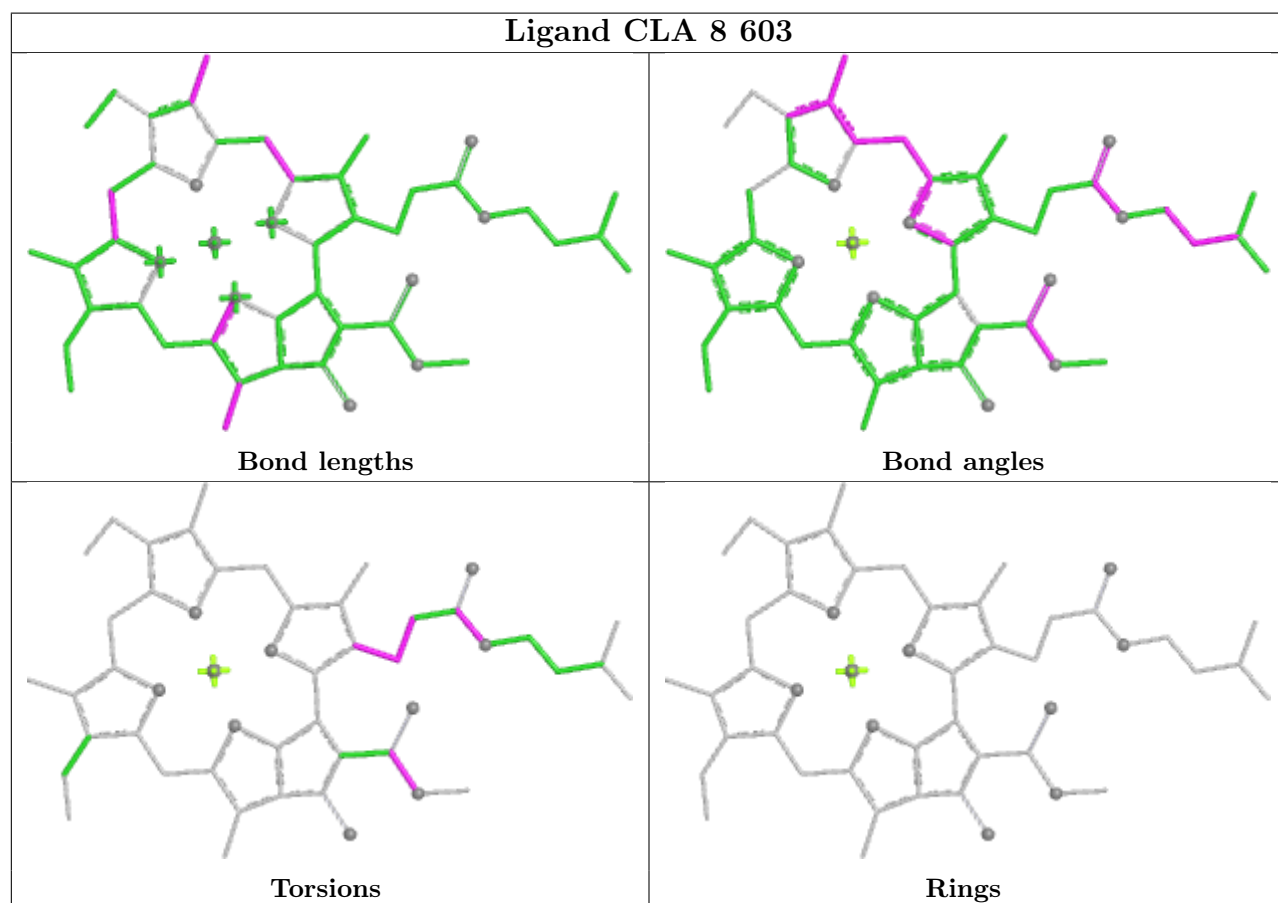
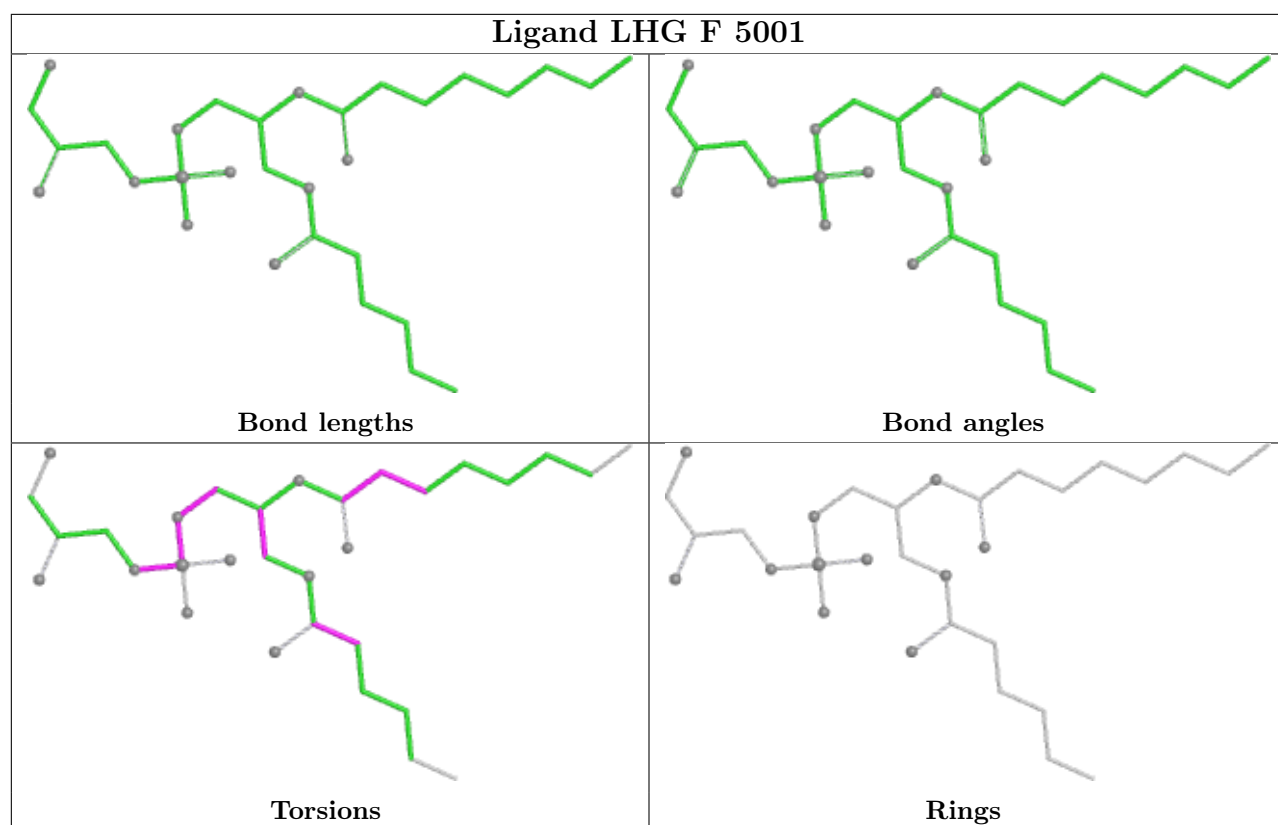


Ligand CHL 8 601

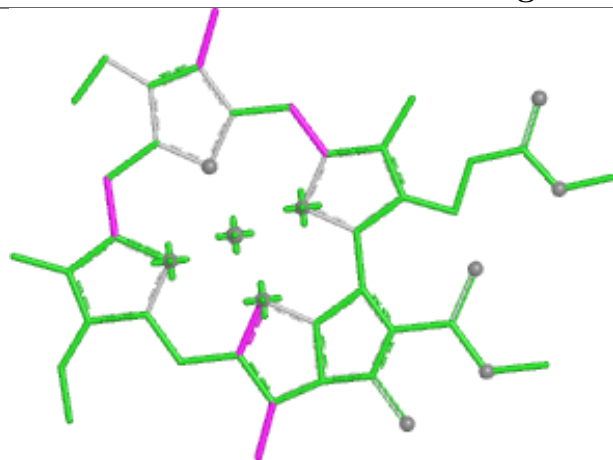


Ligand BCR a 317

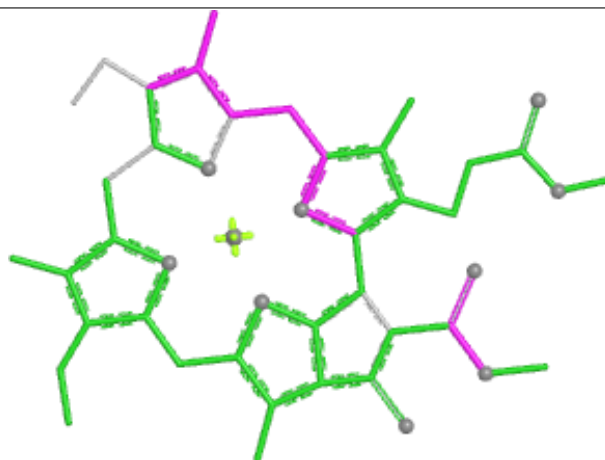




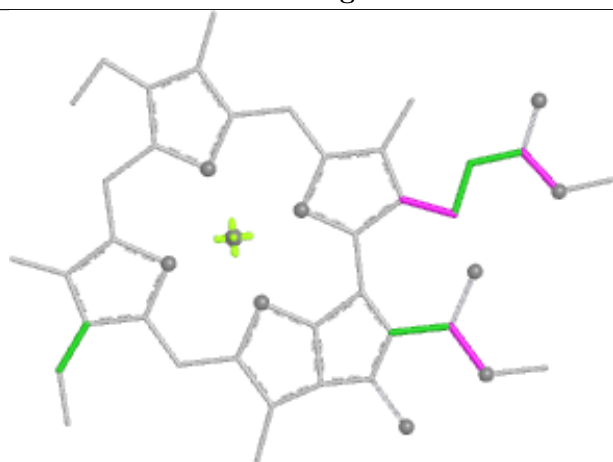
Ligand CLA b 315



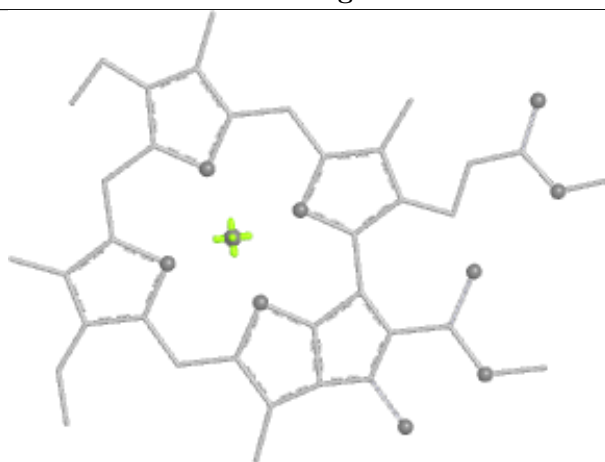
Bond lengths



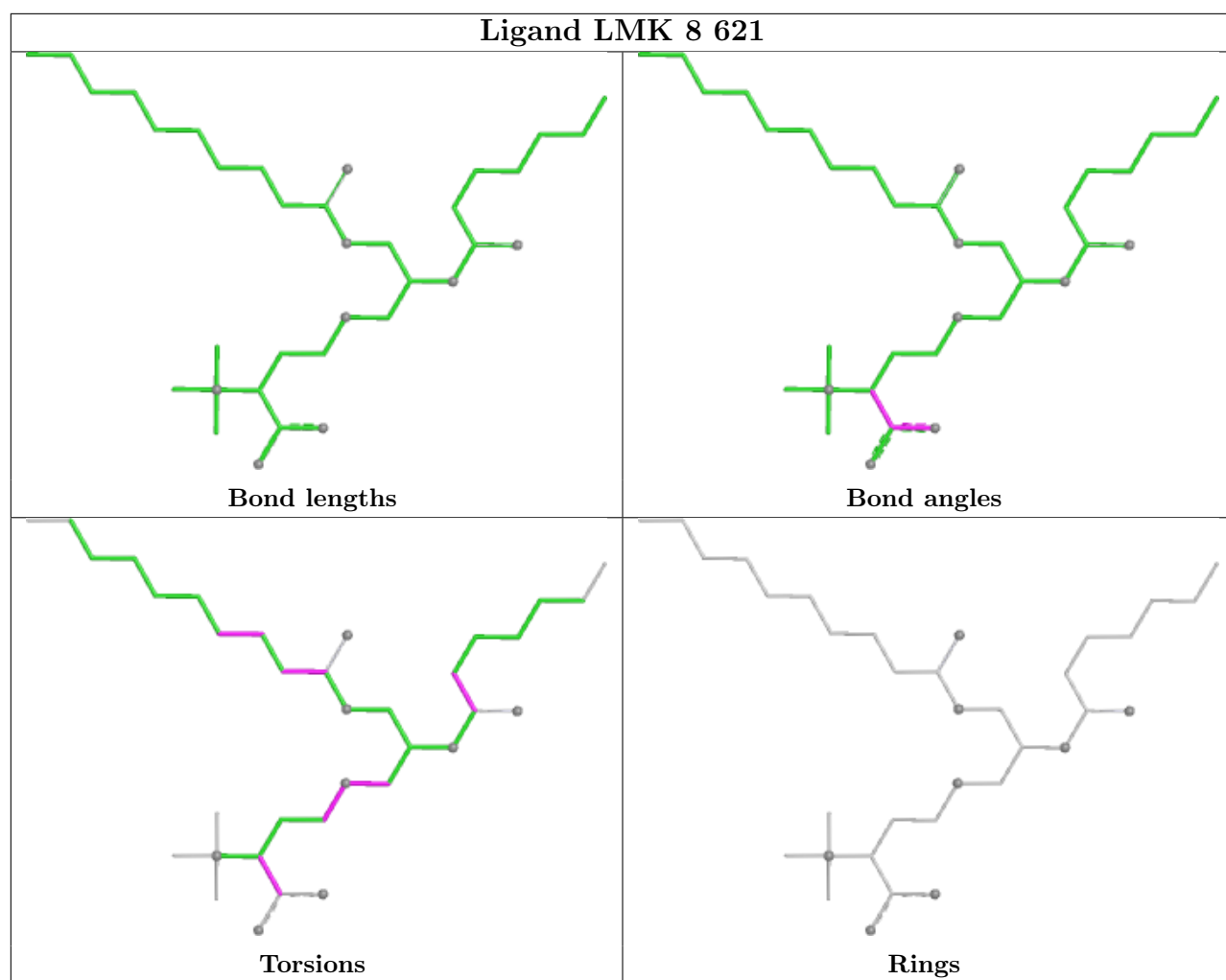
Bond angles



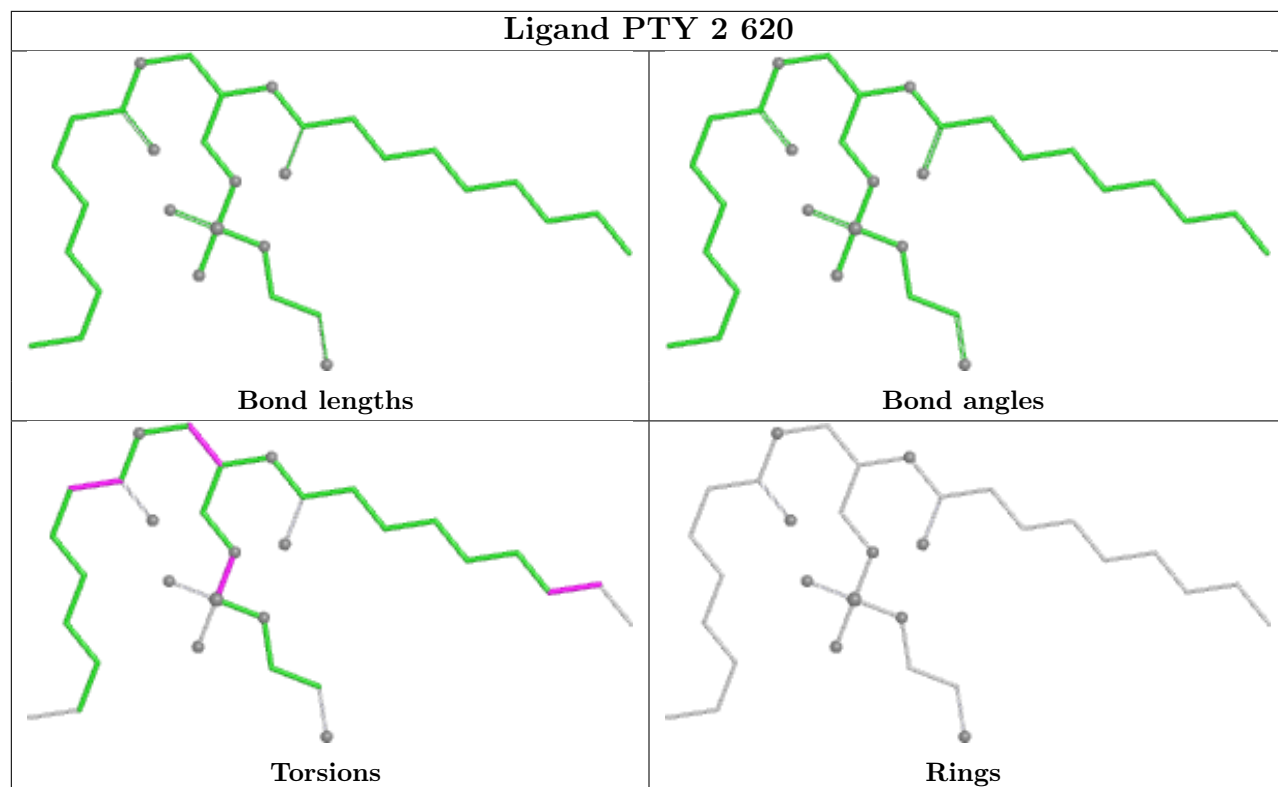
Torsions



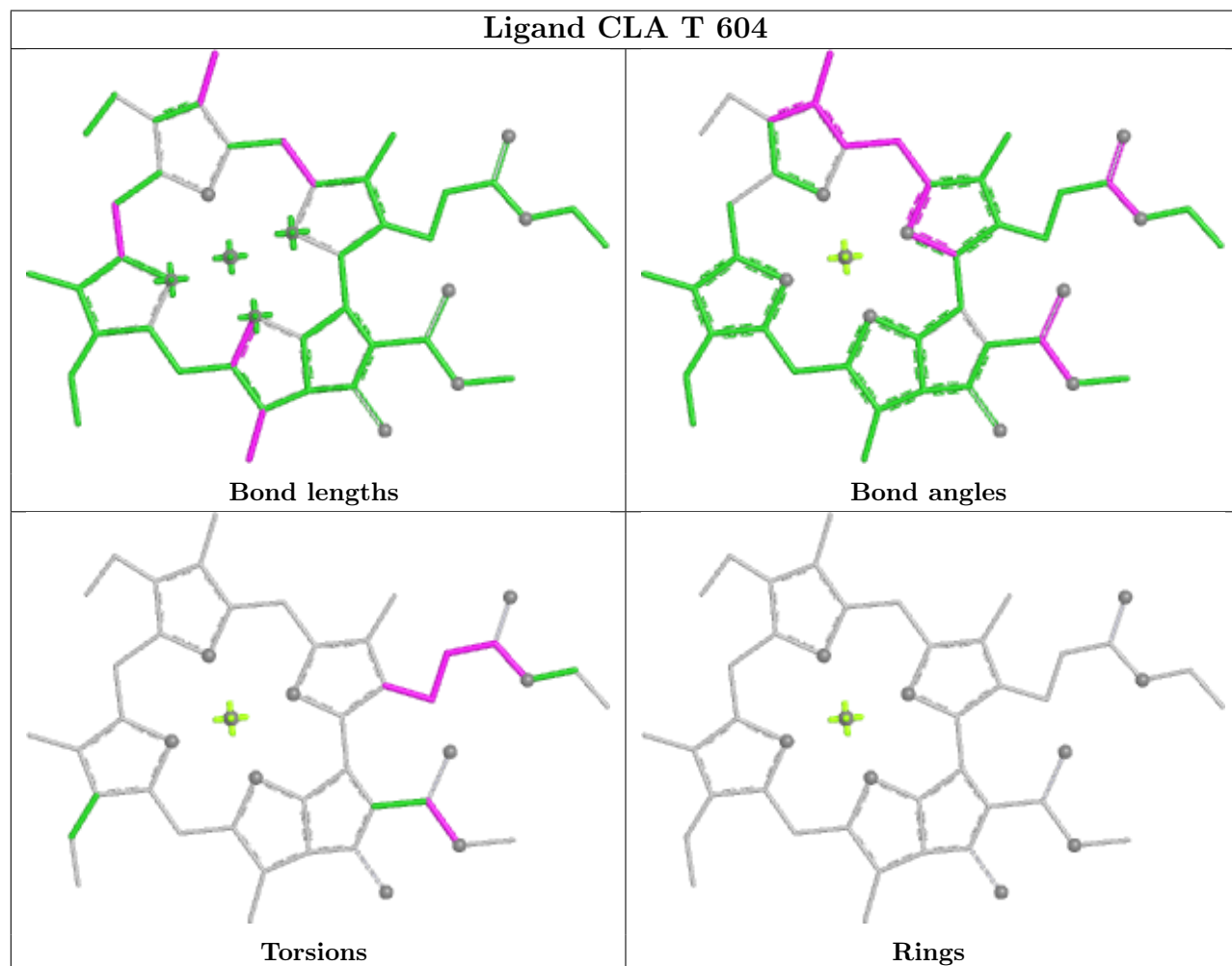
Rings



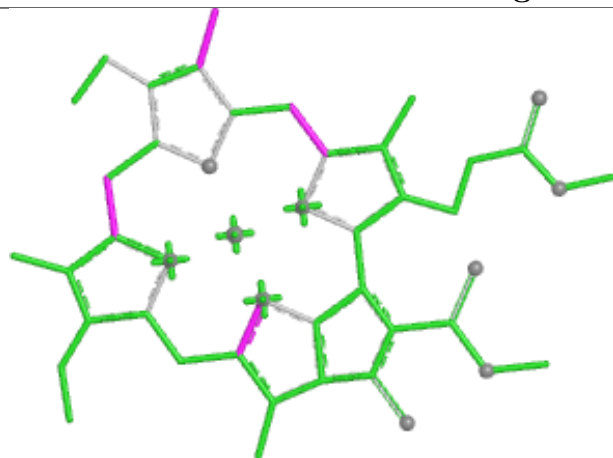
Ligand PTY 2 620



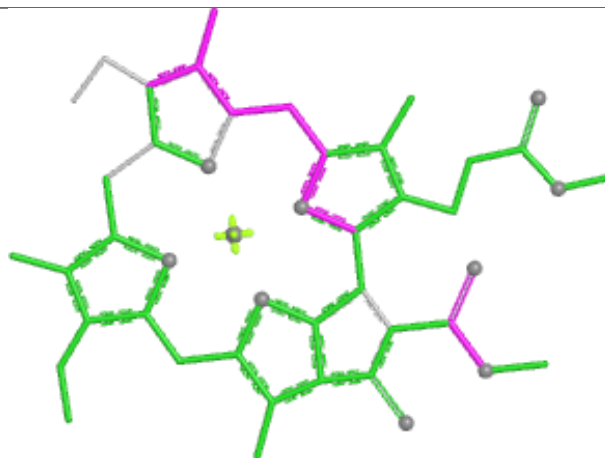
Ligand CLA T 604



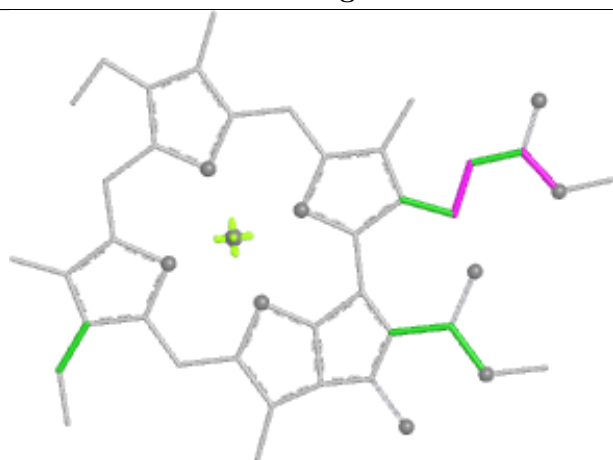
Ligand CLA H 204



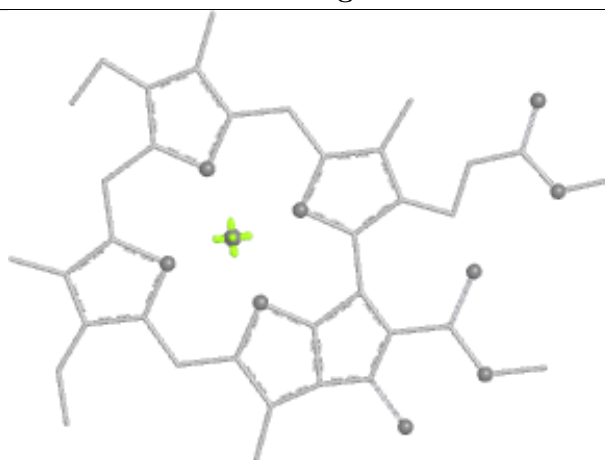
Bond lengths



Bond angles

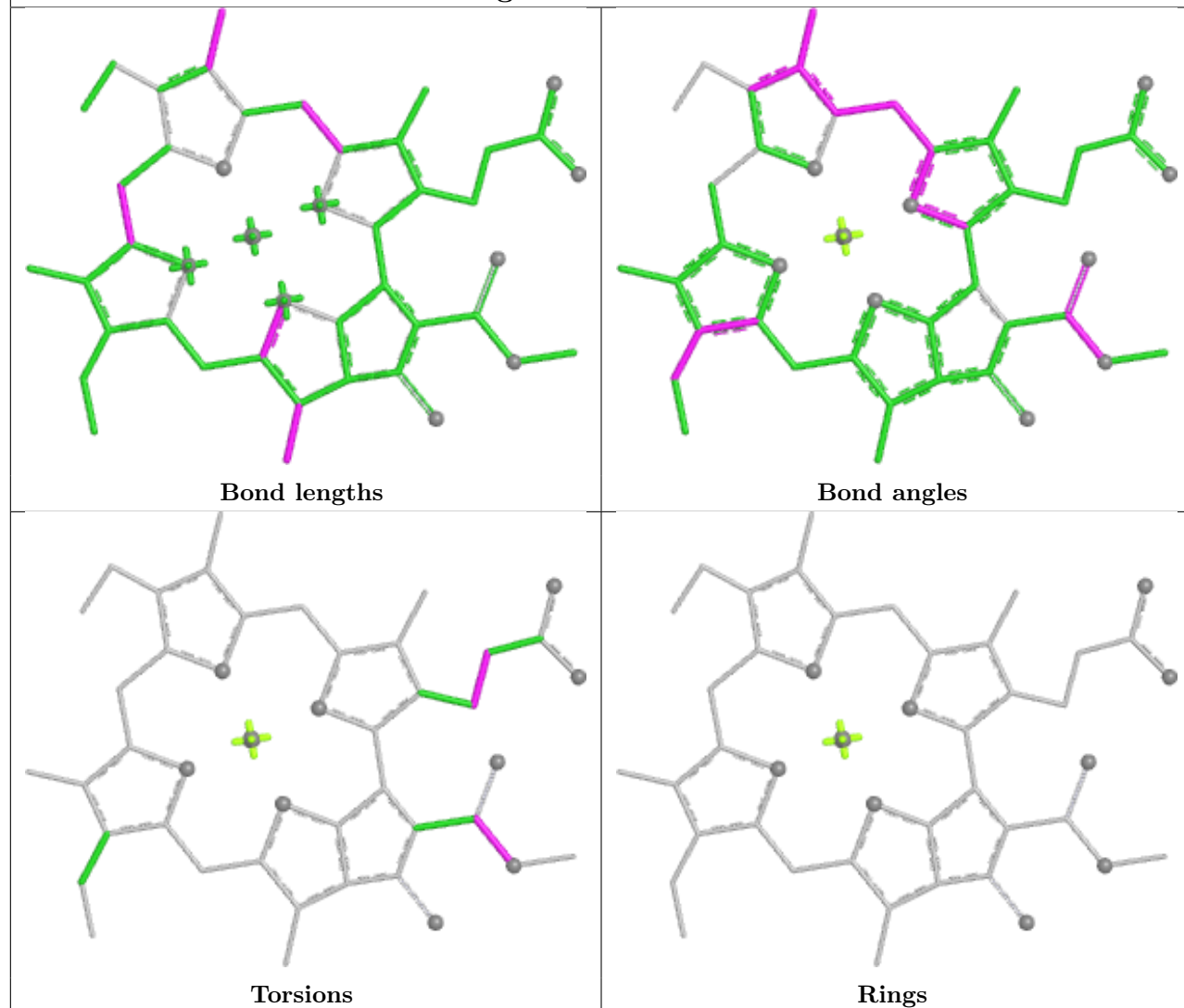


Torsions

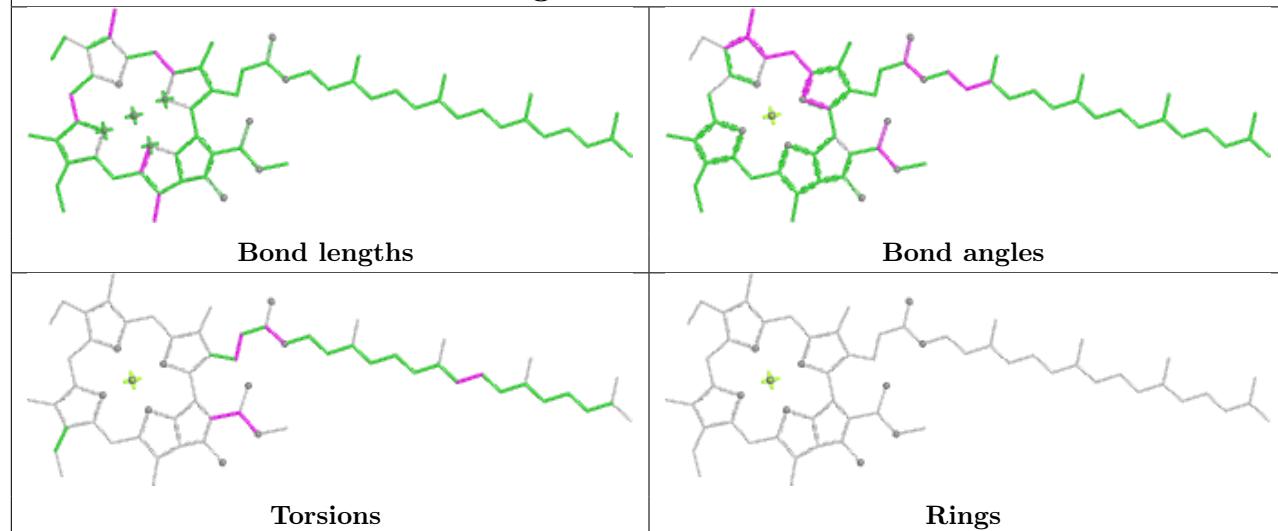


Rings

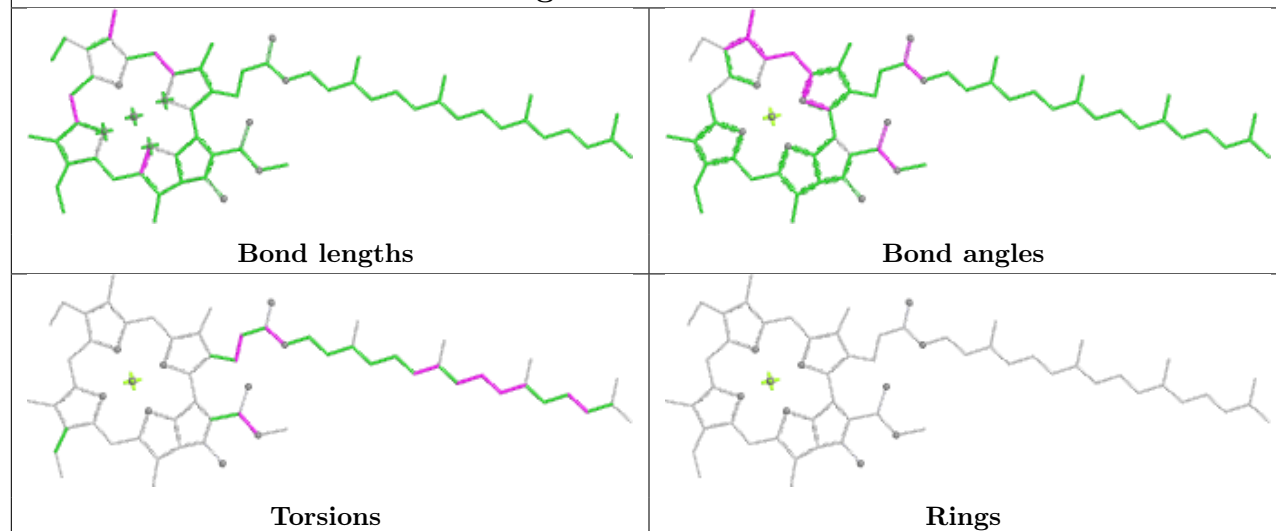
Ligand CLA a 305



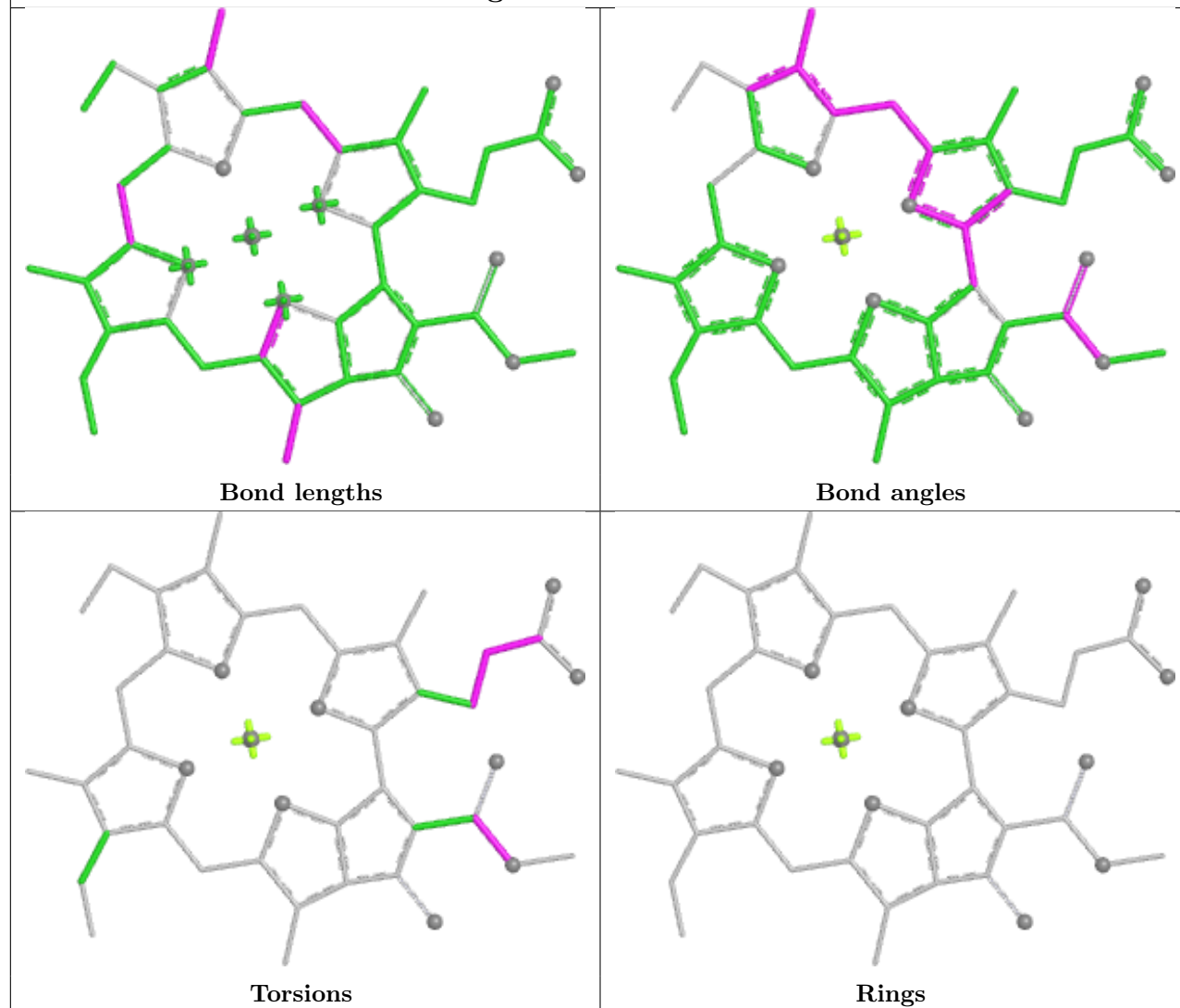
Ligand CLA B 828

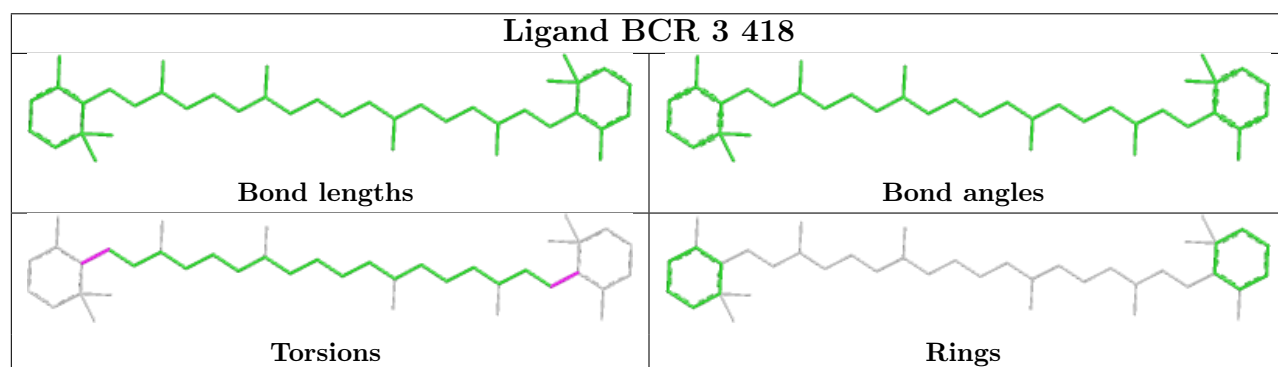
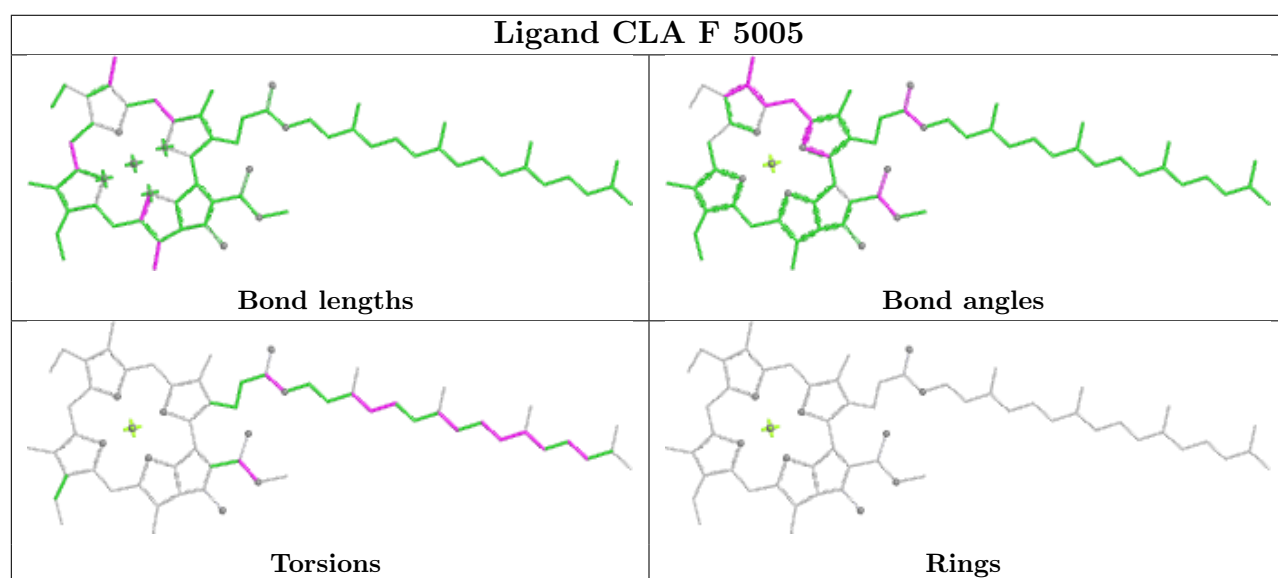
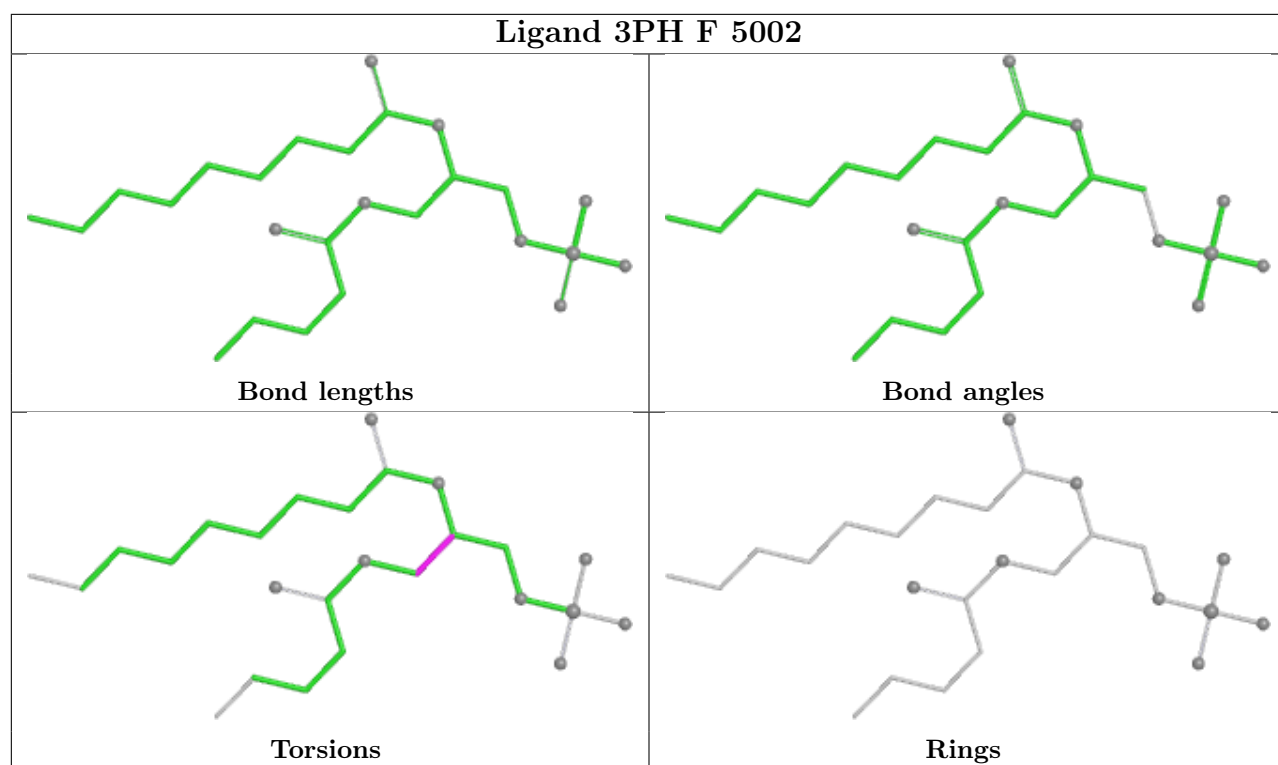


Ligand CLA a 302

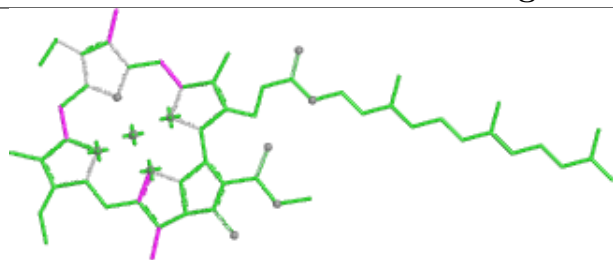


Ligand CLA J 5002

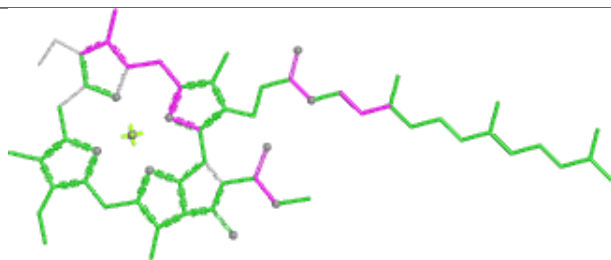




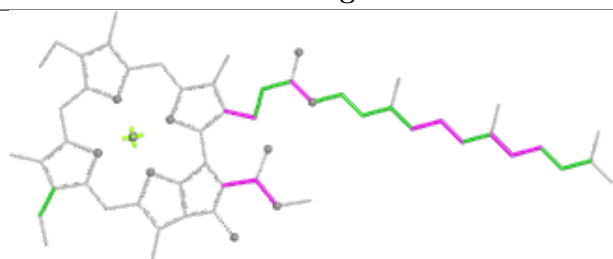
Ligand CLA 3 409



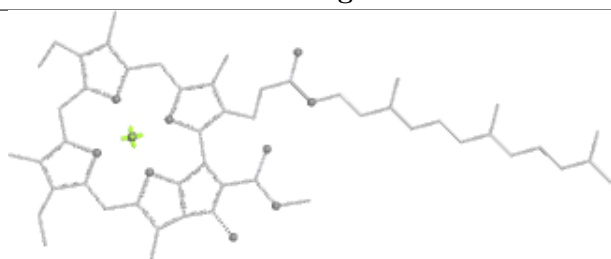
Bond lengths



Bond angles

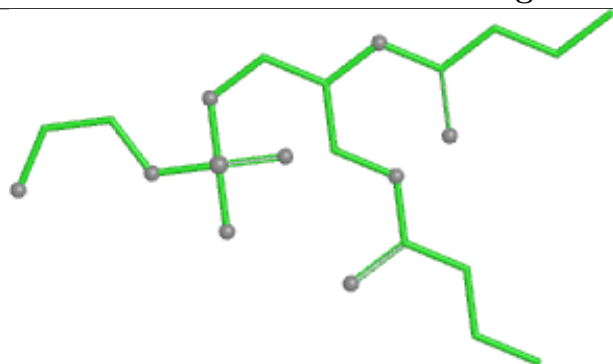


Torsions

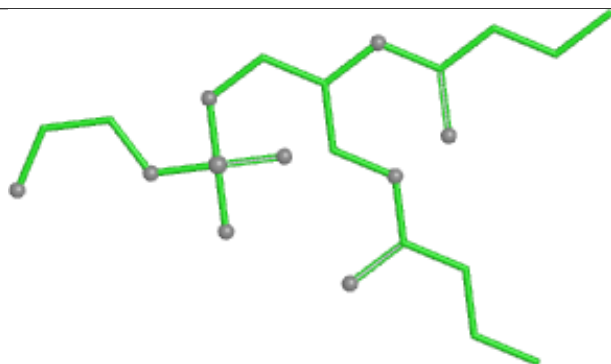


Rings

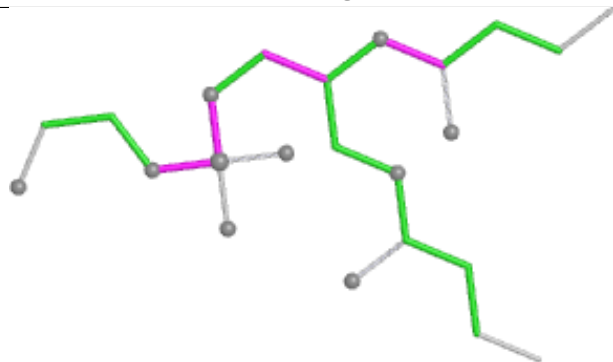
Ligand LHG b 303



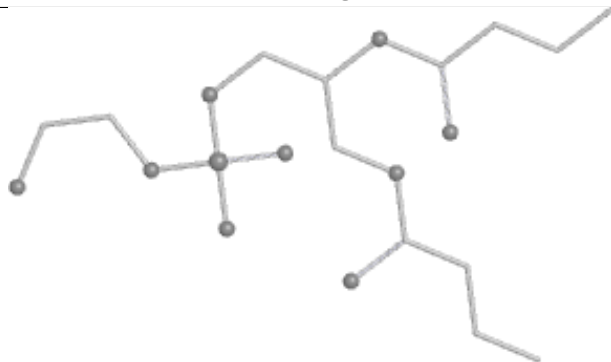
Bond lengths



Bond angles

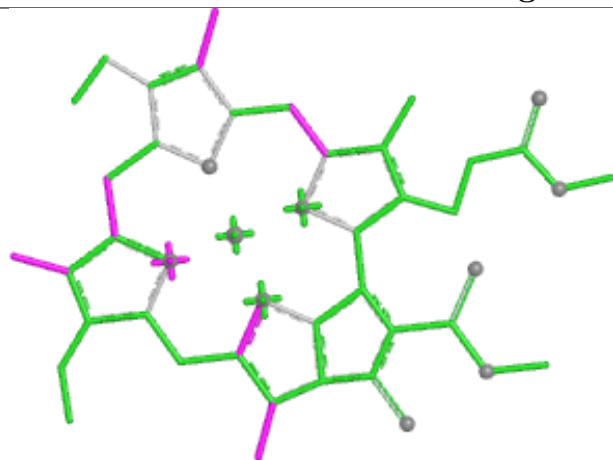


Torsions

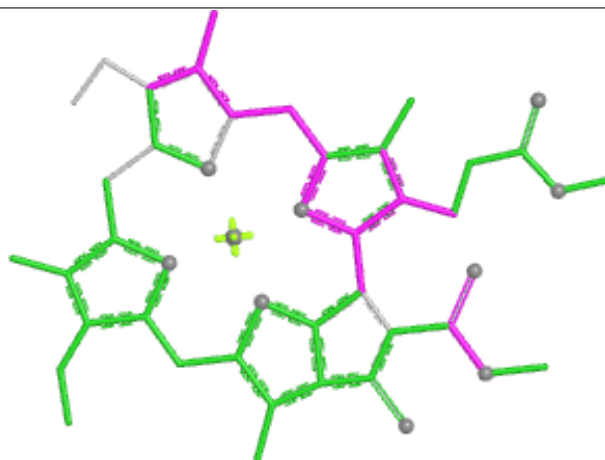


Rings

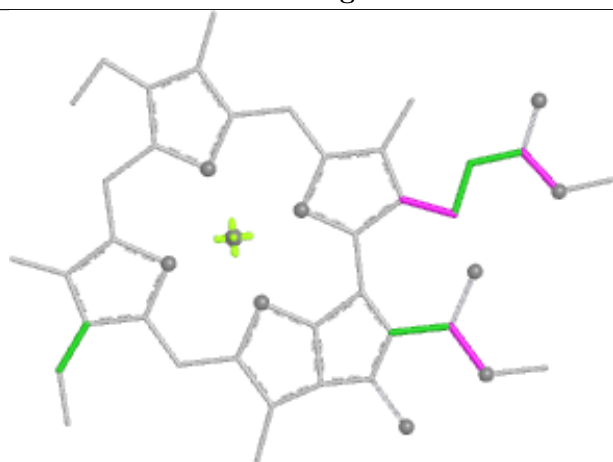
Ligand CLA 1 310



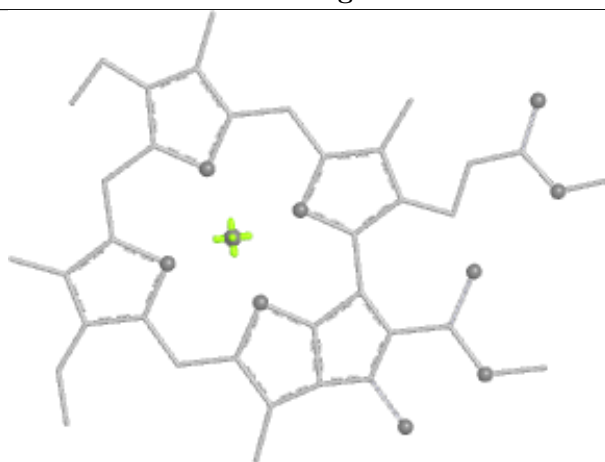
Bond lengths



Bond angles

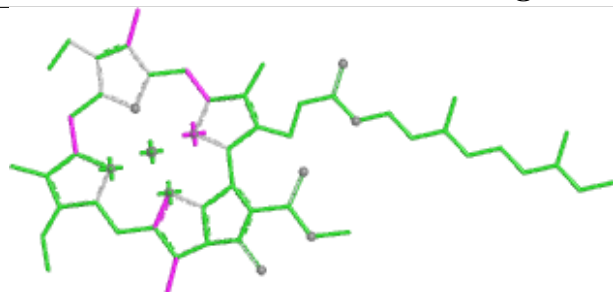


Torsions

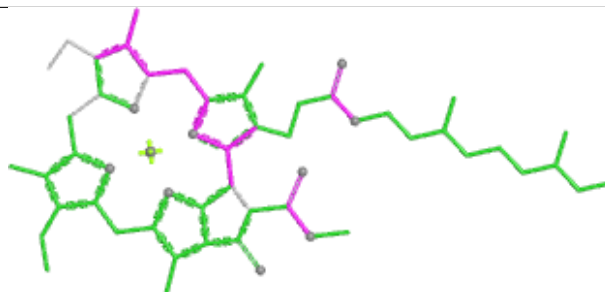


Rings

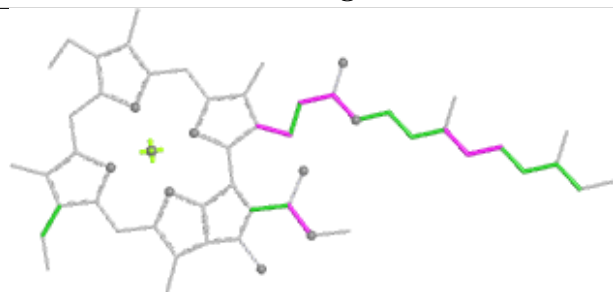
Ligand CLA T 603



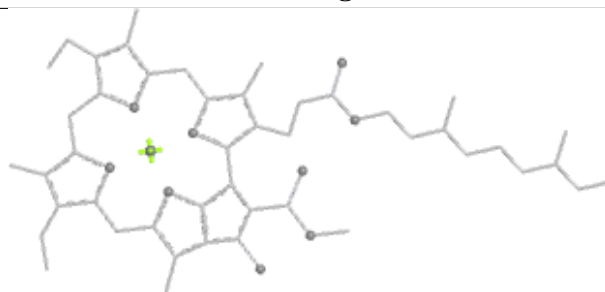
Bond lengths



Bond angles

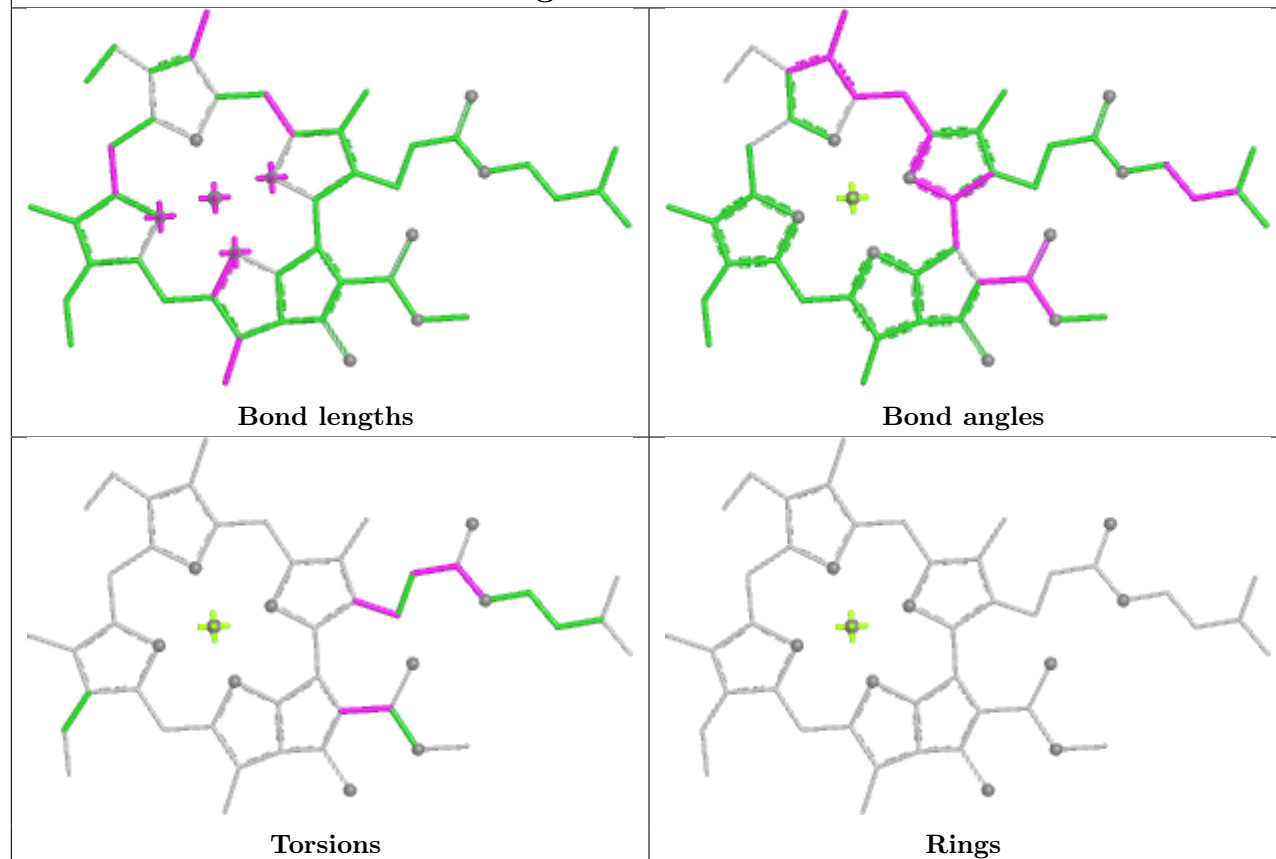


Torsions

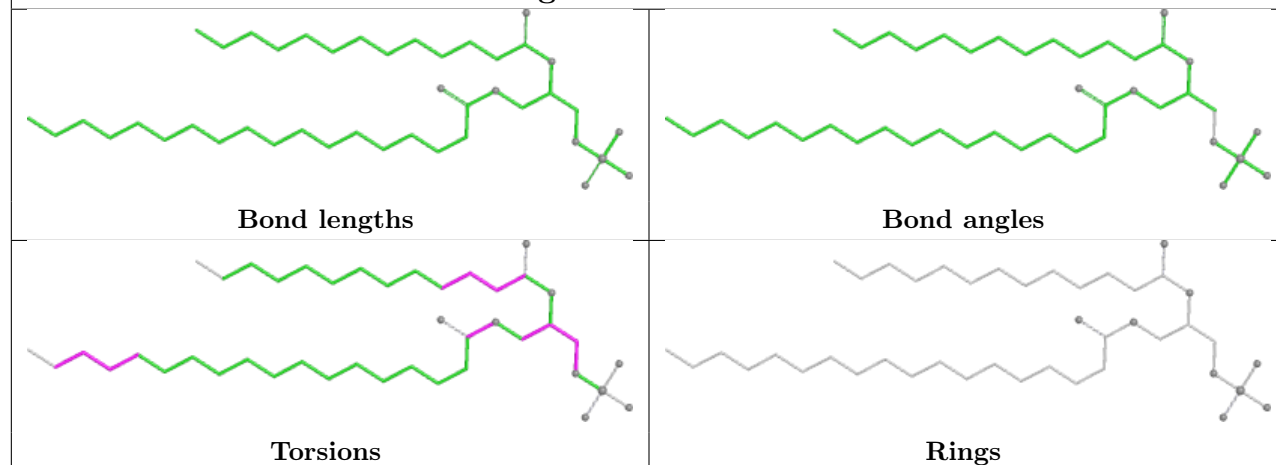


Rings

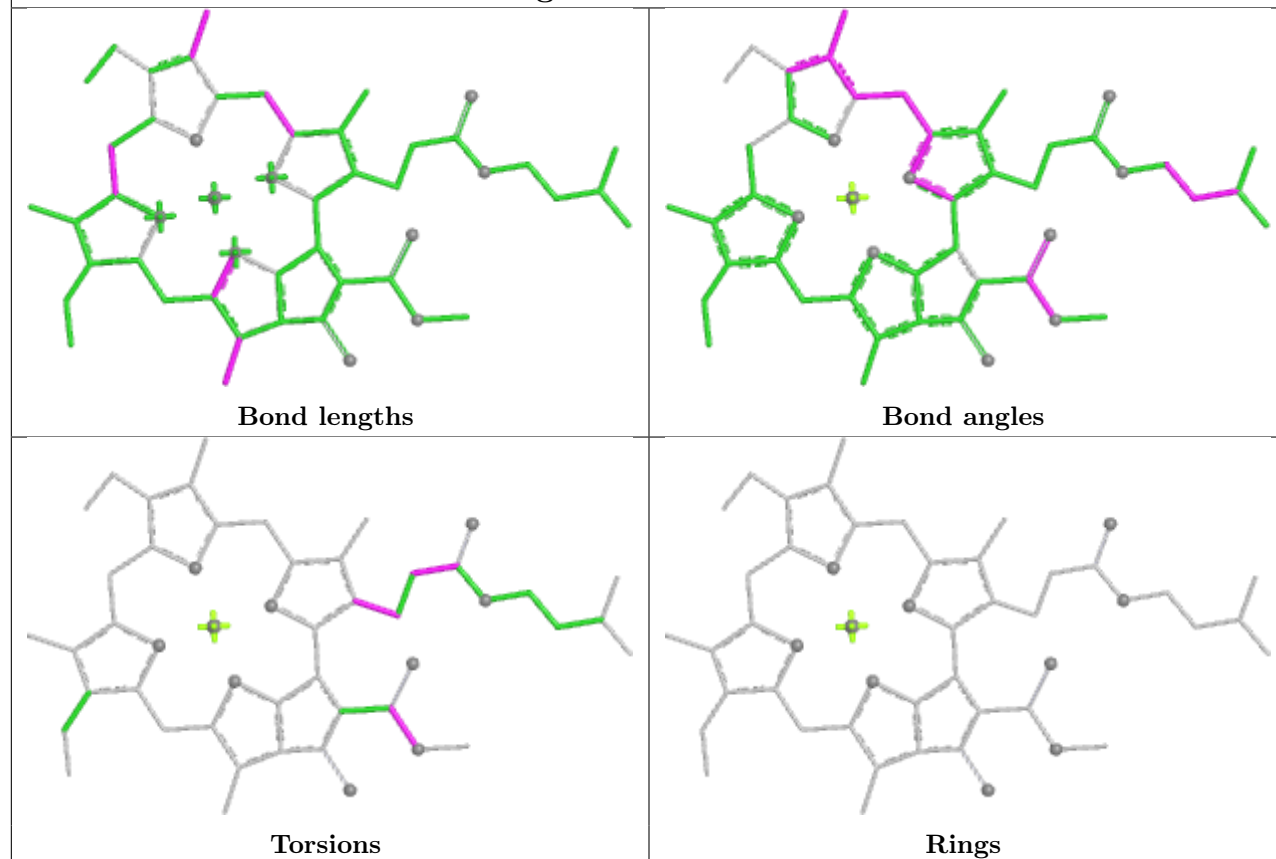
Ligand CLA 8 612



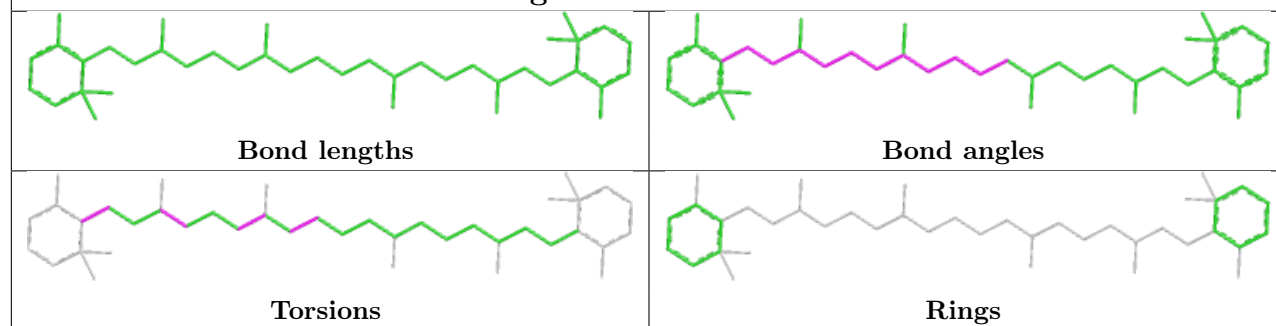
Ligand 3PH 2 619



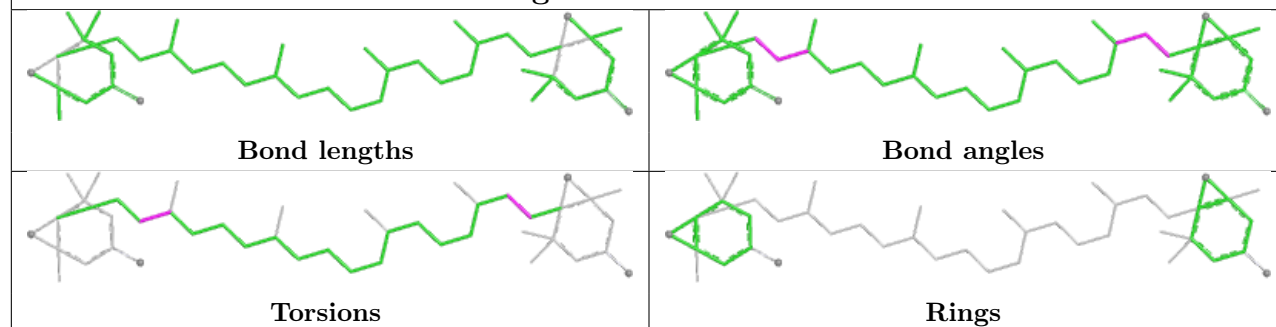
Ligand CLA 9 604

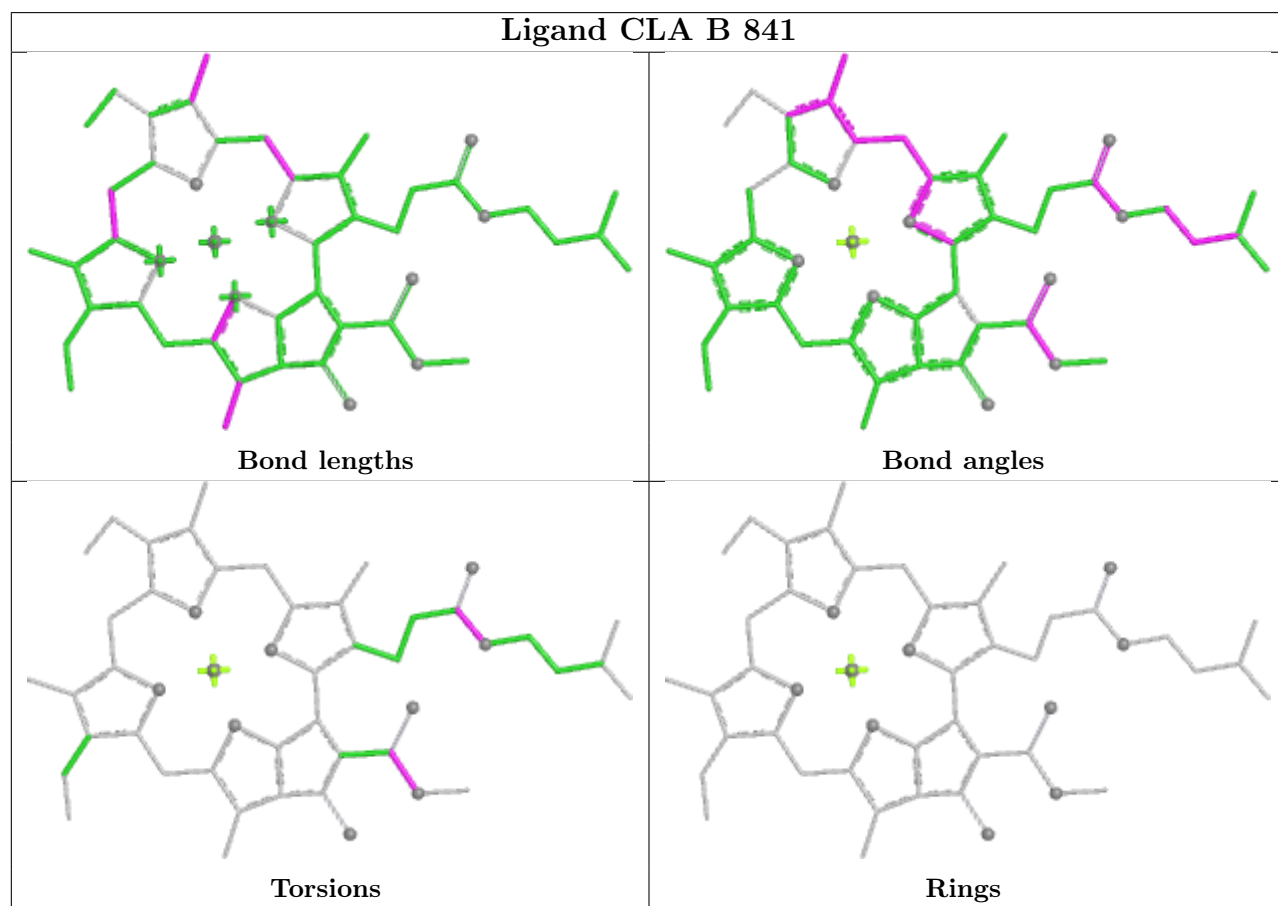
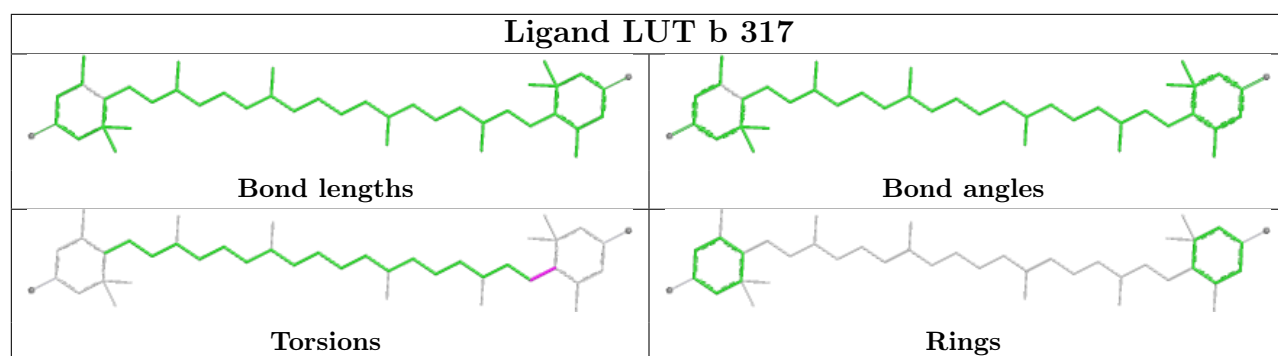


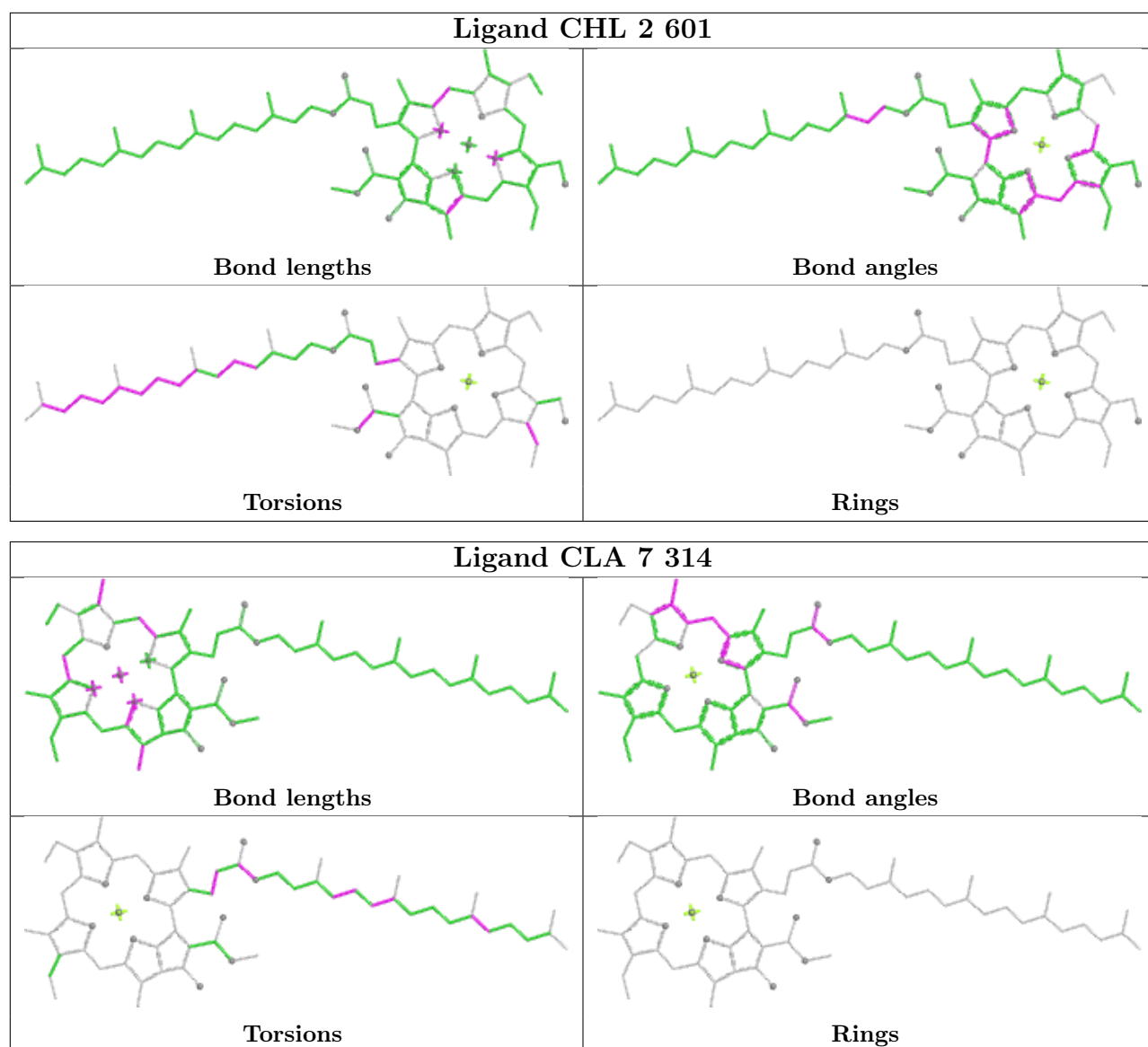
Ligand BCR A 846



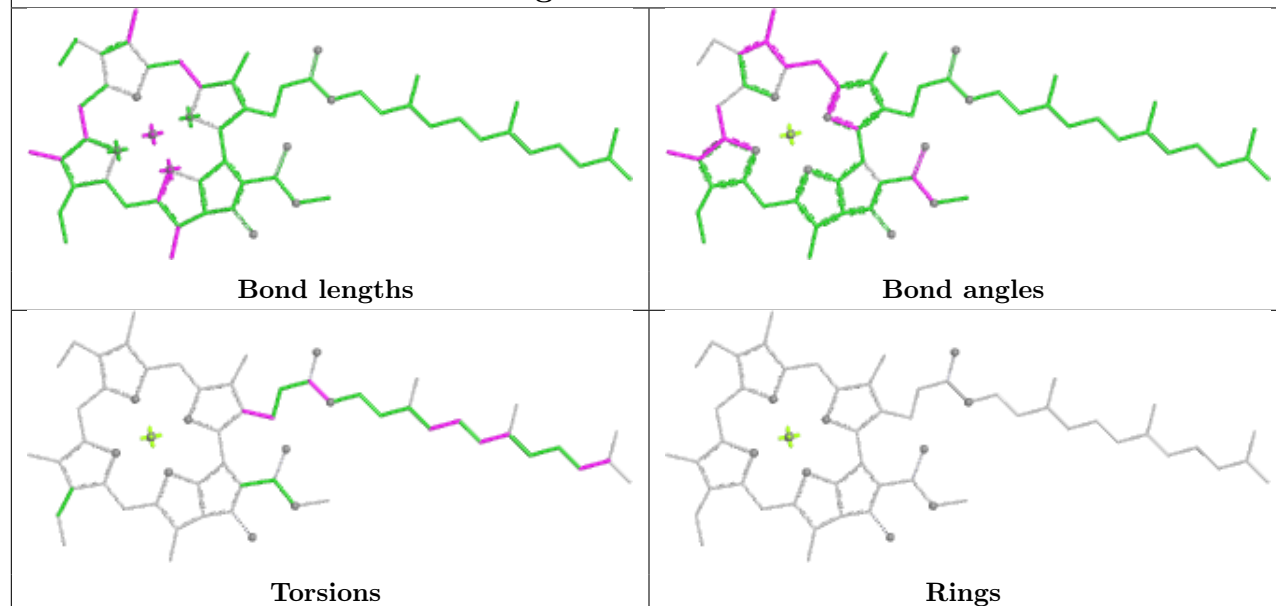
Ligand XAT T 616



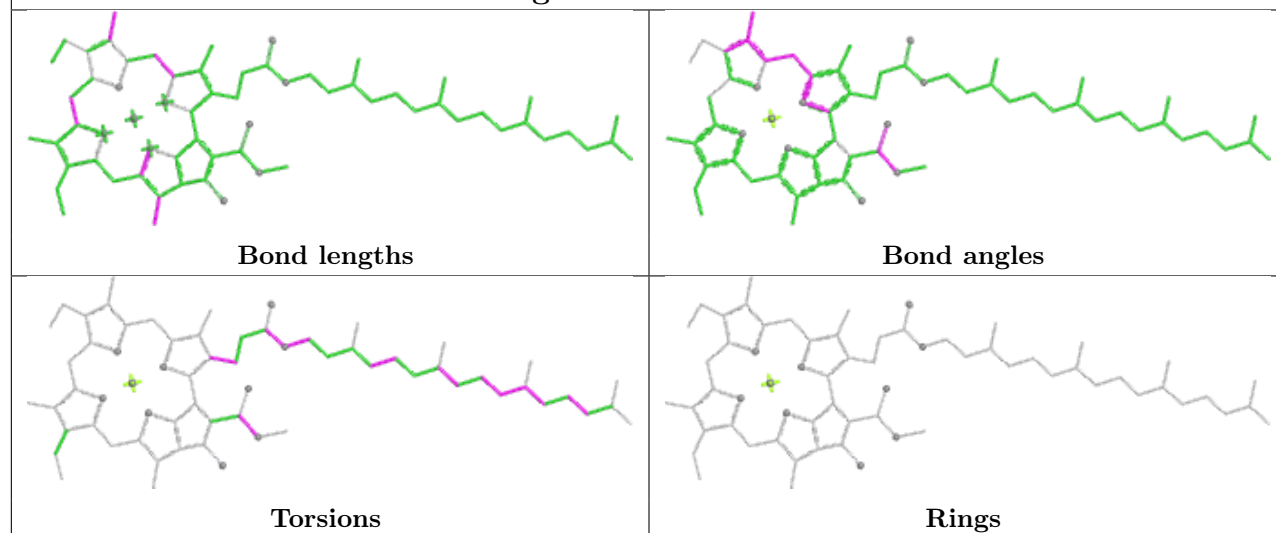




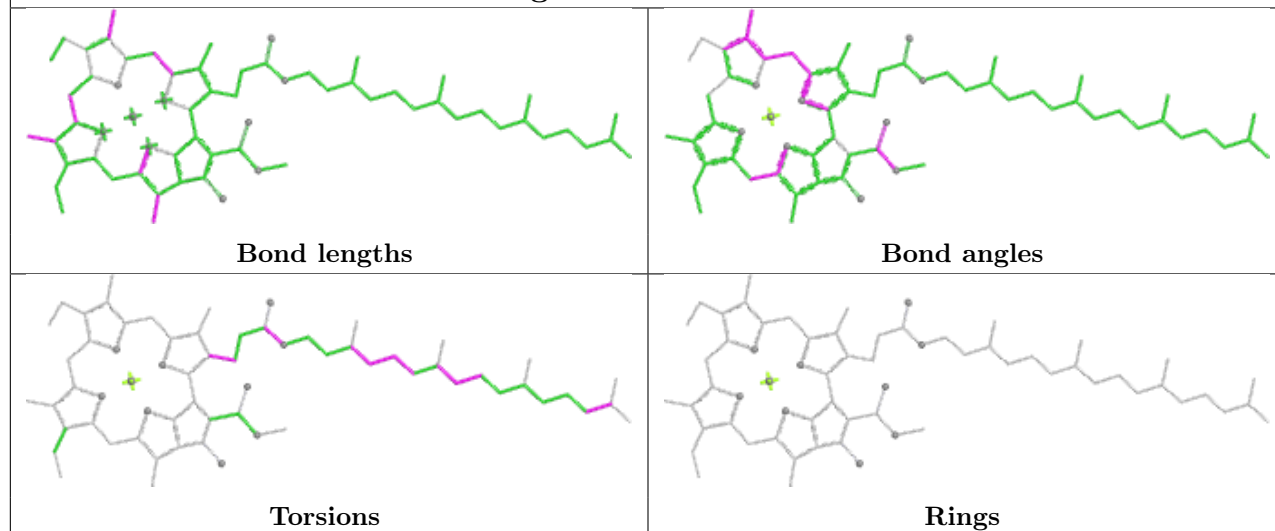
Ligand CLA b 311



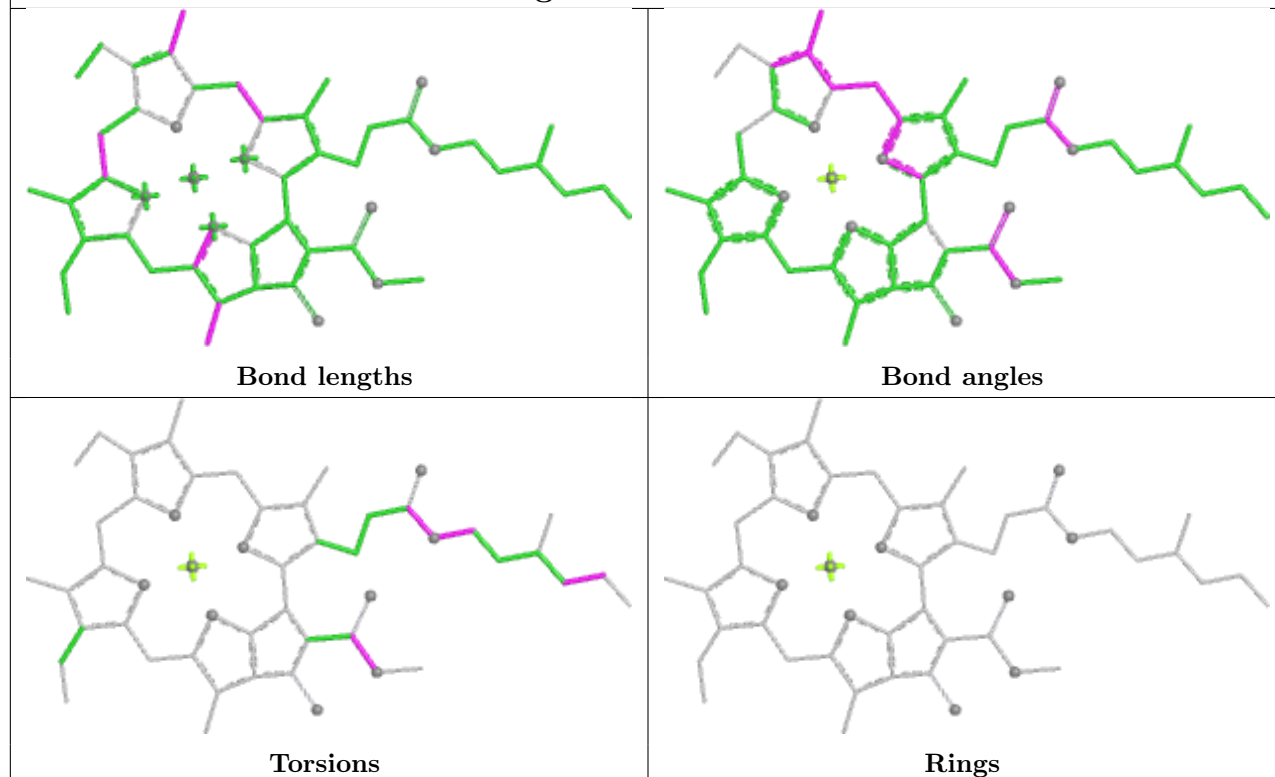
Ligand CLA B 821



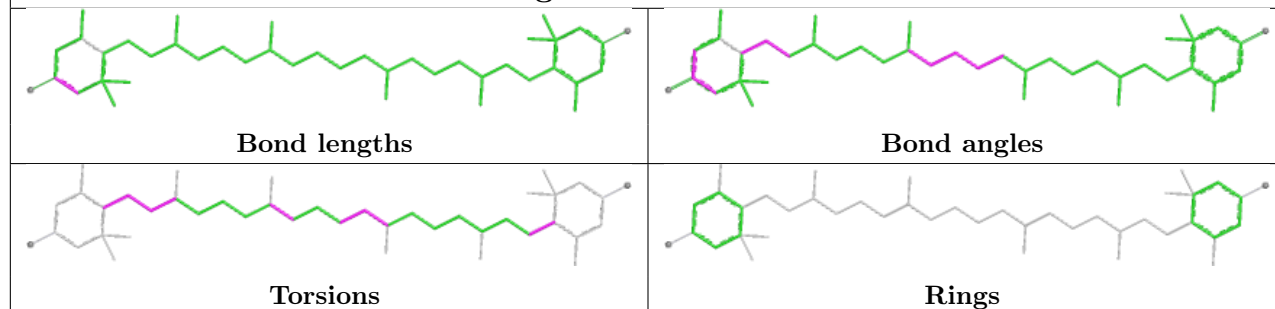
Ligand CLA A 807

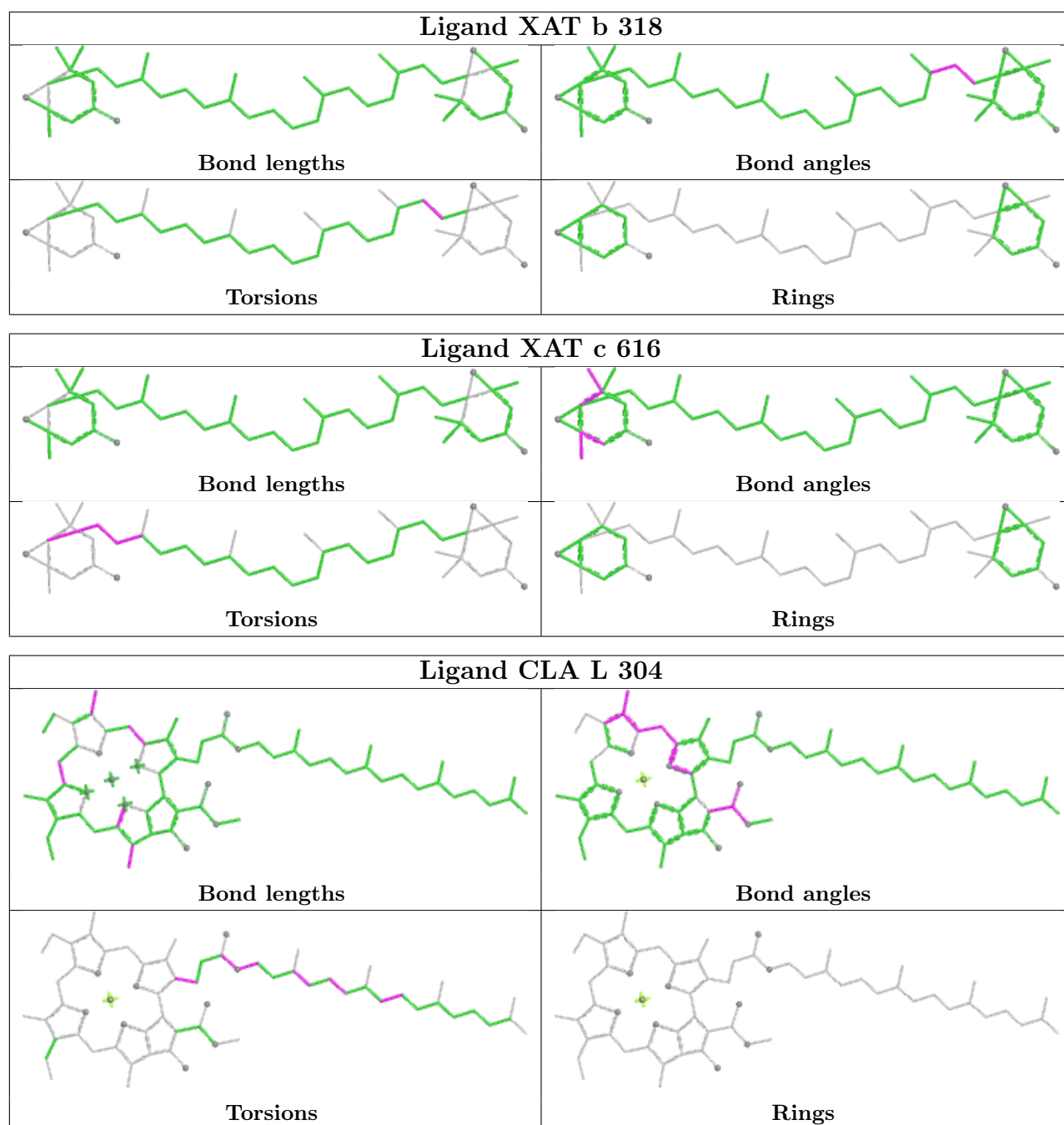


Ligand CLA 7 313

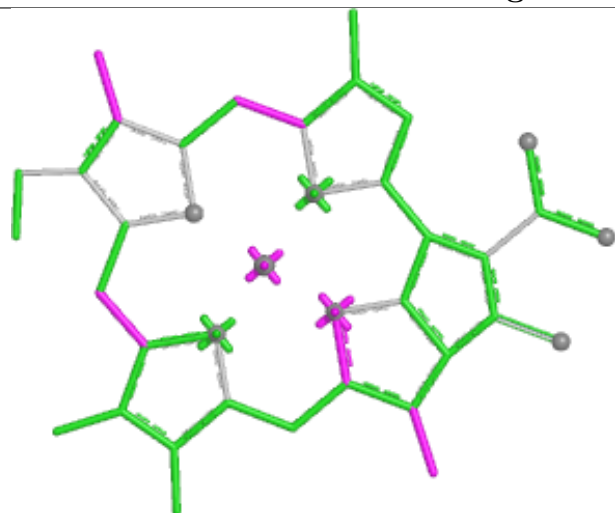


Ligand LUT 1 314

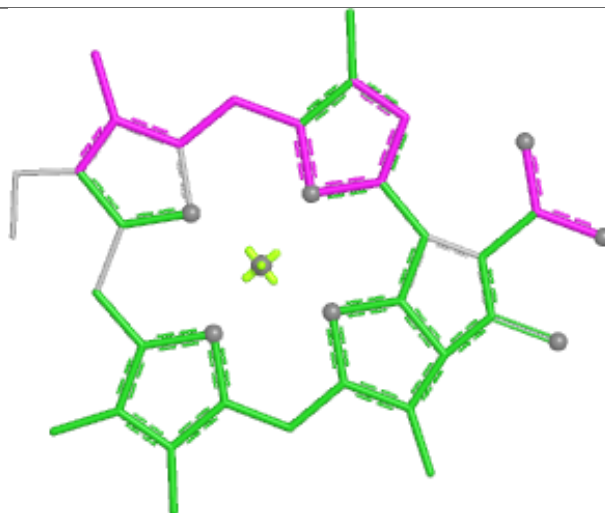




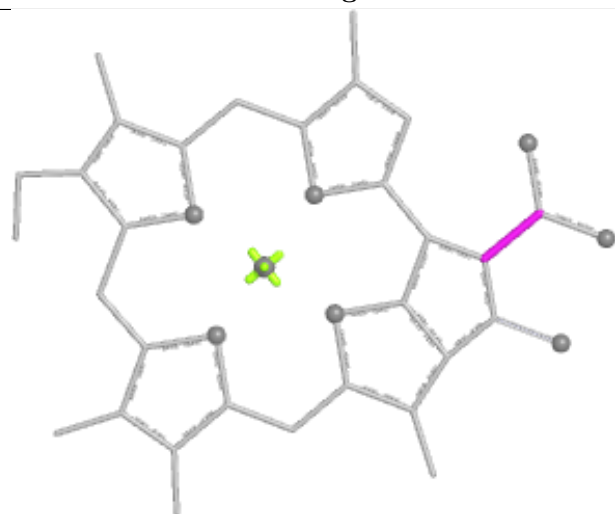
Ligand CLA O 2001



Bond lengths



Bond angles

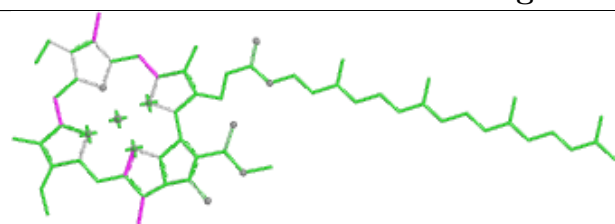


Torsions

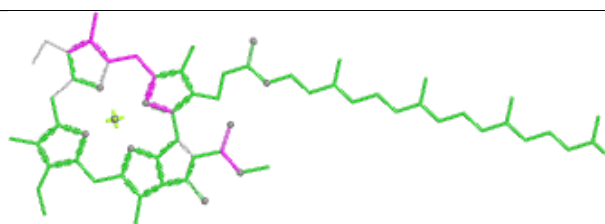


Rings

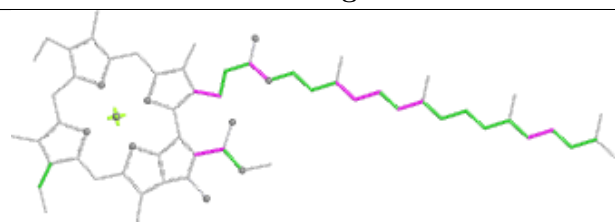
Ligand CLA B 816



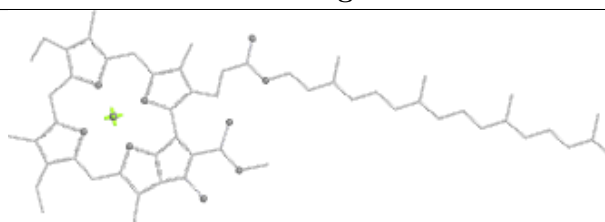
Bond lengths



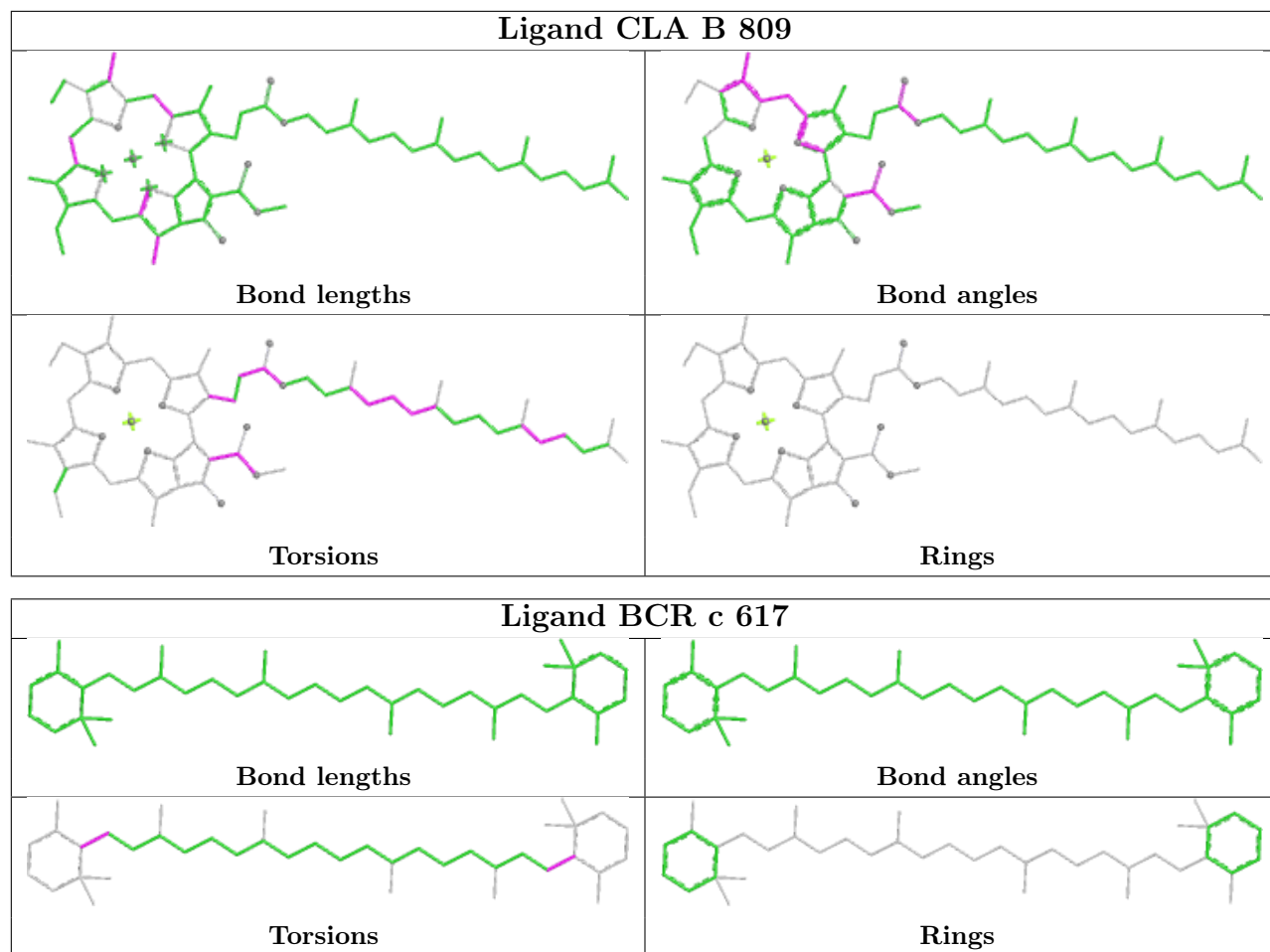
Bond angles



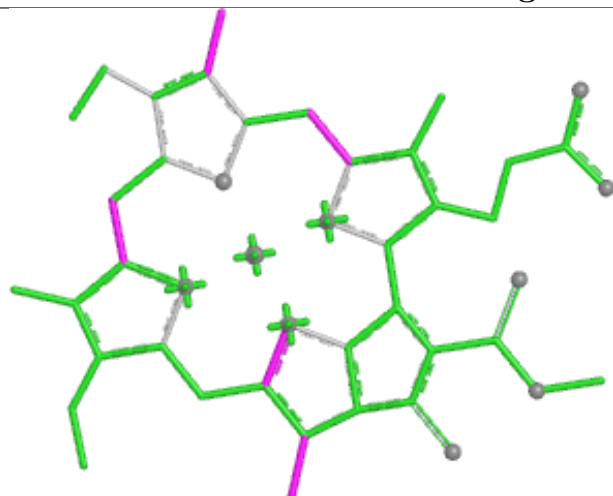
Torsions



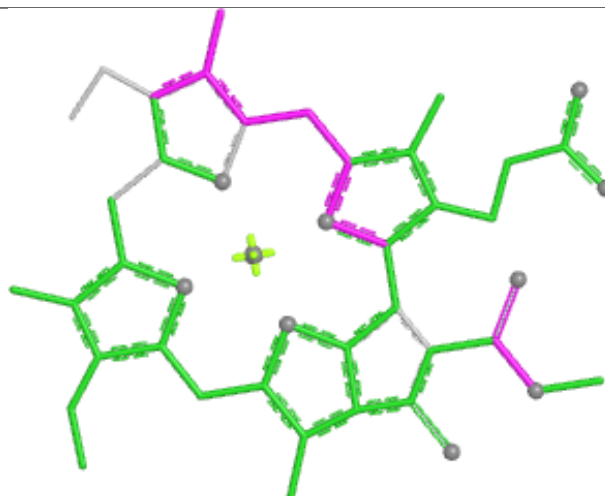
Rings



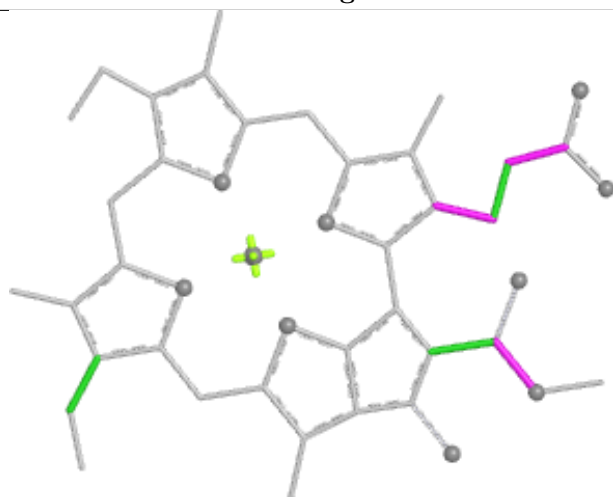
Ligand CLA 1 312



Bond lengths



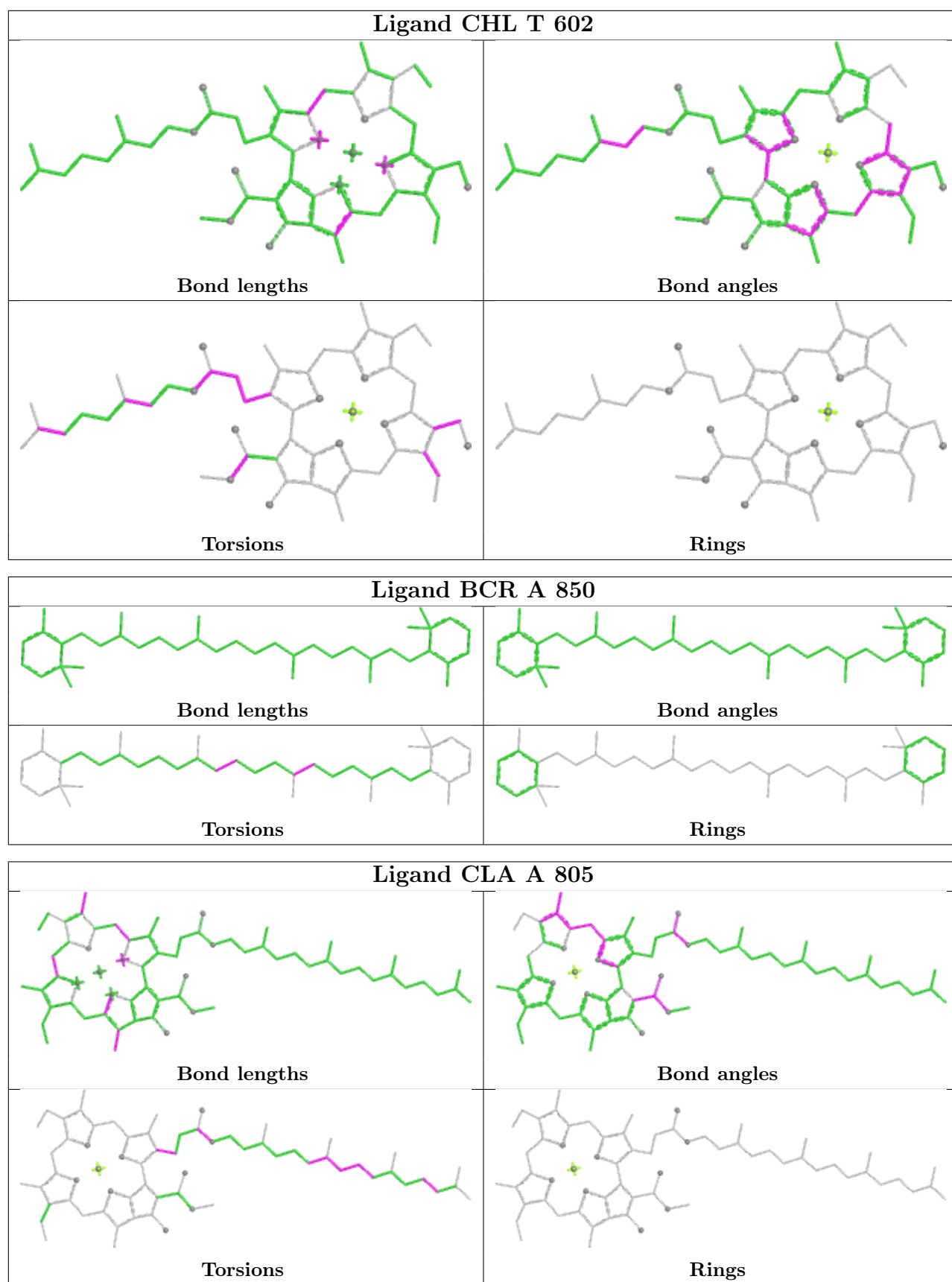
Bond angles

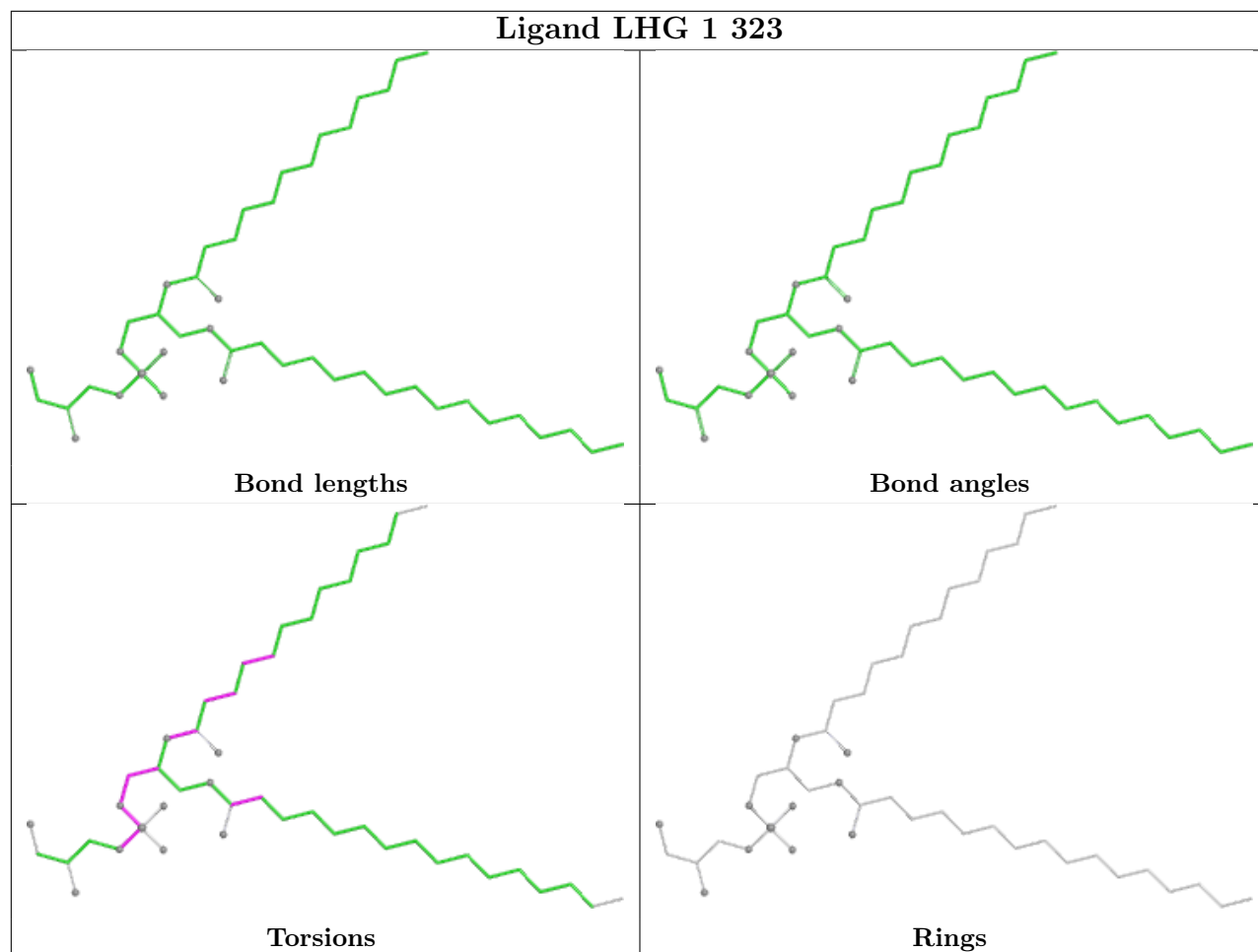
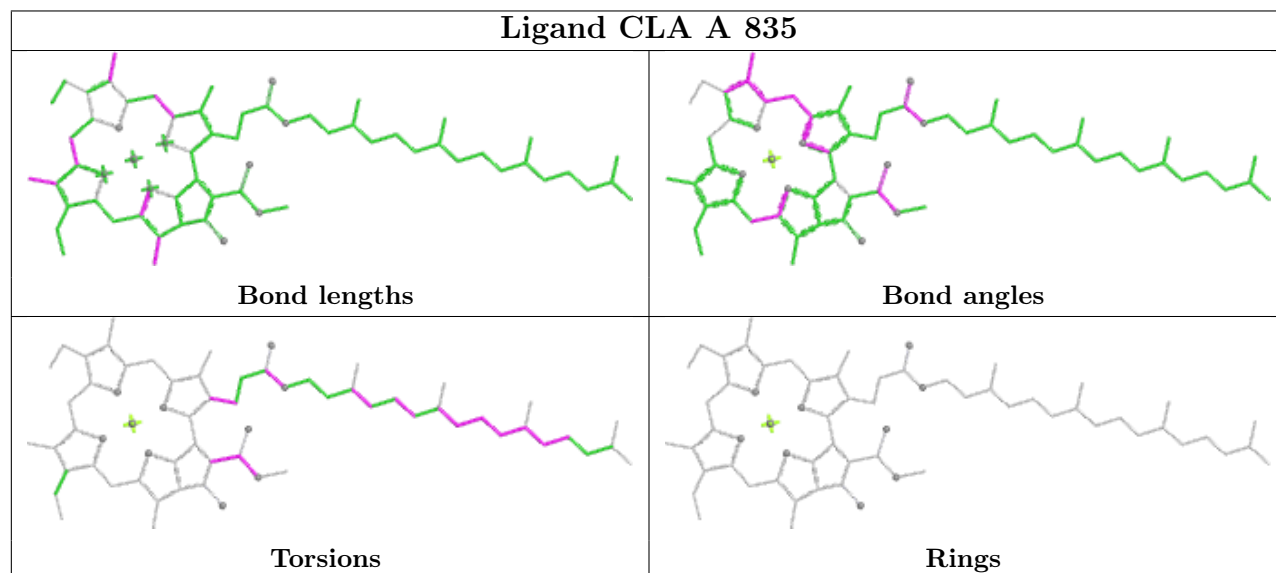


Torsions

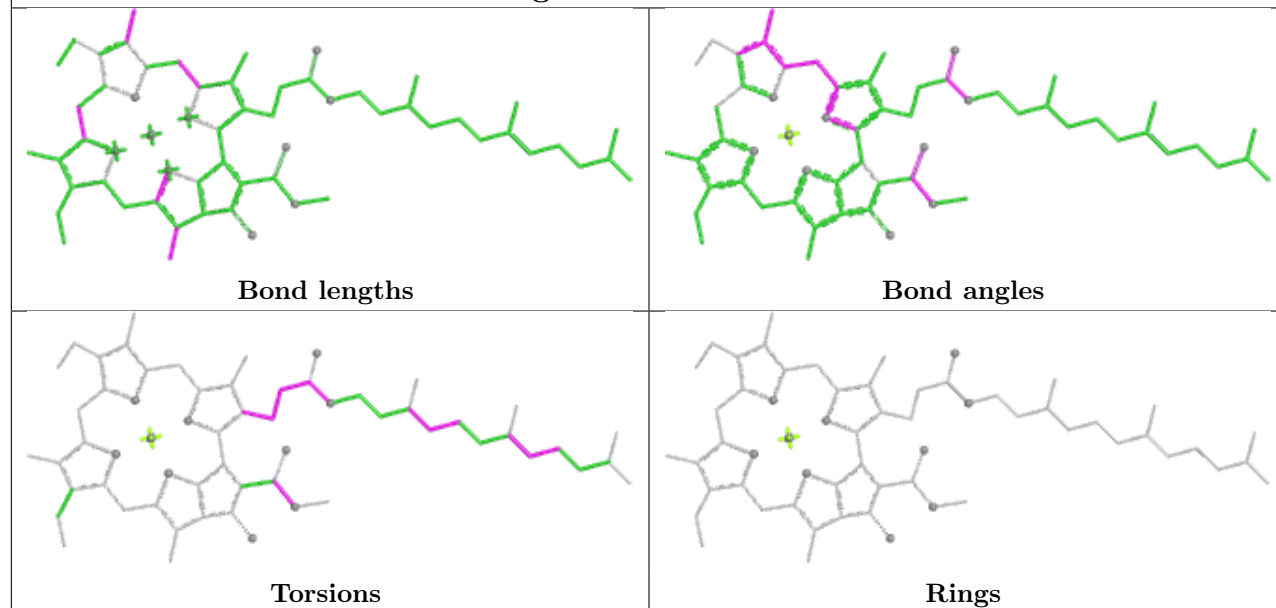


Rings

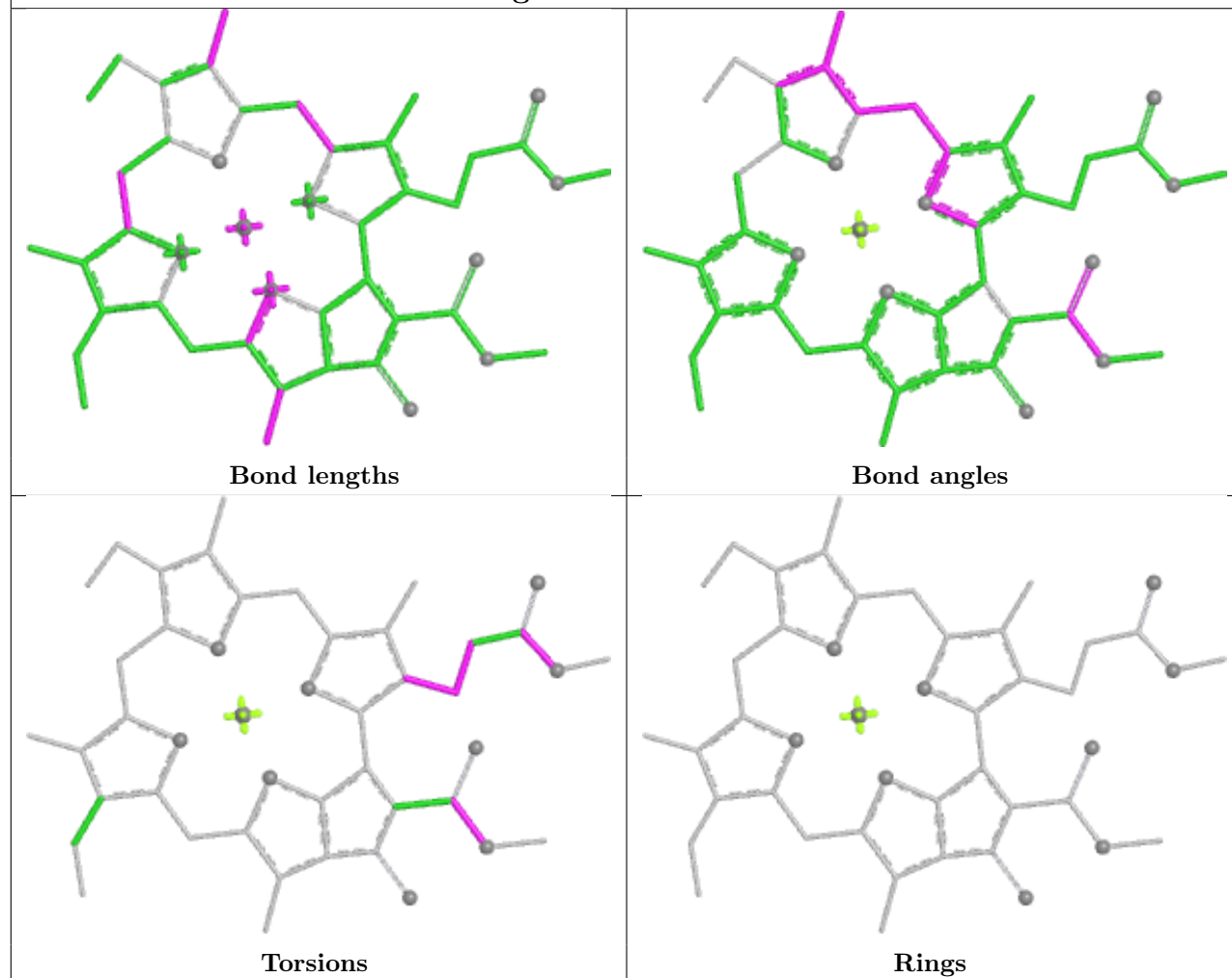


Ligand LHG 1 323**Ligand CLA A 835**

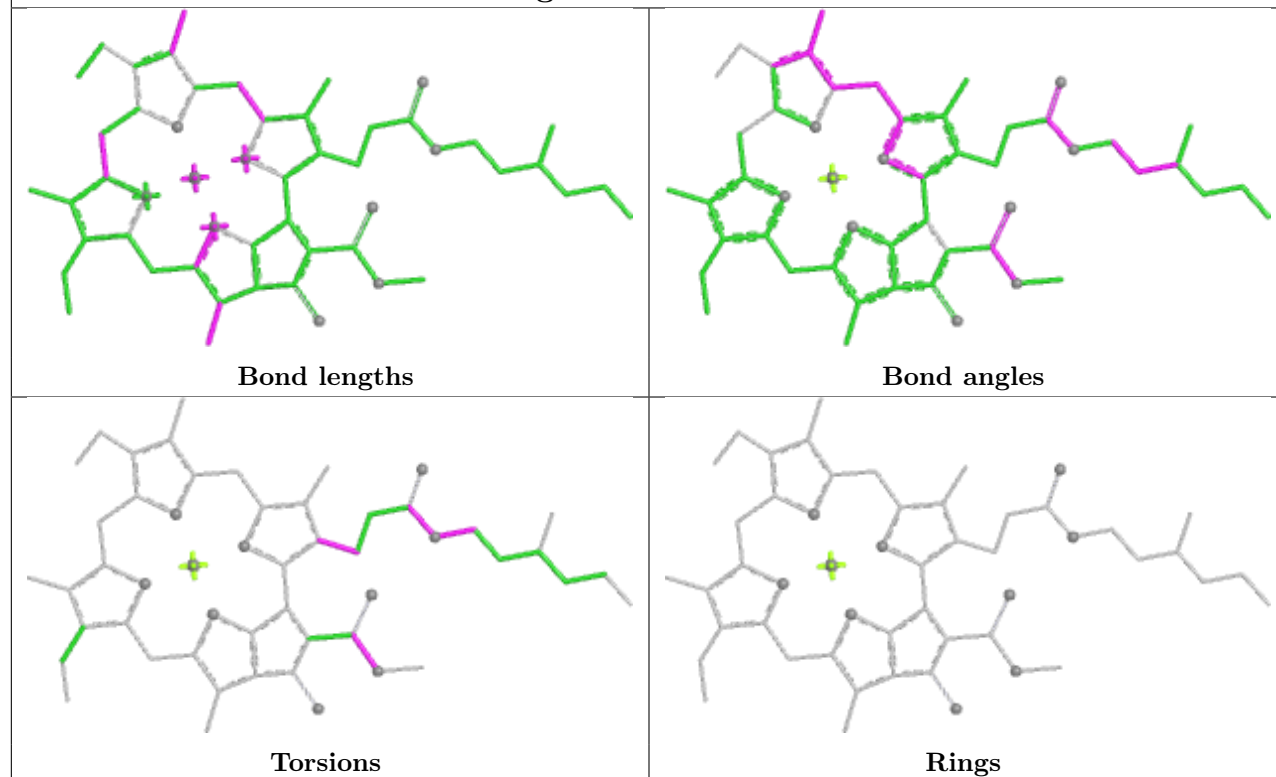
Ligand CLA B 830



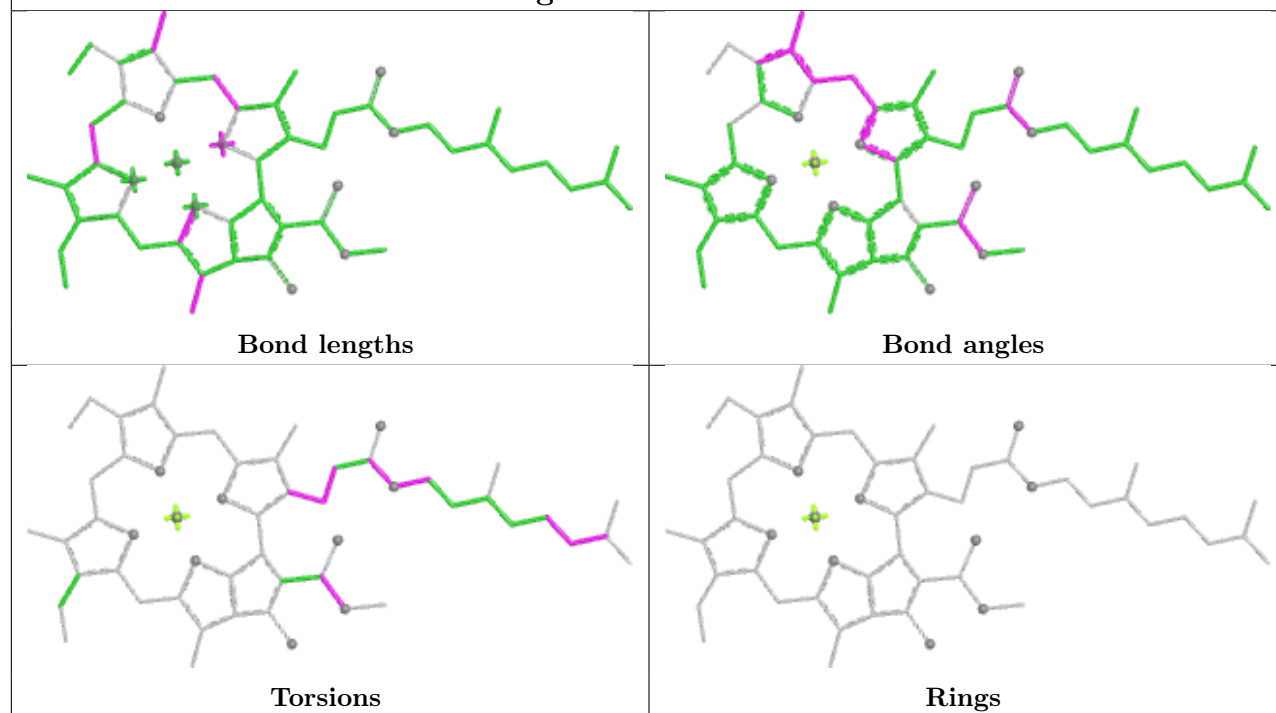
Ligand CLA G 204

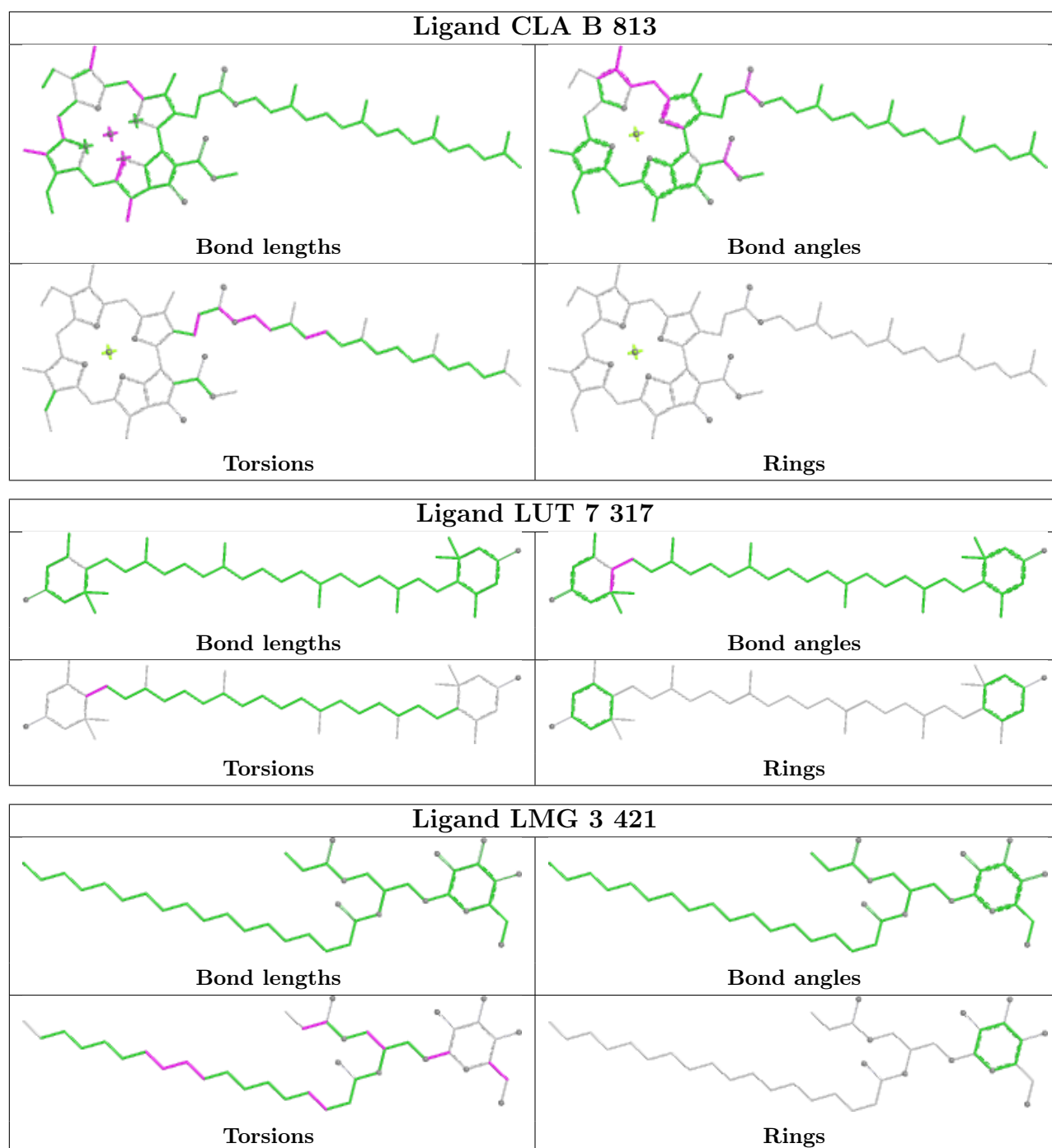


Ligand CLA 3 410

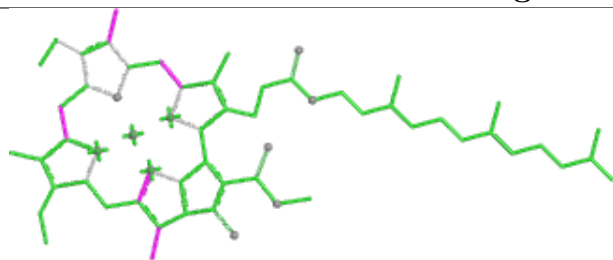


Ligand CLA 7 305

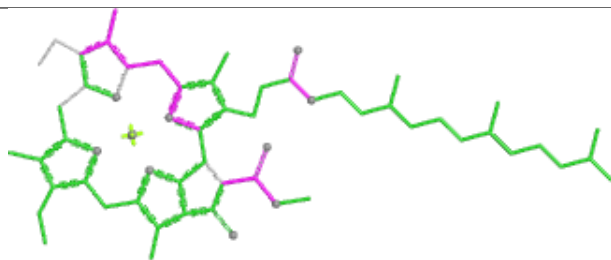




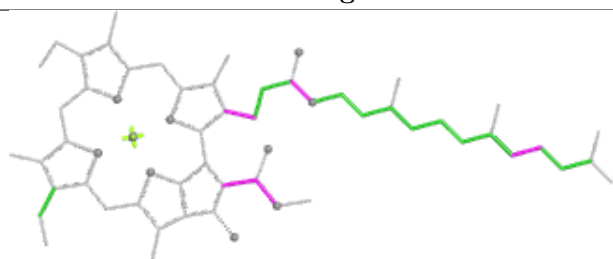
Ligand CLA A 806



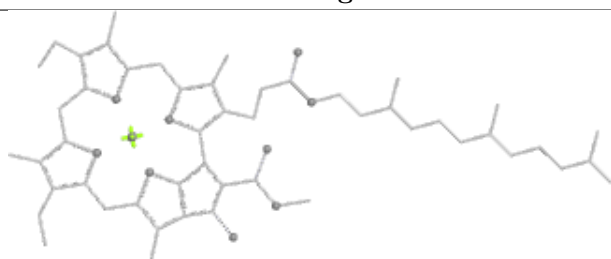
Bond lengths



Bond angles

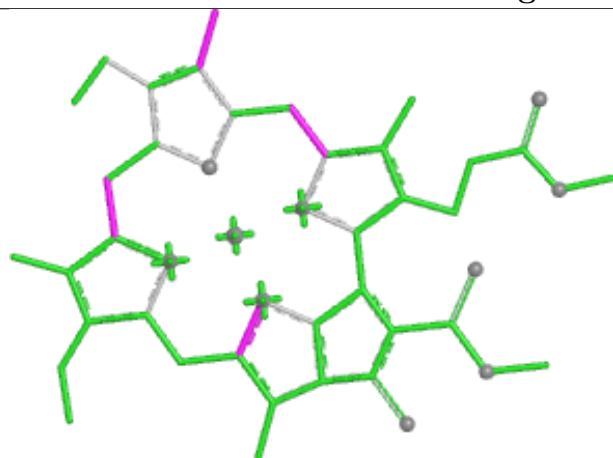


Torsions

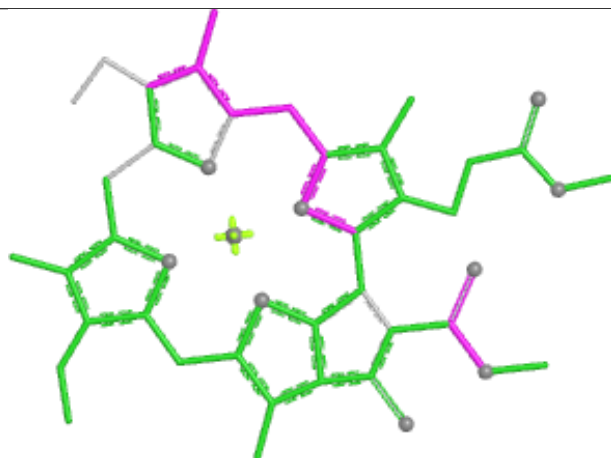


Rings

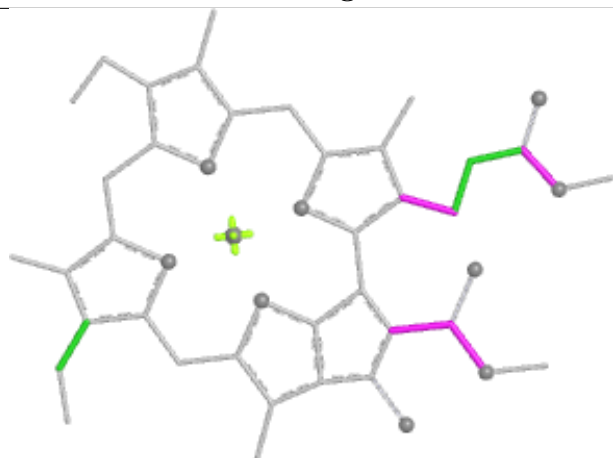
Ligand CLA 9 609



Bond lengths



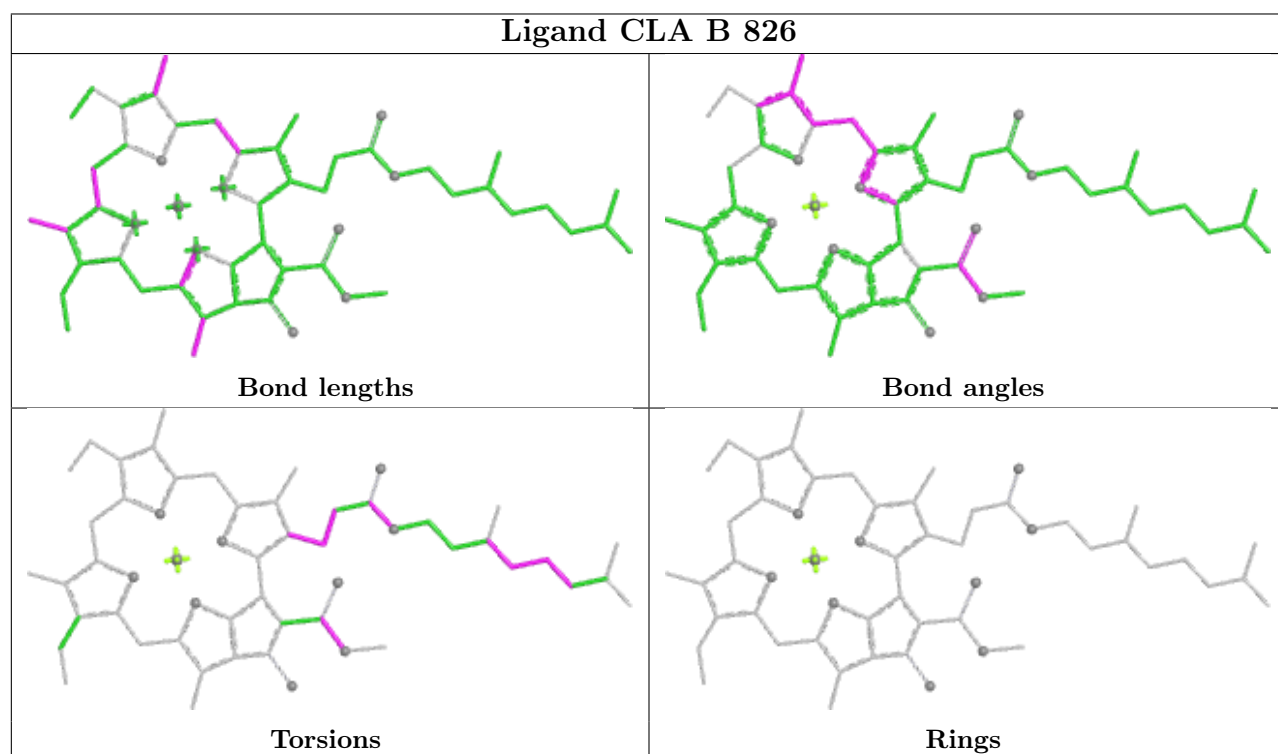
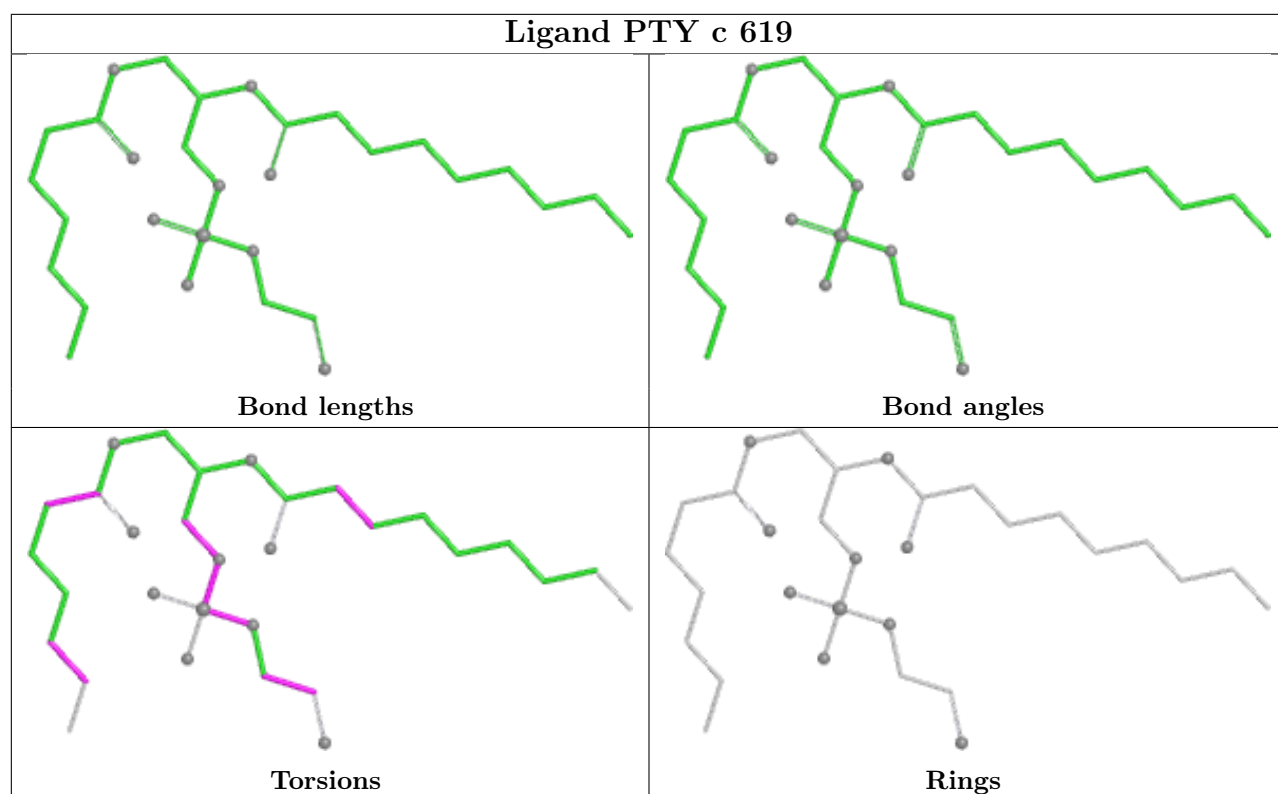
Bond angles



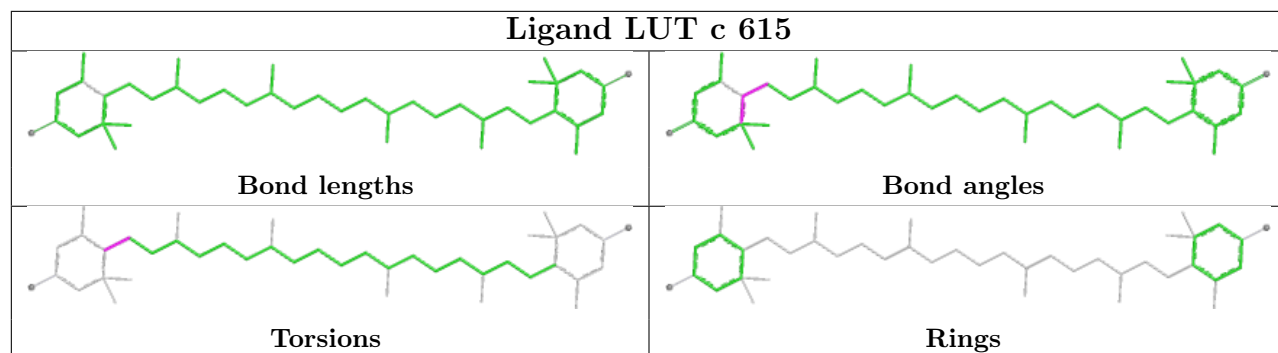
Torsions



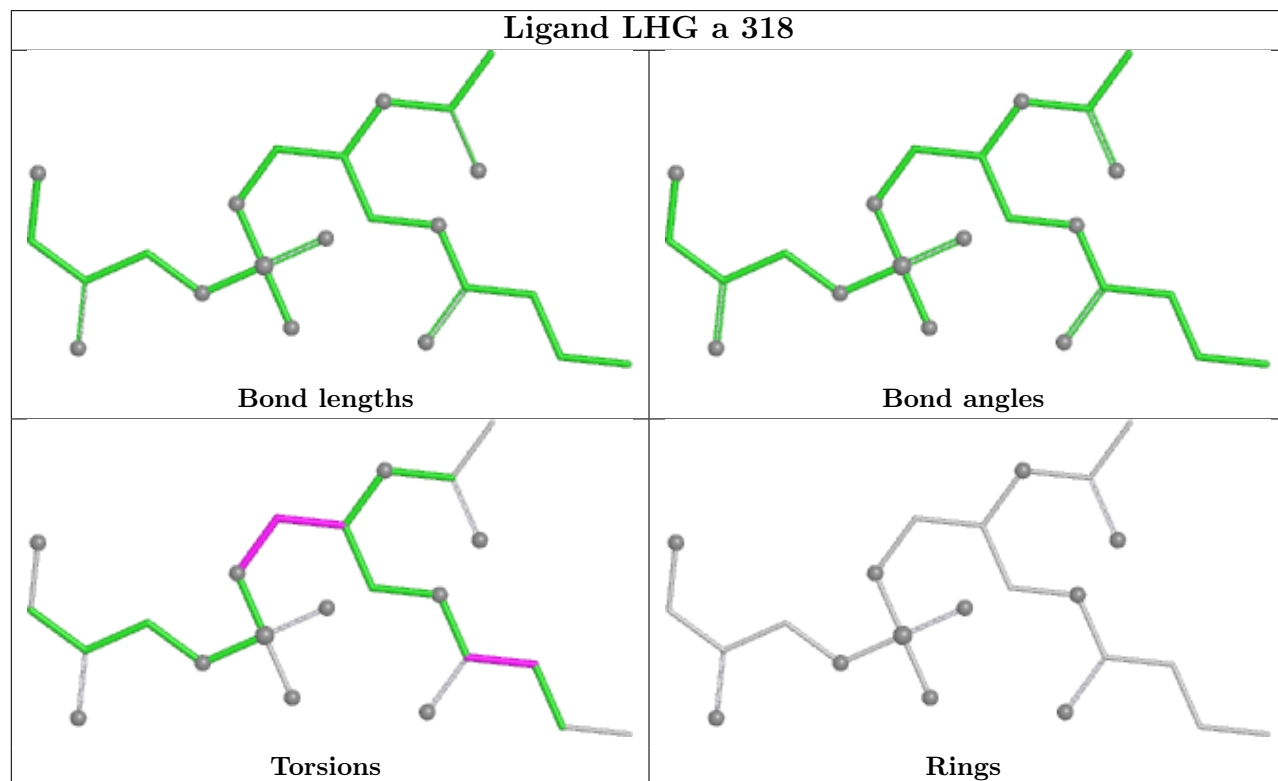
Rings



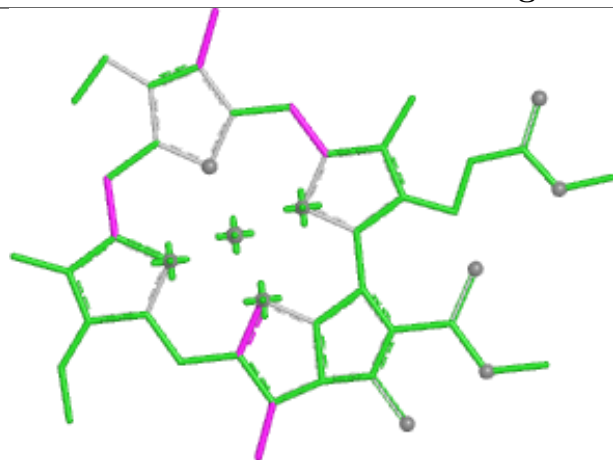
Ligand LUT c 615



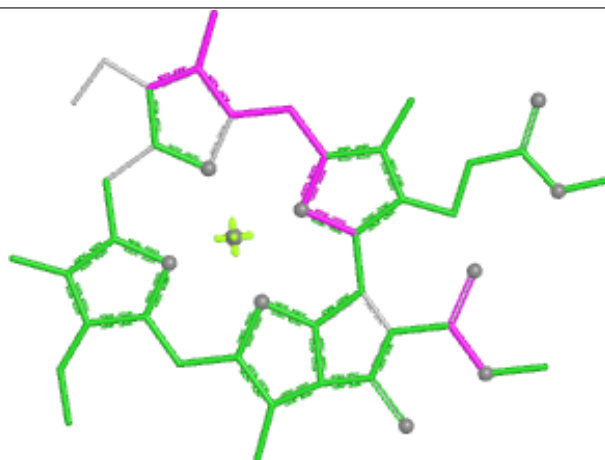
Ligand LHG a 318



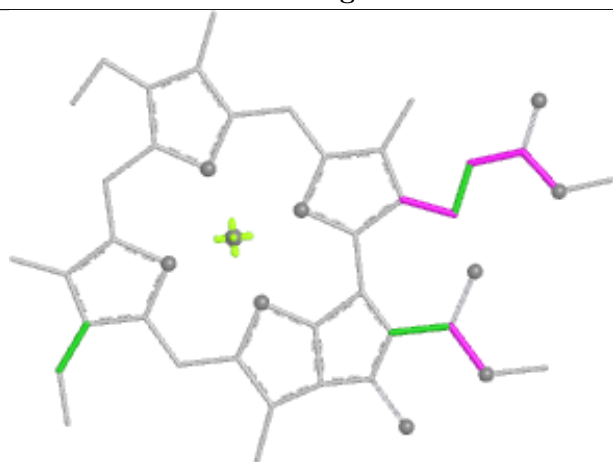
Ligand CLA a 313



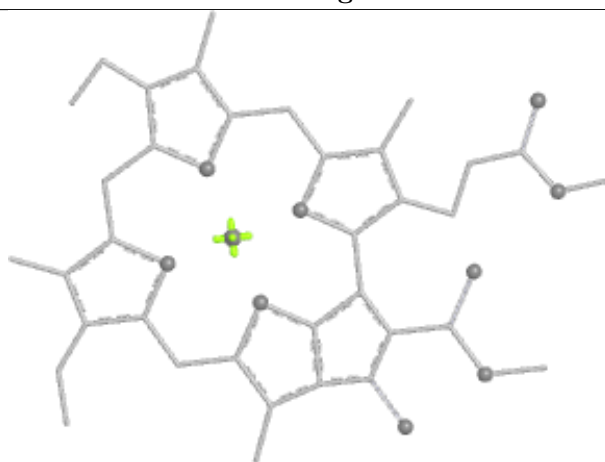
Bond lengths



Bond angles

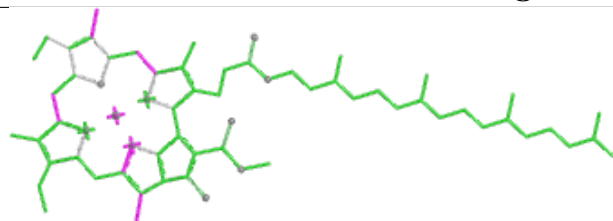


Torsions

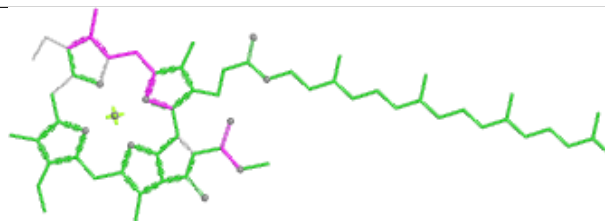


Rings

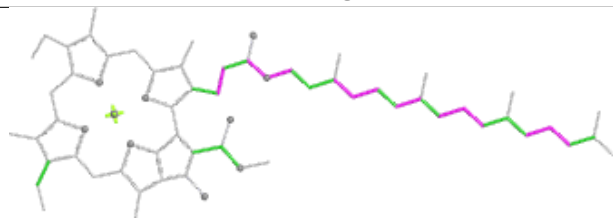
Ligand CLA B 844



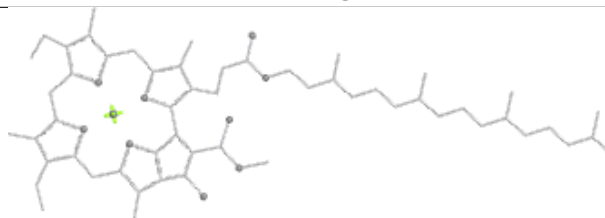
Bond lengths



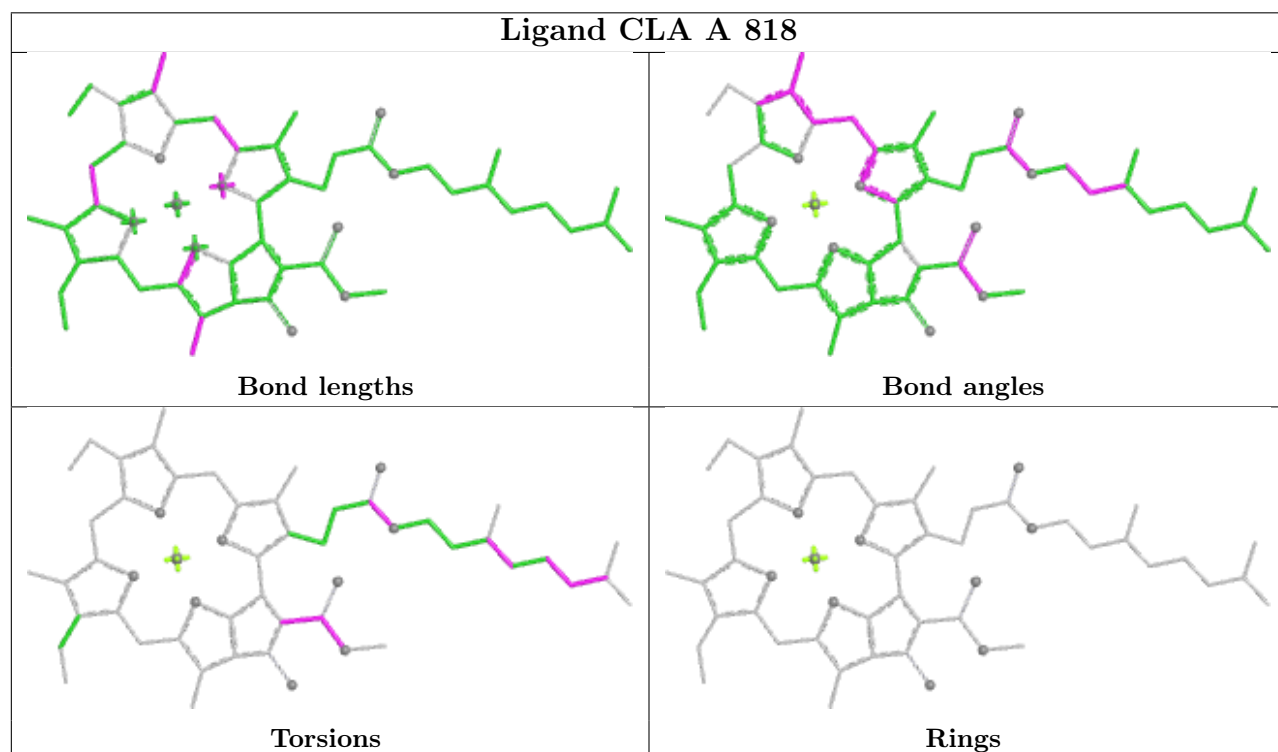
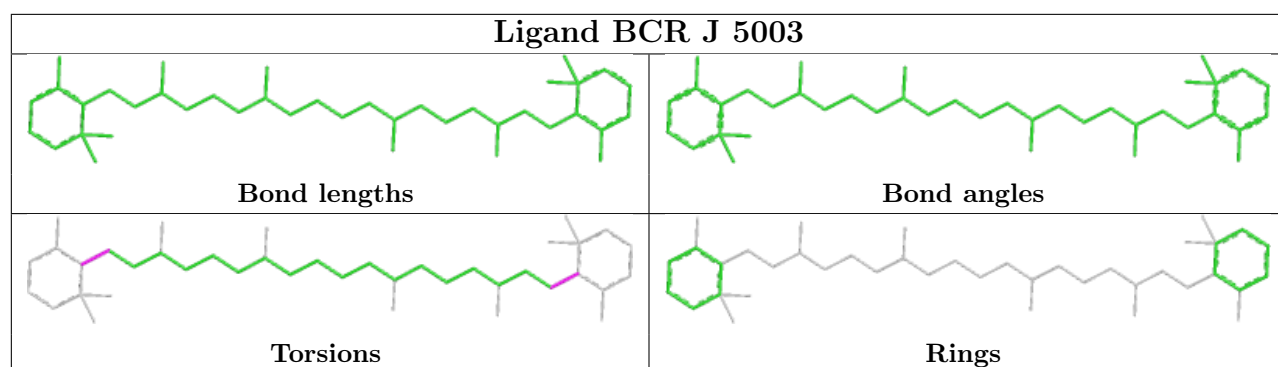
Bond angles



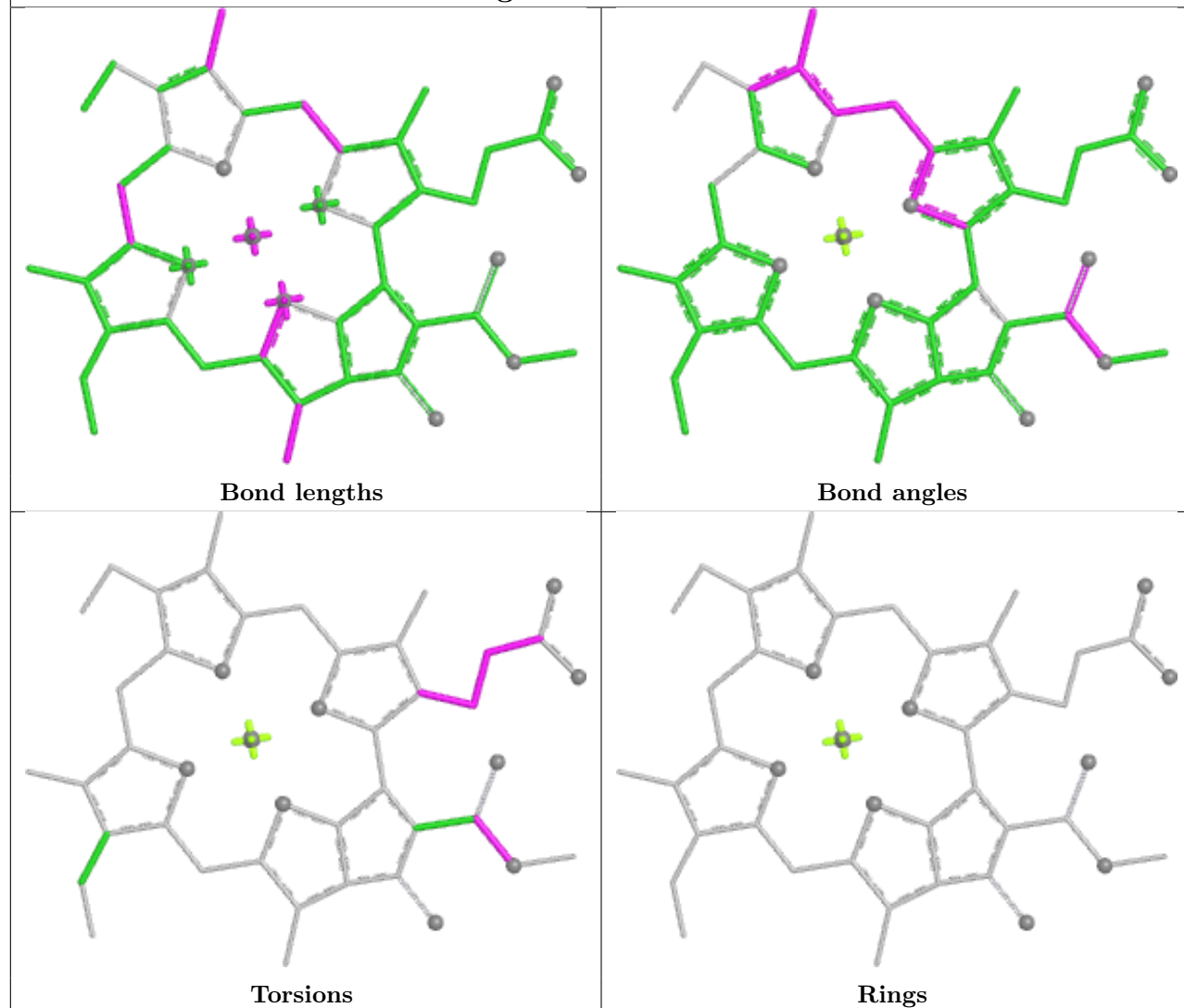
Torsions



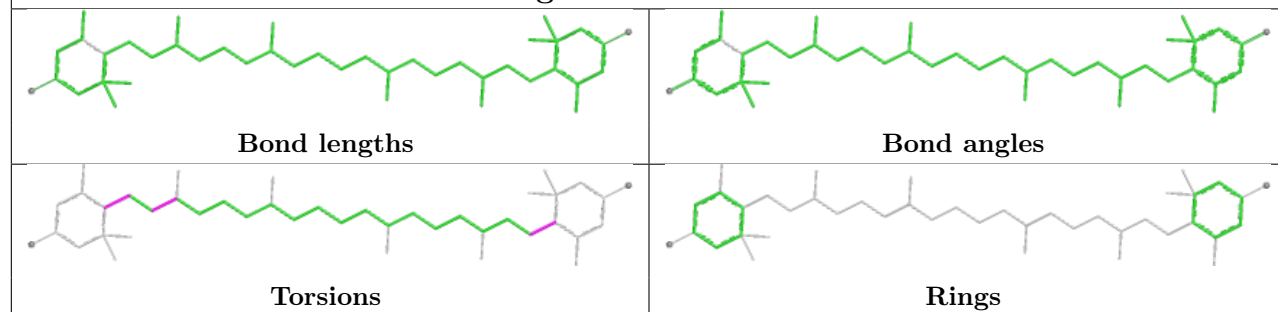
Rings



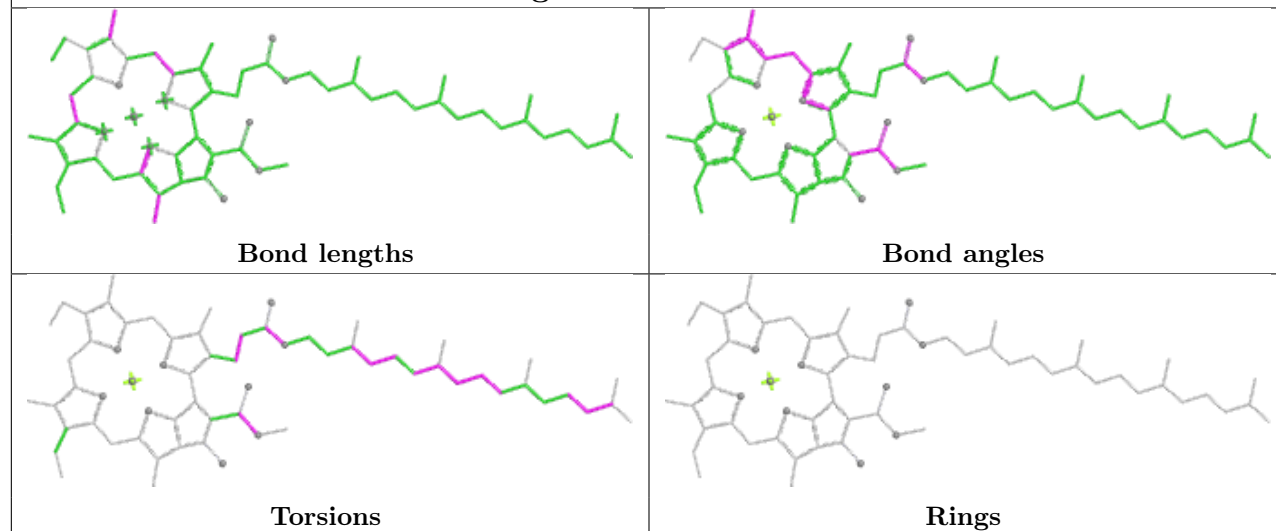
Ligand CLA 1 313



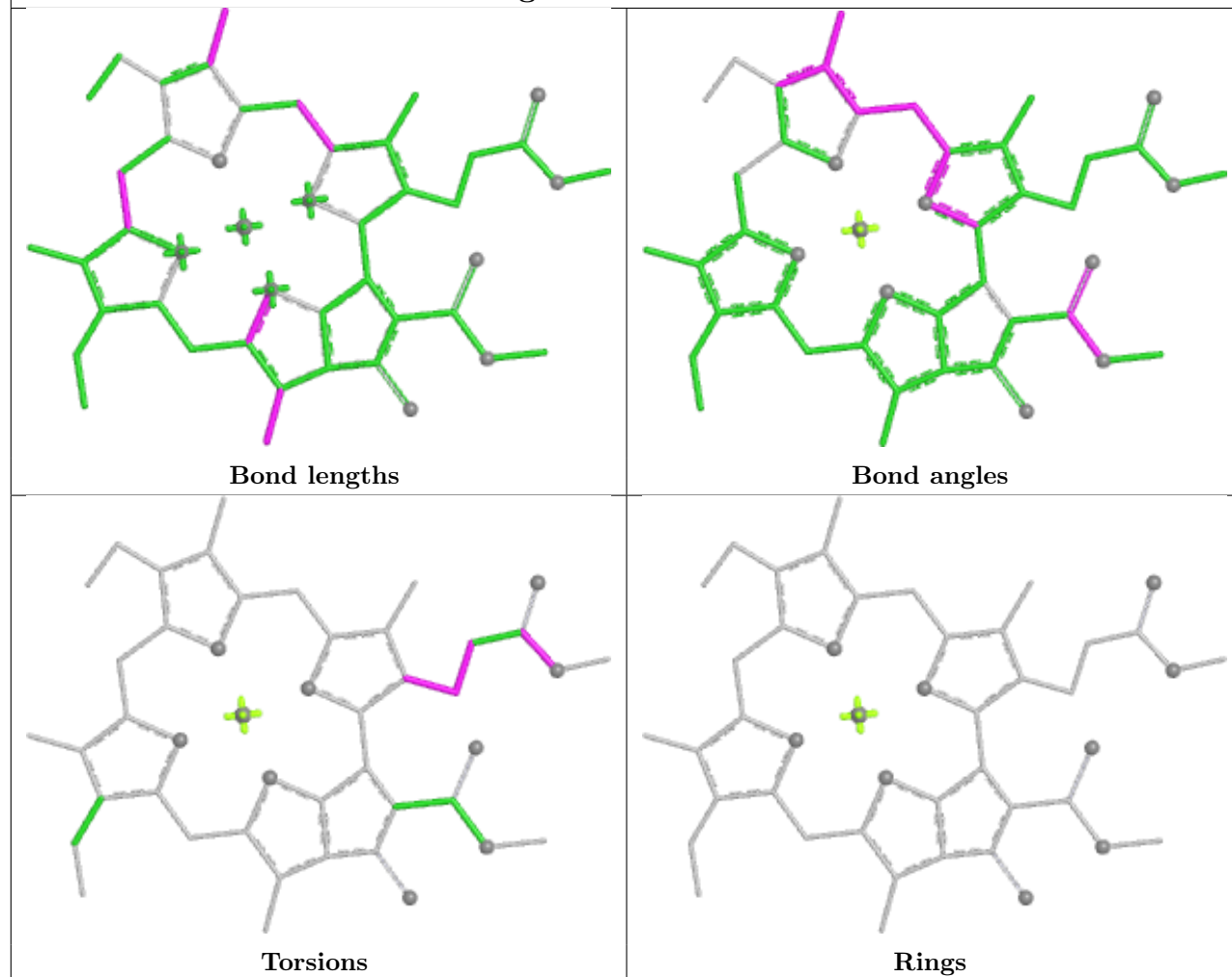
Ligand LUT 3 415

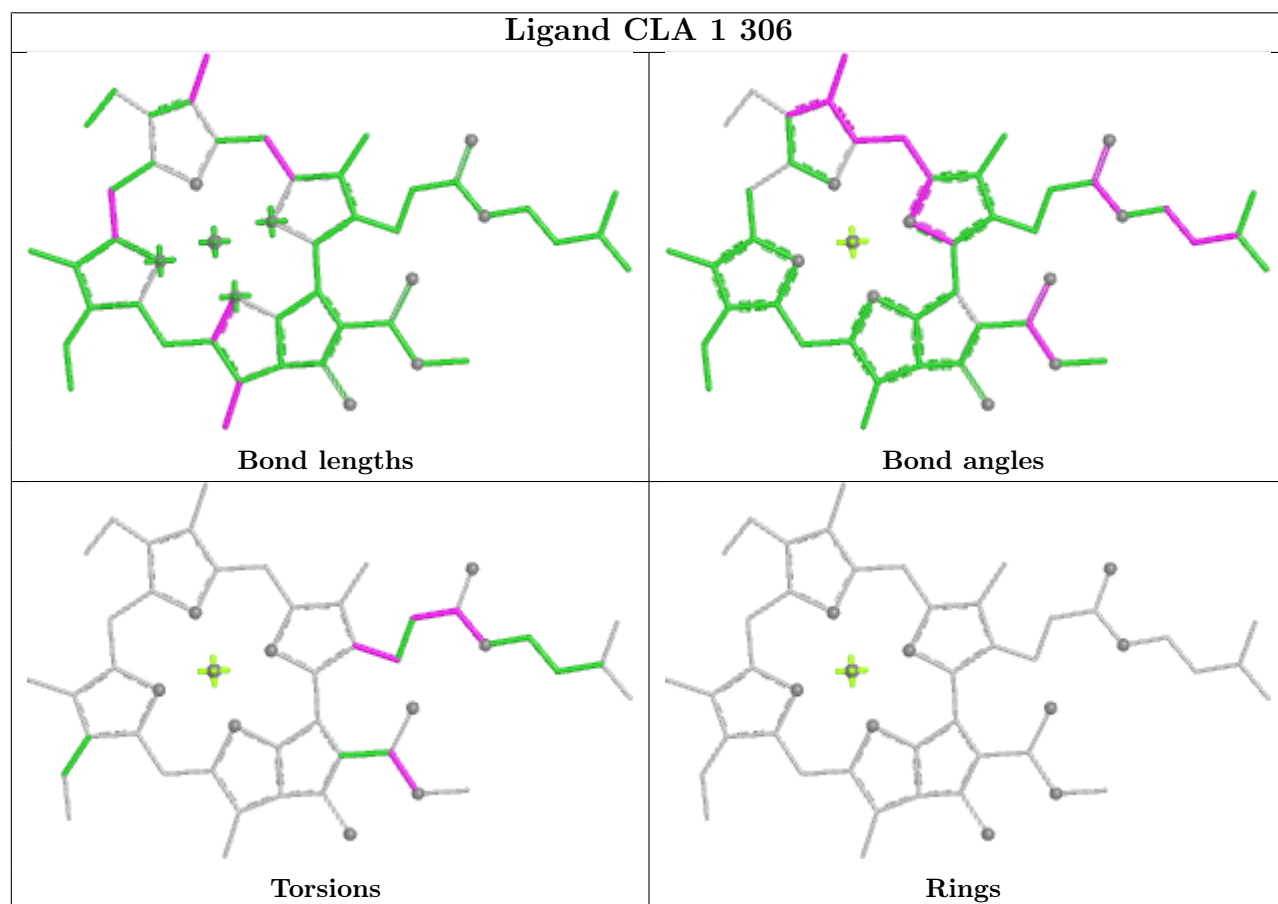
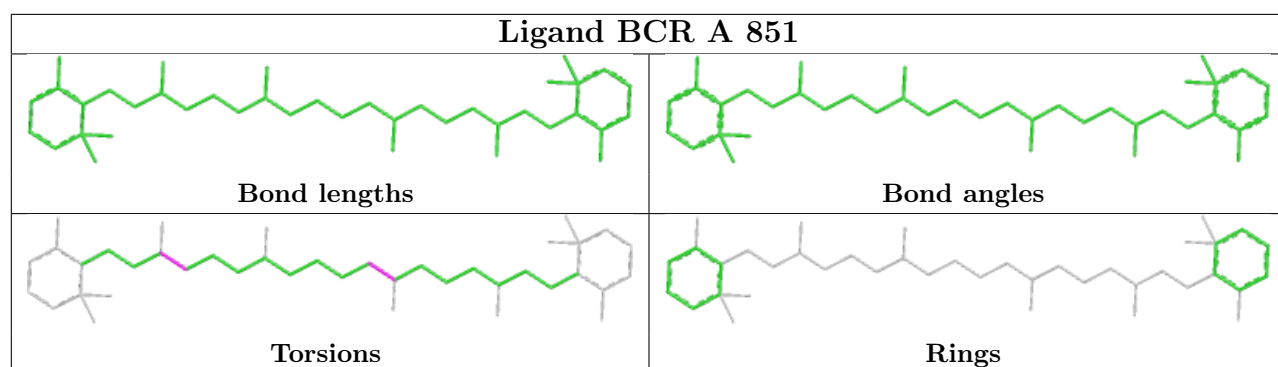


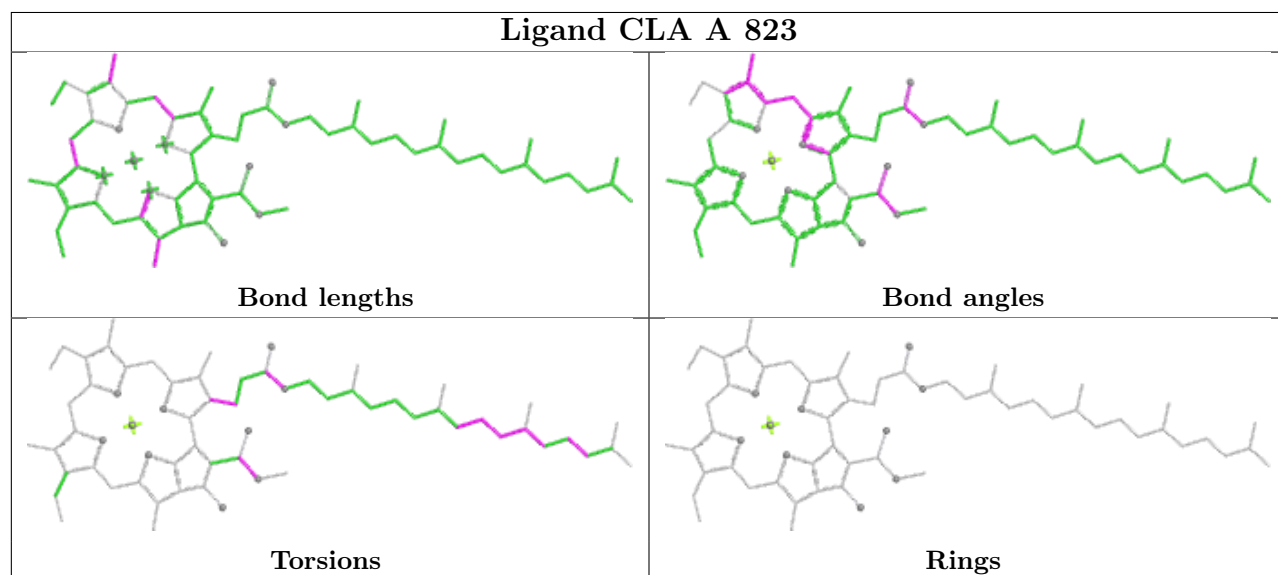
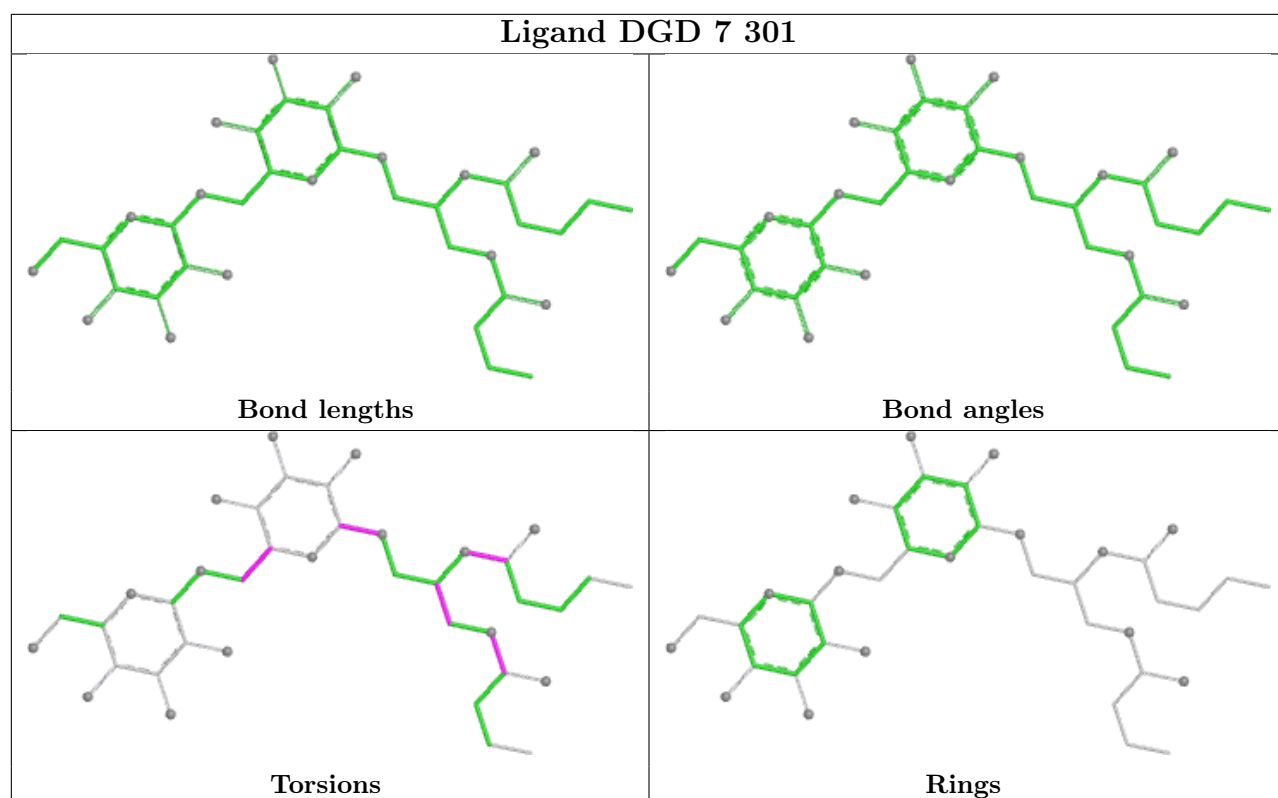
Ligand CLA A 815

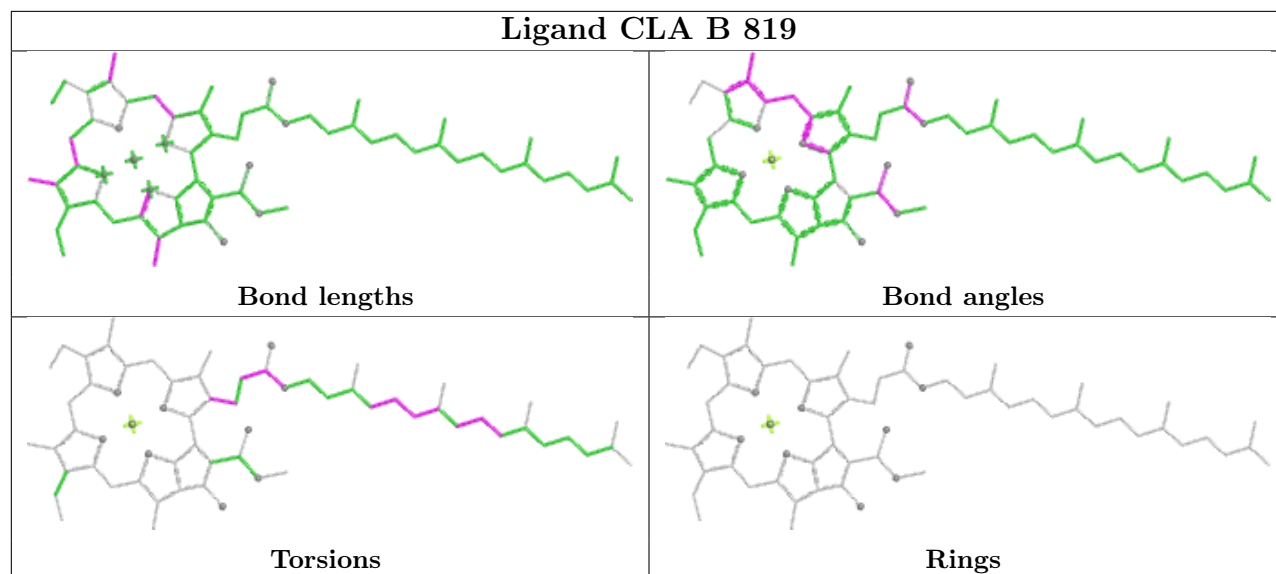
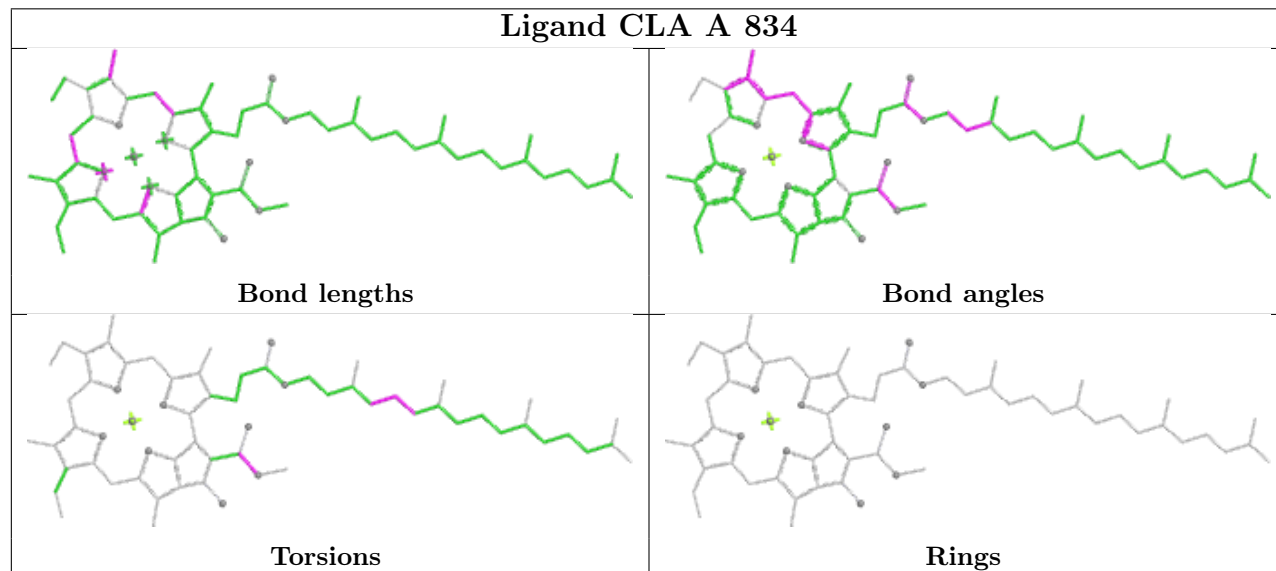


Ligand CLA c 609

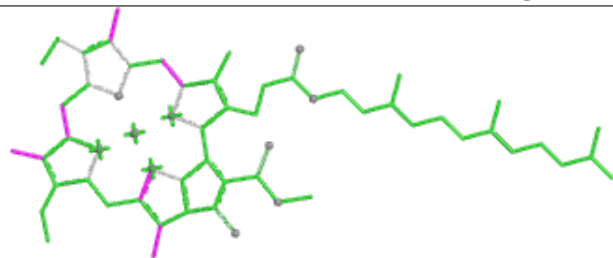




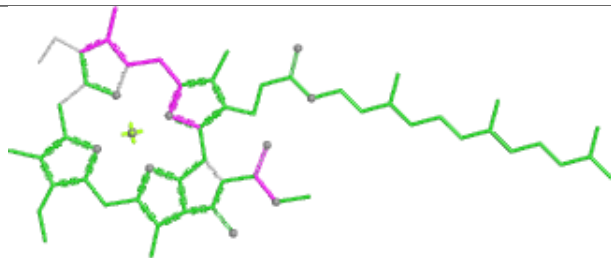


Ligand CLA B 819**Ligand CLA A 834**

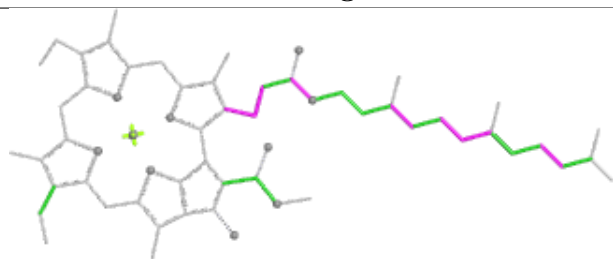
Ligand CLA 1 308



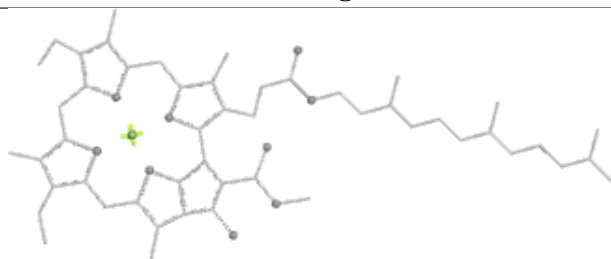
Bond lengths



Bond angles

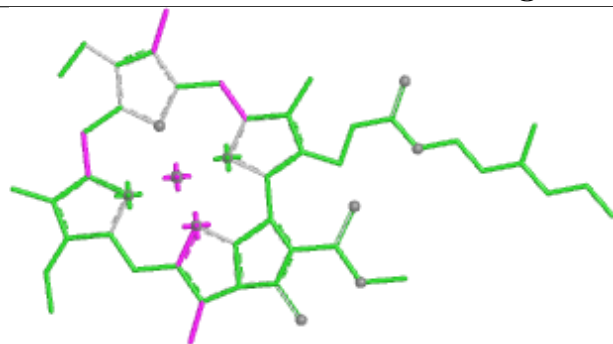


Torsions

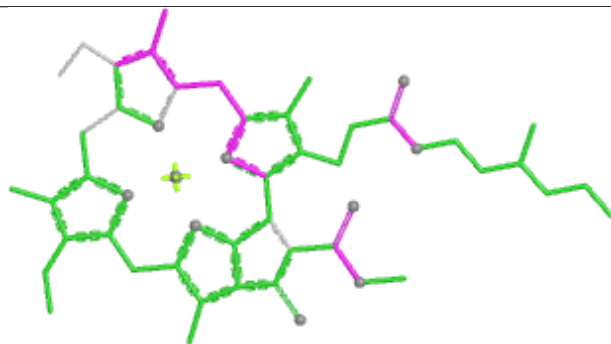


Rings

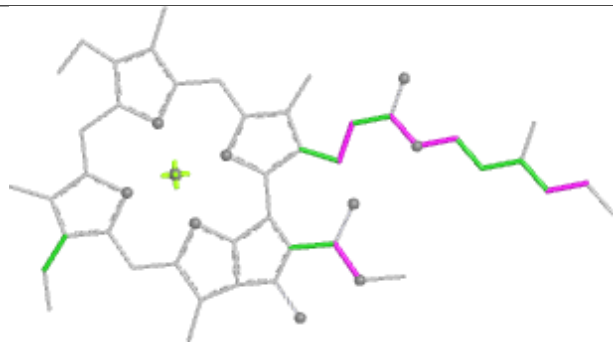
Ligand CLA 8 613



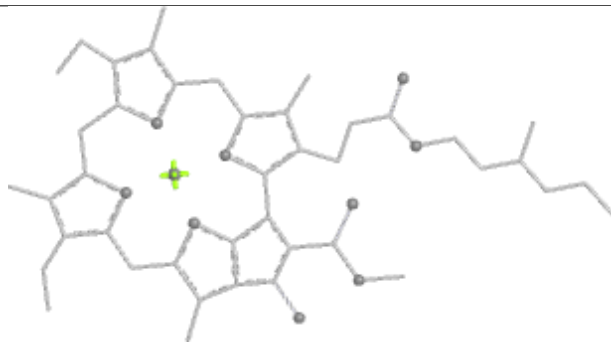
Bond lengths



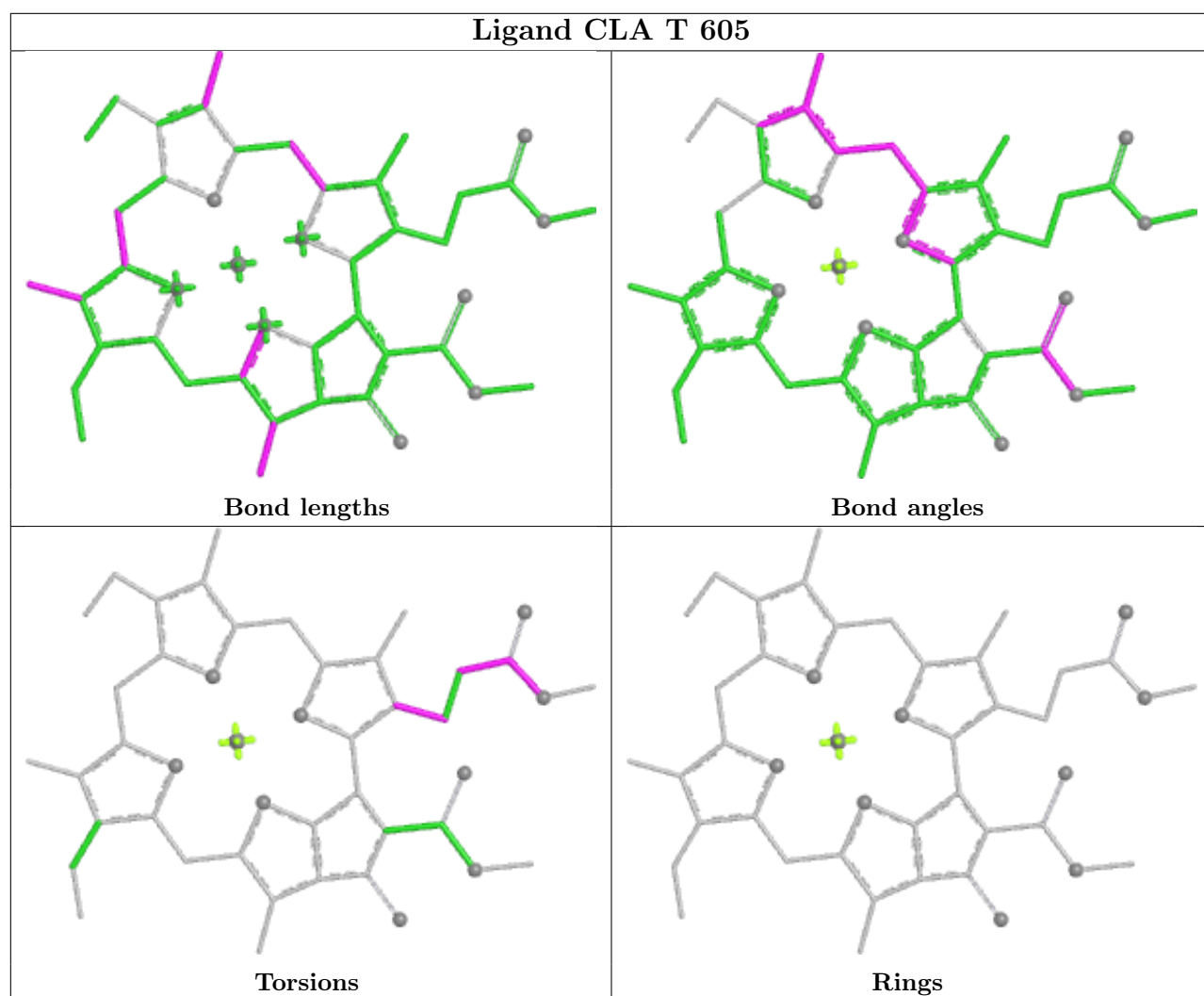
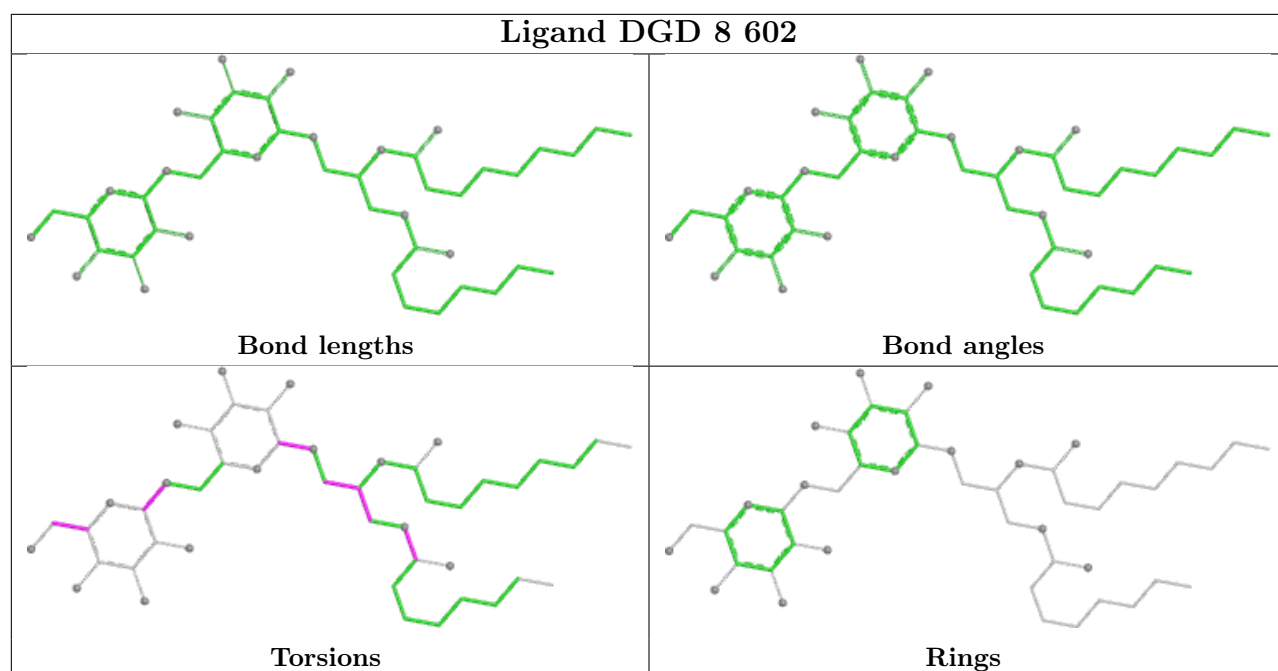
Bond angles

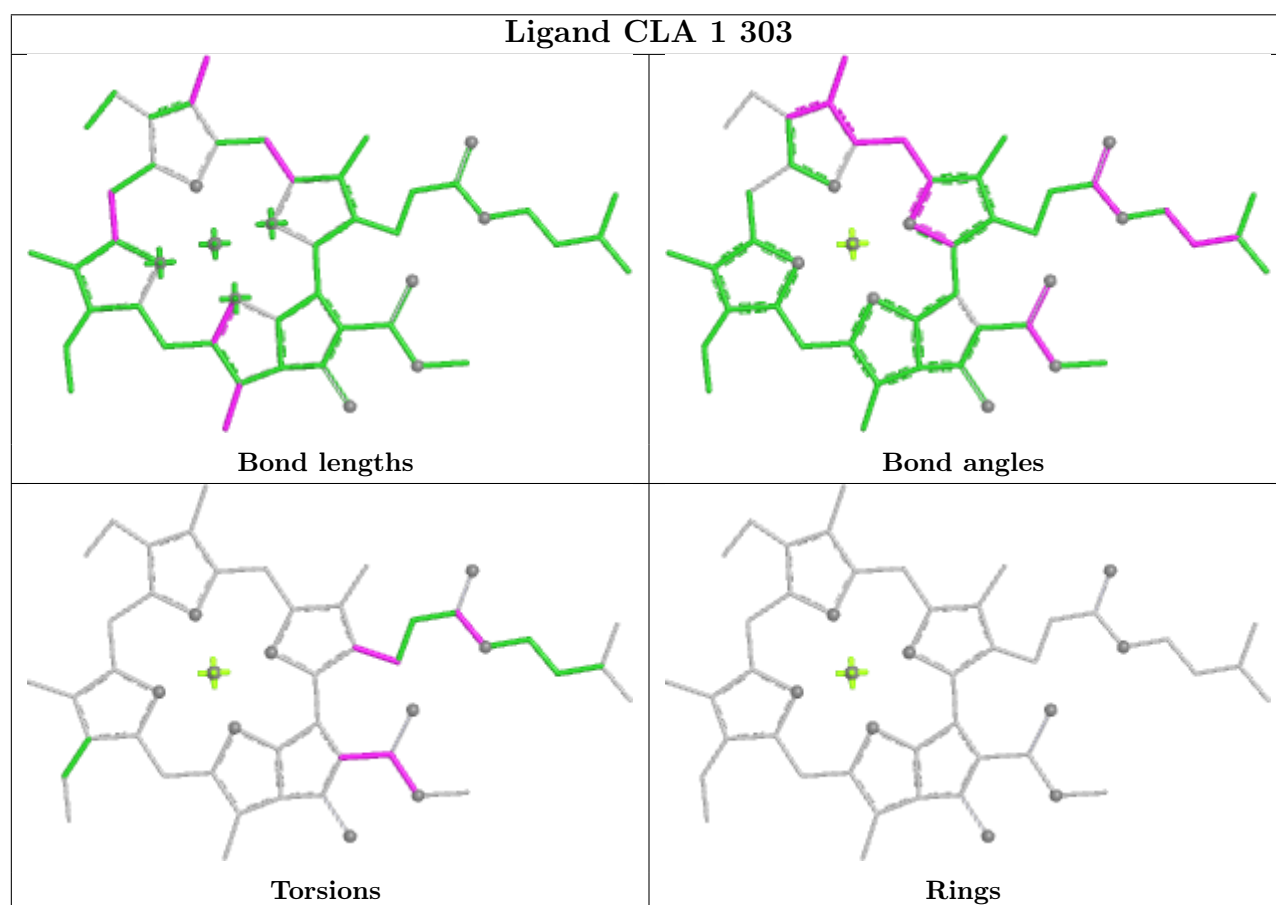
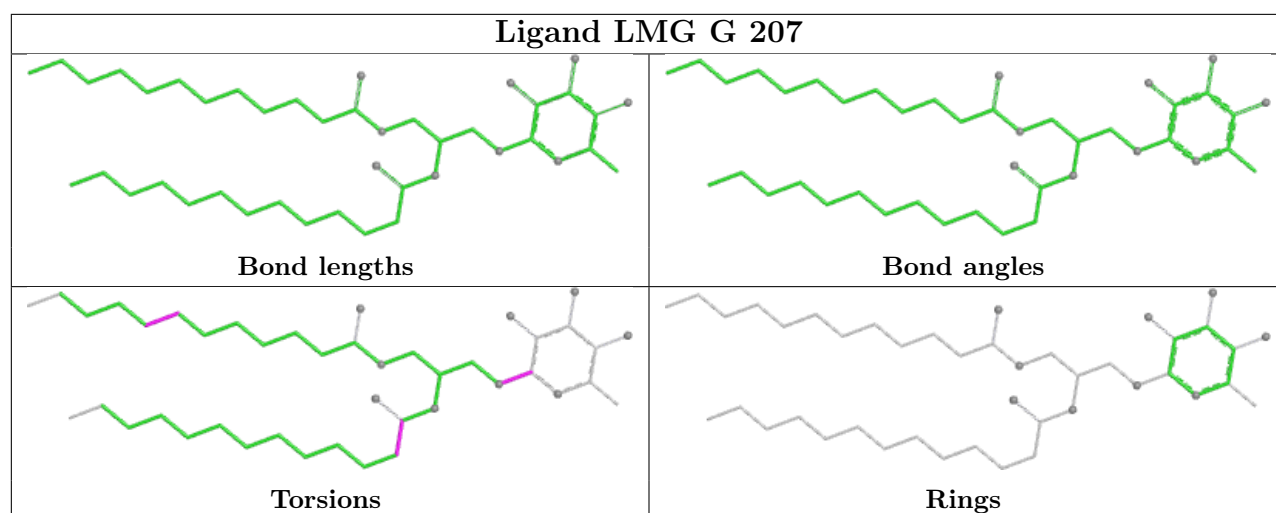


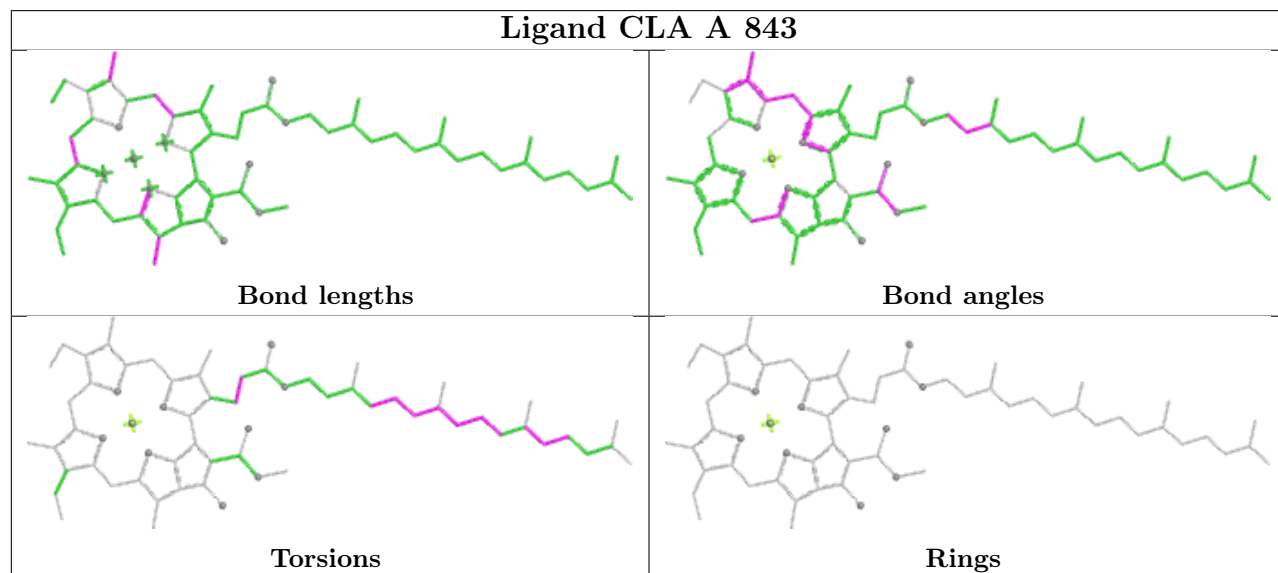
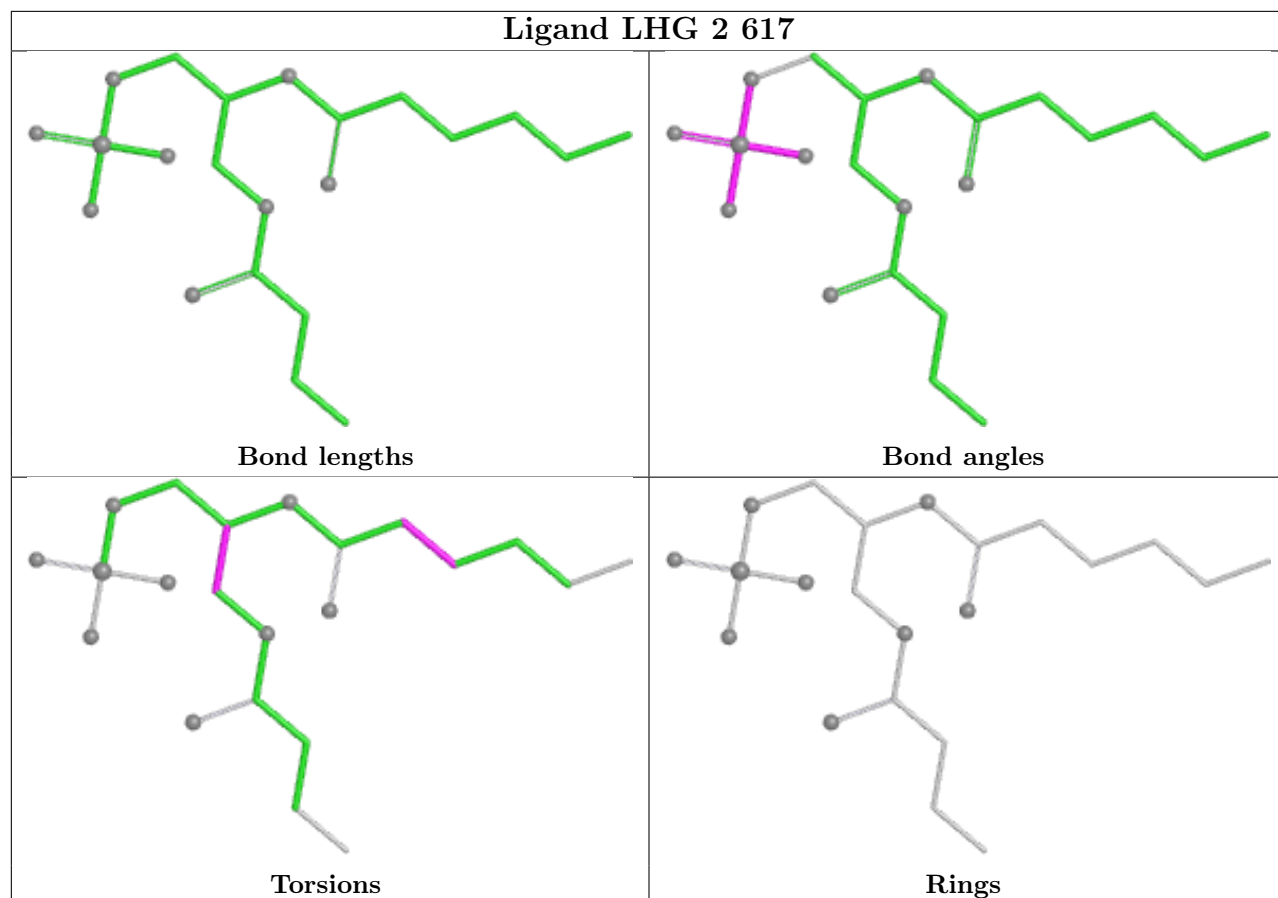
Torsions

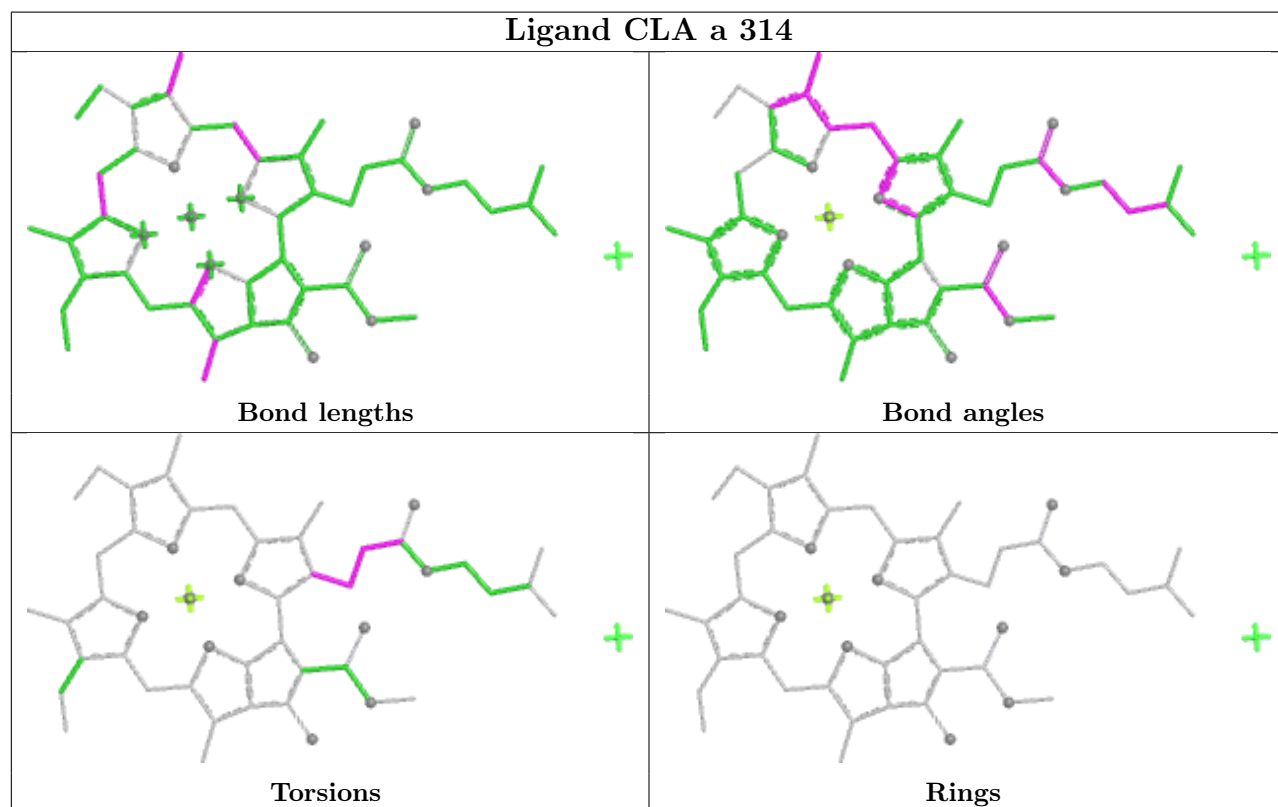
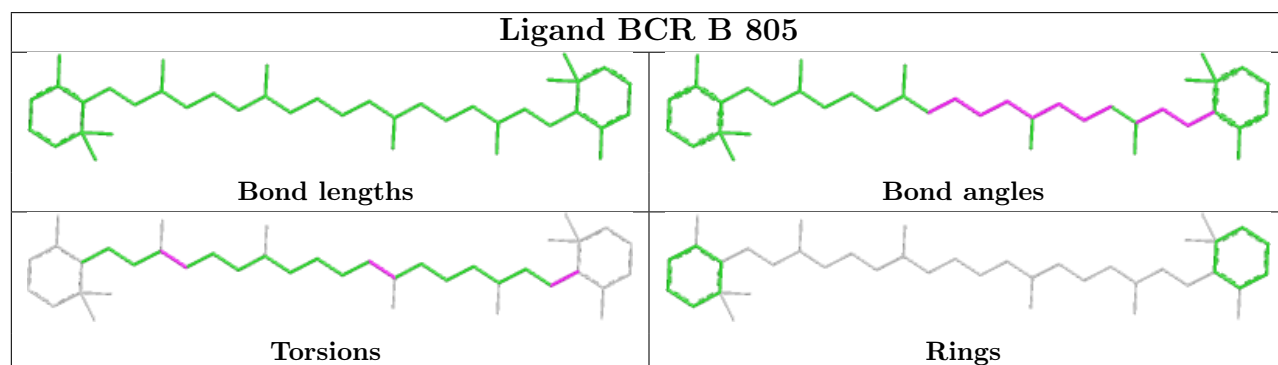
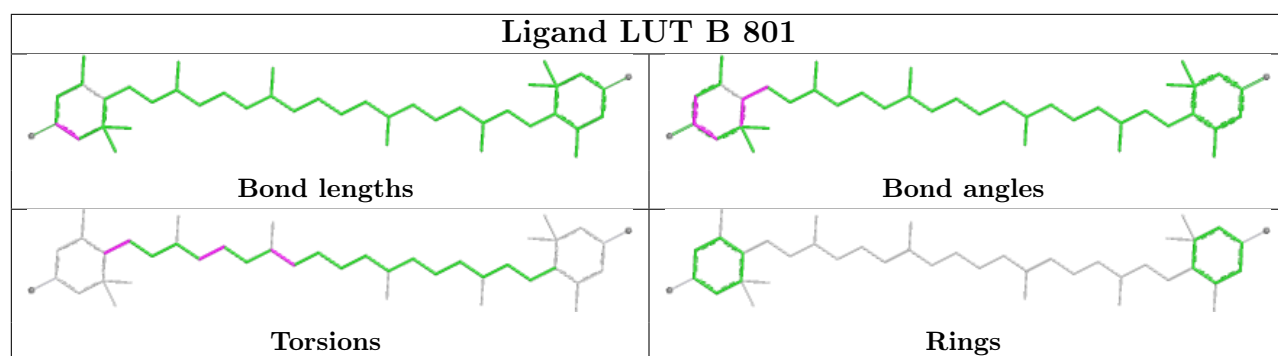


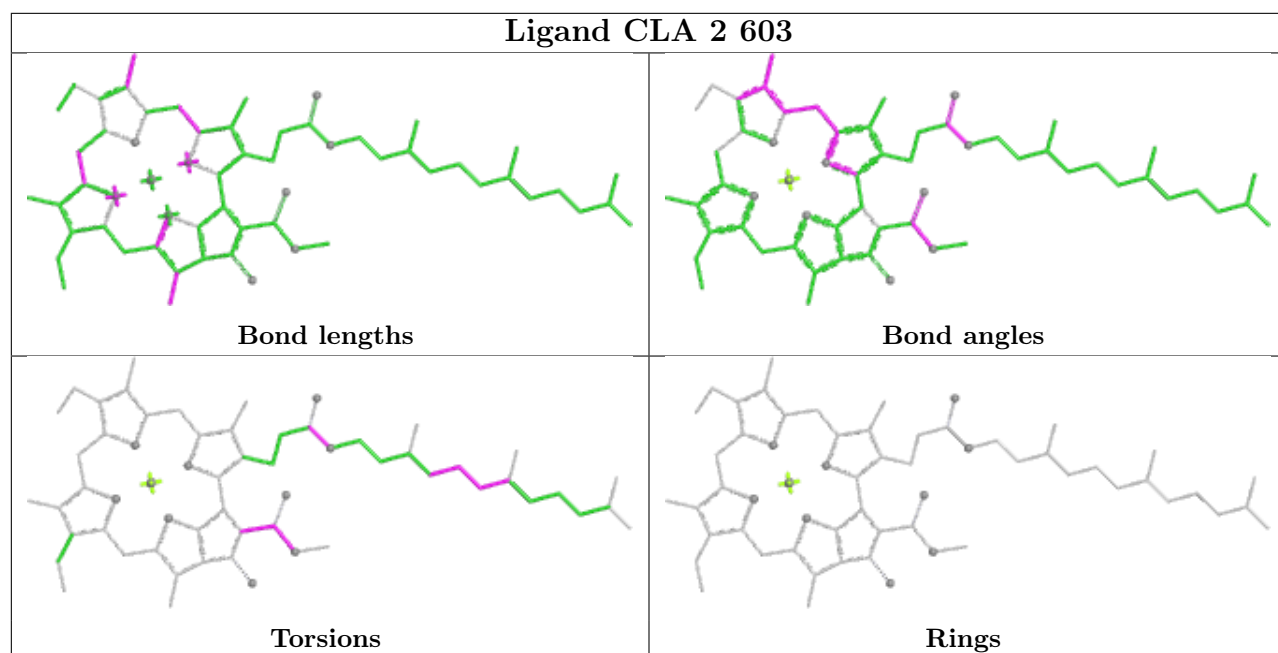
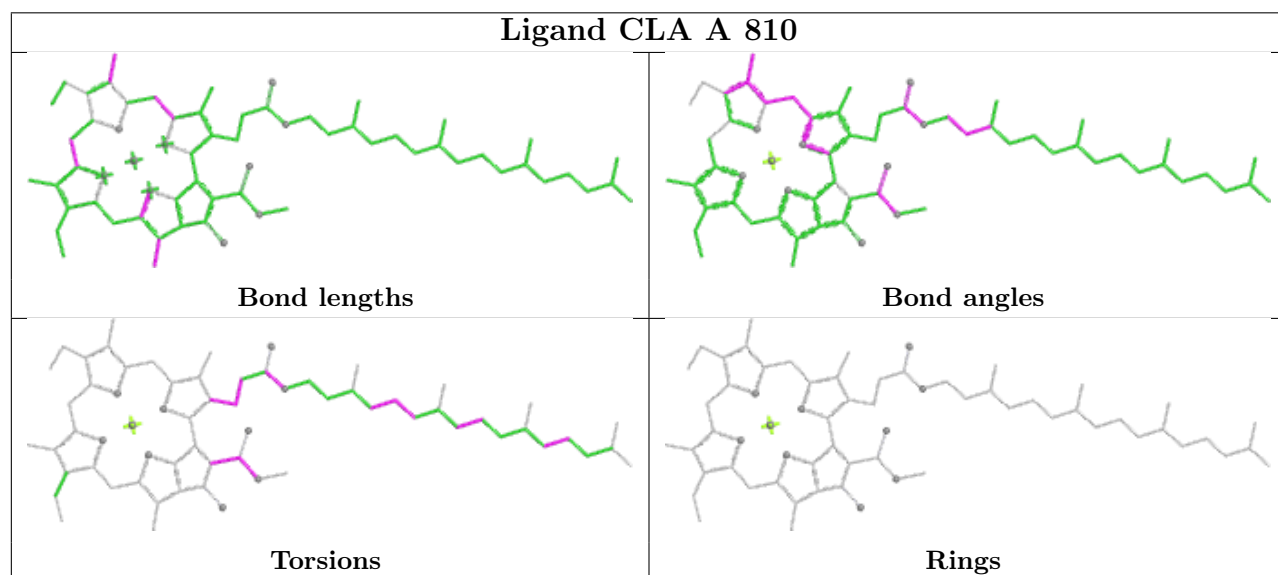
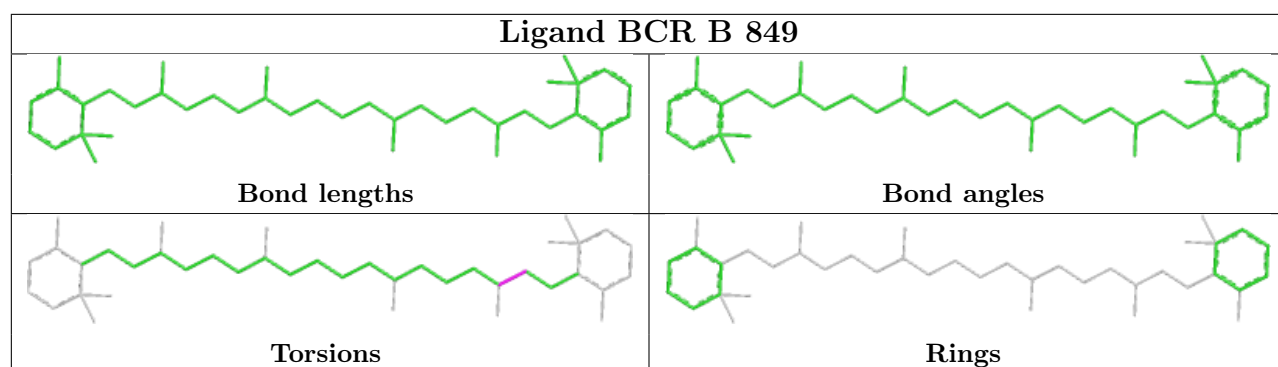
Rings



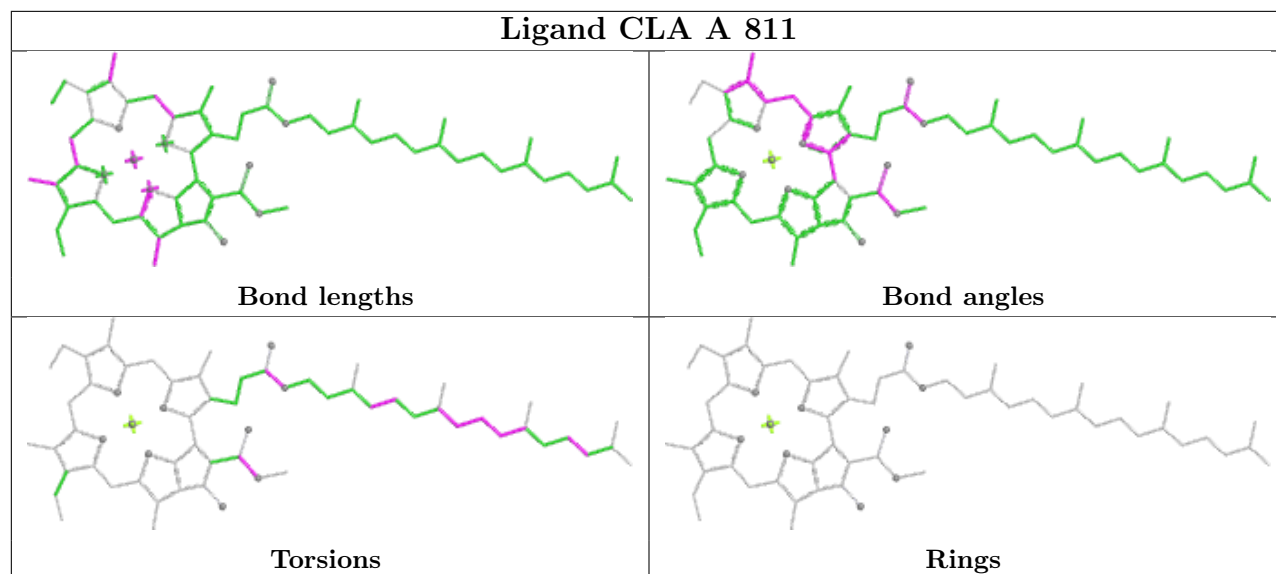




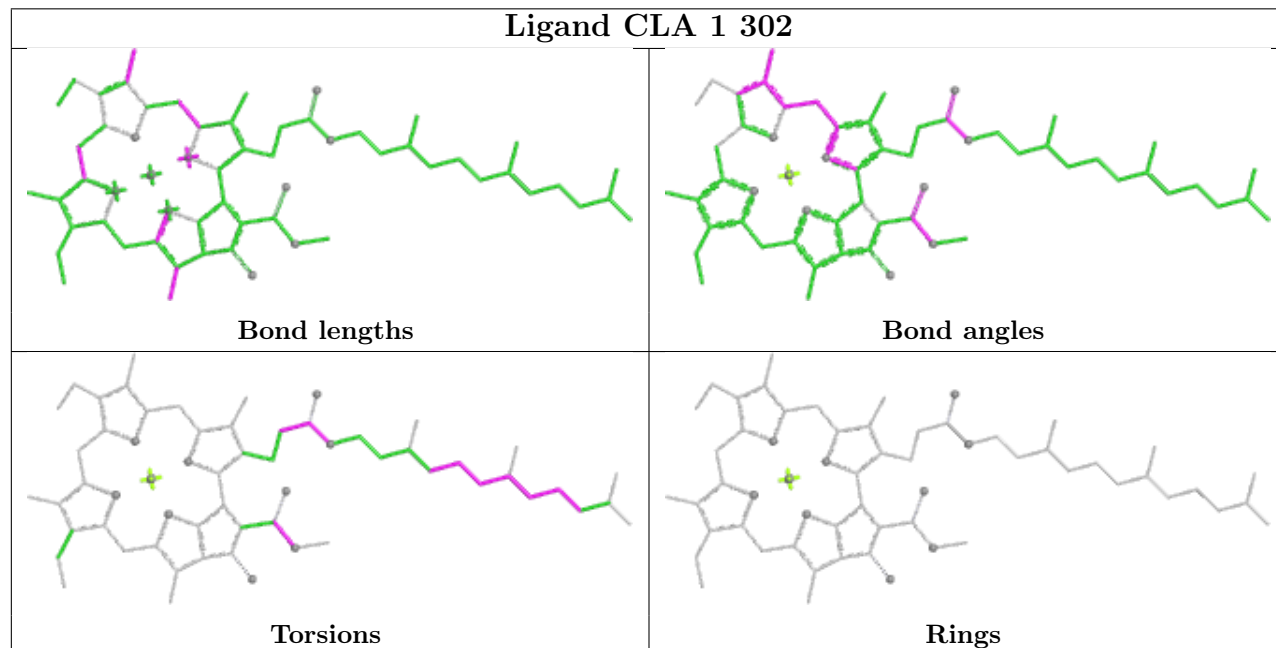


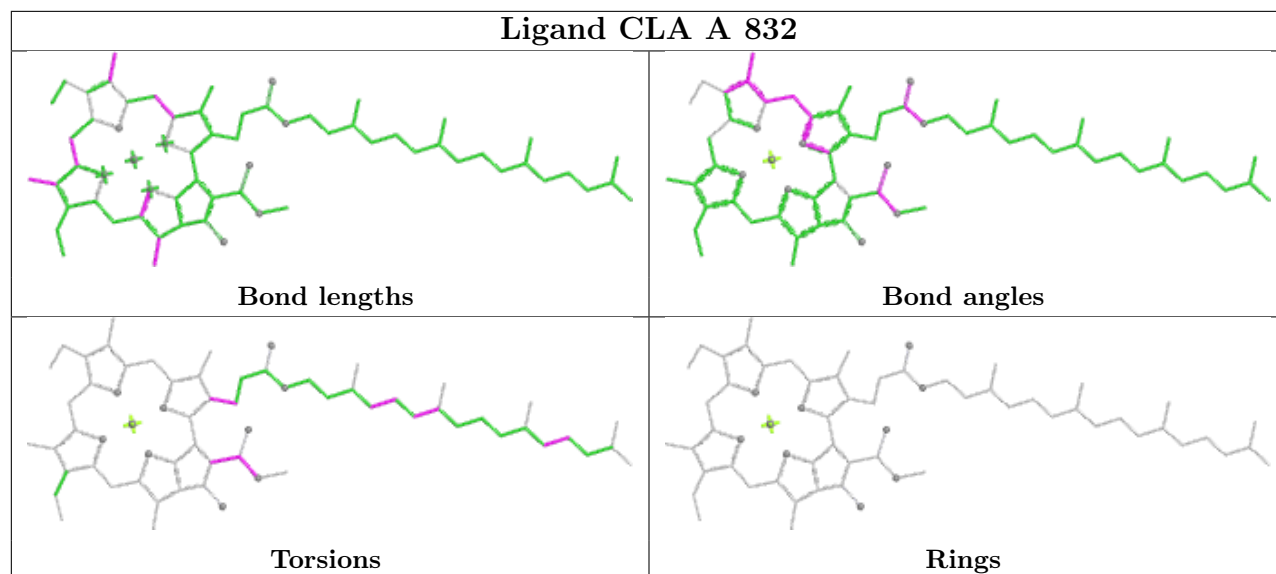
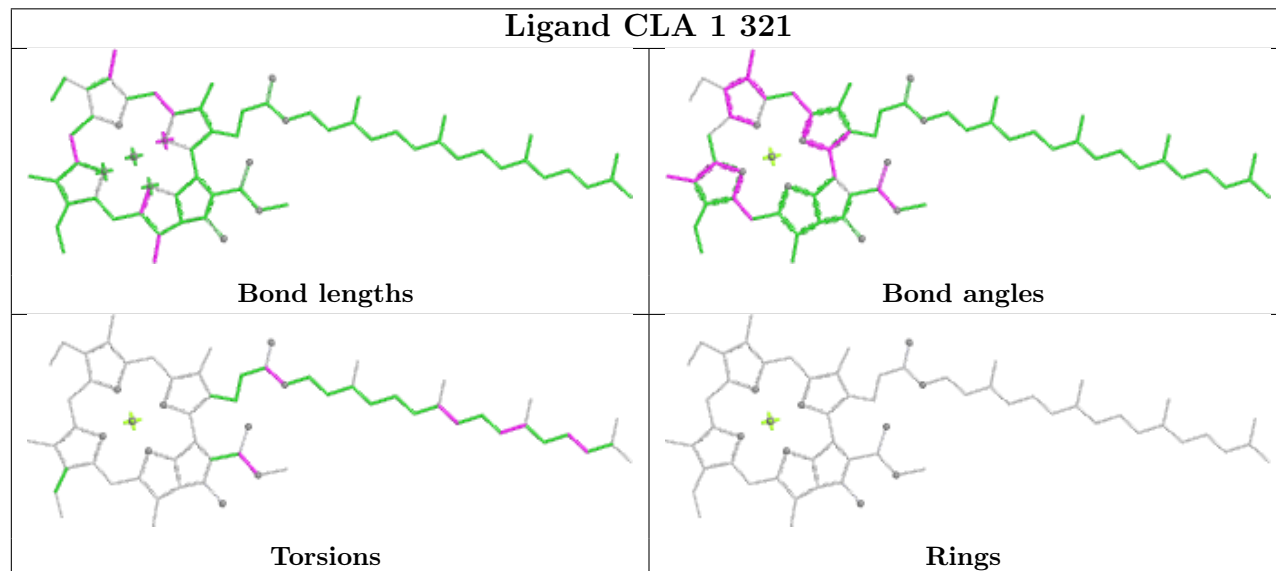


Ligand CLA A 811

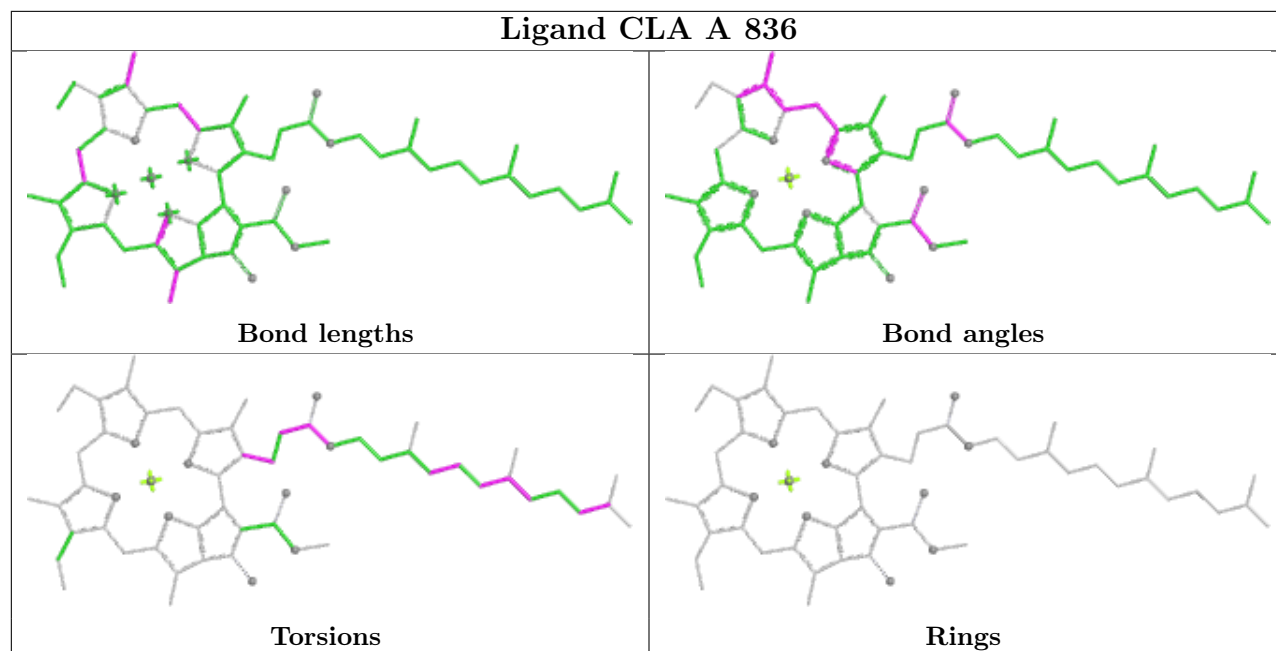


Ligand CLA 1 302

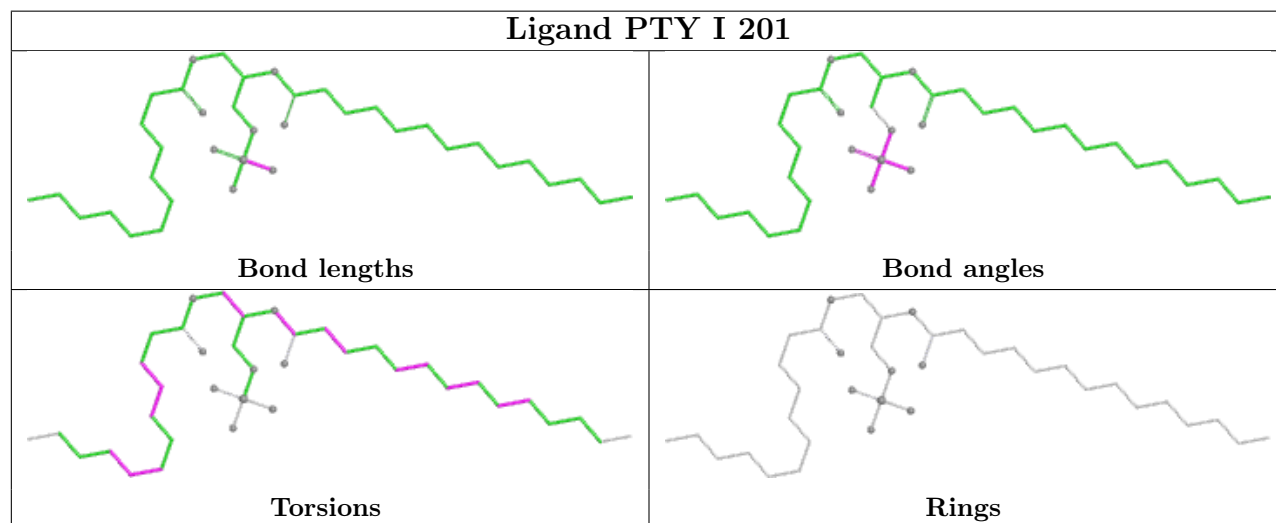


Ligand CLA A 832**Ligand CLA 1 321**

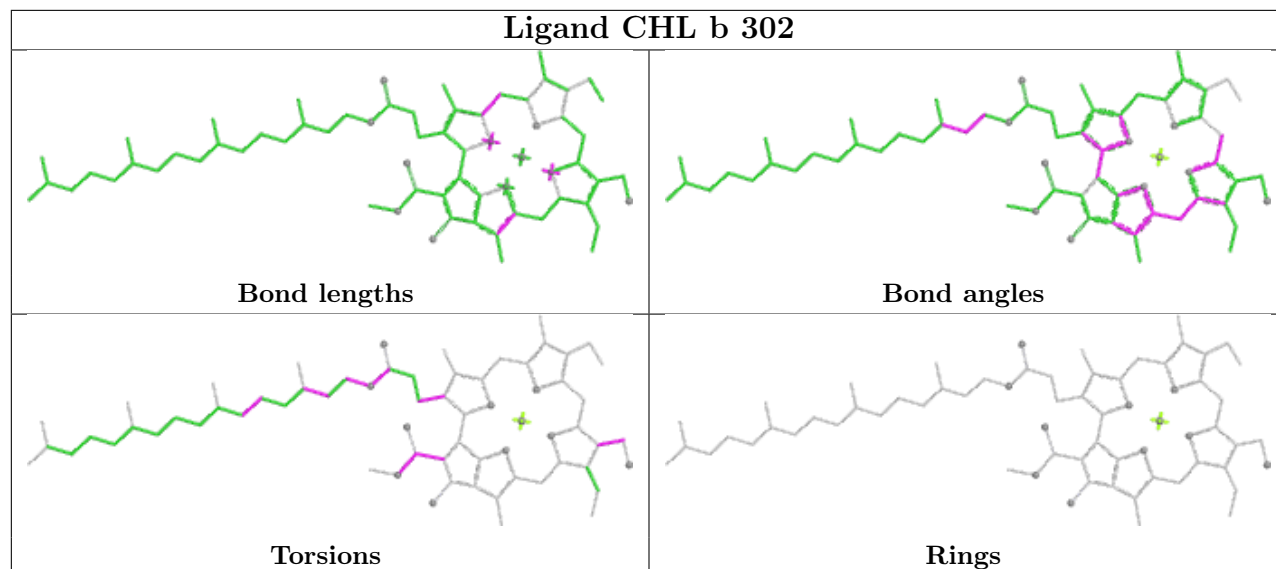
Ligand CLA A 836



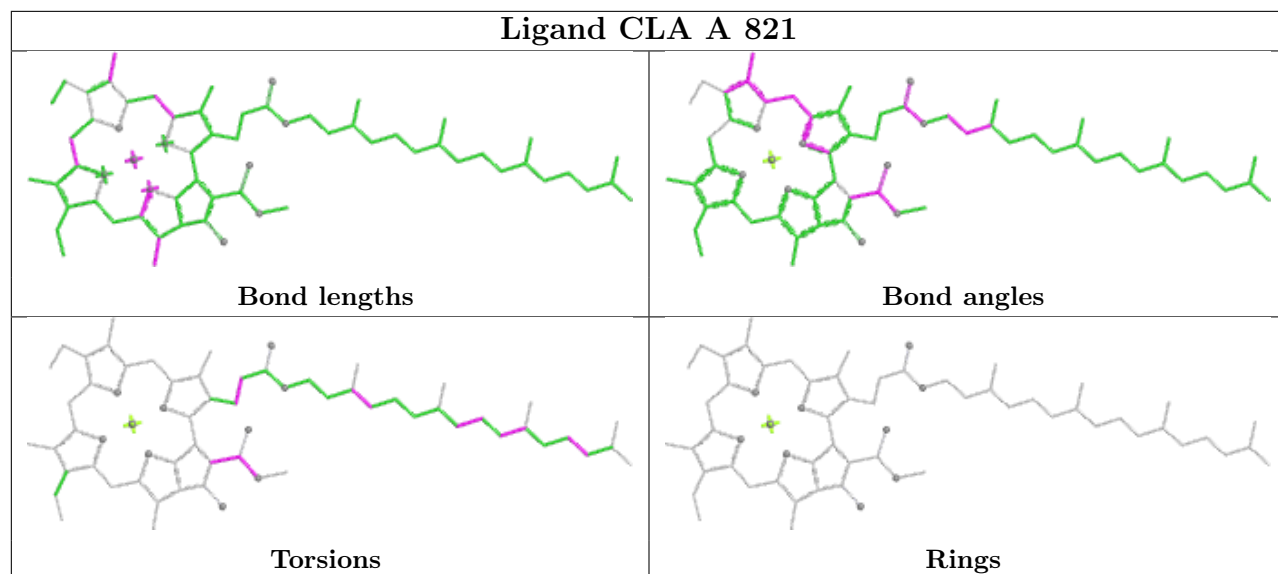
Ligand PTY I 201



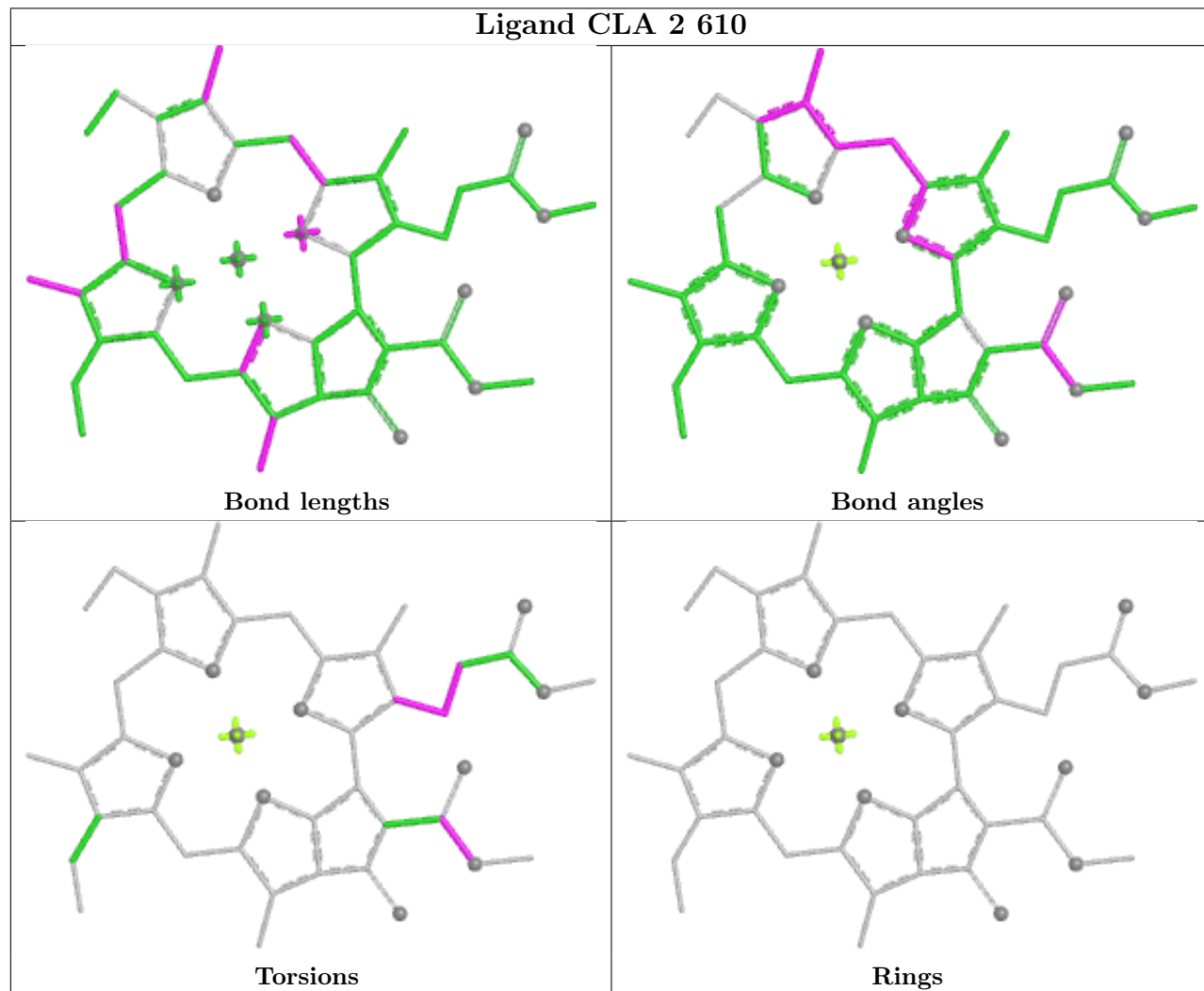
Ligand CHL b 302

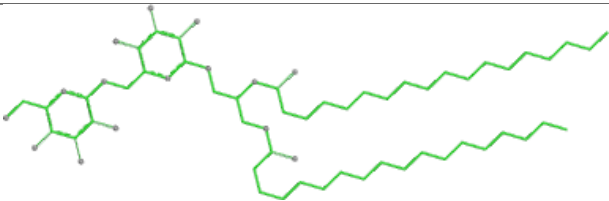
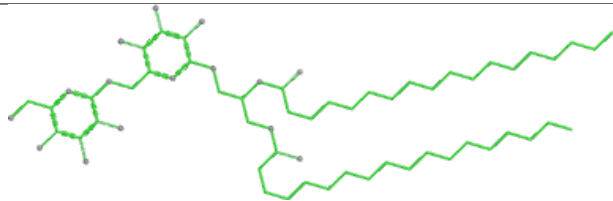
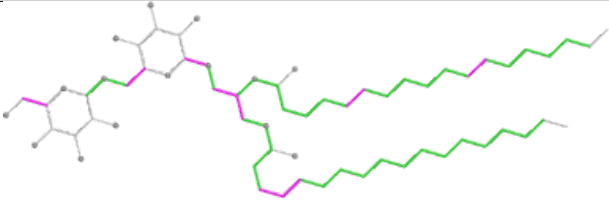
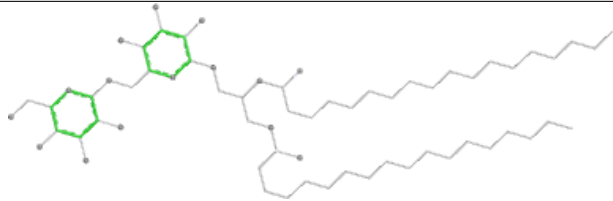


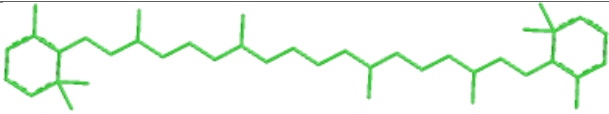
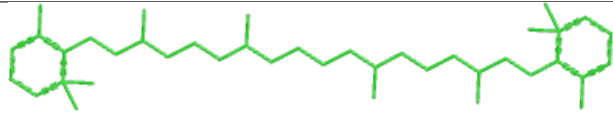
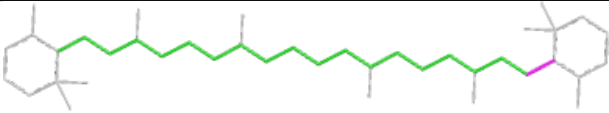
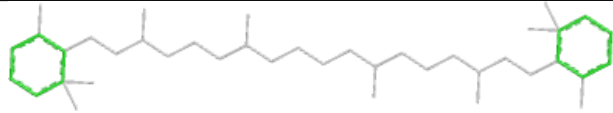
Ligand CLA A 821



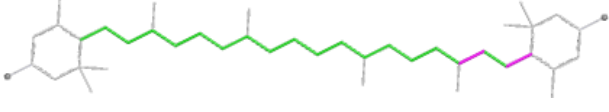
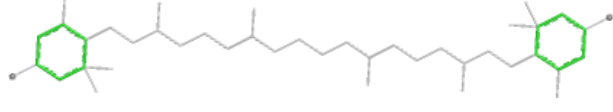


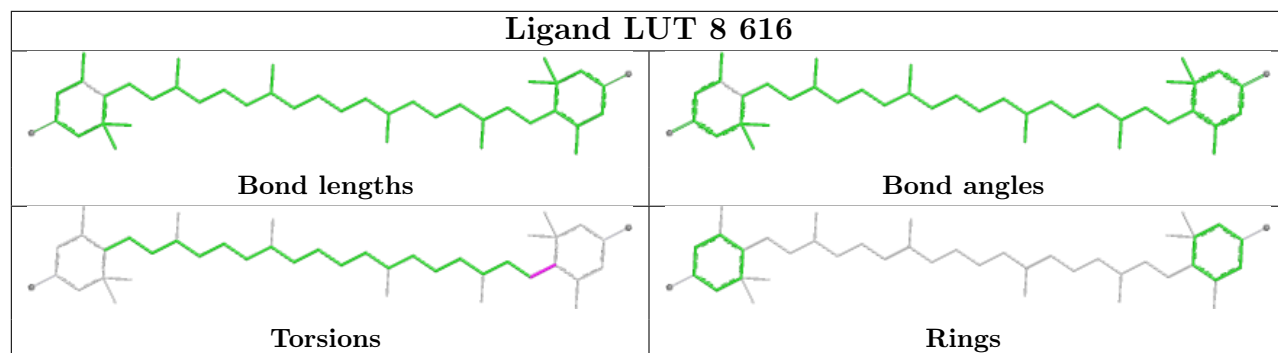
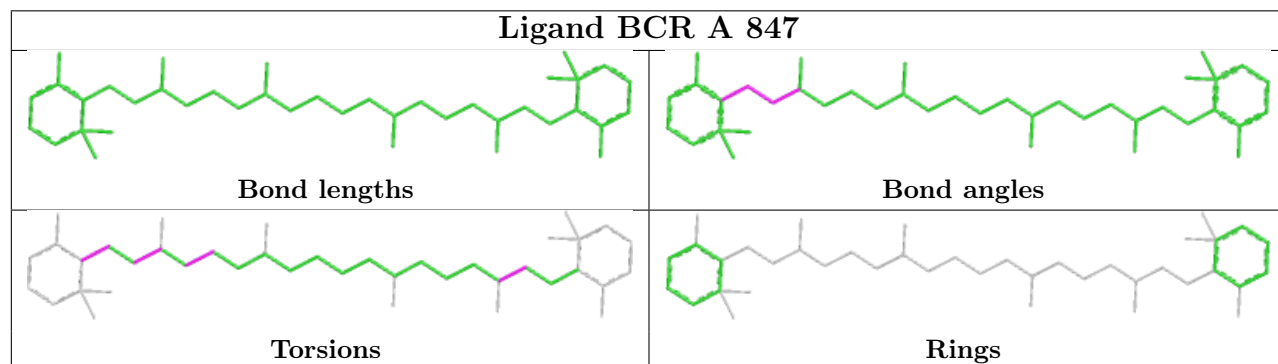
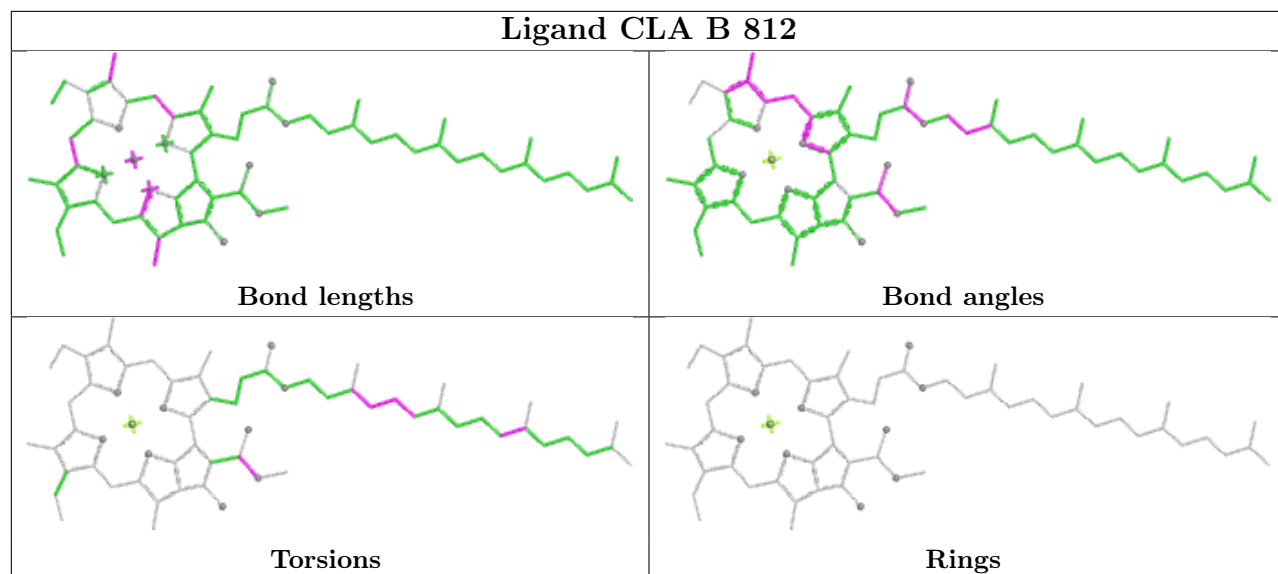
Ligand CLA 2 610

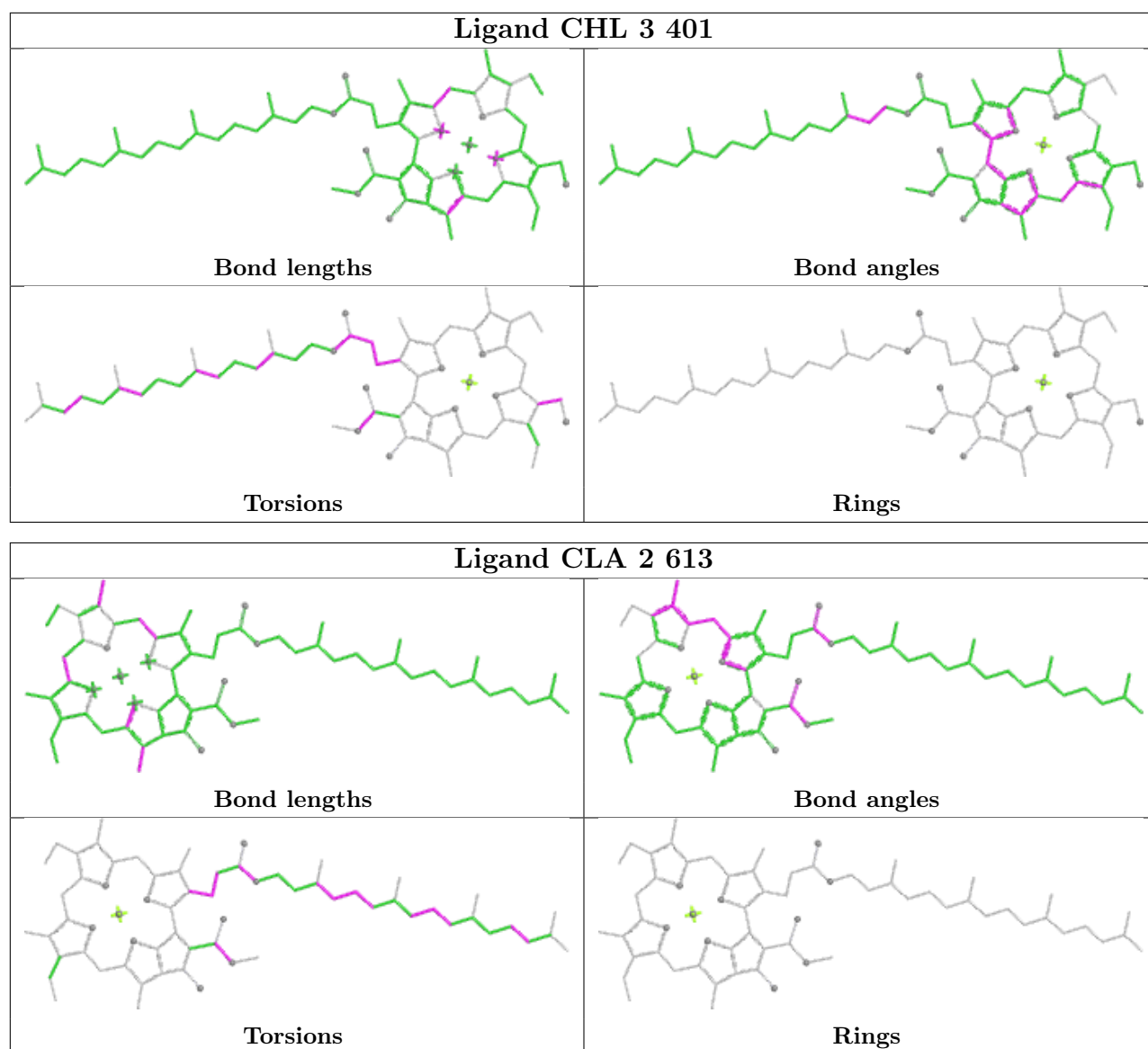


Ligand DGD A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

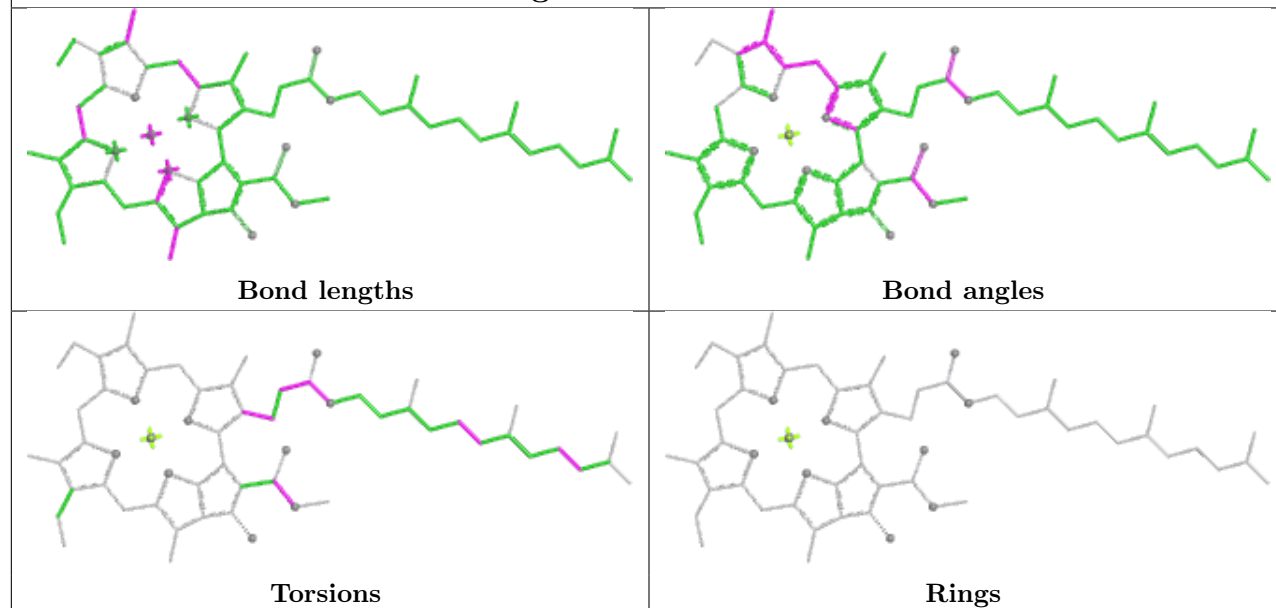
Ligand BCR b 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

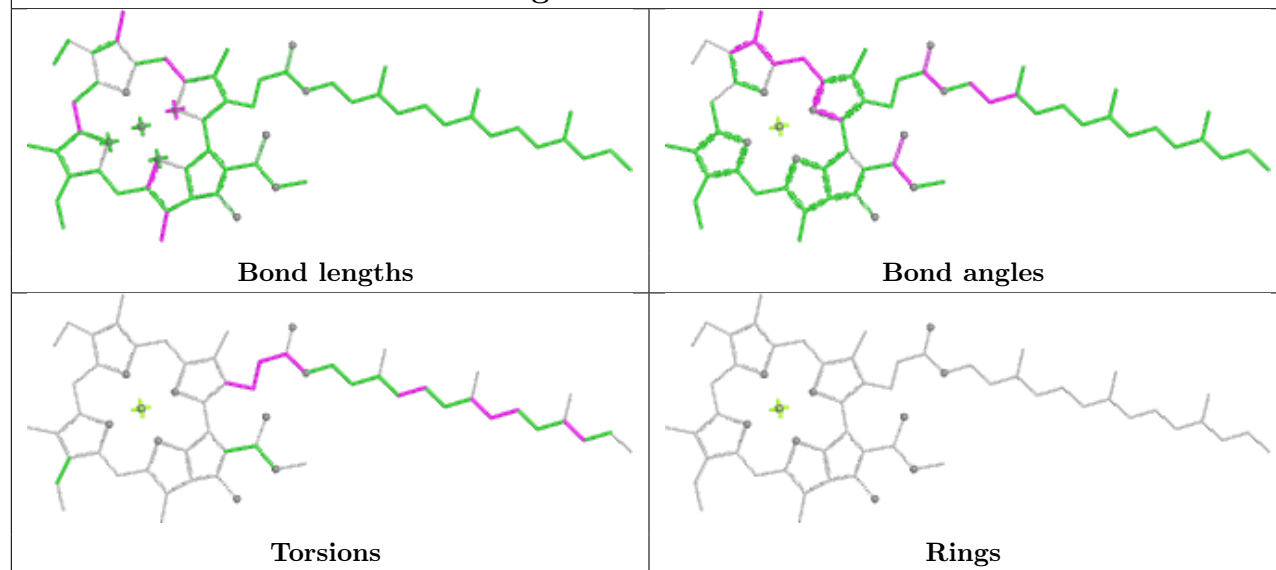


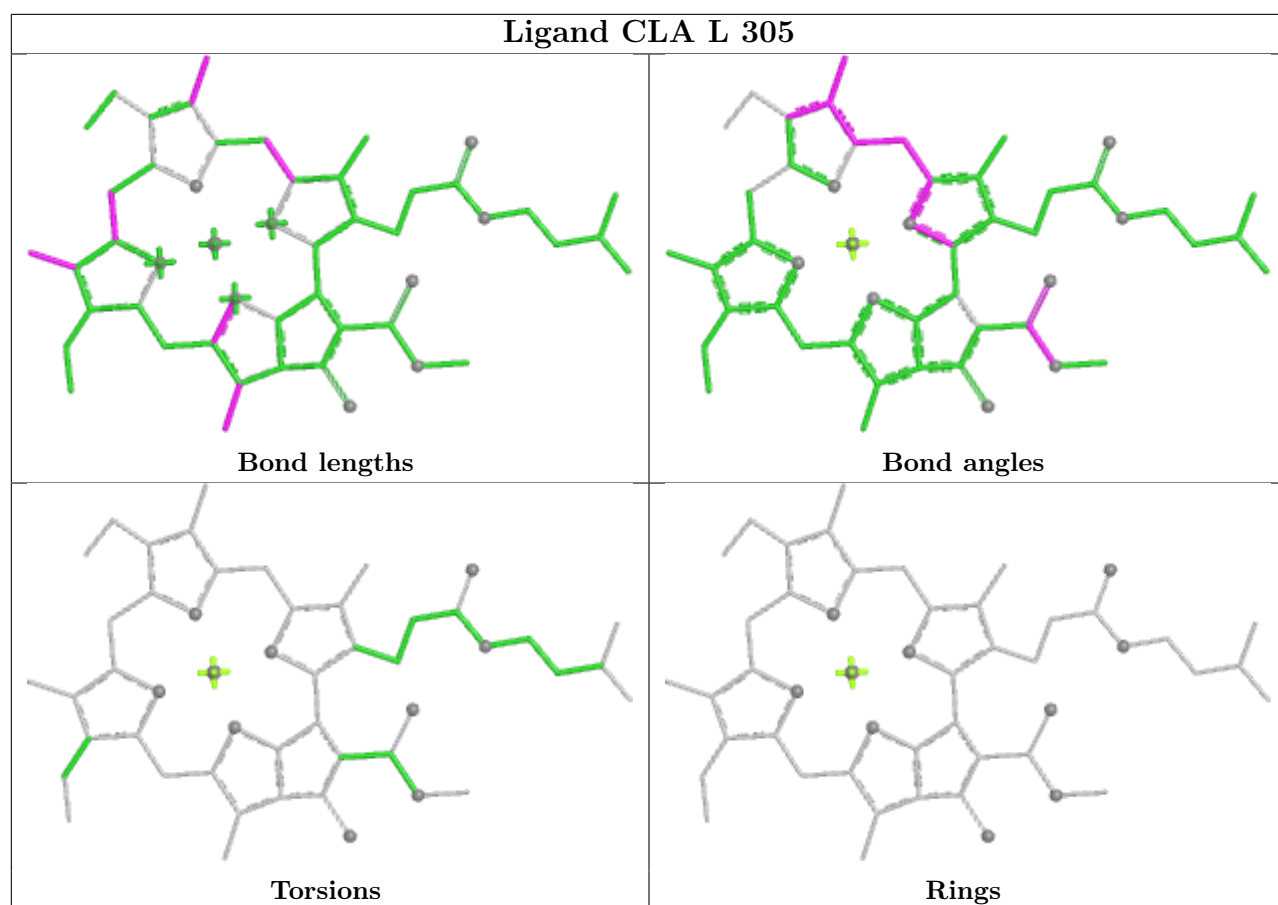


Ligand CLA A 826

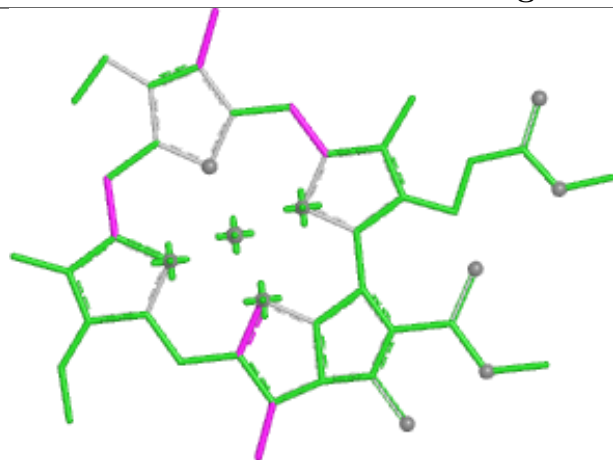


Ligand CLA A 814

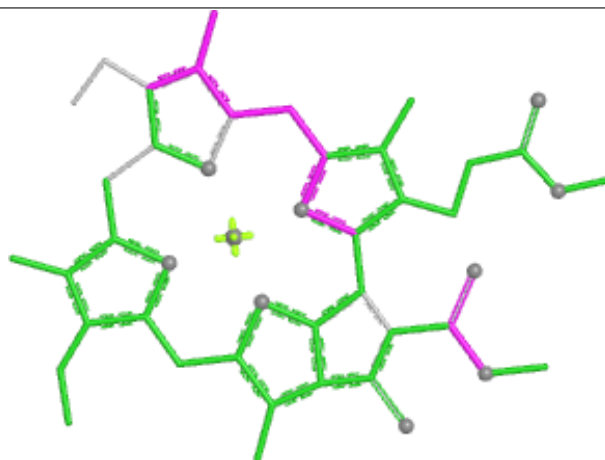




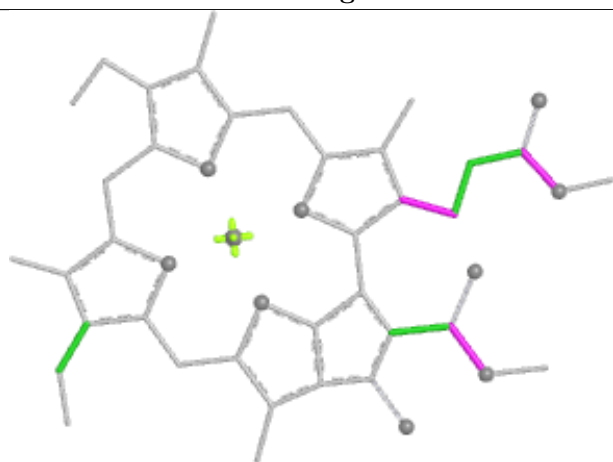
Ligand CLA b 312



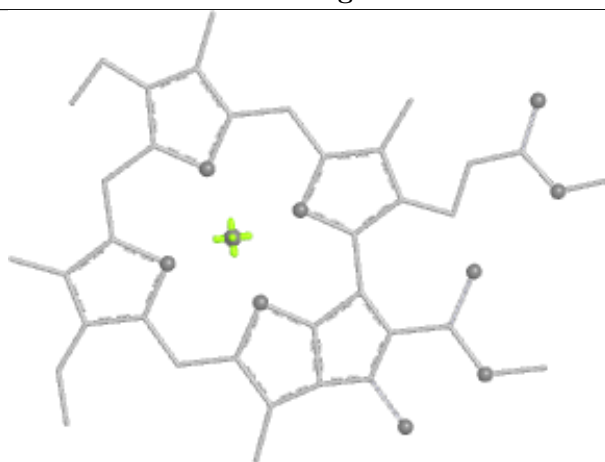
Bond lengths



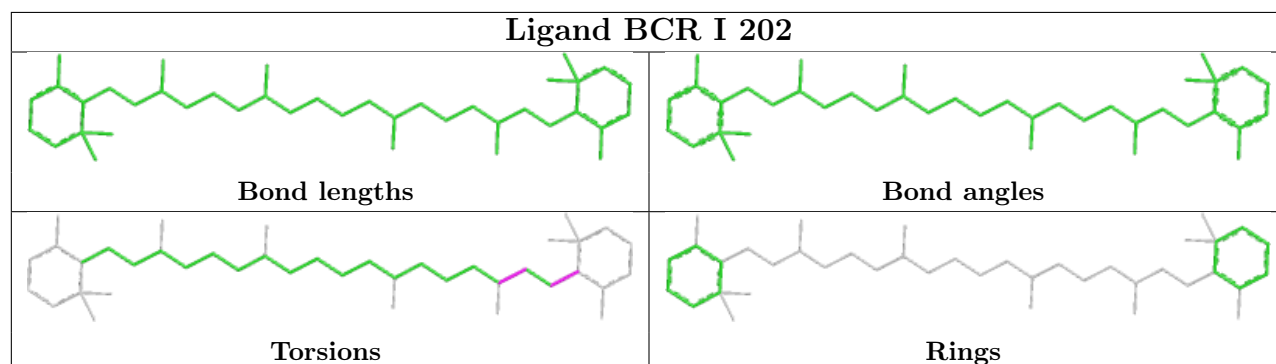
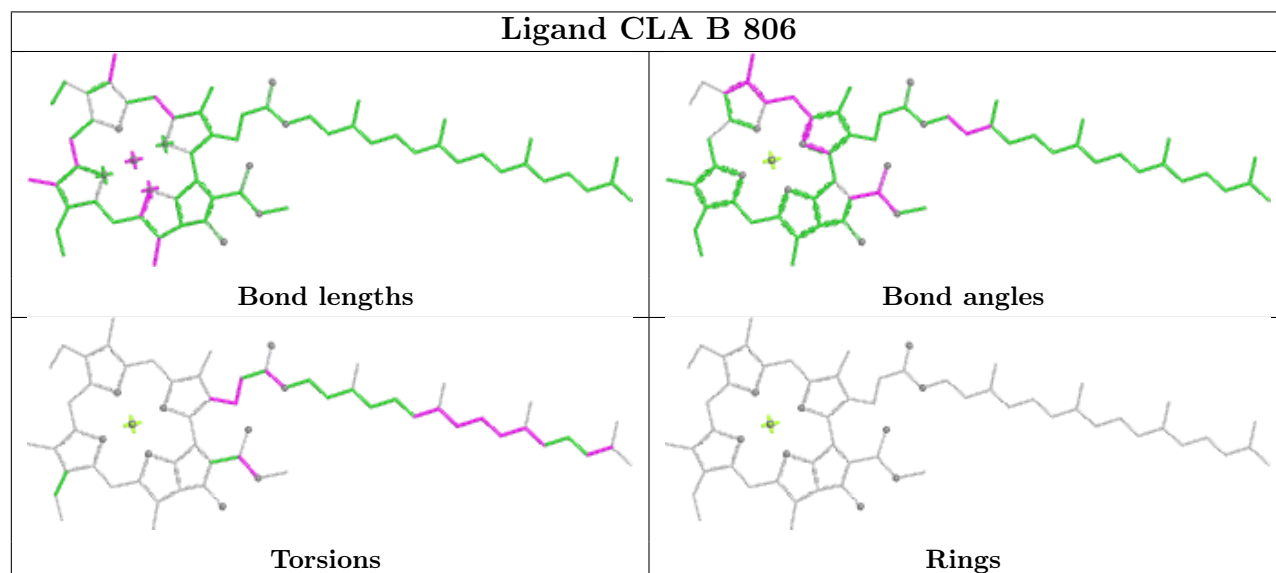
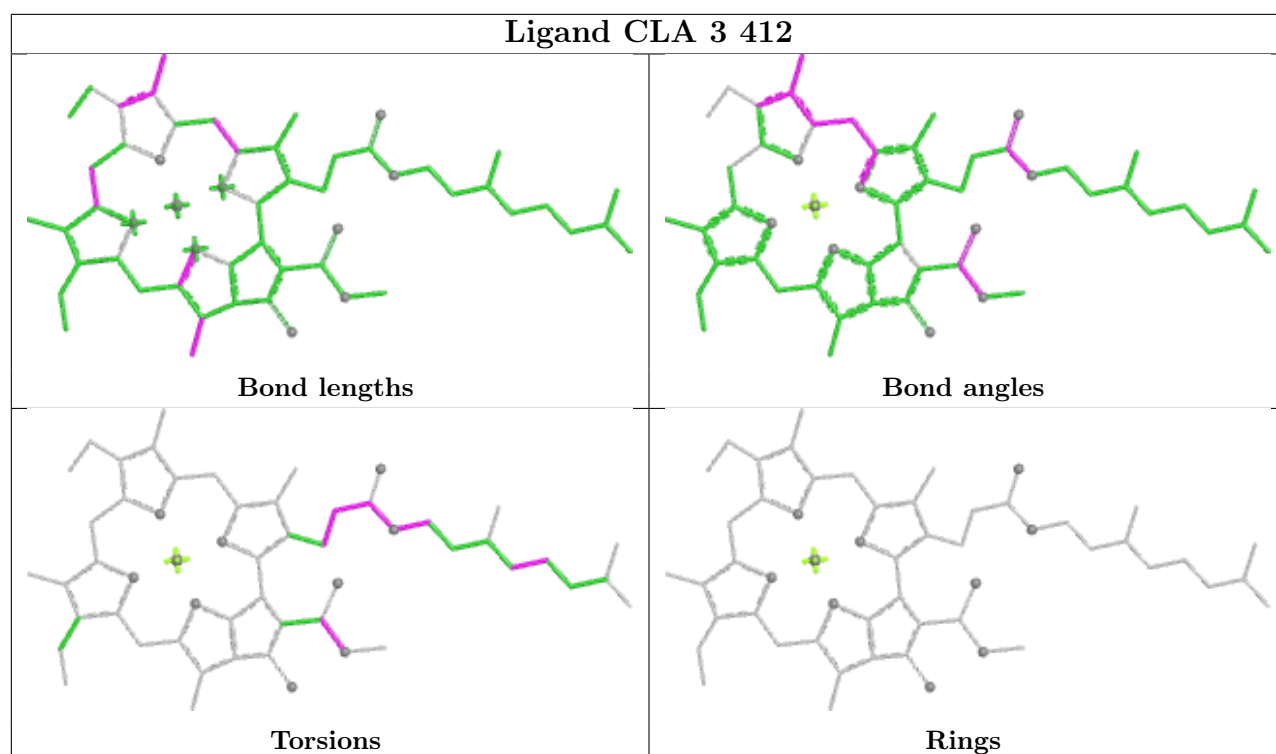
Bond angles



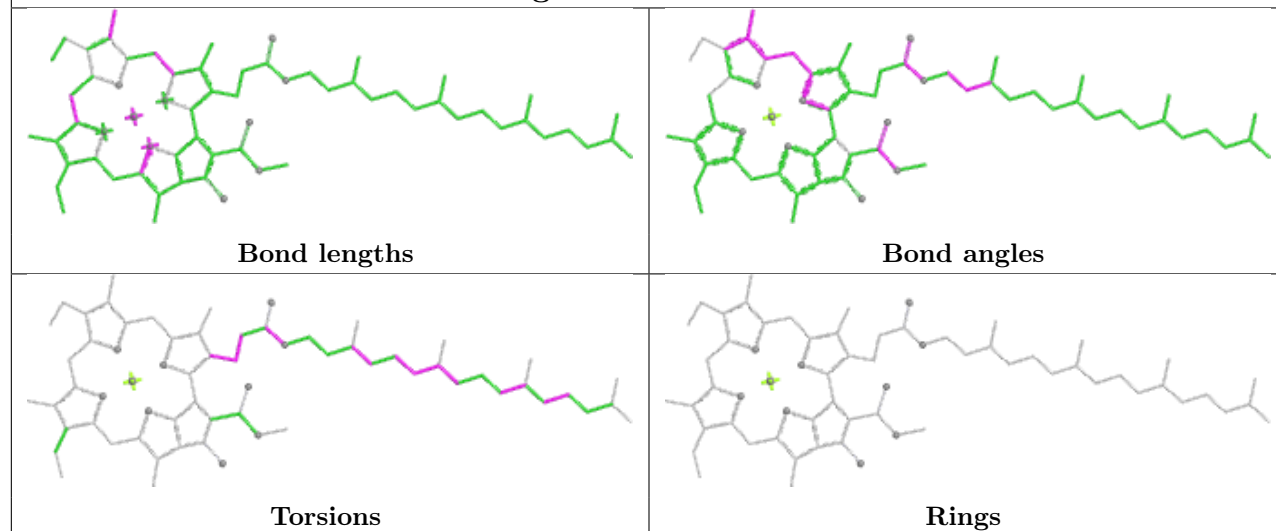
Torsions



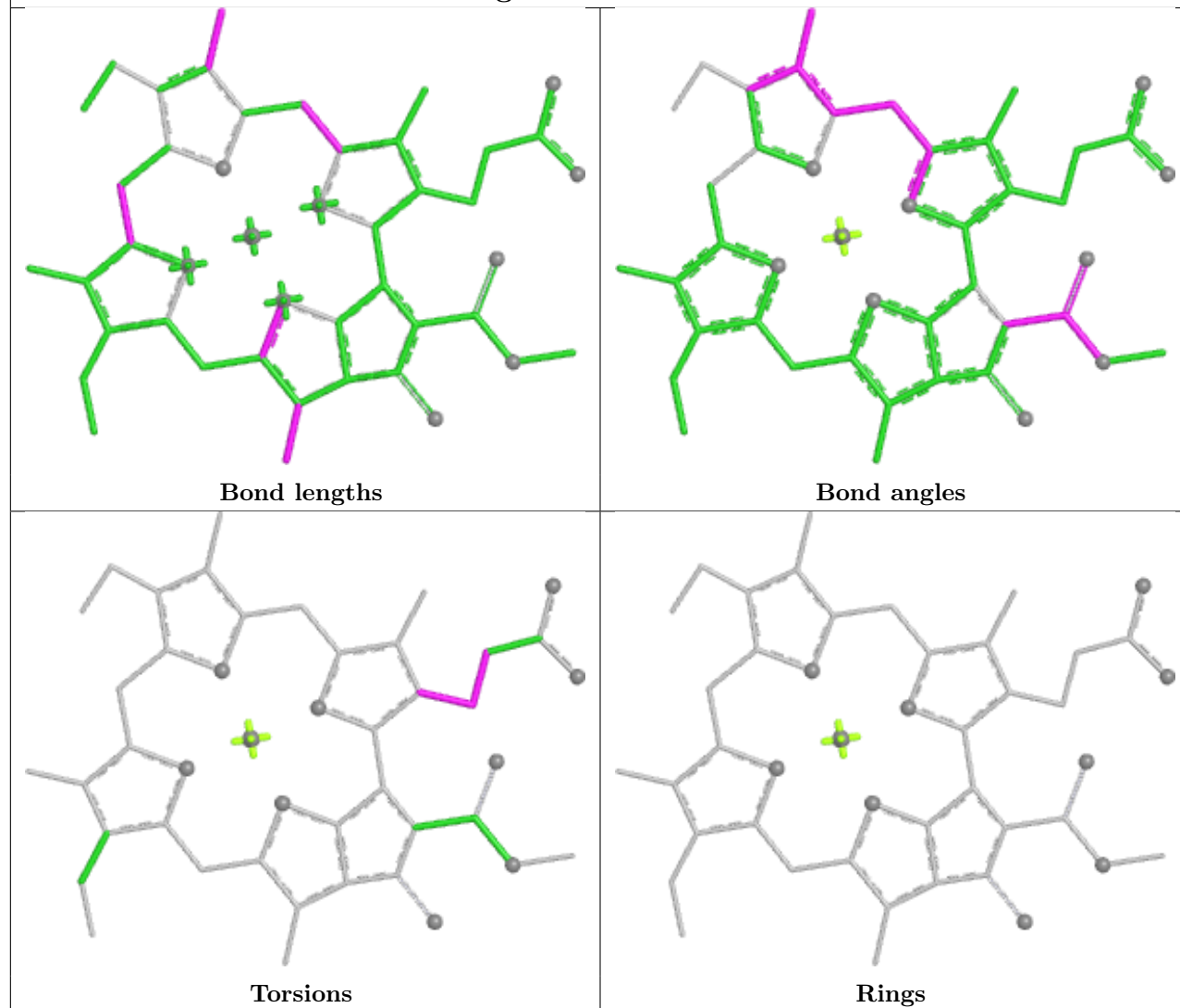
Rings



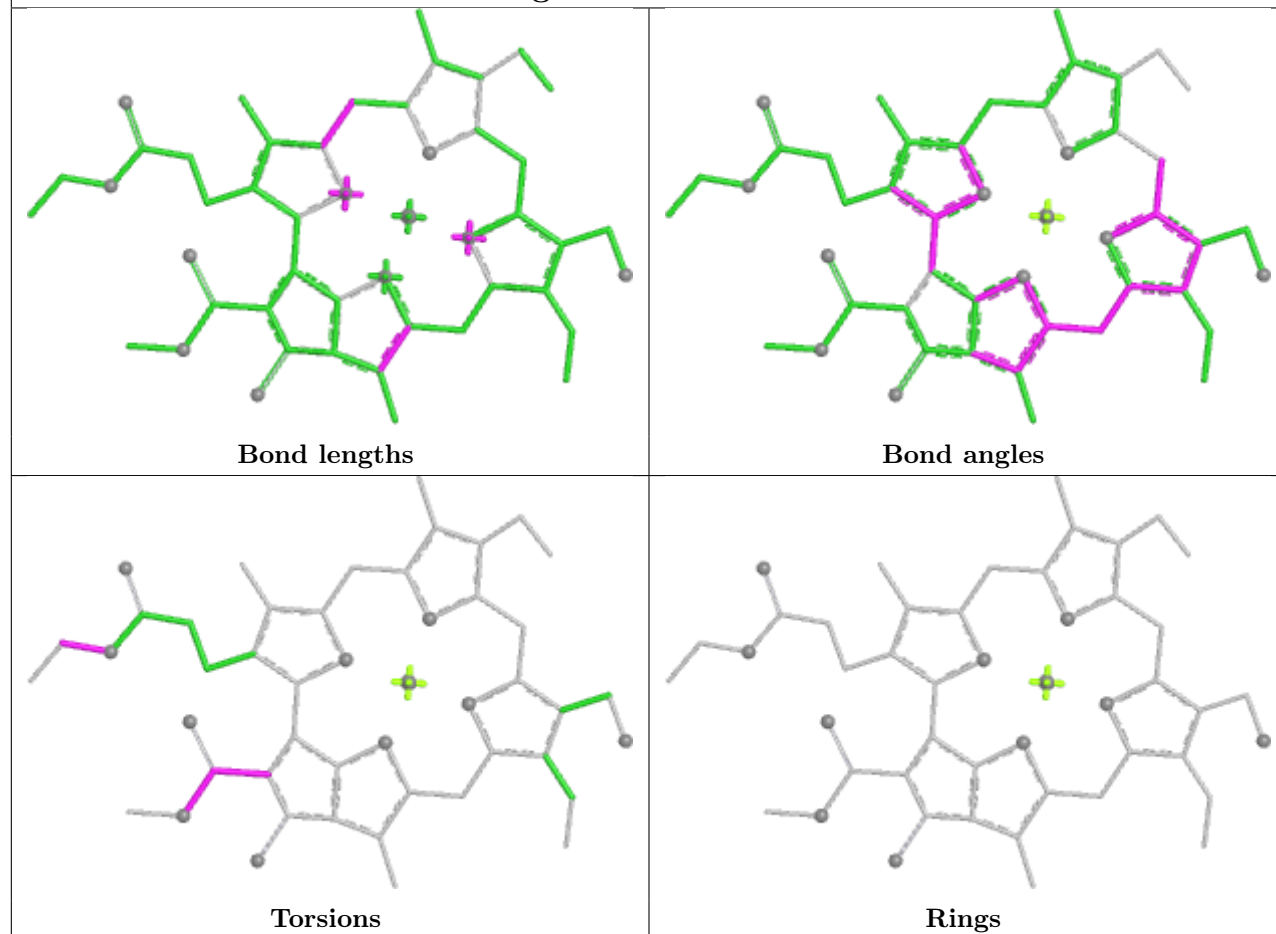
Ligand CLA B 822



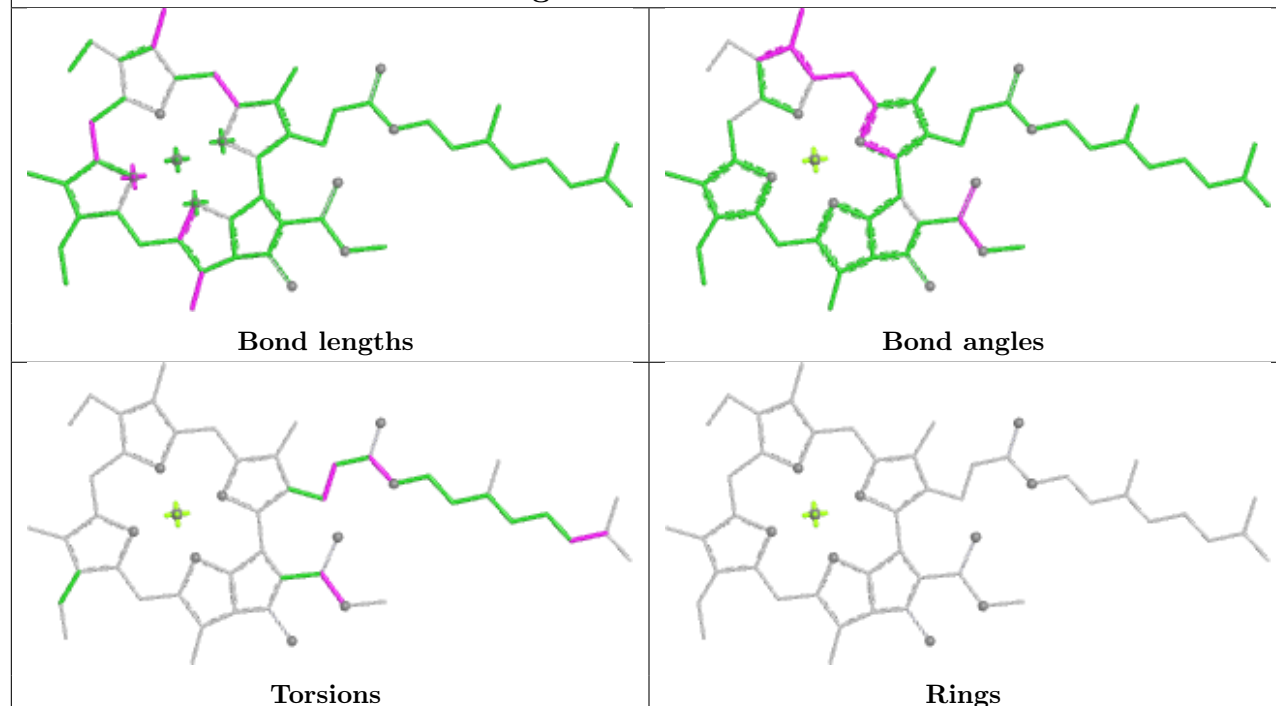
Ligand CLA 2 608



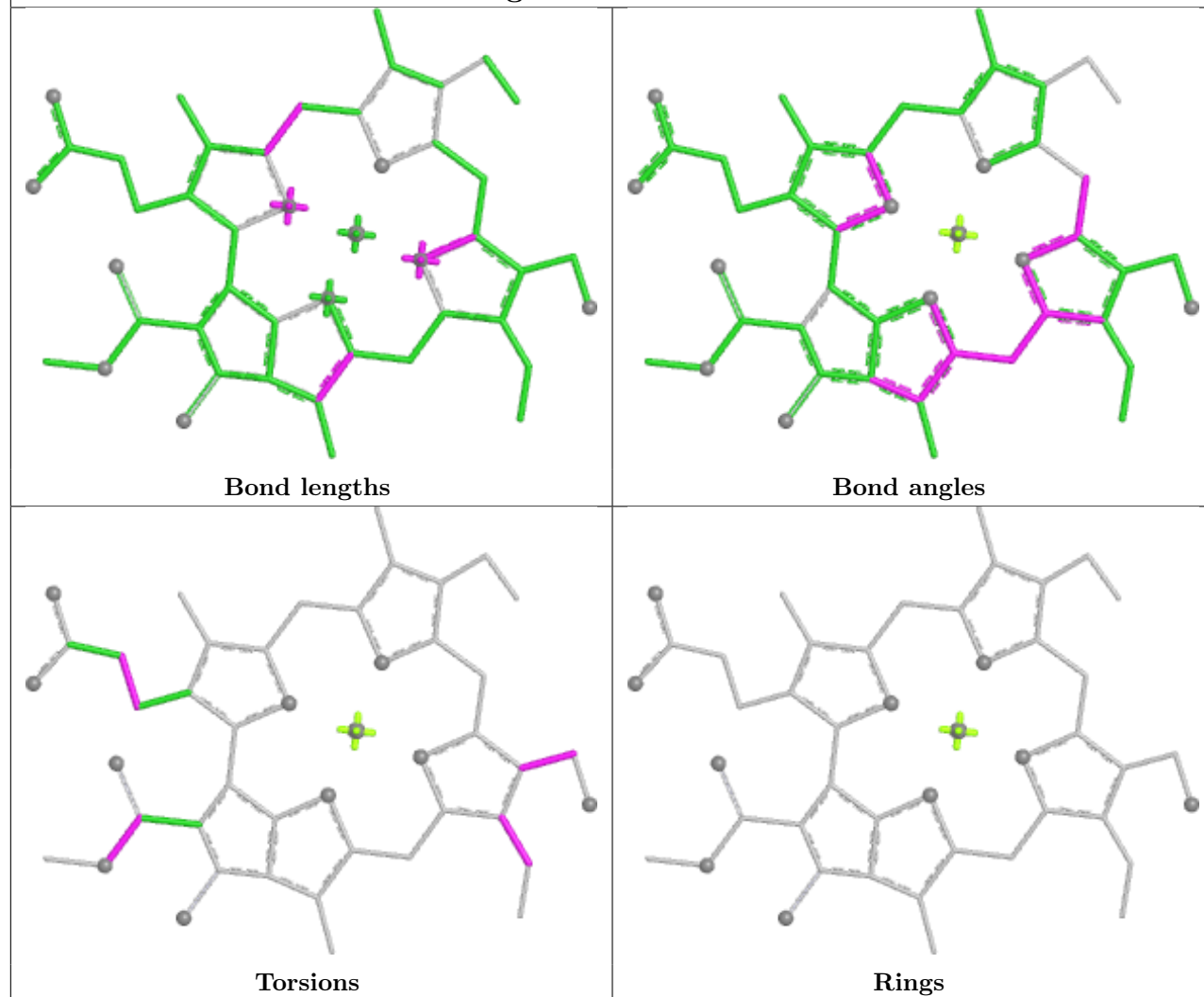
Ligand CHL T 601



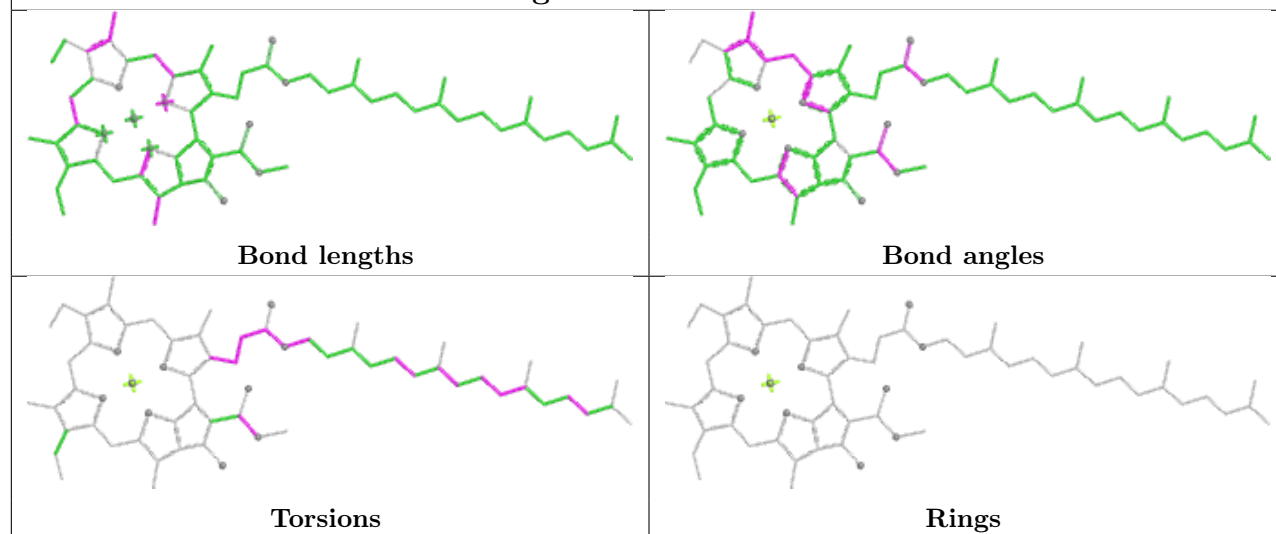
Ligand CLA B 811

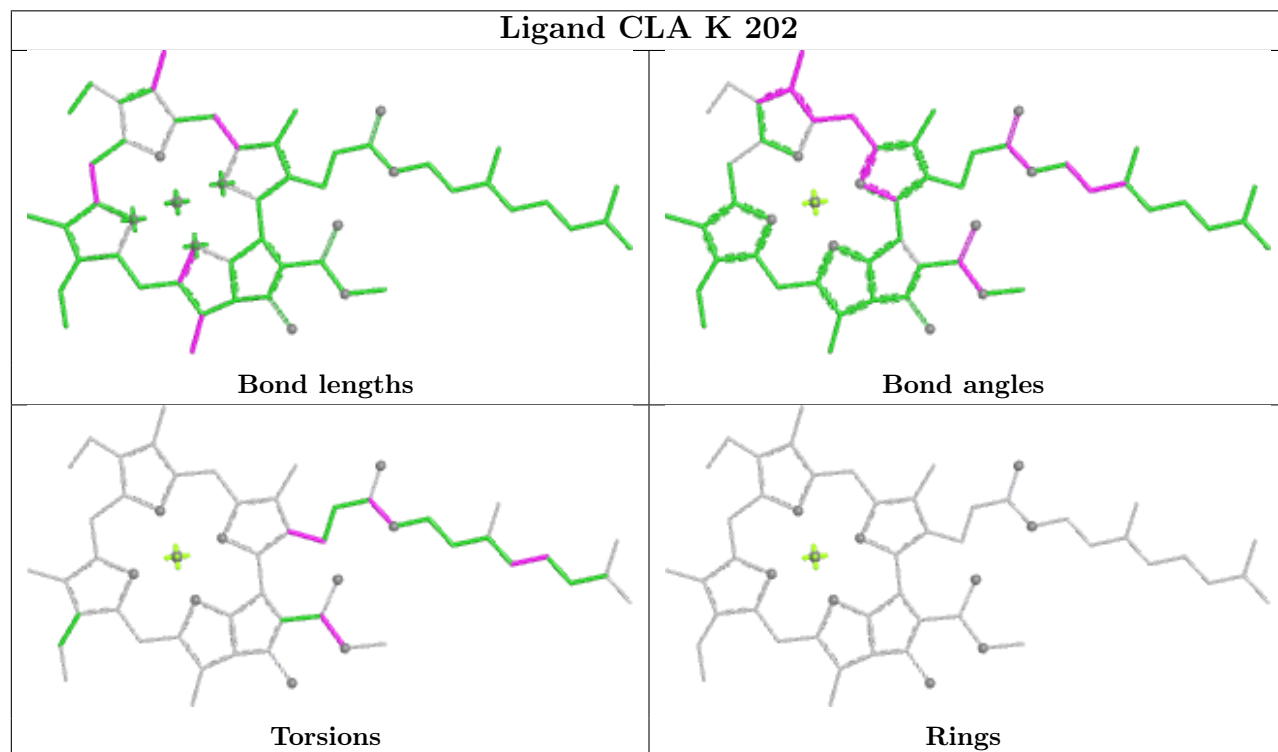
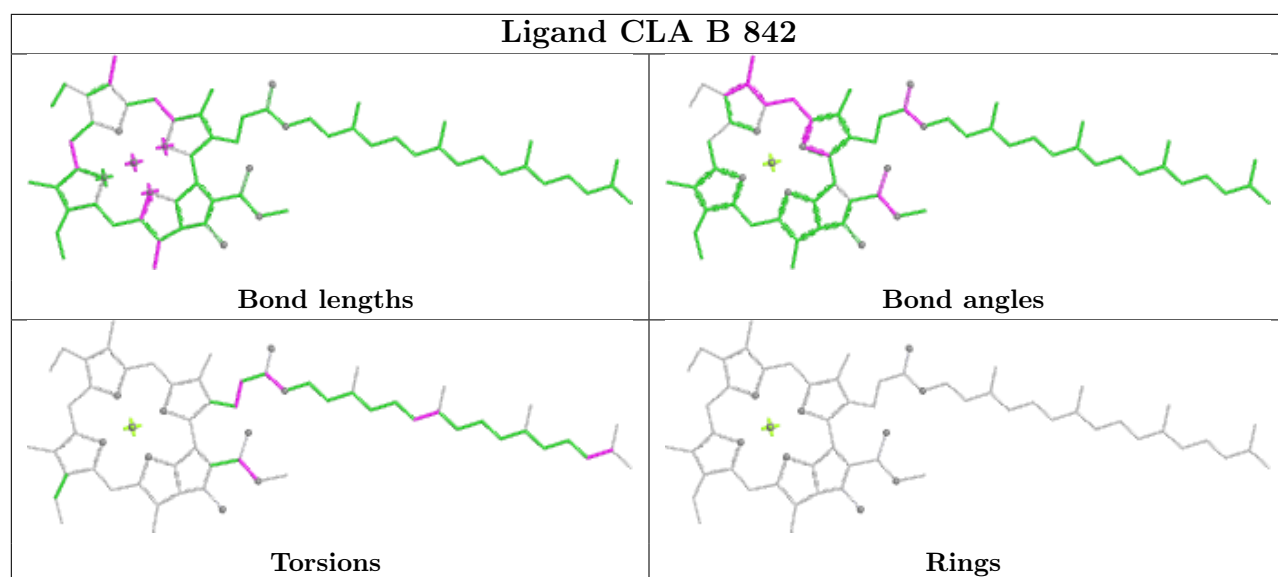


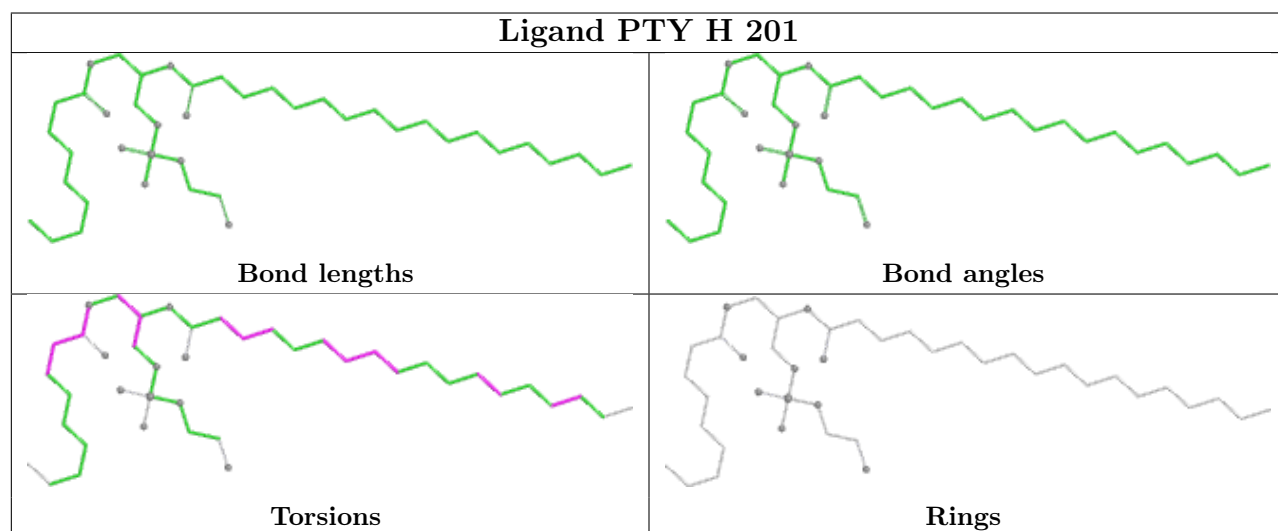
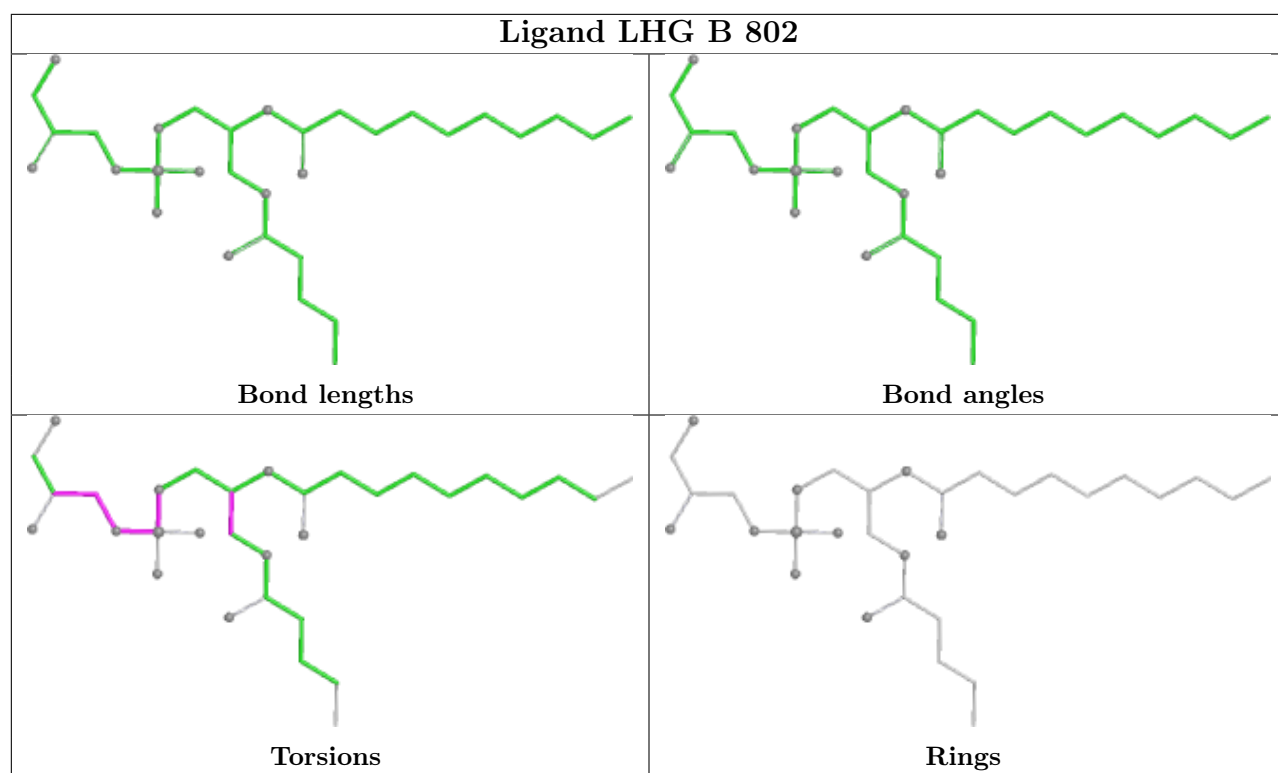
Ligand CHL c 605

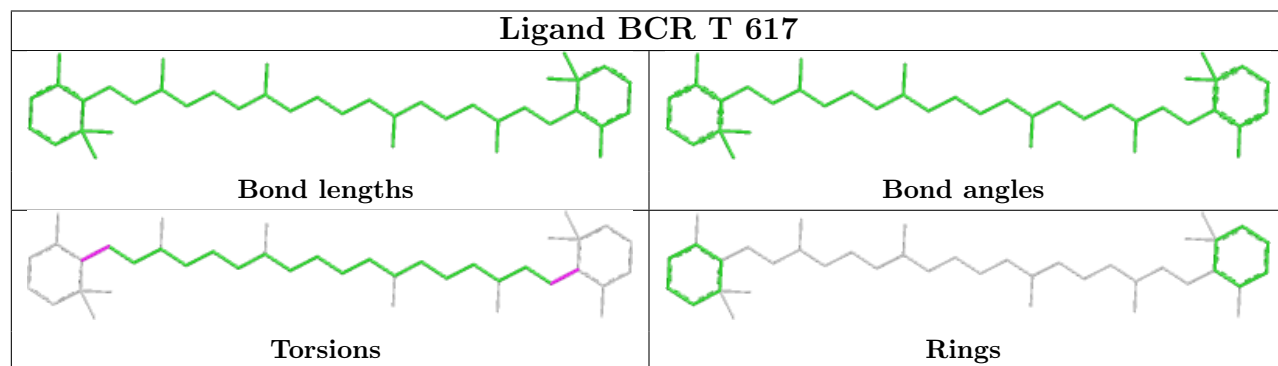
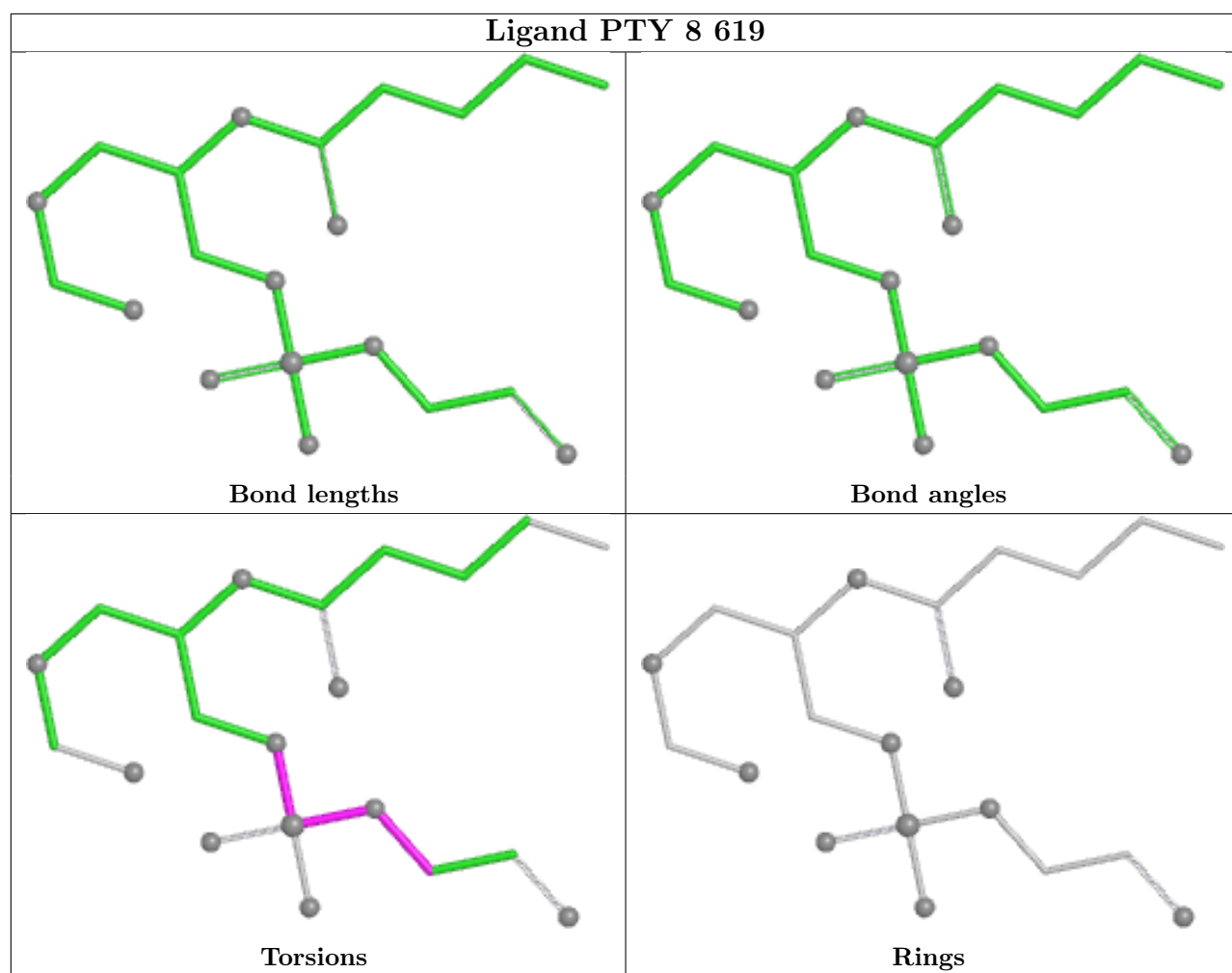


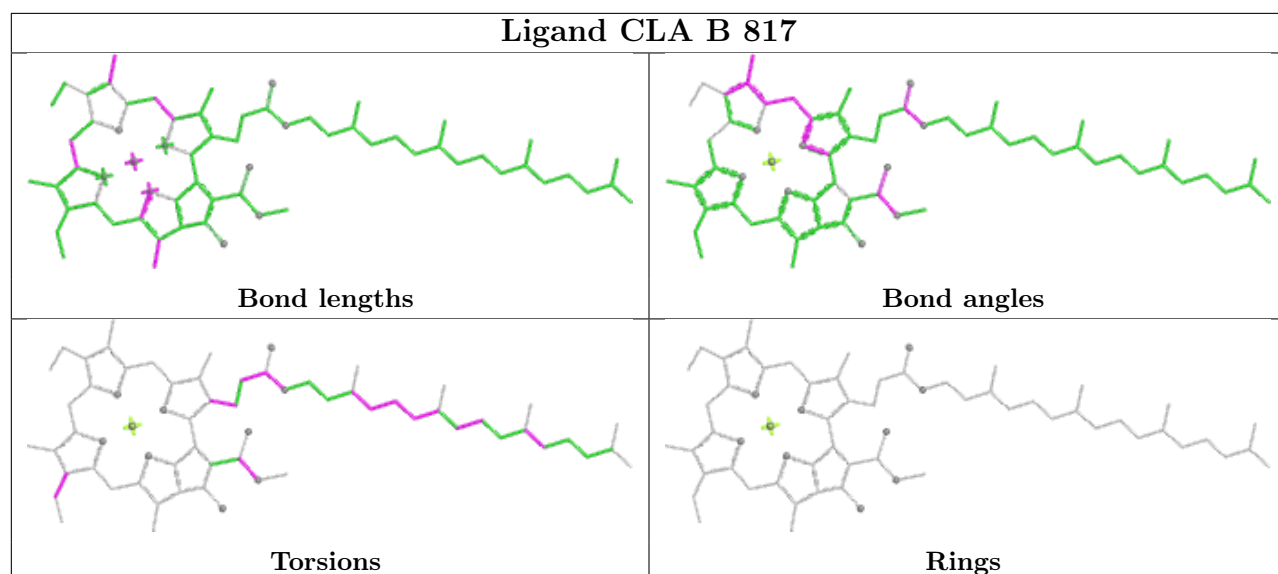
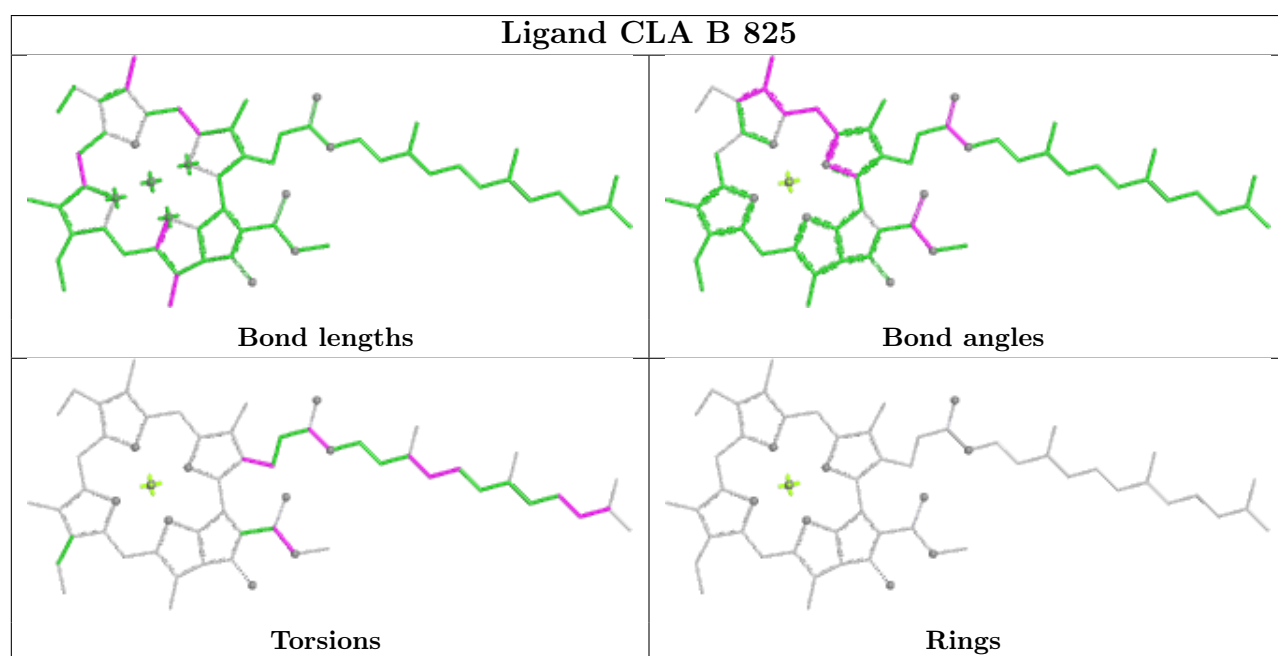
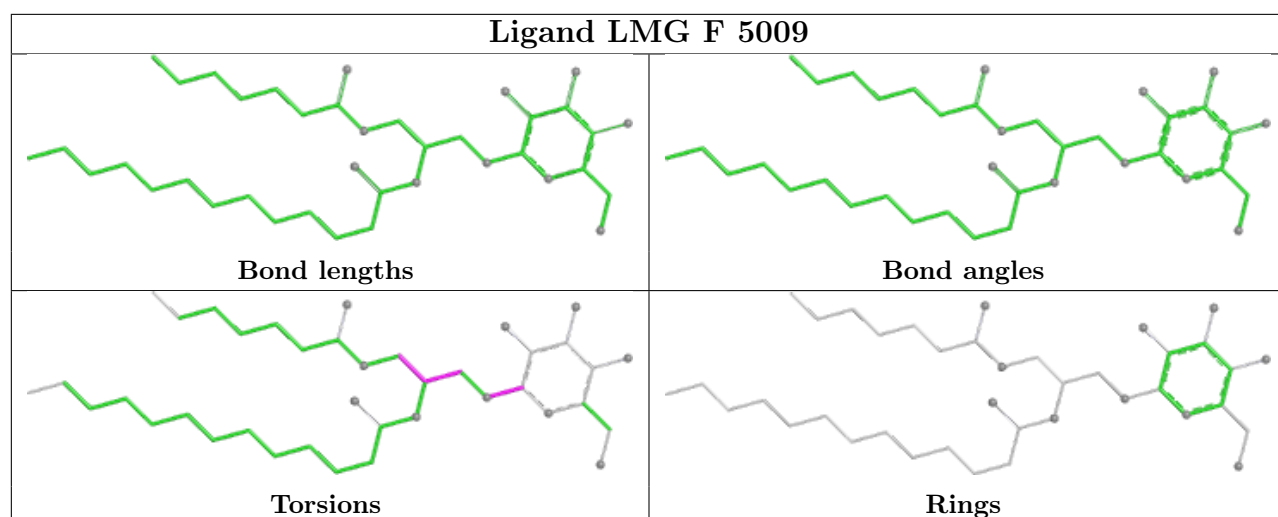
Ligand CLA B 832

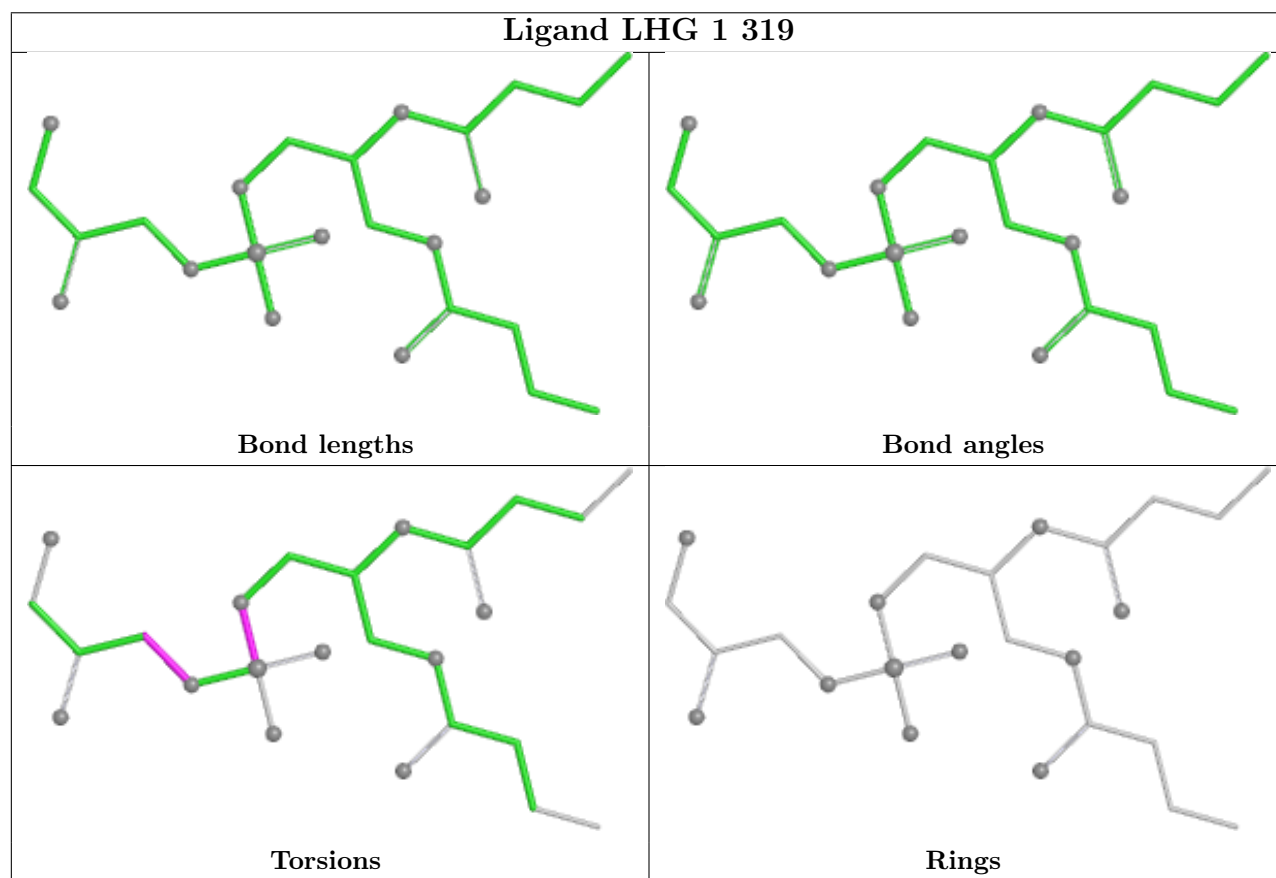
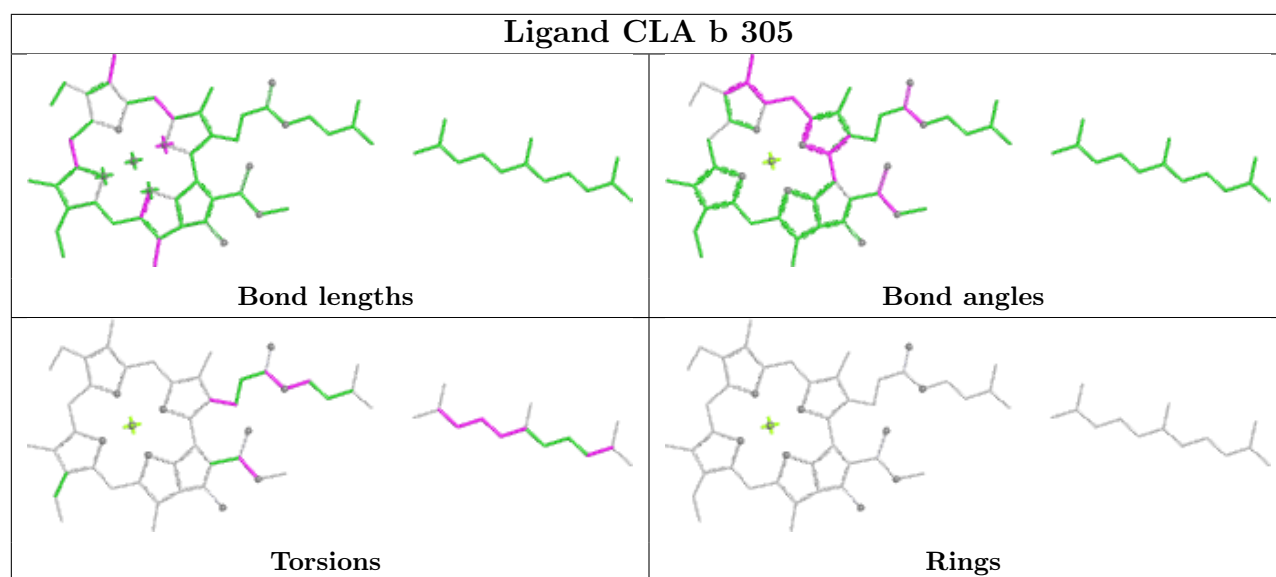




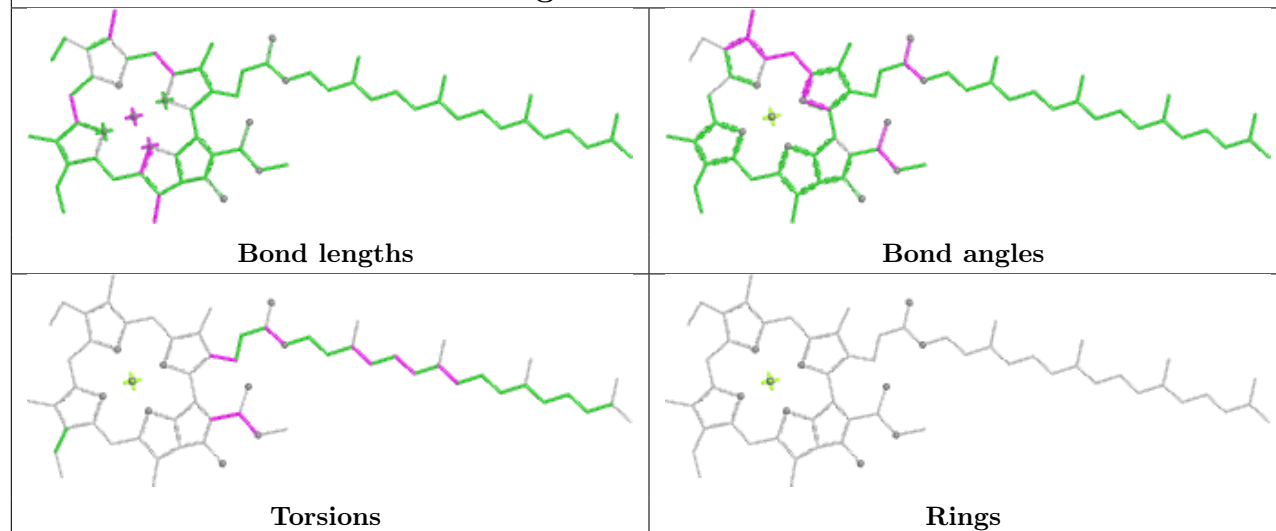




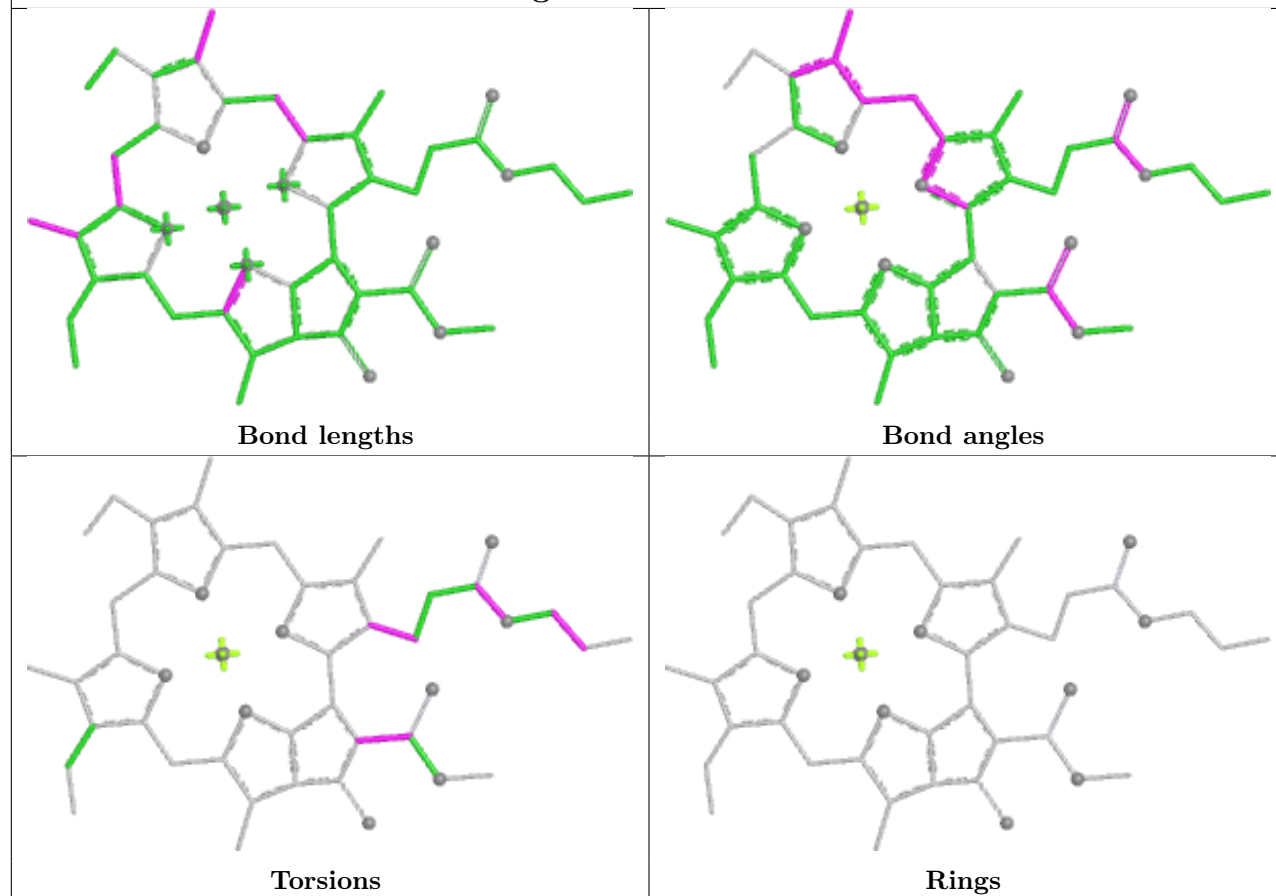


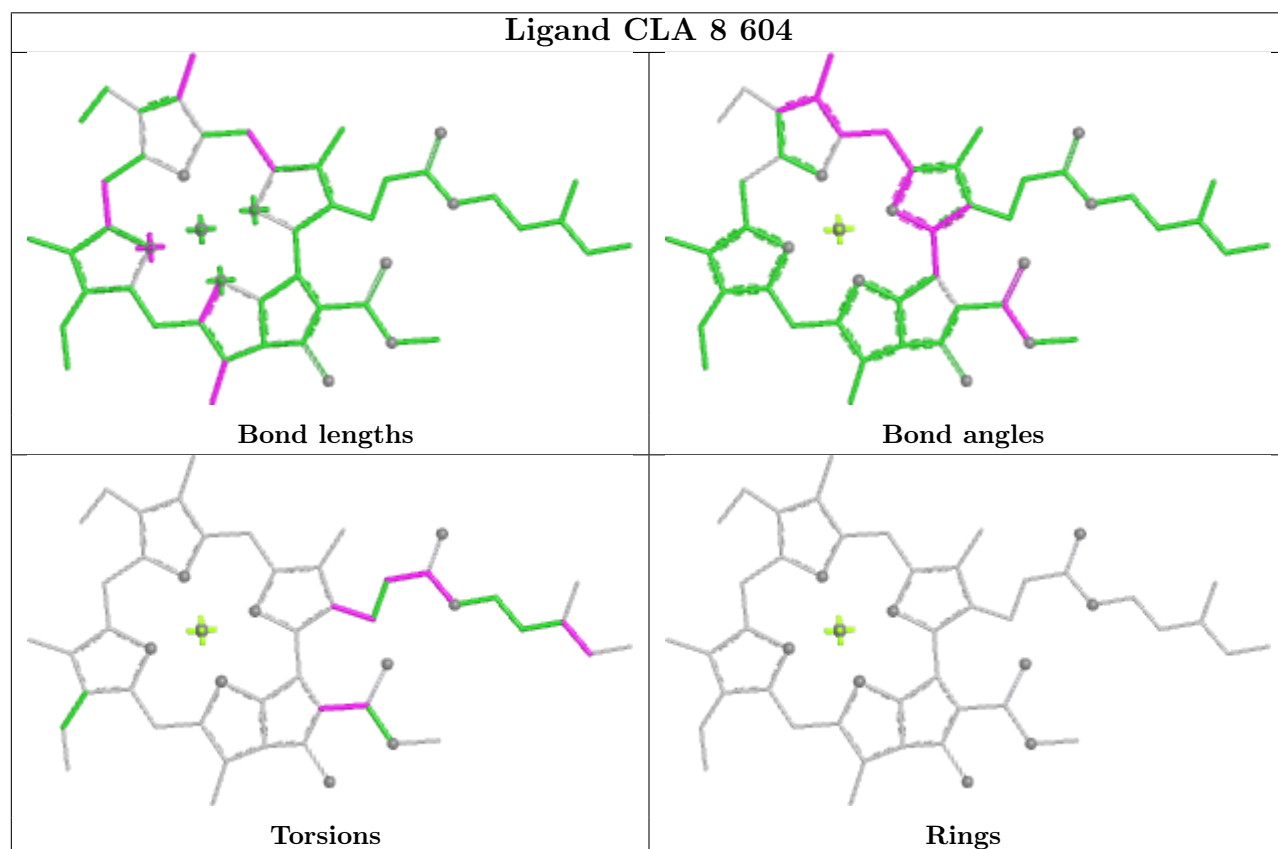
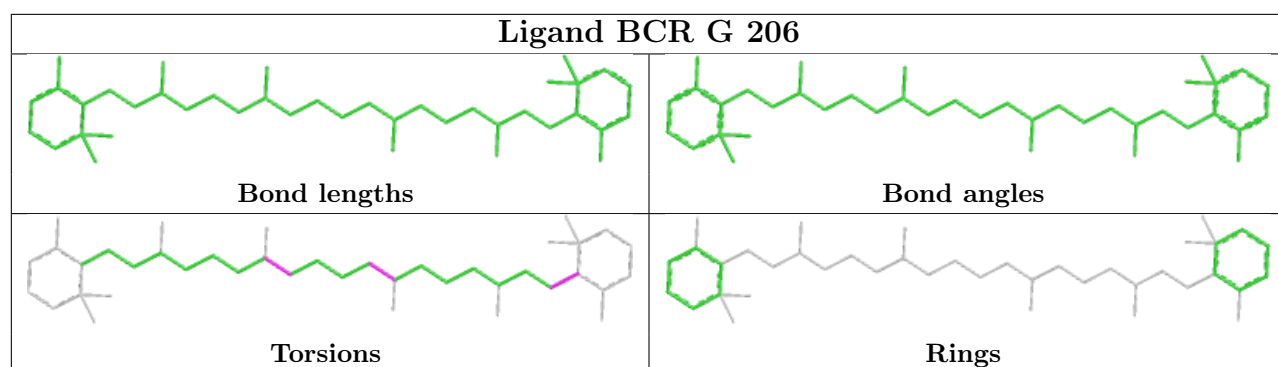


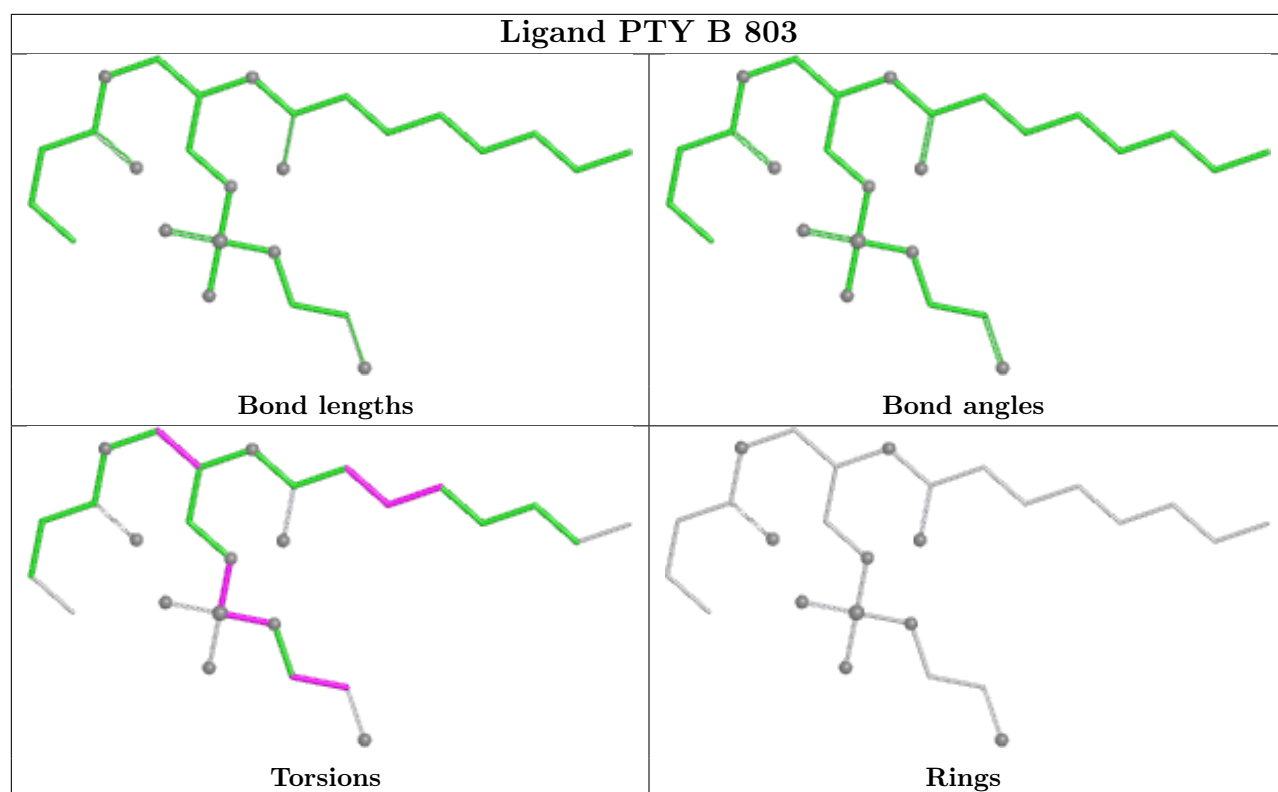
Ligand CLA 3 407



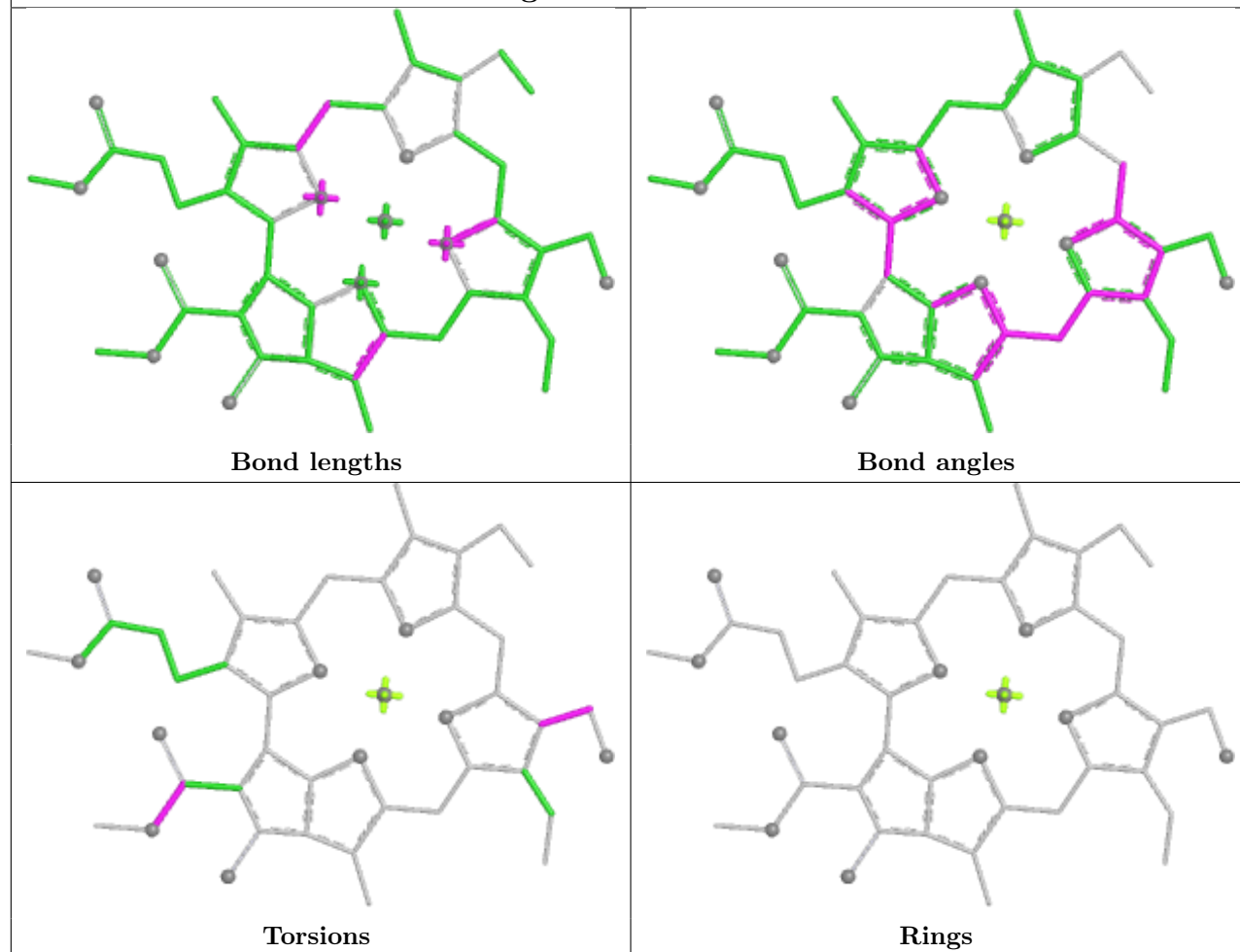
Ligand CLA B 808



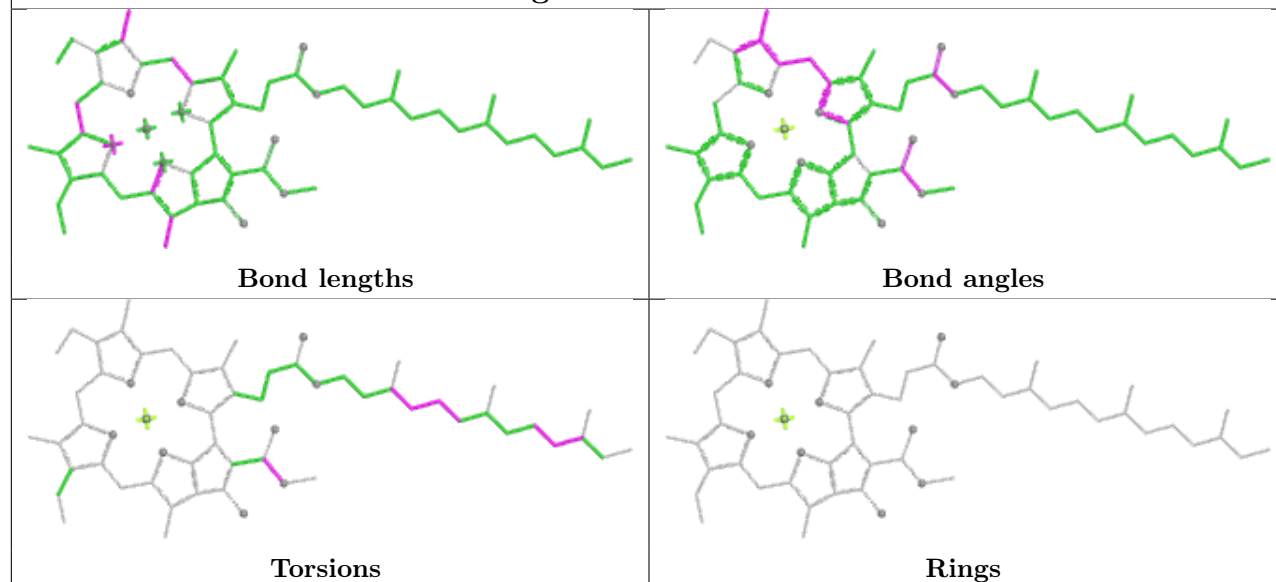


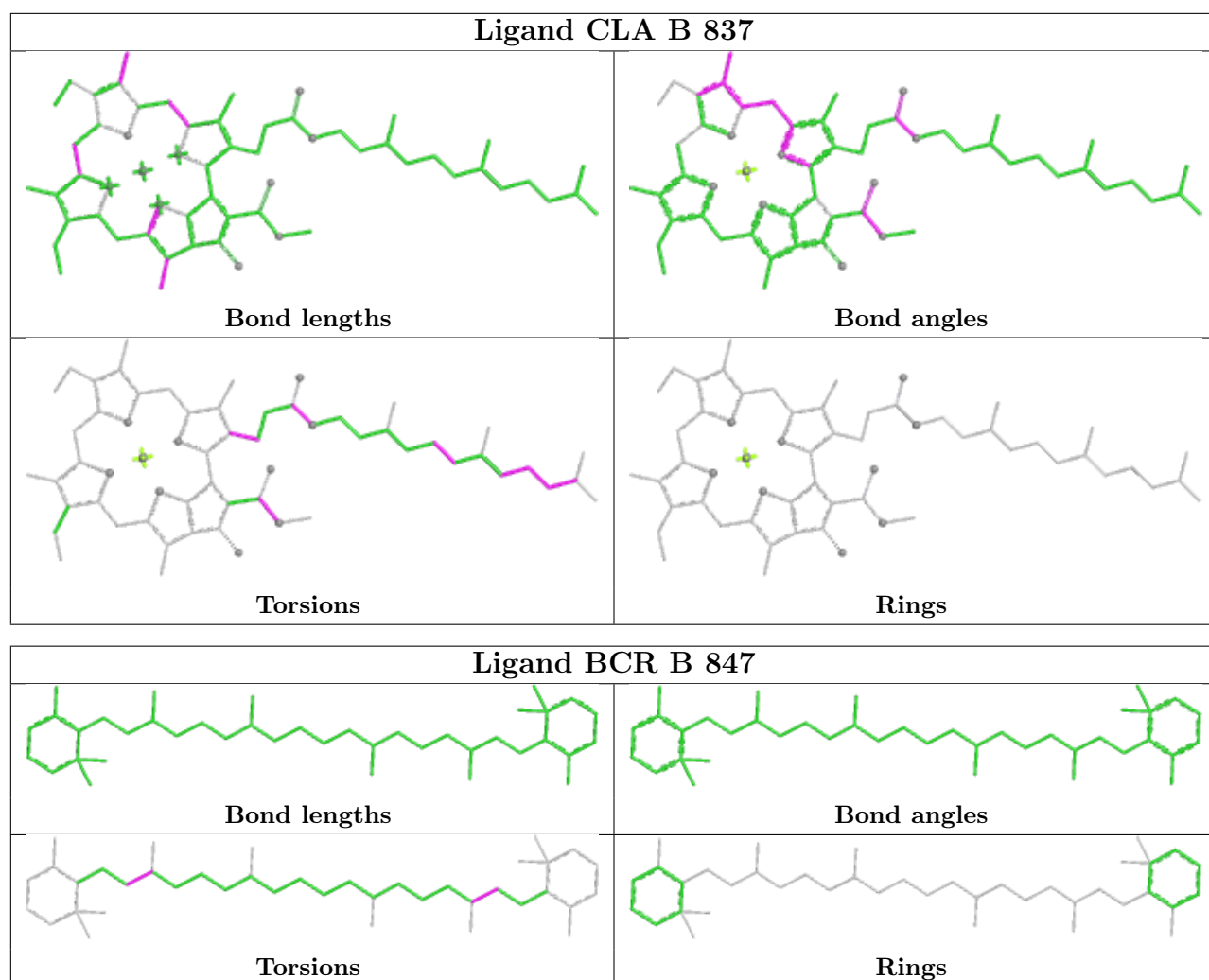


Ligand CHL a 306

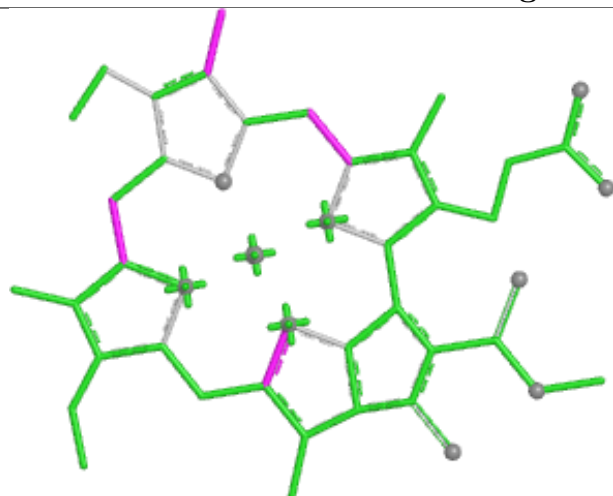


Ligand CLA A 856

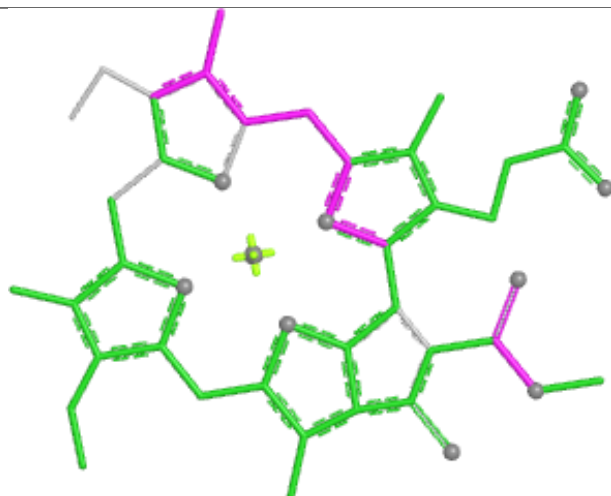




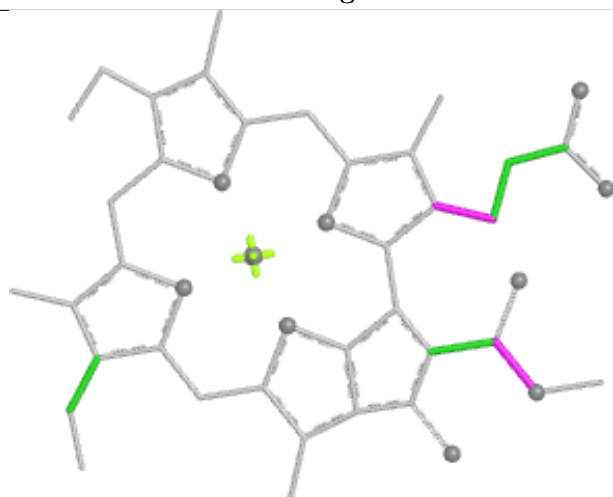
Ligand CLA c 614



Bond lengths



Bond angles

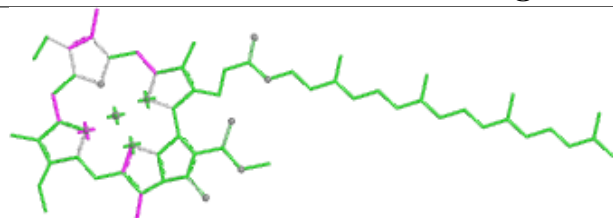


Torsions

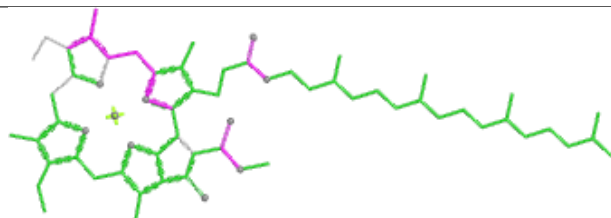


Rings

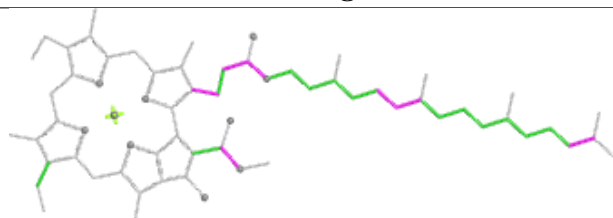
Ligand CLA B 843



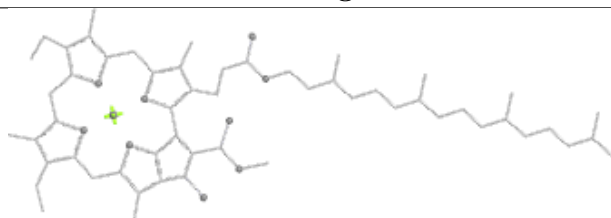
Bond lengths



Bond angles

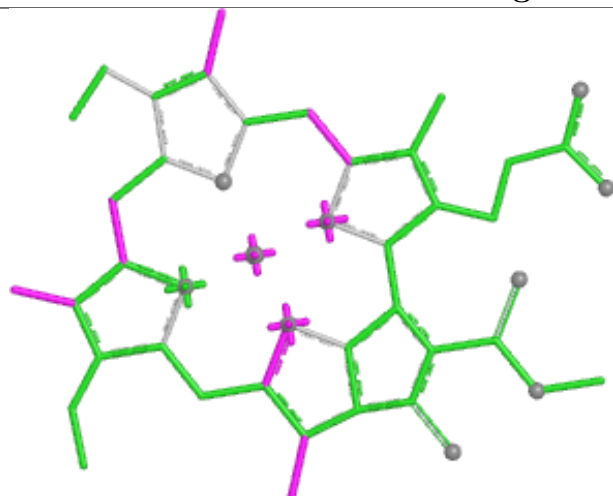


Torsions

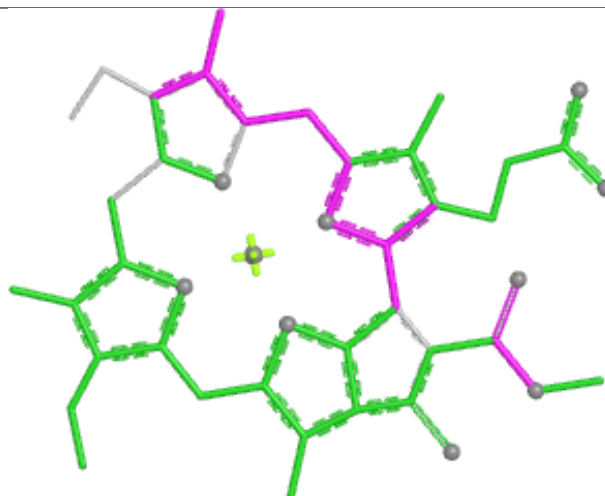


Rings

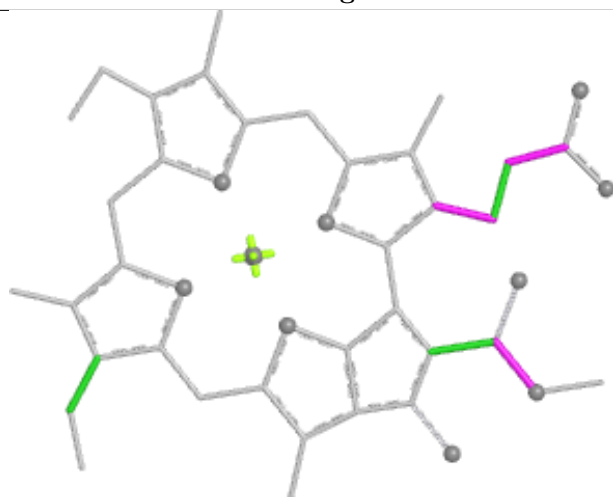
Ligand CLA K 203



Bond lengths



Bond angles

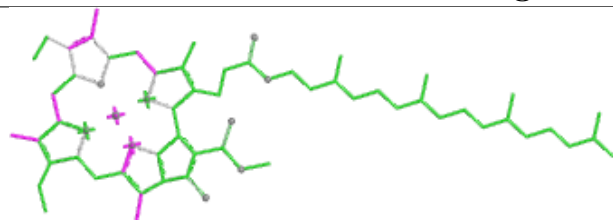


Torsions

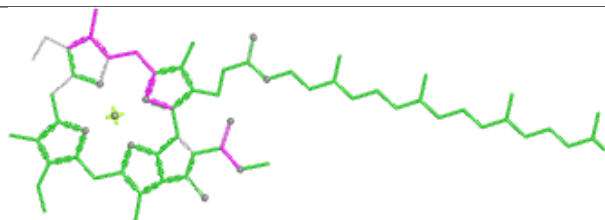


Rings

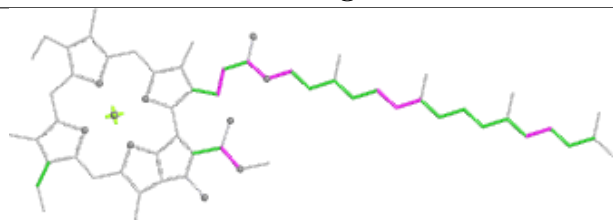
Ligand CLA A 804



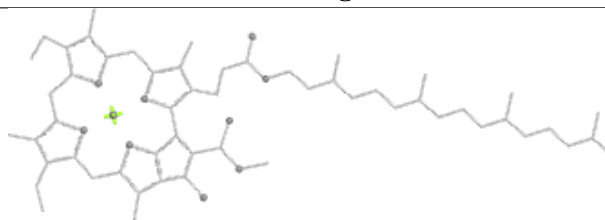
Bond lengths



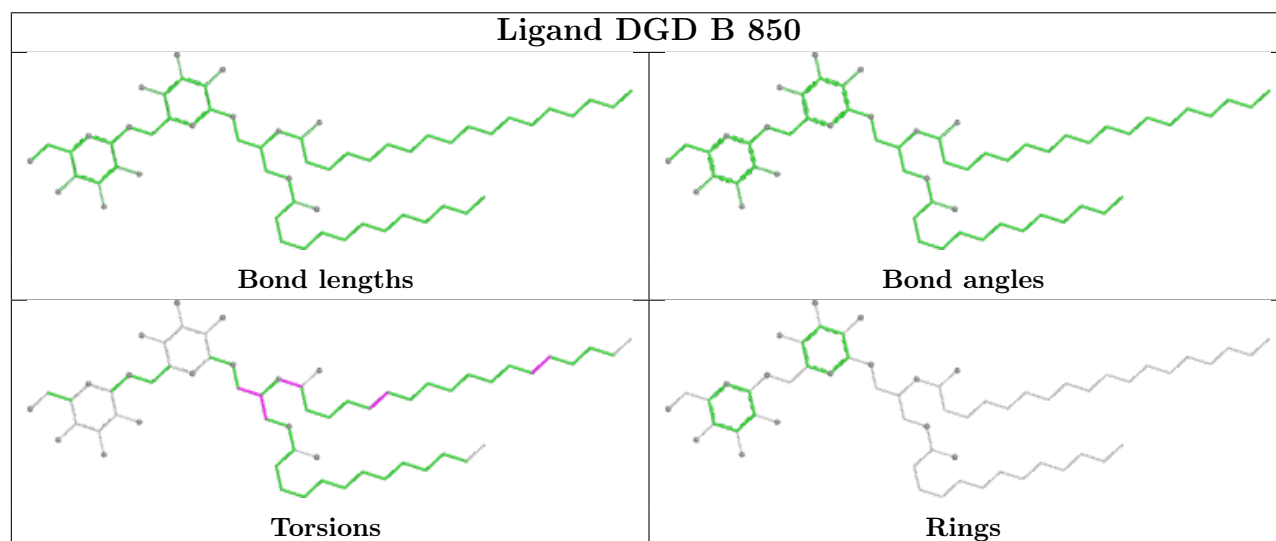
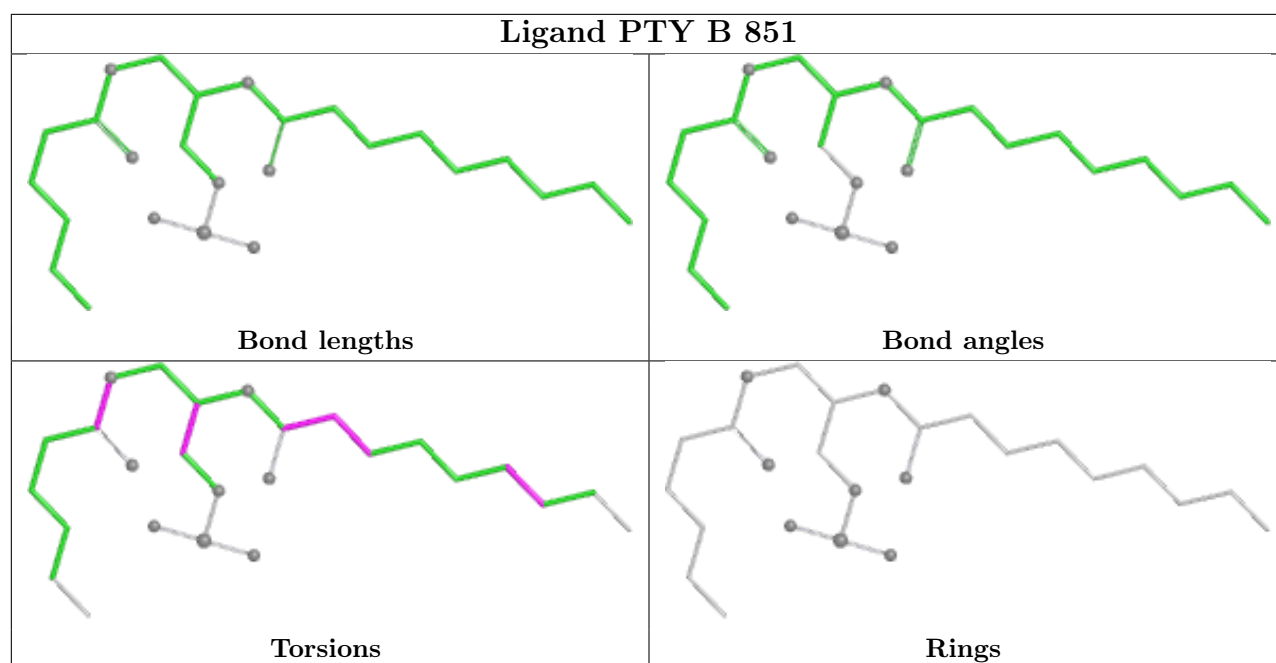
Bond angles



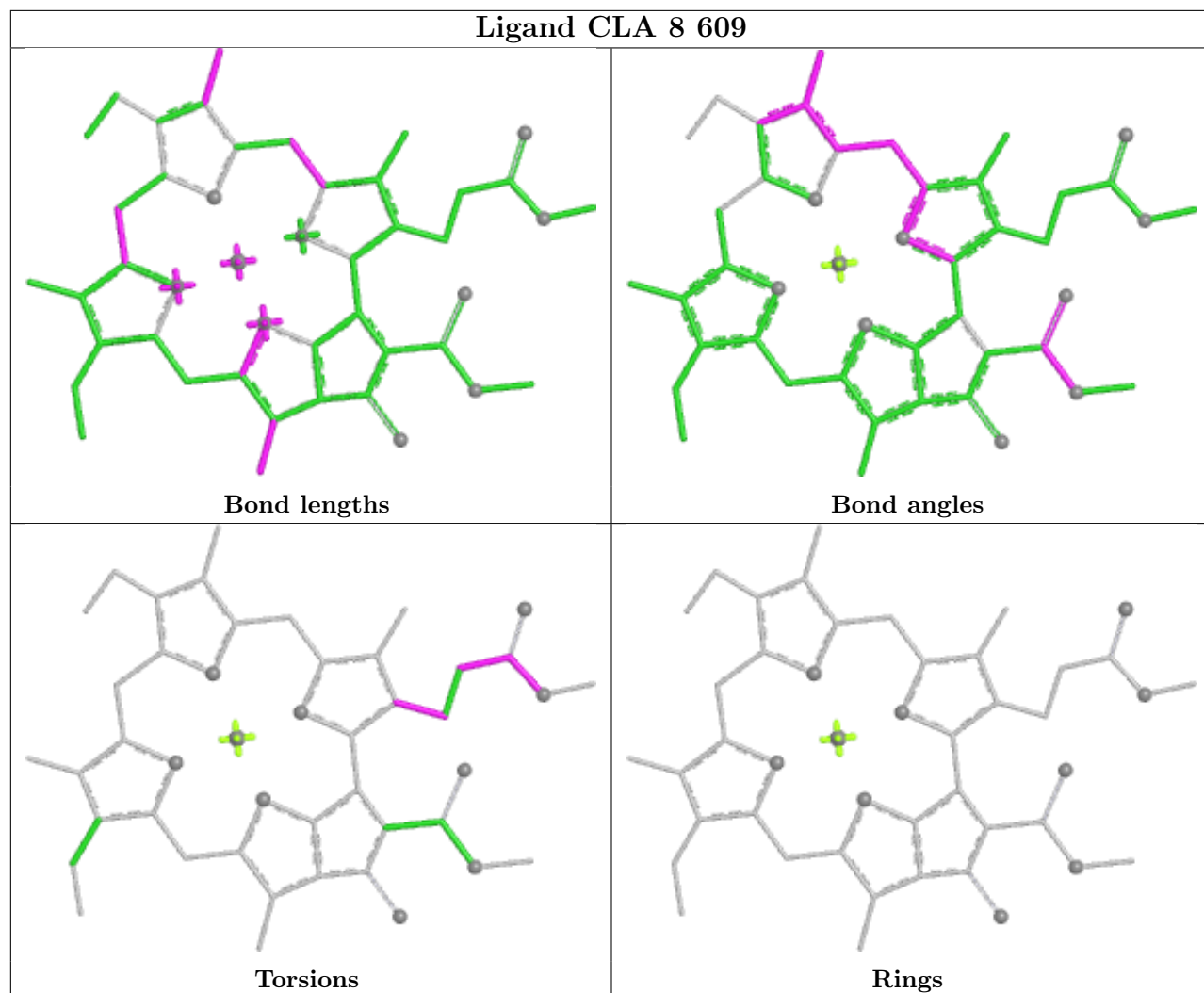
Torsions



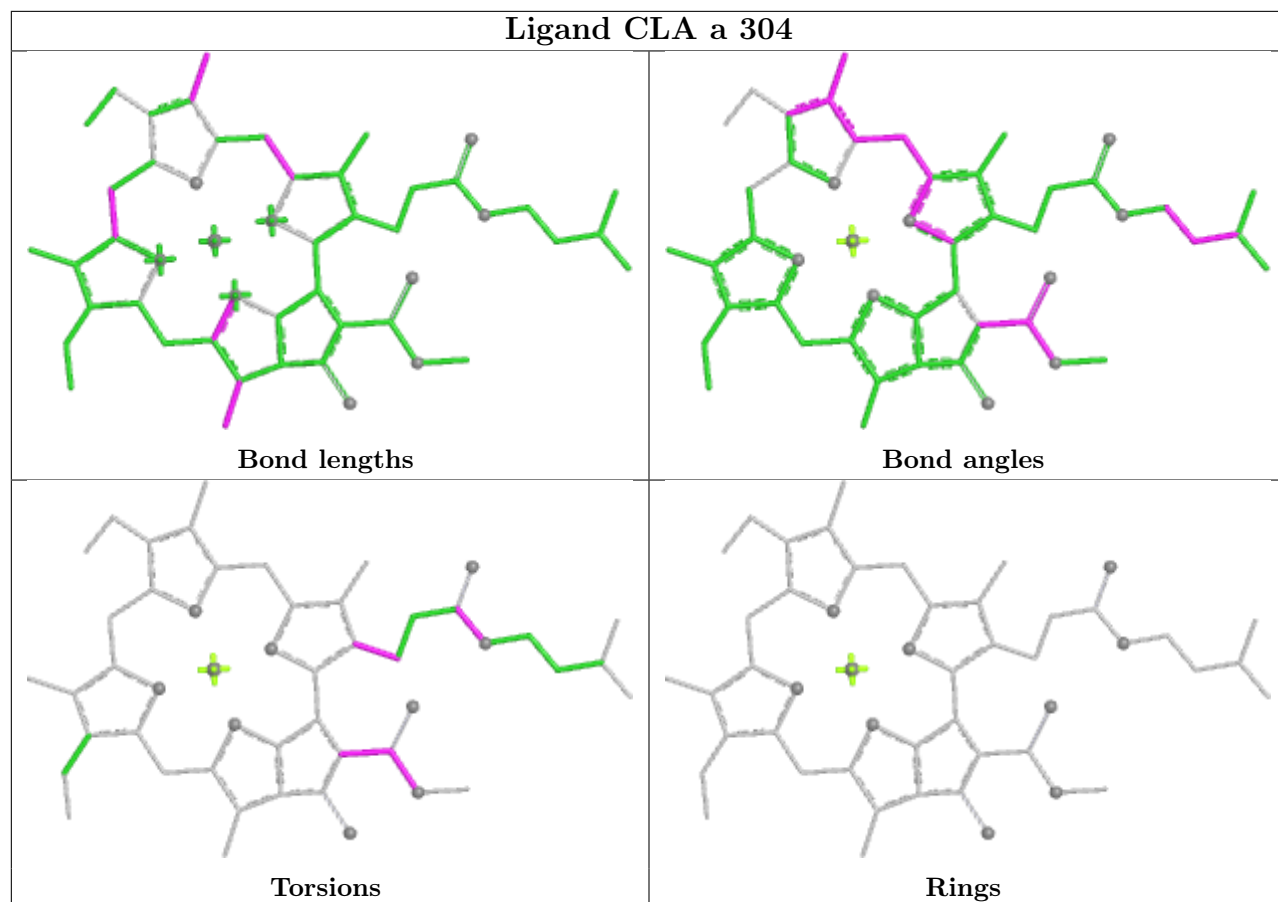
Rings



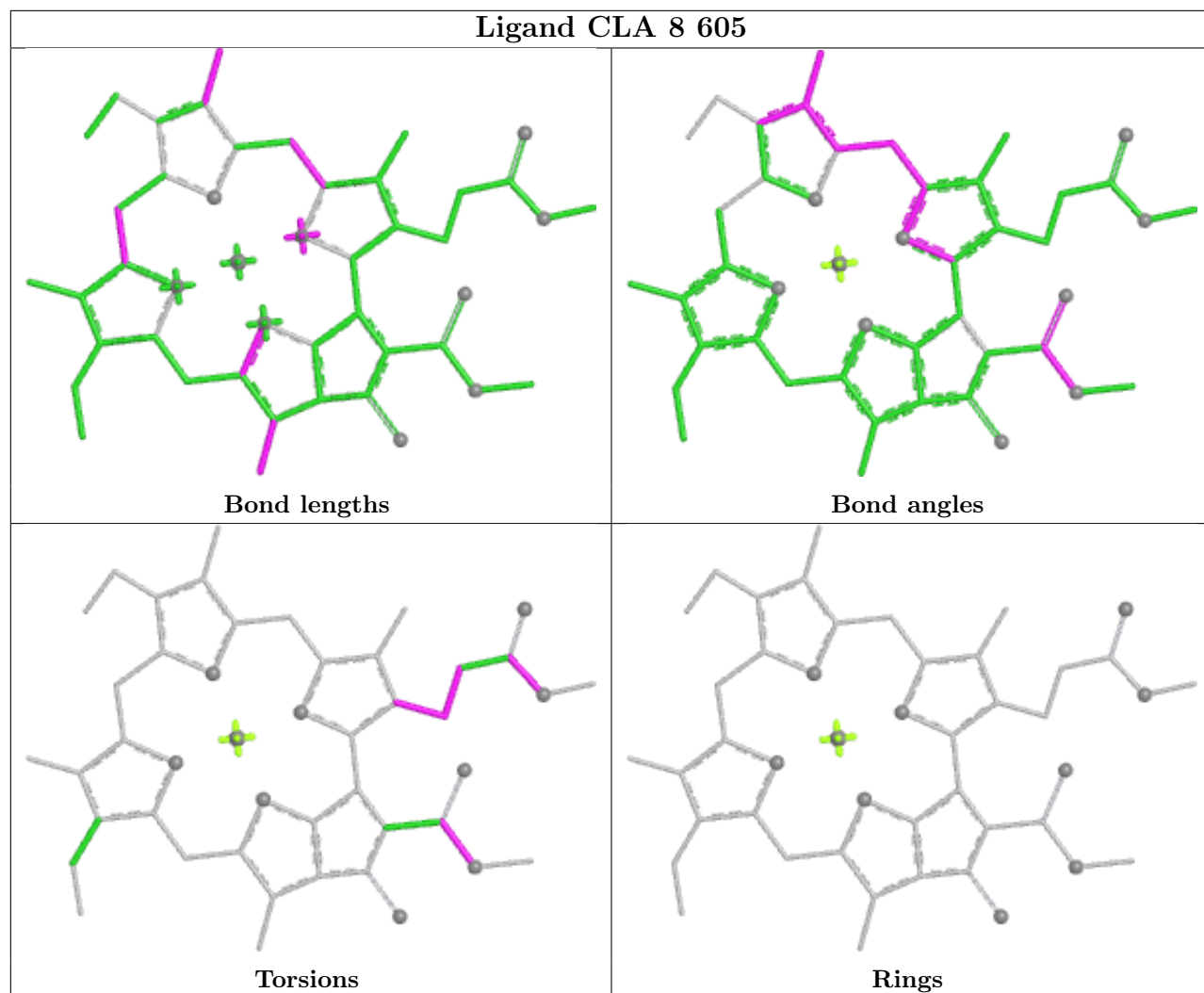
Ligand CLA 8 609

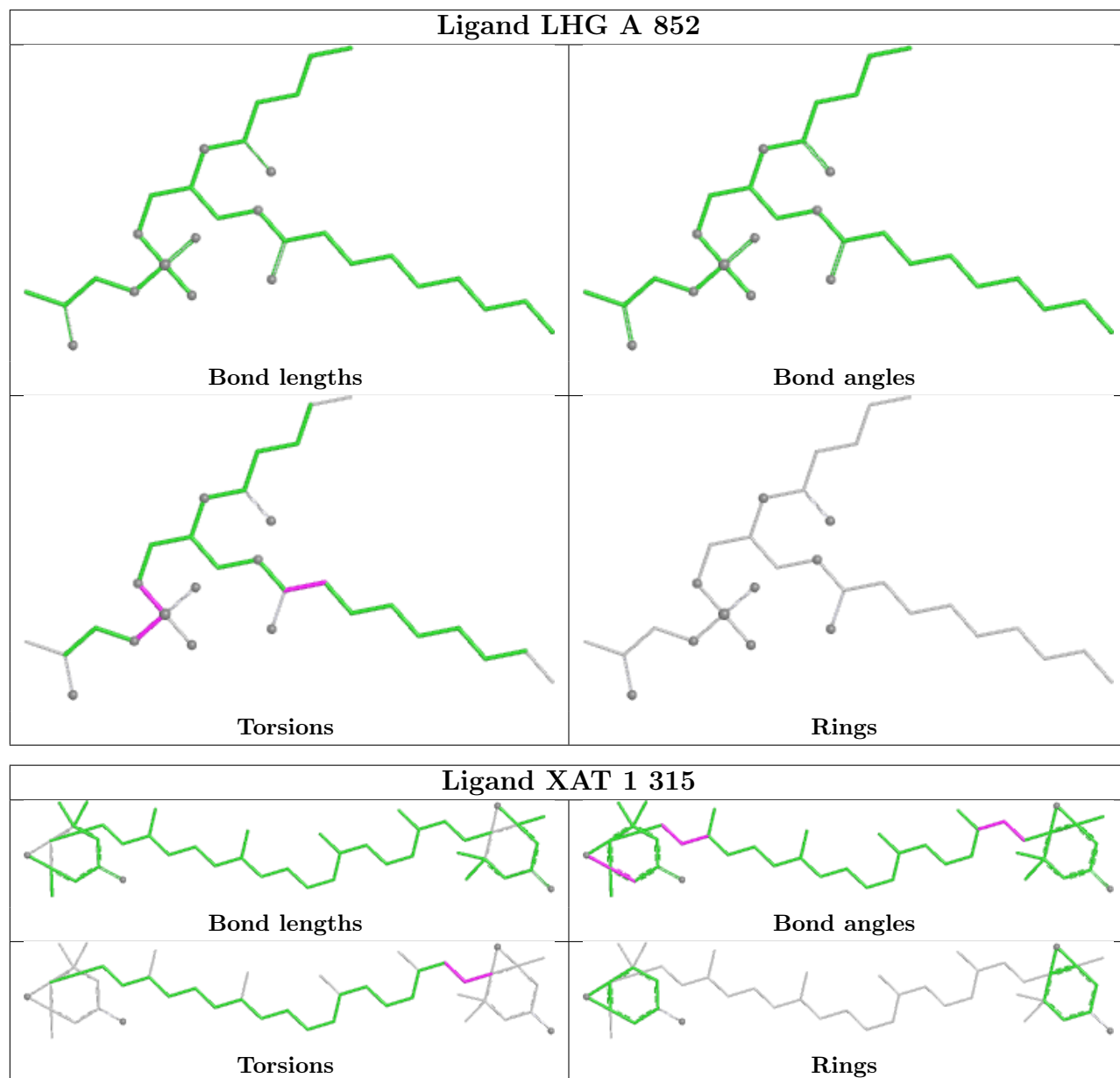


Ligand CLA a 304

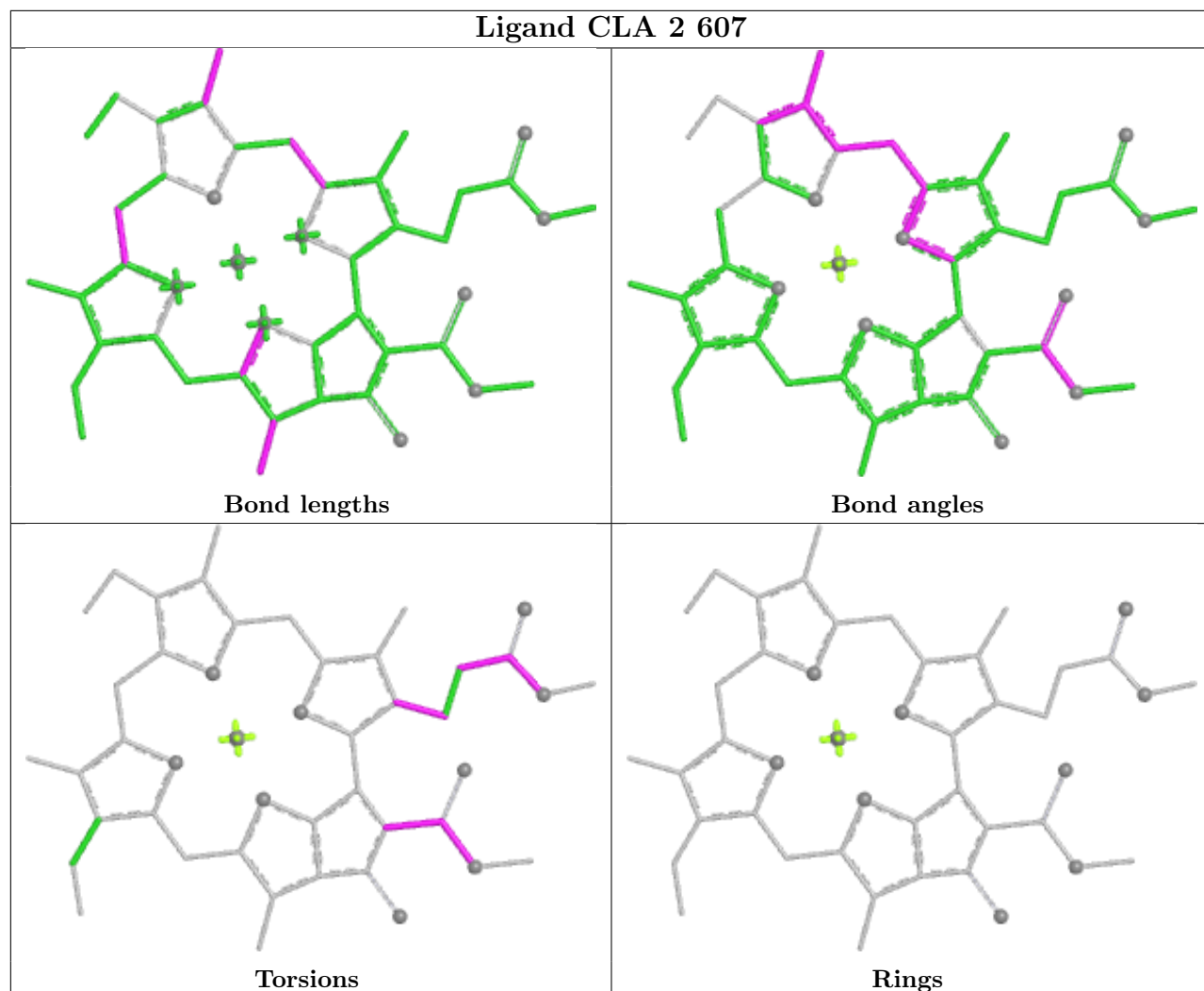


Ligand CLA 8 605

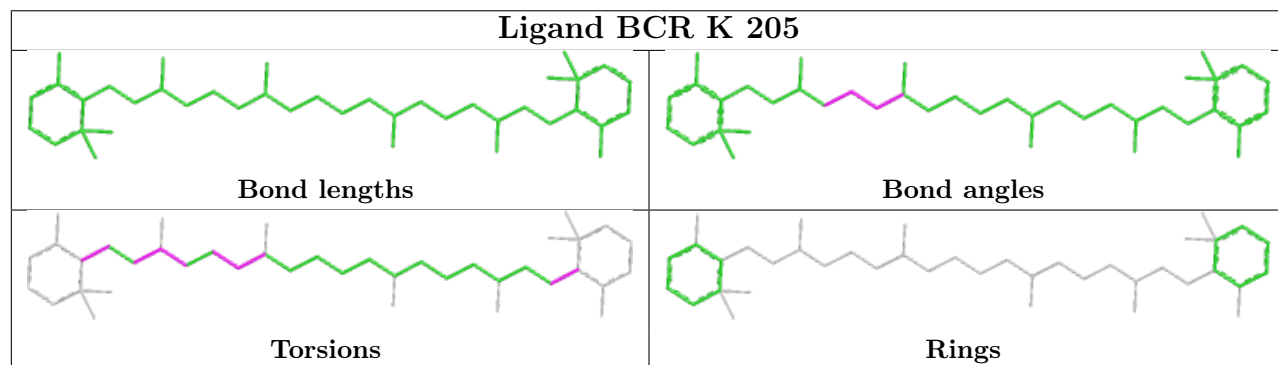


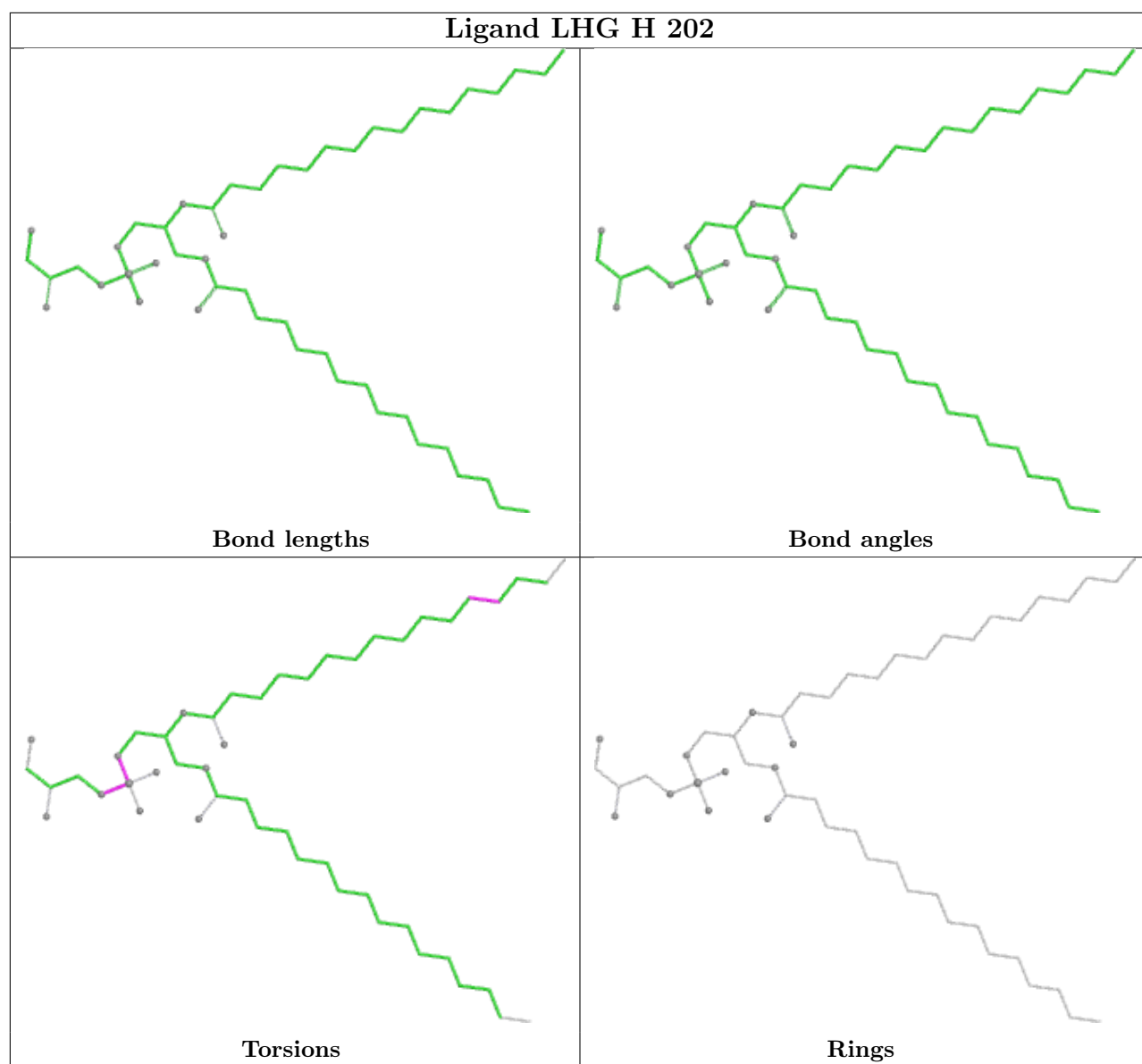


Ligand CLA 2 607

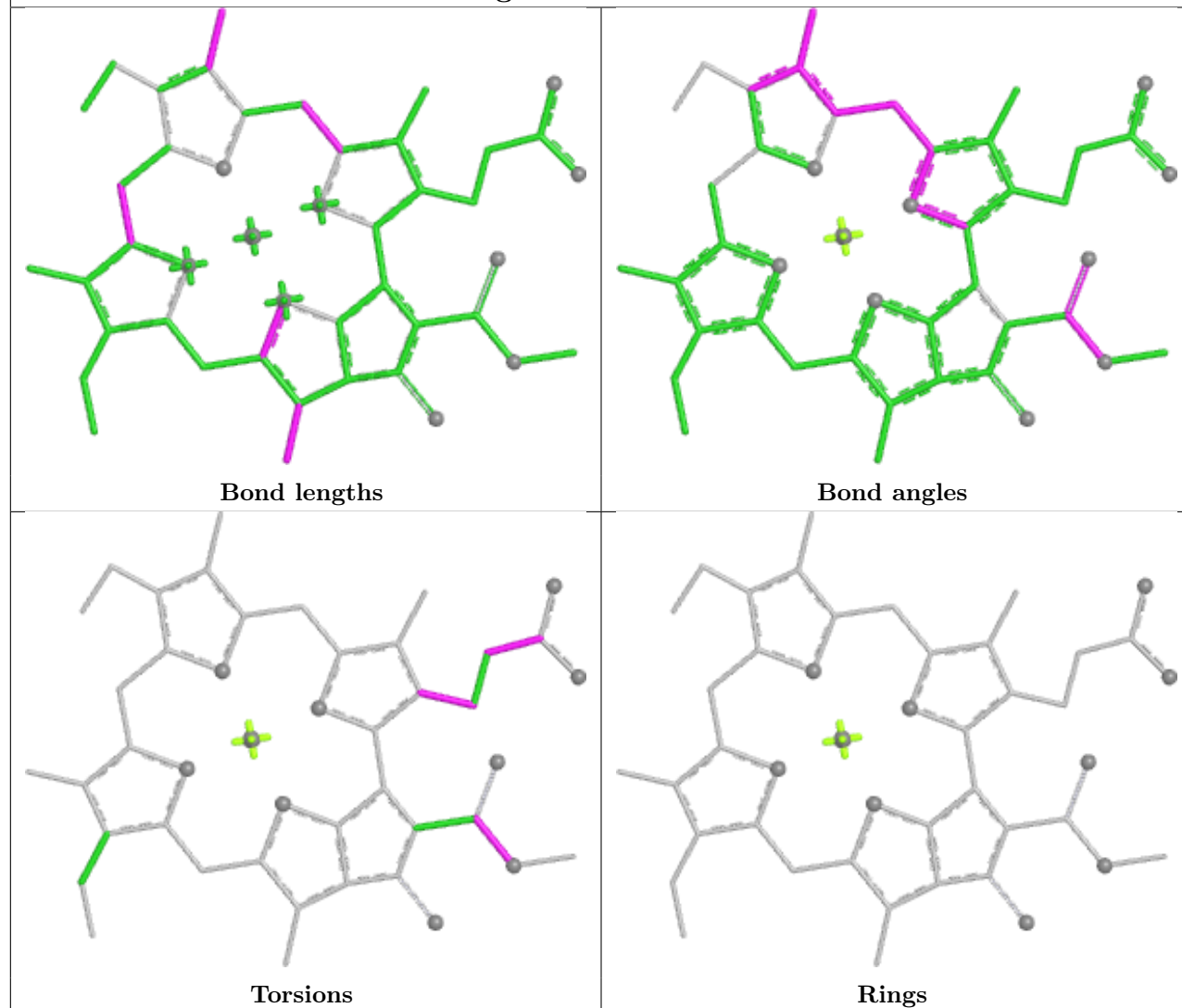


Ligand BCR K 205

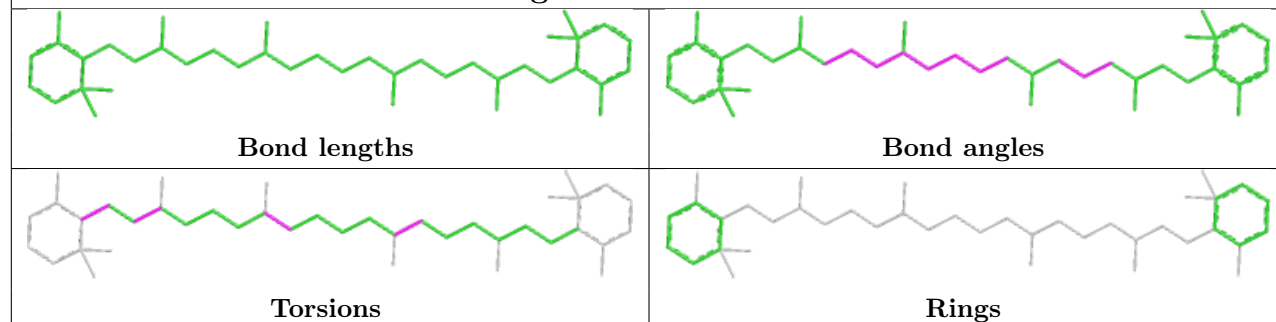


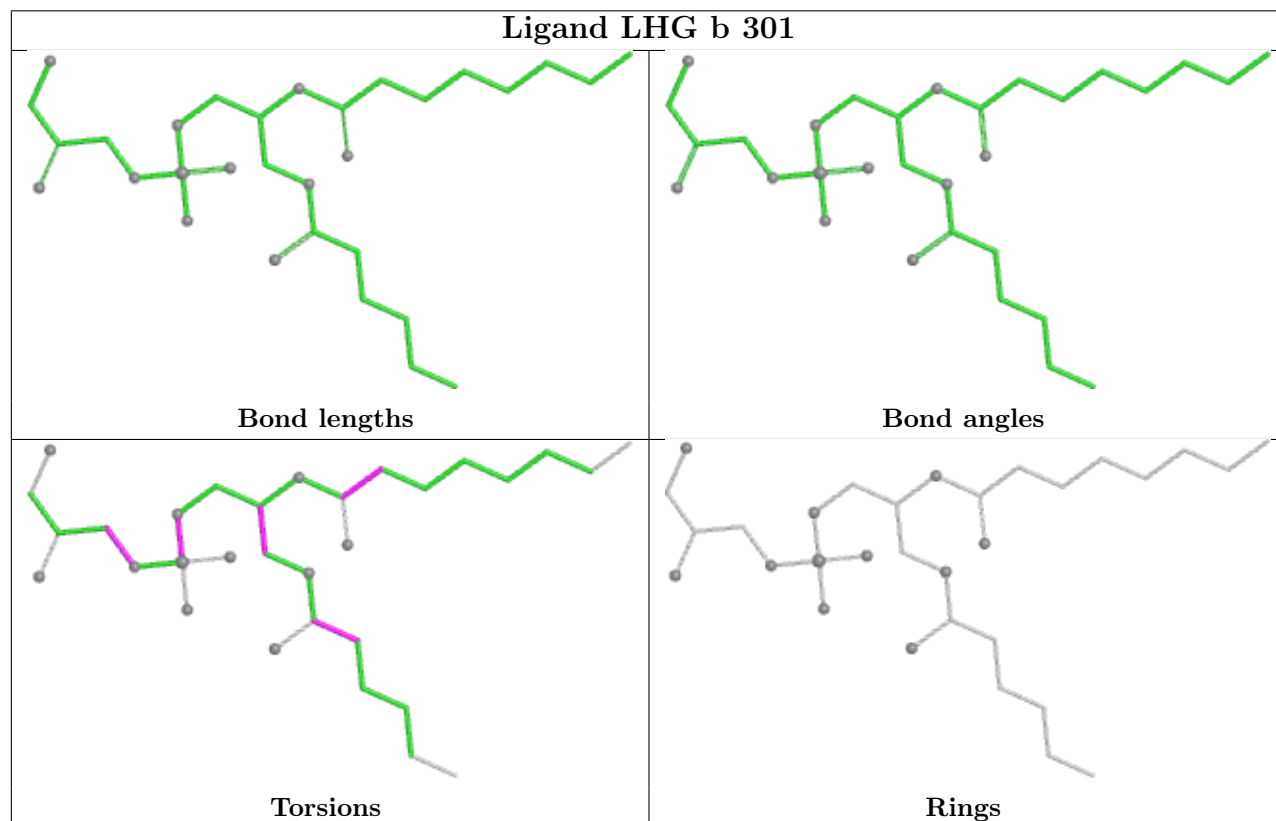
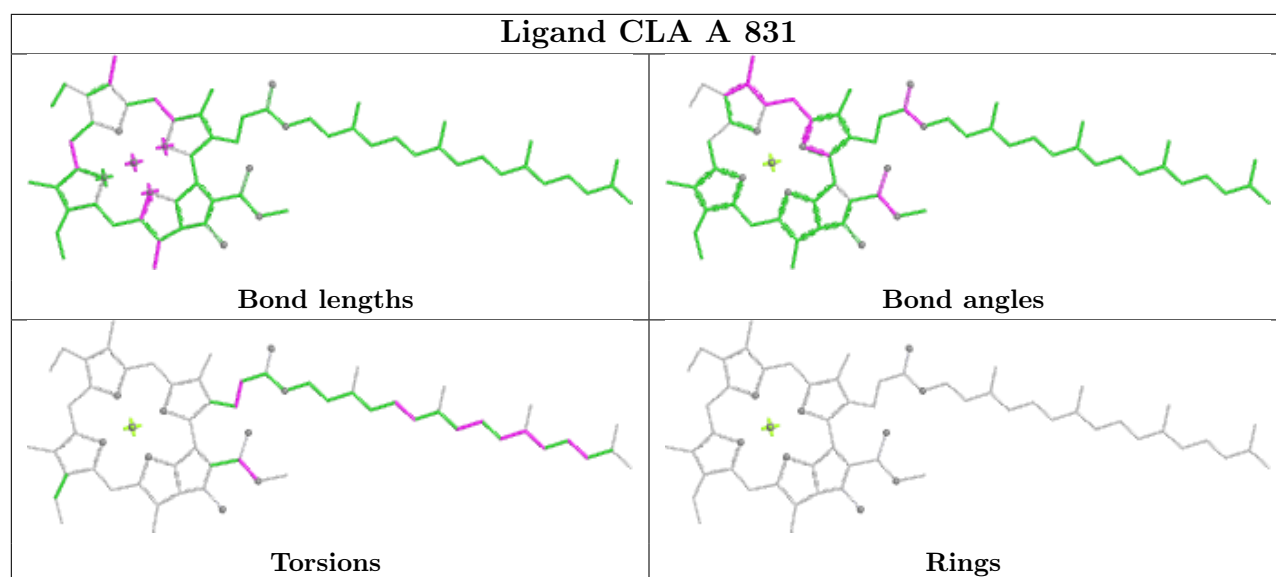


Ligand CLA b 316

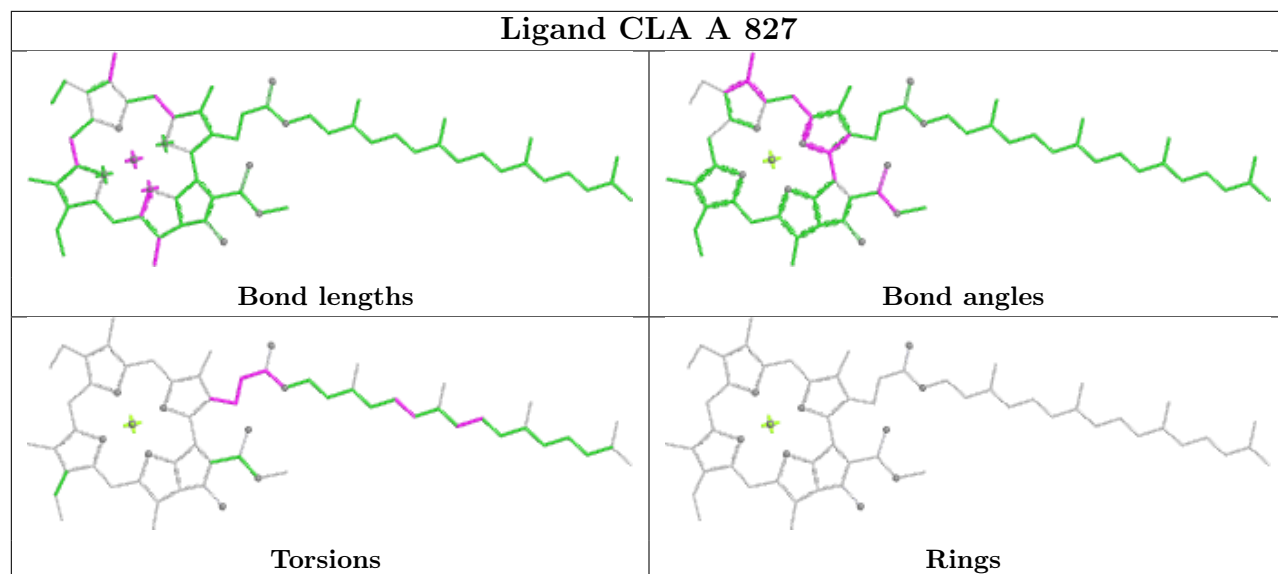


Ligand BCR B 852

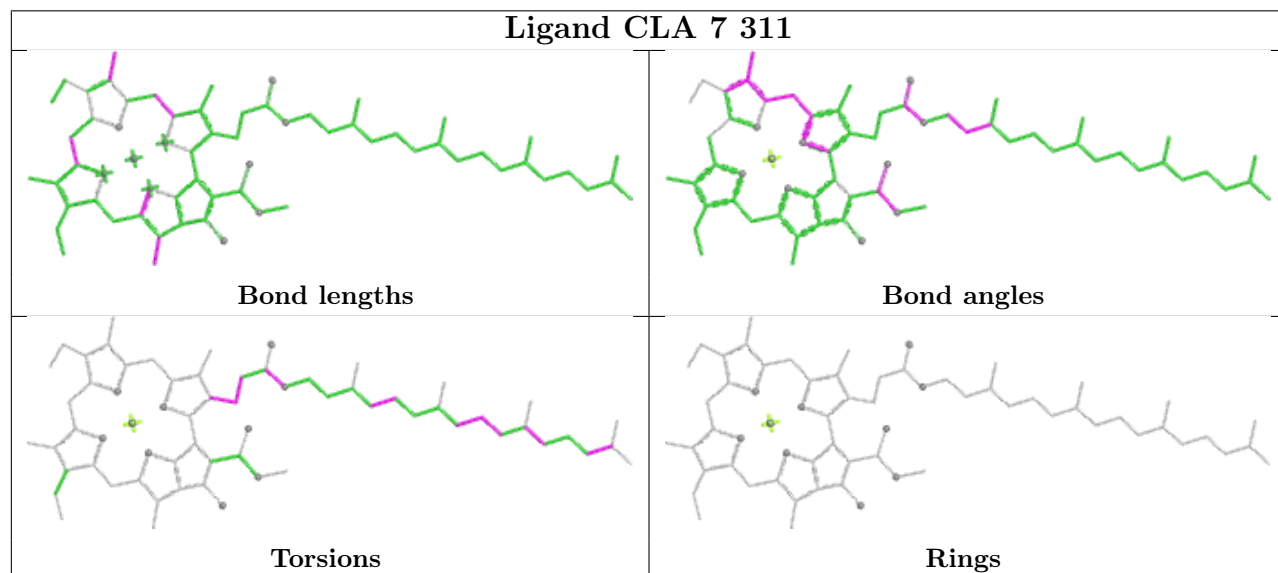




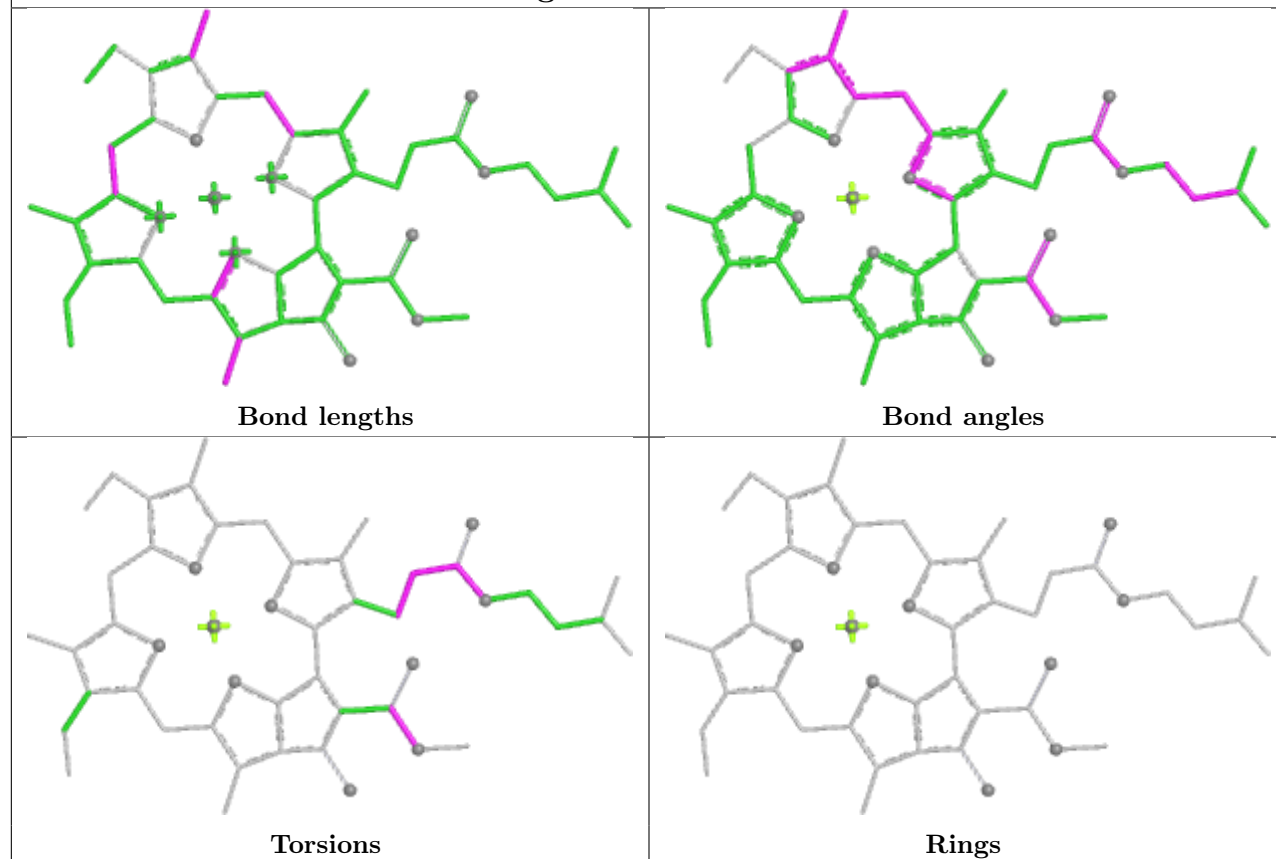
Ligand CLA A 827



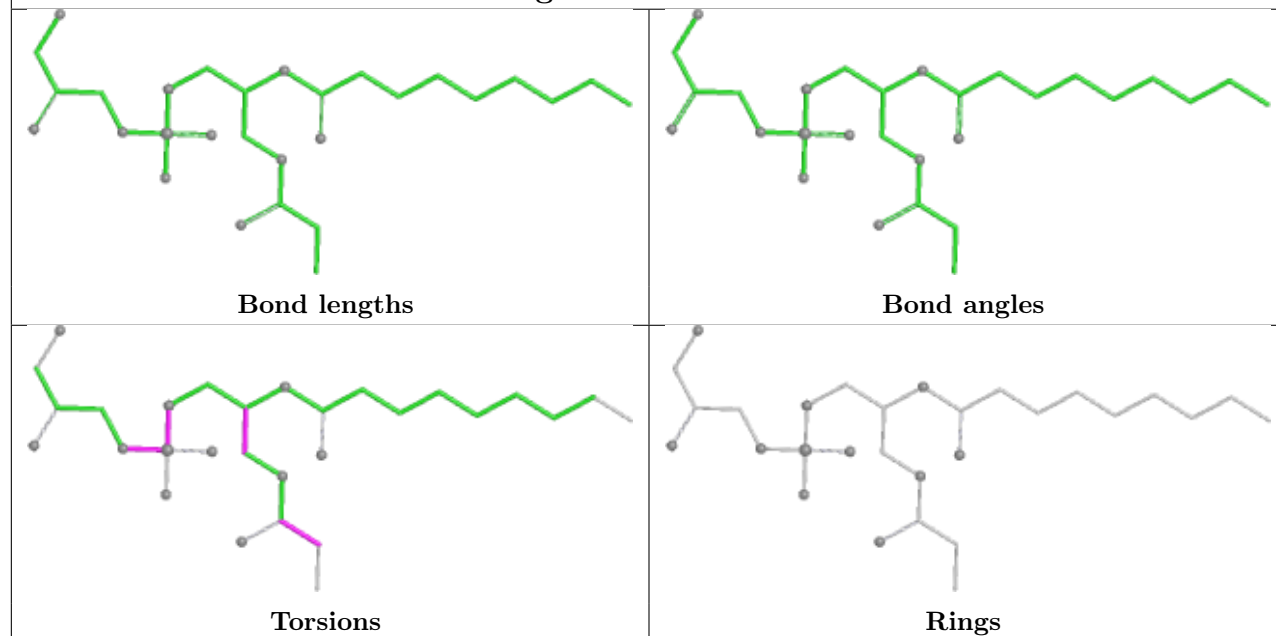
Ligand CLA 7 311

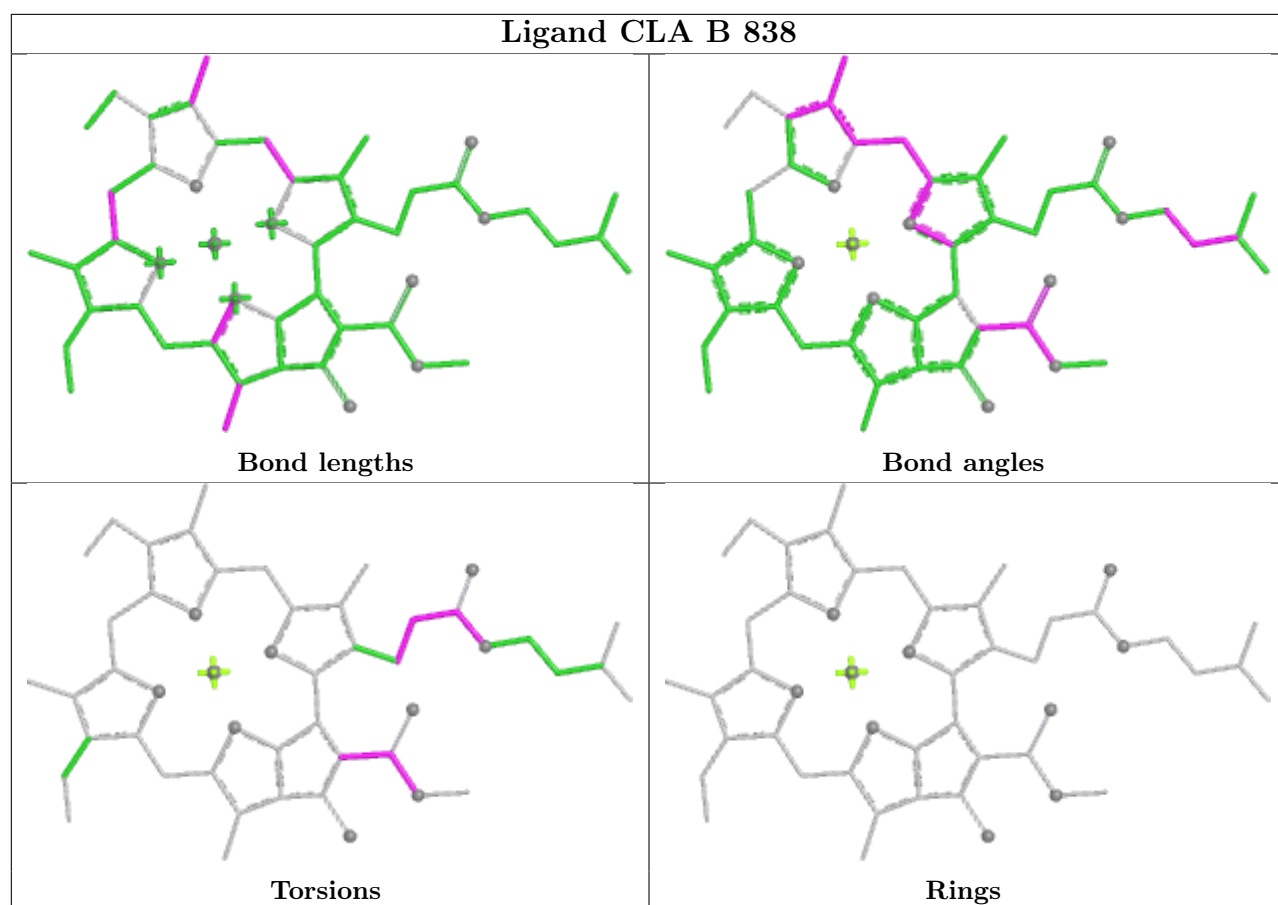


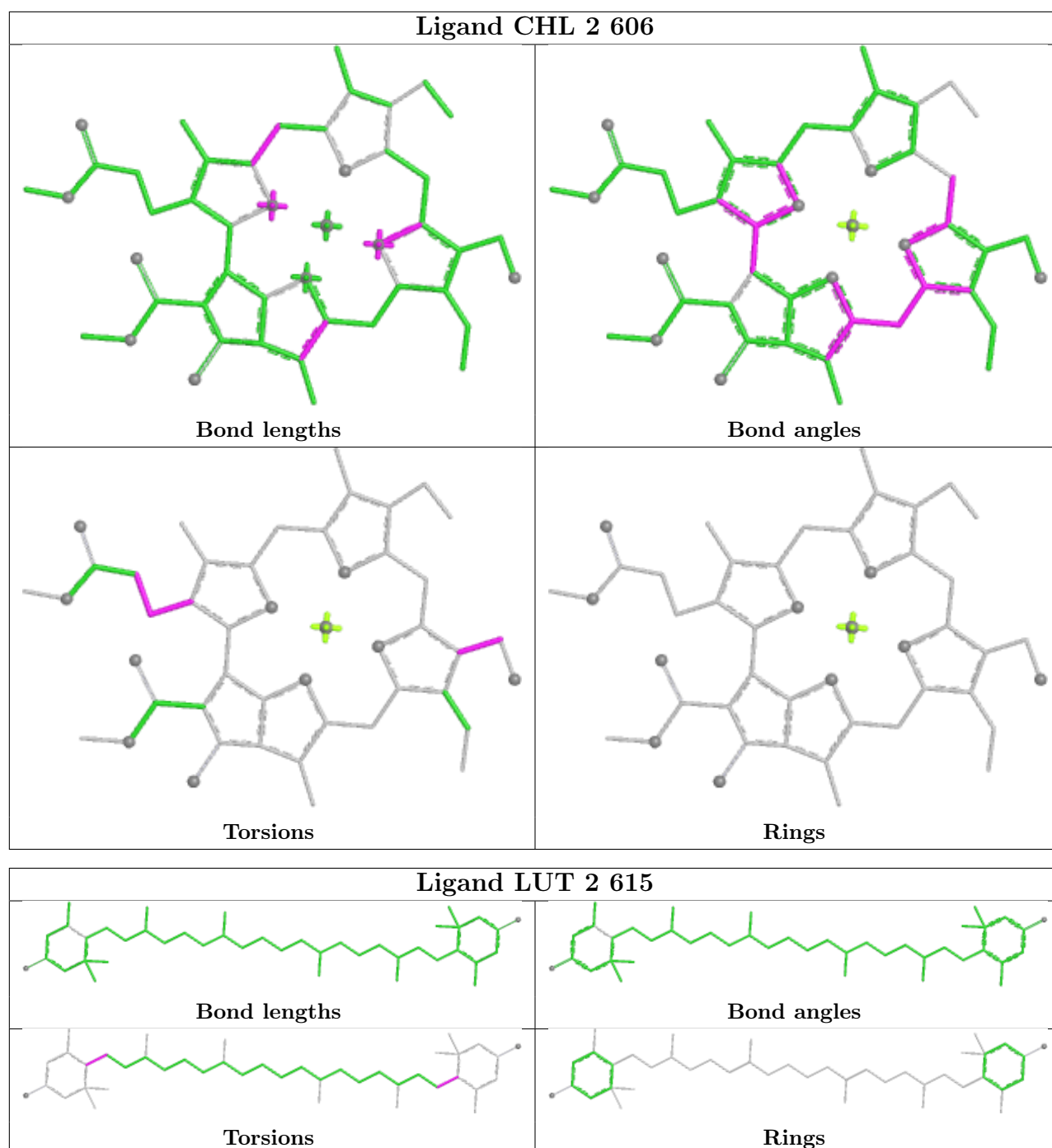
Ligand CLA c 613



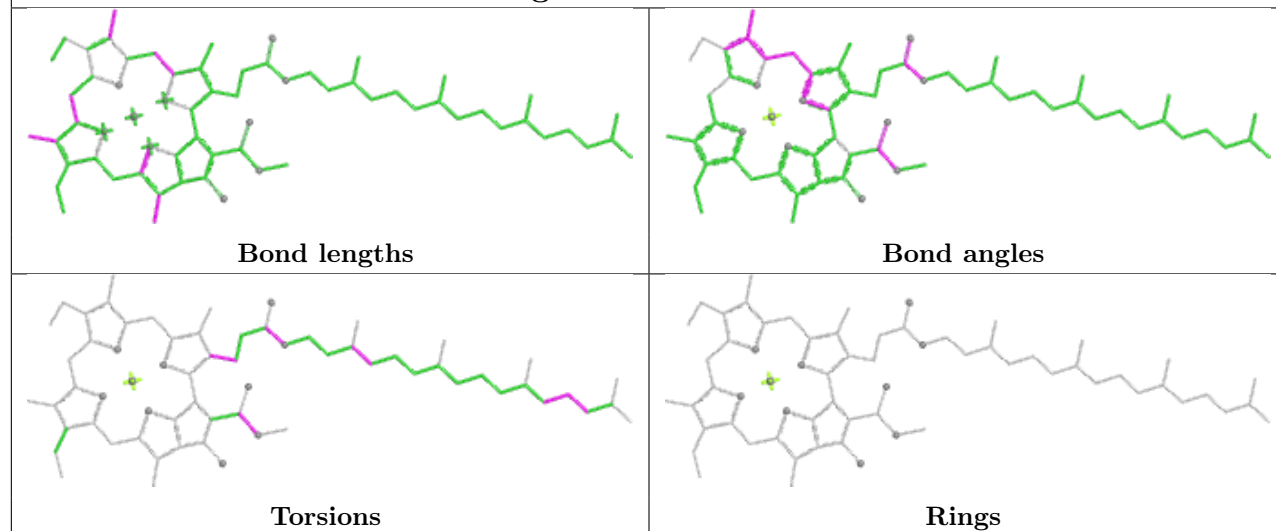
Ligand LHG c 618



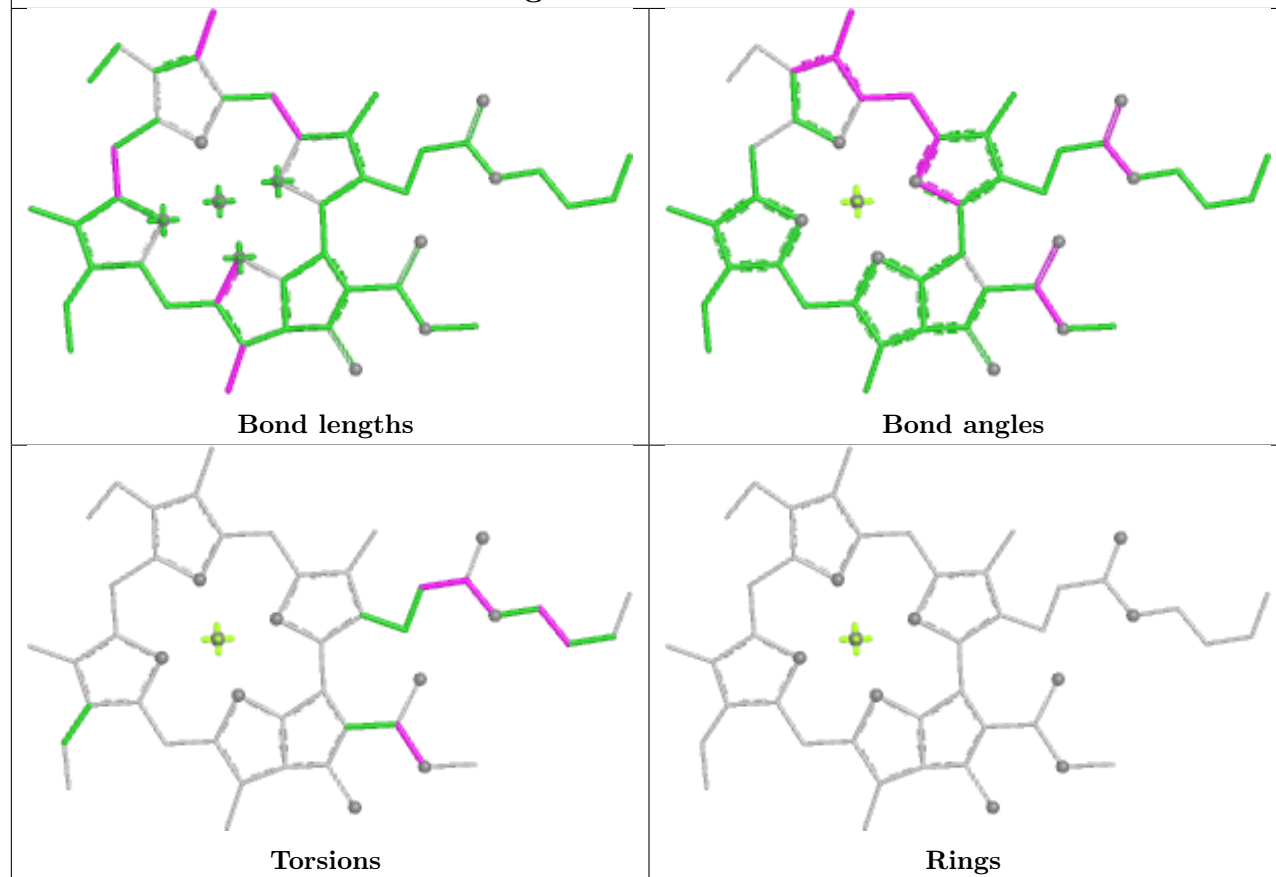




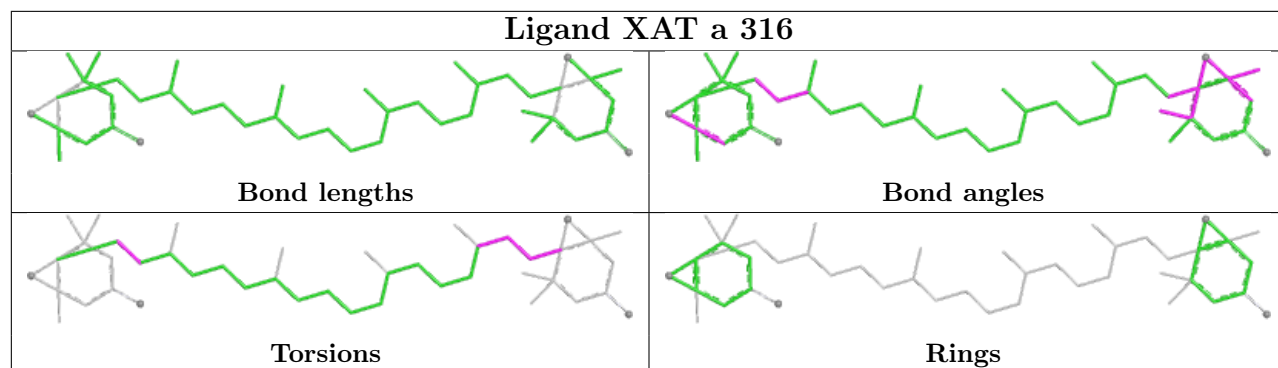
Ligand CLA A 813



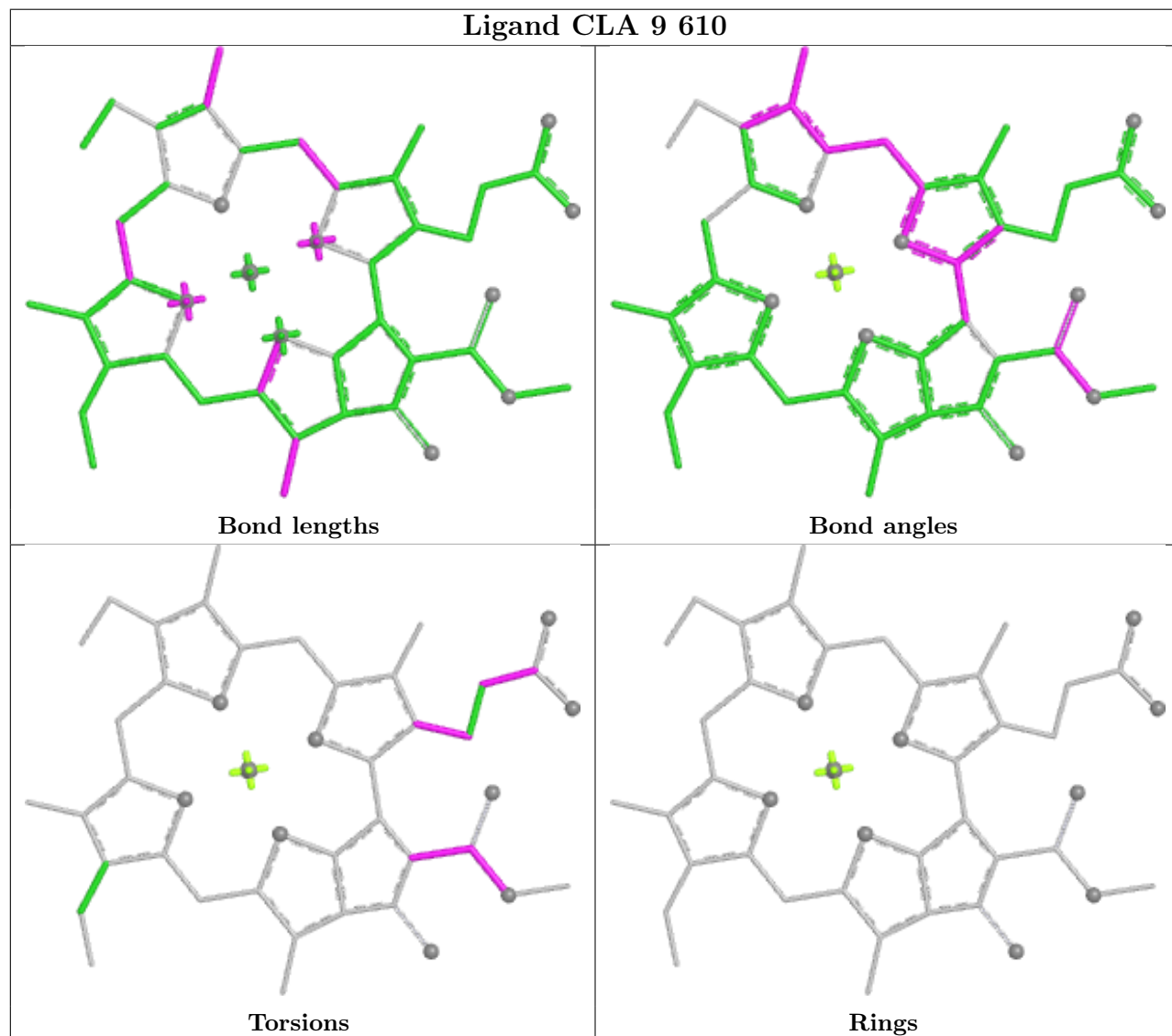
Ligand CLA F 5007

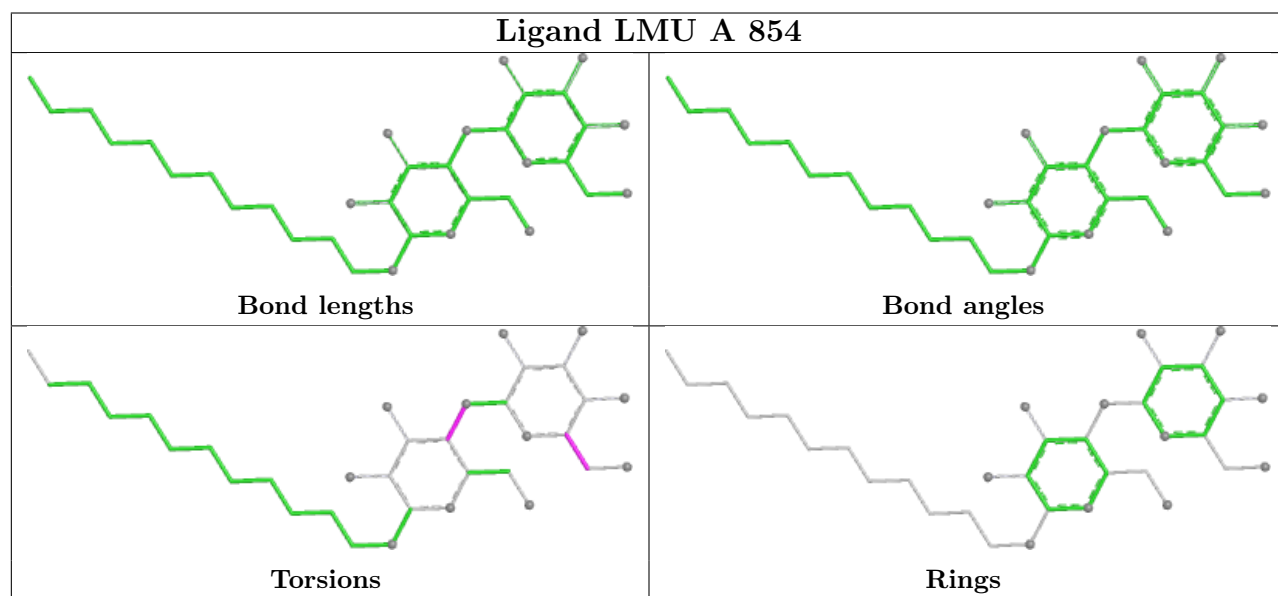
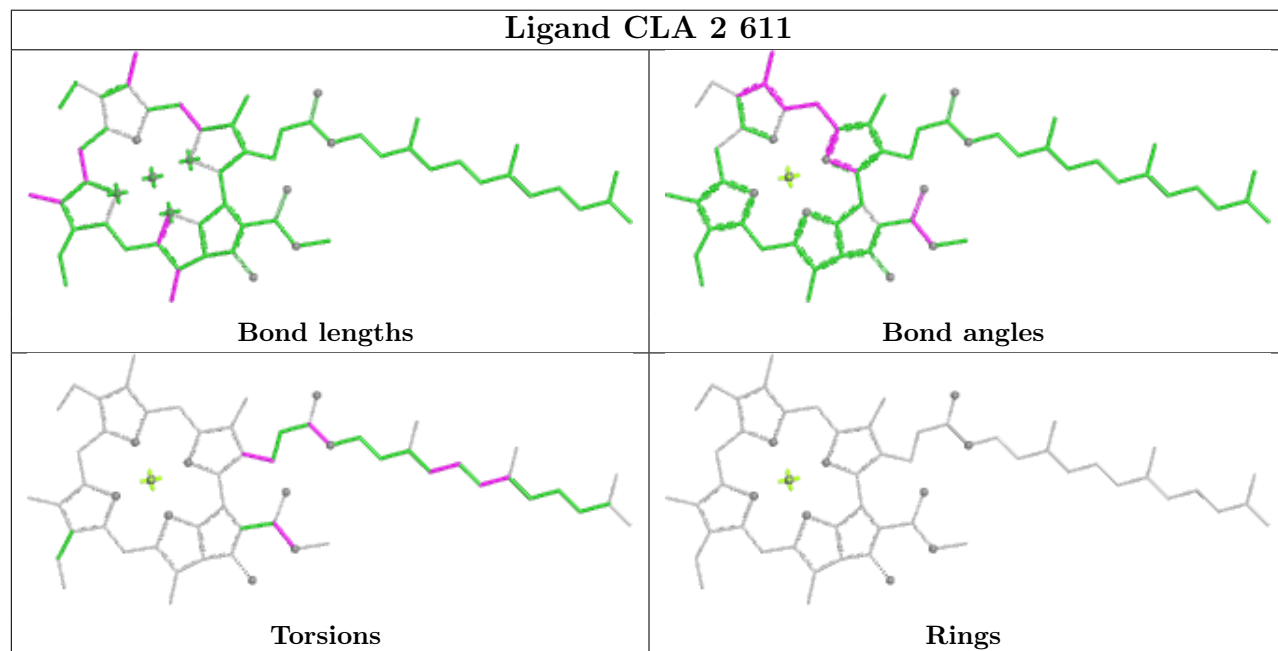
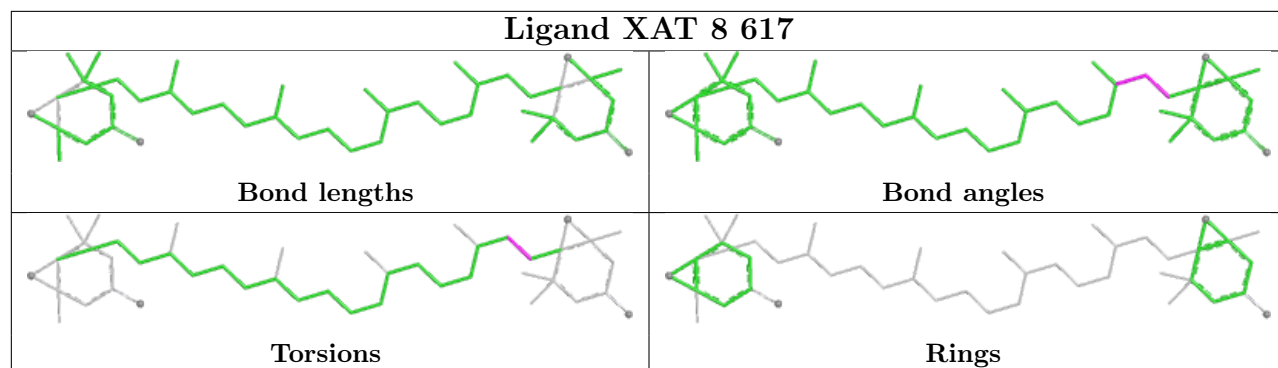


Ligand XAT a 316

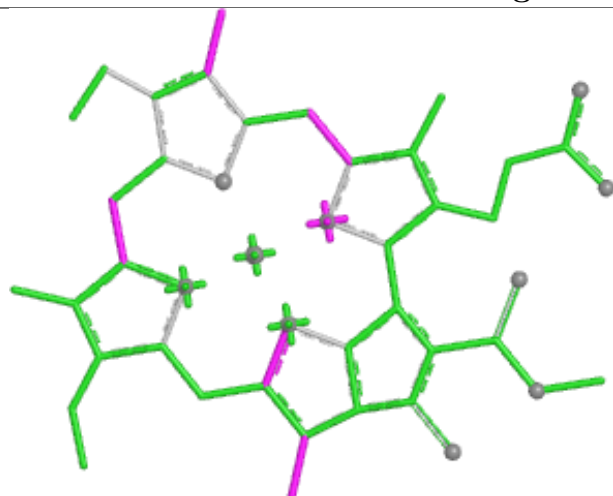


Ligand CLA 9 610

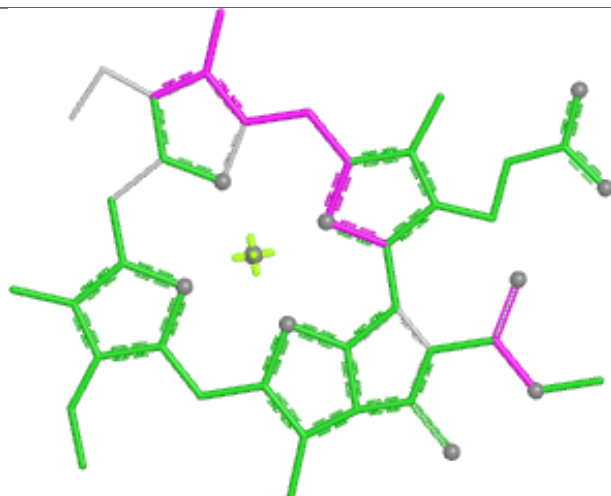




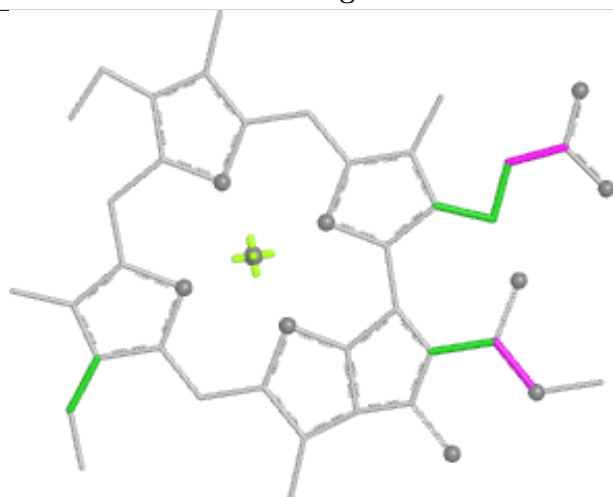
Ligand CLA K 201



Bond lengths



Bond angles

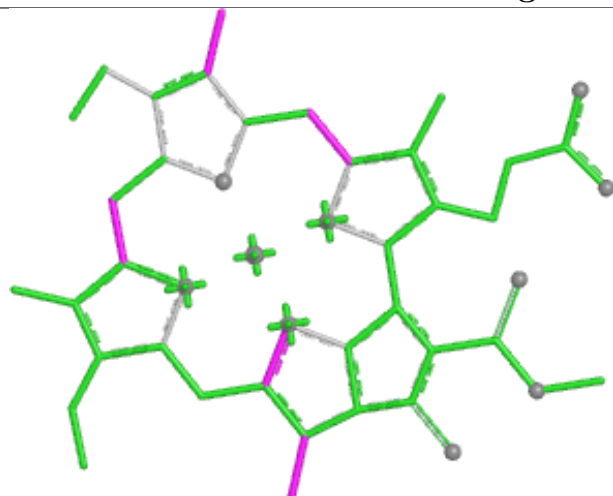


Torsions

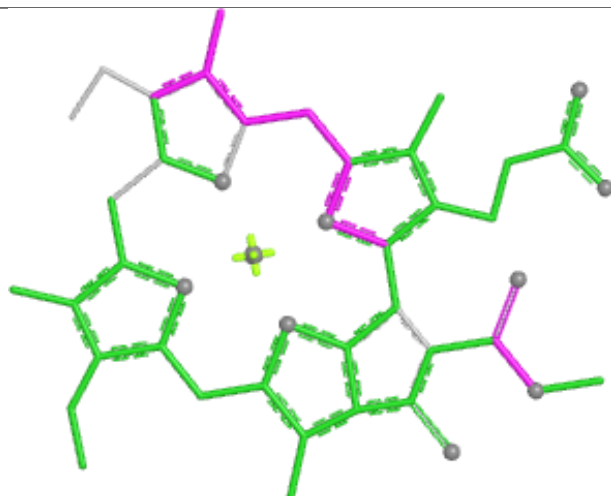


Rings

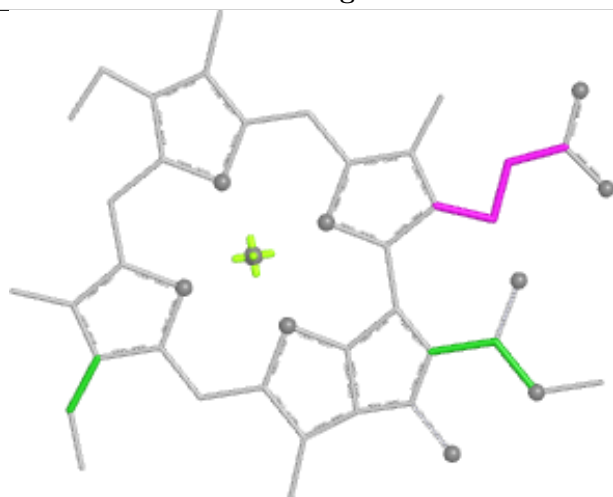
Ligand CLA 8 615



Bond lengths



Bond angles

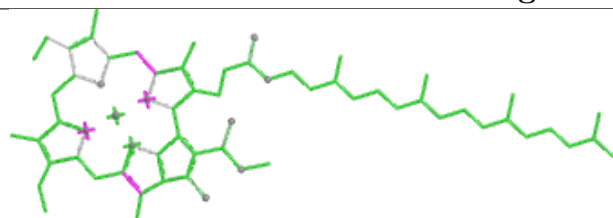


Torsions

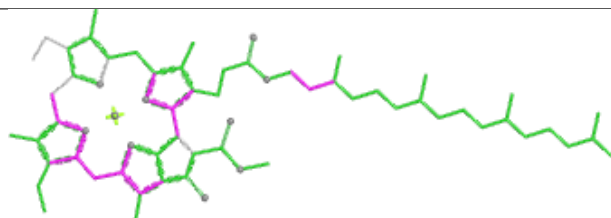


Rings

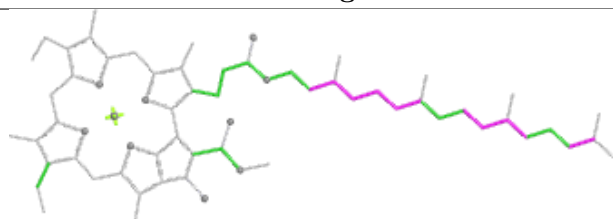
Ligand CL0 A 803



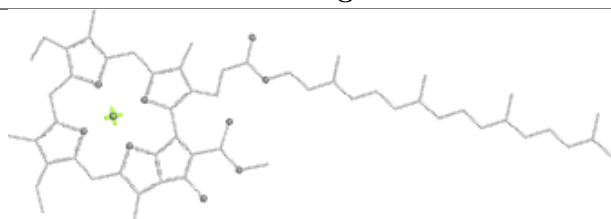
Bond lengths



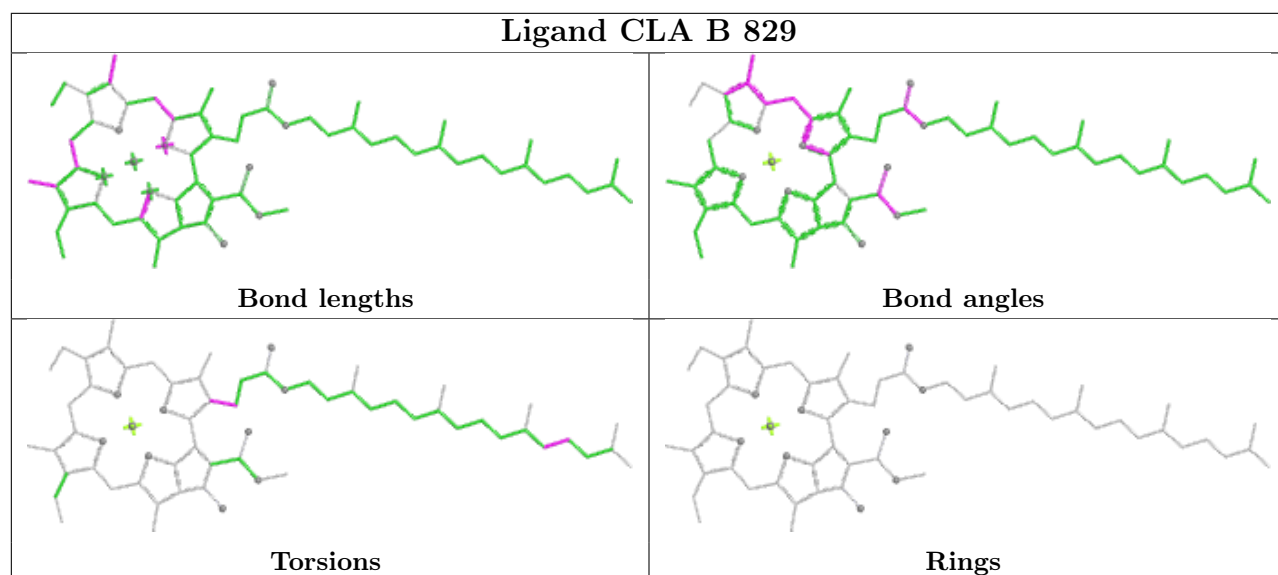
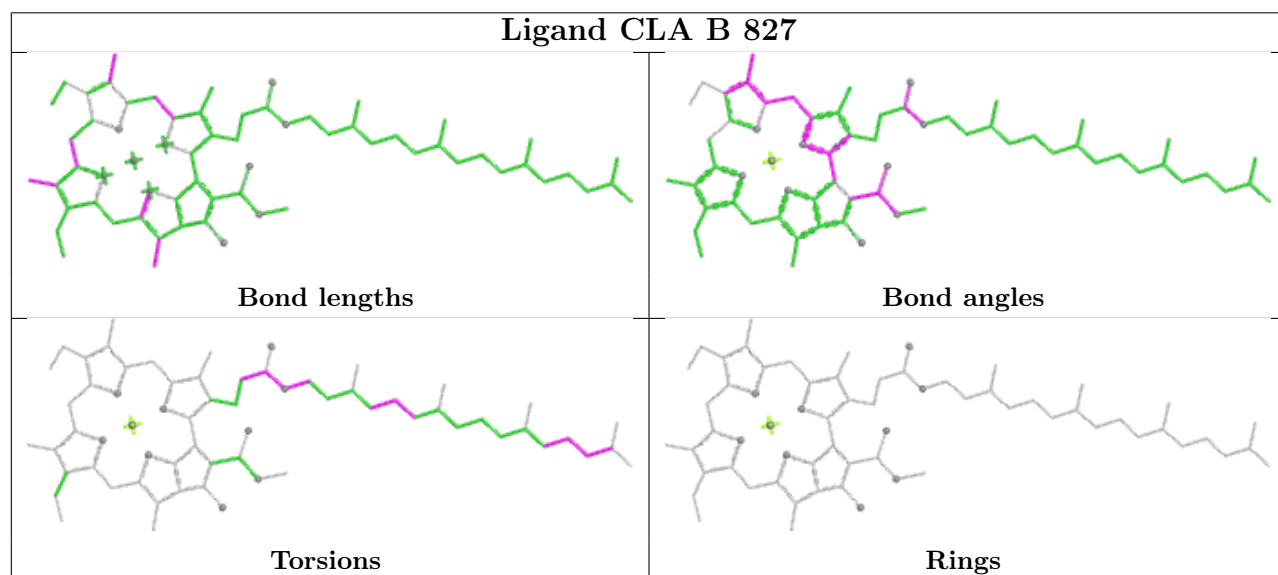
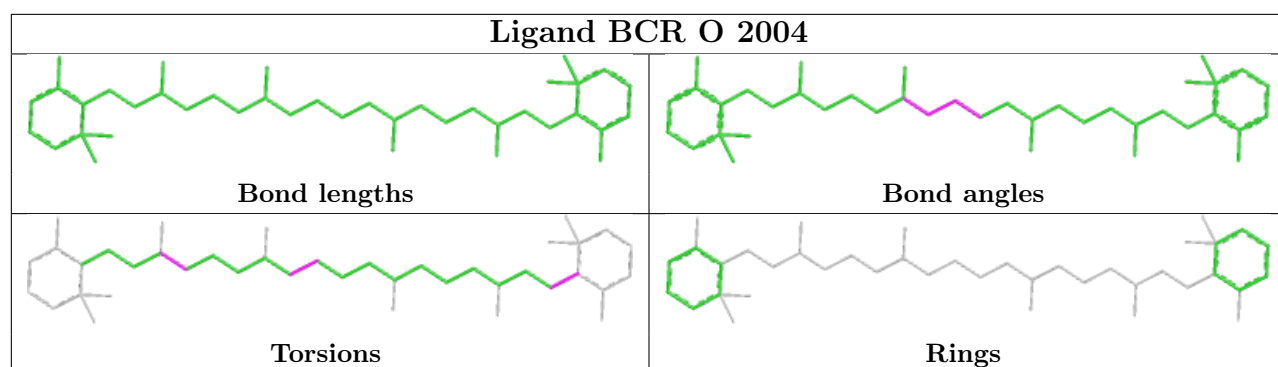
Bond angles

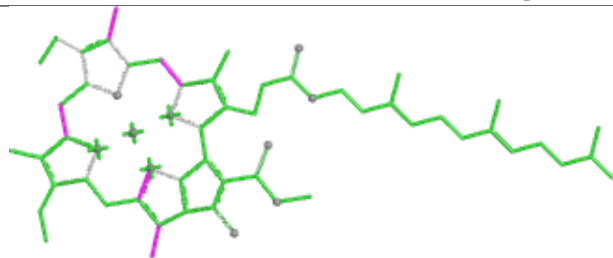
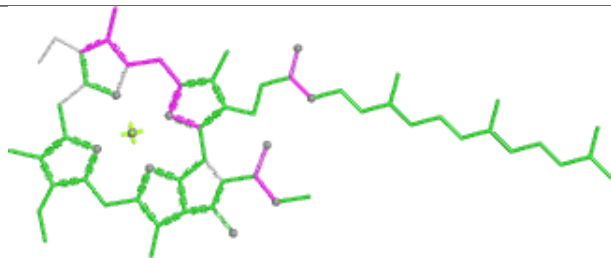
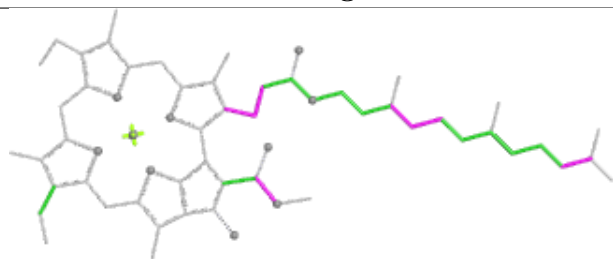
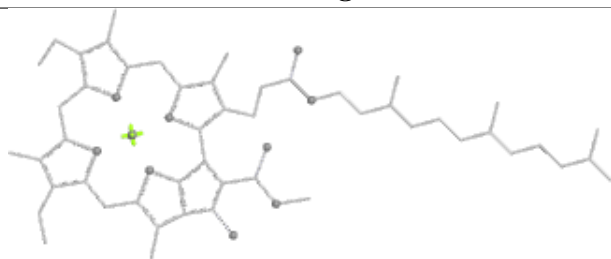
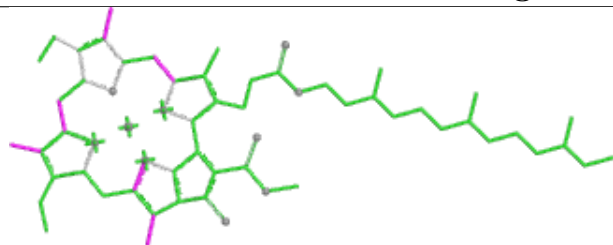
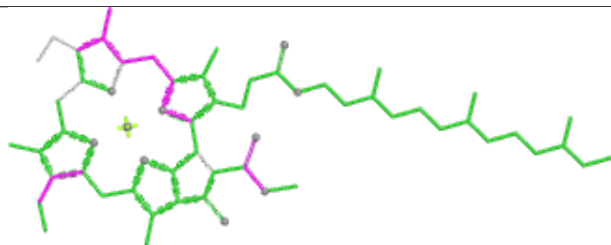
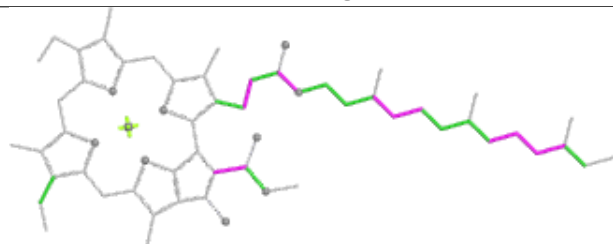
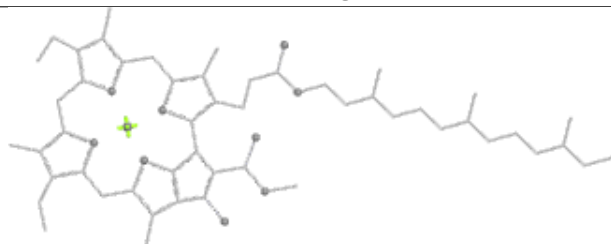


Torsions

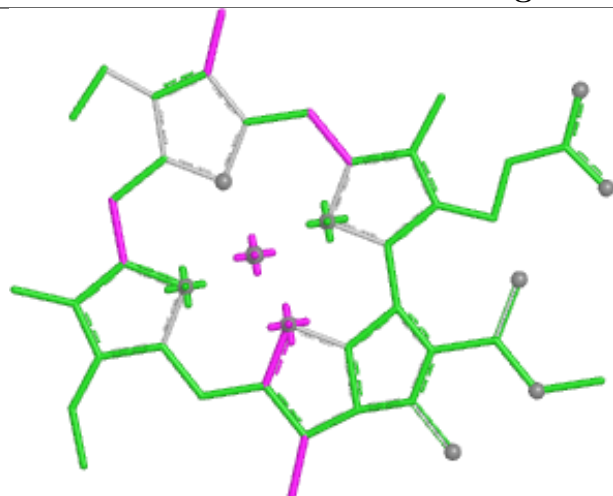


Rings

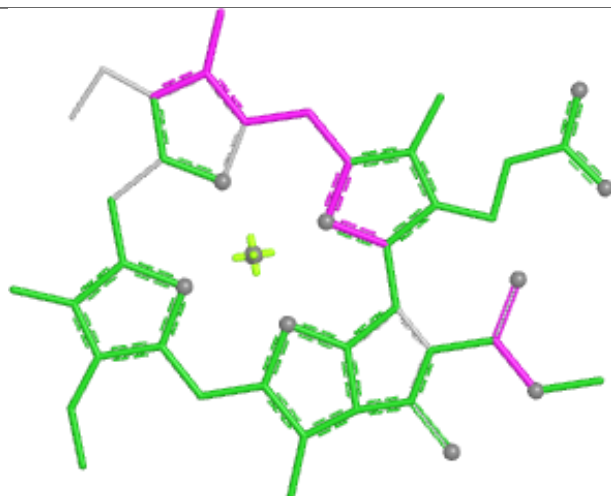


Ligand CLA 9 608**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 820****Bond lengths****Bond angles****Torsions****Rings**

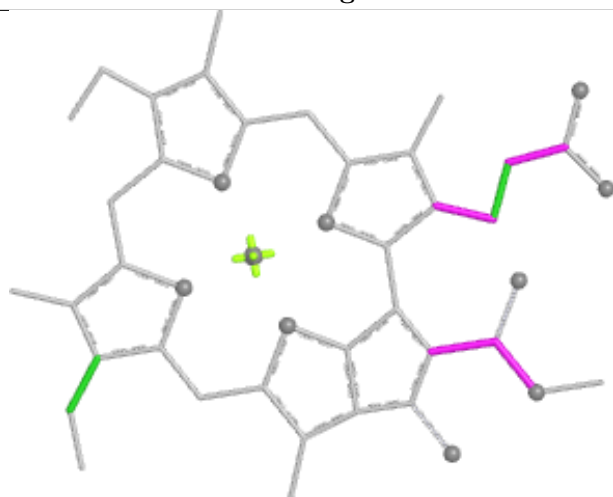
Ligand CLA T 608



Bond lengths



Bond angles

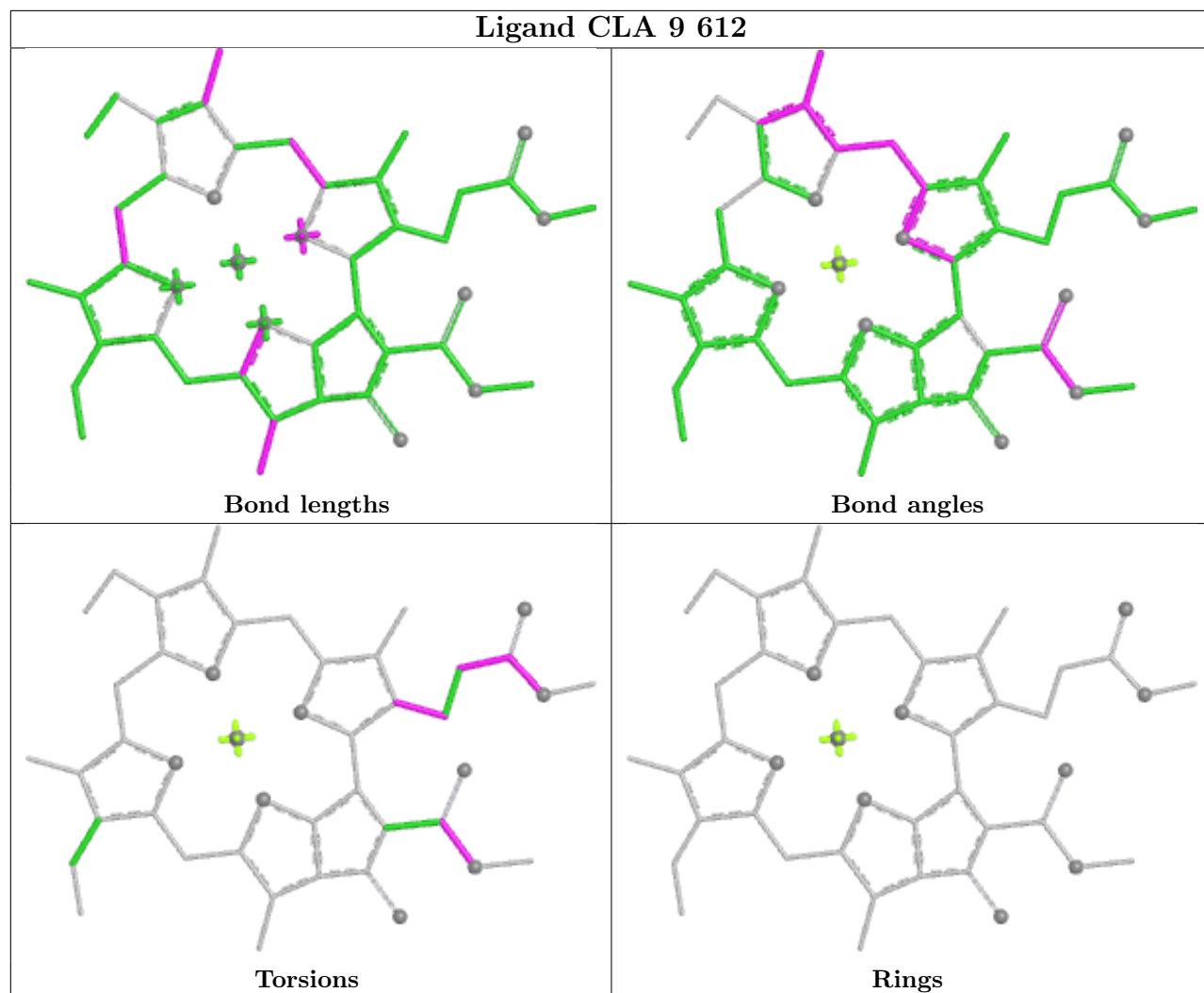


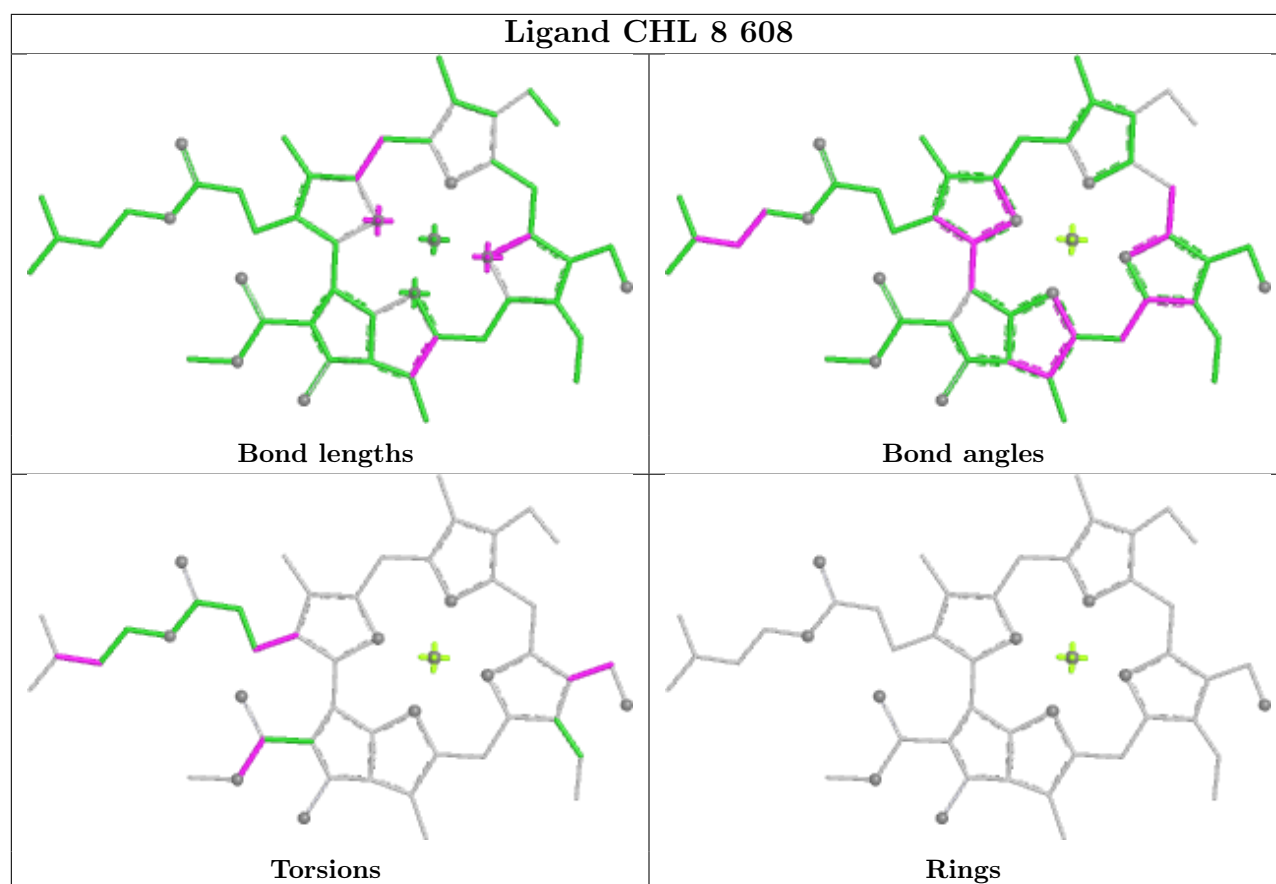
Torsions



Rings

Ligand CLA 9 612





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.

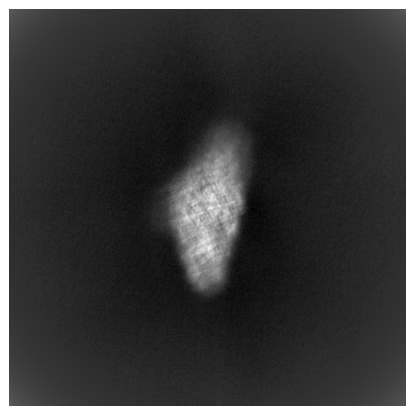
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-48262. These allow visual inspection of the internal detail of the map and identification of artifacts.

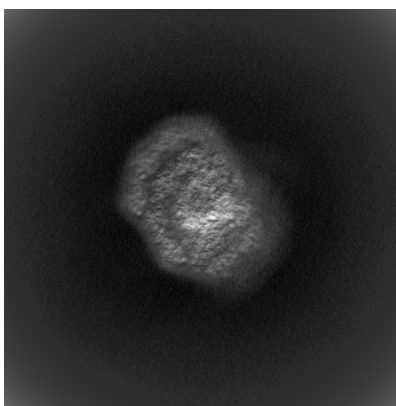
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X

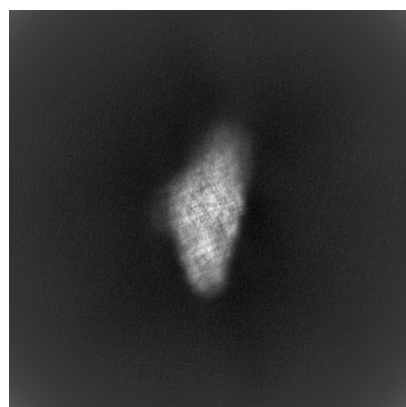


Y

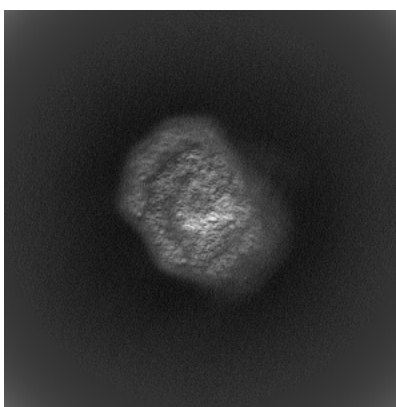


Z

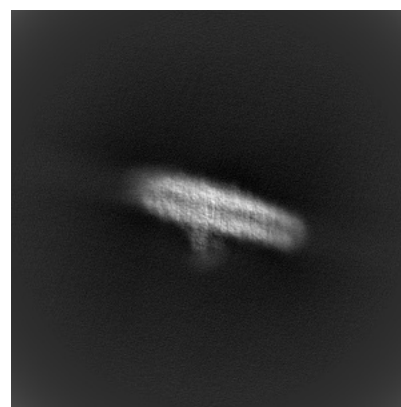
6.1.2 Raw map



X



Y

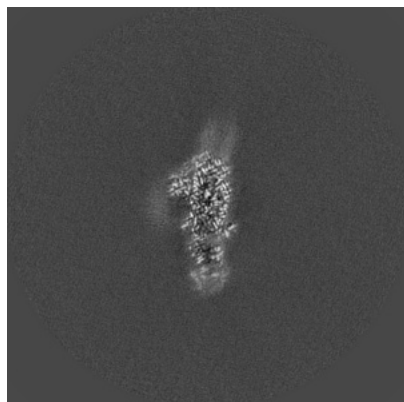


Z

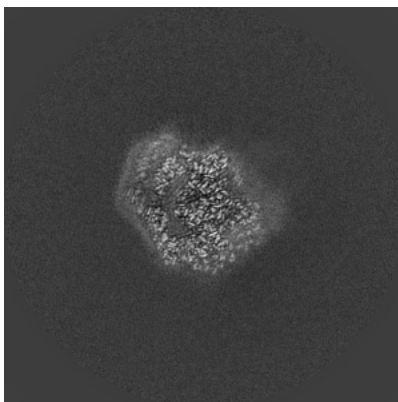
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

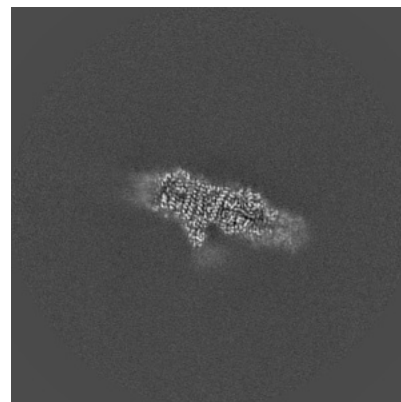
6.2.1 Primary map



X Index: 240

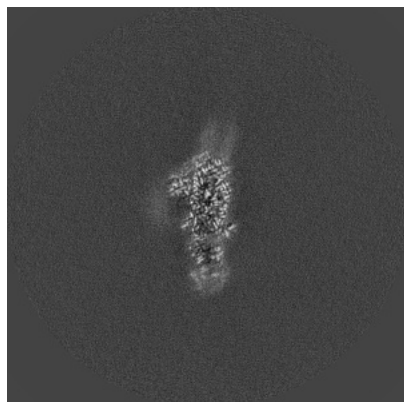


Y Index: 240

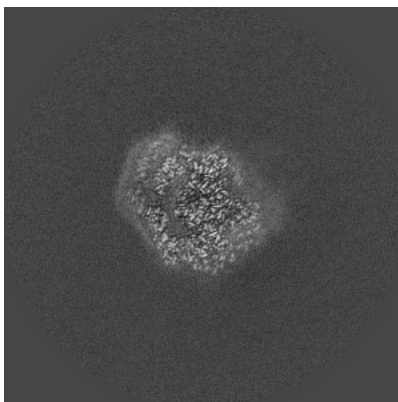


Z Index: 240

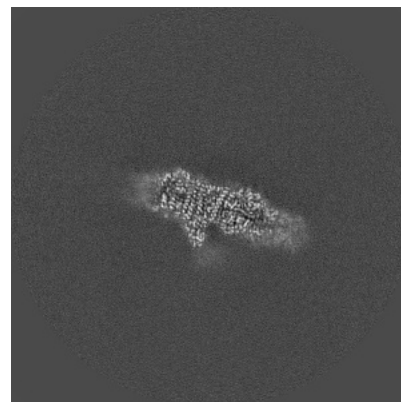
6.2.2 Raw map



X Index: 240



Y Index: 240

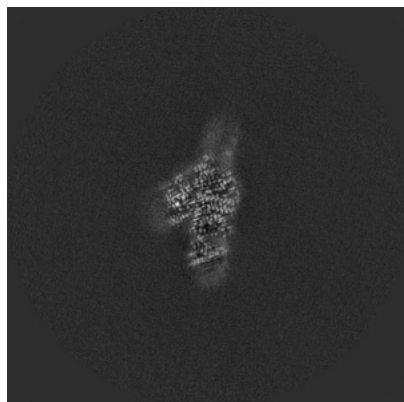


Z Index: 240

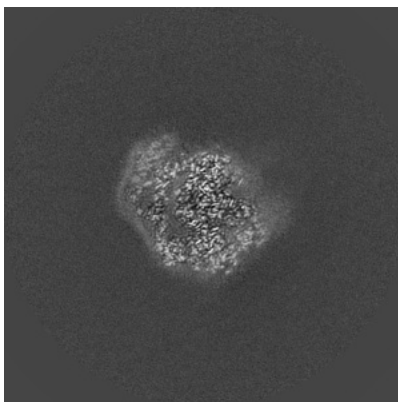
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

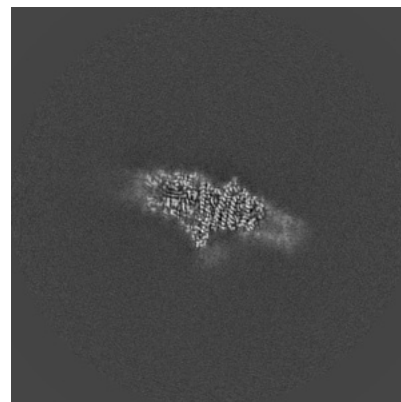
6.3.1 Primary map



X Index: 228

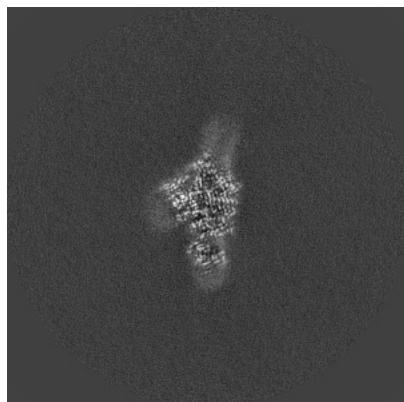


Y Index: 243

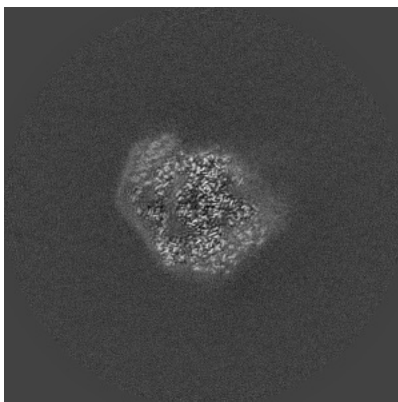


Z Index: 249

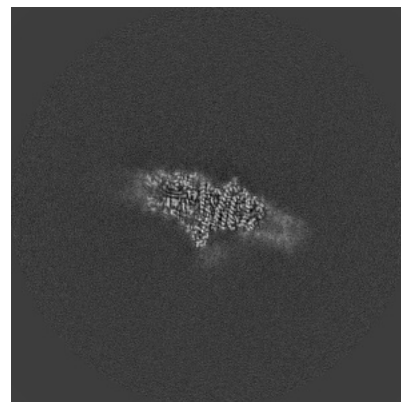
6.3.2 Raw map



X Index: 231



Y Index: 242



Z Index: 249

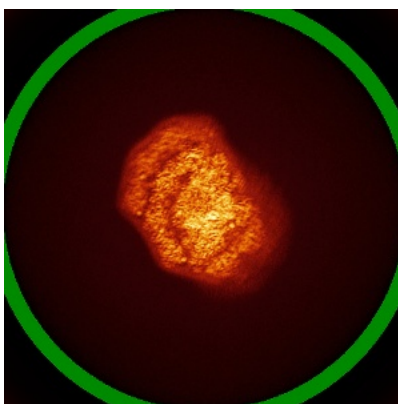
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

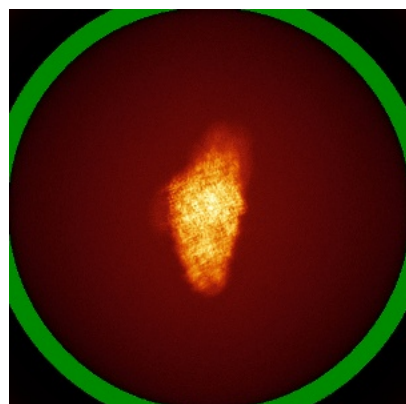


Y

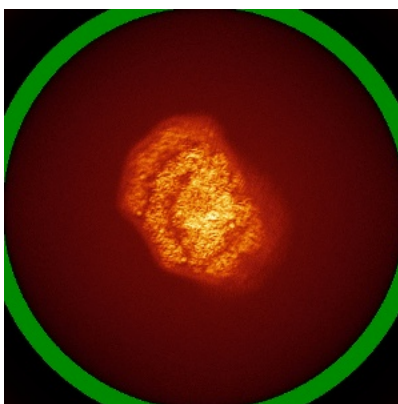


Z

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 0.0128. 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.

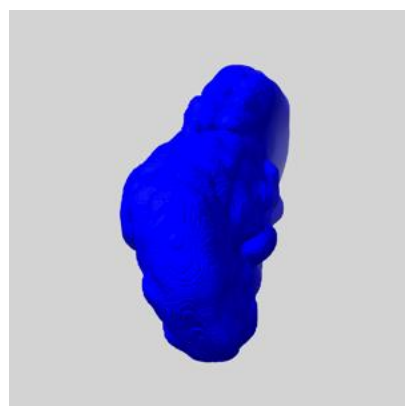
6.6 Mask visualisation [i](#)

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

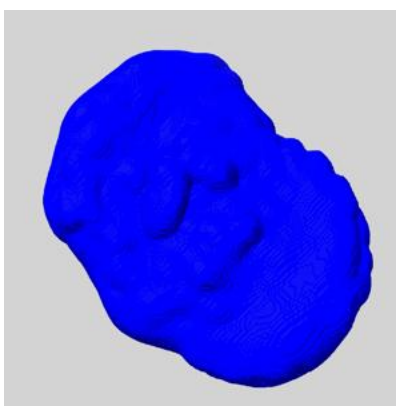
A mask typically either:

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

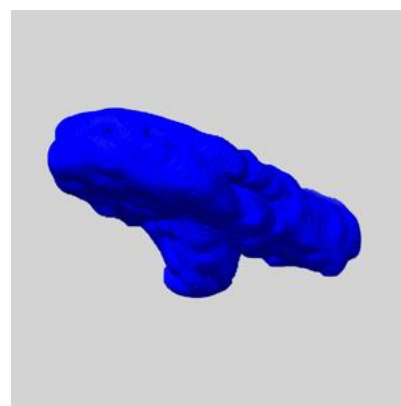
6.6.1 emd_48262_msk_1.map [i](#)



X



Y

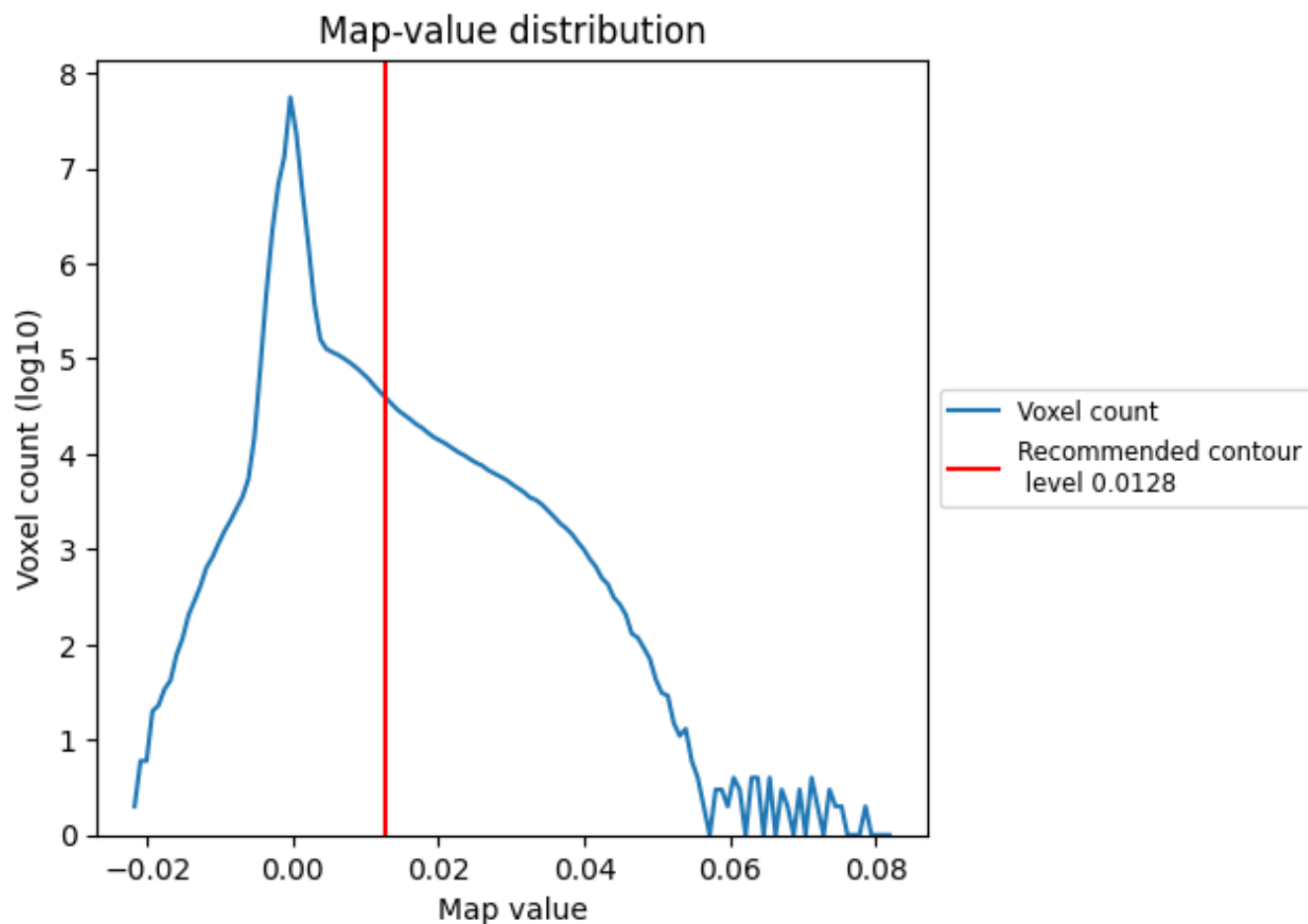


Z

7 Map analysis [i](#)

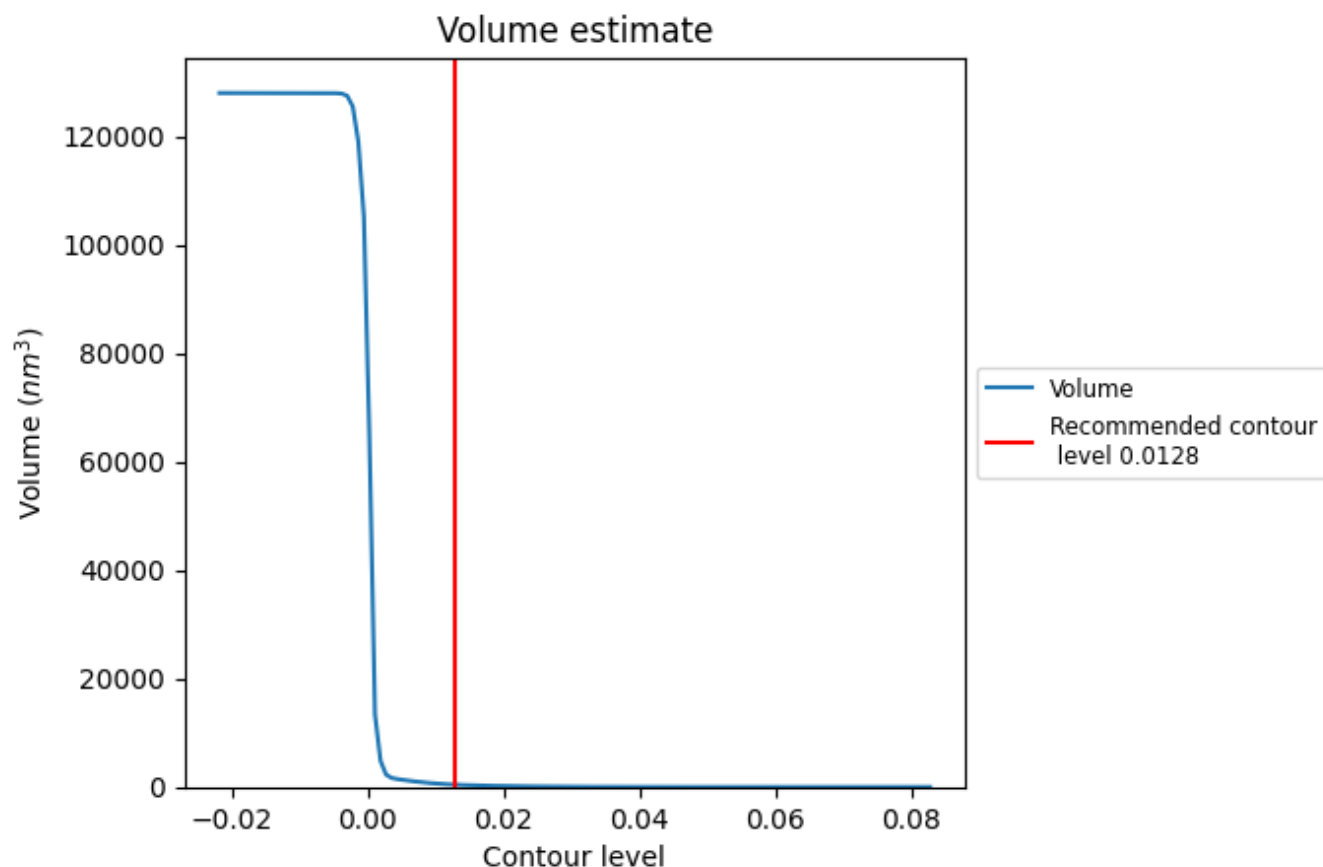
This section contains the results of statistical analysis of the map.

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.

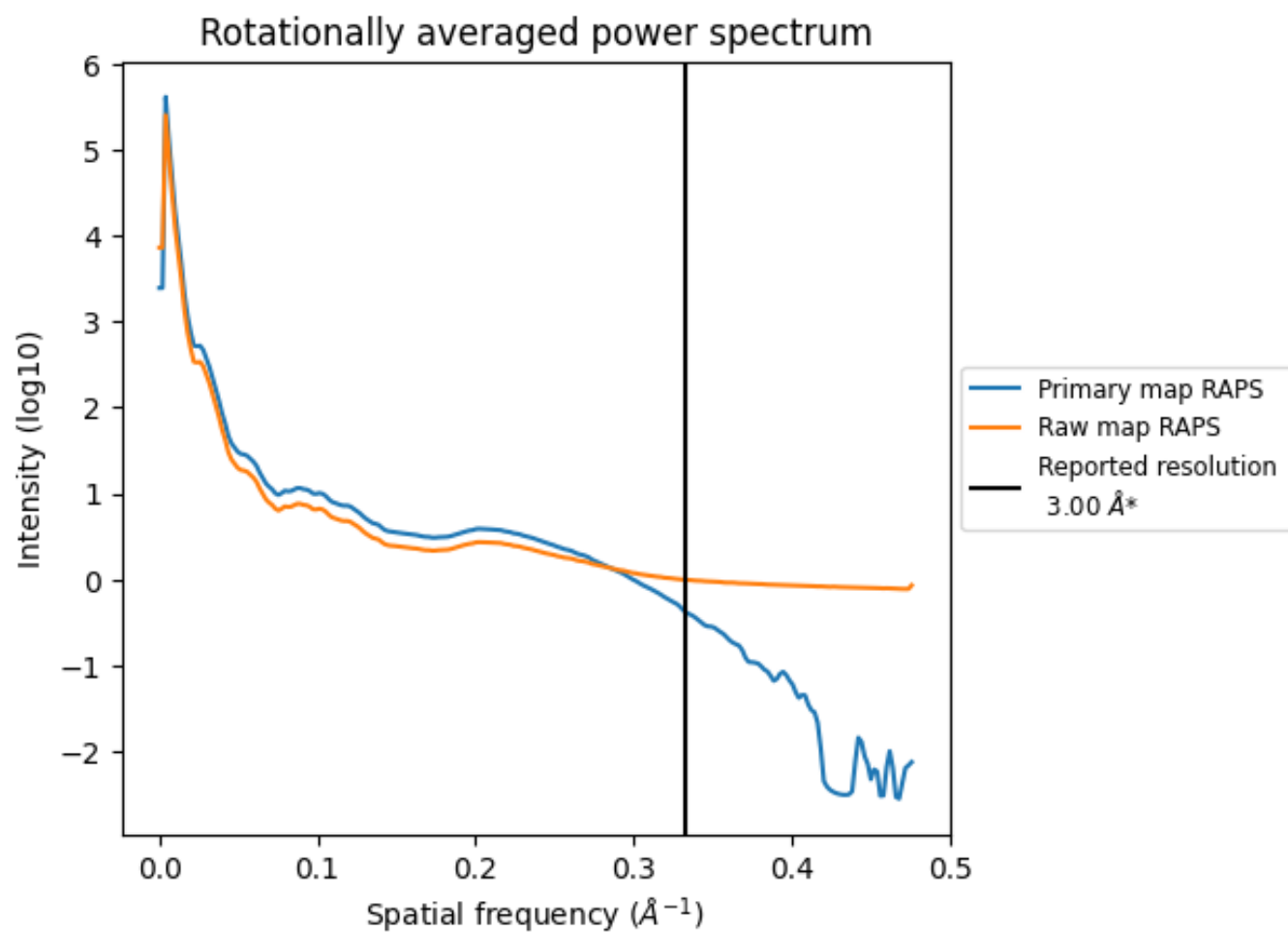
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm^3 ; this corresponds to an approximate mass of 384 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

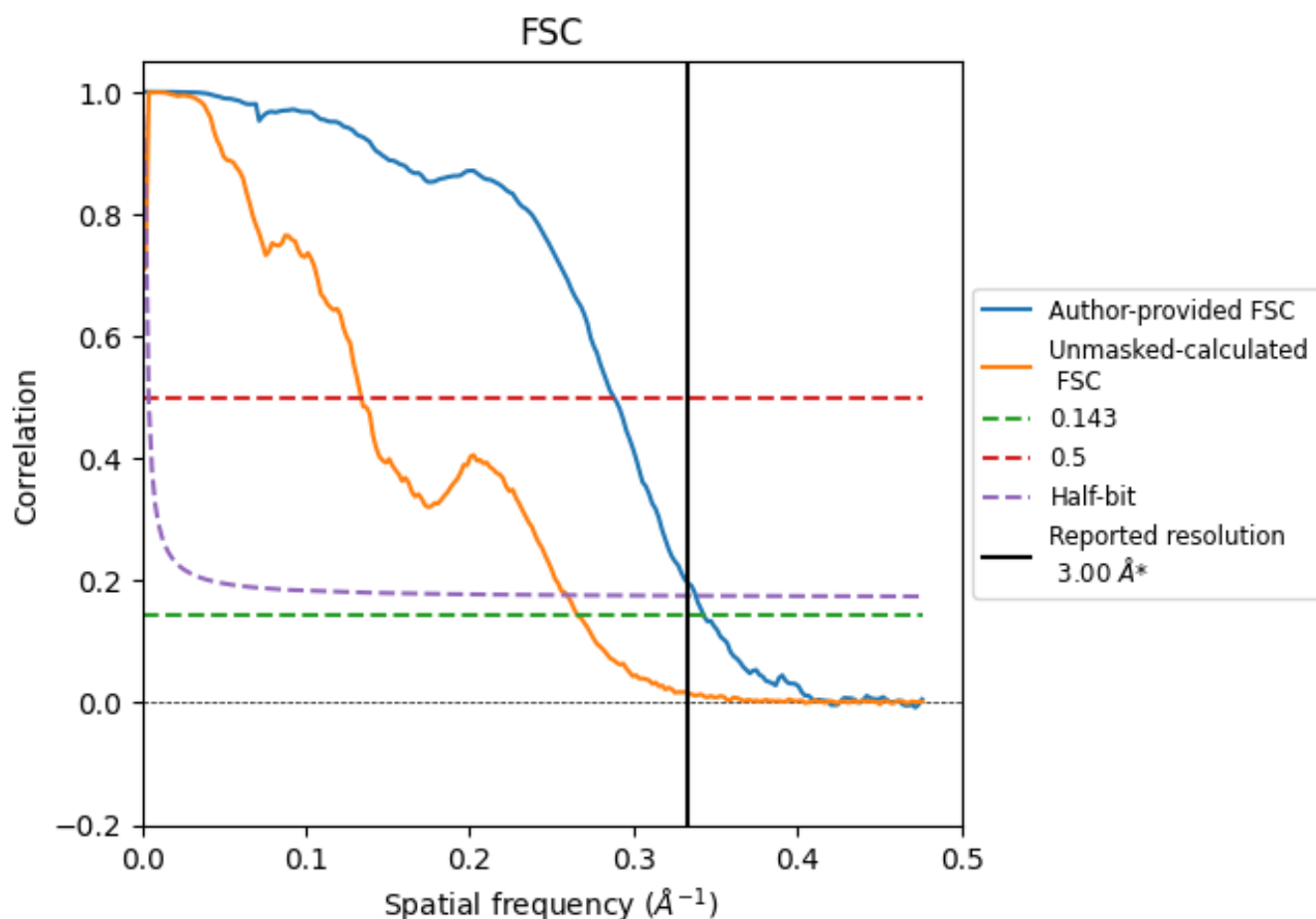


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

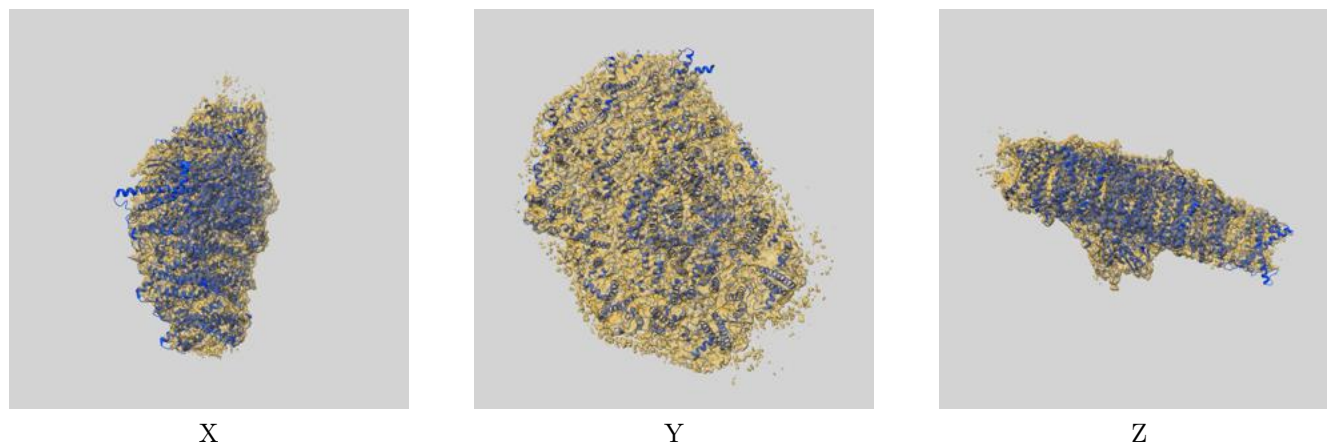
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.92	3.47	2.96
Unmasked-calculated*	3.76	7.47	416.67

*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 3.76 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

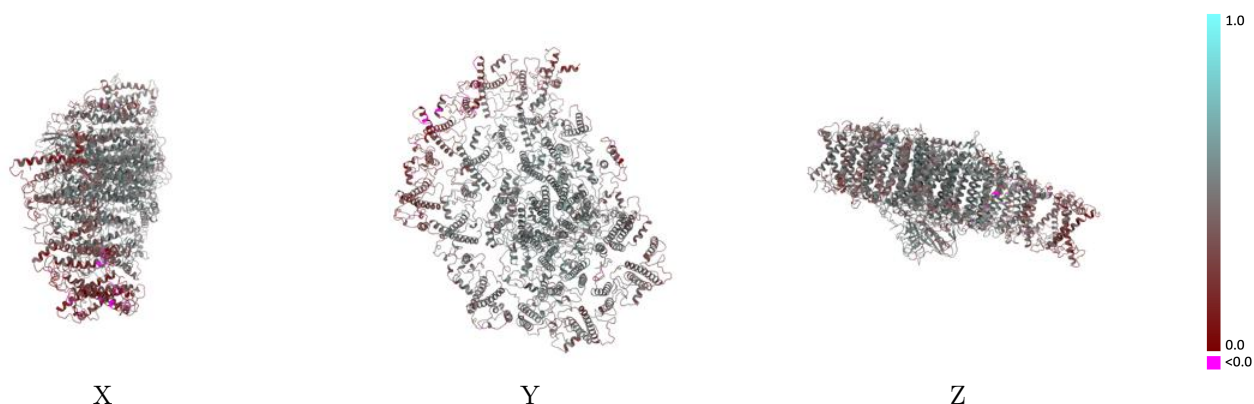
This section contains information regarding the fit between EMDB map EMD-48262 and PDB model 9MGW. Per-residue inclusion information can be found in section [3](#) on page [40](#).

9.1 Map-model overlay [i](#)



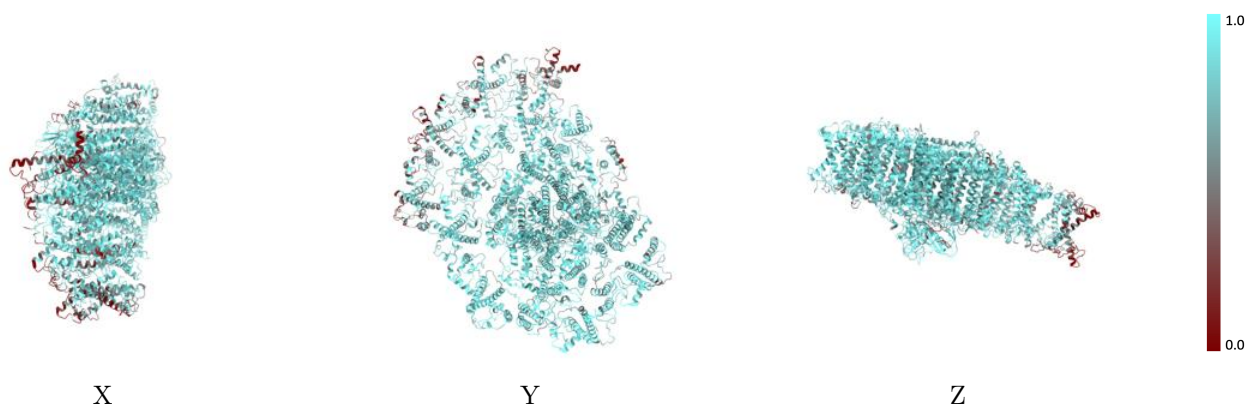
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



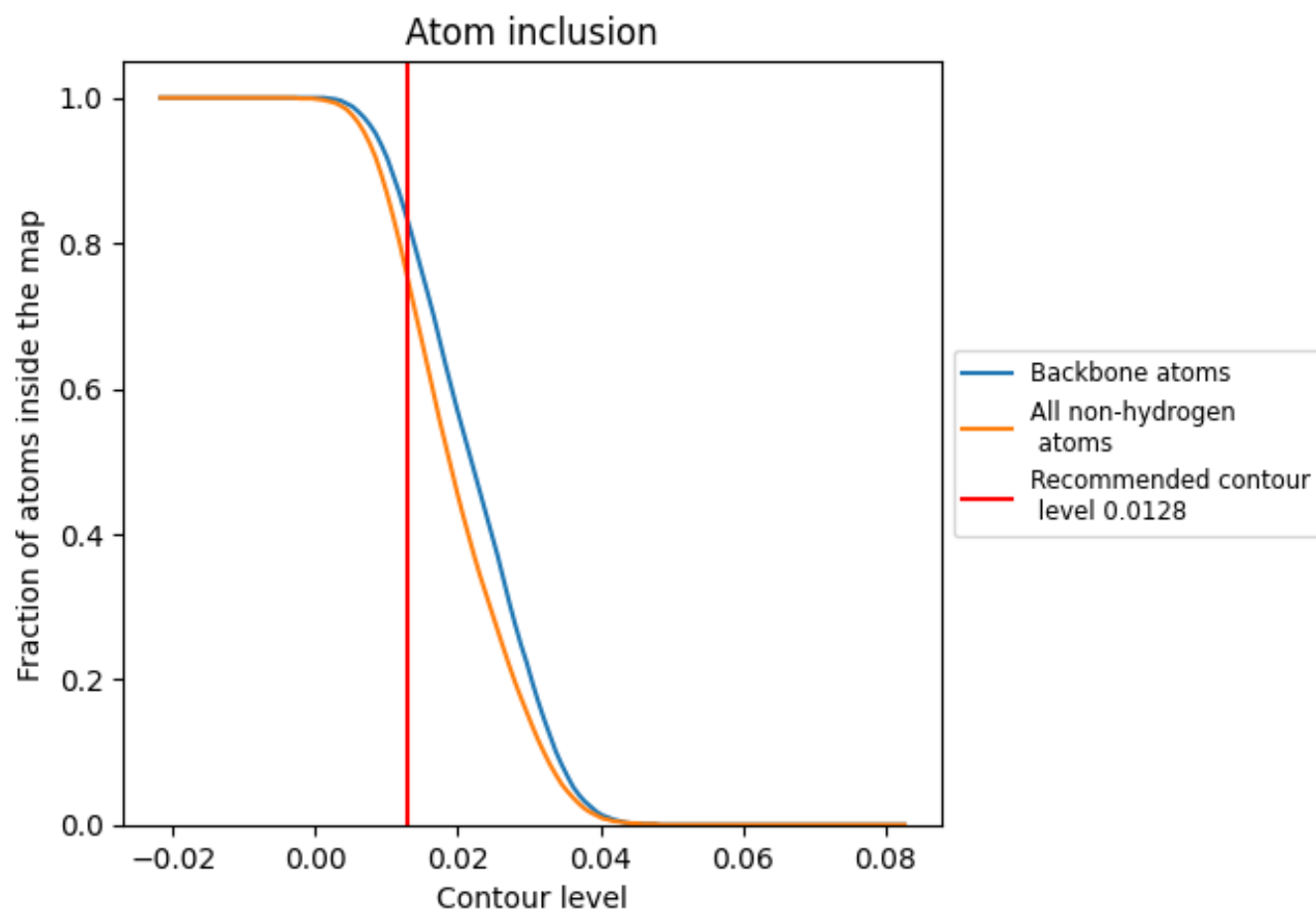
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0128).

















































9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.4180
1	 0.8060	 0.4130
2	 0.7430	 0.3890
3	 0.8160	 0.4590
7	 0.7990	 0.4530
8	 0.7930	 0.4380
9	 0.8030	 0.4050
A	 0.8370	 0.5050
B	 0.8470	 0.4970
C	 0.9190	 0.4990
D	 0.8770	 0.4690
E	 0.8490	 0.4990
F	 0.7890	 0.4480
G	 0.7660	 0.4190
H	 0.6470	 0.3730
I	 0.7740	 0.4220
J	 0.8350	 0.4460
K	 0.7720	 0.3550
L	 0.7530	 0.4130
O	 0.6530	 0.3420
T	 0.3940	 0.2670
a	 0.5860	 0.2630
b	 0.5470	 0.2100
c	 0.6510	 0.2690

