



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 11:23 AM EDT

PDB ID : 9MH1 / pdb\_00009mh1  
EMDB ID : EMD-48266  
Title : Dunaliella tertiolecta PSI-LHCI supercomplex  
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.  
Deposited on : 2024-12-11  
Resolution : 2.10 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](mailto: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>.

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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

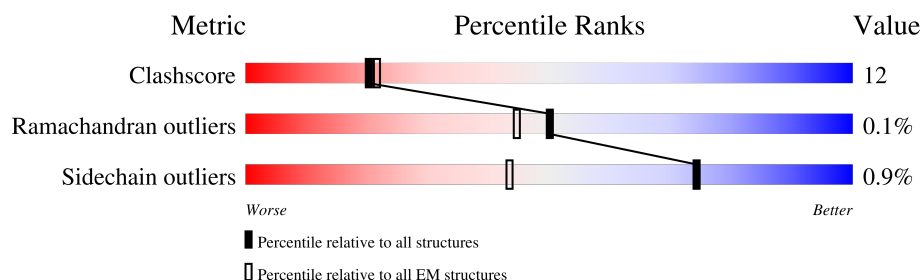
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.10 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.





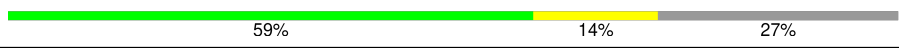



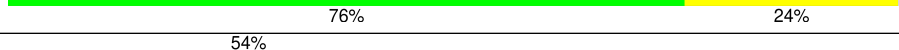


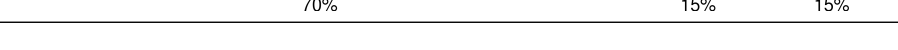
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
2	3	286	
3	7	255	
4	8	254	
5	9	222	
6	A	751	
7	B	735	
8	C	81	

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Mol	Chain	Length	Quality of chain
9	D	193	
10	E	111	
11	F	227	
12	G	141	
13	H	134	
14	I	109	
15	J	41	
16	K	123	
17	L	198	
18	2	261	

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
19	CHL	1	601	X	-	-	-
19	CHL	1	606	X	-	-	-
19	CHL	2	302	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	3	301	X	-	-	-
19	CHL	3	323	X	-	-	-
19	CHL	7	306	X	-	-	-
19	CHL	7	307	X	-	-	-
19	CHL	7	308	X	-	-	-
19	CHL	8	304	X	-	-	-
19	CHL	8	305	X	-	-	-
19	CHL	8	306	X	-	-	-
19	CHL	9	606	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	610	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	2	301	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	313	X	-	-	-
20	CLA	3	302	X	-	-	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	3	324	X	-	-	-
20	CLA	3	325	X	-	-	-
20	CLA	7	303	X	-	-	-
20	CLA	7	304	X	-	-	-
20	CLA	7	305	X	-	-	-
20	CLA	7	309	X	-	-	-
20	CLA	7	310	X	-	-	-
20	CLA	7	311	X	-	-	-
20	CLA	7	312	X	-	-	-
20	CLA	7	313	X	-	-	-
20	CLA	7	314	X	-	-	-
20	CLA	7	315	X	-	-	-
20	CLA	7	323	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	8	301	X	-	-	-
20	CLA	8	302	X	-	-	-
20	CLA	8	303	X	-	-	-
20	CLA	8	307	X	-	-	-
20	CLA	8	308	X	-	-	-
20	CLA	8	309	X	-	-	-
20	CLA	8	310	X	-	-	-
20	CLA	8	311	X	-	-	-
20	CLA	8	312	X	-	-	-
20	CLA	8	313	X	-	-	-
20	CLA	9	601	X	-	-	-
20	CLA	9	602	X	-	-	-
20	CLA	9	603	X	-	-	-
20	CLA	9	604	X	-	-	-
20	CLA	9	605	X	-	-	-
20	CLA	9	607	X	-	-	-
20	CLA	9	608	X	-	-	-
20	CLA	9	609	X	-	-	-
20	CLA	9	610	X	-	-	-
20	CLA	9	611	X	-	-	-
20	CLA	9	612	X	-	-	-
20	CLA	A	5004	X	-	-	-
20	CLA	A	5005	X	-	-	-
20	CLA	A	5006	X	-	-	-
20	CLA	A	5007	X	-	-	-
20	CLA	A	5008	X	-	-	-
20	CLA	A	5009	X	-	-	-
20	CLA	A	5010	X	-	-	-
20	CLA	A	5011	X	-	-	-
20	CLA	A	5012	X	-	-	-
20	CLA	A	5013	X	-	-	-
20	CLA	A	5015	X	-	-	-
20	CLA	A	5016	X	-	-	-
20	CLA	A	5017	X	-	-	-
20	CLA	A	5018	X	-	-	-
20	CLA	A	5019	X	-	-	-
20	CLA	A	5020	X	-	-	-
20	CLA	A	5021	X	-	-	-
20	CLA	A	5022	X	-	-	-
20	CLA	A	5023	X	-	-	-
20	CLA	A	5024	X	-	-	-
20	CLA	A	5025	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	5026	X	-	-	-
20	CLA	A	5027	X	-	-	-
20	CLA	A	5028	X	-	-	-
20	CLA	A	5029	X	-	-	-
20	CLA	A	5030	X	-	-	-
20	CLA	A	5031	X	-	-	-
20	CLA	A	5032	X	-	-	-
20	CLA	A	5033	X	-	-	-
20	CLA	A	5034	X	-	-	-
20	CLA	A	5035	X	-	-	-
20	CLA	A	5036	X	-	-	-
20	CLA	A	5037	X	-	-	-
20	CLA	A	5038	X	-	-	-
20	CLA	A	5039	X	-	-	-
20	CLA	A	5040	X	-	-	-
20	CLA	A	5041	X	-	-	-
20	CLA	A	5042	X	-	-	-
20	CLA	A	5043	X	-	-	-
20	CLA	A	5044	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	306	X	-	-	-
20	CLA	F	307	X	-	-	-
20	CLA	F	308	X	-	-	-
20	CLA	G	201	X	-	-	-
20	CLA	G	202	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	204	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	104	X	-	-	-
20	CLA	K	4002	X	-	-	-
20	CLA	K	4003	X	-	-	-
20	CLA	K	4004	X	-	-	-
20	CLA	K	4005	X	-	-	-
20	CLA	L	201	X	-	-	-
20	CLA	L	202	X	-	-	-
20	CLA	L	204	X	-	-	-
20	CLA	L	205	X	-	-	-
21	LUT	1	615	X	-	-	-
21	LUT	2	314	X	-	-	-
21	LUT	2	315	X	-	-	-
21	LUT	3	315	X	-	-	-
21	LUT	7	316	X	-	-	-
21	LUT	8	314	X	-	-	-
21	LUT	9	613	X	-	-	-
30	CL0	A	5003	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 41548 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
			1505	965	255	278	7		

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	226	Total	C	N	O	S	0	0
			1719	1120	282	312	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	217	Total	C	N	O	S	0	0
			1669	1078	281	304	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	226	Total	C	N	O	S	0	0
			1721	1108	286	320	7		

- Molecule 5 is a protein called LHCA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	187	Total	C	N	O	S	0	0
			1453	945	244	259	5		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

- Molecule 10 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	68	Total	C	N	O	S	0	0
			540	343	95	102			

- Molecule 11 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

- Molecule 12 is a protein called PSAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	105	Total	C	N	O	S	0	0
			794	515	134	142	3		

- Molecule 13 is a protein called PSAH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	47	Total	C	N	O	S	0	0
			349	223	60	66			

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			274	191	40	42	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 PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

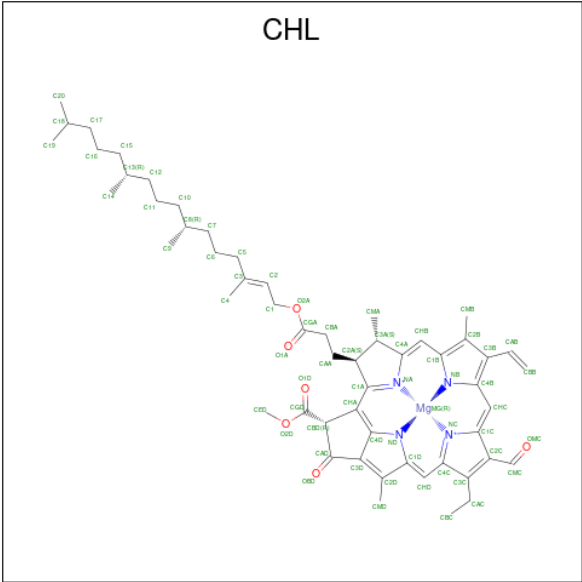
- Molecule 17 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	124	Total	C	N	O	S	0	0
			891	580	146	160	5		

- Molecule 18 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	222	Total	C	N	O	S	0	0
			1728	1125	284	311	8		

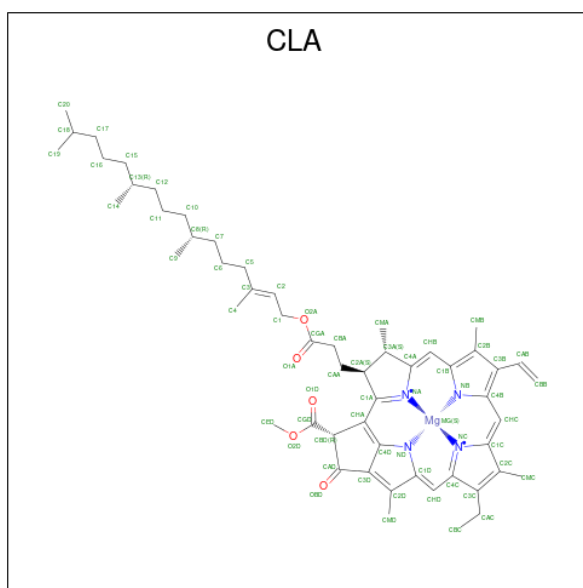
- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	3	1	Total 62	C 51	Mg 1	N 4	O 6	0
19	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
19	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
19	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	7	1	Total 48	C 37	Mg 1	N 4	O 6	0
19	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
19	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
19	2	1	Total 47	C 36	Mg 1	N 4	O 6	0

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 49	C 40	Mg 1	N 4	O 4	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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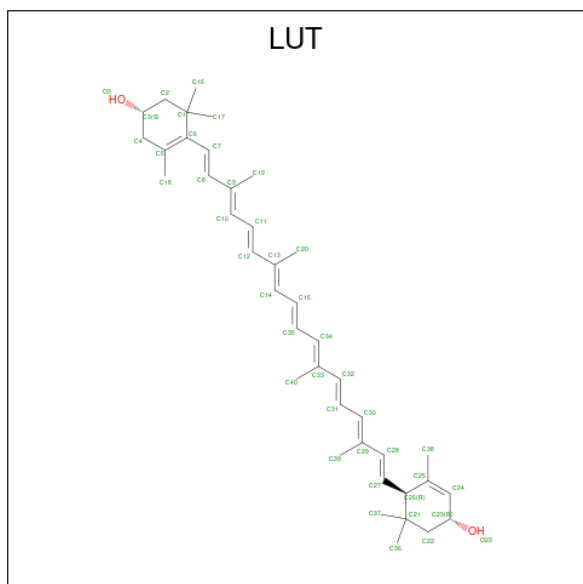
Mol	Chain	Residues	Atoms					AltConf
20	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 21 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
21	1	1	Total	C	O			0
			42	40	2			
21	3	1	Total	C	O			0
			42	40	2			
21	7	1	Total	C	O			0
			42	40	2			

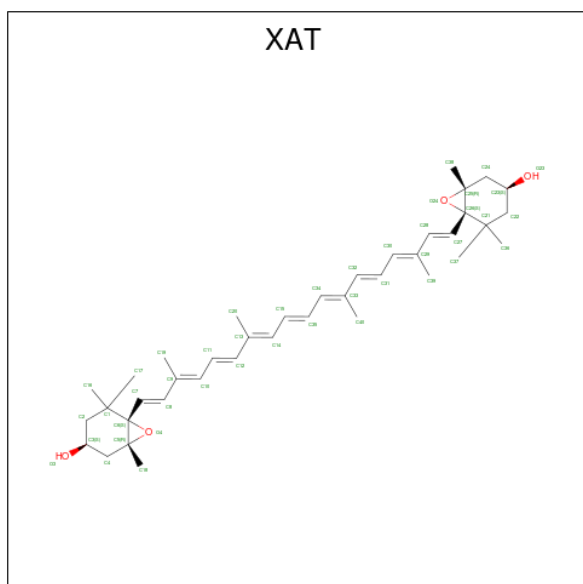
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Mol	Chain	Residues	Atoms			AltConf
21	8	1	Total	C	O	0
			42	40	2	
21	9	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	

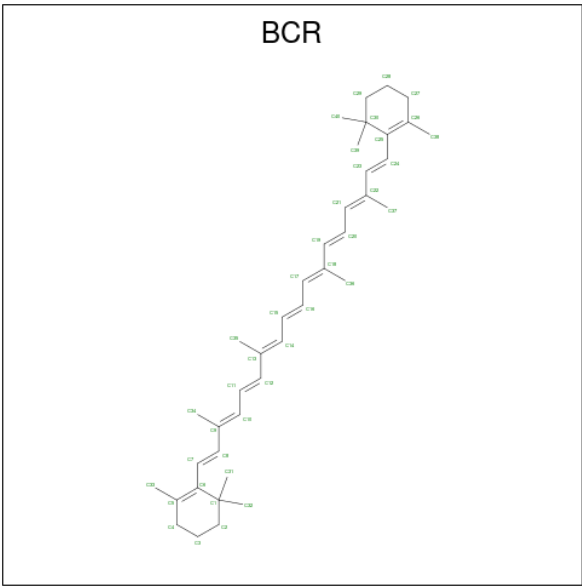
- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	7	1	Total	C	O	0
			44	40	4	
22	8	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand

of Interest" by depositor).



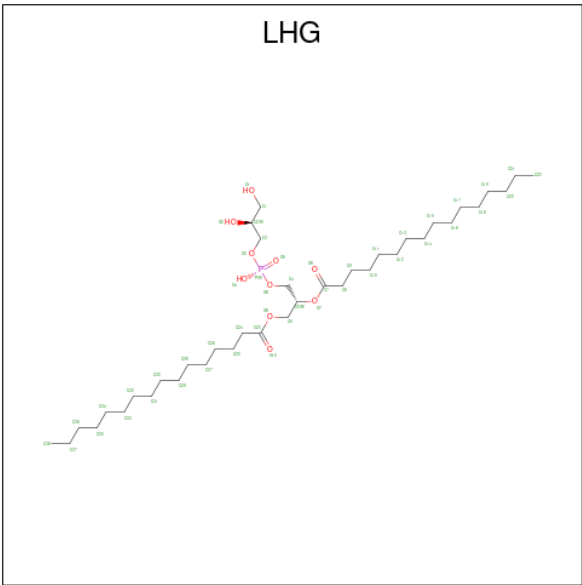
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	8	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 39 39	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



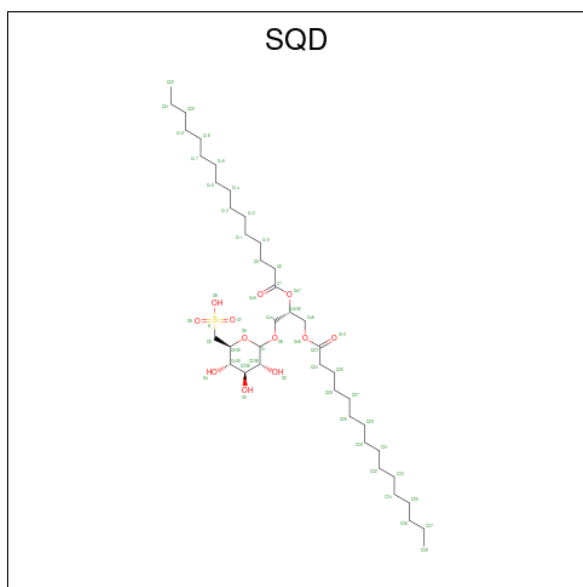
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			26	15	10	1	
24	1	1	Total	C	O	P	0
			46	35	10	1	
24	7	1	Total	C	O	P	0
			22	11	10	1	
24	7	1	Total	C	O	P	0
			34	23	10	1	
24	8	1	Total	C	O	P	0
			29	18	10	1	
24	8	1	Total	C	O	P	0
			38	27	10	1	
24	8	1	Total	C	O	P	0
			43	32	10	1	
24	9	1	Total	C	O	P	0
			36	25	10	1	
24	A	1	Total	C	O	P	0
			36	25	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			28	17	10	1	
24	A	1	Total	C	O	P	0
			34	25	8	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	B	1	Total	C	O	P	0
			30	19	10	1	

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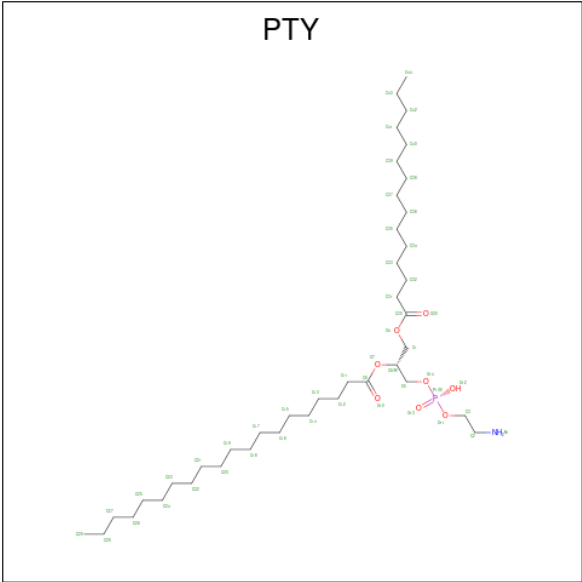
Mol	Chain	Residues	Atoms				AltConf
24	I	1	Total	C	O	P	0
			28	17	10	1	
24	2	1	Total	C	O	P	0
			25	16	8	1	

- Molecule 25 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).



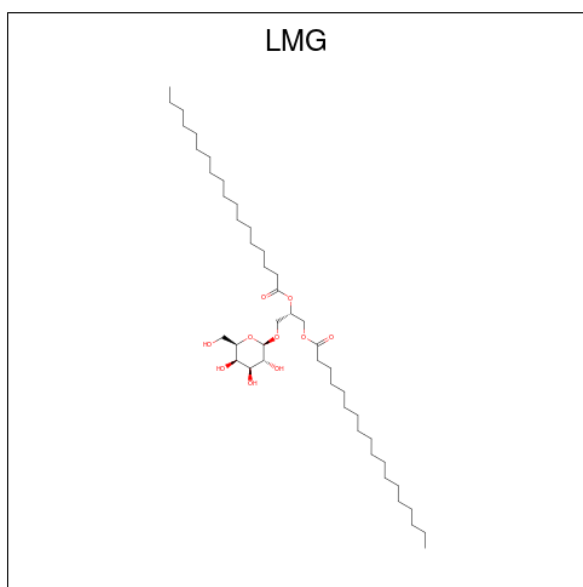
Mol	Chain	Residues	Atoms				AltConf
25	1	1	Total	C	O	S	0
			38	25	12	1	
25	3	1	Total	C	O	S	0
			35	22	12	1	
25	3	1	Total	C	O	S	0
			41	28	12	1	
25	7	1	Total	C	O	S	0
			39	26	12	1	
25	B	1	Total	C	O	S	0
			31	18	12	1	
25	F	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula:  $C_{40}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



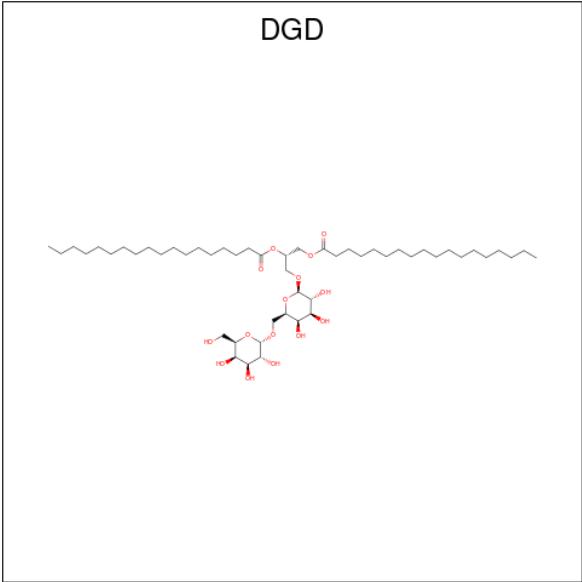
Mol	Chain	Residues	Atoms					AltConf
26	3	1	Total	C	N	O	P	0
			50	40	1	8	1	
26	7	1	Total	C	O	P		0
			15	6	8	1		
26	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
26	F	1	Total	C	N	O	P	0
			29	19	1	8	1	
26	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
26	F	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



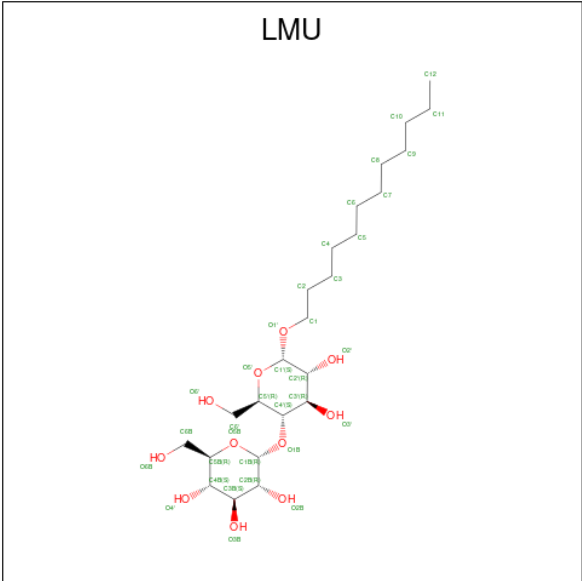
Mol	Chain	Residues	Atoms			AltConf
27	7	1	Total	C	O	0
			50	40	10	
27	7	1	Total	C	O	0
			30	20	10	
27	A	1	Total	C	O	0
			32	22	10	
27	G	1	Total	C	O	0
			43	34	9	
27	J	1	Total	C	O	0
			29	19	10	

- Molecule 28 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
28	7	1	Total	C	O	0
			39	24	15	
28	B	1	Total	C	O	0
			61	46	15	

- Molecule 29 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	7	1	Total	C	O	0
			32	21	11	

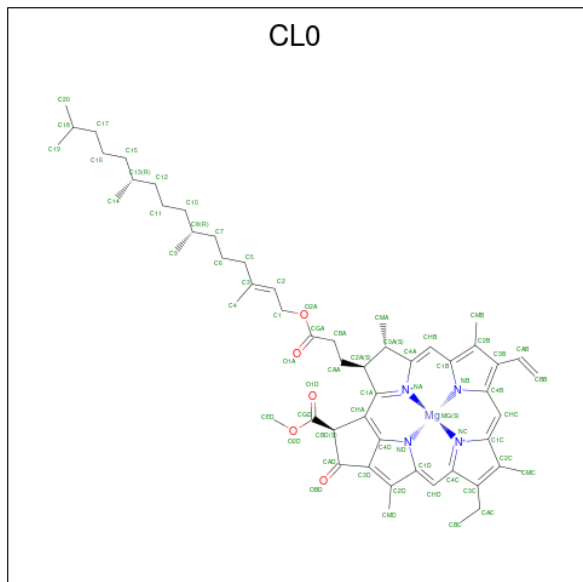
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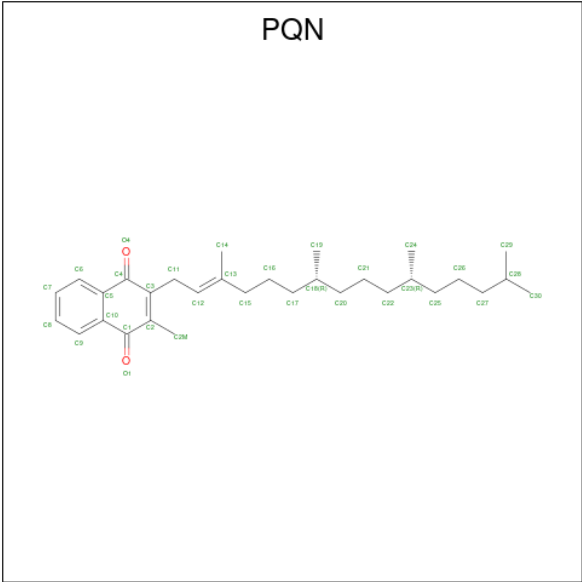
Mol	Chain	Residues	Atoms			AltConf
29	8	1	Total	C	O	0
			33	22	11	
29	8	1	Total	C	O	0
			35	24	11	
29	9	1	Total	C	O	0
			29	18	11	
29	A	1	Total	C	O	0
			35	24	11	
29	F	1	Total	C	O	0
			32	21	11	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



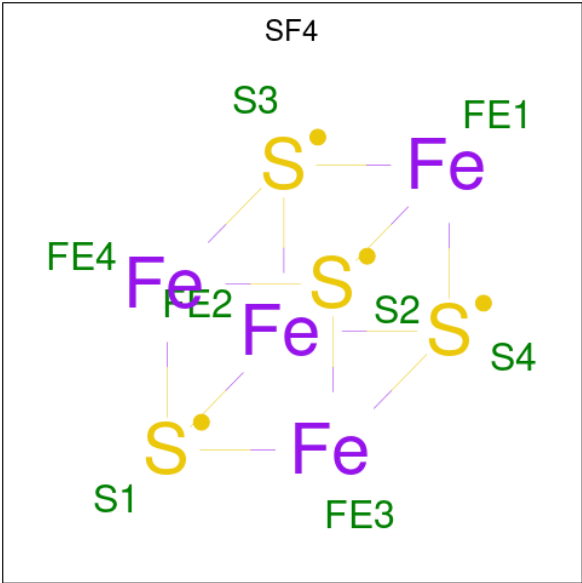
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



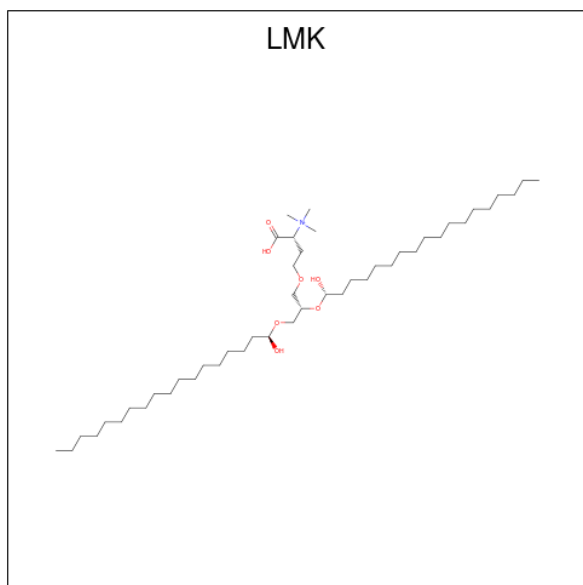
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

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

- 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]azanium (CCD ID: LMK) (formula: C<sub>46</sub>H<sub>94</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).

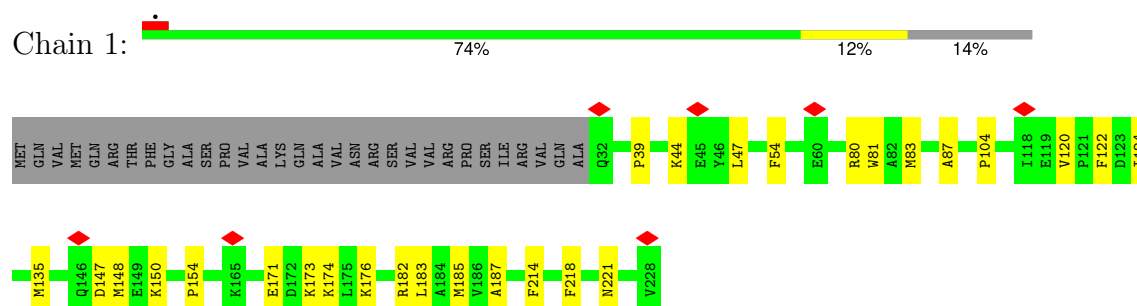


Mol	Chain	Residues	Atoms				AltConf
33	J	1	Total	C	N	O	0
			35	27	1	7	

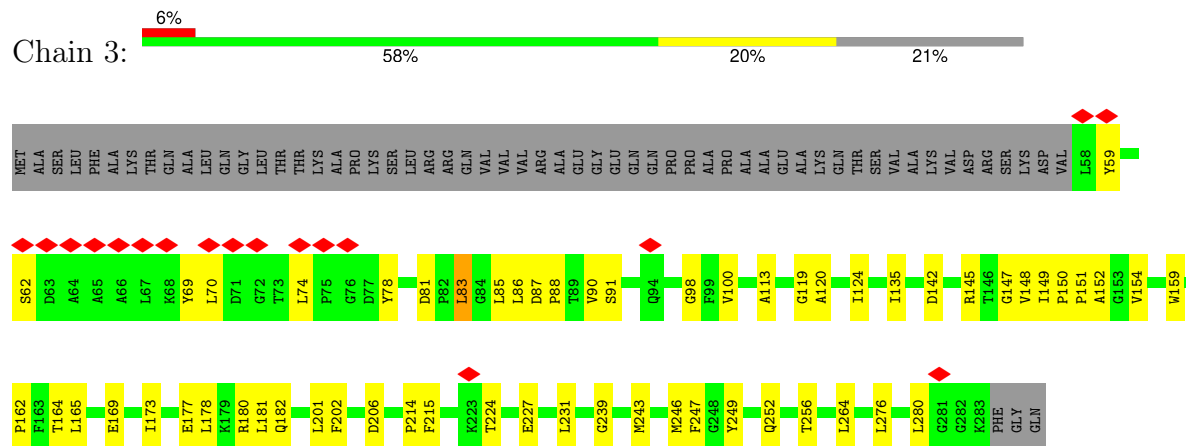
### 3 Residue-property plots

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.

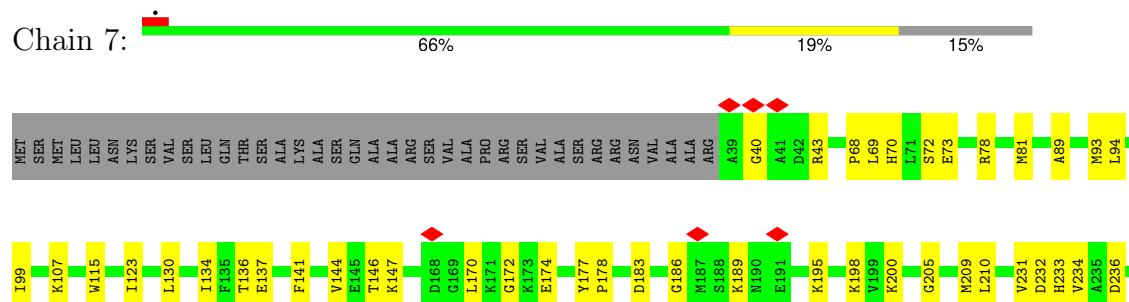
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

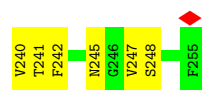


- Molecule 2: LHCA3



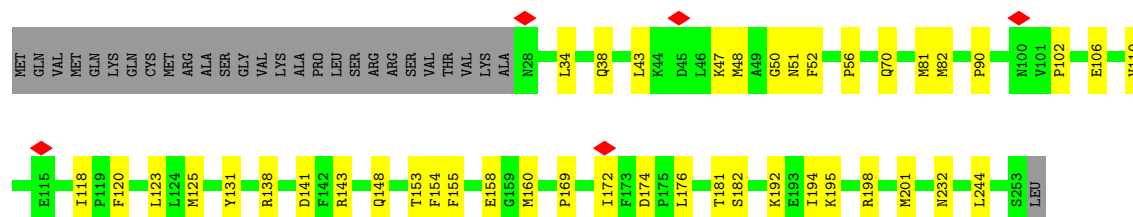
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic





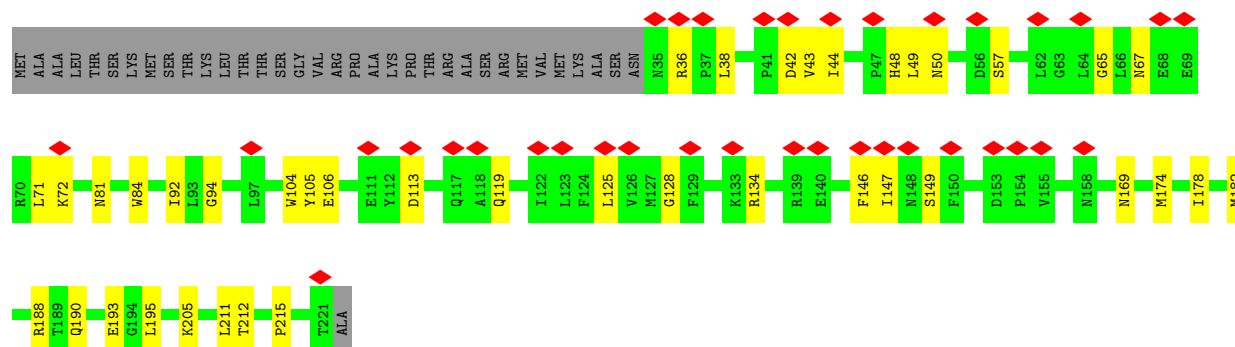
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 72% 17% 11%



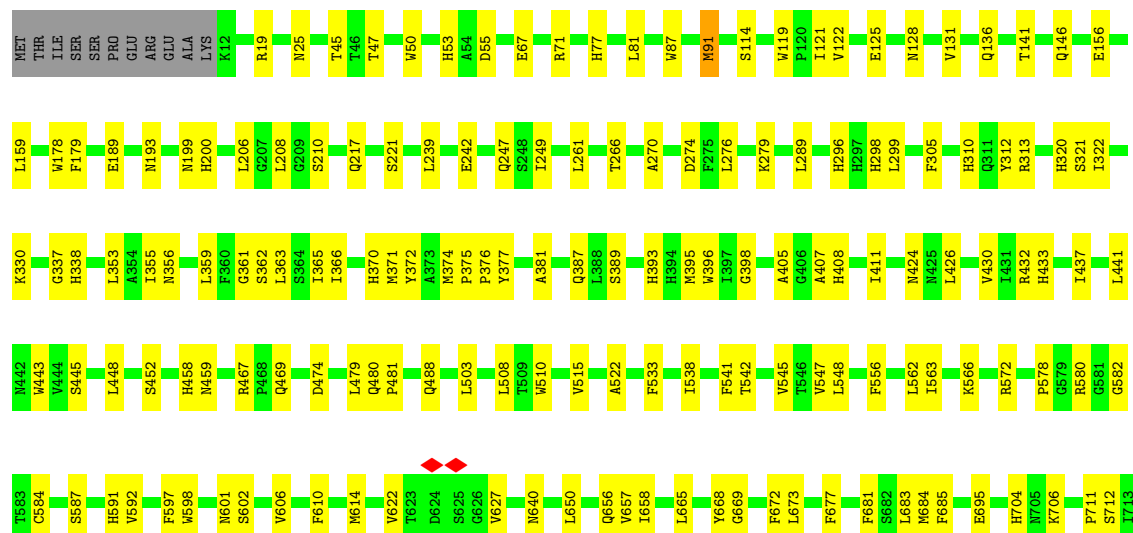
- Molecule 5: LHCA9

Chain 9: 16% 66% 18% 16%

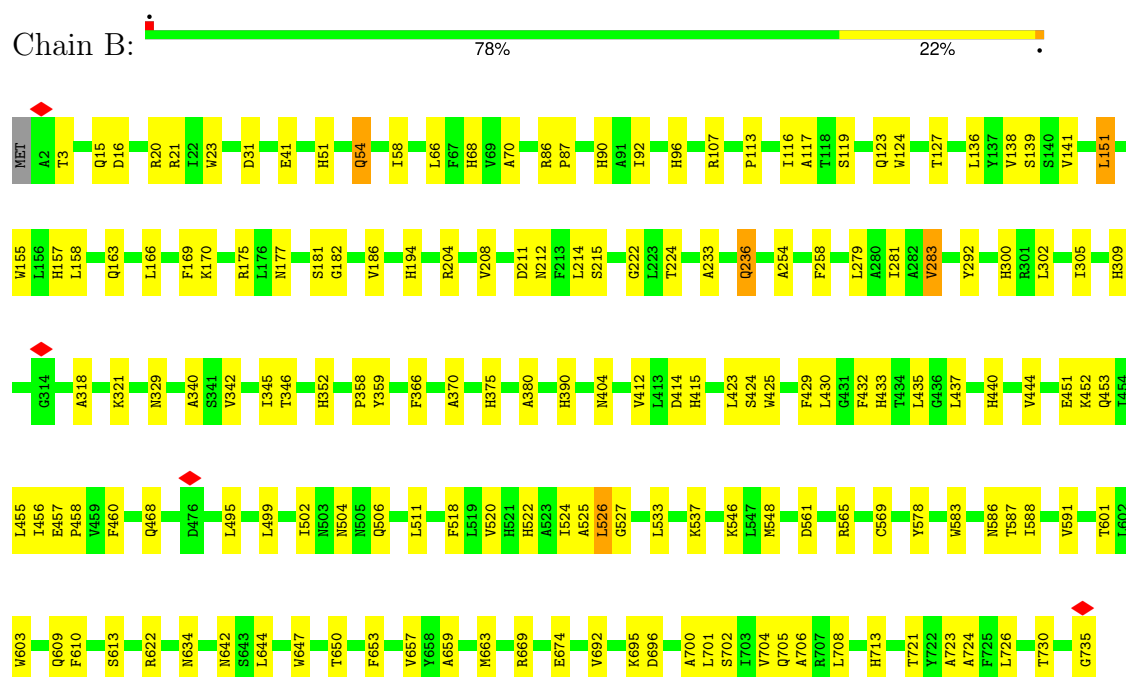


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

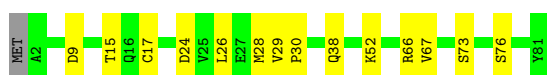
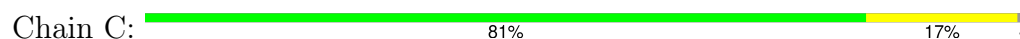
Chain A: 76% 23%



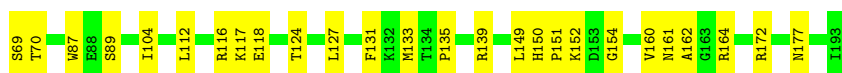
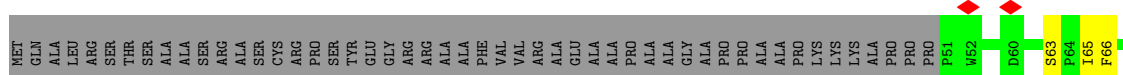
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2



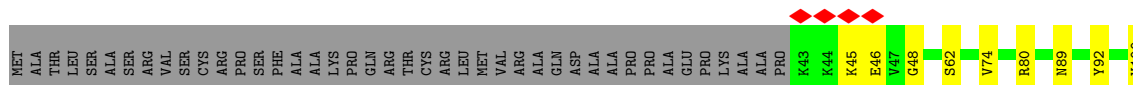
- Molecule 8: Photosystem I iron-sulfur center

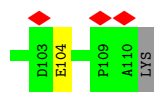


- Molecule 9: Photosystem I reaction center subunit II, chloroplatic



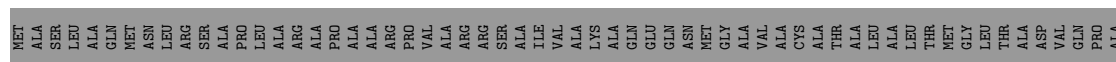
- Molecule 10: Photosystem I reaction center subunit IV





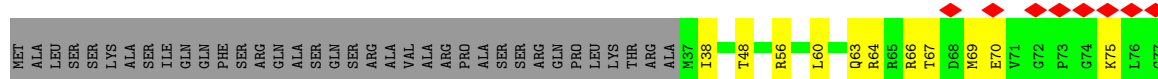
- Molecule 11: PSAF1

Chain F: 59% 14% 27%



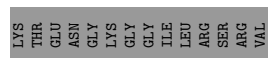
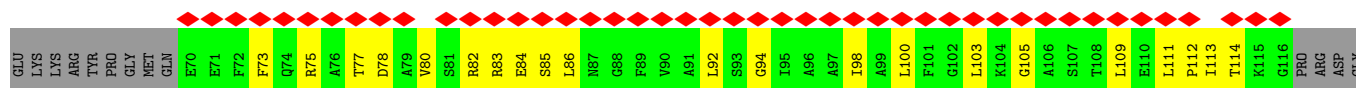
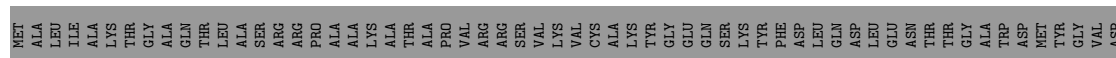
- Molecule 12: PSAG1

Chain G: 21% 60% 14% 26%



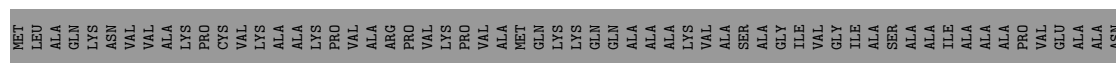
- Molecule 13: PSAH1

Chain H: 34% 19% 16% 65%

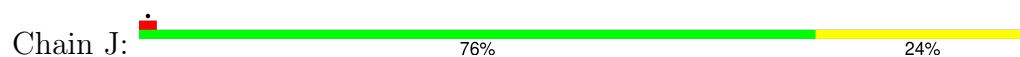


- Molecule 14: Photosystem I reaction center subunit VIII

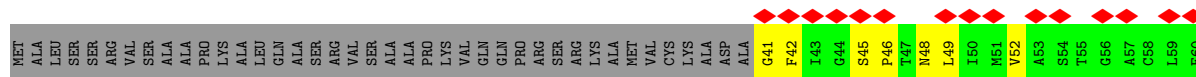
Chain I: 24% 8% 68%



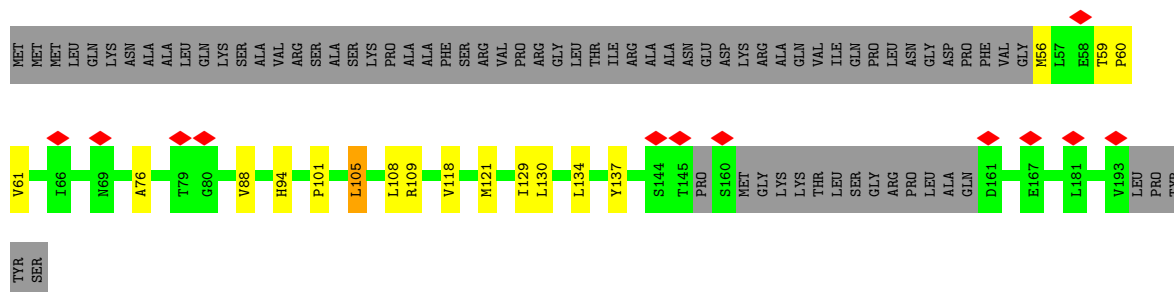
- Molecule 15: Photosystem I reaction center subunit IX



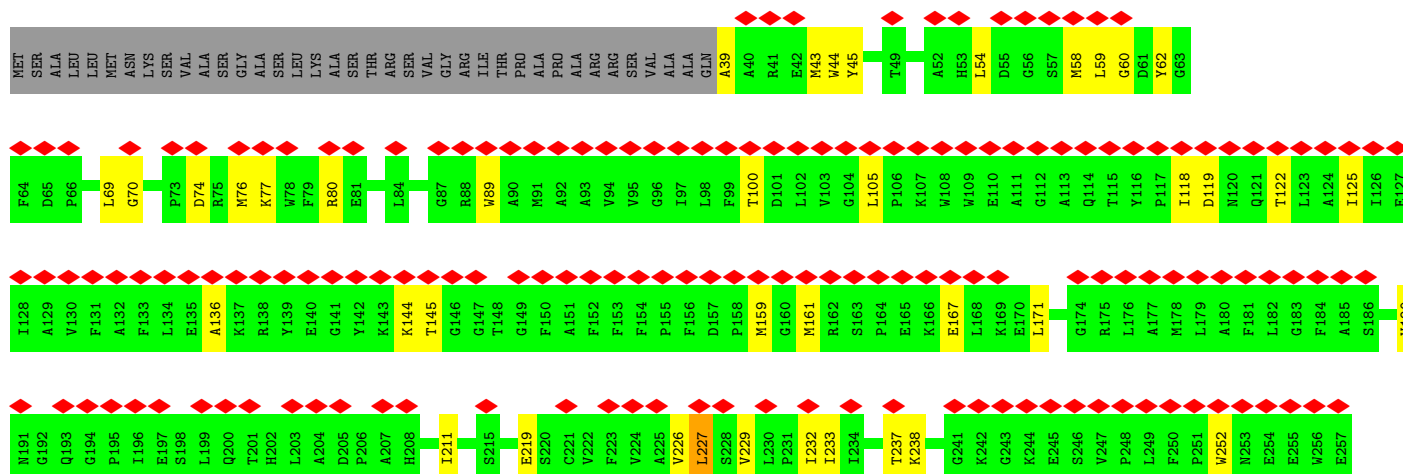
• Molecule 16: PSI-K



• Molecule 17: PSAL1



• Molecule 18: LHCA2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126839	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	0.091	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0172	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

### 5.1 Standard geometry

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

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	0.18	0/1544	0.38	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.15	0/1722	0.39	0/2339
4	8	0.17	0/1770	0.37	0/2401
5	9	0.20	0/1496	0.46	0/2038
6	A	0.14	0/6004	0.33	0/8190
7	B	0.14	0/6026	0.35	1/8235 (0.0%)
8	C	0.12	0/610	0.33	0/828
9	D	0.14	0/1163	0.40	0/1571
10	E	0.10	0/552	0.28	0/750
11	F	0.17	0/1329	0.42	0/1797
12	G	0.17	0/814	0.41	0/1100
13	H	0.18	0/353	0.45	0/474
14	I	0.23	0/286	0.57	0/394
15	J	0.16	0/338	0.43	0/461
16	K	0.22	0/587	0.54	0/795
17	L	0.15	0/911	0.35	0/1244
18	2	0.16	0/1779	0.40	0/2417
All	All	0.16	0/29052	0.38	1/39529 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	54	GLN	CA-CB-CG	6.45	127.00	114.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1468	25	0
2	3	1719	0	1676	60	0
3	7	1669	0	1612	42	0
4	8	1721	0	1661	35	0
5	9	1453	0	1437	34	0
6	A	5808	0	5638	135	0
7	B	5814	0	5556	141	0
8	C	600	0	582	10	0
9	D	1133	0	1138	23	0
10	E	540	0	539	7	0
11	F	1300	0	1322	25	0
12	G	794	0	796	20	0
13	H	349	0	357	18	0
14	I	274	0	282	8	0
15	J	327	0	328	9	0
16	K	579	0	608	19	0
17	L	891	0	908	22	0
18	2	1728	0	1697	59	0
19	1	94	0	62	7	0
19	2	108	0	88	10	0
19	3	123	0	115	22	0
19	7	141	0	95	12	0
19	8	145	0	95	18	0
19	9	47	0	30	2	0
20	1	604	0	486	28	0
20	2	517	0	381	20	0
20	3	769	0	649	36	0
20	7	595	0	533	22	0
20	8	606	0	552	29	0
20	9	563	0	462	29	0
20	A	2475	0	2517	137	0
20	B	2260	0	2330	140	0
20	F	217	0	197	11	0
20	G	203	0	170	17	0
20	H	60	0	57	2	0
20	J	49	0	39	2	0
20	K	193	0	151	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	245	0	249	11	0
21	1	42	0	56	7	0
21	2	84	0	112	2	0
21	3	42	0	56	2	0
21	7	42	0	56	2	0
21	8	42	0	56	4	0
21	9	42	0	56	2	0
22	1	44	0	56	0	0
22	3	44	0	56	7	0
22	7	44	0	56	4	0
22	8	44	0	54	1	0
22	9	88	0	112	2	0
23	1	40	0	56	5	0
23	3	120	0	168	18	0
23	7	40	0	56	3	0
23	8	40	0	56	10	0
23	A	200	0	280	22	0
23	B	279	0	388	23	0
23	F	80	0	112	10	0
23	G	40	0	56	1	0
23	I	40	0	53	1	0
23	J	120	0	168	15	0
23	K	80	0	112	6	0
23	L	80	0	110	5	0
24	1	72	0	87	6	0
24	2	25	0	23	1	0
24	7	56	0	52	6	0
24	8	110	0	132	3	0
24	9	36	0	45	0	0
24	A	147	0	181	8	0
24	B	62	0	63	1	0
24	I	28	0	26	2	0
25	1	38	0	40	2	0
25	3	76	0	78	3	0
25	7	39	0	42	1	0
25	B	31	0	25	0	0
25	F	39	0	42	3	0
26	3	50	0	79	1	0
26	7	15	0	5	1	0
26	B	27	0	27	0	0
26	F	92	0	99	3	0
27	7	80	0	102	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	32	0	34	2	0
27	G	43	0	55	6	0
27	J	29	0	28	0	0
28	7	39	0	36	0	0
28	B	61	0	83	9	0
29	7	32	0	37	0	0
29	8	68	0	85	5	0
29	9	29	0	30	0	0
29	A	35	0	45	2	0
29	F	32	0	37	0	0
30	A	65	0	72	10	0
31	A	33	0	46	3	0
31	B	33	0	46	8	0
32	A	8	0	0	1	0
32	C	16	0	0	1	0
33	J	35	0	0	0	0
All	All	41548	0	40986	992	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 12.

All (992) 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)
20:9:607:CLA:CMB	18:2:232:ILE:HD13	1.11	1.58
20:9:607:CLA:HMB1	18:2:232:ILE:CD1	0.97	1.43
20:9:607:CLA:HMB1	18:2:232:ILE:CG1	1.58	1.31
18:2:161:MET:HG2	20:2:308:CLA:O1A	1.31	1.31
20:9:607:CLA:CMB	18:2:232:ILE:CD1	1.84	1.19
20:9:607:CLA:HMB2	18:2:232:ILE:HD13	1.20	1.17
12:G:108:ILE:CG2	20:G:203:CLA:C1	2.24	1.15
6:A:479:LEU:HD13	6:A:533:PHE:CD2	1.81	1.14
18:2:211:ILE:HD12	20:2:311:CLA:CHD	1.81	1.11
12:G:108:ILE:HG23	20:G:203:CLA:O1A	1.51	1.11
7:B:708:LEU:HD23	28:B:848:DGD:HA21	1.31	1.09
2:3:124:ILE:HD11	2:3:249:TYR:OH	1.57	1.05
2:3:169:GLU:O	2:3:173:ILE:HG22	1.58	1.04
20:9:607:CLA:HMB1	18:2:232:ILE:HD11	1.39	1.03
6:A:362:SER:O	6:A:366:ILE:HD12	1.57	1.02
18:2:211:ILE:HD12	20:2:311:CLA:C4C	1.90	1.01
20:9:607:CLA:CMB	18:2:232:ILE:CG1	2.27	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:5005:CLA:NB	20:B:805:CLA:HBB1	1.78	0.99
19:7:306:CHL:HBC2	19:7:307:CHL:HHD	1.49	0.94
20:9:607:CLA:HBB	18:2:232:ILE:HD11	1.48	0.94
20:A:5005:CLA:C1B	20:B:805:CLA:HBB1	1.99	0.92
18:2:161:MET:CG	20:2:308:CLA:O1A	2.17	0.92
6:A:479:LEU:HD13	6:A:533:PHE:HD2	1.27	0.91
12:G:108:ILE:HG21	20:G:203:CLA:C1	2.01	0.89
23:B:803:BCR:H16C	20:B:839:CLA:HBB1	1.55	0.87
19:8:304:CHL:HBC2	19:8:305:CHL:HHD	1.56	0.87
6:A:408:HIS:HE1	20:A:5031:CLA:NA	1.74	0.84
18:2:58:MET:HE1	18:2:76:MET:CE	2.08	0.84
20:B:836:CLA:HBC2	23:J:102:BCR:H24C	1.59	0.83
6:A:121:ILE:HG13	6:A:122:VAL:HG13	1.61	0.83
2:3:74:LEU:HD12	19:3:301:CHL:HED3	1.62	0.81
7:B:708:LEU:CD2	28:B:848:DGD:HA21	2.11	0.80
20:9:607:CLA:HMB3	18:2:232:ILE:HB	1.64	0.80
12:G:108:ILE:HG22	20:G:203:CLA:C1	2.10	0.80
6:A:91:MET:HE1	20:A:5011:CLA:H2A	1.64	0.79
6:A:479:LEU:CD1	6:A:533:PHE:CD2	2.66	0.79
7:B:708:LEU:HD23	28:B:848:DGD:C2A	2.12	0.79
20:9:607:CLA:HMB1	18:2:232:ILE:HG12	1.64	0.78
20:A:5004:CLA:HBB1	20:A:5044:CLA:C4B	2.12	0.78
20:A:5012:CLA:HBB1	23:J:105:BCR:HC8	1.65	0.78
18:2:211:ILE:CD1	20:2:311:CLA:CHD	2.60	0.77
13:H:94:GLY:O	13:H:98:ILE:HG12	1.85	0.77
6:A:479:LEU:CD1	6:A:533:PHE:HD2	1.97	0.77
18:2:161:MET:HE3	20:2:308:CLA:O1A	1.84	0.76
6:A:479:LEU:HD12	6:A:479:LEU:O	1.86	0.75
17:L:59:THR:HG22	17:L:61:VAL:H	1.51	0.74
2:3:173:ILE:HD13	20:3:307:CLA:HMC3	1.69	0.74
20:1:605:CLA:HAB	19:1:606:CHL:HHC	1.70	0.74
20:B:811:CLA:H3A	20:L:201:CLA:HBB1	1.70	0.73
7:B:404:ASN:OD1	7:B:404:ASN:O	2.07	0.73
20:3:305:CLA:HAB	27:7:301:LMG:H341	1.70	0.73
4:8:160:MET:SD	4:8:172:ILE:HG23	2.29	0.72
18:2:226:VAL:HA	18:2:229:VAL:HG12	1.69	0.72
3:7:147:LYS:HD3	19:7:308:CHL:HHC	1.70	0.72
20:B:819:CLA:H162	20:B:826:CLA:H3A	1.71	0.72
18:2:227:LEU:HD12	19:2:302:CHL:H3A	1.70	0.72
7:B:390:HIS:HE1	20:B:829:CLA:NA	1.86	0.72
20:9:607:CLA:CMB	18:2:232:ILE:HG12	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:243:MET:HE3	19:3:301:CHL:HHC	1.71	0.72
6:A:448:LEU:HB3	6:A:541:PHE:HB2	1.72	0.71
5:9:128:GLY:HA2	20:9:607:CLA:HAB	1.72	0.71
12:G:108:ILE:HG23	20:G:203:CLA:CGA	2.19	0.71
20:K:4004:CLA:H3A	23:K:4006:BCR:H363	1.72	0.71
20:B:838:CLA:HAB	31:B:841:PQN:H141	1.73	0.70
20:A:5004:CLA:H3A	20:A:5004:CLA:H12	1.72	0.70
20:A:5005:CLA:C4B	20:B:805:CLA:HBB1	2.21	0.70
16:K:66:LEU:HG	20:K:4005:CLA:ND	2.06	0.70
20:1:605:CLA:HBB2	19:1:606:CHL:HAB	1.74	0.69
4:8:52:PHE:HB2	20:8:301:CLA:HMD1	1.74	0.69
1:1:87:ALA:HB2	21:1:615:LUT:H15	1.72	0.69
18:2:58:MET:HE1	18:2:76:MET:SD	2.32	0.69
6:A:81:LEU:HD22	20:A:5014:CLA:HED1	1.74	0.69
20:A:5021:CLA:HBB2	23:A:5047:BCR:H281	1.74	0.69
23:3:317:BCR:H333	19:3:323:CHL:HMD2	1.75	0.69
18:2:58:MET:HE1	18:2:76:MET:HE3	1.75	0.69
19:2:302:CHL:HBB2	20:2:303:CLA:HHH	1.74	0.69
20:B:832:CLA:HMA1	23:J:102:BCR:H363	1.76	0.68
13:H:109:LEU:HD12	13:H:109:LEU:O	1.94	0.68
18:2:167:GLU:HB3	20:2:308:CLA:HMA1	1.75	0.68
20:1:605:CLA:HAA1	23:1:617:BCR:H23C	1.75	0.68
19:7:307:CHL:HED3	19:7:307:CHL:H2A	1.76	0.68
20:9:607:CLA:HMB3	18:2:232:ILE:CB	2.24	0.68
20:1:612:CLA:HBC2	20:1:614:CLA:HAB	1.75	0.67
6:A:217:GLN:HA	6:A:221:SER:HB2	1.76	0.67
20:1:611:CLA:HAB	21:1:615:LUT:H12	1.76	0.67
18:2:211:ILE:HG21	20:2:311:CLA:H2	1.76	0.67
1:1:87:ALA:HB2	21:1:615:LUT:H34	1.76	0.67
2:3:120:ALA:O	2:3:124:ILE:HG12	1.95	0.67
7:B:437:LEU:HD12	20:B:832:CLA:HAB	1.75	0.67
7:B:437:LEU:HD21	23:J:102:BCR:H383	1.76	0.67
14:I:87:LEU:HA	14:I:91:VAL:HG22	1.78	0.66
30:A:5003:CL0:H46	20:A:5005:CLA:HED3	1.79	0.65
20:A:5009:CLA:H151	20:A:5030:CLA:HBB2	1.77	0.65
20:9:607:CLA:HMB3	18:2:232:ILE:CG1	2.24	0.65
6:A:393:HIS:HE1	20:A:5029:CLA:ND	1.91	0.65
5:9:92:ILE:HD12	5:9:104:TRP:HB2	1.79	0.64
20:B:834:CLA:HAA1	20:G:204:CLA:HMA1	1.80	0.64
12:G:95:PHE:CZ	12:G:108:ILE:HD11	2.32	0.64
20:1:602:CLA:H41	20:B:840:CLA:HBB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:323:CHL:H51	20:7:313:CLA:H71	1.78	0.64
3:7:137:GLU:O	3:7:141:PHE:HB2	1.96	0.64
20:A:5025:CLA:HBB1	23:A:5049:BCR:H15C	1.77	0.64
7:B:370:ALA:HB1	7:B:726:LEU:HD11	1.80	0.64
17:L:94:HIS:HE1	20:L:204:CLA:ND	1.92	0.64
2:3:173:ILE:HD13	20:3:307:CLA:CMC	2.27	0.64
7:B:119:SER:HA	20:B:827:CLA:HMA2	1.80	0.64
16:K:66:LEU:HD12	20:K:4005:CLA:NA	2.12	0.64
7:B:692:VAL:HG23	17:L:137:TYR:CZ	2.32	0.64
19:3:301:CHL:H11	22:3:316:XAT:H222	1.80	0.64
4:8:141:ASP:HB3	4:8:148:GLN:HG2	1.80	0.64
20:8:301:CLA:HBB1	20:8:301:CLA:H51	1.80	0.64
6:A:296:HIS:HE1	20:A:5018:CLA:ND	1.95	0.64
7:B:437:LEU:CD2	23:J:102:BCR:H383	2.28	0.64
7:B:458:PRO:HB3	7:B:518:PHE:HB2	1.79	0.64
9:D:87:TRP:HB3	9:D:135:PRO:HB3	1.79	0.63
19:3:323:CHL:HMC	24:7:320:LHG:HC61	1.80	0.63
18:2:211:ILE:CD1	20:2:311:CLA:C4C	2.74	0.63
19:1:606:CHL:HMD2	27:G:206:LMG:H171	1.81	0.63
4:8:123:LEU:HD13	19:8:304:CHL:HHH	1.81	0.63
7:B:51:HIS:HB3	20:B:814:CLA:HED3	1.80	0.63
5:9:215:PRO:HD3	7:B:222:GLY:HA3	1.80	0.62
20:7:303:CLA:HBC1	24:7:320:LHG:H291	1.82	0.62
20:B:808:CLA:H151	20:B:828:CLA:HBB2	1.80	0.62
20:1:605:CLA:HBA1	23:1:617:BCR:H21C	1.81	0.62
2:3:98:GLY:HA2	6:A:179:PHE:HZ	1.64	0.62
20:8:303:CLA:H151	19:8:306:CHL:HMA2	1.81	0.62
6:A:396:TRP:CD1	20:A:5029:CLA:HAB	2.34	0.62
20:A:5025:CLA:H2A	20:A:5025:CLA:HED3	1.81	0.62
1:1:83:MET:HG3	21:1:615:LUT:H201	1.81	0.62
20:7:303:CLA:HAB	22:7:317:XAT:H12	1.81	0.62
20:A:5033:CLA:HBB2	23:L:203:BCR:H342	1.82	0.62
7:B:92:ILE:HB	7:B:113:PRO:HB2	1.81	0.62
20:G:204:CLA:C4D	27:G:206:LMG:H381	2.28	0.62
7:B:54:GLN:HG2	20:B:807:CLA:H3A	1.80	0.62
18:2:229:VAL:O	18:2:232:ILE:HG22	2.00	0.62
17:L:59:THR:HG23	17:L:60:PRO:HD2	1.82	0.62
23:B:803:BCR:H19C	31:B:841:PQN:H18	1.82	0.62
7:B:54:GLN:HG2	20:B:807:CLA:HHB	1.82	0.61
20:B:839:CLA:HAA2	28:B:848:DGD:HAW1	1.81	0.61
2:3:246:MET:HE2	22:3:316:XAT:H10	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:338:HIS:H	6:A:426:LEU:HD23	1.64	0.61
7:B:433:HIS:O	7:B:437:LEU:HD13	1.99	0.61
6:A:53:HIS:HE1	20:A:5006:CLA:ND	1.98	0.61
20:B:826:CLA:H13	23:B:846:BCR:H15C	1.81	0.61
20:B:839:CLA:HBC1	31:B:841:PQN:H2M2	1.83	0.61
23:3:318:BCR:H17C	20:A:5016:CLA:H93	1.82	0.61
3:7:81:MET:HB3	20:7:303:CLA:H3A	1.83	0.61
5:9:134:ARG:HH12	20:9:607:CLA:HED1	1.65	0.61
18:2:144:LYS:HG3	18:2:145:THR:HG23	1.83	0.61
5:9:38:LEU:HD13	5:9:44:ILE:H	1.64	0.60
7:B:155:TRP:HD1	23:B:847:BCR:HC32	1.66	0.60
3:7:210:LEU:HD11	24:7:320:LHG:H292	1.83	0.60
4:8:143:ARG:NH2	20:8:321:CLA:OBD	2.34	0.60
20:B:812:CLA:HBB2	20:B:814:CLA:HMA3	1.83	0.60
12:G:108:ILE:HG23	20:G:203:CLA:C1	2.27	0.60
18:2:161:MET:CE	20:2:308:CLA:O1A	2.48	0.60
4:8:198:ARG:HA	4:8:201:MET:HG3	1.84	0.60
2:3:70:LEU:HD13	19:3:301:CHL:HED1	1.84	0.60
5:9:188:ARG:NH1	7:B:214:LEU:O	2.34	0.60
8:C:17:CYS:HB3	32:C:102:SF4:S2	2.42	0.59
17:L:129:ILE:HD11	23:L:203:BCR:H272	1.84	0.59
19:2:306:CHL:HED3	19:2:306:CHL:HBA1	1.82	0.59
14:I:79:TRP:HZ2	20:2:313:CLA:H3A	1.67	0.59
20:A:5030:CLA:H12	23:A:5048:BCR:H392	1.83	0.59
6:A:740:TRP:HB2	20:A:5029:CLA:HBB1	1.83	0.59
2:3:85:LEU:HD22	19:3:301:CHL:H12	1.84	0.59
5:9:195:LEU:HB2	21:9:613:LUT:H21	1.84	0.59
6:A:266:THR:HG22	16:K:41:GLY:HA3	1.84	0.59
7:B:440:HIS:HE1	20:B:832:CLA:NA	1.94	0.59
13:H:100:LEU:O	13:H:105:GLY:N	2.35	0.59
20:A:5023:CLA:HBA2	23:K:4001:BCR:H281	1.84	0.59
20:A:5033:CLA:OBD	17:L:59:THR:HG21	2.03	0.59
20:1:610:CLA:HBC2	24:1:618:LHG:HC81	1.85	0.58
20:A:5012:CLA:HAB	20:B:832:CLA:HMD2	1.85	0.58
6:A:363:LEU:HD11	20:A:5020:CLA:H71	1.84	0.58
6:A:488:GLN:HG2	6:A:510:TRP:HA	1.84	0.58
20:B:823:CLA:H11	20:B:824:CLA:H151	1.85	0.58
23:3:318:BCR:H393	20:A:5016:CLA:H11	1.85	0.58
7:B:208:VAL:HA	7:B:212:ASN:HD21	1.66	0.58
29:8:322:LMU:H31	15:J:32:PHE:HB3	1.86	0.58
20:A:5014:CLA:HAA2	20:A:5026:CLA:H51	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:723:ALA:HB2	20:B:827:CLA:HBB1	1.85	0.58
16:K:46:PRO:HB2	16:K:123:LEU:HD22	1.85	0.58
20:3:306:CLA:HMB1	23:3:319:BCR:HC7	1.84	0.58
19:7:306:CHL:HBB2	19:7:307:CHL:HBB1	1.86	0.58
20:B:807:CLA:H112	20:B:807:CLA:HBD	1.84	0.58
18:2:211:ILE:CG2	20:2:311:CLA:H2	2.33	0.58
25:3:322:SQD:H462	3:7:68:PRO:HB3	1.86	0.58
7:B:451:GLU:OE2	11:F:114:ARG:NH1	2.36	0.58
23:B:803:BCR:H393	31:B:841:PQN:H111	1.84	0.58
7:B:525:ALA:HB2	20:B:836:CLA:HMA1	1.86	0.58
3:7:232:ASP:HB3	3:7:240:VAL:HG11	1.85	0.57
20:B:814:CLA:H202	23:B:843:BCR:HC42	1.86	0.57
19:2:306:CHL:HED3	19:2:306:CHL:H2A	1.87	0.57
1:1:182:ARG:HA	1:1:185:MET:HE3	1.85	0.57
20:9:607:CLA:CMB	18:2:232:ILE:CB	2.82	0.57
12:G:67:THR:HA	12:G:70:GLU:HB3	1.86	0.57
20:1:604:CLA:HMA2	20:1:605:CLA:HBC3	1.85	0.57
20:3:306:CLA:HHB	23:3:319:BCR:H342	1.86	0.57
7:B:16:ASP:HB3	7:B:21:ARG:HB2	1.86	0.57
20:A:5010:CLA:HBA2	29:A:5053:LMU:H62	1.87	0.57
23:A:5051:BCR:H291	23:F:304:BCR:H17C	1.86	0.57
6:A:279:LYS:HB3	6:A:503:LEU:HD12	1.85	0.57
6:A:366:ILE:HG21	20:A:5020:CLA:H201	1.86	0.57
7:B:548:MET:HE2	8:C:66:ARG:HH22	1.70	0.57
8:C:29:VAL:HG12	9:D:164:ARG:HB2	1.85	0.57
20:A:5010:CLA:H2	29:A:5053:LMU:H51	1.87	0.57
23:A:5049:BCR:H361	23:A:5049:BCR:H21C	1.86	0.57
17:L:134:LEU:HD13	23:L:206:BCR:H24C	1.87	0.57
5:9:182:MET:HB3	20:9:611:CLA:HMD3	1.86	0.57
1:1:187:ALA:HB2	21:1:615:LUT:H192	1.85	0.56
2:3:142:ASP:HB2	2:3:145:ARG:HG3	1.86	0.56
5:9:182:MET:HG3	20:9:611:CLA:HAC2	1.87	0.56
3:7:245:ASN:ND2	20:7:313:CLA:OBD	2.38	0.56
6:A:395:MET:HE2	6:A:606:VAL:HG11	1.86	0.56
6:A:441:LEU:HD21	6:A:547:VAL:HG12	1.85	0.56
17:L:121:MET:HE2	20:L:201:CLA:H41	1.87	0.56
3:7:174:GLU:HB2	3:7:177:TYR:HB2	1.88	0.56
19:8:305:CHL:H2A	19:8:305:CHL:HED3	1.87	0.56
16:K:61:ALA:HB1	16:K:66:LEU:HD22	1.88	0.56
3:7:72:SER:HB2	3:7:78:ARG:HA	1.87	0.56
6:A:718:LEU:HB3	6:A:722:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:89:SER:HA	9:D:133:MET:HE1	1.88	0.56
4:8:48:MET:HE1	4:8:70:GLN:HB2	1.88	0.56
6:A:469:GLN:O	17:L:109:ARG:NH2	2.37	0.56
7:B:157:HIS:HE1	20:B:812:CLA:NA	1.98	0.56
20:1:608:CLA:H3A	24:1:620:LHG:H271	1.88	0.56
20:8:302:CLA:HAB	22:8:315:XAT:H403	1.87	0.56
20:A:5005:CLA:C4B	20:B:805:CLA:CBB	2.83	0.56
6:A:467:ARG:NH2	20:A:5035:CLA:OBD	2.38	0.56
18:2:45:TYR:OH	18:2:238:LYS:NZ	2.38	0.56
20:A:5006:CLA:HBB2	20:A:5013:CLA:H102	1.89	0.55
8:C:73:SER:H	8:C:76:SER:HB3	1.71	0.55
20:A:5041:CLA:H91	20:F:307:CLA:HAC2	1.88	0.55
20:9:603:CLA:HBC1	19:9:606:CHL:HBB2	1.86	0.55
20:B:810:CLA:H112	20:B:827:CLA:H122	1.87	0.55
7:B:66:LEU:HD21	23:B:844:BCR:H291	1.89	0.55
7:B:524:ILE:HG12	7:B:591:VAL:HG12	1.88	0.55
7:B:546:LYS:NZ	10:E:62:SER:O	2.39	0.55
20:A:5034:CLA:HBB2	17:L:105:LEU:HD11	1.88	0.55
12:G:102:ASP:HB2	20:G:203:CLA:HAA2	1.88	0.55
2:3:201:LEU:HA	2:3:214:PRO:HD2	1.89	0.55
2:3:162:PRO:HA	2:3:165:LEU:HD12	1.88	0.55
20:B:817:CLA:H11	20:G:204:CLA:HED1	1.88	0.55
18:2:100:THR:HG22	18:2:105:LEU:HD12	1.87	0.55
31:A:5045:PQN:H141	20:F:306:CLA:HBB2	1.89	0.55
16:K:117:LEU:HB3	16:K:122:GLN:HB2	1.89	0.55
3:7:69:LEU:HG	22:7:317:XAT:H21	1.88	0.55
4:8:81:MET:HE1	20:8:308:CLA:HAB	1.89	0.55
1:1:221:ASN:ND2	20:1:612:CLA:OBD	2.39	0.54
29:8:318:LMU:H31	26:F:301:PTY:HC6	1.90	0.54
16:K:49:LEU:O	16:K:52:VAL:HG12	2.07	0.54
20:A:5022:CLA:H101	23:A:5050:BCR:H21C	1.89	0.54
15:J:21:PHE:HA	20:J:104:CLA:HBB2	1.89	0.54
20:A:5035:CLA:H3A	17:L:105:LEU:HD13	1.88	0.54
7:B:182:GLY:HA2	7:B:186:VAL:HG12	1.90	0.54
6:A:87:TRP:HA	20:A:5010:CLA:HBB2	1.88	0.54
6:A:247:GLN:NE2	20:A:5016:CLA:OBD	2.41	0.54
7:B:456:ILE:HD12	23:J:102:BCR:H382	1.87	0.54
5:9:178:ILE:HD11	20:9:603:CLA:HAB	1.87	0.54
7:B:634:ASN:O	7:B:642:ASN:ND2	2.38	0.54
20:B:815:CLA:H3A	23:B:844:BCR:H392	1.90	0.54
20:B:820:CLA:HBC2	20:B:824:CLA:H172	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:82:ARG:HE	13:H:84:GLU:HB2	1.72	0.54
18:2:226:VAL:HA	18:2:229:VAL:CG1	2.35	0.54
3:7:144:VAL:HG13	19:7:308:CHL:C4B	2.15	0.54
6:A:598:TRP:CH2	20:A:5005:CLA:HAB	2.43	0.54
7:B:175:ARG:HB2	20:B:814:CLA:HBC2	1.89	0.54
7:B:453:GLN:HE21	7:B:455:LEU:HD11	1.73	0.54
18:2:62:TYR:HB2	20:2:303:CLA:HMD1	1.88	0.54
20:1:609:CLA:H72	21:1:615:LUT:H30	1.88	0.54
2:3:59:TYR:HB3	2:3:62:SER:HB2	1.90	0.54
20:3:305:CLA:H2	27:7:301:LMG:H252	1.90	0.54
3:7:69:LEU:HD22	24:A:5002:LHG:H281	1.89	0.54
27:7:324:LMG:H112	4:8:56:PRO:HB2	1.90	0.54
6:A:322:ILE:HG21	20:A:5026:CLA:HAC1	1.90	0.54
7:B:696:ASP:OD1	7:B:696:ASP:N	2.40	0.54
18:2:69:LEU:HD13	20:2:303:CLA:H11	1.90	0.54
5:9:146:PHE:HB3	5:9:147:ILE:HD12	1.90	0.54
6:A:445:SER:HB3	6:A:545:VAL:HG22	1.90	0.54
19:3:323:CHL:HBB2	20:7:303:CLA:HAC2	1.90	0.53
5:9:125:LEU:HD11	19:2:302:CHL:HBD	1.89	0.53
6:A:441:LEU:HG	6:A:548:LEU:HB2	1.89	0.53
20:A:5032:CLA:HAA2	17:L:59:THR:HG23	1.90	0.53
7:B:170:LYS:NZ	7:B:329:ASN:OD1	2.40	0.53
7:B:90:HIS:CD2	20:B:810:CLA:NA	2.77	0.53
2:3:246:MET:HG3	22:3:316:XAT:H12	1.90	0.53
20:9:607:CLA:HHB	18:2:232:ILE:CD1	2.31	0.53
3:7:200:LYS:HD3	20:7:312:CLA:HAA2	1.90	0.53
4:8:232:ASN:HB3	20:8:311:CLA:HED1	1.89	0.53
7:B:300:HIS:HE1	20:G:201:CLA:NA	1.99	0.53
11:F:74:LYS:HG3	11:F:78:LYS:HE2	1.90	0.53
6:A:424:ASN:OD1	6:A:432:ARG:NH2	2.42	0.53
30:A:5003:CL0:H36	30:A:5003:CL0:H30	1.91	0.53
7:B:340:ALA:HB2	23:B:846:BCR:H372	1.90	0.53
20:B:810:CLA:HAB	20:B:811:CLA:HAA2	1.90	0.53
13:H:98:ILE:HD12	14:I:90:LEU:HD12	1.90	0.53
6:A:657:VAL:HG22	6:A:745:ALA:HB3	1.89	0.53
2:3:124:ILE:HD11	2:3:249:TYR:CZ	2.43	0.53
3:7:94:LEU:HD13	20:7:305:CLA:HBB2	1.90	0.53
4:8:181:THR:OG1	4:8:182:SER:N	2.42	0.53
15:J:28:GLU:OE1	15:J:31:ARG:NH2	2.42	0.53
20:B:831:CLA:HBA2	23:F:309:BCR:H361	1.89	0.53
1:1:147:ASP:HB3	1:1:150:LYS:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:195:LYS:HA	3:7:198:LYS:HE2	1.92	0.52
6:A:128:ASN:HB3	6:A:136:GLN:HB3	1.91	0.52
24:I:4002:LHG:HC61	18:2:219:GLU:HG2	1.91	0.52
23:B:844:BCR:H10C	23:B:844:BCR:C6	2.39	0.52
6:A:566:LYS:NZ	7:B:674:GLU:OE2	2.38	0.52
20:A:5044:CLA:HBC2	7:B:586:ASN:HB2	1.90	0.52
7:B:669:ARG:NH2	7:B:700:ALA:O	2.42	0.52
24:1:618:LHG:HC82	23:8:316:BCR:H291	1.91	0.52
6:A:189:GLU:O	6:A:193:ASN:ND2	2.43	0.52
3:7:231:VAL:HA	3:7:234:VAL:HG22	1.91	0.52
6:A:67:GLU:OE2	6:A:71:ARG:NH2	2.42	0.52
20:A:5023:CLA:H2	20:K:4005:CLA:HBC3	1.92	0.52
7:B:468:GLN:HE22	20:B:833:CLA:C1B	2.20	0.52
15:J:26:LEU:HD13	23:J:105:BCR:HC7	1.92	0.52
18:2:226:VAL:CA	18:2:229:VAL:HG12	2.38	0.52
20:1:603:CLA:HED1	23:B:845:BCR:H313	1.91	0.52
2:3:113:ALA:HB1	2:3:239:GLY:HA3	1.90	0.52
13:H:73:PHE:HB3	17:L:88:VAL:HG21	1.92	0.52
6:A:356:ASN:HD21	20:A:5026:CLA:H101	1.73	0.52
7:B:124:TRP:NE1	20:B:819:CLA:OBD	2.38	0.52
16:K:95:THR:OG1	16:K:96:ALA:N	2.42	0.52
3:7:172:GLY:HA2	3:7:178:PRO:HA	1.92	0.52
20:1:605:CLA:H3A	23:1:617:BCR:H21C	1.92	0.52
7:B:414:ASP:O	11:F:227:ARG:NH2	2.43	0.52
20:B:815:CLA:HAA2	23:B:844:BCR:H392	1.92	0.52
20:8:321:CLA:HBB2	11:F:204:LEU:HD12	1.93	0.51
6:A:704:HIS:HE1	20:A:5041:CLA:ND	2.08	0.51
2:3:178:LEU:HD13	19:3:323:CHL:HMA2	1.92	0.51
4:8:138:ARG:HH12	20:8:307:CLA:HED2	1.74	0.51
6:A:474:ASP:OD1	6:A:480:GLN:NE2	2.40	0.51
7:B:659:ALA:HB1	20:B:805:CLA:HAB	1.92	0.51
7:B:663:MET:HE1	20:B:805:CLA:C4D	2.37	0.51
20:B:820:CLA:H18	20:B:823:CLA:H61	1.92	0.51
18:2:122:THR:HA	18:2:125:ILE:HG22	1.91	0.51
19:8:304:CHL:HMB3	20:8:307:CLA:HMC1	1.92	0.51
5:9:212:THR:HA	7:B:224:THR:OG1	2.10	0.51
6:A:734:GLY:O	6:A:738:THR:OG1	2.24	0.51
20:B:810:CLA:H111	20:B:811:CLA:H71	1.92	0.51
23:3:318:BCR:H21C	20:A:5016:CLA:H62	1.91	0.51
7:B:520:VAL:HG23	20:B:804:CLA:H141	1.93	0.51
1:1:104:PRO:HB3	20:1:605:CLA:HMC1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:171:GLU:HA	1:1:174:LYS:HE3	1.92	0.51
6:A:47:THR:HA	6:A:50:TRP:HD1	1.76	0.51
7:B:302:LEU:HD13	20:B:824:CLA:HAC2	1.91	0.51
7:B:650:THR:HG23	7:B:724:ALA:HB2	1.91	0.51
17:L:134:LEU:HD22	23:L:206:BCR:H402	1.91	0.51
2:3:78:TYR:HB2	19:3:301:CHL:HMD1	1.93	0.51
20:7:304:CLA:HED1	26:F:302:PTY:H171	1.92	0.51
19:8:304:CHL:HAA2	19:8:304:CHL:HBD	1.93	0.51
7:B:713:HIS:HE1	20:B:839:CLA:ND	2.08	0.51
11:F:78:LYS:HD2	11:F:81:ARG:HH21	1.75	0.51
19:8:304:CHL:HBA2	23:8:316:BCR:H12C	1.92	0.51
20:1:608:CLA:HAA2	24:1:620:LHG:H241	1.93	0.51
6:A:371:MET:O	6:A:387:GLN:NE2	2.44	0.51
6:A:405:ALA:HB1	23:A:5050:BCR:H383	1.93	0.51
6:A:580:ARG:NH2	9:D:118:GLU:OE2	2.42	0.51
5:9:57:SER:HB2	20:9:602:CLA:HMD1	1.92	0.51
6:A:320:HIS:HD2	20:A:5023:CLA:HED3	1.75	0.51
20:A:5029:CLA:H193	23:J:105:BCR:H12C	1.93	0.51
7:B:96:HIS:HE1	20:L:201:CLA:NB	2.09	0.51
20:B:825:CLA:HMA1	23:B:846:BCR:H14C	1.93	0.51
7:B:123:GLN:O	7:B:127:THR:OG1	2.29	0.51
11:F:122:GLY:O	11:F:145:HIS:NE2	2.40	0.51
2:3:100:VAL:HG23	20:3:324:CLA:HBD	1.92	0.50
6:A:572:ARG:NH1	24:A:5052:LHG:O10	2.44	0.50
2:3:276:LEU:HD22	20:3:311:CLA:H2	1.92	0.50
19:3:301:CHL:H43	20:3:302:CLA:HBA1	1.92	0.50
20:7:313:CLA:H2A	20:7:313:CLA:HED3	1.93	0.50
23:A:5049:BCR:H19C	24:A:5054:LHG:HC82	1.94	0.50
7:B:504:ASN:HD21	7:B:506:GLN:HB2	1.76	0.50
29:8:322:LMU:H6E	23:J:102:BCR:H312	1.92	0.50
2:3:206:ASP:OD1	2:3:206:ASP:N	2.44	0.50
2:3:215:PHE:CE2	23:3:319:BCR:HC8	2.46	0.50
5:9:190:GLN:HB2	5:9:193:GLU:HB2	1.94	0.50
2:3:135:ILE:HD13	20:3:313:CLA:C1C	2.42	0.50
20:3:325:CLA:NA	6:A:200:HIS:HE1	2.06	0.50
6:A:114:SER:HB2	6:A:131:VAL:HG11	1.94	0.50
2:3:264:LEU:HB2	21:3:315:LUT:H21	1.92	0.50
30:A:5003:CL0:H70	20:A:5005:CLA:C1B	2.42	0.50
20:A:5043:CLA:HBB1	24:A:5055:LHG:H311	1.92	0.50
7:B:86:ARG:NH1	7:B:735:GLY:O	2.44	0.50
12:G:108:ILE:CG2	20:G:203:CLA:O1A	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:135:ILE:HD12	20:3:313:CLA:C4C	2.40	0.50
2:3:149:ILE:HG22	2:3:152:ALA:H	1.75	0.50
2:3:202:PHE:HZ	23:3:319:BCR:H322	1.76	0.50
4:8:176:LEU:HB2	21:8:314:LUT:H23	1.94	0.50
6:A:685:PHE:HA	31:A:5045:PQN:H9	1.93	0.50
18:2:159:MET:CG	18:2:161:MET:HE2	2.41	0.50
6:A:313:ARG:HH21	6:A:321:SER:HB2	1.76	0.50
6:A:432:ARG:O	9:D:70:THR:OG1	2.23	0.50
20:A:5035:CLA:H162	20:L:204:CLA:HMB2	1.93	0.50
20:A:5043:CLA:NB	24:A:5054:LHG:O5	2.45	0.50
7:B:68:HIS:HE1	20:B:809:CLA:ND	2.10	0.50
20:B:809:CLA:HAA1	14:I:85:VAL:HG22	1.93	0.50
13:H:82:ARG:HG2	13:H:85:SER:H	1.77	0.50
18:2:74:ASP:OD1	18:2:77:LYS:NZ	2.45	0.50
3:7:134:ILE:HD11	4:8:244:LEU:HD11	1.94	0.49
1:1:176:LYS:HD3	20:1:611:CLA:HBA1	1.93	0.49
3:7:70:HIS:NE2	26:7:302:PTY:O12	2.45	0.49
30:A:5003:CL0:H13	20:A:5044:CLA:HMD1	1.94	0.49
7:B:211:ASP:OD1	7:B:211:ASP:N	2.44	0.49
19:3:323:CHL:H52	24:7:320:LHG:H132	1.95	0.49
3:7:146:THR:HG21	20:7:323:CLA:H2A	1.93	0.49
4:8:50:GLY:HA3	4:8:194:ILE:HG21	1.94	0.49
7:B:139:SER:HB3	23:B:844:BCR:H401	1.94	0.49
12:G:60:LEU:HA	12:G:63:GLN:HB2	1.95	0.49
20:J:104:CLA:H3A	20:J:104:CLA:H2	1.93	0.49
20:3:305:CLA:HBB2	20:A:5017:CLA:CHD	2.43	0.49
20:B:807:CLA:H101	20:B:814:CLA:HAA2	1.94	0.49
19:3:301:CHL:H62	20:3:302:CLA:HHB	1.93	0.49
3:7:170:LEU:HB3	19:7:308:CHL:HMC	1.93	0.49
7:B:346:THR:HB	7:B:380:ALA:HB2	1.95	0.49
4:8:43:LEU:HD22	20:8:301:CLA:HED1	1.94	0.49
6:A:305:PHE:HZ	20:A:5020:CLA:H112	1.78	0.49
7:B:359:TYR:OH	20:B:828:CLA:OBD	2.25	0.49
2:3:159:TRP:NE1	20:3:304:CLA:OBD	2.41	0.49
20:3:314:CLA:H2A	20:3:314:CLA:HED3	1.95	0.49
19:3:323:CHL:HBB2	20:7:303:CLA:HHD	1.94	0.49
4:8:102:PRO:HG3	4:8:110:VAL:HG11	1.95	0.49
6:A:622:VAL:HG22	6:A:627:VAL:HG22	1.93	0.49
7:B:3:THR:HG22	7:B:15:GLN:HG2	1.94	0.49
9:D:124:THR:HA	9:D:135:PRO:HG2	1.94	0.49
13:H:80:VAL:HG22	13:H:86:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9:188:ARG:HH12	7:B:215:SER:HA	1.77	0.49
6:A:249:ILE:HD12	6:A:249:ILE:H	1.78	0.49
20:A:5018:CLA:CHD	20:A:5019:CLA:HBB2	2.43	0.49
7:B:352:HIS:CD2	20:B:826:CLA:NC	2.80	0.49
7:B:375:HIS:HB2	20:B:827:CLA:C1B	2.43	0.49
17:L:59:THR:CG2	17:L:60:PRO:HD2	2.43	0.49
1:1:39:PRO:HB3	4:8:153:THR:HG21	1.95	0.49
20:8:303:CLA:H102	23:8:316:BCR:HC8	1.93	0.49
6:A:45:THR:HG22	6:A:714:GLN:HB2	1.93	0.49
7:B:233:ALA:HA	7:B:236:GLN:HG2	1.93	0.49
7:B:457:GLU:OE1	11:F:132:HIS:ND1	2.46	0.49
20:B:822:CLA:H62	20:B:822:CLA:H41	1.55	0.48
25:3:322:SQD:H81	25:3:322:SQD:H45	1.41	0.48
20:B:839:CLA:H11	31:B:841:PQN:H302	1.95	0.48
23:B:847:BCR:H401	24:I:4002:LHG:H242	1.95	0.48
11:F:208:GLN:O	11:F:212:ASN:ND2	2.47	0.48
2:3:247:PHE:HB3	20:3:311:CLA:HMC2	1.95	0.48
2:3:280:LEU:HD11	23:3:318:BCR:H282	1.96	0.48
20:3:324:CLA:H72	20:A:5014:CLA:H18	1.95	0.48
20:B:810:CLA:H71	20:B:810:CLA:HBB1	1.95	0.48
20:B:825:CLA:H72	20:B:835:CLA:H42	1.95	0.48
2:3:119:GLY:HA2	22:3:316:XAT:H181	1.95	0.48
3:7:99:ILE:HG12	3:7:115:TRP:HB2	1.95	0.48
4:8:82:MET:HG3	20:8:303:CLA:H172	1.95	0.48
6:A:353:LEU:HD11	20:A:5031:CLA:HBB1	1.96	0.48
9:D:124:THR:HG23	9:D:135:PRO:HD2	1.94	0.48
13:H:77:THR:HA	13:H:80:VAL:HG12	1.94	0.48
16:K:48:ASN:O	16:K:52:VAL:HG12	2.13	0.48
29:8:322:LMU:H6E	23:J:102:BCR:HC32	1.94	0.48
6:A:125:GLU:OE2	11:F:110:ARG:NH2	2.46	0.48
6:A:695:GLU:OE1	7:B:537:LYS:NZ	2.46	0.48
20:A:5004:CLA:H71	7:B:432:PHE:HE1	1.78	0.48
7:B:258:PHE:CE2	20:B:818:CLA:HBB1	2.49	0.48
12:G:56:ARG:NH1	12:G:102:ASP:OD2	2.47	0.48
2:3:224:THR:OG1	2:3:227:GLU:OE1	2.31	0.48
6:A:706:LYS:NZ	11:F:219:ASP:OD1	2.47	0.48
20:A:5005:CLA:H203	23:B:803:BCR:H321	1.94	0.48
3:7:89:ALA:O	3:7:93:MET:HG3	2.13	0.48
3:7:241:THR:OG1	3:7:242:PHE:N	2.46	0.48
6:A:274:ASP:OD1	6:A:274:ASP:N	2.46	0.48
7:B:650:THR:HA	7:B:653:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:825:CLA:H12	20:B:837:CLA:H11	1.95	0.48
24:8:319:LHG:H281	25:F:311:SQD:H462	1.95	0.48
20:A:5004:CLA:H171	20:A:5044:CLA:H171	1.95	0.48
7:B:345:ILE:HD12	20:B:819:CLA:H71	1.96	0.48
7:B:425:TRP:CE2	20:B:831:CLA:HAB	2.48	0.48
20:B:826:CLA:H2A	20:B:826:CLA:HED2	1.96	0.48
16:K:71:ARG:HA	16:K:81:ASP:HB3	1.95	0.48
6:A:481:PRO:HG3	6:A:533:PHE:HB2	1.96	0.48
12:G:94:SER:O	12:G:98:THR:OG1	2.32	0.48
18:2:69:LEU:HD23	18:2:252:TRP:HD1	1.79	0.48
19:3:301:CHL:H3A	19:3:301:CHL:HBA2	1.60	0.48
25:7:322:SQD:H45	25:7:322:SQD:H82	1.38	0.48
7:B:309:HIS:HE1	20:B:822:CLA:ND	2.12	0.48
7:B:601:THR:HG21	7:B:610:PHE:HB2	1.96	0.48
2:3:83:LEU:HD13	20:3:325:CLA:H52	1.96	0.47
20:9:608:CLA:H3A	20:9:608:CLA:HBA2	1.61	0.47
6:A:330:LYS:HA	6:A:337:GLY:HA3	1.95	0.47
6:A:375:PRO:HG2	6:A:381:ALA:HB2	1.95	0.47
8:C:30:PRO:HG3	9:D:162:ALA:HA	1.95	0.47
2:3:164:THR:HG23	20:7:314:CLA:HED3	1.96	0.47
6:A:363:LEU:HD21	20:A:5020:CLA:H93	1.96	0.47
6:A:556:PHE:O	6:A:566:LYS:NZ	2.44	0.47
20:B:827:CLA:H111	20:B:829:CLA:H171	1.95	0.47
20:B:831:CLA:H2	23:F:309:BCR:H372	1.94	0.47
3:7:136:THR:HG23	20:8:312:CLA:HAA2	1.95	0.47
24:8:319:LHG:H342	25:F:311:SQD:H292	1.96	0.47
6:A:210:SER:OG	6:A:298:HIS:O	2.31	0.47
20:A:5012:CLA:H8	20:A:5012:CLA:H121	1.75	0.47
20:B:808:CLA:H62	20:B:808:CLA:H2	1.63	0.47
16:K:66:LEU:HD21	20:K:4005:CLA:NC	2.29	0.47
16:K:72:LYS:HE2	16:K:72:LYS:HB2	1.66	0.47
2:3:202:PHE:HE1	23:3:319:BCR:H313	1.79	0.47
3:7:115:TRP:O	22:7:317:XAT:O23	2.26	0.47
19:8:306:CHL:H12	21:8:314:LUT:H372	1.95	0.47
6:A:459:ASN:HD22	6:A:640:ASN:HB2	1.79	0.47
19:3:301:CHL:H91	20:3:307:CLA:H193	1.96	0.47
23:3:318:BCR:H23C	20:A:5016:CLA:H42	1.96	0.47
6:A:712:SER:N	11:F:184:GLU:OE2	2.41	0.47
12:G:48:THR:HA	12:G:118:GLY:HA3	1.97	0.47
19:7:307:CHL:H2A	19:7:307:CHL:CED	2.45	0.47
20:8:307:CLA:H3A	20:8:307:CLA:HBA2	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:208:LEU:HD21	20:A:5021:CLA:HMC1	1.96	0.47
20:A:5006:CLA:H92	31:A:5045:PQN:H272	1.96	0.47
7:B:433:HIS:HE1	20:F:303:CLA:C4D	2.28	0.47
20:B:828:CLA:H161	23:B:843:BCR:H363	1.97	0.47
6:A:601:ASN:HD22	30:A:5003:CL0:H37	1.78	0.47
20:A:5005:CLA:H201	20:B:811:CLA:H2	1.97	0.47
20:A:5036:CLA:HBA1	23:A:5050:BCR:H332	1.97	0.47
7:B:70:ALA:HB2	7:B:136:LEU:HB2	1.96	0.47
9:D:131:PHE:HB2	9:D:133:MET:HG2	1.95	0.47
20:F:303:CLA:HBC3	23:J:102:BCR:H392	1.96	0.47
18:2:74:ASP:HA	18:2:77:LYS:HG2	1.97	0.47
19:8:304:CHL:H3A	23:8:316:BCR:C11	2.45	0.47
20:B:819:CLA:H141	20:B:820:CLA:H102	1.96	0.47
20:B:838:CLA:H8	20:B:839:CLA:H121	1.97	0.47
9:D:116:ARG:NH2	9:D:118:GLU:OE1	2.43	0.47
13:H:109:LEU:O	13:H:109:LEU:CD1	2.63	0.47
17:L:108:LEU:HD13	17:L:118:VAL:HG21	1.97	0.47
18:2:89:TRP:HB3	21:2:315:LUT:H391	1.97	0.47
1:1:214:PHE:HB3	4:8:118:ILE:HG23	1.97	0.47
6:A:683:LEU:HB2	20:A:5004:CLA:HMC2	1.97	0.47
7:B:430:LEU:HD11	20:B:836:CLA:HMB2	1.97	0.47
20:B:810:CLA:HBA2	20:B:810:CLA:H141	1.96	0.47
20:B:833:CLA:C4C	20:B:834:CLA:HAB	2.45	0.47
20:G:204:CLA:C1D	27:G:206:LMG:H382	2.35	0.47
18:2:60:GLY:HA3	18:2:171:LEU:HD23	1.95	0.47
19:2:302:CHL:HAC2	24:2:316:LHG:HC5	1.96	0.47
20:8:301:CLA:H3A	20:8:301:CLA:HBA2	1.63	0.47
6:A:25:ASN:ND2	24:A:5002:LHG:O2	2.48	0.47
30:A:5003:CL0:H66	20:A:5005:CLA:C2B	2.45	0.47
20:A:5028:CLA:H112	20:A:5028:CLA:H72	1.45	0.47
7:B:318:ALA:HB1	7:B:321:LYS:HG2	1.97	0.47
28:B:848:DGD:HB22	28:B:848:DGD:HG2	1.41	0.47
18:2:43:MET:HE2	18:2:43:MET:HB3	1.78	0.47
6:A:452:SER:HB2	6:A:538:ILE:HG12	1.97	0.46
7:B:177:ASN:ND2	7:B:292:TYR:O	2.47	0.46
18:2:190:VAL:HG12	18:2:190:VAL:O	2.15	0.46
6:A:119:TRP:HB3	23:J:106:BCR:HC42	1.96	0.46
6:A:338:HIS:CD2	20:A:5025:CLA:ND	2.83	0.46
20:A:5035:CLA:HMA2	17:L:105:LEU:HB2	1.96	0.46
20:A:5041:CLA:HBB2	11:F:167:GLY:HA3	1.97	0.46
20:B:819:CLA:H3A	20:B:819:CLA:HBA2	1.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:830:CLA:H3A	20:B:831:CLA:OBD	2.14	0.46
20:A:5020:CLA:H92	20:A:5030:CLA:H91	1.97	0.46
20:B:804:CLA:H122	20:B:804:CLA:H161	1.60	0.46
10:E:89:ASN:OD1	10:E:89:ASN:N	2.47	0.46
11:F:187:LEU:HD22	15:J:14:VAL:HG21	1.96	0.46
17:L:130:LEU:HD11	20:L:202:CLA:H161	1.97	0.46
1:1:44:LYS:HB2	1:1:47:LEU:HB2	1.97	0.46
1:1:124:ILE:HD13	27:G:206:LMG:H112	1.96	0.46
20:1:607:CLA:HMB2	23:1:617:BCR:H16C	1.97	0.46
3:7:123:ILE:HG23	19:7:306:CHL:HBC1	1.97	0.46
6:A:669:GLY:O	6:A:672:PHE:HB3	2.16	0.46
20:A:5011:CLA:HAB	20:A:5029:CLA:H13	1.97	0.46
9:D:172:ARG:NE	9:D:177:ASN:OD1	2.44	0.46
8:C:9:ASP:HB2	10:E:80:ARG:HD3	1.96	0.46
19:7:306:CHL:C2C	19:7:307:CHL:HAC2	2.46	0.46
4:8:48:MET:HG2	20:8:301:CLA:HED2	1.97	0.46
6:A:199:ASN:ND2	6:A:312:TYR:O	2.43	0.46
20:A:5027:CLA:H91	20:A:5040:CLA:H93	1.97	0.46
20:A:5028:CLA:H121	20:A:5036:CLA:H101	1.98	0.46
2:3:215:PHE:HE2	23:3:319:BCR:HC8	1.81	0.46
20:A:5042:CLA:H72	20:A:5044:CLA:H193	1.98	0.46
20:B:825:CLA:H92	20:B:840:CLA:H193	1.97	0.46
12:G:97:GLU:N	12:G:97:GLU:OE2	2.48	0.46
16:K:52:VAL:HG23	20:K:4004:CLA:CGA	2.46	0.46
18:2:233:ILE:O	18:2:237:THR:HG23	2.15	0.46
2:3:87:ASP:HB3	2:3:90:VAL:HG23	1.98	0.46
6:A:289:LEU:HD12	6:A:376:PRO:HB3	1.98	0.46
20:A:5010:CLA:H2A	20:A:5012:CLA:HED1	1.98	0.46
20:B:821:CLA:H3A	20:B:821:CLA:HBA2	1.52	0.46
12:G:66:ARG:HE	20:G:201:CLA:HMA2	1.81	0.46
4:8:192:LYS:NZ	20:8:310:CLA:O1D	2.44	0.46
19:8:305:CHL:H3A	26:F:301:PTY:H112	1.98	0.46
19:8:306:CHL:HMA3	23:8:316:BCR:H353	1.98	0.46
7:B:23:TRP:HB3	28:B:848:DGD:HA31	1.98	0.46
20:B:814:CLA:H62	20:B:814:CLA:H2	1.58	0.46
9:D:139:ARG:HB2	9:D:149:LEU:HD11	1.98	0.46
3:7:247:VAL:HG12	3:7:248:SER:H	1.81	0.46
20:8:309:CLA:H2	20:8:310:CLA:HMD2	1.98	0.46
17:L:101:PRO:HG3	20:L:205:CLA:HBB1	1.97	0.46
27:7:301:LMG:H392	20:A:5017:CLA:HBB1	1.98	0.45
6:A:515:VAL:HG12	6:A:522:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:107:ARG:HH21	7:B:116:ILE:HG12	1.80	0.45
7:B:342:VAL:O	7:B:346:THR:OG1	2.31	0.45
20:B:805:CLA:H141	20:L:201:CLA:HBC1	1.98	0.45
10:E:45:LYS:HD3	10:E:46:GLU:H	1.82	0.45
20:H:201:CLA:H62	20:H:201:CLA:H41	1.66	0.45
6:A:443:TRP:CE2	20:A:5033:CLA:HAB	2.52	0.45
20:A:5004:CLA:H62	20:A:5004:CLA:H41	1.64	0.45
24:A:5055:LHG:HC81	24:A:5055:LHG:HC5	1.37	0.45
23:B:842:BCR:HC7	20:G:201:CLA:HMD2	1.98	0.45
9:D:151:PRO:HB2	9:D:154:GLY:HA2	1.98	0.45
11:F:85:LYS:HG2	11:F:89:LYS:HE3	1.98	0.45
13:H:98:ILE:HG23	14:I:86:PRO:HB3	1.98	0.45
14:I:106:LYS:HA	14:I:106:LYS:HD3	1.80	0.45
18:2:119:ASP:HB3	18:2:122:THR:HG22	1.98	0.45
19:1:601:CHL:HBC1	24:1:618:LHG:HC31	1.98	0.45
20:A:5007:CLA:HAA1	20:A:5013:CLA:H51	1.99	0.45
20:A:5012:CLA:H61	20:A:5012:CLA:H2	1.63	0.45
7:B:704:VAL:HG12	28:B:848:DGD:HG12	1.98	0.45
16:K:66:LEU:HD23	16:K:67:ALA:N	2.32	0.45
16:K:82:ARG:HD3	16:K:84:VAL:HG23	1.98	0.45
20:1:607:CLA:HBA2	20:1:607:CLA:H3A	1.70	0.45
3:7:183:ASP:OD1	21:7:316:LUT:O3	2.32	0.45
3:7:186:GLY:HA3	3:7:189:LYS:HZ2	1.81	0.45
20:8:302:CLA:HBC1	19:8:305:CHL:HBB2	1.98	0.45
20:B:816:CLA:H62	20:B:816:CLA:H2	1.64	0.45
27:7:324:LMG:HC92	27:7:324:LMG:H291	1.35	0.45
5:9:67:ASN:OD1	5:9:71:LEU:N	2.49	0.45
5:9:195:LEU:HD22	21:9:613:LUT:H163	1.98	0.45
30:A:5003:CL0:H2	20:B:804:CLA:NC	2.31	0.45
7:B:58:ILE:HG12	20:B:808:CLA:C2C	2.46	0.45
11:F:75:ALA:HA	11:F:78:LYS:HG2	1.98	0.45
15:J:12:PRO:HB2	23:J:106:BCR:H391	1.99	0.45
20:3:302:CLA:H152	20:3:302:CLA:H112	1.61	0.45
20:3:305:CLA:H12	27:7:301:LMG:H141	1.97	0.45
6:A:711:PRO:HG2	6:A:715:PRO:HD3	1.99	0.45
20:A:5007:CLA:HAB	20:A:5013:CLA:H122	1.97	0.45
7:B:182:GLY:HA3	20:B:814:CLA:HBB1	1.98	0.45
20:K:4004:CLA:HBB1	23:K:4006:BCR:H352	1.98	0.45
18:2:59:LEU:O	18:2:80:ARG:NH1	2.50	0.45
5:9:113:ASP:N	5:9:113:ASP:OD1	2.46	0.45
20:A:5029:CLA:H3A	20:A:5029:CLA:HBA2	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:430:LEU:HB3	7:B:526:LEU:HB2	1.98	0.45
9:D:69:SER:H	17:L:56:MET:HB3	1.82	0.45
20:1:610:CLA:HAB	4:8:155:PHE:HE1	1.80	0.45
20:1:612:CLA:H62	20:1:612:CLA:H41	1.66	0.45
6:A:361:GLY:HA2	6:A:398:GLY:HA2	1.99	0.45
20:A:5011:CLA:H143	20:A:5011:CLA:H111	1.82	0.45
7:B:546:LYS:HE3	11:F:223:THR:HG22	1.99	0.45
20:B:832:CLA:H91	20:F:307:CLA:H12	1.99	0.45
18:2:44:TRP:H	18:2:44:TRP:CD1	2.34	0.45
20:1:612:CLA:HMB3	21:1:615:LUT:H22	1.99	0.45
20:3:307:CLA:H141	23:3:318:BCR:H14C	1.99	0.45
19:8:304:CHL:H3A	23:8:316:BCR:C10	2.46	0.45
23:8:316:BCR:H24C	23:8:316:BCR:H371	1.81	0.45
6:A:578:PRO:HA	6:A:582:GLY:HA2	1.99	0.45
20:A:5040:CLA:H11	23:A:5050:BCR:H14C	1.99	0.45
20:A:5033:CLA:H72	20:L:204:CLA:H11	1.98	0.45
10:E:100:TYR:HB3	10:E:104:GLU:HG3	1.98	0.45
2:3:178:LEU:HB3	19:3:323:CHL:HED2	1.99	0.44
4:8:169:PRO:HG3	19:8:306:CHL:HMD2	1.98	0.44
5:9:42:ASP:OD1	5:9:43:VAL:N	2.50	0.44
6:A:208:LEU:HD22	23:A:5047:BCR:H361	1.99	0.44
6:A:650:LEU:HD11	30:A:5003:CL0:H42	2.00	0.44
24:B:849:LHG:HC81	24:B:849:LHG:HC5	1.46	0.44
9:D:117:LYS:HE3	9:D:149:LEU:HD13	1.99	0.44
13:H:83:ARG:HH11	13:H:84:GLU:HG2	1.81	0.44
20:7:310:CLA:H3A	20:7:310:CLA:HBA2	1.49	0.44
4:8:174:ASP:OD1	21:8:314:LUT:O23	2.30	0.44
5:9:48:HIS:HD2	5:9:49:LEU:HG	1.83	0.44
5:9:72:LYS:N	5:9:72:LYS:HE2	2.32	0.44
22:9:615:XAT:H171	22:9:615:XAT:H193	1.99	0.44
20:A:5020:CLA:HAB	20:A:5020:CLA:H8	1.99	0.44
20:A:5025:CLA:H92	20:A:5025:CLA:H61	1.83	0.44
23:A:5049:BCR:H24C	23:A:5049:BCR:H371	1.82	0.44
23:A:5051:BCR:H373	7:B:435:LEU:HD23	1.98	0.44
7:B:138:VAL:HA	7:B:141:VAL:HG22	1.98	0.44
20:B:807:CLA:H3A	20:B:807:CLA:HBA1	1.65	0.44
3:7:233:HIS:CD2	20:7:314:CLA:NC	2.85	0.44
20:7:305:CLA:C4B	23:7:318:BCR:H281	2.31	0.44
24:7:319:LHG:HC5	24:7:319:LHG:HC82	1.53	0.44
23:8:316:BCR:H20C	23:8:316:BCR:H361	1.85	0.44
20:A:5042:CLA:H92	20:A:5042:CLA:H62	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:825:CLA:HED2	20:B:826:CLA:HBD	1.99	0.44
2:3:177:GLU:OE2	2:3:180:ARG:NH1	2.51	0.44
2:3:252:GLN:O	2:3:256:THR:OG1	2.28	0.44
5:9:50:ASN:OD1	5:9:50:ASN:N	2.50	0.44
20:B:826:CLA:H141	20:B:826:CLA:H162	1.81	0.44
9:D:127:LEU:HB3	9:D:133:MET:HB2	1.98	0.44
3:7:115:TRP:HE3	22:7:317:XAT:H242	1.82	0.44
6:A:146:GLN:HB3	6:A:377:TYR:HB3	1.99	0.44
20:B:826:CLA:H152	20:B:826:CLA:H112	1.81	0.44
11:F:159:VAL:HG22	20:F:307:CLA:HBA2	2.00	0.44
19:7:306:CHL:HBA1	23:7:318:BCR:H19C	1.99	0.44
20:A:5028:CLA:H142	20:A:5028:CLA:H111	1.75	0.44
20:A:5041:CLA:OBD	7:B:424:SER:OG	2.33	0.44
7:B:20:ARG:HA	7:B:23:TRP:HD1	1.82	0.44
7:B:281:ILE:HD13	7:B:281:ILE:HA	1.86	0.44
7:B:527:GLY:HA2	7:B:583:TRP:HZ3	1.81	0.44
20:B:806:CLA:CHB	23:B:847:BCR:HC8	2.48	0.44
10:E:48:GLY:HA3	10:E:74:VAL:HG11	2.00	0.44
11:F:205:ALA:O	11:F:209:GLU:HG3	2.18	0.44
2:3:231:LEU:HB3	20:3:308:CLA:H3A	1.98	0.44
20:9:603:CLA:HMD1	20:9:607:CLA:HBC2	2.00	0.44
6:A:261:LEU:HD21	23:K:4001:BCR:HC42	1.99	0.44
19:2:306:CHL:HBA1	19:2:306:CHL:CED	2.48	0.44
20:A:5011:CLA:H192	20:A:5042:CLA:H101	1.99	0.44
20:A:5041:CLA:H121	20:F:307:CLA:HAC1	2.00	0.44
20:A:5043:CLA:HBA2	20:A:5043:CLA:H3A	1.76	0.44
20:G:204:CLA:HMD2	27:G:206:LMG:H162	2.00	0.44
19:3:301:CHL:H61	20:3:302:CLA:HMA1	2.00	0.44
6:A:610:PHE:O	6:A:614:MET:HG2	2.18	0.44
13:H:80:VAL:HG22	13:H:80:VAL:O	2.18	0.44
18:2:211:ILE:N	20:2:311:CLA:O1A	2.49	0.44
2:3:98:GLY:HA2	6:A:179:PHE:CZ	2.49	0.43
22:3:316:XAT:H171	20:A:5016:CLA:H191	1.99	0.43
7:B:87:PRO:HB2	7:B:117:ALA:HB3	1.99	0.43
7:B:692:VAL:HG11	20:L:202:CLA:HMB2	2.00	0.43
7:B:726:LEU:O	7:B:730:THR:OG1	2.28	0.43
20:B:828:CLA:H3A	20:B:828:CLA:HBA2	1.57	0.43
23:F:309:BCR:H24C	23:F:309:BCR:H371	1.79	0.43
20:K:4002:CLA:C4D	23:K:4006:BCR:H281	2.48	0.43
1:1:150:LYS:HG3	1:1:154:PRO:HA	1.99	0.43
23:1:617:BCR:H24C	23:1:617:BCR:H371	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:306:CLA:H43	23:3:319:BCR:H12C	2.00	0.43
20:7:313:CLA:H152	20:7:313:CLA:H112	1.83	0.43
20:A:5044:CLA:HAB	7:B:583:TRP:CH2	2.53	0.43
7:B:702:SER:O	7:B:706:ALA:N	2.42	0.43
6:A:178:TRP:CD2	27:A:5001:LMG:H162	2.53	0.43
20:A:5025:CLA:H62	20:A:5025:CLA:H41	1.89	0.43
7:B:158:LEU:O	7:B:163:GLN:NE2	2.48	0.43
5:9:84:TRP:CD1	20:9:607:CLA:HMD3	2.53	0.43
5:9:211:LEU:HD11	20:B:816:CLA:H42	1.99	0.43
6:A:141:THR:O	6:A:389:SER:OG	2.37	0.43
6:A:407:ALA:HB2	6:A:592:VAL:HG11	2.00	0.43
6:A:408:HIS:HA	6:A:411:ILE:HD12	1.99	0.43
20:A:5018:CLA:H51	20:A:5018:CLA:H11	1.80	0.43
20:A:5035:CLA:H111	20:A:5035:CLA:H71	1.84	0.43
20:B:824:CLA:HMA1	20:B:824:CLA:H52	1.99	0.43
2:3:181:LEU:HD11	25:3:320:SQD:H82	2.01	0.43
2:3:276:LEU:N	20:3:311:CLA:O1A	2.51	0.43
6:A:239:LEU:N	6:A:242:GLU:OE1	2.51	0.43
6:A:393:HIS:HE1	20:A:5029:CLA:C1D	2.30	0.43
6:A:441:LEU:HB2	20:A:5040:CLA:HBB1	2.00	0.43
6:A:597:PHE:HB2	20:B:805:CLA:HBC3	1.99	0.43
20:A:5027:CLA:H2A	20:A:5027:CLA:HED2	2.00	0.43
20:F:306:CLA:H51	20:F:306:CLA:H11	1.84	0.43
16:K:42:PHE:HB3	16:K:45:SER:HB3	1.99	0.43
2:3:91:SER:O	6:A:19:ARG:NH1	2.51	0.43
7:B:653:PHE:O	7:B:657:VAL:HG23	2.18	0.43
9:D:87:TRP:HH2	9:D:112:LEU:HD12	1.83	0.43
19:2:302:CHL:H72	19:2:302:CHL:H111	1.53	0.43
5:9:81:ASN:HB3	5:9:174:MET:HE2	2.01	0.43
5:9:106:GLU:HG3	19:9:606:CHL:HED3	2.01	0.43
6:A:355:ILE:HD11	23:A:5049:BCR:HC7	2.00	0.43
6:A:433:HIS:CE1	20:A:5032:CLA:ND	2.86	0.43
20:A:5040:CLA:H62	20:A:5040:CLA:H41	1.75	0.43
7:B:169:PHE:O	7:B:175:ARG:NH1	2.52	0.43
7:B:279:LEU:O	7:B:283:VAL:HG12	2.19	0.43
7:B:561:ASP:OD1	8:C:52:LYS:NZ	2.40	0.43
11:F:87:LEU:HD13	11:F:108:LYS:HA	2.00	0.43
1:1:81:TRP:HZ2	1:1:135:MET:HE1	1.82	0.43
19:3:301:CHL:H61	19:3:301:CHL:H41	1.47	0.43
20:A:5041:CLA:H3A	20:A:5041:CLA:HBA2	1.79	0.43
20:B:814:CLA:H112	20:B:814:CLA:H72	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:311:SQD:H241	25:F:311:SQD:H461	1.37	0.43
25:1:619:SQD:H92	20:B:830:CLA:H52	2.01	0.43
20:7:310:CLA:H91	20:7:310:CLA:H111	1.82	0.43
4:8:154:PHE:N	4:8:158:GLU:OE1	2.47	0.43
20:8:303:CLA:H142	20:8:303:CLA:H112	1.79	0.43
6:A:289:LEU:HB2	6:A:376:PRO:HA	2.00	0.43
6:A:310:HIS:HD2	20:A:5021:CLA:NA	2.11	0.43
6:A:656:GLN:H	6:A:656:GLN:HG2	1.63	0.43
20:A:5042:CLA:HAC2	23:F:304:BCR:H342	2.00	0.43
7:B:151:LEU:HD23	23:B:847:BCR:H14C	2.01	0.43
4:8:195:LYS:NZ	20:8:309:CLA:O1D	2.46	0.43
20:A:5019:CLA:HBA2	20:A:5019:CLA:H3A	1.64	0.43
7:B:644:LEU:HA	7:B:647:TRP:HD1	1.84	0.43
11:F:95:GLU:O	11:F:98:SER:OG	2.30	0.43
12:G:69:MET:SD	12:G:69:MET:N	2.87	0.43
1:1:183:LEU:HD12	1:1:183:LEU:HA	1.89	0.42
7:B:588:ILE:HA	7:B:591:VAL:HG22	2.01	0.42
20:B:823:CLA:O1A	23:B:845:BCR:H14C	2.19	0.42
27:G:206:LMG:H362	27:G:206:LMG:H182	2.01	0.42
14:I:101:PHE:HB2	23:L:206:BCR:H12C	2.00	0.42
16:K:49:LEU:HA	16:K:52:VAL:HG12	2.00	0.42
19:1:601:CHL:HMD2	23:8:316:BCR:H381	2.00	0.42
3:7:236:ASP:HB3	3:7:240:VAL:HG23	2.01	0.42
6:A:724:ARG:NH2	32:A:5046:SF4:S2	2.92	0.42
7:B:358:PRO:HG3	20:B:819:CLA:HBA1	2.01	0.42
2:3:182:GLN:HG3	19:3:323:CHL:HED1	2.00	0.42
2:3:239:GLY:O	2:3:243:MET:HG2	2.19	0.42
5:9:36:ARG:NH1	5:9:50:ASN:O	2.53	0.42
20:A:5008:CLA:HBC2	20:A:5031:CLA:HMA1	2.02	0.42
20:A:5040:CLA:H62	20:A:5040:CLA:H92	1.90	0.42
7:B:695:LYS:HA	7:B:695:LYS:HD2	1.79	0.42
20:B:804:CLA:HED2	20:B:804:CLA:HBD	1.89	0.42
20:B:840:CLA:H2	20:B:840:CLA:H62	1.65	0.42
23:F:304:BCR:H20C	23:F:304:BCR:H361	1.91	0.42
20:1:610:CLA:HBA2	20:1:611:CLA:HMD3	2.01	0.42
24:1:620:LHG:HC82	24:1:620:LHG:HC5	1.45	0.42
2:3:81:ASP:OD1	22:3:316:XAT:O23	2.37	0.42
2:3:181:LEU:HD13	20:3:307:CLA:HMA2	2.01	0.42
3:7:73:GLU:O	3:7:78:ARG:NH2	2.50	0.42
20:9:611:CLA:H92	20:9:611:CLA:HMC1	2.00	0.42
7:B:204:ARG:HH12	7:B:254:ALA:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:452:LYS:HB3	7:B:452:LYS:HE2	1.86	0.42
7:B:499:LEU:HA	7:B:502:ILE:HG22	2.00	0.42
20:B:804:CLA:H202	20:B:804:CLA:H162	1.81	0.42
20:B:822:CLA:HAA1	12:G:66:ARG:HH22	1.83	0.42
20:B:839:CLA:H3A	20:B:839:CLA:HBA2	1.65	0.42
19:2:306:CHL:C1B	21:2:315:LUT:H24	2.49	0.42
19:8:304:CHL:C3C	19:8:305:CHL:HAC2	2.49	0.42
7:B:41:GLU:HG3	7:B:166:LEU:HB2	2.01	0.42
20:8:309:CLA:HBC3	24:8:317:LHG:HC82	2.01	0.42
5:9:71:LEU:HB3	5:9:72:LYS:HE2	2.02	0.42
6:A:276:LEU:HD21	6:A:299:LEU:HD23	2.01	0.42
20:A:5018:CLA:H61	20:A:5018:CLA:H41	1.84	0.42
7:B:31:ASP:HB2	20:B:829:CLA:HAA2	2.02	0.42
20:B:821:CLA:H92	20:B:821:CLA:H61	1.93	0.42
8:C:38:GLN:HG2	9:D:160:VAL:HG11	2.02	0.42
2:3:151:PRO:O	26:3:321:PTY:N1	2.45	0.42
4:8:47:LYS:HA	4:8:47:LYS:HD3	1.81	0.42
30:A:5003:CL0:H33	20:A:5005:CLA:C1D	2.50	0.42
7:B:68:HIS:HE1	20:B:809:CLA:C4D	2.33	0.42
20:B:840:CLA:H202	20:B:840:CLA:H162	1.81	0.42
9:D:160:VAL:HG23	9:D:161:ASN:N	2.35	0.42
6:A:747:ILE:HD12	6:A:747:ILE:HA	1.90	0.42
7:B:54:GLN:HG2	20:B:807:CLA:C3A	2.48	0.42
7:B:460:PHE:HE1	11:F:136:ASP:HB2	1.84	0.42
20:B:808:CLA:H91	28:B:848:DGD:HBN1	2.00	0.42
20:B:831:CLA:HAA2	11:F:216:LEU:HD21	2.01	0.42
20:K:4002:CLA:H3A	20:K:4002:CLA:HBA1	1.76	0.42
18:2:59:LEU:HD12	18:2:59:LEU:C	2.44	0.42
6:A:458:HIS:HE1	20:A:5035:CLA:NA	2.14	0.42
6:A:673:LEU:HD23	6:A:673:LEU:HA	1.89	0.42
6:A:677:PHE:CG	23:A:5051:BCR:H363	2.55	0.42
6:A:730:HIS:HE1	20:A:5042:CLA:ND	2.16	0.42
23:A:5047:BCR:H361	23:A:5047:BCR:H20C	1.84	0.42
7:B:214:LEU:HD23	20:B:816:CLA:HMA2	2.02	0.42
7:B:663:MET:HB2	20:B:805:CLA:C4B	2.50	0.42
20:B:809:CLA:H2	14:I:88:THR:HG21	2.01	0.42
20:B:820:CLA:HAA2	20:B:824:CLA:C3B	2.49	0.42
20:B:827:CLA:H3A	20:B:827:CLA:HBA2	1.63	0.42
1:1:80:ARG:NH1	20:1:607:CLA:OBD	2.53	0.42
2:3:147:GLY:HA2	2:3:154:VAL:HG22	2.02	0.42
20:3:307:CLA:H203	23:A:5048:BCR:H321	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:7:318:BCR:H24C	23:7:318:BCR:H371	1.89	0.42
20:8:308:CLA:O1A	21:8:314:LUT:O23	2.38	0.42
6:A:77:HIS:ND1	20:A:5014:CLA:OBD	2.46	0.42
6:A:370:HIS:CD2	20:A:5028:CLA:NC	2.88	0.42
20:A:5011:CLA:H61	20:A:5011:CLA:H101	1.78	0.42
7:B:587:THR:O	7:B:591:VAL:HG13	2.19	0.42
20:B:806:CLA:HHC	20:B:808:CLA:OBD	2.20	0.42
20:B:832:CLA:H121	15:J:25:LEU:HD11	2.02	0.42
9:D:65:ILE:N	9:D:104:ILE:O	2.51	0.42
23:G:205:BCR:H24C	23:G:205:BCR:H371	1.82	0.42
13:H:113:ILE:HG23	13:H:114:THR:HG23	2.01	0.42
16:K:78:LYS:HE2	16:K:78:LYS:HB2	1.90	0.42
1:1:173:LYS:HD3	20:1:609:CLA:H11	2.02	0.41
20:3:311:CLA:H11	20:3:311:CLA:H51	1.85	0.41
5:9:147:ILE:O	5:9:149:SER:N	2.52	0.41
6:A:53:HIS:HB3	24:A:5052:LHG:H111	2.01	0.41
6:A:206:LEU:HD11	20:A:5030:CLA:H192	2.02	0.41
6:A:587:SER:O	6:A:591:HIS:ND1	2.37	0.41
7:B:366:PHE:HB3	7:B:603:TRP:CZ3	2.55	0.41
7:B:444:VAL:HG11	7:B:453:GLN:N	2.35	0.41
20:F:307:CLA:HBA1	20:F:307:CLA:H3A	1.51	0.41
20:1:608:CLA:H2A	20:1:608:CLA:HED2	2.02	0.41
20:1:608:CLA:HBB1	20:G:201:CLA:H151	2.01	0.41
20:7:310:CLA:H43	21:7:316:LUT:H8	2.01	0.41
4:8:154:PHE:CZ	19:8:306:CHL:HBB2	2.55	0.41
20:A:5029:CLA:H61	20:A:5029:CLA:H41	1.54	0.41
23:A:5047:BCR:H382	23:K:4001:BCR:HC8	2.02	0.41
7:B:412:VAL:HA	7:B:415:HIS:CE1	2.56	0.41
13:H:92:LEU:HD21	20:H:201:CLA:H51	2.02	0.41
18:2:226:VAL:O	18:2:229:VAL:HG12	2.20	0.41
2:3:150:PRO:HA	2:3:154:VAL:HG23	2.02	0.41
5:9:94:GLY:HA3	20:9:604:CLA:HBC3	2.00	0.41
6:A:270:ALA:HA	20:A:5018:CLA:HAA2	2.01	0.41
6:A:542:THR:HB	6:A:602:SER:HB2	2.01	0.41
20:A:5016:CLA:H3A	20:A:5016:CLA:HBA2	1.71	0.41
20:A:5036:CLA:H41	20:A:5036:CLA:H61	1.84	0.41
7:B:300:HIS:HB3	7:B:305:ILE:HD11	2.01	0.41
7:B:701:LEU:HD21	31:B:841:PQN:H151	2.03	0.41
20:B:807:CLA:H8	20:B:807:CLA:H121	1.88	0.41
15:J:31:ARG:HD3	23:J:106:BCR:H332	2.02	0.41
17:L:76:ALA:HB2	20:L:204:CLA:HMD1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:54:PHE:HE1	19:1:601:CHL:HBC2	1.85	0.41
3:7:210:LEU:HD13	20:7:313:CLA:H102	2.02	0.41
7:B:565:ARG:HB3	10:E:92:TYR:HB2	2.02	0.41
20:B:829:CLA:H111	20:B:829:CLA:H151	1.80	0.41
20:B:836:CLA:H121	23:F:309:BCR:H323	2.02	0.41
11:F:157:LEU:HD22	20:F:303:CLA:H152	2.01	0.41
13:H:111:LEU:HA	13:H:112:PRO:HD3	1.87	0.41
20:7:311:CLA:NA	24:7:320:LHG:O4	2.54	0.41
20:9:602:CLA:CBB	22:9:614:XAT:H32	2.50	0.41
7:B:548:MET:HE3	7:B:548:MET:HB2	1.88	0.41
7:B:705:GLN:HG3	28:B:848:DGD:HA22	2.02	0.41
13:H:103:LEU:HD23	13:H:103:LEU:H	1.86	0.41
18:2:136:ALA:HB2	20:2:301:CLA:HAA1	2.02	0.41
20:7:323:CLA:HMA3	4:8:34:LEU:HD13	2.01	0.41
4:8:125:MET:HE3	4:8:125:MET:HB3	1.85	0.41
20:8:309:CLA:H2	20:8:309:CLA:H61	1.89	0.41
6:A:720:ILE:H	6:A:720:ILE:HG13	1.64	0.41
20:A:5011:CLA:H42	23:A:5051:BCR:H321	2.02	0.41
20:B:805:CLA:HED2	20:B:805:CLA:HBD	1.78	0.41
9:D:152:LYS:HD2	9:D:152:LYS:HA	1.84	0.41
23:F:304:BCR:H24C	23:F:304:BCR:H371	1.87	0.41
23:I:4001:BCR:H20C	23:I:4001:BCR:H361	1.85	0.41
16:K:49:LEU:C	16:K:52:VAL:HG12	2.45	0.41
1:1:54:PHE:CE1	19:1:601:CHL:HBC2	2.55	0.41
1:1:148:MET:HE3	1:1:148:MET:HA	2.02	0.41
20:3:314:CLA:HBB2	27:7:301:LMG:H273	2.02	0.41
21:3:315:LUT:H402	23:3:319:BCR:H361	2.03	0.41
4:8:106:GLU:O	4:8:110:VAL:HG12	2.21	0.41
20:8:308:CLA:H51	20:8:308:CLA:HBB1	2.02	0.41
5:9:65:GLY:HA3	5:9:71:LEU:HD13	2.02	0.41
20:9:603:CLA:H41	20:B:812:CLA:H12	2.03	0.41
6:A:156:GLU:HA	6:A:159:LEU:HD12	2.03	0.41
7:B:429:PHE:CZ	23:J:102:BCR:H291	2.56	0.41
7:B:659:ALA:HB1	20:B:805:CLA:CAB	2.51	0.41
9:D:66:PHE:HE2	9:D:69:SER:HB2	1.86	0.41
18:2:39:ALA:HB2	18:2:54:LEU:HB3	2.01	0.41
2:3:148:VAL:HG21	22:3:316:XAT:H172	2.02	0.41
20:3:302:CLA:H143	20:3:307:CLA:H42	2.03	0.41
4:8:51:ASN:HA	20:8:301:CLA:CGD	2.51	0.41
6:A:508:LEU:HD23	6:A:508:LEU:HA	1.91	0.41
6:A:562:LEU:HG	6:A:563:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:5001:LMG:H111	27:A:5001:LMG:HC8	1.42	0.41
20:A:5032:CLA:H3A	20:A:5033:CLA:OBD	2.21	0.41
20:A:5044:CLA:HAB	7:B:583:TRP:CZ2	2.55	0.41
23:A:5048:BCR:H24C	23:A:5048:BCR:H371	1.86	0.41
7:B:511:LEU:HD12	7:B:511:LEU:H	1.85	0.41
20:B:831:CLA:ND	23:F:309:BCR:H363	2.36	0.41
1:1:135:MET:HE2	1:1:135:MET:HB3	1.89	0.41
1:1:218:PHE:CD1	20:1:612:CLA:H2	2.56	0.41
19:3:301:CHL:H8	20:3:302:CLA:HMB3	2.03	0.41
3:7:40:GLY:HA2	3:7:43:ARG:HD3	2.02	0.41
3:7:123:ILE:HG21	3:7:130:LEU:HD13	2.03	0.41
3:7:134:ILE:HG22	19:7:307:CHL:HBC3	2.03	0.41
20:8:303:CLA:C4B	23:8:316:BCR:HC32	2.36	0.41
29:8:322:LMU:H122	15:J:29:ILE:HG13	2.02	0.41
6:A:433:HIS:CE1	6:A:437:ILE:HD11	2.56	0.41
6:A:681:PHE:HZ	20:A:5042:CLA:HBC2	1.86	0.41
20:A:5005:CLA:C1B	20:B:805:CLA:CBB	2.84	0.41
11:F:74:LYS:HD3	11:F:74:LYS:HA	1.76	0.41
11:F:206:ALA:HB1	23:F:309:BCR:H391	2.03	0.41
18:2:70:GLY:O	18:2:76:MET:SD	2.79	0.41
6:A:684:MET:HE1	20:A:5004:CLA:C4A	2.29	0.41
7:B:423:LEU:HD13	7:B:533:LEU:HA	2.03	0.41
20:B:807:CLA:H12	23:B:843:BCR:H343	2.03	0.41
8:C:15:THR:HG22	8:C:28:MET:HE2	2.03	0.41
12:G:64:ARG:NH2	12:G:105:GLY:O	2.54	0.41
2:3:69:TYR:HB2	2:3:88:PRO:HD2	2.01	0.40
2:3:124:ILE:HD11	2:3:249:TYR:HH	1.76	0.40
20:3:306:CLA:H12	23:3:319:BCR:H12C	2.03	0.40
4:8:120:PHE:CD1	19:8:305:CHL:HMD2	2.57	0.40
6:A:361:GLY:O	6:A:365:ILE:HG12	2.20	0.40
20:B:832:CLA:H151	20:F:307:CLA:H11	2.02	0.40
13:H:75:ARG:HA	13:H:78:ASP:HB2	2.01	0.40
25:1:619:SQD:H241	25:1:619:SQD:H461	1.70	0.40
3:7:107:LYS:HE2	3:7:107:LYS:HB2	1.90	0.40
5:9:211:LEU:HD23	5:9:211:LEU:HA	1.87	0.40
6:A:601:ASN:HD21	30:A:5003:CL0:H68	1.87	0.40
20:A:5041:CLA:H162	20:A:5041:CLA:H202	1.86	0.40
20:B:828:CLA:H122	20:B:828:CLA:H162	1.89	0.40
20:B:829:CLA:H141	20:B:829:CLA:H161	1.88	0.40
20:2:305:CLA:C3C	19:2:306:CHL:HBC3	2.52	0.40
20:2:311:CLA:H3A	20:2:311:CLA:HBA2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:307:CLA:H192	23:A:5048:BCR:H311	2.02	0.40
23:3:318:BCR:H403	23:A:5047:BCR:H402	2.02	0.40
19:8:304:CHL:HBB2	19:8:305:CHL:HBB1	2.03	0.40
20:A:5005:CLA:H93	20:B:839:CLA:HBB2	2.04	0.40
7:B:194:HIS:HB2	20:B:815:CLA:C1C	2.52	0.40
7:B:522:HIS:CD2	20:B:836:CLA:NA	2.87	0.40
20:B:817:CLA:HBA2	20:B:817:CLA:H3A	1.79	0.40
20:B:832:CLA:H151	20:B:832:CLA:H111	1.86	0.40
20:B:839:CLA:H42	31:B:841:PQN:H302	2.03	0.40
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.87	0.40
8:C:24:ASP:OD2	9:D:150:HIS:ND1	2.48	0.40
20:2:307:CLA:HBA2	20:2:307:CLA:H3A	1.64	0.40
1:1:120:VAL:HG22	1:1:122:PHE:HD1	1.86	0.40
2:3:86:LEU:HD23	2:3:86:LEU:HA	1.92	0.40
2:3:202:PHE:CE1	23:3:319:BCR:H313	2.55	0.40
3:7:89:ALA:HB1	3:7:205:GLY:HA3	2.03	0.40
3:7:137:GLU:OE1	19:7:307:CHL:HMC	2.21	0.40
4:8:90:PRO:HD3	20:8:303:CLA:HBC3	2.03	0.40
5:9:205:LYS:HD3	5:9:205:LYS:HA	1.88	0.40
6:A:665:LEU:O	6:A:668:TYR:HB2	2.21	0.40
7:B:548:MET:HE1	7:B:561:ASP:HB2	2.03	0.40
20:B:822:CLA:H201	12:G:120:VAL:HG11	2.03	0.40
20:B:826:CLA:H162	20:B:826:CLA:H192	1.89	0.40
2:3:202:PHE:CZ	20:3:306:CLA:HAB	2.55	0.40
3:7:205:GLY:O	3:7:209:MET:HG2	2.22	0.40
6:A:359:LEU:HG	20:A:5026:CLA:HMA3	2.04	0.40
6:A:430:VAL:HA	6:A:433:HIS:CE1	2.56	0.40
6:A:658:ILE:HB	7:B:622:ARG:HB2	2.03	0.40
7:B:609:GLN:O	7:B:613:SER:CB	2.69	0.40
7:B:657:VAL:HG13	7:B:713:HIS:HD2	1.87	0.40
31:B:841:PQN:H261	31:B:841:PQN:H222	1.69	0.40
17:L:59:THR:HG22	17:L:60:PRO:N	2.37	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%)	185 (95%)	10 (5%)	0	100	100
2	3	224/286 (78%)	212 (95%)	12 (5%)	0	100	100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100	100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100	100
5	9	185/222 (83%)	173 (94%)	12 (6%)	0	100	100
6	A	738/751 (98%)	711 (96%)	27 (4%)	0	100	100
7	B	732/735 (100%)	710 (97%)	22 (3%)	0	100	100
8	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
9	D	141/193 (73%)	129 (92%)	12 (8%)	0	100	100
10	E	66/111 (60%)	64 (97%)	2 (3%)	0	100	100
11	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
12	G	103/141 (73%)	97 (94%)	5 (5%)	1 (1%)	13	9
13	H	45/134 (34%)	42 (93%)	3 (7%)	0	100	100
14	I	33/109 (30%)	33 (100%)	0	0	100	100
15	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
16	K	81/123 (66%)	65 (80%)	14 (17%)	2 (2%)	4	2
17	L	120/198 (61%)	117 (98%)	3 (2%)	0	100	100
18	2	220/261 (84%)	211 (96%)	8 (4%)	1 (0%)	25	23
All	All	3602/4350 (83%)	3442 (96%)	156 (4%)	4 (0%)	50	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	74	ALA
16	K	66	LEU
18	2	118	ILE
12	G	38	ILE

### 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	153/179 (86%)	153 (100%)	0	100	100
2	3	170/217 (78%)	169 (99%)	1 (1%)	84	89
3	7	171/201 (85%)	171 (100%)	0	100	100
4	8	173/197 (88%)	171 (99%)	2 (1%)	67	74
5	9	152/180 (84%)	149 (98%)	3 (2%)	50	57
6	A	599/609 (98%)	594 (99%)	5 (1%)	79	84
7	B	595/596 (100%)	586 (98%)	9 (2%)	60	67
8	C	68/69 (99%)	66 (97%)	2 (3%)	37	41
9	D	123/156 (79%)	122 (99%)	1 (1%)	79	84
10	E	60/93 (64%)	60 (100%)	0	100	100
11	F	136/177 (77%)	136 (100%)	0	100	100
12	G	82/111 (74%)	81 (99%)	1 (1%)	67	74
13	H	35/103 (34%)	35 (100%)	0	100	100
14	I	28/77 (36%)	28 (100%)	0	100	100
15	J	36/36 (100%)	35 (97%)	1 (3%)	38	43
16	K	58/88 (66%)	58 (100%)	0	100	100
17	L	91/150 (61%)	90 (99%)	1 (1%)	70	77
18	2	176/205 (86%)	175 (99%)	1 (1%)	84	89
All	All	2906/3444 (84%)	2879 (99%)	27 (1%)	74	82

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	83	LEU
4	8	38	GLN
4	8	131	TYR
5	9	105	TYR
5	9	119	GLN
5	9	169	ASN
6	A	55	ASP
6	A	91	MET
6	A	372	TYR

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Mol	Chain	Res	Type
6	A	374	MET
6	A	584	CYS
7	B	151	LEU
7	B	181	SER
7	B	236	GLN
7	B	283	VAL
7	B	495	LEU
7	B	526	LEU
7	B	569	CYS
7	B	578	TYR
7	B	721	THR
8	C	26	LEU
8	C	67	VAL
9	D	63	SER
12	G	75	LYS
15	J	5	THR
17	L	105	LEU
18	2	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	55	ASN
1	1	146	GLN
1	1	216	ASN
2	3	106	GLN
2	3	220	ASN
2	3	238	ASN
3	7	204	ASN
3	7	220	HIS
5	9	165	ASN
5	9	183	GLN
6	A	25	ASN
6	A	182	HIS
6	A	311	GLN
6	A	387	GLN
6	A	421	ASN
6	A	478	GLN
6	A	637	GLN
6	A	659	GLN
7	B	11	GLN
7	B	236	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	B	404	ASN
7	B	631	GLN
7	B	683	HIS
8	C	16	GLN
14	I	105	GLN
15	J	30	ASN
18	2	53	HIS

### 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](#)

270 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	$\# Z  > 2$
20	CLA	B	819	7	63,73,73	1.33	5 (7%)	74,113,113	1.33	7 (9%)
20	CLA	3	305	2	48,58,73	1.47	5 (10%)	56,95,113	1.46	8 (14%)
20	CLA	A	5035	6	63,73,73	1.35	5 (7%)	74,113,113	1.27	6 (8%)
32	SF4	C	102	8	0,12,12	-	-	-		
29	LMU	8	322	-	36,36,36	0.12	0	47,47,47	0.20	0
20	CLA	3	309	2	44,54,73	1.58	5 (11%)	51,90,113	1.38	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
31	PQN	B	841	-	34,34,34	0.29	0	43,45,45	0.55	1 (2%)
20	CLA	B	837	7	53,63,73	1.42	5 (9%)	62,101,113	1.43	8 (12%)
21	LUT	1	615	-	42,43,43	0.19	0	51,60,60	1.43	7 (13%)
31	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.56	1 (2%)
22	XAT	8	315	-	41,47,47	0.16	0	54,74,74	0.83	1 (1%)
23	BCR	L	203	-	41,41,41	0.14	0	56,56,56	0.25	0
20	CLA	B	810	7	63,73,73	1.31	7 (11%)	74,113,113	1.26	8 (10%)
20	CLA	9	612	5	44,54,73	1.60	5 (11%)	51,90,113	1.37	6 (11%)
20	CLA	A	5040	-	58,68,73	1.40	5 (8%)	68,107,113	1.28	6 (8%)
27	LMG	7	324	-	30,30,55	0.24	0	38,38,63	0.24	0
20	CLA	B	829	7	63,73,73	1.39	5 (7%)	74,113,113	1.28	8 (10%)
20	CLA	K	4005	-	46,56,73	1.67	6 (13%)	53,92,113	1.56	7 (13%)
20	CLA	K	4002	-	43,53,73	1.70	4 (9%)	50,89,113	1.50	6 (12%)
20	CLA	F	303	7	63,73,73	1.41	7 (11%)	74,113,113	1.69	13 (17%)
20	CLA	A	5017	-	53,63,73	1.48	5 (9%)	62,101,113	1.44	7 (11%)
20	CLA	8	308	4	58,68,73	1.36	5 (8%)	68,107,113	1.22	6 (8%)
25	SQD	3	322	-	39,41,54	0.22	0	49,52,65	0.26	0
20	CLA	1	614	1	44,54,73	1.58	4 (9%)	51,90,113	1.51	6 (11%)
20	CLA	2	312	18	40,52,73	1.66	5 (12%)	45,87,113	1.50	6 (13%)
20	CLA	A	5014	-	63,73,73	1.33	6 (9%)	74,113,113	1.39	8 (10%)
20	CLA	7	314	3	48,58,73	1.54	5 (10%)	56,95,113	1.43	8 (14%)
20	CLA	9	605	5	43,53,73	1.65	5 (11%)	50,89,113	1.62	5 (10%)
23	BCR	A	5049	-	41,41,41	0.27	0	56,56,56	1.03	5 (8%)
23	BCR	3	319	-	41,41,41	1.38	8 (19%)	56,56,56	1.53	12 (21%)
27	LMG	G	206	-	43,43,55	0.19	0	51,51,63	0.18	0
23	BCR	L	206	-	41,41,41	0.17	0	56,56,56	0.48	0
20	CLA	1	607	-	48,58,73	1.54	5 (10%)	56,95,113	1.38	8 (14%)
20	CLA	3	325	6	53,63,73	1.48	5 (9%)	62,101,113	1.37	6 (9%)
19	CHL	1	601	-	45,55,74	1.53	4 (8%)	48,91,114	1.66	9 (18%)
26	PTY	3	321	-	49,49,49	0.44	0	52,54,54	0.78	2 (3%)
23	BCR	K	4006	-	41,41,41	0.17	0	56,56,56	0.32	0
23	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
23	BCR	J	106	-	41,41,41	0.17	0	56,56,56	0.36	0
27	LMG	J	103	-	29,29,55	0.20	0	37,37,63	0.14	0
20	CLA	7	303	3	58,68,73	1.39	6 (10%)	68,107,113	1.22	7 (10%)
20	CLA	3	311	-	53,63,73	1.46	5 (9%)	62,101,113	1.39	7 (11%)
28	DGD	7	321	-	40,40,67	0.24	0	54,54,81	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	8	307	4	45,55,73	1.81	9 (20%)	52,91,113	2.04	13 (25%)
19	CHL	1	606	-	45,55,74	1.61	4 (8%)	48,91,114	1.99	9 (18%)
20	CLA	2	313	-	48,58,73	1.53	5 (10%)	56,95,113	1.47	8 (14%)
20	CLA	1	603	1	53,63,73	1.49	6 (11%)	62,101,113	1.39	7 (11%)
20	CLA	B	833	7	58,68,73	1.41	5 (8%)	68,107,113	1.39	6 (8%)
24	LHG	9	617	20	35,35,48	0.35	0	38,41,54	0.36	0
20	CLA	B	815	-	63,73,73	1.30	6 (9%)	74,113,113	1.27	7 (9%)
23	BCR	J	105	-	41,41,41	0.15	0	56,56,56	0.27	0
24	LHG	A	5052	-	48,48,48	0.29	0	51,54,54	0.28	0
20	CLA	B	821	-	53,63,73	1.46	5 (9%)	62,101,113	1.38	7 (11%)
20	CLA	B	840	-	63,73,73	1.32	5 (7%)	74,113,113	1.21	7 (9%)
20	CLA	3	310	2	44,54,73	1.62	7 (15%)	51,90,113	1.58	6 (11%)
20	CLA	2	309	-	43,53,73	1.62	5 (11%)	50,89,113	1.45	6 (12%)
22	XAT	9	614	-	41,47,47	0.14	0	54,74,74	0.75	3 (5%)
20	CLA	A	5025	6	58,68,73	1.40	6 (10%)	68,107,113	1.26	4 (5%)
24	LHG	7	319	-	21,21,48	0.41	0	24,27,54	0.45	0
26	PTY	B	802	-	26,26,49	0.61	0	29,31,54	0.50	0
26	PTY	F	302	-	31,31,49	0.56	0	34,36,54	0.46	0
20	CLA	H	201	18	58,68,73	1.54	6 (10%)	68,107,113	1.33	9 (13%)
20	CLA	L	204	17	63,73,73	1.33	5 (7%)	74,113,113	1.19	7 (9%)
29	LMU	8	318	-	34,34,36	0.13	0	45,45,47	0.14	0
20	CLA	1	604	-	48,58,73	1.45	5 (10%)	56,95,113	1.46	8 (14%)
19	CHL	2	306	-	45,55,74	1.16	5 (11%)	48,91,114	2.14	12 (25%)
20	CLA	8	310	4	44,54,73	1.64	8 (18%)	51,90,113	1.57	7 (13%)
20	CLA	8	301	4	58,68,73	1.38	5 (8%)	68,107,113	1.29	8 (11%)
24	LHG	2	316	-	24,24,48	0.55	0	27,29,54	0.84	2 (7%)
20	CLA	A	5021	6	48,58,73	1.53	6 (12%)	56,95,113	1.39	8 (14%)
20	CLA	B	825	-	63,73,73	1.33	7 (11%)	74,113,113	1.19	7 (9%)
20	CLA	7	323	4	45,55,73	1.59	6 (13%)	52,91,113	1.45	8 (15%)
23	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.56	2 (3%)
20	CLA	A	5034	6	63,73,73	1.35	5 (7%)	74,113,113	1.34	8 (10%)
20	CLA	1	612	-	58,68,73	1.43	5 (8%)	68,107,113	1.32	6 (8%)
20	CLA	8	313	4	44,54,73	1.60	6 (13%)	51,90,113	1.39	6 (11%)
21	LUT	2	315	-	42,43,43	0.20	0	51,60,60	0.74	2 (3%)
20	CLA	G	204	-	43,53,73	1.86	7 (16%)	50,89,113	1.48	5 (10%)
20	CLA	B	832	7	63,73,73	1.35	6 (9%)	74,113,113	1.25	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	3	303	-	44,54,73	1.59	5 (11%)	51,90,113	1.50	6 (11%)
20	CLA	A	5019	6	53,63,73	1.48	7 (13%)	62,101,113	1.36	7 (11%)
20	CLA	7	309	3	44,54,73	1.59	5 (11%)	51,90,113	1.46	6 (11%)
20	CLA	B	818	7	63,73,73	1.32	6 (9%)	74,113,113	1.27	6 (8%)
20	CLA	A	5033	6	53,63,73	1.44	5 (9%)	62,101,113	1.33	7 (11%)
23	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.37	0
20	CLA	B	823	7	53,63,73	1.45	6 (11%)	62,101,113	1.25	8 (12%)
29	LMU	9	616	-	30,30,36	0.19	0	41,41,47	0.86	2 (4%)
20	CLA	2	301	-	44,54,73	1.57	5 (11%)	51,90,113	1.40	6 (11%)
20	CLA	8	303	-	63,73,73	1.37	7 (11%)	74,113,113	1.15	6 (8%)
20	CLA	A	5007	6,20	63,73,73	1.31	6 (9%)	74,113,113	1.20	7 (9%)
20	CLA	3	314	2	44,54,73	1.60	5 (11%)	51,90,113	1.44	6 (11%)
20	CLA	7	313	3	63,73,73	1.42	6 (9%)	74,113,113	1.32	7 (9%)
20	CLA	B	812	7	53,63,73	1.48	5 (9%)	62,101,113	1.33	6 (9%)
20	CLA	B	813	7	44,54,73	1.60	6 (13%)	51,90,113	1.42	6 (11%)
21	LUT	2	314	-	42,43,43	0.29	0	51,60,60	1.04	3 (5%)
20	CLA	A	5042	6	58,68,73	1.41	6 (10%)	68,107,113	1.32	8 (11%)
20	CLA	1	605	-	43,53,73	1.63	6 (13%)	50,89,113	1.58	6 (12%)
29	LMU	F	305	-	33,33,36	0.16	0	44,44,47	0.48	0
19	CHL	3	301	2	60,70,74	1.21	4 (6%)	66,109,114	1.95	8 (12%)
19	CHL	7	307	-	45,55,74	1.27	4 (8%)	48,91,114	2.47	9 (18%)
20	CLA	A	5008	6	63,73,73	1.32	6 (9%)	74,113,113	1.27	7 (9%)
20	CLA	9	610	5	48,58,73	1.59	7 (14%)	56,95,113	1.56	9 (16%)
20	CLA	3	324	6	53,63,73	1.47	5 (9%)	62,101,113	1.37	7 (11%)
20	CLA	F	307	-	45,55,73	1.57	5 (11%)	52,91,113	1.40	7 (13%)
23	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.34	0
23	BCR	A	5047	-	41,41,41	0.29	0	56,56,56	0.54	0
24	LHG	I	4002	-	27,27,48	0.38	0	30,33,54	0.36	0
25	SQD	7	322	-	37,39,54	0.23	0	47,50,65	0.24	0
20	CLA	B	811	7	63,73,73	1.35	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	A	5028	6	63,73,73	1.37	7 (11%)	74,113,113	1.37	7 (9%)
20	CLA	L	202	-	63,73,73	1.34	5 (7%)	74,113,113	1.24	7 (9%)
28	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.19	0
20	CLA	L	201	7	63,73,73	1.35	5 (7%)	74,113,113	1.33	8 (10%)
20	CLA	B	809	7	63,73,73	1.32	5 (7%)	74,113,113	1.29	7 (9%)
22	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.81	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	8	311	4	63,73,73	1.38	6 (9%)	74,113,113	1.25	7 (9%)
20	CLA	G	203	12	44,54,73	1.62	5 (11%)	51,90,113	1.45	6 (11%)
24	LHG	A	5055	-	33,33,48	0.45	0	36,38,54	0.65	2 (5%)
20	CLA	F	306	-	58,68,73	1.37	5 (8%)	68,107,113	1.25	7 (10%)
19	CHL	2	302	18	59,69,74	1.19	4 (6%)	65,108,114	1.91	8 (12%)
20	CLA	A	5032	6	48,58,73	1.63	7 (14%)	56,95,113	1.44	8 (14%)
20	CLA	B	836	7	58,68,73	1.37	5 (8%)	68,107,113	1.27	8 (11%)
23	BCR	A	5050	-	41,41,41	0.13	0	56,56,56	0.39	0
24	LHG	8	319	-	37,37,48	0.33	0	40,43,54	0.31	0
20	CLA	7	304	3	53,63,73	1.50	6 (11%)	62,101,113	1.37	7 (11%)
23	BCR	J	102	-	41,41,41	0.24	0	56,56,56	0.93	4 (7%)
19	CHL	8	306	-	49,59,74	1.65	4 (8%)	53,96,114	2.07	8 (15%)
26	PTY	F	310	-	30,30,49	0.56	0	33,35,54	0.55	0
20	CLA	7	310	3	63,73,73	1.29	5 (7%)	74,113,113	1.20	7 (9%)
20	CLA	B	824	-	63,73,73	1.32	7 (11%)	74,113,113	1.41	9 (12%)
30	CL0	A	5003	6	63,73,73	1.14	4 (6%)	74,113,113	1.84	7 (9%)
24	LHG	1	620	-	45,45,48	0.31	0	48,51,54	0.34	0
20	CLA	A	5010	-	49,59,73	1.53	5 (10%)	56,96,113	1.47	8 (14%)
20	CLA	2	308	-	43,53,73	1.62	5 (11%)	50,89,113	1.42	8 (16%)
19	CHL	3	323	-	59,69,74	1.30	4 (6%)	65,108,114	2.18	8 (12%)
19	CHL	7	306	-	44,54,74	1.40	5 (11%)	47,90,114	2.16	6 (12%)
20	CLA	A	5018	6	58,68,73	1.39	6 (10%)	68,107,113	1.32	6 (8%)
20	CLA	A	5023	6	48,58,73	1.52	5 (10%)	56,95,113	1.57	9 (16%)
23	BCR	K	4001	-	41,41,41	0.18	0	56,56,56	0.35	0
26	PTY	F	301	-	28,28,49	0.59	0	31,33,54	0.50	0
20	CLA	A	5020	6	63,73,73	1.33	5 (7%)	74,113,113	1.30	9 (12%)
20	CLA	8	309	24	58,68,73	1.43	7 (12%)	68,107,113	1.31	7 (10%)
20	CLA	A	5027	-	54,64,73	1.51	7 (12%)	63,102,113	1.34	8 (12%)
20	CLA	A	5039	6	53,63,73	1.45	6 (11%)	62,101,113	1.35	8 (12%)
20	CLA	2	304	-	48,58,73	1.50	5 (10%)	56,95,113	1.38	8 (14%)
20	CLA	B	830	7	63,73,73	1.37	5 (7%)	74,113,113	1.29	8 (10%)
20	CLA	1	602	1	53,63,73	1.47	5 (9%)	62,101,113	1.41	8 (12%)
24	LHG	1	618	20	25,25,48	0.41	0	28,31,54	0.40	0
24	LHG	8	320	-	42,42,48	0.31	0	45,48,54	0.30	0
25	SQD	3	320	-	33,35,54	0.27	0	43,46,65	0.39	0
20	CLA	8	312	4	44,54,73	1.59	5 (11%)	51,90,113	1.49	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	8	321	-	44,54,73	1.64	5 (11%)	51,90,113	1.56	8 (15%)
20	CLA	B	827	-	63,73,73	1.32	5 (7%)	74,113,113	1.28	7 (9%)
23	BCR	F	304	-	41,41,41	0.17	0	56,56,56	0.30	0
20	CLA	9	602	5	58,68,73	1.35	5 (8%)	68,107,113	1.27	8 (11%)
25	SQD	1	619	-	36,38,54	0.27	0	46,49,65	0.52	1 (2%)
20	CLA	A	5016	6	63,73,73	1.34	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	B	820	-	63,73,73	1.38	8 (12%)	74,113,113	1.39	6 (8%)
20	CLA	A	5005	-	63,73,73	1.34	6 (9%)	74,113,113	1.27	5 (6%)
19	CHL	8	305	-	45,55,74	1.50	4 (8%)	48,91,114	2.43	6 (12%)
20	CLA	G	201	7	63,73,73	1.35	5 (7%)	74,113,113	1.21	6 (8%)
20	CLA	2	303	18	48,58,73	1.59	7 (14%)	56,95,113	1.51	10 (17%)
20	CLA	J	104	15	47,57,73	1.55	5 (10%)	53,93,113	1.45	6 (11%)
20	CLA	9	611	-	53,63,73	1.48	6 (11%)	62,101,113	1.45	7 (11%)
24	LHG	7	320	20	33,33,48	0.34	0	36,39,54	0.33	0
20	CLA	2	305	-	43,53,73	1.64	5 (11%)	50,89,113	1.45	6 (12%)
32	SF4	A	5046	7,6	0,12,12	-	-	-	-	-
20	CLA	7	312	3	50,60,73	1.52	7 (14%)	57,97,113	1.52	8 (14%)
20	CLA	A	5041	6	63,73,73	1.32	6 (9%)	74,113,113	1.29	8 (10%)
20	CLA	A	5038	6	48,58,73	1.52	6 (12%)	56,95,113	1.53	7 (12%)
23	BCR	B	845	-	40,40,41	0.17	0	54,54,56	0.48	1 (1%)
20	CLA	B	839	7	63,73,73	1.33	6 (9%)	74,113,113	1.21	8 (10%)
20	CLA	B	805	-	63,73,73	1.33	7 (11%)	74,113,113	1.40	9 (12%)
23	BCR	7	318	-	41,41,41	0.14	0	56,56,56	0.38	0
23	BCR	B	844	-	41,41,41	0.34	0	56,56,56	1.11	6 (10%)
20	CLA	K	4003	-	53,63,73	1.48	5 (9%)	62,101,113	1.31	7 (11%)
20	CLA	L	205	-	48,58,73	1.50	5 (10%)	56,95,113	1.43	8 (14%)
21	LUT	9	613	-	42,43,43	0.26	0	51,60,60	0.30	0
26	PTY	7	302	-	14,14,49	1.11	2 (14%)	15,18,54	1.70	2 (13%)
20	CLA	7	305	-	48,58,73	1.57	6 (12%)	56,95,113	1.45	7 (12%)
23	BCR	F	309	-	41,41,41	0.17	0	56,56,56	0.40	0
20	CLA	B	816	-	53,63,73	1.45	5 (9%)	62,101,113	1.43	8 (12%)
20	CLA	B	828	-	63,73,73	1.39	7 (11%)	74,113,113	1.31	6 (8%)
29	LMU	7	325	-	33,33,36	0.13	0	44,44,47	0.15	0
20	CLA	B	834	-	48,58,73	1.52	5 (10%)	56,95,113	1.47	9 (16%)
24	LHG	A	5054	20	27,27,48	0.42	0	30,33,54	0.49	0
20	CLA	9	601	5	44,54,73	1.58	5 (11%)	51,90,113	1.36	7 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	B	803	-	41,41,41	0.26	0	56,56,56	0.63	1 (1%)
22	XAT	1	616	-	41,47,47	0.14	0	54,74,74	0.84	2 (3%)
22	XAT	9	615	-	41,47,47	0.18	0	54,74,74	0.79	3 (5%)
20	CLA	A	5036	6	62,72,73	1.33	5 (8%)	72,111,113	1.33	6 (8%)
21	LUT	7	316	-	42,43,43	0.35	0	51,60,60	0.53	1 (1%)
20	CLA	B	838	-	53,63,73	1.52	7 (13%)	62,101,113	1.43	7 (11%)
25	SQD	F	311	-	37,39,54	0.26	0	47,50,65	0.49	1 (2%)
20	CLA	8	302	4	63,73,73	1.38	6 (9%)	74,113,113	1.35	7 (9%)
20	CLA	1	611	1	44,54,73	1.63	6 (13%)	51,90,113	1.58	9 (17%)
27	LMG	A	5001	-	32,32,55	0.20	0	40,40,63	0.31	0
20	CLA	3	312	2	44,54,73	1.59	5 (11%)	51,90,113	1.37	6 (11%)
20	CLA	9	604	5	48,58,73	1.54	5 (10%)	56,95,113	1.33	7 (12%)
20	CLA	1	610	24	44,54,73	1.57	5 (11%)	51,90,113	1.38	6 (11%)
29	LMU	A	5053	-	36,36,36	0.13	0	47,47,47	0.15	0
20	CLA	9	603	-	53,63,73	1.51	6 (11%)	62,101,113	1.49	7 (11%)
20	CLA	1	613	1	48,58,73	1.56	6 (12%)	56,95,113	1.52	7 (12%)
20	CLA	B	817	-	58,68,73	1.42	7 (12%)	68,107,113	1.36	6 (8%)
20	CLA	1	609	1	53,63,73	1.45	6 (11%)	62,101,113	1.32	6 (9%)
21	LUT	8	314	-	42,43,43	0.27	0	51,60,60	0.42	0
20	CLA	A	5043	24	47,57,73	1.52	5 (10%)	54,93,113	1.44	7 (12%)
24	LHG	B	801	-	31,31,48	0.36	0	34,37,54	0.33	0
23	BCR	A	5048	-	41,41,41	0.17	0	56,56,56	0.24	0
20	CLA	9	608	5	48,58,73	1.52	6 (12%)	56,95,113	1.35	7 (12%)
20	CLA	A	5012	6	63,73,73	1.34	6 (9%)	74,113,113	1.17	7 (9%)
24	LHG	8	317	20	28,28,48	0.38	0	31,34,54	0.34	0
19	CHL	7	308	-	46,56,74	1.51	4 (8%)	49,92,114	1.96	8 (16%)
20	CLA	A	5029	6	63,73,73	1.31	6 (9%)	74,113,113	1.28	8 (10%)
20	CLA	A	5006	6	63,73,73	1.32	6 (9%)	74,113,113	1.32	8 (10%)
19	CHL	8	304	4	45,55,74	2.22	4 (8%)	48,91,114	2.67	10 (20%)
23	BCR	G	205	-	41,41,41	0.21	0	56,56,56	0.49	0
23	BCR	B	843	-	41,41,41	0.22	0	56,56,56	0.40	0
20	CLA	B	814	7	63,73,73	1.37	6 (9%)	74,113,113	1.31	7 (9%)
20	CLA	K	4004	16	43,53,73	1.67	7 (16%)	50,89,113	1.56	6 (12%)
22	XAT	7	317	-	41,47,47	0.17	0	54,74,74	0.86	3 (5%)
20	CLA	A	5013	6,20	63,73,73	1.33	5 (7%)	74,113,113	1.25	7 (9%)
23	BCR	1	617	-	41,41,41	0.18	0	56,56,56	0.26	0
25	SQD	B	850	-	29,31,54	0.21	0	39,42,65	0.25	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	826	7	63,73,73	1.39	7 (11%)	74,113,113	1.37	8 (10%)
20	CLA	3	302	2	63,73,73	1.35	6 (9%)	74,113,113	1.32	7 (9%)
24	LHG	A	5002	-	35,35,48	0.36	0	38,41,54	0.40	0
20	CLA	3	308	2	53,63,73	1.44	5 (9%)	62,101,113	1.27	7 (11%)
20	CLA	A	5009	6	63,73,73	1.35	6 (9%)	74,113,113	1.38	8 (10%)
24	LHG	B	849	-	29,29,48	0.40	0	32,35,54	0.42	0
20	CLA	A	5011	6	63,73,73	1.32	5 (7%)	74,113,113	1.24	6 (8%)
20	CLA	A	5031	6	63,73,73	1.38	5 (7%)	74,113,113	1.29	7 (9%)
23	BCR	3	317	-	41,41,41	0.16	0	56,56,56	0.32	0
20	CLA	G	202	12	45,55,73	1.60	6 (13%)	52,91,113	1.58	7 (13%)
27	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
20	CLA	3	313	-	40,50,73	1.68	6 (15%)	45,85,113	1.40	6 (13%)
20	CLA	3	304	-	44,54,73	1.57	6 (13%)	51,90,113	1.43	6 (11%)
33	LMK	J	101	-	34,34,53	0.42	0	34,41,60	0.52	1 (2%)
23	BCR	8	316	-	41,41,41	0.16	0	56,56,56	0.40	0
32	SF4	C	101	8	0,12,12	-	-	-	-	-
20	CLA	A	5030	-	63,73,73	1.35	6 (9%)	74,113,113	1.37	8 (10%)
20	CLA	2	307	18	44,54,73	1.61	5 (11%)	51,90,113	1.36	6 (11%)
20	CLA	7	315	3	43,53,73	1.61	5 (11%)	50,89,113	1.52	6 (12%)
20	CLA	2	310	18	44,54,73	1.64	6 (13%)	51,90,113	1.60	8 (15%)
20	CLA	9	609	24	44,54,73	1.58	5 (11%)	51,90,113	1.42	6 (11%)
20	CLA	7	311	24	58,68,73	1.42	7 (12%)	68,107,113	1.33	8 (11%)
20	CLA	3	306	-	49,59,73	1.50	5 (10%)	56,96,113	1.41	8 (14%)
20	CLA	9	607	5	58,68,73	1.33	6 (10%)	68,107,113	1.25	6 (8%)
20	CLA	A	5004	-	63,73,73	1.34	6 (9%)	74,113,113	1.26	7 (9%)
23	BCR	B	842	-	41,41,41	0.19	0	56,56,56	0.33	0
20	CLA	B	835	7	49,59,73	1.52	5 (10%)	56,96,113	1.61	6 (10%)
20	CLA	A	5024	6	58,68,73	1.39	5 (8%)	68,107,113	1.22	7 (10%)
20	CLA	A	5037	6	48,58,73	1.54	5 (10%)	56,95,113	1.41	9 (16%)
20	CLA	B	807	-	63,73,73	1.32	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	A	5022	-	63,73,73	1.32	6 (9%)	74,113,113	1.30	6 (8%)
20	CLA	2	311	-	48,58,73	1.56	4 (8%)	56,95,113	1.52	8 (14%)
20	CLA	B	808	7	63,73,73	1.97	6 (9%)	74,113,113	1.22	10 (13%)
20	CLA	B	804	7	63,73,73	1.37	7 (11%)	74,113,113	1.14	6 (8%)
20	CLA	1	608	1	44,54,73	1.57	5 (11%)	51,90,113	1.47	7 (13%)
19	CHL	9	606	-	45,55,74	1.50	4 (8%)	48,91,114	2.07	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	5044	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	8 (10%)
20	CLA	B	806	7	46,56,73	1.52	5 (10%)	53,92,113	1.48	8 (15%)
20	CLA	A	5015	-	53,63,73	1.44	5 (9%)	62,101,113	1.45	7 (11%)
20	CLA	3	307	2	63,73,73	1.35	5 (7%)	74,113,113	1.26	8 (10%)
20	CLA	A	5026	-	63,73,73	1.37	6 (9%)	74,113,113	1.44	6 (8%)
20	CLA	B	822	7	63,73,73	1.33	5 (7%)	74,113,113	1.32	7 (9%)
20	CLA	F	308	11	43,53,73	1.62	5 (11%)	50,89,113	1.49	6 (12%)
20	CLA	B	831	7	58,68,73	1.39	6 (10%)	68,107,113	1.33	7 (10%)
21	LUT	3	315	-	42,43,43	0.31	0	51,60,60	0.38	0
23	BCR	I	4001	-	41,41,41	0.17	0	56,56,56	0.29	0

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
20	CLA	B	819	7	1/1/15/20	11/37/115/115	-
20	CLA	3	305	2	1/1/12/20	5/19/97/115	-
20	CLA	A	5035	6	1/1/15/20	15/37/115/115	-
32	SF4	C	102	8	-	-	0/6/5/5
29	LMU	8	322	-	-	6/21/61/61	0/2/2/2
20	CLA	3	309	2	1/1/11/20	8/15/93/115	-
31	PQN	B	841	-	-	5/23/43/43	0/2/2/2
21	LUT	1	615	-	3/3/12/27	8/29/67/67	0/2/2/2
20	CLA	B	837	7	-	1/25/103/115	-
31	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
22	XAT	8	315	-	-	1/31/93/93	0/4/4/4
23	BCR	L	203	-	-	4/29/63/63	0/2/2/2
20	CLA	B	810	7	1/1/15/20	11/37/115/115	-
20	CLA	9	612	5	1/1/11/20	6/15/93/115	-
20	CLA	A	5040	-	1/1/14/20	7/31/109/115	-
27	LMG	7	324	-	-	10/25/45/70	0/1/1/1
20	CLA	B	829	7	1/1/15/20	16/37/115/115	-
20	CLA	K	4005	-	1/1/11/20	9/17/95/115	-
20	CLA	K	4002	-	1/1/11/20	6/13/91/115	-
20	CLA	F	303	7	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5017	-	1/1/13/20	11/25/103/115	-
20	CLA	8	308	4	1/1/14/20	11/31/109/115	-
25	SQD	3	322	-	-	14/36/56/69	0/1/1/1
20	CLA	1	614	1	1/1/11/20	8/15/93/115	-
20	CLA	2	312	18	1/1/11/20	5/13/91/115	-
20	CLA	A	5014	-	-	11/37/115/115	-
20	CLA	7	314	3	1/1/12/20	5/19/97/115	-
20	CLA	9	605	5	1/1/11/20	4/13/91/115	-
23	BCR	A	5049	-	-	4/29/63/63	0/2/2/2
23	BCR	3	319	-	-	23/29/63/63	0/2/2/2
27	LMG	G	206	-	-	6/37/57/70	0/1/1/1
23	BCR	L	206	-	-	6/29/63/63	0/2/2/2
20	CLA	1	607	-	1/1/12/20	7/19/97/115	-
20	CLA	3	325	6	1/1/13/20	4/25/103/115	-
19	CHL	1	601	-	1/1/16/26	6/17/115/137	-
26	PTY	3	321	-	-	24/53/53/53	-
23	BCR	K	4006	-	-	4/29/63/63	0/2/2/2
23	BCR	A	5051	-	-	4/29/63/63	0/2/2/2
23	BCR	J	106	-	-	2/29/63/63	0/2/2/2
27	LMG	J	103	-	-	3/24/44/70	0/1/1/1
20	CLA	7	303	3	1/1/14/20	11/31/109/115	-
20	CLA	3	311	-	1/1/13/20	8/25/103/115	-
28	DGD	7	321	-	-	8/28/68/95	0/2/2/2
20	CLA	8	307	4	1/1/11/20	6/16/94/115	-
19	CHL	1	606	-	1/1/16/26	10/17/115/137	-
20	CLA	2	313	-	1/1/12/20	5/19/97/115	-
20	CLA	1	603	1	1/1/13/20	11/25/103/115	-
20	CLA	B	833	7	1/1/14/20	10/31/109/115	-
24	LHG	9	617	20	-	15/40/40/53	-
20	CLA	B	815	-	1/1/15/20	10/37/115/115	-
23	BCR	J	105	-	-	4/29/63/63	0/2/2/2
24	LHG	A	5052	-	-	12/53/53/53	-
20	CLA	B	821	-	1/1/13/20	8/25/103/115	-
20	CLA	B	840	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	310	2	1/1/11/20	5/15/93/115	-
20	CLA	2	309	-	1/1/11/20	2/13/91/115	-
22	XAT	9	614	-	-	0/31/93/93	0/4/4/4
20	CLA	A	5025	6	1/1/14/20	11/31/109/115	-
24	LHG	7	319	-	-	7/25/25/53	-
26	PTY	B	802	-	-	12/30/30/53	-
26	PTY	F	302	-	-	16/35/35/53	-
20	CLA	H	201	18	1/1/14/20	17/31/109/115	-
20	CLA	L	204	17	1/1/15/20	10/37/115/115	-
29	LMU	8	318	-	-	2/19/59/61	0/2/2/2
20	CLA	1	604	-	1/1/12/20	5/19/97/115	-
19	CHL	2	306	-	2/2/16/26	7/17/115/137	-
20	CLA	8	310	4	1/1/11/20	7/15/93/115	-
20	CLA	8	301	4	1/1/14/20	9/31/109/115	-
24	LHG	2	316	-	-	4/26/26/53	-
20	CLA	A	5021	6	1/1/12/20	6/19/97/115	-
20	CLA	B	825	-	1/1/15/20	9/37/115/115	-
20	CLA	7	323	4	1/1/11/20	8/16/94/115	-
23	BCR	B	847	-	-	5/29/63/63	0/2/2/2
20	CLA	A	5034	6	1/1/15/20	2/37/115/115	-
20	CLA	1	612	-	1/1/14/20	11/31/109/115	-
20	CLA	8	313	4	1/1/11/20	5/15/93/115	-
21	LUT	2	315	-	3/3/12/27	12/29/67/67	0/2/2/2
20	CLA	G	204	-	1/1/11/20	5/13/91/115	-
20	CLA	B	832	7	1/1/15/20	12/37/115/115	-
20	CLA	3	303	-	1/1/11/20	4/15/93/115	-
20	CLA	A	5019	6	1/1/13/20	9/25/103/115	-
20	CLA	7	309	3	1/1/11/20	4/15/93/115	-
20	CLA	B	818	7	1/1/15/20	15/37/115/115	-
20	CLA	A	5033	6	1/1/13/20	1/25/103/115	-
23	BCR	B	846	-	-	0/29/63/63	0/2/2/2
20	CLA	B	823	7	1/1/13/20	10/25/103/115	-
29	LMU	9	616	-	-	5/15/55/61	0/2/2/2
20	CLA	2	301	-	1/1/11/20	4/15/93/115	-
20	CLA	8	303	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5007	6,20	1/1/15/20	8/37/115/115	-
20	CLA	3	314	2	1/1/11/20	5/15/93/115	-
20	CLA	7	313	3	1/1/15/20	11/37/115/115	-
20	CLA	B	812	7	1/1/13/20	4/25/103/115	-
20	CLA	B	813	7	1/1/11/20	2/15/93/115	-
21	LUT	2	314	-	3/3/12/27	4/29/67/67	0/2/2/2
20	CLA	A	5042	6	1/1/14/20	6/31/109/115	-
20	CLA	1	605	-	1/1/11/20	4/13/91/115	-
29	LMU	F	305	-	-	7/18/58/61	0/2/2/2
19	CHL	3	301	2	2/2/19/26	20/35/133/137	-
19	CHL	7	307	-	2/2/16/26	5/17/115/137	-
20	CLA	A	5008	6	1/1/15/20	11/37/115/115	-
20	CLA	9	610	5	1/1/12/20	10/19/97/115	-
20	CLA	3	324	6	1/1/13/20	10/25/103/115	-
20	CLA	F	307	-	1/1/11/20	5/16/94/115	-
23	BCR	3	318	-	-	3/29/63/63	0/2/2/2
23	BCR	A	5047	-	-	5/29/63/63	0/2/2/2
24	LHG	I	4002	-	-	6/32/32/53	-
25	SQD	7	322	-	-	4/34/54/69	0/1/1/1
20	CLA	B	811	7	1/1/15/20	7/37/115/115	-
20	CLA	A	5028	6	1/1/15/20	15/37/115/115	-
20	CLA	L	202	-	1/1/15/20	14/37/115/115	-
28	DGD	B	848	-	-	12/50/90/95	0/2/2/2
20	CLA	L	201	7	1/1/15/20	13/37/115/115	-
20	CLA	B	809	7	1/1/15/20	14/37/115/115	-
22	XAT	3	316	-	-	3/31/93/93	0/4/4/4
20	CLA	8	311	4	1/1/15/20	17/37/115/115	-
20	CLA	G	203	12	1/1/11/20	6/15/93/115	-
24	LHG	A	5055	-	-	4/35/35/53	-
20	CLA	F	306	-	1/1/14/20	10/31/109/115	-
19	CHL	2	302	18	2/2/19/26	16/33/131/137	-
20	CLA	A	5032	6	1/1/12/20	2/19/97/115	-
20	CLA	B	836	7	1/1/14/20	4/31/109/115	-
23	BCR	A	5050	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	8	319	-	-	8/42/42/53	-
20	CLA	7	304	3	1/1/13/20	2/25/103/115	-
23	BCR	J	102	-	-	8/29/63/63	0/2/2/2
19	CHL	8	306	-	2/2/17/26	8/21/119/137	-
26	PTY	F	310	-	-	13/34/34/53	-
20	CLA	7	310	3	1/1/15/20	14/37/115/115	-
20	CLA	B	824	-	1/1/15/20	10/37/115/115	-
30	CL0	A	5003	6	1/1/20/25	21/37/135/135	-
24	LHG	1	620	-	-	13/50/50/53	-
20	CLA	A	5010	-	1/1/12/20	2/21/99/115	-
20	CLA	2	308	-	1/1/11/20	3/13/91/115	-
19	CHL	3	323	-	3/3/19/26	16/33/131/137	-
19	CHL	7	306	-	1/1/16/26	2/15/113/137	-
20	CLA	A	5018	6	1/1/14/20	9/31/109/115	-
20	CLA	A	5023	6	1/1/12/20	5/19/97/115	-
23	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
26	PTY	F	301	-	-	14/32/32/53	-
20	CLA	A	5020	6	1/1/15/20	13/37/115/115	-
20	CLA	8	309	24	1/1/14/20	10/31/109/115	-
20	CLA	A	5027	-	1/1/13/20	8/27/105/115	-
20	CLA	A	5039	6	1/1/13/20	3/25/103/115	-
20	CLA	2	304	-	1/1/12/20	8/19/97/115	-
20	CLA	B	830	7	1/1/15/20	14/37/115/115	-
20	CLA	1	602	1	1/1/13/20	11/25/103/115	-
24	LHG	1	618	20	-	5/30/30/53	-
24	LHG	8	320	-	-	6/47/47/53	-
25	SQD	3	320	-	-	4/30/50/69	0/1/1/1
20	CLA	8	312	4	1/1/11/20	7/15/93/115	-
20	CLA	B	827	-	1/1/15/20	10/37/115/115	-
20	CLA	8	321	-	-	9/15/93/115	-
23	BCR	F	304	-	-	0/29/63/63	0/2/2/2
20	CLA	9	602	5	1/1/14/20	10/31/109/115	-
25	SQD	1	619	-	-	14/33/53/69	0/1/1/1
20	CLA	A	5016	6	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	820	-	1/1/15/20	11/37/115/115	-
20	CLA	A	5005	-	1/1/15/20	6/37/115/115	-
19	CHL	8	305	-	1/1/16/26	4/17/115/137	-
20	CLA	G	201	7	1/1/15/20	13/37/115/115	-
20	CLA	2	303	18	1/1/12/20	4/19/97/115	-
20	CLA	J	104	15	1/1/11/20	4/18/96/115	-
20	CLA	9	611	-	1/1/13/20	5/25/103/115	-
24	LHG	7	320	20	-	9/38/38/53	-
20	CLA	2	305	-	1/1/11/20	6/13/91/115	-
32	SF4	A	5046	7,6	-	-	0/6/5/5
20	CLA	7	312	3	1/1/12/20	5/22/100/115	-
20	CLA	A	5041	6	1/1/15/20	6/37/115/115	-
20	CLA	A	5038	6	1/1/12/20	5/19/97/115	-
23	BCR	B	845	-	-	2/27/61/63	0/2/2/2
20	CLA	B	839	7	1/1/15/20	8/37/115/115	-
20	CLA	B	805	-	1/1/15/20	14/37/115/115	-
23	BCR	7	318	-	-	2/29/63/63	0/2/2/2
23	BCR	B	844	-	-	10/29/63/63	0/2/2/2
20	CLA	K	4003	-	1/1/13/20	11/25/103/115	-
20	CLA	L	205	-	1/1/12/20	6/19/97/115	-
21	LUT	9	613	-	3/3/12/27	2/29/67/67	0/2/2/2
26	PTY	7	302	-	-	8/14/14/53	-
20	CLA	7	305	-	1/1/12/20	4/19/97/115	-
23	BCR	F	309	-	-	4/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	9/25/103/115	-
20	CLA	B	828	-	1/1/15/20	16/37/115/115	-
29	LMU	7	325	-	-	4/18/58/61	0/2/2/2
20	CLA	B	834	-	1/1/12/20	11/19/97/115	-
24	LHG	A	5054	20	-	9/32/32/53	-
20	CLA	9	601	5	1/1/11/20	9/15/93/115	-
23	BCR	B	803	-	-	3/29/63/63	0/2/2/2
22	XAT	1	616	-	-	2/31/93/93	0/4/4/4
22	XAT	9	615	-	-	5/31/93/93	0/4/4/4
20	CLA	A	5036	6	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LUT	7	316	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	B	838	-	1/1/13/20	5/25/103/115	-
25	SQD	F	311	-	-	6/34/54/69	0/1/1/1
20	CLA	8	302	4	1/1/15/20	11/37/115/115	-
20	CLA	1	611	1	1/1/11/20	6/15/93/115	-
27	LMG	A	5001	-	-	6/26/46/70	0/1/1/1
20	CLA	3	312	2	1/1/11/20	7/15/93/115	-
20	CLA	9	604	5	1/1/12/20	4/19/97/115	-
20	CLA	1	610	24	1/1/11/20	7/15/93/115	-
29	LMU	A	5053	-	-	3/21/61/61	0/2/2/2
20	CLA	9	603	-	1/1/13/20	10/25/103/115	-
20	CLA	1	613	1	1/1/12/20	6/19/97/115	-
20	CLA	B	817	-	1/1/14/20	7/31/109/115	-
20	CLA	1	609	1	1/1/13/20	6/25/103/115	-
21	LUT	8	314	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	A	5043	24	1/1/11/20	5/17/95/115	-
24	LHG	B	801	-	-	8/36/36/53	-
23	BCR	A	5048	-	-	0/29/63/63	0/2/2/2
20	CLA	9	608	5	1/1/12/20	6/19/97/115	-
20	CLA	A	5012	6	1/1/15/20	10/37/115/115	-
24	LHG	8	317	20	-	5/33/33/53	-
19	CHL	7	308	-	2/2/16/26	6/18/116/137	-
20	CLA	A	5029	6	1/1/15/20	16/37/115/115	-
20	CLA	A	5006	6	1/1/15/20	14/37/115/115	-
19	CHL	8	304	4	1/1/16/26	7/17/115/137	-
23	BCR	G	205	-	-	6/29/63/63	0/2/2/2
23	BCR	B	843	-	-	0/29/63/63	0/2/2/2
20	CLA	B	814	7	1/1/15/20	15/37/115/115	-
20	CLA	K	4004	16	1/1/11/20	6/13/91/115	-
22	XAT	7	317	-	-	3/31/93/93	0/4/4/4
20	CLA	A	5013	6,20	1/1/15/20	11/37/115/115	-
23	BCR	1	617	-	-	0/29/63/63	0/2/2/2
25	SQD	B	850	-	-	10/25/45/69	0/1/1/1
20	CLA	B	826	7	1/1/15/20	9/37/115/115	-
20	CLA	3	302	2	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	A	5002	-	-	10/40/40/53	-
20	CLA	3	308	2	1/1/13/20	8/25/103/115	-
20	CLA	A	5009	6	1/1/15/20	14/37/115/115	-
24	LHG	B	849	-	-	8/34/34/53	-
20	CLA	A	5011	6	1/1/15/20	11/37/115/115	-
20	CLA	A	5031	6	1/1/15/20	7/37/115/115	-
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
20	CLA	G	202	12	1/1/11/20	5/16/94/115	-
27	LMG	7	301	-	-	10/45/65/70	0/1/1/1
20	CLA	3	313	-	1/1/10/20	0/10/88/115	-
20	CLA	3	304	-	1/1/11/20	6/15/93/115	-
33	LMK	J	101	-	-	5/41/41/60	-
23	BCR	8	316	-	-	2/29/63/63	0/2/2/2
32	SF4	C	101	8	-	-	0/6/5/5
20	CLA	A	5030	-	1/1/15/20	12/37/115/115	-
20	CLA	2	307	18	1/1/11/20	9/15/93/115	-
20	CLA	7	315	3	1/1/11/20	4/13/91/115	-
20	CLA	2	310	18	1/1/11/20	8/15/93/115	-
20	CLA	9	609	24	1/1/11/20	8/15/93/115	-
20	CLA	7	311	24	1/1/14/20	8/31/109/115	-
20	CLA	3	306	-	1/1/12/20	6/21/99/115	-
20	CLA	9	607	5	1/1/14/20	13/31/109/115	-
20	CLA	A	5004	-	1/1/15/20	13/37/115/115	-
23	BCR	B	842	-	-	2/29/63/63	0/2/2/2
20	CLA	B	835	7	1/1/12/20	5/21/99/115	-
20	CLA	A	5024	6	1/1/14/20	14/31/109/115	-
20	CLA	A	5037	6	1/1/12/20	7/19/97/115	-
20	CLA	B	807	-	1/1/15/20	12/37/115/115	-
20	CLA	A	5022	-	1/1/15/20	6/37/115/115	-
20	CLA	2	311	-	1/1/12/20	8/19/97/115	-
20	CLA	B	808	7	1/1/15/20	11/37/115/115	-
20	CLA	B	804	7	1/1/15/20	17/37/115/115	-
20	CLA	1	608	1	1/1/11/20	6/15/93/115	-
19	CHL	9	606	-	2/2/16/26	11/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5044	-	1/1/15/20	10/37/115/115	-
20	CLA	B	806	7	1/1/11/20	9/17/95/115	-
20	CLA	A	5015	-	1/1/13/20	8/25/103/115	-
20	CLA	3	307	2	1/1/15/20	13/37/115/115	-
20	CLA	A	5026	-	1/1/15/20	10/37/115/115	-
20	CLA	B	822	7	1/1/15/20	13/37/115/115	-
20	CLA	F	308	11	1/1/11/20	3/13/91/115	-
20	CLA	B	831	7	1/1/14/20	8/31/109/115	-
21	LUT	3	315	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	I	4001	-	-	4/29/63/63	0/2/2/2

All (1012) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	MG-NA	11.87	2.34	2.06
19	8	304	CHL	MG-NC	11.84	2.34	2.06
19	1	606	CHL	MG-NA	8.23	2.25	2.06
20	G	204	CLA	CHB-C4A	7.79	1.40	1.33
19	8	306	CHL	MG-NA	7.43	2.23	2.06
19	8	304	CHL	MG-NA	7.10	2.23	2.06
19	1	601	CHL	MG-NA	6.96	2.22	2.06
20	A	5031	CLA	CHB-C4A	6.79	1.39	1.33
20	B	829	CLA	CHB-C4A	6.74	1.39	1.33
20	K	4002	CLA	CHB-C4A	6.66	1.39	1.33
20	B	805	CLA	CHB-C4A	6.53	1.39	1.33
20	K	4005	CLA	CHB-C4A	6.50	1.39	1.33
19	8	306	CHL	MG-NC	6.42	2.21	2.06
20	A	5026	CLA	CHB-C4A	6.31	1.38	1.33
20	8	321	CLA	CHB-C4A	6.31	1.38	1.33
19	3	301	CHL	MG-NC	6.29	2.21	2.06
20	8	303	CLA	CHB-C4A	6.28	1.38	1.33
20	A	5017	CLA	CHB-C4A	6.26	1.38	1.33
20	G	203	CLA	CHB-C4A	6.26	1.38	1.33
19	9	606	CHL	MG-NA	6.26	2.21	2.06
20	9	605	CLA	CHB-C4A	6.25	1.38	1.33
20	B	812	CLA	CHB-C4A	6.25	1.38	1.33
20	2	305	CLA	CHB-C4A	6.24	1.38	1.33
20	K	4003	CLA	CHB-C4A	6.22	1.38	1.33
20	2	307	CLA	CHB-C4A	6.22	1.38	1.33
19	7	308	CHL	MG-NC	6.22	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	305	CHL	MG-NA	6.22	2.21	2.06
20	A	5036	CLA	CHB-C4A	6.22	1.38	1.33
20	B	823	CLA	CHB-C4A	6.22	1.38	1.33
20	2	313	CLA	CHB-C4A	6.22	1.38	1.33
20	3	313	CLA	CHB-C4A	6.21	1.38	1.33
20	2	310	CLA	CHB-C4A	6.20	1.38	1.33
20	1	605	CLA	CHB-C4A	6.19	1.38	1.33
20	B	830	CLA	CHB-C4A	6.19	1.38	1.33
20	A	5008	CLA	CHB-C4A	6.19	1.38	1.33
20	3	324	CLA	CHB-C4A	6.19	1.38	1.33
20	2	311	CLA	CHB-C4A	6.19	1.38	1.33
20	9	611	CLA	CHB-C4A	6.19	1.38	1.33
20	B	833	CLA	CHB-C4A	6.19	1.38	1.33
20	A	5037	CLA	CHB-C4A	6.19	1.38	1.33
20	8	302	CLA	CHB-C4A	6.19	1.38	1.33
20	9	601	CLA	CHB-C4A	6.19	1.38	1.33
20	2	309	CLA	CHB-C4A	6.18	1.38	1.33
20	J	104	CLA	CHB-C4A	6.18	1.38	1.33
20	2	303	CLA	CHB-C4A	6.18	1.38	1.33
20	7	305	CLA	CHB-C4A	6.18	1.38	1.33
20	1	607	CLA	CHB-C4A	6.16	1.38	1.33
20	B	820	CLA	CHB-C4A	6.16	1.38	1.33
20	B	807	CLA	CHB-C4A	6.16	1.38	1.33
20	1	612	CLA	CHB-C4A	6.16	1.38	1.33
20	3	309	CLA	CHB-C4A	6.15	1.38	1.33
20	9	609	CLA	CHB-C4A	6.15	1.38	1.33
20	B	827	CLA	CHB-C4A	6.15	1.38	1.33
20	2	312	CLA	CHB-C4A	6.15	1.38	1.33
20	A	5016	CLA	CHB-C4A	6.15	1.38	1.33
20	3	314	CLA	CHB-C4A	6.15	1.38	1.33
19	7	306	CHL	MG-NA	6.14	2.20	2.06
20	8	310	CLA	CHB-C4A	6.14	1.38	1.33
20	3	307	CLA	CHB-C4A	6.14	1.38	1.33
20	B	832	CLA	CHB-C4A	6.14	1.38	1.33
19	3	323	CHL	MG-NA	6.13	2.20	2.06
20	9	610	CLA	CHB-C4A	6.13	1.38	1.33
20	7	313	CLA	CHB-C4A	6.13	1.38	1.33
20	1	611	CLA	CHB-C4A	6.13	1.38	1.33
20	7	309	CLA	CHB-C4A	6.13	1.38	1.33
20	1	608	CLA	CHB-C4A	6.12	1.38	1.33
20	3	310	CLA	CHB-C4A	6.12	1.38	1.33
20	1	602	CLA	CHB-C4A	6.12	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	9	604	CLA	CHB-C4A	6.12	1.38	1.33
20	B	826	CLA	CHB-C4A	6.12	1.38	1.33
20	7	311	CLA	CHB-C4A	6.12	1.38	1.33
20	8	301	CLA	CHB-C4A	6.11	1.38	1.33
20	F	307	CLA	CHB-C4A	6.11	1.38	1.33
20	A	5034	CLA	CHB-C4A	6.11	1.38	1.33
20	A	5018	CLA	CHB-C4A	6.10	1.38	1.33
20	9	603	CLA	CHB-C4A	6.10	1.38	1.33
20	A	5035	CLA	CHB-C4A	6.10	1.38	1.33
20	7	323	CLA	CHB-C4A	6.10	1.38	1.33
20	7	312	CLA	CHB-C4A	6.09	1.38	1.33
20	9	612	CLA	CHB-C4A	6.09	1.38	1.33
20	3	312	CLA	CHB-C4A	6.09	1.38	1.33
19	7	308	CHL	MG-NA	6.09	2.20	2.06
20	F	308	CLA	CHB-C4A	6.08	1.38	1.33
20	3	311	CLA	CHB-C4A	6.08	1.38	1.33
20	1	610	CLA	CHB-C4A	6.08	1.38	1.33
20	B	809	CLA	CHB-C4A	6.08	1.38	1.33
20	F	303	CLA	CHB-C4A	6.08	1.38	1.33
20	A	5042	CLA	CHB-C4A	6.07	1.38	1.33
20	A	5025	CLA	CHB-C4A	6.07	1.38	1.33
20	B	822	CLA	CHB-C4A	6.06	1.38	1.33
20	H	201	CLA	CHB-C4A	6.06	1.38	1.33
20	L	201	CLA	CHB-C4A	6.06	1.38	1.33
20	B	828	CLA	CHB-C4A	6.06	1.38	1.33
20	2	308	CLA	CHB-C4A	6.05	1.38	1.33
20	7	303	CLA	CHB-C4A	6.05	1.38	1.33
20	3	325	CLA	CHB-C4A	6.05	1.38	1.33
20	G	202	CLA	CHB-C4A	6.05	1.38	1.33
20	A	5010	CLA	CHB-C4A	6.04	1.38	1.33
20	8	313	CLA	CHB-C4A	6.04	1.38	1.33
20	B	821	CLA	CHB-C4A	6.04	1.38	1.33
20	A	5009	CLA	CHB-C4A	6.03	1.38	1.33
20	A	5032	CLA	CHB-C4A	6.03	1.38	1.33
20	B	817	CLA	CHB-C4A	6.03	1.38	1.33
20	8	311	CLA	CHB-C4A	6.03	1.38	1.33
20	B	811	CLA	CHB-C4A	6.03	1.38	1.33
20	2	301	CLA	CHB-C4A	6.03	1.38	1.33
20	7	314	CLA	CHB-C4A	6.02	1.38	1.33
20	1	609	CLA	CHB-C4A	6.01	1.38	1.33
20	9	608	CLA	CHB-C4A	6.01	1.38	1.33
20	7	304	CLA	CHB-C4A	6.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5043	CLA	CHB-C4A	6.01	1.38	1.33
20	A	5006	CLA	CHB-C4A	6.00	1.38	1.33
20	A	5021	CLA	CHB-C4A	6.00	1.38	1.33
20	A	5004	CLA	CHB-C4A	6.00	1.38	1.33
20	A	5030	CLA	CHB-C4A	5.99	1.38	1.33
20	B	835	CLA	CHB-C4A	5.99	1.38	1.33
20	L	204	CLA	CHB-C4A	5.99	1.38	1.33
20	B	819	CLA	CHB-C4A	5.98	1.38	1.33
20	A	5040	CLA	CHB-C4A	5.98	1.38	1.33
20	B	818	CLA	CHB-C4A	5.98	1.38	1.33
20	A	5027	CLA	CHB-C4A	5.98	1.38	1.33
20	8	309	CLA	CHB-C4A	5.97	1.38	1.33
20	A	5024	CLA	CHB-C4A	5.97	1.38	1.33
20	8	312	CLA	CHB-C4A	5.96	1.38	1.33
20	A	5041	CLA	CHB-C4A	5.96	1.38	1.33
20	3	304	CLA	CHB-C4A	5.95	1.38	1.33
20	1	603	CLA	CHB-C4A	5.95	1.38	1.33
20	3	303	CLA	CHB-C4A	5.95	1.38	1.33
20	F	306	CLA	CHB-C4A	5.95	1.38	1.33
20	A	5019	CLA	CHB-C4A	5.95	1.38	1.33
20	A	5039	CLA	CHB-C4A	5.95	1.38	1.33
20	1	613	CLA	CHB-C4A	5.95	1.38	1.33
20	A	5028	CLA	CHB-C4A	5.95	1.38	1.33
20	A	5023	CLA	CHB-C4A	5.95	1.38	1.33
20	L	202	CLA	CHB-C4A	5.95	1.38	1.33
20	2	304	CLA	CHB-C4A	5.94	1.38	1.33
20	A	5022	CLA	CHB-C4A	5.94	1.38	1.33
20	A	5013	CLA	CHB-C4A	5.94	1.38	1.33
20	B	813	CLA	CHB-C4A	5.94	1.38	1.33
20	3	302	CLA	CHB-C4A	5.93	1.38	1.33
20	A	5014	CLA	CHB-C4A	5.93	1.38	1.33
20	B	814	CLA	CHB-C4A	5.93	1.38	1.33
20	A	5012	CLA	CHB-C4A	5.93	1.38	1.33
20	B	831	CLA	CHB-C4A	5.92	1.38	1.33
20	B	837	CLA	CHB-C4A	5.92	1.38	1.33
20	3	306	CLA	CHB-C4A	5.91	1.38	1.33
20	B	804	CLA	CHB-C4A	5.91	1.38	1.33
19	2	302	CHL	MG-NC	5.91	2.20	2.06
20	B	815	CLA	CHB-C4A	5.91	1.38	1.33
20	7	315	CLA	CHB-C4A	5.90	1.38	1.33
20	A	5029	CLA	CHB-C4A	5.90	1.38	1.33
20	G	201	CLA	CHB-C4A	5.90	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	CHB-C4A	5.89	1.38	1.33
20	A	5011	CLA	CHB-C4A	5.89	1.38	1.33
20	B	839	CLA	CHB-C4A	5.87	1.38	1.33
20	B	836	CLA	CHB-C4A	5.86	1.38	1.33
20	B	816	CLA	CHB-C4A	5.84	1.38	1.33
20	K	4004	CLA	CHB-C4A	5.83	1.38	1.33
20	A	5020	CLA	CHB-C4A	5.83	1.38	1.33
20	B	840	CLA	CHB-C4A	5.83	1.38	1.33
20	3	308	CLA	CHB-C4A	5.82	1.38	1.33
20	1	614	CLA	CHB-C4A	5.82	1.38	1.33
20	A	5033	CLA	CHB-C4A	5.79	1.38	1.33
20	B	810	CLA	CHB-C4A	5.79	1.38	1.33
20	A	5007	CLA	CHB-C4A	5.78	1.38	1.33
20	A	5015	CLA	CHB-C4A	5.78	1.38	1.33
20	B	825	CLA	CHB-C4A	5.74	1.38	1.33
20	8	308	CLA	CHB-C4A	5.74	1.38	1.33
20	B	808	CLA	CHB-C4A	5.71	1.38	1.33
20	L	205	CLA	CHB-C4A	5.70	1.38	1.33
20	A	5038	CLA	CHB-C4A	5.69	1.38	1.33
20	9	602	CLA	CHB-C4A	5.68	1.38	1.33
20	B	806	CLA	CHB-C4A	5.67	1.38	1.33
30	A	5003	CL0	MG-NA	5.67	2.19	2.06
20	A	5044	CLA	CHB-C4A	5.63	1.38	1.33
20	B	838	CLA	CHB-C4A	5.62	1.38	1.33
20	3	305	CLA	CHB-C4A	5.60	1.38	1.33
20	8	307	CLA	CHB-C4A	5.59	1.38	1.33
20	B	824	CLA	CHB-C4A	5.53	1.38	1.33
20	7	310	CLA	CHB-C4A	5.52	1.38	1.33
20	A	5005	CLA	CHB-C4A	5.49	1.38	1.33
19	9	606	CHL	MG-NC	5.46	2.19	2.06
19	8	305	CHL	MG-NC	5.38	2.19	2.06
20	1	604	CLA	CHB-C4A	5.36	1.38	1.33
19	3	323	CHL	MG-NC	5.32	2.18	2.06
19	1	601	CHL	MG-NC	5.30	2.18	2.06
19	7	307	CHL	MG-NA	4.89	2.17	2.06
20	9	607	CLA	CHB-C4A	4.80	1.37	1.33
20	H	201	CLA	MG-NC	4.72	2.17	2.06
20	8	307	CLA	C3C-C2C	4.49	1.46	1.36
19	1	606	CHL	MG-NC	4.47	2.16	2.06
30	A	5003	CL0	MG-NC	4.46	2.16	2.06
19	3	301	CHL	MG-NA	4.38	2.16	2.06
19	2	306	CHL	MG-NA	4.11	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	306	CHL	MG-NC	4.08	2.16	2.06
19	7	307	CHL	MG-NC	4.05	2.15	2.06
19	2	302	CHL	MG-NA	3.95	2.15	2.06
20	8	307	CLA	CHC-C1C	3.90	1.44	1.34
20	H	201	CLA	C1D-ND	3.85	1.42	1.37
20	K	4005	CLA	MG-NC	3.76	2.15	2.06
20	8	321	CLA	C1D-ND	3.76	1.42	1.37
20	2	311	CLA	C1D-ND	3.72	1.42	1.37
20	A	5032	CLA	MG-ND	-3.72	1.98	2.05
20	8	307	CLA	C1D-ND	3.71	1.42	1.37
20	9	610	CLA	C1D-ND	3.70	1.42	1.37
20	9	607	CLA	C1D-ND	3.64	1.42	1.37
20	B	817	CLA	C1D-ND	3.63	1.42	1.37
20	G	204	CLA	C1D-ND	3.62	1.42	1.37
20	K	4004	CLA	C1D-ND	3.62	1.42	1.37
20	A	5038	CLA	C1D-ND	3.62	1.42	1.37
20	9	605	CLA	C1D-ND	3.62	1.42	1.37
20	1	612	CLA	C1D-ND	3.62	1.42	1.37
20	A	5007	CLA	CHC-C1C	3.60	1.43	1.34
20	2	310	CLA	C1D-ND	3.60	1.42	1.37
20	3	307	CLA	C1D-ND	3.60	1.42	1.37
20	7	304	CLA	C1D-ND	3.59	1.42	1.37
20	K	4002	CLA	C1D-ND	3.59	1.42	1.37
20	G	202	CLA	C1D-ND	3.59	1.42	1.37
20	9	601	CLA	C1D-ND	3.58	1.42	1.37
20	B	820	CLA	C1D-ND	3.58	1.42	1.37
20	K	4005	CLA	C1D-ND	3.58	1.42	1.37
20	B	824	CLA	CHC-C1C	3.58	1.43	1.34
20	9	603	CLA	C1D-ND	3.58	1.42	1.37
20	B	822	CLA	C1D-ND	3.57	1.42	1.37
20	F	303	CLA	C1D-ND	3.57	1.42	1.37
20	3	308	CLA	C1D-ND	3.56	1.42	1.37
20	3	309	CLA	C1D-ND	3.56	1.42	1.37
20	B	814	CLA	C1D-ND	3.56	1.42	1.37
20	7	310	CLA	CHC-C1C	3.56	1.43	1.34
20	8	310	CLA	C1D-ND	3.56	1.42	1.37
20	1	603	CLA	C1D-ND	3.56	1.42	1.37
20	9	609	CLA	C1D-ND	3.56	1.42	1.37
20	B	806	CLA	CHC-C1C	3.55	1.43	1.34
20	A	5044	CLA	CHC-C1C	3.55	1.43	1.34
20	A	5019	CLA	C1D-ND	3.55	1.42	1.37
20	3	314	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	302	CLA	C1D-ND	3.55	1.42	1.37
20	1	608	CLA	C1D-ND	3.54	1.42	1.37
20	L	205	CLA	C1D-ND	3.54	1.42	1.37
20	K	4003	CLA	C1D-ND	3.53	1.42	1.37
20	A	5008	CLA	CHC-C1C	3.53	1.43	1.34
20	1	611	CLA	C1D-ND	3.53	1.42	1.37
20	8	303	CLA	CHC-C1C	3.53	1.43	1.34
20	7	311	CLA	C1D-ND	3.53	1.42	1.37
20	7	323	CLA	C1D-ND	3.53	1.42	1.37
20	7	312	CLA	C1D-ND	3.53	1.42	1.37
20	A	5025	CLA	C1D-ND	3.53	1.42	1.37
20	1	604	CLA	CHC-C1C	3.53	1.43	1.34
20	3	304	CLA	C1D-ND	3.53	1.42	1.37
20	7	305	CLA	C1D-ND	3.53	1.42	1.37
20	B	817	CLA	CHC-C1C	3.53	1.43	1.34
20	B	838	CLA	C1D-ND	3.52	1.42	1.37
20	8	302	CLA	C1D-ND	3.52	1.42	1.37
20	7	303	CLA	CHC-C1C	3.52	1.43	1.34
20	K	4002	CLA	CHC-C1C	3.52	1.43	1.34
20	7	313	CLA	C1D-ND	3.51	1.42	1.37
20	A	5014	CLA	C1D-ND	3.51	1.42	1.37
20	9	602	CLA	CHC-C1C	3.51	1.43	1.34
20	9	604	CLA	C1D-ND	3.51	1.42	1.37
20	3	310	CLA	C1D-ND	3.51	1.42	1.37
20	A	5029	CLA	C1D-ND	3.51	1.42	1.37
20	1	613	CLA	C1D-ND	3.51	1.42	1.37
20	A	5028	CLA	CHC-C1C	3.51	1.43	1.34
20	3	304	CLA	CHC-C1C	3.51	1.43	1.34
20	3	312	CLA	C1D-ND	3.51	1.42	1.37
20	8	309	CLA	C1D-ND	3.51	1.42	1.37
20	B	835	CLA	C1D-ND	3.50	1.42	1.37
20	2	305	CLA	C1D-ND	3.50	1.42	1.37
20	B	838	CLA	CHC-C1C	3.50	1.43	1.34
20	B	826	CLA	C1D-ND	3.50	1.42	1.37
20	2	301	CLA	C1D-ND	3.50	1.42	1.37
20	2	313	CLA	C1D-ND	3.50	1.42	1.37
20	2	307	CLA	C1D-ND	3.50	1.42	1.37
20	L	201	CLA	C1D-ND	3.50	1.42	1.37
20	2	312	CLA	C2D-C1D	3.50	1.48	1.42
20	A	5015	CLA	CHC-C1C	3.50	1.43	1.34
20	A	5026	CLA	C1D-ND	3.50	1.42	1.37
20	2	308	CLA	CHC-C1C	3.50	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	829	CLA	CHC-C1C	3.49	1.43	1.34
20	K	4003	CLA	CHC-C1C	3.49	1.43	1.34
20	A	5010	CLA	C1D-ND	3.49	1.42	1.37
20	2	309	CLA	C1D-ND	3.49	1.42	1.37
20	7	311	CLA	CHC-C1C	3.49	1.43	1.34
20	7	309	CLA	C1D-ND	3.49	1.42	1.37
20	B	805	CLA	CHC-C1C	3.49	1.43	1.34
20	7	314	CLA	C1D-ND	3.49	1.42	1.37
20	A	5039	CLA	C1D-ND	3.49	1.42	1.37
20	9	612	CLA	C1D-ND	3.49	1.42	1.37
20	9	601	CLA	CHC-C1C	3.49	1.43	1.34
20	2	311	CLA	CHC-C1C	3.49	1.43	1.34
20	1	610	CLA	C1D-ND	3.49	1.42	1.37
20	F	308	CLA	C1D-ND	3.49	1.42	1.37
20	J	104	CLA	C1D-ND	3.49	1.42	1.37
20	2	301	CLA	CHC-C1C	3.49	1.43	1.34
20	A	5014	CLA	CHC-C1C	3.49	1.43	1.34
20	9	608	CLA	C1D-ND	3.49	1.42	1.37
20	G	203	CLA	C1D-ND	3.48	1.42	1.37
20	A	5019	CLA	CHC-C1C	3.48	1.43	1.34
20	B	821	CLA	C1D-ND	3.48	1.42	1.37
20	G	204	CLA	CHC-C1C	3.48	1.43	1.34
20	A	5013	CLA	C1D-ND	3.48	1.42	1.37
20	B	811	CLA	C1D-ND	3.48	1.42	1.37
20	A	5040	CLA	C1D-ND	3.48	1.42	1.37
20	8	311	CLA	C1D-ND	3.48	1.42	1.37
20	7	309	CLA	CHC-C1C	3.48	1.43	1.34
20	2	304	CLA	CHC-C1C	3.47	1.43	1.34
20	A	5024	CLA	C1D-ND	3.47	1.42	1.37
20	B	813	CLA	C1D-ND	3.47	1.42	1.37
20	A	5029	CLA	CHC-C1C	3.47	1.43	1.34
20	F	307	CLA	C1D-ND	3.47	1.42	1.37
20	A	5032	CLA	C1D-ND	3.47	1.42	1.37
20	B	816	CLA	C1D-ND	3.47	1.42	1.37
20	B	828	CLA	CHC-C1C	3.47	1.43	1.34
20	9	608	CLA	CHC-C1C	3.47	1.43	1.34
20	A	5041	CLA	CHC-C1C	3.47	1.43	1.34
20	K	4005	CLA	CHC-C1C	3.47	1.43	1.34
20	A	5009	CLA	C1D-ND	3.47	1.42	1.37
20	A	5020	CLA	C1D-ND	3.46	1.42	1.37
20	2	308	CLA	C1D-ND	3.46	1.42	1.37
20	1	602	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	605	CLA	CHC-C1C	3.46	1.43	1.34
20	L	202	CLA	C1D-ND	3.46	1.42	1.37
20	7	314	CLA	CHC-C1C	3.46	1.43	1.34
20	A	5010	CLA	CHC-C1C	3.46	1.43	1.34
20	2	307	CLA	CHC-C1C	3.46	1.43	1.34
20	B	807	CLA	CHC-C1C	3.46	1.43	1.34
20	2	310	CLA	CHC-C1C	3.46	1.43	1.34
20	B	813	CLA	CHC-C1C	3.46	1.43	1.34
20	3	310	CLA	CHC-C1C	3.46	1.43	1.34
20	J	104	CLA	CHC-C1C	3.46	1.43	1.34
20	A	5037	CLA	CHC-C1C	3.46	1.43	1.34
20	A	5017	CLA	C1D-ND	3.46	1.42	1.37
20	G	203	CLA	CHC-C1C	3.46	1.43	1.34
20	A	5016	CLA	CHC-C1C	3.46	1.43	1.34
20	A	5031	CLA	C1D-ND	3.46	1.42	1.37
20	L	204	CLA	CHC-C1C	3.46	1.43	1.34
20	B	819	CLA	C1D-ND	3.46	1.42	1.37
20	9	609	CLA	CHC-C1C	3.46	1.43	1.34
20	3	312	CLA	CHC-C1C	3.46	1.43	1.34
20	9	603	CLA	CHC-C1C	3.46	1.43	1.34
20	G	201	CLA	C1D-ND	3.46	1.42	1.37
20	B	840	CLA	CHC-C1C	3.46	1.43	1.34
20	B	833	CLA	CHC-C1C	3.45	1.43	1.34
20	B	829	CLA	C1D-ND	3.45	1.42	1.37
20	A	5024	CLA	CHC-C1C	3.45	1.43	1.34
20	B	818	CLA	C1D-ND	3.45	1.42	1.37
20	G	201	CLA	CHC-C1C	3.45	1.43	1.34
20	8	312	CLA	C1D-ND	3.45	1.42	1.37
20	9	604	CLA	CHC-C1C	3.45	1.43	1.34
20	A	5006	CLA	CHC-C1C	3.45	1.43	1.34
20	7	315	CLA	C1D-ND	3.45	1.42	1.37
20	A	5037	CLA	C1D-ND	3.45	1.42	1.37
20	9	612	CLA	CHC-C1C	3.45	1.43	1.34
20	B	816	CLA	CHC-C1C	3.45	1.43	1.34
20	A	5005	CLA	C1D-ND	3.45	1.42	1.37
20	8	309	CLA	CHC-C1C	3.45	1.43	1.34
20	1	607	CLA	C1D-ND	3.45	1.42	1.37
20	B	809	CLA	C1D-ND	3.45	1.42	1.37
20	B	833	CLA	C1D-ND	3.45	1.42	1.37
20	1	609	CLA	CHC-C1C	3.45	1.43	1.34
20	8	312	CLA	CHC-C1C	3.45	1.43	1.34
20	A	5012	CLA	CHC-C1C	3.45	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	CHC-C1C	3.45	1.43	1.34
20	2	309	CLA	CHC-C1C	3.45	1.43	1.34
20	9	605	CLA	CHC-C1C	3.45	1.43	1.34
20	3	325	CLA	CHC-C1C	3.44	1.43	1.34
20	B	831	CLA	CHC-C1C	3.44	1.43	1.34
20	8	310	CLA	CHC-C1C	3.44	1.43	1.34
20	B	836	CLA	CHC-C1C	3.44	1.43	1.34
20	2	305	CLA	CHC-C1C	3.44	1.43	1.34
20	2	312	CLA	CHC-C1C	3.44	1.43	1.34
20	9	611	CLA	CHC-C1C	3.44	1.43	1.34
20	F	306	CLA	CHC-C1C	3.44	1.43	1.34
20	A	5043	CLA	C1D-ND	3.44	1.42	1.37
20	B	834	CLA	C1D-ND	3.44	1.42	1.37
20	B	826	CLA	CHC-C1C	3.44	1.43	1.34
20	1	613	CLA	CHC-C1C	3.44	1.43	1.34
20	3	313	CLA	CHC-C1C	3.44	1.43	1.34
20	2	304	CLA	C1D-ND	3.44	1.42	1.37
20	9	607	CLA	CHC-C1C	3.44	1.43	1.34
20	A	5028	CLA	C1D-ND	3.44	1.42	1.37
20	3	313	CLA	C1D-ND	3.44	1.42	1.37
20	A	5004	CLA	C1D-ND	3.44	1.42	1.37
20	1	614	CLA	C1D-ND	3.44	1.42	1.37
20	A	5013	CLA	CHC-C1C	3.44	1.43	1.34
20	9	611	CLA	C1D-ND	3.44	1.42	1.37
20	9	602	CLA	C1D-ND	3.44	1.42	1.37
20	B	840	CLA	C1D-ND	3.44	1.42	1.37
20	1	611	CLA	CHC-C1C	3.43	1.43	1.34
20	A	5033	CLA	C1D-ND	3.43	1.42	1.37
20	1	602	CLA	CHC-C1C	3.43	1.43	1.34
20	B	815	CLA	CHC-C1C	3.43	1.43	1.34
20	L	205	CLA	CHC-C1C	3.43	1.43	1.34
20	3	309	CLA	CHC-C1C	3.43	1.43	1.34
20	F	307	CLA	CHC-C1C	3.43	1.43	1.34
20	A	5023	CLA	CHC-C1C	3.43	1.43	1.34
20	1	607	CLA	CHC-C1C	3.43	1.43	1.34
20	A	5011	CLA	CHC-C1C	3.43	1.43	1.34
20	3	302	CLA	CHC-C1C	3.43	1.43	1.34
20	F	308	CLA	CHC-C1C	3.43	1.43	1.34
20	A	5020	CLA	CHC-C1C	3.43	1.43	1.34
20	B	806	CLA	C1D-ND	3.43	1.42	1.37
20	B	825	CLA	CHC-C1C	3.43	1.43	1.34
20	A	5040	CLA	CHC-C1C	3.43	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5044	CLA	C1D-ND	3.43	1.42	1.37
20	A	5033	CLA	CHC-C1C	3.42	1.43	1.34
20	1	603	CLA	CHC-C1C	3.42	1.43	1.34
20	A	5030	CLA	C1D-ND	3.42	1.42	1.37
20	A	5042	CLA	C1D-ND	3.42	1.42	1.37
20	B	804	CLA	C1D-ND	3.42	1.42	1.37
20	3	303	CLA	C1D-ND	3.42	1.42	1.37
20	3	311	CLA	C1D-ND	3.42	1.42	1.37
20	8	308	CLA	C1D-ND	3.42	1.42	1.37
20	2	313	CLA	CHC-C1C	3.42	1.43	1.34
20	A	5034	CLA	C1D-ND	3.42	1.42	1.37
20	B	830	CLA	C1D-ND	3.42	1.42	1.37
20	7	310	CLA	C1D-ND	3.42	1.42	1.37
20	A	5018	CLA	C1D-ND	3.42	1.42	1.37
20	8	308	CLA	CHC-C1C	3.42	1.43	1.34
20	B	818	CLA	CHC-C1C	3.42	1.43	1.34
20	A	5030	CLA	CHC-C1C	3.42	1.43	1.34
20	1	609	CLA	C1D-ND	3.42	1.42	1.37
20	B	812	CLA	CHC-C1C	3.42	1.43	1.34
20	B	832	CLA	CHC-C1C	3.42	1.43	1.34
20	3	314	CLA	CHC-C1C	3.42	1.43	1.34
20	L	202	CLA	CHC-C1C	3.42	1.43	1.34
20	A	5016	CLA	C1D-ND	3.41	1.42	1.37
20	A	5036	CLA	C1D-ND	3.41	1.42	1.37
20	7	315	CLA	CHC-C1C	3.41	1.43	1.34
20	8	313	CLA	C1D-ND	3.41	1.42	1.37
20	A	5004	CLA	CHC-C1C	3.41	1.43	1.34
20	8	302	CLA	CHC-C1C	3.41	1.43	1.34
20	B	832	CLA	C1D-ND	3.41	1.42	1.37
20	1	605	CLA	C1D-ND	3.41	1.42	1.37
20	A	5023	CLA	C1D-ND	3.40	1.42	1.37
20	3	311	CLA	CHC-C1C	3.40	1.42	1.34
20	K	4004	CLA	MG-NA	3.40	2.14	2.06
20	A	5027	CLA	CHC-C1C	3.40	1.42	1.34
20	7	312	CLA	CHC-C1C	3.40	1.42	1.34
20	B	804	CLA	CHC-C1C	3.40	1.42	1.34
20	3	307	CLA	CHC-C1C	3.40	1.42	1.34
20	9	610	CLA	CHC-C1C	3.40	1.42	1.34
20	A	5039	CLA	CHC-C1C	3.40	1.42	1.34
20	1	604	CLA	C1D-ND	3.40	1.42	1.37
20	B	830	CLA	CHC-C1C	3.40	1.42	1.34
20	B	823	CLA	CHC-C1C	3.40	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	303	CLA	CHC-C1C	3.40	1.42	1.34
20	1	610	CLA	CHC-C1C	3.40	1.42	1.34
20	B	824	CLA	C1D-ND	3.40	1.42	1.37
20	3	325	CLA	C1D-ND	3.39	1.42	1.37
20	A	5022	CLA	CHC-C1C	3.39	1.42	1.34
20	1	614	CLA	CHC-C1C	3.39	1.42	1.34
20	8	311	CLA	CHC-C1C	3.39	1.42	1.34
20	B	810	CLA	C1D-ND	3.39	1.42	1.37
20	B	808	CLA	CHC-C1C	3.39	1.42	1.34
20	B	837	CLA	C1D-ND	3.39	1.42	1.37
20	A	5021	CLA	C1D-ND	3.39	1.42	1.37
20	7	313	CLA	MG-ND	-3.39	1.99	2.05
20	G	202	CLA	CHC-C1C	3.39	1.42	1.34
20	A	5034	CLA	CHC-C1C	3.38	1.42	1.34
20	B	821	CLA	CHC-C1C	3.38	1.42	1.34
20	F	306	CLA	C1D-ND	3.38	1.42	1.37
20	7	303	CLA	C1D-ND	3.38	1.42	1.37
20	A	5018	CLA	CHC-C1C	3.38	1.42	1.34
20	B	837	CLA	CHC-C1C	3.38	1.42	1.34
20	A	5006	CLA	C1D-ND	3.38	1.42	1.37
20	7	313	CLA	CHC-C1C	3.38	1.42	1.34
20	7	305	CLA	CHC-C1C	3.38	1.42	1.34
20	8	313	CLA	CHC-C1C	3.38	1.42	1.34
20	8	301	CLA	CHC-C1C	3.37	1.42	1.34
20	A	5015	CLA	C1D-ND	3.37	1.42	1.37
20	B	812	CLA	C1D-ND	3.37	1.42	1.37
20	8	321	CLA	CHC-C1C	3.37	1.42	1.34
20	A	5031	CLA	CHC-C1C	3.37	1.42	1.34
20	3	306	CLA	CHC-C1C	3.37	1.42	1.34
20	A	5035	CLA	CHC-C1C	3.37	1.42	1.34
20	A	5035	CLA	C1D-ND	3.37	1.42	1.37
20	A	5021	CLA	CHC-C1C	3.37	1.42	1.34
20	A	5043	CLA	CHC-C1C	3.37	1.42	1.34
20	B	828	CLA	C1D-ND	3.37	1.42	1.37
20	A	5042	CLA	CHC-C1C	3.37	1.42	1.34
20	B	827	CLA	CHC-C1C	3.37	1.42	1.34
20	1	612	CLA	CHC-C1C	3.36	1.42	1.34
20	H	201	CLA	CHC-C1C	3.36	1.42	1.34
20	L	204	CLA	C1D-ND	3.36	1.42	1.37
20	7	323	CLA	CHC-C1C	3.36	1.42	1.34
20	A	5022	CLA	C1D-ND	3.36	1.42	1.37
20	7	304	CLA	CHC-C1C	3.36	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5011	CLA	C1D-ND	3.36	1.42	1.37
20	A	5041	CLA	C1D-ND	3.36	1.42	1.37
20	A	5017	CLA	CHC-C1C	3.36	1.42	1.34
20	A	5009	CLA	CHC-C1C	3.36	1.42	1.34
20	B	814	CLA	CHC-C1C	3.35	1.42	1.34
20	8	303	CLA	C1D-ND	3.35	1.42	1.37
20	K	4004	CLA	CHC-C1C	3.35	1.42	1.34
20	A	5012	CLA	C1D-ND	3.35	1.42	1.37
20	B	831	CLA	C1D-ND	3.35	1.42	1.37
20	L	201	CLA	CHC-C1C	3.35	1.42	1.34
20	3	306	CLA	C1D-ND	3.35	1.42	1.37
20	B	809	CLA	CHC-C1C	3.35	1.42	1.34
20	3	305	CLA	C1D-ND	3.34	1.42	1.37
20	A	5032	CLA	CHC-C1C	3.34	1.42	1.34
20	A	5026	CLA	CHC-C1C	3.34	1.42	1.34
20	B	839	CLA	C1D-ND	3.33	1.42	1.37
20	B	822	CLA	CHC-C1C	3.33	1.42	1.34
20	3	303	CLA	CHC-C1C	3.33	1.42	1.34
20	B	815	CLA	C1D-ND	3.32	1.42	1.37
20	B	825	CLA	C1D-ND	3.32	1.42	1.37
20	A	5025	CLA	CHC-C1C	3.32	1.42	1.34
20	B	819	CLA	CHC-C1C	3.32	1.42	1.34
20	3	324	CLA	CHC-C1C	3.32	1.42	1.34
20	3	305	CLA	CHC-C1C	3.31	1.42	1.34
20	A	5007	CLA	C1D-ND	3.31	1.42	1.37
20	3	308	CLA	CHC-C1C	3.31	1.42	1.34
20	A	5038	CLA	CHC-C1C	3.30	1.42	1.34
20	A	5005	CLA	CHC-C1C	3.30	1.42	1.34
20	1	608	CLA	CHC-C1C	3.30	1.42	1.34
20	B	810	CLA	CHC-C1C	3.29	1.42	1.34
20	A	5027	CLA	MG-ND	-3.29	1.99	2.05
20	B	823	CLA	C1D-ND	3.28	1.42	1.37
19	8	306	CHL	C1D-C2D	-3.28	1.38	1.45
20	B	835	CLA	CHC-C1C	3.28	1.42	1.34
19	3	323	CHL	C1D-C2D	-3.28	1.38	1.45
20	F	303	CLA	CHC-C1C	3.26	1.42	1.34
20	B	807	CLA	C1D-ND	3.25	1.42	1.37
20	B	820	CLA	CHC-C1C	3.24	1.42	1.34
20	B	811	CLA	CHC-C1C	3.24	1.42	1.34
20	A	5028	CLA	MG-NA	3.24	2.14	2.06
20	A	5027	CLA	C1D-ND	3.23	1.42	1.37
20	B	826	CLA	MG-NA	3.22	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	836	CLA	C1D-ND	3.21	1.42	1.37
20	A	5008	CLA	C1D-ND	3.19	1.42	1.37
20	B	804	CLA	MG-NC	3.15	2.13	2.06
20	F	303	CLA	MG-NC	3.14	2.13	2.06
20	B	827	CLA	C1D-ND	3.14	1.42	1.37
20	B	839	CLA	CHC-C1C	3.13	1.42	1.34
20	2	303	CLA	C1D-ND	3.12	1.42	1.37
19	7	307	CHL	CHB-C4A	3.09	1.35	1.33
23	3	319	BCR	C8-C9	-3.09	1.39	1.46
20	8	301	CLA	C1D-ND	3.08	1.41	1.37
20	2	303	CLA	MG-NA	3.07	2.13	2.06
20	B	839	CLA	CMB-C2B	-3.07	1.45	1.51
20	A	5004	CLA	CMB-C2B	-3.07	1.45	1.51
19	8	305	CHL	CHB-C4A	3.05	1.35	1.33
19	2	302	CHL	C1D-C2D	-3.03	1.39	1.45
20	B	808	CLA	C1D-ND	3.03	1.41	1.37
20	7	304	CLA	MG-NA	3.01	2.13	2.06
20	B	838	CLA	MG-ND	-2.99	1.99	2.05
19	2	306	CHL	CHB-C4A	2.99	1.35	1.33
20	B	828	CLA	MG-NA	2.98	2.13	2.06
20	3	324	CLA	C1D-ND	2.97	1.41	1.37
19	2	306	CHL	MG-NC	2.96	2.13	2.06
20	8	307	CLA	MG-ND	-2.95	1.99	2.05
30	A	5003	CL0	C1D-C2D	-2.95	1.39	1.45
19	8	305	CHL	C1D-C2D	-2.95	1.39	1.45
19	8	304	CHL	CHB-C4A	2.94	1.35	1.33
30	A	5003	CL0	CHB-C4A	2.94	1.35	1.33
19	9	606	CHL	C1D-C2D	-2.94	1.39	1.45
23	3	319	BCR	C23-C22	-2.90	1.39	1.46
20	A	5036	CLA	C2C-C1C	2.90	1.46	1.40
19	2	302	CHL	CHB-C4A	2.90	1.35	1.33
19	8	306	CHL	CHB-C4A	2.89	1.35	1.33
19	3	301	CHL	C1D-C2D	-2.89	1.39	1.45
19	2	306	CHL	C1D-C2D	-2.89	1.39	1.45
19	9	606	CHL	CHB-C4A	2.88	1.35	1.33
19	3	323	CHL	CHB-C4A	2.87	1.35	1.33
19	7	308	CHL	C1D-C2D	-2.86	1.39	1.45
20	1	603	CLA	MG-NA	2.85	2.13	2.06
19	1	606	CHL	C1D-C2D	-2.80	1.39	1.45
20	B	820	CLA	CMB-C2B	-2.80	1.46	1.51
19	7	306	CHL	CHB-C4A	2.80	1.35	1.33
19	1	601	CHL	CHB-C4A	2.78	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5005	CLA	CMB-C2B	-2.78	1.46	1.51
20	A	5005	CLA	MG-ND	-2.76	2.00	2.05
19	7	306	CHL	C1D-C2D	-2.74	1.39	1.45
19	1	601	CHL	C1D-C2D	-2.74	1.39	1.45
19	8	304	CHL	C1D-C2D	-2.74	1.39	1.45
20	B	811	CLA	CMB-C2B	-2.74	1.46	1.51
20	A	5042	CLA	CMB-C2B	-2.73	1.46	1.51
20	A	5032	CLA	CMB-C2B	-2.71	1.46	1.51
19	1	606	CHL	CHB-C4A	2.71	1.35	1.33
20	B	828	CLA	CMB-C2B	-2.71	1.46	1.51
20	9	610	CLA	MG-NC	2.71	2.12	2.06
19	7	308	CHL	CHB-C4A	2.71	1.35	1.33
20	3	303	CLA	CMB-C2B	-2.70	1.46	1.51
20	8	307	CLA	MG-NC	2.70	2.12	2.06
20	3	306	CLA	CMB-C2B	-2.69	1.46	1.51
19	7	307	CHL	C1D-C2D	-2.68	1.40	1.45
20	9	607	CLA	CMB-C2B	-2.67	1.46	1.51
20	8	311	CLA	MG-ND	-2.66	2.00	2.05
20	A	5022	CLA	CMB-C2B	-2.66	1.46	1.51
20	A	5027	CLA	CMD-C2D	-2.65	1.45	1.50
20	A	5036	CLA	CMB-C2B	-2.65	1.46	1.51
20	8	302	CLA	CMB-C2B	-2.65	1.46	1.51
20	1	613	CLA	MG-NA	2.64	2.12	2.06
19	3	301	CHL	CHB-C4A	2.64	1.35	1.33
20	B	838	CLA	CMB-C2B	-2.64	1.46	1.51
20	A	5020	CLA	CMB-C2B	-2.64	1.46	1.51
20	8	302	CLA	MG-NA	2.63	2.12	2.06
20	B	834	CLA	CMB-C2B	-2.63	1.46	1.51
20	A	5032	CLA	CMD-C2D	-2.63	1.45	1.50
20	A	5017	CLA	CMB-C2B	-2.63	1.46	1.51
20	3	305	CLA	CMB-C2B	-2.63	1.46	1.51
20	B	836	CLA	CMB-C2B	-2.62	1.46	1.51
20	8	308	CLA	CMB-C2B	-2.62	1.46	1.51
20	1	612	CLA	CMB-C2B	-2.62	1.46	1.51
20	8	309	CLA	MG-NA	2.62	2.12	2.06
20	9	608	CLA	CMB-C2B	-2.61	1.46	1.51
20	2	303	CLA	CMB-C2B	-2.60	1.46	1.51
20	3	324	CLA	CMB-C2B	-2.60	1.46	1.51
20	7	305	CLA	CMB-C2B	-2.59	1.46	1.51
20	B	826	CLA	CMB-C2B	-2.59	1.46	1.51
20	B	821	CLA	CMB-C2B	-2.59	1.46	1.51
20	2	307	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	614	CLA	CMB-C2B	-2.59	1.46	1.51
20	7	315	CLA	CMB-C2B	-2.59	1.46	1.51
20	3	302	CLA	MG-NA	2.58	2.12	2.06
20	A	5025	CLA	CMB-C2B	-2.58	1.46	1.51
20	F	308	CLA	CMB-C2B	-2.58	1.46	1.51
20	B	804	CLA	CMB-C2B	-2.58	1.46	1.51
20	L	202	CLA	CMB-C2B	-2.58	1.46	1.51
20	A	5015	CLA	CMB-C2B	-2.58	1.46	1.51
20	1	607	CLA	CMB-C2B	-2.57	1.46	1.51
20	B	822	CLA	CMB-C2B	-2.57	1.46	1.51
20	A	5010	CLA	CMB-C2B	-2.57	1.46	1.51
20	K	4002	CLA	CMB-C2B	-2.57	1.46	1.51
20	A	5027	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	812	CLA	CMB-C2B	-2.56	1.46	1.51
20	A	5023	CLA	CMB-C2B	-2.56	1.46	1.51
20	A	5034	CLA	CMB-C2B	-2.56	1.46	1.51
20	8	321	CLA	CMB-C2B	-2.56	1.46	1.51
20	7	310	CLA	CMB-C2B	-2.56	1.46	1.51
20	8	301	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	825	CLA	CMB-C2B	-2.56	1.46	1.51
20	G	203	CLA	CMB-C2B	-2.56	1.46	1.51
20	3	325	CLA	CMB-C2B	-2.56	1.46	1.51
20	3	307	CLA	CMB-C2B	-2.56	1.46	1.51
20	A	5013	CLA	CMB-C2B	-2.56	1.46	1.51
20	A	5021	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	833	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	816	CLA	CMB-C2B	-2.55	1.46	1.51
20	L	205	CLA	CMB-C2B	-2.55	1.46	1.51
20	A	5037	CLA	CMB-C2B	-2.55	1.46	1.51
20	G	201	CLA	CMB-C2B	-2.55	1.46	1.51
20	A	5035	CLA	CMB-C2B	-2.55	1.46	1.51
20	A	5043	CLA	CMB-C2B	-2.55	1.46	1.51
20	7	304	CLA	CMB-C2B	-2.55	1.46	1.51
20	3	314	CLA	CMB-C2B	-2.55	1.46	1.51
20	H	201	CLA	CMB-C2B	-2.55	1.46	1.51
20	B	831	CLA	CMB-C2B	-2.55	1.46	1.51
20	A	5028	CLA	CMB-C2B	-2.54	1.46	1.51
20	A	5041	CLA	CMB-C2B	-2.54	1.46	1.51
20	B	805	CLA	CMB-C2B	-2.54	1.46	1.51
20	2	304	CLA	CMB-C2B	-2.54	1.46	1.51
20	B	830	CLA	CMB-C2B	-2.54	1.46	1.51
20	1	608	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5019	CLA	CMB-C2B	-2.54	1.46	1.51
20	B	817	CLA	CMB-C2B	-2.54	1.46	1.51
20	2	301	CLA	CMB-C2B	-2.54	1.46	1.51
20	2	305	CLA	CMB-C2B	-2.54	1.46	1.51
20	A	5024	CLA	CMB-C2B	-2.53	1.46	1.51
20	B	818	CLA	CMB-C2B	-2.53	1.46	1.51
20	8	303	CLA	CMB-C2B	-2.53	1.46	1.51
20	J	104	CLA	CMB-C2B	-2.53	1.46	1.51
20	7	313	CLA	CMB-C2B	-2.53	1.46	1.51
20	B	810	CLA	CMB-C2B	-2.53	1.46	1.51
20	8	311	CLA	CMB-C2B	-2.53	1.46	1.51
20	A	5040	CLA	CMB-C2B	-2.53	1.46	1.51
20	B	823	CLA	CMB-C2B	-2.53	1.46	1.51
20	3	313	CLA	CMB-C2B	-2.53	1.46	1.51
20	3	311	CLA	CMB-C2B	-2.52	1.46	1.51
20	8	309	CLA	CMB-C2B	-2.52	1.46	1.51
20	7	309	CLA	CMB-C2B	-2.52	1.46	1.51
20	2	308	CLA	CMB-C2B	-2.52	1.46	1.51
20	8	312	CLA	CMB-C2B	-2.52	1.46	1.51
20	9	611	CLA	CMB-C2B	-2.52	1.46	1.51
20	2	309	CLA	CMB-C2B	-2.52	1.46	1.51
20	9	604	CLA	CMB-C2B	-2.52	1.46	1.51
20	7	323	CLA	CMB-C2B	-2.52	1.46	1.51
20	8	313	CLA	CMB-C2B	-2.52	1.46	1.51
20	F	307	CLA	CMB-C2B	-2.52	1.46	1.51
20	B	813	CLA	CMB-C2B	-2.52	1.46	1.51
20	B	809	CLA	CMB-C2B	-2.52	1.46	1.51
20	A	5039	CLA	CMB-C2B	-2.52	1.46	1.51
26	7	302	PTY	P1-O11	2.52	1.64	1.54
20	9	603	CLA	CMB-C2B	-2.51	1.46	1.51
20	7	314	CLA	CMB-C2B	-2.51	1.46	1.51
20	A	5011	CLA	CMB-C2B	-2.51	1.46	1.51
20	L	201	CLA	CMB-C2B	-2.51	1.46	1.51
20	A	5029	CLA	CMB-C2B	-2.51	1.46	1.51
20	1	613	CLA	CMB-C2B	-2.51	1.46	1.51
20	A	5014	CLA	CMB-C2B	-2.51	1.46	1.51
20	B	835	CLA	CMB-C2B	-2.51	1.46	1.51
20	F	306	CLA	CMB-C2B	-2.51	1.46	1.51
20	8	303	CLA	MG-NA	2.51	2.12	2.06
20	A	5006	CLA	CMB-C2B	-2.51	1.46	1.51
20	A	5018	CLA	CMB-C2B	-2.51	1.46	1.51
20	B	808	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	312	CLA	CMB-C2B	-2.51	1.46	1.51
20	1	609	CLA	CMB-C2B	-2.51	1.46	1.51
20	7	303	CLA	CMB-C2B	-2.51	1.46	1.51
20	9	609	CLA	CMB-C2B	-2.51	1.46	1.51
20	B	815	CLA	CMB-C2B	-2.50	1.46	1.51
20	K	4004	CLA	CMB-C2B	-2.50	1.46	1.51
20	B	814	CLA	CMB-C2B	-2.50	1.46	1.51
20	2	311	CLA	CMB-C2B	-2.50	1.46	1.51
20	3	308	CLA	CMB-C2B	-2.50	1.46	1.51
20	3	302	CLA	CMB-C2B	-2.50	1.46	1.51
20	B	832	CLA	CMB-C2B	-2.50	1.46	1.51
20	1	603	CLA	CMB-C2B	-2.50	1.46	1.51
20	B	840	CLA	CMB-C2B	-2.50	1.46	1.51
20	A	5030	CLA	CMB-C2B	-2.50	1.46	1.51
20	A	5033	CLA	CMB-C2B	-2.50	1.46	1.51
20	A	5009	CLA	CMB-C2B	-2.50	1.46	1.51
20	7	312	CLA	CMB-C2B	-2.50	1.46	1.51
20	B	837	CLA	CMB-C2B	-2.50	1.46	1.51
20	2	312	CLA	MG-NA	2.50	2.12	2.06
20	9	612	CLA	CMB-C2B	-2.49	1.46	1.51
20	1	611	CLA	CMB-C2B	-2.49	1.46	1.51
20	9	605	CLA	CMB-C2B	-2.49	1.46	1.51
20	7	311	CLA	CMB-C2B	-2.49	1.46	1.51
20	A	5026	CLA	CMB-C2B	-2.49	1.46	1.51
20	G	202	CLA	CMB-C2B	-2.49	1.46	1.51
20	3	310	CLA	CMB-C2B	-2.49	1.46	1.51
20	2	313	CLA	CMB-C2B	-2.49	1.46	1.51
20	3	309	CLA	CMB-C2B	-2.49	1.46	1.51
20	1	605	CLA	CMB-C2B	-2.48	1.46	1.51
20	1	604	CLA	CMB-C2B	-2.48	1.46	1.51
20	L	204	CLA	CMB-C2B	-2.48	1.46	1.51
20	1	602	CLA	CMB-C2B	-2.48	1.46	1.51
20	3	304	CLA	CMB-C2B	-2.48	1.46	1.51
20	K	4005	CLA	CMB-C2B	-2.48	1.46	1.51
20	9	603	CLA	MG-ND	-2.48	2.00	2.05
20	A	5016	CLA	CMB-C2B	-2.48	1.46	1.51
20	K	4003	CLA	CMB-C2B	-2.48	1.46	1.51
20	A	5007	CLA	CMB-C2B	-2.47	1.46	1.51
20	F	303	CLA	CMB-C2B	-2.47	1.46	1.51
20	G	204	CLA	CMB-C2B	-2.47	1.46	1.51
20	9	610	CLA	CMB-C2B	-2.47	1.46	1.51
20	A	5012	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	310	CLA	CMB-C2B	-2.47	1.46	1.51
20	G	202	CLA	MG-NA	2.47	2.12	2.06
20	9	601	CLA	CMB-C2B	-2.46	1.46	1.51
20	2	312	CLA	CMB-C2B	-2.46	1.46	1.51
20	9	602	CLA	CMB-C2B	-2.46	1.46	1.51
20	B	827	CLA	CMB-C2B	-2.46	1.46	1.51
20	B	838	CLA	MG-NA	2.46	2.12	2.06
20	1	610	CLA	CMB-C2B	-2.46	1.46	1.51
20	B	819	CLA	CMB-C2B	-2.46	1.46	1.51
20	G	204	CLA	MG-ND	-2.46	2.00	2.05
20	B	824	CLA	CMB-C2B	-2.46	1.46	1.51
20	2	310	CLA	CMB-C2B	-2.45	1.46	1.51
20	B	806	CLA	CMB-C2B	-2.44	1.46	1.51
20	8	307	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	5038	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	5008	CLA	CMB-C2B	-2.43	1.46	1.51
20	8	310	CLA	MG-NA	2.42	2.12	2.06
20	B	805	CLA	C1D-ND	2.42	1.41	1.37
19	2	306	CHL	C1C-NC	-2.41	1.34	1.37
20	B	825	CLA	MG-ND	-2.40	2.01	2.05
23	3	319	BCR	C12-C13	-2.39	1.40	1.46
20	A	5044	CLA	CMB-C2B	-2.38	1.46	1.51
20	B	814	CLA	MG-ND	-2.38	2.01	2.05
20	7	305	CLA	MG-NA	2.36	2.11	2.06
20	B	807	CLA	CMB-C2B	-2.36	1.46	1.51
20	3	324	CLA	CMD-C2D	-2.33	1.46	1.50
20	A	5021	CLA	MG-ND	-2.33	2.01	2.05
20	8	313	CLA	MG-ND	-2.32	2.01	2.05
20	8	307	CLA	C4C-C3C	2.32	1.49	1.45
20	A	5031	CLA	CMB-C2B	-2.32	1.47	1.51
20	B	829	CLA	CMD-C2D	-2.31	1.46	1.50
23	3	319	BCR	C21-C22	2.29	1.41	1.35
20	G	204	CLA	MG-NA	2.29	2.11	2.06
20	B	827	CLA	CMD-C2D	-2.28	1.46	1.50
20	B	824	CLA	MG-NA	2.28	2.11	2.06
20	B	820	CLA	C3B-C2B	-2.26	1.37	1.40
20	B	825	CLA	CMD-C2D	-2.26	1.46	1.50
26	7	302	PTY	O7-C6	-2.25	1.43	1.46
20	A	5005	CLA	CMD-C2D	-2.25	1.46	1.50
20	1	612	CLA	CMD-C2D	-2.25	1.46	1.50
20	A	5012	CLA	CMD-C2D	-2.25	1.46	1.50
20	7	311	CLA	MG-ND	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	CMD-C2D	-2.24	1.46	1.50
23	3	319	BCR	C19-C18	-2.23	1.41	1.46
19	7	306	CHL	C1C-NC	-2.23	1.34	1.37
20	A	5008	CLA	CMC-C2C	-2.22	1.46	1.50
20	B	820	CLA	CMC-C2C	-2.22	1.46	1.50
20	A	5004	CLA	CMC-C2C	-2.21	1.46	1.50
20	B	824	CLA	CMD-C2D	-2.20	1.46	1.50
20	8	321	CLA	MG-NA	2.20	2.11	2.06
20	B	838	CLA	CMD-C2D	-2.20	1.46	1.50
20	3	310	CLA	MG-NA	2.20	2.11	2.06
20	A	5028	CLA	CMC-C2C	-2.20	1.46	1.50
20	8	301	CLA	CMD-C2D	-2.20	1.46	1.50
20	8	313	CLA	CMD-C2D	-2.19	1.46	1.50
20	B	829	CLA	CMB-C2B	-2.19	1.47	1.51
20	K	4004	CLA	CMC-C2C	-2.18	1.46	1.50
20	B	815	CLA	CMD-C2D	-2.18	1.46	1.50
20	A	5021	CLA	CMD-C2D	-2.18	1.46	1.50
23	3	319	BCR	C17-C18	2.18	1.40	1.35
20	7	303	CLA	CMC-C2C	-2.18	1.46	1.50
20	L	202	CLA	CMD-C2D	-2.17	1.46	1.50
20	B	839	CLA	C3B-C2B	-2.17	1.37	1.40
20	B	836	CLA	CMD-C2D	-2.16	1.46	1.50
20	F	306	CLA	CMD-C2D	-2.16	1.46	1.50
20	A	5004	CLA	CMD-C2D	-2.16	1.46	1.50
20	9	610	CLA	MG-NA	2.16	2.11	2.06
20	A	5006	CLA	CMD-C2D	-2.16	1.46	1.50
20	3	302	CLA	CMD-C2D	-2.15	1.46	1.50
20	9	607	CLA	C3B-C2B	-2.15	1.37	1.40
20	A	5030	CLA	CMD-C2D	-2.15	1.46	1.50
20	A	5012	CLA	CMC-C2C	-2.15	1.46	1.50
20	A	5013	CLA	CMD-C2D	-2.15	1.46	1.50
20	B	805	CLA	CMD-C2D	-2.15	1.46	1.50
20	B	833	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	810	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	832	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	810	CLA	MG-ND	-2.14	2.01	2.05
20	3	306	CLA	CMD-C2D	-2.14	1.46	1.50
20	A	5014	CLA	CMC-C2C	-2.14	1.46	1.50
20	9	607	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	808	CLA	CMD-C2D	-2.13	1.46	1.50
20	B	804	CLA	CMD-C2D	-2.13	1.46	1.50
20	B	837	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5039	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	804	CLA	CMC-C2C	-2.12	1.46	1.50
23	3	319	BCR	C14-C13	2.12	1.40	1.35
23	3	319	BCR	C10-C9	2.12	1.40	1.35
20	A	5035	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	814	CLA	CMD-C2D	-2.12	1.46	1.50
20	1	611	CLA	CMC-C2C	-2.12	1.46	1.50
20	2	307	CLA	CMD-C2D	-2.12	1.46	1.50
20	2	303	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	826	CLA	CMC-C2C	-2.12	1.46	1.50
20	A	5030	CLA	MG-ND	-2.12	2.01	2.05
20	A	5024	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	807	CLA	CMC-C2C	-2.11	1.46	1.50
20	A	5044	CLA	CMD-C2D	-2.11	1.46	1.50
20	3	311	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	5011	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	5042	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	5029	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	817	CLA	CMC-C2C	-2.11	1.46	1.50
20	B	830	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	5019	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	5017	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	821	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	5041	CLA	MG-NC	2.10	2.11	2.06
20	8	310	CLA	CMD-C2D	-2.10	1.46	1.50
20	1	609	CLA	CMD-C2D	-2.10	1.46	1.50
20	7	312	CLA	MG-NA	2.10	2.11	2.06
20	9	603	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	5008	CLA	CMD-C2D	-2.10	1.46	1.50
20	3	325	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	810	CLA	CMC-C2C	-2.09	1.46	1.50
20	K	4004	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	5014	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	5026	CLA	CMD-C2D	-2.09	1.46	1.50
20	1	602	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	824	CLA	CMC-C2C	-2.09	1.46	1.50
20	7	312	CLA	CMD-C2D	-2.09	1.46	1.50
20	3	313	CLA	MG-NA	2.09	2.11	2.06
20	1	609	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	831	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	806	CLA	CMD-C2D	-2.08	1.46	1.50
20	7	315	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5018	CLA	CMC-C2C	-2.08	1.46	1.50
20	9	612	CLA	CMD-C2D	-2.08	1.46	1.50
20	G	204	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	5038	CLA	MG-ND	-2.07	2.01	2.05
20	L	201	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	823	CLA	CMD-C2D	-2.07	1.46	1.50
20	8	308	CLA	CMD-C2D	-2.07	1.46	1.50
20	9	608	CLA	CMD-C2D	-2.07	1.46	1.50
20	7	311	CLA	CMD-C2D	-2.07	1.46	1.50
20	1	605	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	312	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	815	CLA	CMC-C2C	-2.07	1.46	1.50
20	8	311	CLA	CMD-C2D	-2.07	1.46	1.50
20	F	308	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	818	CLA	CMD-C2D	-2.07	1.46	1.50
20	1	604	CLA	CMD-C2D	-2.07	1.46	1.50
20	9	610	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	305	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	5009	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	828	CLA	CMC-C2C	-2.06	1.46	1.50
20	B	812	CLA	CMD-C2D	-2.06	1.46	1.50
20	F	307	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	807	CLA	CMD-C2D	-2.06	1.46	1.50
20	8	312	CLA	CMD-C2D	-2.06	1.46	1.50
20	3	313	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	823	CLA	CMC-C2C	-2.06	1.46	1.50
20	9	608	CLA	CMC-C2C	-2.06	1.46	1.50
20	3	310	CLA	CMD-C2D	-2.05	1.46	1.50
20	1	610	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	304	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5031	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5040	CLA	CMD-C2D	-2.05	1.46	1.50
20	7	314	CLA	CMD-C2D	-2.05	1.46	1.50
20	7	323	CLA	CMD-C2D	-2.05	1.46	1.50
20	9	611	CLA	CMD-C2D	-2.05	1.46	1.50
20	2	308	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	309	CLA	CMD-C2D	-2.05	1.46	1.50
20	9	601	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5025	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	840	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	303	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	611	CLA	CMD-C2D	-2.05	1.46	1.50
20	1	608	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5034	CLA	CMD-C2D	-2.05	1.46	1.50
20	8	307	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5020	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	817	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	839	CLA	CMD-C2D	-2.05	1.46	1.50
20	G	202	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5010	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	832	CLA	CMC-C2C	-2.05	1.46	1.50
20	1	613	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5009	CLA	CMC-C2C	-2.05	1.46	1.50
20	A	5033	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	5041	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	811	CLA	CMC-C2C	-2.05	1.46	1.50
20	7	309	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	826	CLA	CMD-C2D	-2.04	1.46	1.50
20	G	203	CLA	CMD-C2D	-2.04	1.46	1.50
20	8	302	CLA	CMD-C2D	-2.04	1.46	1.50
20	8	310	CLA	MG-NC	2.04	2.11	2.06
20	3	314	CLA	CMD-C2D	-2.04	1.46	1.50
20	7	310	CLA	CMD-C2D	-2.04	1.46	1.50
20	8	309	CLA	CMD-C2D	-2.04	1.46	1.50
20	1	603	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	813	CLA	MG-ND	-2.04	2.01	2.05
20	3	307	CLA	CMD-C2D	-2.04	1.46	1.50
20	J	104	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	5037	CLA	CMD-C2D	-2.04	1.46	1.50
20	2	303	CLA	C3D-C4D	2.04	1.48	1.44
20	K	4003	CLA	CMD-C2D	-2.04	1.46	1.50
20	2	309	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	816	CLA	CMD-C2D	-2.04	1.46	1.50
20	G	201	CLA	CMD-C2D	-2.03	1.46	1.50
20	H	201	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5044	CLA	MG-NA	2.03	2.11	2.06
20	2	305	CLA	CMD-C2D	-2.03	1.46	1.50
20	7	312	CLA	CMC-C2C	-2.03	1.46	1.50
20	7	303	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5038	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	805	CLA	CMC-C2C	-2.03	1.46	1.50
20	A	5023	CLA	CMD-C2D	-2.03	1.46	1.50
20	F	303	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	308	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	820	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	822	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	835	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	313	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5015	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5032	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	819	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5036	CLA	CMD-C2D	-2.03	1.46	1.50
20	8	303	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5016	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5022	CLA	CMC-C2C	-2.03	1.46	1.50
20	A	5028	CLA	CMD-C2D	-2.03	1.46	1.50
20	3	304	CLA	CMC-C2C	-2.03	1.46	1.50
20	A	5018	CLA	CMD-C2D	-2.03	1.46	1.50
20	L	204	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	811	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	5029	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	825	CLA	CMC-C2C	-2.02	1.46	1.50
20	2	304	CLA	CMD-C2D	-2.02	1.46	1.50
20	B	817	CLA	MG-ND	-2.02	2.01	2.05
20	B	805	CLA	MG-NA	-2.02	2.01	2.06
20	2	301	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	5042	CLA	MG-NC	2.02	2.11	2.06
20	A	5007	CLA	CMD-C2D	-2.02	1.46	1.50
20	F	303	CLA	MG-NA	2.02	2.11	2.06
20	A	5006	CLA	CMC-C2C	-2.02	1.46	1.50
20	A	5039	CLA	CMC-C2C	-2.02	1.46	1.50
20	A	5022	CLA	CMD-C2D	-2.02	1.46	1.50
20	L	205	CLA	CMD-C2D	-2.02	1.46	1.50
20	7	323	CLA	MG-ND	-2.02	2.01	2.05
20	3	310	CLA	CMC-C2C	-2.02	1.46	1.50
20	7	313	CLA	CMD-C2D	-2.02	1.46	1.50
20	8	303	CLA	CMC-C2C	-2.02	1.46	1.50
20	9	604	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	5026	CLA	MG-ND	-2.02	2.01	2.05
20	7	305	CLA	CMD-C2D	-2.02	1.46	1.50
20	B	809	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	5016	CLA	CMC-C2C	-2.02	1.46	1.50
20	A	5019	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	820	CLA	MG-ND	-2.02	2.01	2.05
20	8	310	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	9	611	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	818	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	5027	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	5007	CLA	CMC-C2C	-2.01	1.46	1.50
20	2	310	CLA	CMC-C2C	-2.01	1.46	1.50
20	7	304	CLA	CMD-C2D	-2.01	1.46	1.50
20	9	602	CLA	CMD-C2D	-2.01	1.46	1.50
20	1	607	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	5019	CLA	MG-ND	-2.01	2.01	2.05
20	2	310	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	834	CLA	CMD-C2D	-2.01	1.46	1.50
20	7	311	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	5043	CLA	CMD-C2D	-2.01	1.46	1.50
20	8	309	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	831	CLA	CMC-C2C	-2.00	1.46	1.50
20	K	4005	CLA	CMD-C2D	-2.00	1.46	1.50
20	9	609	CLA	CMD-C2D	-2.00	1.46	1.50
20	A	5025	CLA	CMC-C2C	-2.00	1.46	1.50
20	1	605	CLA	CMC-C2C	-2.00	1.46	1.50
20	9	605	CLA	CMD-C2D	-2.00	1.46	1.50

All (1380) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	304	CHL	C4A-NA-C1A	15.46	113.73	106.68
19	7	307	CHL	C4A-NA-C1A	14.62	113.35	106.68
19	3	323	CHL	C4A-NA-C1A	14.54	113.31	106.68
19	8	305	CHL	C4A-NA-C1A	14.54	113.31	106.68
30	A	5003	CL0	C4A-NA-C1A	12.73	112.49	106.68
19	3	301	CHL	C4A-NA-C1A	12.66	112.45	106.68
19	2	302	CHL	C4A-NA-C1A	12.08	112.19	106.68
19	7	306	CHL	C4A-NA-C1A	12.02	112.16	106.68
19	2	306	CHL	C4A-NA-C1A	11.13	111.75	106.68
19	7	308	CHL	C4A-NA-C1A	10.92	111.66	106.68
19	9	606	CHL	C4A-NA-C1A	10.77	111.59	106.68
19	8	306	CHL	C4A-NA-C1A	10.74	111.58	106.68
19	1	606	CHL	C4A-NA-C1A	9.94	111.22	106.68
20	F	303	CLA	C4A-NA-C1A	7.46	110.08	106.68
20	A	5026	CLA	C4A-NA-C1A	7.35	110.03	106.68
20	B	820	CLA	C4A-NA-C1A	7.16	109.95	106.68
20	9	605	CLA	C4A-NA-C1A	6.81	109.78	106.68
20	K	4005	CLA	C4A-NA-C1A	6.78	109.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	835	CLA	C4A-NA-C1A	6.75	109.76	106.68
20	3	310	CLA	C4A-NA-C1A	6.73	109.75	106.68
20	9	603	CLA	C4A-NA-C1A	6.71	109.74	106.68
20	8	310	CLA	C4A-NA-C1A	6.69	109.73	106.68
20	9	611	CLA	C4A-NA-C1A	6.65	109.71	106.68
20	A	5023	CLA	C4A-NA-C1A	6.64	109.71	106.68
19	1	601	CHL	C4A-NA-C1A	6.63	109.70	106.68
20	2	310	CLA	C4A-NA-C1A	6.62	109.70	106.68
20	A	5017	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	8	307	CLA	C1C-C2C-C3C	-6.56	100.08	106.98
20	A	5028	CLA	C4A-NA-C1A	6.48	109.64	106.68
20	A	5009	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	7	312	CLA	C4A-NA-C1A	6.41	109.60	106.68
20	8	302	CLA	C4A-NA-C1A	6.38	109.59	106.68
20	G	202	CLA	C4A-NA-C1A	6.30	109.55	106.68
20	A	5030	CLA	C4A-NA-C1A	6.28	109.55	106.68
20	1	611	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	B	833	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	A	5015	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	7	305	CLA	C4A-NA-C1A	6.18	109.50	106.68
20	1	605	CLA	C4A-NA-C1A	6.15	109.48	106.68
20	1	613	CLA	C4A-NA-C1A	6.12	109.47	106.68
20	2	313	CLA	C4A-NA-C1A	6.09	109.46	106.68
20	A	5014	CLA	C4A-NA-C1A	6.06	109.44	106.68
20	B	826	CLA	C4A-NA-C1A	6.03	109.43	106.68
20	B	817	CLA	C4A-NA-C1A	5.96	109.40	106.68
20	K	4002	CLA	C4A-NA-C1A	5.96	109.40	106.68
20	B	837	CLA	C4A-NA-C1A	5.94	109.39	106.68
20	A	5031	CLA	C4A-NA-C1A	5.94	109.39	106.68
20	9	610	CLA	C4A-NA-C1A	5.93	109.38	106.68
20	B	811	CLA	C4A-NA-C1A	5.92	109.38	106.68
20	3	303	CLA	C4A-NA-C1A	5.92	109.38	106.68
20	K	4004	CLA	C4A-NA-C1A	5.88	109.36	106.68
20	8	312	CLA	C4A-NA-C1A	5.85	109.35	106.68
20	B	824	CLA	C4A-NA-C1A	5.83	109.34	106.68
20	3	311	CLA	C4A-NA-C1A	5.82	109.34	106.68
20	7	315	CLA	C4A-NA-C1A	5.78	109.32	106.68
20	A	5010	CLA	C4A-NA-C1A	5.76	109.31	106.68
20	B	821	CLA	C4A-NA-C1A	5.75	109.30	106.68
20	1	602	CLA	C4A-NA-C1A	5.73	109.30	106.68
20	A	5034	CLA	C4A-NA-C1A	5.72	109.29	106.68
20	B	809	CLA	C4A-NA-C1A	5.70	109.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	313	CLA	C4A-NA-C1A	5.67	109.27	106.68
20	2	303	CLA	C4A-NA-C1A	5.61	109.24	106.68
20	A	5018	CLA	C4A-NA-C1A	5.60	109.24	106.68
20	F	308	CLA	C4A-NA-C1A	5.58	109.22	106.68
20	7	311	CLA	C4A-NA-C1A	5.56	109.22	106.68
20	B	814	CLA	C4A-NA-C1A	5.55	109.21	106.68
20	J	104	CLA	C4A-NA-C1A	5.55	109.21	106.68
20	A	5038	CLA	C4A-NA-C1A	5.53	109.20	106.68
20	A	5032	CLA	C4A-NA-C1A	5.53	109.20	106.68
20	B	830	CLA	C4A-NA-C1A	5.52	109.20	106.68
20	A	5042	CLA	C4A-NA-C1A	5.51	109.19	106.68
20	8	309	CLA	C4A-NA-C1A	5.50	109.19	106.68
20	1	614	CLA	C4A-NA-C1A	5.50	109.19	106.68
20	B	816	CLA	C4A-NA-C1A	5.48	109.18	106.68
20	A	5036	CLA	C4A-NA-C1A	5.48	109.18	106.68
20	B	822	CLA	C4A-NA-C1A	5.48	109.18	106.68
20	A	5006	CLA	C4A-NA-C1A	5.46	109.17	106.68
20	7	323	CLA	C4A-NA-C1A	5.43	109.16	106.68
20	3	302	CLA	C4A-NA-C1A	5.43	109.16	106.68
20	2	311	CLA	C4A-NA-C1A	5.43	109.16	106.68
26	7	302	PTY	O11-P1-O14	-5.42	92.53	106.67
20	3	325	CLA	C4A-NA-C1A	5.41	109.15	106.68
20	L	201	CLA	C4A-NA-C1A	5.40	109.14	106.68
20	1	603	CLA	C4A-NA-C1A	5.34	109.12	106.68
20	A	5019	CLA	C4A-NA-C1A	5.34	109.11	106.68
20	B	838	CLA	C4A-NA-C1A	5.32	109.11	106.68
20	7	304	CLA	C4A-NA-C1A	5.32	109.11	106.68
20	3	314	CLA	C4A-NA-C1A	5.30	109.10	106.68
20	B	828	CLA	C4A-NA-C1A	5.30	109.09	106.68
20	G	203	CLA	C4A-NA-C1A	5.27	109.08	106.68
20	A	5041	CLA	C4A-NA-C1A	5.26	109.08	106.68
20	1	608	CLA	C4A-NA-C1A	5.20	109.05	106.68
20	A	5039	CLA	C4A-NA-C1A	5.17	109.04	106.68
20	2	312	CLA	C4A-NA-C1A	5.14	109.03	106.68
20	B	819	CLA	C4A-NA-C1A	5.13	109.02	106.68
20	7	309	CLA	C4A-NA-C1A	5.13	109.02	106.68
20	A	5027	CLA	C4A-NA-C1A	5.12	109.02	106.68
20	A	5025	CLA	C4A-NA-C1A	5.08	109.00	106.68
20	B	831	CLA	C4A-NA-C1A	5.05	108.98	106.68
20	B	813	CLA	C4A-NA-C1A	5.05	108.98	106.68
20	B	834	CLA	C4A-NA-C1A	5.05	108.98	106.68
20	B	812	CLA	C4A-NA-C1A	5.02	108.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5022	CLA	C4A-NA-C1A	5.02	108.97	106.68
20	1	612	CLA	C4A-NA-C1A	5.01	108.97	106.68
20	7	314	CLA	C4A-NA-C1A	5.01	108.96	106.68
20	L	205	CLA	C4A-NA-C1A	5.00	108.96	106.68
20	B	829	CLA	C4A-NA-C1A	4.95	108.94	106.68
20	A	5044	CLA	CMB-C2B-C1B	-4.94	121.22	128.46
20	A	5035	CLA	C4A-NA-C1A	4.93	108.93	106.68
20	F	307	CLA	C4A-NA-C1A	4.91	108.92	106.68
20	G	204	CLA	C4A-NA-C1A	4.91	108.92	106.68
21	1	615	LUT	C35-C15-C14	4.91	133.56	123.52
20	2	309	CLA	C4A-NA-C1A	4.90	108.92	106.68
20	9	609	CLA	C4A-NA-C1A	4.88	108.91	106.68
20	A	5016	CLA	C4A-NA-C1A	4.86	108.90	106.68
20	8	307	CLA	C4A-NA-C1A	4.82	108.88	106.68
20	A	5033	CLA	C4A-NA-C1A	4.82	108.88	106.68
20	2	305	CLA	C4A-NA-C1A	4.79	108.86	106.68
20	3	306	CLA	C4A-NA-C1A	4.77	108.86	106.68
20	8	313	CLA	C4A-NA-C1A	4.71	108.83	106.68
20	3	324	CLA	C4A-NA-C1A	4.69	108.82	106.68
20	8	311	CLA	C4A-NA-C1A	4.68	108.81	106.68
20	A	5020	CLA	C4A-NA-C1A	4.67	108.81	106.68
20	A	5043	CLA	C4A-NA-C1A	4.67	108.81	106.68
20	3	304	CLA	C4A-NA-C1A	4.64	108.80	106.68
20	A	5004	CLA	CMB-C2B-C1B	-4.62	121.68	128.46
20	B	806	CLA	C4A-NA-C1A	4.62	108.79	106.68
20	B	807	CLA	CMB-C2B-C1B	-4.62	121.69	128.46
20	1	609	CLA	C4A-NA-C1A	4.61	108.78	106.68
21	2	314	LUT	C26-C27-C28	4.58	131.70	124.58
20	1	610	CLA	C4A-NA-C1A	4.55	108.75	106.68
20	A	5037	CLA	C4A-NA-C1A	4.55	108.75	106.68
20	A	5044	CLA	C4A-NA-C1A	4.54	108.75	106.68
20	L	202	CLA	C4A-NA-C1A	4.53	108.75	106.68
20	3	305	CLA	C4A-NA-C1A	4.50	108.73	106.68
19	8	304	CHL	C1D-CHD-C4C	-4.47	116.51	126.02
21	1	615	LUT	C15-C35-C34	-4.46	114.39	123.52
20	3	309	CLA	C4A-NA-C1A	4.46	108.71	106.68
20	8	321	CLA	CHB-C4A-NA	4.45	130.83	124.40
20	B	806	CLA	CMB-C2B-C1B	-4.45	121.93	128.46
20	A	5016	CLA	CMB-C2B-C1B	-4.45	121.94	128.46
20	F	303	CLA	CMB-C2B-C1B	-4.44	121.95	128.46
20	2	307	CLA	C4A-NA-C1A	4.42	108.69	106.68
20	3	307	CLA	C4A-NA-C1A	4.36	108.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	827	CLA	C4A-NA-C1A	4.36	108.67	106.68
20	A	5008	CLA	CMB-C2B-C1B	-4.34	122.10	128.46
20	2	301	CLA	C4A-NA-C1A	4.34	108.66	106.68
20	B	807	CLA	C4A-NA-C1A	4.30	108.64	106.68
26	3	321	PTY	C6-O7-C8	4.30	128.08	117.80
21	2	314	LUT	C21-C26-C27	4.29	117.76	112.83
20	1	607	CLA	C4A-NA-C1A	4.28	108.63	106.68
20	B	805	CLA	CMB-C2B-C1B	-4.28	122.18	128.46
20	B	816	CLA	CMB-C2B-C1B	-4.27	122.19	128.46
20	8	307	CLA	CHC-C1C-NC	-4.27	117.88	124.31
19	8	306	CHL	C1-C2-C3	-4.27	119.86	126.76
20	A	5013	CLA	C4A-NA-C1A	4.23	108.61	106.68
20	A	5040	CLA	C4A-NA-C1A	4.23	108.61	106.68
20	3	305	CLA	CMB-C2B-C1B	-4.23	122.27	128.46
20	H	201	CLA	C4A-NA-C1A	4.22	108.60	106.68
20	A	5021	CLA	C4A-NA-C1A	4.20	108.60	106.68
20	1	604	CLA	CMB-C2B-C1B	-4.19	122.32	128.46
20	A	5005	CLA	CMB-C2B-C1B	-4.19	122.32	128.46
20	3	312	CLA	C4A-NA-C1A	4.18	108.59	106.68
20	A	5011	CLA	C4A-NA-C1A	4.18	108.59	106.68
20	9	602	CLA	CMB-C2B-C1B	-4.18	122.33	128.46
20	B	838	CLA	CMB-C2B-C1B	-4.12	122.42	128.46
20	A	5029	CLA	C4A-NA-C1A	4.12	108.56	106.68
20	B	826	CLA	CMB-C2B-C1B	-4.11	122.44	128.46
20	A	5005	CLA	C4A-NA-C1A	4.11	108.55	106.68
19	3	301	CHL	C1-C2-C3	-4.10	119.48	126.20
20	A	5038	CLA	CMB-C2B-C1B	-4.09	122.46	128.46
20	9	612	CLA	C4A-NA-C1A	4.09	108.54	106.68
20	A	5007	CLA	CMB-C2B-C1B	-4.07	122.49	128.46
20	B	824	CLA	CMB-C2B-C1B	-4.07	122.50	128.46
20	B	818	CLA	C4A-NA-C1A	4.05	108.53	106.68
20	B	835	CLA	CMB-C2B-C1B	-4.03	122.55	128.46
19	2	306	CHL	CHD-C4C-C3C	4.03	130.64	124.77
20	1	605	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
20	1	614	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
20	A	5043	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
20	B	815	CLA	C4A-NA-C1A	4.01	108.51	106.68
20	3	304	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
20	3	313	CLA	C4A-NA-C1A	4.01	108.51	106.68
20	B	827	CLA	CMB-C2B-C1B	-3.98	122.63	128.46
20	A	5022	CLA	CMB-C2B-C1B	-3.97	122.64	128.46
20	8	307	CLA	CMB-C2B-C1B	-3.97	122.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	321	CLA	C2A-C1A-CHA	3.96	130.74	123.87
20	A	5026	CLA	CMB-C2B-C1B	-3.96	122.66	128.46
20	B	839	CLA	CMB-C2B-C1B	-3.95	122.66	128.46
20	8	321	CLA	C4A-NA-C1A	3.95	108.48	106.68
20	B	831	CLA	CMB-C2B-C1B	-3.95	122.67	128.46
23	3	319	BCR	C16-C15-C14	3.94	131.58	123.52
23	J	102	BCR	C23-C24-C25	3.94	137.52	127.00
20	K	4003	CLA	C4A-NA-C1A	3.93	108.47	106.68
20	A	5029	CLA	CMB-C2B-C1B	-3.93	122.70	128.46
20	B	815	CLA	CMB-C2B-C1B	-3.93	122.70	128.46
20	F	306	CLA	CMB-C2B-C1B	-3.89	122.76	128.46
20	B	805	CLA	C4A-NA-C1A	-3.88	104.91	106.68
20	3	306	CLA	CMB-C2B-C1B	-3.87	122.79	128.46
20	9	610	CLA	CMB-C2B-C1B	-3.87	122.79	128.46
20	A	5014	CLA	CMB-C2B-C1B	-3.86	122.80	128.46
19	7	307	CHL	CHD-C4C-C3C	3.84	130.37	124.77
20	B	828	CLA	CMB-C2B-C1B	-3.84	122.83	128.46
20	B	818	CLA	CMB-C2B-C1B	-3.83	122.84	128.46
20	8	307	CLA	CMC-C2C-C1C	3.83	131.02	125.03
20	2	304	CLA	CMB-C2B-C1B	-3.83	122.85	128.46
20	A	5044	CLA	CMB-C2B-C3B	3.83	132.33	124.68
20	9	601	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
20	L	205	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
20	9	607	CLA	CMB-C2B-C1B	-3.82	122.86	128.46
19	8	304	CHL	CHD-C4C-C3C	3.81	130.34	124.77
20	B	817	CLA	CMB-C2B-C1B	-3.81	122.87	128.46
19	3	323	CHL	C1-C2-C3	-3.80	119.96	126.20
20	B	834	CLA	CMB-C2B-C1B	-3.80	122.89	128.46
20	A	5013	CLA	CMB-C2B-C1B	-3.80	122.89	128.46
20	1	609	CLA	CMB-C2B-C1B	-3.79	122.90	128.46
20	B	819	CLA	CMB-C2B-C1B	-3.78	122.92	128.46
20	A	5020	CLA	CMB-C2B-C1B	-3.78	122.92	128.46
20	3	302	CLA	CMB-C2B-C1B	-3.77	122.93	128.46
20	1	604	CLA	C4A-NA-C1A	3.77	108.40	106.68
20	G	202	CLA	CMB-C2B-C1B	-3.77	122.94	128.46
20	A	5028	CLA	CMB-C2B-C1B	-3.76	122.94	128.46
20	A	5030	CLA	CMB-C2B-C1B	-3.76	122.95	128.46
20	9	608	CLA	CMB-C2B-C1B	-3.76	122.95	128.46
20	A	5015	CLA	CMB-C2B-C1B	-3.75	122.96	128.46
20	L	202	CLA	CMB-C2B-C1B	-3.75	122.96	128.46
20	7	315	CLA	CMB-C2B-C1B	-3.75	122.97	128.46
19	2	302	CHL	C1-C2-C3	-3.74	120.06	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	5003	CL0	C1-C2-C3	-3.74	120.07	126.20
20	B	825	CLA	CMB-C2B-C1B	-3.74	122.98	128.46
20	3	303	CLA	CMB-C2B-C1B	-3.73	122.98	128.46
19	8	306	CHL	CHD-C4C-C3C	3.73	130.22	124.77
20	7	310	CLA	CMB-C2B-C1B	-3.73	122.99	128.46
20	L	204	CLA	CMB-C2B-C1B	-3.73	122.99	128.46
20	A	5027	CLA	CMB-C2B-C1B	-3.73	123.00	128.46
20	3	325	CLA	CMB-C2B-C1B	-3.72	123.00	128.46
20	B	813	CLA	CMB-C2B-C1B	-3.72	123.01	128.46
30	A	5003	CL0	CHD-C4C-C3C	3.72	130.19	124.77
20	2	305	CLA	CMB-C2B-C1B	-3.71	123.01	128.46
20	9	608	CLA	C4A-NA-C1A	3.71	108.37	106.68
19	9	606	CHL	C2D-C1D-ND	-3.71	106.46	110.13
20	A	5040	CLA	CMB-C2B-C1B	-3.70	123.03	128.46
20	8	307	CLA	C1B-CHB-C4A	-3.69	123.01	130.04
20	F	306	CLA	C4A-NA-C1A	3.69	108.36	106.68
20	1	602	CLA	CMB-C2B-C1B	-3.69	123.06	128.46
20	A	5039	CLA	CMB-C2B-C1B	-3.67	123.08	128.46
20	3	308	CLA	CMB-C2B-C1B	-3.66	123.09	128.46
20	B	837	CLA	CMB-C2B-C1B	-3.66	123.09	128.46
19	8	306	CHL	C2D-C1D-ND	-3.66	106.50	110.13
20	A	5010	CLA	CMB-C2B-C1B	-3.66	123.09	128.46
20	A	5023	CLA	CMB-C2B-C1B	-3.66	123.09	128.46
20	A	5037	CLA	CMB-C2B-C1B	-3.66	123.09	128.46
20	B	836	CLA	CMB-C2B-C1B	-3.66	123.10	128.46
20	8	308	CLA	CMB-C2B-C1B	-3.65	123.11	128.46
20	9	605	CLA	CMB-C2B-C1B	-3.65	123.11	128.46
23	3	319	BCR	C15-C16-C17	3.65	130.98	123.52
20	A	5042	CLA	CMB-C2B-C1B	-3.64	123.12	128.46
20	B	808	CLA	CMB-C2B-C1B	-3.64	123.12	128.46
20	A	5032	CLA	CMB-C2B-C1B	-3.63	123.13	128.46
19	3	323	CHL	CHD-C4C-C3C	3.63	130.07	124.77
19	3	323	CHL	C2D-C1D-ND	-3.63	106.53	110.13
20	2	310	CLA	CMB-C2B-C1B	-3.62	123.15	128.46
20	G	201	CLA	CMB-C2B-C1B	-3.61	123.17	128.46
20	7	303	CLA	CMB-C2B-C1B	-3.61	123.17	128.46
19	8	305	CHL	CHD-C4C-C3C	3.60	130.03	124.77
20	A	5011	CLA	CMB-C2B-C1B	-3.60	123.18	128.46
20	A	5018	CLA	CMB-C2B-C1B	-3.60	123.18	128.46
19	2	302	CHL	CHD-C4C-C3C	3.60	130.02	124.77
20	7	309	CLA	CMB-C2B-C1B	-3.60	123.19	128.46
20	A	5034	CLA	CMB-C2B-C1B	-3.59	123.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	303	CLA	CMB-C2B-C1B	-3.59	123.19	128.46
20	3	310	CLA	CMB-C2B-C1B	-3.59	123.20	128.46
20	F	308	CLA	CMB-C2B-C1B	-3.58	123.20	128.46
23	A	5049	BCR	C16-C15-C14	3.58	130.85	123.52
20	7	314	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
20	7	311	CLA	CMB-C2B-C1B	-3.58	123.21	128.46
20	1	603	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
20	1	607	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
20	9	604	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
20	A	5012	CLA	CMB-C2B-C1B	-3.58	123.22	128.46
20	B	810	CLA	CMB-C2B-C1B	-3.57	123.22	128.46
20	1	610	CLA	CMB-C2B-C1B	-3.57	123.23	128.46
19	1	601	CHL	C2A-C1A-CHA	3.57	130.06	123.87
20	8	312	CLA	CMB-C2B-C1B	-3.57	123.23	128.46
20	2	312	CLA	CMB-C2B-C1B	-3.56	123.24	128.46
20	3	314	CLA	CMB-C2B-C1B	-3.56	123.24	128.46
20	1	613	CLA	CMB-C2B-C1B	-3.56	123.25	128.46
20	K	4003	CLA	CMB-C2B-C1B	-3.56	123.25	128.46
20	2	308	CLA	CMB-C2B-C1B	-3.55	123.25	128.46
20	B	840	CLA	CMB-C2B-C1B	-3.55	123.25	128.46
20	B	814	CLA	CMB-C2B-C1B	-3.55	123.25	128.46
20	7	323	CLA	CMB-C2B-C1B	-3.55	123.25	128.46
20	8	310	CLA	CMB-C2B-C1B	-3.55	123.26	128.46
19	1	606	CHL	CHD-C4C-C3C	3.54	129.94	124.77
20	B	805	CLA	CMB-C2B-C3B	3.54	131.76	124.68
20	8	309	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
23	3	319	BCR	C34-C9-C10	-3.53	117.09	122.82
20	9	612	CLA	CMB-C2B-C1B	-3.53	123.28	128.46
20	B	832	CLA	C4A-NA-C1A	3.53	108.29	106.68
20	3	312	CLA	CMB-C2B-C1B	-3.53	123.28	128.46
20	9	609	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
20	G	203	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
20	A	5041	CLA	CMB-C2B-C1B	-3.53	123.29	128.46
20	B	807	CLA	CMB-C2B-C3B	3.53	131.73	124.68
20	A	5033	CLA	CMB-C2B-C1B	-3.52	123.29	128.46
20	7	312	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
20	A	5036	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
20	2	311	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
20	K	4004	CLA	CMB-C2B-C1B	-3.52	123.30	128.46
20	F	307	CLA	CMB-C2B-C1B	-3.52	123.31	128.46
20	3	309	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
20	A	5019	CLA	CMB-C2B-C1B	-3.51	123.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	306	CHL	CHD-C4C-C3C	3.51	129.89	124.77
20	7	304	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
20	B	821	CLA	CMB-C2B-C1B	-3.51	123.31	128.46
20	1	611	CLA	CMB-C2B-C1B	-3.51	123.32	128.46
20	K	4005	CLA	CMB-C2B-C1B	-3.51	123.32	128.46
20	1	608	CLA	CMB-C2B-C1B	-3.50	123.32	128.46
20	9	611	CLA	CMB-C2B-C1B	-3.50	123.32	128.46
20	B	833	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
20	2	303	CLA	CMB-C2B-C1B	-3.50	123.33	128.46
20	8	311	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
20	8	301	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
20	2	309	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
20	A	5006	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
20	2	313	CLA	CMB-C2B-C1B	-3.49	123.34	128.46
20	A	5024	CLA	CMB-C2B-C1B	-3.48	123.35	128.46
20	B	811	CLA	CMB-C2B-C1B	-3.48	123.35	128.46
20	J	104	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
20	A	5021	CLA	CMB-C2B-C1B	-3.48	123.36	128.46
20	B	809	CLA	CMB-C2B-C1B	-3.47	123.36	128.46
20	8	313	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
20	3	313	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
20	A	5009	CLA	CMB-C2B-C1B	-3.47	123.38	128.46
20	3	311	CLA	CMB-C2B-C1B	-3.46	123.38	128.46
20	2	301	CLA	CMB-C2B-C1B	-3.46	123.39	128.46
20	L	201	CLA	CMB-C2B-C1B	-3.44	123.41	128.46
22	1	616	XAT	C27-C28-C29	3.44	130.87	125.53
20	F	303	CLA	CMB-C2B-C3B	3.44	131.56	124.68
20	8	302	CLA	CMB-C2B-C1B	-3.44	123.42	128.46
20	9	604	CLA	C4A-NA-C1A	3.44	108.25	106.68
20	B	823	CLA	CMB-C2B-C1B	-3.43	123.43	128.46
20	9	603	CLA	CMB-C2B-C1B	-3.43	123.44	128.46
20	B	806	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
20	A	5044	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
20	A	5006	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
20	B	822	CLA	CMB-C2B-C1B	-3.39	123.49	128.46
20	3	307	CLA	CMB-C2B-C1B	-3.39	123.50	128.46
20	3	324	CLA	CMB-C2B-C1B	-3.38	123.50	128.46
20	8	307	CLA	C2C-C1C-NC	3.38	113.54	109.98
20	B	810	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
23	3	319	BCR	C37-C22-C21	-3.38	117.34	122.82
20	7	313	CLA	CMB-C2B-C1B	-3.38	123.50	128.46
20	H	201	CLA	CMB-C2B-C1B	-3.38	123.51	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	5049	BCR	C21-C20-C19	3.37	132.97	123.20
20	A	5023	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
20	B	810	CLA	C4A-NA-C1A	3.37	108.22	106.68
23	3	319	BCR	C19-C18-C17	3.37	124.30	119.01
20	B	830	CLA	CMB-C2B-C1B	-3.37	123.53	128.46
20	B	824	CLA	CHB-C4A-NA	3.36	129.25	124.40
20	1	612	CLA	CMB-C2B-C1B	-3.35	123.54	128.46
20	A	5017	CLA	CMB-C2B-C1B	-3.35	123.55	128.46
20	B	806	CLA	CMB-C2B-C3B	3.35	131.38	124.68
20	B	836	CLA	C4A-NA-C1A	3.35	108.21	106.68
20	H	201	CLA	C2A-C1A-CHA	3.35	129.67	123.87
20	2	307	CLA	CMB-C2B-C1B	-3.35	123.56	128.46
20	B	829	CLA	CMB-C2B-C1B	-3.33	123.58	128.46
20	A	5005	CLA	C1B-CHB-C4A	-3.32	123.70	130.04
20	A	5035	CLA	CMB-C2B-C1B	-3.32	123.60	128.46
20	A	5038	CLA	CMB-C2B-C3B	3.31	131.30	124.68
20	A	5004	CLA	C1B-CHB-C4A	-3.31	123.73	130.04
19	1	601	CHL	C2D-C1D-ND	-3.31	106.86	110.13
20	B	832	CLA	CMB-C2B-C1B	-3.29	123.63	128.46
20	B	812	CLA	CMB-C2B-C1B	-3.29	123.64	128.46
20	8	308	CLA	CHB-C4A-NA	3.28	129.13	124.40
20	1	604	CLA	CHB-C4A-NA	3.28	129.13	124.40
19	1	601	CHL	CHD-C4C-C3C	3.27	129.54	124.77
23	3	319	BCR	C36-C18-C17	-3.26	117.53	122.82
20	A	5008	CLA	CMB-C2B-C3B	3.25	131.18	124.68
20	A	5014	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
20	8	301	CLA	CHB-C4A-NA	3.25	129.09	124.40
20	A	5016	CLA	CMB-C2B-C3B	3.25	131.18	124.68
20	8	301	CLA	C4A-NA-C1A	3.25	108.16	106.68
20	1	604	CLA	CMB-C2B-C3B	3.24	131.16	124.68
19	9	606	CHL	CHD-C4C-C3C	3.24	129.49	124.77
20	K	4002	CLA	CMB-C2B-C1B	-3.23	123.72	128.46
20	B	804	CLA	CMB-C2B-C1B	-3.22	123.73	128.46
19	7	308	CHL	CHD-C4C-C3C	3.22	129.47	124.77
20	3	308	CLA	CHB-C4A-NA	3.22	129.04	124.40
19	2	306	CHL	C2D-C1D-ND	-3.22	106.94	110.13
20	9	602	CLA	CMB-C2B-C3B	3.21	131.10	124.68
20	7	305	CLA	CMB-C2B-C1B	-3.21	123.75	128.46
19	8	305	CHL	C2D-C1D-ND	-3.21	106.95	110.13
20	B	815	CLA	CHB-C4A-NA	3.21	129.03	124.40
20	B	827	CLA	CHB-C4A-NA	3.21	129.03	124.40
20	L	201	CLA	O2D-CGD-O1D	-3.20	117.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	606	CHL	C1D-ND-C4D	3.20	108.55	106.31
20	9	601	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
19	9	606	CHL	C2A-C1A-CHA	3.18	129.39	123.87
20	3	324	CLA	CHB-C4A-NA	3.18	128.99	124.40
20	B	834	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
20	A	5037	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
20	A	5020	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
20	7	303	CLA	CHB-C4A-NA	3.17	128.98	124.40
20	B	804	CLA	C1B-CHB-C4A	-3.17	123.99	130.04
20	8	321	CLA	CMB-C2B-C1B	-3.17	123.81	128.46
19	2	302	CHL	C2D-C1D-ND	-3.17	106.99	110.13
22	9	615	XAT	C7-C8-C9	3.17	130.45	125.53
20	9	607	CLA	C1B-CHB-C4A	-3.16	124.01	130.04
20	B	823	CLA	C4A-NA-C1A	3.16	108.12	106.68
20	B	808	CLA	C4A-NA-C1A	3.16	108.12	106.68
20	B	816	CLA	CMB-C2B-C3B	3.15	130.99	124.68
20	B	832	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
20	K	4003	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
20	9	607	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
20	7	310	CLA	CHB-C4A-NA	3.14	128.94	124.40
20	B	835	CLA	CMB-C2B-C3B	3.14	130.96	124.68
20	3	305	CLA	CMB-C2B-C3B	3.14	130.95	124.68
20	F	303	CLA	CAC-C3C-C4C	3.14	128.87	124.79
20	3	307	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
20	A	5007	CLA	CMB-C2B-C3B	3.11	130.89	124.68
20	A	5035	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
20	B	839	CLA	C4A-NA-C1A	3.09	108.09	106.68
20	9	611	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
20	A	5035	CLA	CHB-C4A-NA	3.09	128.86	124.40
20	B	824	CLA	CMB-C2B-C3B	3.09	130.85	124.68
22	3	316	XAT	C27-C28-C29	3.08	130.31	125.53
20	B	817	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
20	1	608	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
20	A	5043	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
19	1	606	CHL	C2D-C1D-ND	-3.06	107.09	110.13
20	B	824	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
20	2	308	CLA	C1B-CHB-C4A	-3.06	124.20	130.04
19	7	306	CHL	C3D-C2D-C1D	3.06	110.00	105.83
20	G	204	CLA	C1B-CHB-C4A	-3.05	124.22	130.04
20	8	307	CLA	CMB-C2B-C3B	3.05	130.78	124.68
20	2	304	CLA	C1B-CHB-C4A	-3.05	124.23	130.04
20	B	807	CLA	CHB-C4A-NA	3.05	128.80	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	308	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
31	B	841	PQN	C11-C3-C4	-3.04	115.38	118.58
31	A	5045	PQN	C11-C3-C4	-3.04	115.38	118.58
20	G	203	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	A	5036	CLA	CHB-C4A-NA	3.04	128.78	124.40
20	2	308	CLA	CHB-C4A-NA	3.04	128.78	124.40
20	F	303	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
19	3	301	CHL	C3D-C2D-C1D	3.04	109.97	105.83
20	B	827	CLA	CMB-C2B-C3B	3.03	130.75	124.68
20	B	838	CLA	CMB-C2B-C3B	3.03	130.75	124.68
20	B	815	CLA	CMB-C2B-C3B	3.03	130.74	124.68
19	3	301	CHL	CHD-C4C-C3C	3.03	129.19	124.77
20	A	5010	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
20	3	307	CLA	CHB-C4A-NA	3.02	128.76	124.40
19	1	601	CHL	C1D-ND-C4D	3.02	108.43	106.31
20	9	605	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
20	9	604	CLA	CHB-C4A-NA	3.01	128.75	124.40
20	B	826	CLA	CMB-C2B-C3B	3.01	130.70	124.68
20	A	5029	CLA	CMB-C2B-C3B	3.01	130.69	124.68
20	B	833	CLA	CHB-C4A-NA	3.00	128.73	124.40
19	8	306	CHL	C1D-CHD-C4C	-3.00	119.64	126.02
20	A	5021	CLA	CHB-C4A-NA	3.00	128.73	124.40
20	9	601	CLA	C4A-NA-C1A	3.00	108.05	106.68
20	B	838	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
20	9	605	CLA	CHB-C4A-NA	2.99	128.72	124.40
20	A	5005	CLA	CMB-C2B-C3B	2.99	130.66	124.68
20	L	204	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	1	604	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
20	B	805	CLA	CHB-C4A-NA	2.98	128.71	124.40
20	1	614	CLA	CMB-C2B-C3B	2.98	130.64	124.68
20	7	314	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	3	304	CLA	CMB-C2B-C3B	2.98	130.64	124.68
20	2	308	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	9	610	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	B	814	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	H	201	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	B	840	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	8	301	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	A	5024	CLA	C4A-NA-C1A	2.98	108.04	106.68
20	B	840	CLA	C4A-NA-C1A	2.98	108.04	106.68
20	1	613	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
20	B	821	CLA	O2D-CGD-O1D	-2.97	118.07	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	602	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	B	810	CLA	CHB-C4A-NA	2.97	128.68	124.40
20	A	5009	CLA	CHB-C4A-NA	2.96	128.68	124.40
20	B	805	CLA	C1B-CHB-C4A	-2.96	124.39	130.04
20	7	309	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	1	605	CLA	CMB-C2B-C3B	2.96	130.60	124.68
20	G	204	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	1	609	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	B	825	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	1	612	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	8	307	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
20	G	204	CLA	CHB-C4A-NA	2.95	128.66	124.40
20	A	5024	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	B	835	CLA	CHB-C4A-NA	2.95	128.66	124.40
20	B	823	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	8	307	CLA	CBC-CAC-C3C	2.95	120.41	112.42
20	J	104	CLA	CHB-C4A-NA	2.94	128.65	124.40
20	A	5008	CLA	CHB-C4A-NA	2.94	128.64	124.40
23	B	844	BCR	C8-C7-C6	2.94	134.85	127.00
20	9	602	CLA	CHB-C4A-NA	2.94	128.64	124.40
20	B	826	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	3	324	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	1	611	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	A	5007	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	2	304	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	A	5008	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	B	809	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	B	837	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	1	615	LUT	C30-C31-C32	2.93	131.69	123.20
20	F	306	CLA	CMB-C2B-C3B	2.93	130.54	124.68
20	9	610	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	9	610	CLA	CMB-C2B-C3B	2.93	130.53	124.68
20	8	312	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	A	5008	CLA	C4A-NA-C1A	2.93	108.01	106.68
20	B	816	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	A	5014	CLA	CMB-C2B-C3B	2.93	130.53	124.68
20	A	5023	CLA	CHB-C4A-NA	2.92	128.62	124.40
20	3	305	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	L	205	CLA	C1B-CHB-C4A	-2.92	124.47	130.04
20	2	301	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	A	5041	CLA	CHB-C4A-NA	2.92	128.61	124.40
20	1	611	CLA	C2A-C1A-CHA	2.92	128.93	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5022	CLA	CHB-C4A-NA	2.92	128.61	124.40
20	A	5042	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	B	812	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	7	307	CHL	C2D-C1D-ND	-2.92	107.24	110.13
20	B	819	CLA	CMB-C2B-C3B	2.92	130.51	124.68
20	A	5040	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	A	5012	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	A	5011	CLA	CHB-C4A-NA	2.92	128.61	124.40
20	A	5039	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	2	306	CHL	C1D-CHD-C4C	-2.91	119.83	126.02
20	9	609	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	7	309	CLA	CHB-C4A-NA	2.91	128.59	124.40
20	B	831	CLA	CMB-C2B-C3B	2.91	130.49	124.68
20	9	607	CLA	CMB-C2B-C3B	2.90	130.49	124.68
20	1	603	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
20	A	5015	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
20	A	5025	CLA	CHB-C4A-NA	2.90	128.59	124.40
20	8	313	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	A	5031	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	A	5038	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	9	601	CLA	CHB-C4A-NA	2.90	128.58	124.40
20	A	5026	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
20	B	818	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
20	L	205	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
20	A	5007	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
20	A	5026	CLA	CMB-C2B-C3B	2.89	130.47	124.68
20	A	5043	CLA	CMB-C2B-C3B	2.89	130.47	124.68
20	7	313	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	3	312	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	2	311	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	2	307	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	A	5022	CLA	CMB-C2B-C3B	2.89	130.45	124.68
20	9	610	CLA	C2A-C1A-CHA	2.88	128.87	123.87
20	A	5004	CLA	CMB-C2B-C3B	2.88	130.44	124.68
20	A	5017	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
20	A	5004	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	1	616	XAT	O24-C25-C24	-2.88	110.79	113.49
20	8	308	CLA	C1B-CHB-C4A	-2.88	124.55	130.04
20	2	303	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	3	306	CLA	CHB-C4A-NA	2.88	128.55	124.40
20	1	607	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	2	310	CLA	CHB-C4A-NA	2.88	128.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	202	CLA	CMB-C2B-C3B	2.88	130.43	124.68
20	B	836	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	7	315	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	B	835	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	J	104	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	B	836	CLA	CHB-C4A-NA	2.87	128.53	124.40
20	K	4005	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	A	5049	BCR	C20-C19-C18	2.86	134.22	126.36
20	B	808	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
20	B	829	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	9	603	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	F	303	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	A	5030	CLA	CMB-C2B-C3B	2.86	130.40	124.68
20	7	312	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	9	602	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	J	102	BCR	C24-C23-C22	2.86	130.47	126.23
20	3	308	CLA	CMB-C2B-C3B	2.86	130.39	124.68
20	8	310	CLA	CHB-C4A-NA	2.86	128.52	124.40
20	L	202	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
20	B	818	CLA	CHB-C4A-NA	2.86	128.52	124.40
20	K	4005	CLA	C1B-CHB-C4A	-2.86	124.59	130.04
20	A	5018	CLA	CHB-C4A-NA	2.85	128.52	124.40
20	B	818	CLA	CMB-C2B-C3B	2.85	130.38	124.68
20	K	4004	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	B	822	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	B	829	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	2	304	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	1	605	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	9	601	CLA	CMB-C2B-C3B	2.85	130.38	124.68
22	3	316	XAT	C7-C8-C9	2.85	129.95	125.53
20	A	5027	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	A	5013	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	B	819	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	K	4003	CLA	CHB-C4A-NA	2.85	128.51	124.40
20	2	304	CLA	CMB-C2B-C3B	2.85	130.37	124.68
20	1	608	CLA	CHB-C4A-NA	2.85	128.51	124.40
20	B	815	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	A	5016	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	9	612	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	1	603	CLA	C1B-CHB-C4A	-2.84	124.62	130.04
20	B	823	CLA	CHB-C4A-NA	2.84	128.50	124.40
20	L	205	CLA	CMB-C2B-C3B	2.84	130.36	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	311	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	7	310	CLA	C1B-CHB-C4A	-2.84	124.62	130.04
20	8	308	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	A	5028	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
30	A	5003	CL0	C2D-C1D-ND	-2.84	107.32	110.13
20	F	308	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	1	614	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
20	A	5018	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
20	A	5032	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
20	3	302	CLA	CMB-C2B-C3B	2.84	130.35	124.68
19	8	304	CHL	CHD-C1D-C2D	2.84	131.38	125.49
20	7	305	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
19	8	306	CHL	C1C-C2C-C3C	-2.84	104.67	107.28
20	1	610	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	2	305	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	A	5025	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	B	813	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	1	611	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	3	306	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	A	5016	CLA	CHB-C4A-NA	2.83	128.49	124.40
20	3	309	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	3	325	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
30	A	5003	CL0	C3D-C2D-C1D	2.83	109.69	105.83
20	3	302	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	9	603	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	B	831	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	B	820	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	F	306	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	7	311	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	A	5021	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	9	608	CLA	CHB-C4A-NA	2.83	128.48	124.40
20	A	5022	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
20	7	313	CLA	CHB-C4A-NA	2.82	128.48	124.40
20	A	5029	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
19	7	308	CHL	C2D-C1D-ND	-2.82	107.33	110.13
20	A	5029	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	3	314	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	8	309	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	A	5034	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	8	321	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	8	303	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	2	312	CLA	O2D-CGD-O1D	-2.82	118.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	303	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	B	807	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	A	5031	CLA	CMB-C2B-C1B	-2.81	124.34	128.46
20	A	5012	CLA	CHB-C4A-NA	2.81	128.45	124.40
20	B	825	CLA	C4A-NA-C1A	2.81	107.96	106.68
20	G	202	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
20	2	301	CLA	CHB-C4A-NA	2.80	128.45	124.40
20	K	4002	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	3	303	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	A	5013	CLA	CMB-C2B-C3B	2.80	130.28	124.68
20	8	303	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
20	2	309	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
20	1	609	CLA	CMB-C2B-C3B	2.80	130.28	124.68
20	8	311	CLA	CHB-C4A-NA	2.80	128.44	124.40
20	B	832	CLA	CHB-C4A-NA	2.80	128.44	124.40
20	9	602	CLA	C1B-CHB-C4A	-2.80	124.70	130.04
20	B	817	CLA	CMB-C2B-C3B	2.80	130.27	124.68
20	B	839	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
20	1	602	CLA	CMB-C2B-C3B	2.80	130.27	124.68
20	3	313	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
19	8	304	CHL	C2D-C1D-ND	-2.80	107.36	110.13
20	B	816	CLA	CHB-C4A-NA	2.79	128.43	124.40
20	3	310	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	7	312	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	A	5015	CLA	CMB-C2B-C3B	2.79	130.26	124.68
20	2	311	CLA	CHB-C4A-NA	2.79	128.43	124.40
20	G	201	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	A	5041	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	3	304	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	7	310	CLA	C1-C2-C3	-2.79	121.63	126.20
20	A	5040	CLA	CMB-C2B-C3B	2.79	130.25	124.68
20	7	304	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	9	608	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	8	306	CHL	CHD-C1D-C2D	2.79	131.28	125.49
20	A	5036	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	B	840	CLA	CHB-C4A-NA	2.78	128.41	124.40
20	B	837	CLA	CMB-C2B-C3B	2.78	130.24	124.68
20	B	828	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	B	805	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	B	811	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	G	204	CLA	CBC-CAC-C3C	2.77	119.94	112.42
20	B	812	CLA	CHB-C4A-NA	2.77	128.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5009	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	3	308	CLA	C1B-CHB-C4A	-2.77	124.75	130.04
20	A	5019	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	A	5013	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	B	804	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	H	201	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	3	311	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	B	825	CLA	CMB-C2B-C3B	2.77	130.21	124.68
20	2	310	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
20	8	310	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	8	311	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	B	827	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	A	5026	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	L	204	CLA	CMB-C2B-C3B	2.76	130.20	124.68
20	A	5033	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	2	313	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	3	301	CHL	C2A-C1A-CHA	2.76	128.66	123.87
20	8	302	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	B	828	CLA	CMB-C2B-C3B	2.76	130.20	124.68
20	A	5028	CLA	CMB-C2B-C3B	2.76	130.20	124.68
20	F	307	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
20	G	201	CLA	CHB-C4A-NA	2.76	128.38	124.40
20	A	5012	CLA	C1B-CHB-C4A	-2.76	124.78	130.04
23	B	844	BCR	C7-C8-C9	2.76	130.31	126.23
20	B	805	CLA	C2A-C3A-C4A	-2.75	97.42	101.87
20	7	310	CLA	CMB-C2B-C3B	2.75	130.18	124.68
19	2	302	CHL	C1D-CHD-C4C	-2.75	120.17	126.02
20	3	309	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	9	606	CHL	CHD-C1D-C2D	2.75	131.21	125.49
20	8	308	CLA	CMB-C2B-C3B	2.75	130.18	124.68
20	L	204	CLA	CHB-C4A-NA	2.75	128.37	124.40
20	A	5011	CLA	CMB-C2B-C3B	2.75	130.17	124.68
20	A	5017	CLA	CHB-C4A-NA	2.74	128.36	124.40
20	L	202	CLA	CMB-C2B-C3B	2.74	130.17	124.68
20	B	814	CLA	CMB-C2B-C3B	2.74	130.16	124.68
20	3	310	CLA	CHB-C4A-NA	2.74	128.36	124.40
21	1	615	LUT	C35-C34-C33	2.74	131.12	127.28
20	K	4004	CLA	C1B-CHB-C4A	-2.74	124.81	130.04
20	3	305	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	A	5020	CLA	CMB-C2B-C3B	2.74	130.16	124.68
20	A	5012	CLA	CMB-C2B-C3B	2.74	130.16	124.68
20	B	825	CLA	CHB-C4A-NA	2.74	128.35	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5027	CLA	CMB-C2B-C3B	2.74	130.15	124.68
20	9	611	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	7	315	CLA	CMB-C2B-C3B	2.73	130.15	124.68
20	1	604	CLA	C1B-CHB-C4A	-2.73	124.83	130.04
20	1	609	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	7	323	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
20	1	611	CLA	C1B-CHB-C4A	-2.73	124.83	130.04
20	G	201	CLA	C4A-NA-C1A	2.73	107.92	106.68
20	A	5030	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
20	3	308	CLA	C4A-NA-C1A	2.73	107.92	106.68
20	1	610	CLA	CHB-C4A-NA	2.73	128.33	124.40
20	2	305	CLA	CMB-C2B-C3B	2.72	130.13	124.68
20	B	813	CLA	CMB-C2B-C3B	2.72	130.12	124.68
20	A	5040	CLA	C1B-CHB-C4A	-2.72	124.85	130.04
19	1	606	CHL	C1D-CHD-C4C	-2.72	120.23	126.02
20	A	5037	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	F	307	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	G	203	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	3	325	CLA	CMB-C2B-C3B	2.72	130.12	124.68
20	B	819	CLA	C1B-CHB-C4A	-2.72	124.85	130.04
20	B	822	CLA	C1B-CHB-C4A	-2.72	124.85	130.04
20	B	840	CLA	C1B-CHB-C4A	-2.72	124.86	130.04
20	A	5029	CLA	C1B-CHB-C4A	-2.72	124.86	130.04
20	2	310	CLA	CMB-C2B-C3B	2.72	130.11	124.68
20	B	806	CLA	O2D-CGD-CBD	2.72	115.98	111.23
23	B	844	BCR	C10-C11-C12	2.71	131.06	123.20
20	B	832	CLA	C1B-CHB-C4A	-2.71	124.86	130.04
20	B	831	CLA	CHB-C4A-NA	2.71	128.31	124.40
20	A	5011	CLA	C1B-CHB-C4A	-2.71	124.87	130.04
20	3	306	CLA	CMB-C2B-C3B	2.71	130.10	124.68
20	9	608	CLA	CMB-C2B-C3B	2.71	130.09	124.68
20	B	810	CLA	CMB-C2B-C3B	2.71	130.09	124.68
20	B	834	CLA	CHB-C4A-NA	2.71	128.31	124.40
20	K	4005	CLA	CHB-C4A-NA	2.71	128.31	124.40
20	A	5033	CLA	CMB-C2B-C3B	2.71	130.09	124.68
20	A	5024	CLA	CHB-C4A-NA	2.71	128.30	124.40
23	3	319	BCR	C23-C22-C21	2.71	123.26	119.01
22	7	317	XAT	C38-C25-C24	-2.70	111.20	114.24
20	7	309	CLA	CMB-C2B-C3B	2.70	130.09	124.68
20	B	838	CLA	CHB-C4A-NA	2.70	128.30	124.40
20	A	5038	CLA	C1B-CHB-C4A	-2.70	124.89	130.04
20	B	836	CLA	C1B-CHB-C4A	-2.70	124.89	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	605	CLA	CMB-C2B-C3B	2.70	130.08	124.68
20	B	840	CLA	CMB-C2B-C3B	2.70	130.08	124.68
20	9	604	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
19	2	302	CHL	CHD-C1D-C2D	2.70	131.10	125.49
20	A	5010	CLA	CMB-C2B-C3B	2.70	130.08	124.68
20	A	5019	CLA	CMB-C2B-C3B	2.70	130.08	124.68
20	B	834	CLA	CMB-C2B-C3B	2.70	130.07	124.68
20	A	5011	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
20	A	5043	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	2	309	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	B	818	CLA	C1B-CHB-C4A	-2.69	124.90	130.04
20	A	5005	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
20	A	5039	CLA	CMB-C2B-C3B	2.69	130.06	124.68
20	B	820	CLA	CMB-C2B-C1B	-2.69	124.52	128.46
20	7	303	CLA	CMB-C2B-C3B	2.69	130.06	124.68
20	A	5018	CLA	CMB-C2B-C3B	2.69	130.06	124.68
20	B	830	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
20	L	202	CLA	C1B-CHB-C4A	-2.69	124.91	130.04
20	G	201	CLA	CMB-C2B-C3B	2.69	130.05	124.68
20	L	201	CLA	CMB-C2B-C3B	2.69	130.05	124.68
21	1	615	LUT	C26-C27-C28	2.69	128.76	124.58
19	2	306	CHL	CHD-C1D-C2D	2.69	131.07	125.49
20	7	304	CLA	C1B-CHB-C4A	-2.69	124.92	130.04
20	A	5024	CLA	C1B-CHB-C4A	-2.69	124.92	130.04
20	1	603	CLA	CMB-C2B-C3B	2.68	130.05	124.68
20	7	323	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	B	822	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	A	5023	CLA	CMB-C2B-C3B	2.68	130.04	124.68
20	F	306	CLA	CHB-C4A-NA	2.68	128.27	124.40
19	3	323	CHL	CHD-C1D-C2D	2.68	131.06	125.49
20	2	311	CLA	CMB-C2B-C3B	2.68	130.04	124.68
20	1	605	CLA	CHB-C4A-NA	2.68	128.26	124.40
20	A	5028	CLA	CHB-C4A-NA	2.68	128.26	124.40
20	B	836	CLA	CMB-C2B-C3B	2.68	130.03	124.68
19	2	306	CHL	C2A-C1A-CHA	2.68	128.51	123.87
20	7	310	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
20	A	5041	CLA	CMB-C2B-C3B	2.67	130.02	124.68
20	K	4004	CLA	CMB-C2B-C3B	2.67	130.02	124.68
20	A	5037	CLA	CMB-C2B-C3B	2.67	130.02	124.68
20	7	323	CLA	CMB-C2B-C3B	2.67	130.02	124.68
20	3	302	CLA	CHB-C4A-NA	2.67	128.25	124.40
19	2	302	CHL	C2A-C1A-CHA	2.67	128.50	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	313	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	A	5023	CLA	O2D-CGD-CBD	2.67	115.89	111.23
23	3	319	BCR	C8-C9-C10	2.67	123.20	119.01
20	A	5033	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	2	308	CLA	CMB-C2B-C3B	2.67	130.01	124.68
20	2	301	CLA	CMB-C2B-C3B	2.67	130.01	124.68
20	1	607	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	3	314	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	A	5040	CLA	CHB-C4A-NA	2.66	128.25	124.40
20	B	837	CLA	C1B-CHB-C4A	-2.66	124.96	130.04
20	8	312	CLA	CMB-C2B-C3B	2.66	130.00	124.68
19	7	307	CHL	C2A-C1A-CHA	2.66	128.48	123.87
30	A	5003	CL0	C2A-C1A-CHA	2.66	128.48	123.87
23	3	319	BCR	C35-C13-C14	-2.65	118.52	122.82
20	A	5015	CLA	CHB-C4A-NA	2.65	128.23	124.40
20	B	809	CLA	CHB-C4A-NA	2.65	128.23	124.40
20	F	306	CLA	C1B-CHB-C4A	-2.65	124.98	130.04
20	3	310	CLA	CMB-C2B-C3B	2.65	129.98	124.68
20	B	839	CLA	C1B-CHB-C4A	-2.65	124.98	130.04
20	A	5014	CLA	O2D-CGD-CBD	2.65	115.87	111.23
20	1	612	CLA	CHB-C4A-NA	2.65	128.22	124.40
20	9	604	CLA	CMB-C2B-C3B	2.65	129.97	124.68
19	3	323	CHL	C1D-CHD-C4C	-2.65	120.39	126.02
20	1	613	CLA	CMB-C2B-C3B	2.65	129.97	124.68
20	7	311	CLA	CMB-C2B-C3B	2.65	129.97	124.68
20	8	301	CLA	CMB-C2B-C3B	2.64	129.97	124.68
20	B	829	CLA	CMB-C2B-C3B	2.64	129.97	124.68
20	A	5031	CLA	CHB-C4A-NA	2.64	128.22	124.40
20	A	5007	CLA	C1B-CHB-C4A	-2.64	125.00	130.04
20	9	609	CLA	CMB-C2B-C3B	2.64	129.96	124.68
20	A	5034	CLA	CMB-C2B-C3B	2.64	129.96	124.68
20	B	810	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
20	A	5020	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
20	3	305	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
20	G	201	CLA	C1B-CHB-C4A	-2.64	125.01	130.04
20	B	806	CLA	CHB-C4A-NA	2.64	128.21	124.40
20	1	614	CLA	CHB-C4A-NA	2.64	128.21	124.40
20	1	610	CLA	CMB-C2B-C3B	2.64	129.95	124.68
20	8	310	CLA	CMB-C2B-C3B	2.63	129.95	124.68
20	F	308	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	B	838	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
20	1	602	CLA	CHB-C4A-NA	2.63	128.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	B	809	CLA	C1B-CHB-C4A	-2.63	125.02	130.04
20	1	611	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	J	104	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	2	307	CLA	C1B-CHB-C4A	-2.63	125.03	130.04
20	8	309	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	7	314	CLA	CHB-C4A-NA	2.63	128.19	124.40
20	2	312	CLA	CMB-C2B-C3B	2.63	129.94	124.68
20	7	314	CLA	CMB-C2B-C3B	2.63	129.93	124.68
20	8	303	CLA	CMB-C2B-C3B	2.63	129.93	124.68
20	B	814	CLA	C1B-CHB-C4A	-2.63	125.03	130.04
20	K	4003	CLA	CMB-C2B-C3B	2.63	129.93	124.68
20	7	303	CLA	C1B-CHB-C4A	-2.63	125.03	130.04
29	9	616	LMU	C1B-O5B-C5B	2.63	118.85	113.72
20	A	5009	CLA	CMB-C2B-C3B	2.63	129.93	124.68
20	B	819	CLA	C1-C2-C3	-2.63	121.90	126.20
20	3	312	CLA	CMB-C2B-C3B	2.62	129.93	124.68
20	2	307	CLA	CHB-C4A-NA	2.62	128.19	124.40
20	A	5014	CLA	CHB-C4A-NA	2.62	128.19	124.40
20	9	612	CLA	CMB-C2B-C3B	2.62	129.92	124.68
20	B	828	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	1	608	CLA	CMB-C2B-C3B	2.62	129.92	124.68
20	B	811	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	A	5039	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	9	609	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	A	5019	CLA	C1B-CHB-C4A	-2.62	125.05	130.04
20	B	830	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	A	5006	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	2	313	CLA	CMB-C2B-C3B	2.62	129.91	124.68
20	A	5006	CLA	CMB-C2B-C3B	2.61	129.91	124.68
20	2	305	CLA	CHB-C4A-NA	2.61	128.17	124.40
20	7	312	CLA	CMB-C2B-C3B	2.61	129.90	124.68
20	A	5020	CLA	CHB-C4A-NA	2.61	128.17	124.40
23	B	847	BCR	C7-C8-C9	2.61	130.10	126.23
20	3	314	CLA	CMB-C2B-C3B	2.61	129.89	124.68
20	A	5032	CLA	CMB-C2B-C3B	2.61	129.89	124.68
20	3	325	CLA	CHB-C4A-NA	2.61	128.16	124.40
20	A	5024	CLA	CMB-C2B-C3B	2.60	129.89	124.68
20	B	804	CLA	C4A-NA-C1A	2.60	107.87	106.68
20	3	303	CLA	CMB-C2B-C3B	2.60	129.89	124.68
20	B	826	CLA	CHB-C4A-NA	2.60	128.16	124.40
20	8	313	CLA	CMB-C2B-C3B	2.60	129.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	307	CHL	C3D-C2D-C1D	2.60	109.38	105.83
20	G	202	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	2	309	CLA	CMB-C2B-C3B	2.60	129.88	124.68
20	F	307	CLA	CMB-C2B-C3B	2.60	129.87	124.68
20	A	5034	CLA	C1B-CHB-C4A	-2.60	125.09	130.04
19	7	308	CHL	C3D-C2D-C1D	2.60	109.37	105.83
20	K	4002	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	8	311	CLA	CMB-C2B-C3B	2.59	129.86	124.68
20	8	313	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	9	614	XAT	C7-C8-C9	2.59	129.55	125.53
20	8	312	CLA	CHB-C4A-NA	2.59	128.14	124.40
20	A	5036	CLA	CMB-C2B-C3B	2.59	129.86	124.68
20	L	201	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	B	814	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	B	833	CLA	CMB-C2B-C3B	2.59	129.85	124.68
20	3	309	CLA	CMB-C2B-C3B	2.58	129.85	124.68
20	A	5021	CLA	CMB-C2B-C3B	2.58	129.85	124.68
20	8	313	CLA	C1B-CHB-C4A	-2.58	125.12	130.04
20	2	313	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	3	307	CLA	C1B-CHB-C4A	-2.58	125.12	130.04
20	K	4005	CLA	CMB-C2B-C3B	2.58	129.84	124.68
20	1	607	CLA	CMB-C2B-C3B	2.58	129.84	124.68
20	A	5044	CLA	C1B-CHB-C4A	-2.58	125.12	130.04
20	2	313	CLA	C1B-CHB-C4A	-2.58	125.13	130.04
20	A	5004	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	G	203	CLA	CMB-C2B-C3B	2.57	129.83	124.68
20	B	821	CLA	CHB-C4A-NA	2.57	128.11	124.40
20	B	810	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
20	8	321	CLA	CHA-C1A-NA	-2.57	120.58	126.39
20	A	5021	CLA	C1B-CHB-C4A	-2.57	125.15	130.04
20	9	603	CLA	CMB-C2B-C3B	2.56	129.81	124.68
20	3	312	CLA	CHB-C4A-NA	2.56	128.10	124.40
20	A	5010	CLA	CHB-C4A-NA	2.56	128.10	124.40
20	7	304	CLA	CMB-C2B-C3B	2.56	129.80	124.68
20	B	821	CLA	CMB-C2B-C3B	2.56	129.80	124.68
23	B	844	BCR	C21-C20-C19	2.56	130.62	123.20
20	3	312	CLA	C1B-CHB-C4A	-2.56	125.16	130.04
20	A	5039	CLA	C1B-CHB-C4A	-2.56	125.16	130.04
20	B	817	CLA	CHB-C4A-NA	2.56	128.09	124.40
20	B	809	CLA	CMB-C2B-C3B	2.56	129.79	124.68
19	1	606	CHL	C2A-C1A-CHA	2.55	128.30	123.87
20	B	833	CLA	O2D-CGD-O1D	-2.55	118.88	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	201	CLA	CMB-C2B-C3B	2.55	129.79	124.68
20	B	837	CLA	CHB-C4A-NA	2.55	128.09	124.40
19	1	606	CHL	CHD-C1D-C2D	2.55	130.79	125.49
20	2	301	CLA	C1B-CHB-C4A	-2.55	125.18	130.04
19	8	304	CHL	C2A-C1A-CHA	2.55	128.29	123.87
20	B	839	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	B	823	CLA	CMB-C2B-C3B	2.54	129.76	124.68
20	9	612	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	A	5030	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	B	819	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	B	815	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
20	9	611	CLA	CMB-C2B-C3B	2.54	129.76	124.68
20	3	307	CLA	CMB-C2B-C3B	2.54	129.76	124.68
20	9	608	CLA	C1B-CHB-C4A	-2.54	125.20	130.04
20	9	609	CLA	C1B-CHB-C4A	-2.54	125.20	130.04
20	3	311	CLA	CMB-C2B-C3B	2.54	129.75	124.68
20	1	613	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	A	5035	CLA	C1B-CHB-C4A	-2.54	125.20	130.04
20	A	5034	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	A	5042	CLA	CMB-C2B-C3B	2.54	129.75	124.68
20	2	303	CLA	CMB-C2B-C3B	2.54	129.75	124.68
20	A	5020	CLA	C1-C2-C3	-2.53	122.05	126.20
20	7	311	CLA	CHB-C4A-NA	2.53	128.06	124.40
20	9	612	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
20	A	5033	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
20	A	5007	CLA	C4A-NA-C1A	2.53	107.83	106.68
20	F	308	CLA	C1B-CHB-C4A	-2.53	125.21	130.04
20	3	313	CLA	CMB-C2B-C3B	2.53	129.74	124.68
19	8	304	CHL	CHD-C1D-ND	-2.53	121.24	124.80
20	A	5032	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
20	A	5043	CLA	C1B-CHB-C4A	-2.53	125.22	130.04
20	B	813	CLA	CHB-C4A-NA	2.53	128.04	124.40
19	7	306	CHL	C2D-C1D-ND	-2.52	107.63	110.13
20	F	303	CLA	CAA-CBA-CGA	-2.52	106.05	113.21
20	B	832	CLA	CMB-C2B-C3B	2.52	129.72	124.68
20	A	5041	CLA	C1B-CHB-C4A	-2.52	125.23	130.04
20	F	308	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	7	315	CLA	CHB-C4A-NA	2.52	128.03	124.40
20	2	303	CLA	C1B-CHB-C4A	-2.52	125.24	130.04
20	8	302	CLA	CMB-C2B-C3B	2.52	129.71	124.68
20	A	5014	CLA	C1B-CHB-C4A	-2.51	125.24	130.04
20	H	201	CLA	C1B-CHB-C4A	-2.51	125.25	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	311	CLA	C1B-CHB-C4A	-2.51	125.25	130.04
20	B	822	CLA	CMB-C2B-C3B	2.51	129.70	124.68
20	A	5037	CLA	C1B-CHB-C4A	-2.51	125.25	130.04
20	2	310	CLA	C2A-C1A-CHA	2.51	128.22	123.87
20	8	303	CLA	C1B-CHB-C4A	-2.51	125.25	130.04
20	3	304	CLA	C1B-CHB-C4A	-2.51	125.26	130.04
20	8	309	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	B	811	CLA	C1B-CHB-C4A	-2.50	125.26	130.04
20	B	804	CLA	CMB-C2B-C3B	2.50	129.69	124.68
20	8	321	CLA	CMB-C2B-C3B	2.50	129.69	124.68
20	A	5042	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	3	321	PTY	O7-C6-C5	2.50	117.31	108.34
20	3	303	CLA	CHB-C4A-NA	2.50	128.00	124.40
20	7	315	CLA	C1B-CHB-C4A	-2.50	125.28	130.04
23	J	102	BCR	C10-C11-C12	2.49	130.43	123.20
20	8	302	CLA	CHB-C4A-NA	2.49	128.00	124.40
20	F	303	CLA	C1B-CHB-C4A	-2.49	125.29	130.04
20	A	5006	CLA	C1B-CHB-C4A	-2.49	125.29	130.04
20	G	202	CLA	C1B-CHB-C4A	-2.49	125.29	130.04
19	1	601	CHL	CHD-C1D-C2D	2.49	130.66	125.49
20	7	304	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	B	845	BCR	C8-C9-C10	-2.49	118.97	124.72
20	7	309	CLA	C1B-CHB-C4A	-2.48	125.30	130.04
20	A	5035	CLA	CMB-C2B-C3B	2.48	129.65	124.68
20	3	324	CLA	CMB-C2B-C3B	2.48	129.64	124.68
20	3	303	CLA	C1B-CHB-C4A	-2.48	125.31	130.04
20	B	813	CLA	C1B-CHB-C4A	-2.48	125.32	130.04
23	3	319	BCR	C12-C13-C14	2.48	122.90	119.01
20	1	607	CLA	C1B-CHB-C4A	-2.47	125.32	130.04
19	7	307	CHL	CHD-C1D-C2D	2.47	130.63	125.49
20	A	5027	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	3	302	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
20	1	609	CLA	C1B-CHB-C4A	-2.47	125.33	130.04
20	A	5022	CLA	C1B-CHB-C4A	-2.46	125.34	130.04
20	8	301	CLA	C1B-CHB-C4A	-2.46	125.34	130.04
20	L	204	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
20	1	614	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
20	A	5008	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
20	B	821	CLA	C1B-CHB-C4A	-2.46	125.35	130.04
20	2	312	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	2	307	CLA	CMB-C2B-C3B	2.46	129.59	124.68
20	A	5013	CLA	C1B-CHB-C4A	-2.45	125.36	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5038	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	A	5042	CLA	C1B-CHB-C4A	-2.45	125.37	130.04
20	B	810	CLA	C1-C2-C3	-2.45	122.19	126.20
20	B	825	CLA	C1B-CHB-C4A	-2.45	125.38	130.04
20	9	601	CLA	O2D-CGD-CBD	2.45	115.50	111.23
22	9	614	XAT	C27-C28-C29	2.45	129.32	125.53
20	7	313	CLA	CMB-C2B-C3B	2.44	129.57	124.68
20	9	610	CLA	C1B-CHB-C4A	-2.44	125.38	130.04
20	B	831	CLA	C1B-CHB-C4A	-2.44	125.38	130.04
20	B	811	CLA	CMB-C2B-C3B	2.44	129.56	124.68
20	3	309	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
20	B	830	CLA	CMB-C2B-C3B	2.44	129.56	124.68
20	A	5036	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
19	3	301	CHL	C2D-C1D-ND	-2.44	107.71	110.13
20	B	823	CLA	C1B-CHB-C4A	-2.44	125.39	130.04
20	1	603	CLA	CHB-C4A-NA	2.44	127.91	124.40
23	3	319	BCR	C1-C6-C5	-2.43	119.31	122.64
20	B	834	CLA	C1B-CHB-C4A	-2.43	125.40	130.04
20	B	811	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
20	A	5010	CLA	C1B-CHB-C4A	-2.43	125.40	130.04
20	F	303	CLA	C1D-ND-C4D	2.43	108.02	106.31
20	B	839	CLA	CMB-C2B-C3B	2.43	129.54	124.68
20	8	311	CLA	C1B-CHB-C4A	-2.43	125.41	130.04
20	B	820	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	9	615	XAT	C38-C25-C24	-2.43	111.52	114.24
19	7	308	CHL	C1C-C2C-C3C	-2.42	105.05	107.28
20	A	5027	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
20	F	307	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
20	3	313	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
20	9	601	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
20	L	202	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	2	316	LHG	O3-P-O6	-2.42	100.36	106.67
20	1	612	CLA	CMB-C2B-C3B	2.42	129.51	124.68
20	1	610	CLA	C1B-CHB-C4A	-2.42	125.43	130.04
19	2	306	CHL	CHC-C1C-NC	-2.42	120.67	124.31
20	7	313	CLA	C1B-CHB-C4A	-2.42	125.43	130.04
20	3	304	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	F	303	CLA	C2D-C1D-ND	-2.41	107.74	110.13
20	A	5017	CLA	CMB-C2B-C3B	2.41	129.50	124.68
20	7	323	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
20	K	4003	CLA	C1B-CHB-C4A	-2.41	125.44	130.04
20	3	306	CLA	C1B-CHB-C4A	-2.41	125.45	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	608	CLA	C1B-CHB-C4A	-2.41	125.45	130.04
20	L	201	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
20	B	812	CLA	CMB-C2B-C3B	2.40	129.48	124.68
20	9	604	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
20	A	5019	CLA	CHB-C4A-NA	2.40	127.86	124.40
20	A	5044	CLA	C1-C2-C3	-2.40	122.27	126.20
20	8	302	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
20	B	835	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
20	2	305	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
20	7	314	CLA	C1B-CHB-C4A	-2.39	125.47	130.04
20	2	309	CLA	C1B-CHB-C4A	-2.39	125.48	130.04
20	8	312	CLA	C1B-CHB-C4A	-2.39	125.48	130.04
24	A	5055	LHG	O3-P-O6	-2.39	100.44	106.67
19	1	606	CHL	C1C-C2C-C3C	-2.39	105.09	107.28
20	A	5004	CLA	C4A-NA-C1A	2.38	107.77	106.68
20	7	305	CLA	CHB-C4A-NA	2.38	127.84	124.40
20	B	807	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
20	3	325	CLA	C1B-CHB-C4A	-2.38	125.51	130.04
19	3	323	CHL	C2A-C1A-CHA	2.38	127.99	123.87
22	7	317	XAT	O4-C5-C4	-2.37	111.27	113.49
20	B	812	CLA	C1B-CHB-C4A	-2.37	125.51	130.04
20	B	826	CLA	C1B-CHB-C4A	-2.37	125.51	130.04
20	B	805	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	A	5032	CLA	CHB-C4A-NA	2.37	127.82	124.40
20	7	305	CLA	CMB-C2B-C3B	2.37	129.42	124.68
20	9	608	CLA	C1-C2-C3	-2.37	122.93	126.76
20	9	604	CLA	C1-C2-C3	-2.37	122.94	126.76
20	2	303	CLA	C1-C2-C3	-2.36	122.94	126.76
20	B	830	CLA	C1B-CHB-C4A	-2.36	125.54	130.04
20	A	5016	CLA	C1B-CHB-C4A	-2.36	125.54	130.04
20	B	827	CLA	C1B-CHB-C4A	-2.36	125.54	130.04
23	B	844	BCR	C20-C19-C18	2.35	132.82	126.36
20	2	312	CLA	C1B-CHB-C4A	-2.35	125.55	130.04
19	3	301	CHL	C1C-C2C-C3C	-2.35	105.12	107.28
23	J	102	BCR	C11-C12-C13	2.35	132.82	126.36
20	1	602	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
20	B	820	CLA	C1B-CHB-C4A	-2.35	125.56	130.04
21	1	615	LUT	C21-C26-C27	2.35	115.53	112.83
20	K	4002	CLA	CMB-C2B-C3B	2.34	129.37	124.68
20	A	5009	CLA	C1-C2-C3	-2.34	122.36	126.20
20	H	201	CLA	CHA-C1A-NA	-2.34	121.10	126.39
20	B	828	CLA	C1B-CHB-C4A	-2.33	125.59	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	306	CHL	CHC-C1C-NC	-2.33	120.80	124.31
20	A	5034	CLA	C1-C2-C3	-2.33	122.38	126.20
19	7	307	CHL	C1D-CHD-C4C	-2.33	121.06	126.02
20	9	607	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	B	804	CLA	CHB-C4A-NA	2.33	127.76	124.40
21	1	615	LUT	C32-C33-C34	2.33	122.67	119.01
20	A	5021	CLA	C1-C2-C3	-2.32	123.00	126.76
20	G	203	CLA	C1B-CHB-C4A	-2.32	125.61	130.04
20	3	314	CLA	C1B-CHB-C4A	-2.32	125.61	130.04
20	B	808	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
20	1	612	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
20	A	5031	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
20	A	5008	CLA	CHD-C1D-ND	-2.31	121.55	124.80
20	A	5030	CLA	C1-C2-C3	-2.31	122.41	126.20
20	2	311	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
20	3	311	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
19	8	305	CHL	C3D-C2D-C1D	2.31	108.98	105.83
20	9	602	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
20	B	833	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
20	B	808	CLA	CHD-C1D-ND	-2.31	121.55	124.80
23	3	319	BCR	C30-C25-C26	-2.30	119.49	122.64
20	7	314	CLA	C1-C2-C3	-2.30	123.04	126.76
20	1	607	CLA	C1-C2-C3	-2.30	123.04	126.76
20	A	5030	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
20	A	5032	CLA	C1-C2-C3	-2.29	123.06	126.76
20	1	608	CLA	O2D-CGD-CBD	2.29	115.23	111.23
20	7	312	CLA	C1B-CHB-C4A	-2.29	125.68	130.04
20	A	5025	CLA	CMB-C2B-C1B	-2.29	125.11	128.46
22	7	317	XAT	C36-C21-C26	2.28	116.21	110.05
19	7	308	CHL	C2A-C1A-CHA	2.28	127.83	123.87
20	L	205	CLA	CHB-C4A-NA	2.28	127.70	124.40
20	8	309	CLA	C1B-CHB-C4A	-2.28	125.69	130.04
20	2	310	CLA	C1B-CHB-C4A	-2.28	125.69	130.04
20	1	611	CLA	CHA-C1A-NA	-2.28	121.23	126.39
20	9	610	CLA	C1-C2-C3	-2.28	123.08	126.76
20	F	303	CLA	C2A-C1A-CHA	2.28	127.82	123.87
20	2	308	CLA	C2A-C3A-C4A	-2.28	98.19	101.87
26	7	302	PTY	O12-P1-O13	2.28	119.70	110.83
20	B	816	CLA	C1B-CHB-C4A	-2.28	125.70	130.04
20	7	311	CLA	C1B-CHB-C4A	-2.28	125.70	130.04
19	8	305	CHL	CHD-C1D-C2D	2.27	130.22	125.49
20	9	602	CLA	C1-C2-C3	-2.27	122.47	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	CHB-C4A-NA	2.27	127.67	124.40
20	9	603	CLA	C1B-CHB-C4A	-2.27	125.71	130.04
20	3	324	CLA	C1B-CHB-C4A	-2.27	125.72	130.04
19	2	306	CHL	CHD-C4C-NC	-2.27	120.72	124.23
20	L	204	CLA	C4A-NA-C1A	2.26	107.71	106.68
20	B	830	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
20	1	604	CLA	C1-C2-C3	-2.26	123.10	126.76
21	7	316	LUT	C21-C26-C27	2.26	115.42	112.83
20	J	104	CLA	C1B-CHB-C4A	-2.26	125.73	130.04
20	A	5037	CLA	C1-C2-C3	-2.26	123.11	126.76
20	B	817	CLA	C1B-CHB-C4A	-2.25	125.74	130.04
20	B	829	CLA	C1B-CHB-C4A	-2.25	125.74	130.04
20	B	806	CLA	C1B-CHB-C4A	-2.25	125.75	130.04
20	A	5012	CLA	C4A-NA-C1A	2.25	107.71	106.68
19	1	601	CHL	C3D-C2D-C1D	2.25	108.89	105.83
20	2	304	CLA	C2A-C1A-CHA	2.24	127.76	123.87
19	2	306	CHL	C1D-ND-C4D	2.24	107.88	106.31
20	A	5043	CLA	C1-C2-C3	-2.24	123.14	126.76
30	A	5003	CL0	CHC-C1C-NC	-2.24	120.94	124.31
20	3	305	CLA	C1-C2-C3	-2.24	123.14	126.76
20	A	5044	CLA	CHB-C4A-NA	2.23	127.62	124.40
20	8	321	CLA	C1B-CHB-C4A	-2.23	125.78	130.04
20	8	308	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
20	A	5023	CLA	C1B-CHB-C4A	-2.23	125.79	130.04
20	1	613	CLA	C1B-CHB-C4A	-2.23	125.79	130.04
20	2	303	CLA	CMA-C3A-C4A	2.23	117.76	111.77
20	2	304	CLA	C1-C2-C3	-2.22	123.16	126.76
22	8	315	XAT	C7-C8-C9	2.22	128.98	125.53
20	A	5018	CLA	C1B-CHB-C4A	-2.22	125.80	130.04
20	L	205	CLA	C1-C2-C3	-2.22	123.17	126.76
29	9	616	LMU	O5B-C5B-C4B	2.22	113.70	109.70
23	B	847	BCR	C8-C7-C6	2.22	132.93	127.00
23	A	5049	BCR	C15-C16-C17	-2.22	118.98	123.52
20	B	836	CLA	CHD-C1D-ND	-2.22	121.68	124.80
20	K	4002	CLA	C1B-CHB-C4A	-2.22	125.81	130.04
20	K	4004	CLA	CHB-C4A-NA	2.22	127.60	124.40
20	B	834	CLA	C1-C2-C3	-2.21	123.18	126.76
23	B	844	BCR	C11-C10-C9	2.21	130.38	127.28
20	A	5031	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	8	304	CHL	CHD-C4C-NC	-2.21	120.81	124.23
24	2	316	LHG	O4-P-O5	2.21	119.43	110.83
19	9	606	CHL	C1D-CHD-C4C	-2.21	121.33	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	602	CLA	C4A-NA-C1A	2.20	107.68	106.68
20	A	5037	CLA	O2D-CGD-CBD	2.20	115.08	111.23
20	8	303	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
22	9	615	XAT	C18-C5-C4	-2.20	111.77	114.24
20	1	613	CLA	C1-C2-C3	-2.20	123.20	126.76
19	3	323	CHL	C1C-C2C-C3C	-2.20	105.26	107.28
20	B	824	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
19	1	601	CHL	C1D-CHD-C4C	-2.20	121.35	126.02
20	3	305	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
20	A	5028	CLA	C1B-CHB-C4A	-2.19	125.86	130.04
20	2	313	CLA	C1-C2-C3	-2.19	123.22	126.76
20	9	610	CLA	CHA-C1A-NA	-2.19	121.43	126.39
20	7	311	CLA	C1-C2-C3	-2.19	122.62	126.20
20	3	310	CLA	C1B-CHB-C4A	-2.18	125.87	130.04
24	A	5055	LHG	O4-P-O5	2.18	119.34	110.83
19	7	306	CHL	C2A-C1A-CHA	2.18	127.65	123.87
20	8	301	CLA	O2D-CGD-CBD	2.18	115.04	111.23
20	3	308	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
20	A	5027	CLA	C1-C2-C3	-2.17	122.63	126.20
20	A	5009	CLA	C1B-CHB-C4A	-2.17	125.89	130.04
20	7	311	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	8	309	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	B	815	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
33	J	101	LMK	O2-C4-C3	2.17	116.90	111.88
20	1	605	CLA	C1B-CHB-C4A	-2.17	125.90	130.04
19	9	606	CHL	C1C-C2C-C3C	-2.17	105.29	107.28
20	9	611	CLA	C1B-CHB-C4A	-2.17	125.91	130.04
20	1	602	CLA	C1-C2-C3	-2.17	122.65	126.20
20	A	5041	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
20	B	830	CLA	C1-C2-C3	-2.16	122.65	126.20
20	B	808	CLA	C1-C2-C3	-2.16	122.66	126.20
20	2	308	CLA	C2A-C1A-CHA	2.16	127.61	123.87
19	8	305	CHL	C1D-CHD-C4C	-2.16	121.44	126.02
20	A	5006	CLA	O2D-CGD-CBD	2.16	115.00	111.23
20	B	805	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
21	2	314	LUT	C36-C21-C26	2.16	112.81	109.55
20	1	611	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
19	7	307	CHL	CHD-C4C-NC	-2.15	120.89	124.23
20	F	303	CLA	O2D-CGD-CBD	2.15	115.00	111.23
20	L	201	CLA	C1-C2-C3	-2.15	122.67	126.20
20	A	5031	CLA	CMB-C2B-C3B	2.15	128.98	124.68
20	A	5020	CLA	O2D-CGD-CBD	2.15	114.99	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	606	CHL	C1D-ND-C4D	-2.15	104.81	106.31
21	2	315	LUT	C30-C31-C32	2.15	129.42	123.20
20	3	311	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
20	A	5041	CLA	C1-C2-C3	-2.14	122.69	126.20
20	7	310	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
20	B	824	CLA	C1B-CHB-C4A	-2.14	125.96	130.04
23	A	5049	BCR	C15-C14-C13	2.14	130.28	127.28
20	A	5010	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	7	312	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	7	307	CHL	CHC-C1C-NC	-2.13	121.10	124.31
20	A	5017	CLA	C1B-CHB-C4A	-2.13	125.97	130.04
20	A	5024	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
20	A	5044	CLA	O2D-CGD-CBD	2.13	114.96	111.23
20	2	303	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	B	832	CLA	O1D-CGD-CBD	2.13	128.71	124.52
20	A	5038	CLA	C1-C2-C3	-2.13	123.32	126.76
20	3	306	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
20	A	5029	CLA	CHD-C1D-ND	-2.12	121.81	124.80
20	A	5039	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
20	B	829	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
20	8	310	CLA	C1B-CHB-C4A	-2.11	126.01	130.04
20	8	311	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
20	3	307	CLA	O2D-CGD-CBD	2.11	114.92	111.23
20	B	837	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
19	3	301	CHL	CHC-C1C-NC	-2.11	121.14	124.31
20	A	5006	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	B	827	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	A	5030	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
20	F	303	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
20	B	839	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
20	7	303	CLA	C2A-C1A-CHA	2.10	127.52	123.87
20	B	823	CLA	C1-C2-C3	-2.10	122.75	126.20
23	B	803	BCR	C15-C16-C17	2.10	127.81	123.52
19	1	601	CHL	CHC-C1C-NC	-2.10	121.15	124.31
20	A	5020	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
20	A	5026	CLA	C1B-CHB-C4A	-2.10	126.04	130.04
19	2	306	CHL	C1C-C2C-C3C	-2.10	105.35	107.28
20	B	834	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
20	7	305	CLA	C1-C2-C3	-2.09	123.37	126.76
20	9	611	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
20	B	836	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
20	A	5034	CLA	O2A-CGA-O1A	-2.09	118.41	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5015	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	G	202	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	L	201	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
20	B	816	CLA	C1-C2-C3	-2.08	122.78	126.20
20	2	303	CLA	CHB-C4A-NA	2.08	127.41	124.40
20	A	5021	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	A	5023	CLA	C1-C2-C3	-2.08	123.39	126.76
20	A	5037	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	F	307	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	8	304	CHL	C1C-C2C-C3C	-2.08	105.37	107.28
20	L	205	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
22	9	614	XAT	O4-C5-C4	-2.08	111.54	113.49
21	2	315	LUT	C21-C26-C27	2.08	115.21	112.83
20	9	607	CLA	CHA-C1A-NA	-2.08	121.69	126.39
20	9	603	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	A	5009	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	A	5028	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	1	604	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
20	A	5004	CLA	O1D-CGD-CBD	2.07	128.61	124.52
20	A	5016	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
20	7	304	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	2	308	CLA	O2D-CGD-CBD	2.07	114.85	111.23
20	L	204	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	7	323	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	A	5012	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	K	4005	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	7	308	CHL	CHD-C1D-C2D	2.06	129.78	125.49
20	A	5039	CLA	C1-C2-C3	-2.06	122.82	126.20
20	A	5014	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	A	5019	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	1	607	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	K	4003	CLA	O2D-CGD-CBD	2.06	114.83	111.23
20	A	5015	CLA	C1-C2-C3	-2.06	122.83	126.20
20	A	5042	CLA	O2D-CGD-CBD	2.06	114.83	111.23
20	B	824	CLA	O2D-CGD-CBD	2.06	114.83	111.23
20	F	306	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
20	B	834	CLA	O2D-CGD-CBD	2.06	114.83	111.23
19	2	302	CHL	CHD-C1D-ND	-2.06	121.91	124.80
20	B	826	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
20	B	806	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
20	B	823	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
20	B	825	CLA	O2A-CGA-O1A	-2.05	118.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	323	CLA	O1D-CGD-CBD	2.05	128.57	124.52
20	A	5013	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
20	A	5027	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	B	839	CLA	CHD-C1D-ND	-2.05	121.92	124.80
20	3	307	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
19	1	606	CHL	C3D-C2D-C1D	2.05	108.62	105.83
20	B	824	CLA	CHA-C1A-NA	-2.05	121.76	126.39
20	B	820	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
20	A	5042	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
20	H	201	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
20	2	311	CLA	C1-C2-C3	-2.04	123.45	126.76
20	B	837	CLA	C1-C2-C3	-2.04	122.85	126.20
20	B	807	CLA	CHD-C1D-ND	-2.04	121.93	124.80
20	7	314	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	2	313	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	A	5007	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	A	5029	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	B	838	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	B	831	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	B	826	CLA	C1-C2-C3	-2.04	122.86	126.20
20	A	5023	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	2	310	CLA	CHA-C1A-NA	-2.03	121.79	126.39
20	B	814	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	8	307	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	L	202	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	B	829	CLA	C1-C2-C3	-2.03	122.87	126.20
20	B	821	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
20	8	310	CLA	C2A-C1A-CHA	2.03	127.39	123.87
20	B	808	CLA	CHA-C1A-NA	-2.03	121.80	126.39
20	2	303	CLA	O2D-CGD-CBD	2.03	114.77	111.23
20	8	307	CLA	CHA-C1A-NA	-2.03	121.80	126.39
20	A	5032	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
20	A	5010	CLA	C1-C2-C3	-2.03	122.88	126.20
20	3	324	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
20	7	305	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
19	7	308	CHL	CHC-C1C-NC	-2.02	121.27	124.31
20	B	816	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
20	2	304	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
20	3	306	CLA	C1-C2-C3	-2.02	122.89	126.20
20	B	822	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
20	8	307	CLA	O2D-CGD-CBD	2.02	114.76	111.23
20	7	313	CLA	O2A-CGA-O1A	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	5033	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
20	B	808	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
20	7	312	CLA	C2A-C1A-CHA	2.02	127.37	123.87
20	8	301	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
19	8	306	CHL	CHD-C4C-NC	-2.02	121.11	124.23
19	2	306	CHL	C3D-C2D-C1D	2.02	108.58	105.83
20	1	603	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
19	8	304	CHL	C3D-C2D-C1D	2.01	108.58	105.83
20	1	602	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
20	A	5017	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	1	619	SQD	C1-O5-C5	2.01	117.64	113.72
20	7	303	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
20	3	302	CLA	C1-C2-C3	-2.01	122.91	126.20
20	B	809	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
20	B	840	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
20	8	302	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
19	2	306	CHL	CHD-C1D-ND	-2.00	121.98	124.80
25	F	311	SQD	C1-O5-C5	2.00	117.63	113.72

All (208) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	601	CHL	ND
19	1	606	CHL	ND
19	3	301	CHL	C8
19	3	301	CHL	NC
19	3	323	CHL	C8
19	3	323	CHL	ND
19	3	323	CHL	NA
19	7	306	CHL	NC
19	7	307	CHL	NC
19	7	307	CHL	NA
19	7	308	CHL	NA
19	7	308	CHL	NC
19	8	304	CHL	ND
19	8	305	CHL	NC
19	8	306	CHL	NA
19	8	306	CHL	NC
19	9	606	CHL	NA
19	9	606	CHL	NC
19	2	302	CHL	C8
19	2	302	CHL	NC

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Mol	Chain	Res	Type	Atom
19	2	306	CHL	NC
19	2	306	CHL	C3A
20	1	602	CLA	ND
20	1	603	CLA	ND
20	1	604	CLA	ND
20	1	605	CLA	ND
20	1	607	CLA	ND
20	1	608	CLA	ND
20	1	609	CLA	ND
20	1	610	CLA	ND
20	1	611	CLA	ND
20	1	612	CLA	ND
20	1	613	CLA	ND
20	1	614	CLA	ND
20	3	302	CLA	ND
20	3	303	CLA	ND
20	3	304	CLA	ND
20	3	305	CLA	ND
20	3	306	CLA	ND
20	3	307	CLA	ND
20	3	308	CLA	ND
20	3	309	CLA	ND
20	3	310	CLA	ND
20	3	311	CLA	ND
20	3	312	CLA	ND
20	3	313	CLA	ND
20	3	314	CLA	ND
20	3	324	CLA	ND
20	3	325	CLA	ND
20	7	303	CLA	ND
20	7	304	CLA	ND
20	7	305	CLA	ND
20	7	309	CLA	ND
20	7	310	CLA	ND
20	7	311	CLA	ND
20	7	312	CLA	ND
20	7	313	CLA	ND
20	7	314	CLA	ND
20	7	315	CLA	ND
20	7	323	CLA	ND
20	8	301	CLA	ND
20	8	302	CLA	ND

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Mol	Chain	Res	Type	Atom
20	8	303	CLA	ND
20	8	307	CLA	ND
20	8	308	CLA	ND
20	8	309	CLA	ND
20	8	310	CLA	ND
20	8	311	CLA	ND
20	8	312	CLA	ND
20	8	313	CLA	ND
20	9	601	CLA	ND
20	9	602	CLA	ND
20	9	603	CLA	ND
20	9	604	CLA	ND
20	9	605	CLA	ND
20	9	607	CLA	ND
20	9	608	CLA	ND
20	9	609	CLA	ND
20	9	610	CLA	ND
20	9	611	CLA	ND
20	9	612	CLA	ND
20	A	5004	CLA	ND
20	A	5005	CLA	ND
20	A	5006	CLA	ND
20	A	5007	CLA	ND
20	A	5008	CLA	ND
20	A	5009	CLA	ND
20	A	5010	CLA	ND
20	A	5011	CLA	ND
20	A	5012	CLA	ND
20	A	5013	CLA	ND
20	A	5015	CLA	ND
20	A	5016	CLA	ND
20	A	5017	CLA	ND
20	A	5018	CLA	ND
20	A	5019	CLA	ND
20	A	5020	CLA	ND
20	A	5021	CLA	ND
20	A	5022	CLA	ND
20	A	5023	CLA	ND
20	A	5024	CLA	ND
20	A	5025	CLA	ND
20	A	5026	CLA	ND
20	A	5027	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	5028	CLA	ND
20	A	5029	CLA	ND
20	A	5030	CLA	ND
20	A	5031	CLA	ND
20	A	5032	CLA	ND
20	A	5033	CLA	ND
20	A	5034	CLA	ND
20	A	5035	CLA	ND
20	A	5036	CLA	ND
20	A	5037	CLA	ND
20	A	5038	CLA	ND
20	A	5039	CLA	ND
20	A	5040	CLA	ND
20	A	5041	CLA	ND
20	A	5042	CLA	ND
20	A	5043	CLA	ND
20	A	5044	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND
20	B	806	CLA	ND
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	809	CLA	ND
20	B	810	CLA	ND
20	B	811	CLA	ND
20	B	812	CLA	ND
20	B	813	CLA	ND
20	B	814	CLA	ND
20	B	815	CLA	ND
20	B	816	CLA	ND
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	820	CLA	ND
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	824	CLA	ND
20	B	825	CLA	ND
20	B	826	CLA	ND
20	B	827	CLA	ND
20	B	828	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	829	CLA	ND
20	B	830	CLA	ND
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	835	CLA	ND
20	B	836	CLA	ND
20	B	838	CLA	ND
20	B	839	CLA	ND
20	B	840	CLA	ND
20	F	303	CLA	ND
20	F	306	CLA	ND
20	F	307	CLA	ND
20	F	308	CLA	ND
20	G	201	CLA	ND
20	G	202	CLA	ND
20	G	203	CLA	ND
20	G	204	CLA	ND
20	H	201	CLA	ND
20	J	104	CLA	ND
20	K	4002	CLA	ND
20	K	4003	CLA	ND
20	K	4004	CLA	ND
20	K	4005	CLA	ND
20	L	201	CLA	ND
20	L	202	CLA	ND
20	L	204	CLA	ND
20	L	205	CLA	ND
20	2	301	CLA	ND
20	2	303	CLA	ND
20	2	304	CLA	ND
20	2	305	CLA	ND
20	2	307	CLA	ND
20	2	308	CLA	ND
20	2	309	CLA	ND
20	2	310	CLA	ND
20	2	311	CLA	ND
20	2	312	CLA	ND
20	2	313	CLA	ND
21	1	615	LUT	C23
21	1	615	LUT	C26

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Mol	Chain	Res	Type	Atom
21	1	615	LUT	C3
21	3	315	LUT	C23
21	3	315	LUT	C26
21	3	315	LUT	C3
21	7	316	LUT	C23
21	7	316	LUT	C26
21	7	316	LUT	C3
21	8	314	LUT	C23
21	8	314	LUT	C26
21	8	314	LUT	C3
21	9	613	LUT	C23
21	9	613	LUT	C26
21	9	613	LUT	C3
21	2	314	LUT	C23
21	2	314	LUT	C26
21	2	314	LUT	C3
21	2	315	LUT	C23
21	2	315	LUT	C26
21	2	315	LUT	C3
30	A	5003	CL0	NA

All (2063) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	601	CHL	C3A-C2A-CAA-CBA
19	1	601	CHL	CHA-CBD-CGD-O1D
19	1	601	CHL	CHA-CBD-CGD-O2D
19	1	601	CHL	CBD-CGD-O2D-CED
19	1	606	CHL	C1C-C2C-CMC-OMC
19	1	606	CHL	C3C-C2C-CMC-OMC
19	1	606	CHL	CBD-CGD-O2D-CED
19	3	301	CHL	C3A-C2A-CAA-CBA
19	3	301	CHL	C1C-C2C-CMC-OMC
19	3	301	CHL	C1-C2-C3-C4
19	3	323	CHL	C3C-C2C-CMC-OMC
19	7	306	CHL	C1C-C2C-CMC-OMC
19	7	306	CHL	C3C-C2C-CMC-OMC
19	7	307	CHL	C1A-C2A-CAA-CBA
19	7	307	CHL	CBD-CGD-O2D-CED
19	7	308	CHL	C1C-C2C-CMC-OMC
19	7	308	CHL	C3C-C2C-CMC-OMC
19	8	304	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	8	305	CHL	CBD-CGD-O2D-CED
19	9	606	CHL	CBA-CGA-O2A-C1
19	9	606	CHL	C1C-C2C-CMC-OMC
19	9	606	CHL	C3C-C2C-CMC-OMC
19	2	302	CHL	C1A-C2A-CAA-CBA
19	2	302	CHL	CBD-CGD-O2D-CED
19	2	306	CHL	C1C-C2C-CMC-OMC
19	2	306	CHL	C3C-C2C-CMC-OMC
19	2	306	CHL	CBD-CGD-O2D-CED
20	1	602	CLA	CHA-CBD-CGD-O1D
20	1	602	CLA	CHA-CBD-CGD-O2D
20	1	603	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	CAD-CBD-CGD-O1D
20	1	604	CLA	CAD-CBD-CGD-O2D
20	1	605	CLA	CBD-CGD-O2D-CED
20	1	608	CLA	CHA-CBD-CGD-O1D
20	1	608	CLA	CHA-CBD-CGD-O2D
20	1	609	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	C1A-C2A-CAA-CBA
20	1	611	CLA	CBA-CGA-O2A-C1
20	1	612	CLA	C1A-C2A-CAA-CBA
20	1	612	CLA	CBD-CGD-O2D-CED
20	1	612	CLA	C2-C3-C5-C6
20	1	612	CLA	C4-C3-C5-C6
20	1	613	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	C1A-C2A-CAA-CBA
20	1	614	CLA	C3A-C2A-CAA-CBA
20	3	302	CLA	CBD-CGD-O2D-CED
20	3	303	CLA	CBA-CGA-O2A-C1
20	3	304	CLA	CBA-CGA-O2A-C1
20	3	304	CLA	O1A-CGA-O2A-C1
20	3	306	CLA	C1A-C2A-CAA-CBA
20	3	306	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	CHA-CBD-CGD-O1D
20	3	307	CLA	CHA-CBD-CGD-O2D
20	3	309	CLA	CBD-CGD-O2D-CED
20	3	312	CLA	CBD-CGD-O2D-CED
20	3	314	CLA	CBA-CGA-O2A-C1
20	3	314	CLA	O1A-CGA-O2A-C1
20	3	314	CLA	CBD-CGD-O2D-CED
20	3	324	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	3	324	CLA	C3A-C2A-CAA-CBA
20	3	325	CLA	C1A-C2A-CAA-CBA
20	7	303	CLA	C1A-C2A-CAA-CBA
20	7	303	CLA	C3A-C2A-CAA-CBA
20	7	309	CLA	C1A-C2A-CAA-CBA
20	7	309	CLA	C3A-C2A-CAA-CBA
20	7	310	CLA	C1A-C2A-CAA-CBA
20	7	310	CLA	C3A-C2A-CAA-CBA
20	7	312	CLA	C3-C5-C6-C7
20	7	323	CLA	C1A-C2A-CAA-CBA
20	7	323	CLA	C3A-C2A-CAA-CBA
20	7	323	CLA	CBD-CGD-O2D-CED
20	8	301	CLA	C3A-C2A-CAA-CBA
20	8	302	CLA	CBD-CGD-O2D-CED
20	8	303	CLA	C1A-C2A-CAA-CBA
20	8	303	CLA	C3A-C2A-CAA-CBA
20	8	307	CLA	C1A-C2A-CAA-CBA
20	8	307	CLA	C3A-C2A-CAA-CBA
20	8	308	CLA	C1A-C2A-CAA-CBA
20	8	310	CLA	CHA-CBD-CGD-O1D
20	8	310	CLA	CHA-CBD-CGD-O2D
20	8	321	CLA	C1A-C2A-CAA-CBA
20	8	321	CLA	C3A-C2A-CAA-CBA
20	9	601	CLA	C1A-C2A-CAA-CBA
20	9	601	CLA	C3A-C2A-CAA-CBA
20	9	601	CLA	CHA-CBD-CGD-O1D
20	9	601	CLA	CHA-CBD-CGD-O2D
20	9	602	CLA	CAD-CBD-CGD-O2D
20	9	604	CLA	C1A-C2A-CAA-CBA
20	9	607	CLA	C1A-C2A-CAA-CBA
20	9	607	CLA	C3A-C2A-CAA-CBA
20	9	608	CLA	C1A-C2A-CAA-CBA
20	9	608	CLA	C3A-C2A-CAA-CBA
20	9	610	CLA	CHA-CBD-CGD-O1D
20	9	610	CLA	CHA-CBD-CGD-O2D
20	9	612	CLA	CBA-CGA-O2A-C1
20	9	612	CLA	O1A-CGA-O2A-C1
20	A	5004	CLA	CBD-CGD-O2D-CED
20	A	5004	CLA	C2-C3-C5-C6
20	A	5004	CLA	C4-C3-C5-C6
20	A	5007	CLA	C3A-C2A-CAA-CBA
20	A	5008	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	5008	CLA	C3A-C2A-CAA-CBA
20	A	5008	CLA	CAD-CBD-CGD-O1D
20	A	5008	CLA	CAD-CBD-CGD-O2D
20	A	5011	CLA	C1A-C2A-CAA-CBA
20	A	5011	CLA	C3A-C2A-CAA-CBA
20	A	5011	CLA	CHA-CBD-CGD-O1D
20	A	5011	CLA	CHA-CBD-CGD-O2D
20	A	5012	CLA	C1A-C2A-CAA-CBA
20	A	5012	CLA	C3A-C2A-CAA-CBA
20	A	5016	CLA	C1A-C2A-CAA-CBA
20	A	5016	CLA	C3A-C2A-CAA-CBA
20	A	5016	CLA	CBD-CGD-O2D-CED
20	A	5019	CLA	C1A-C2A-CAA-CBA
20	A	5019	CLA	C3A-C2A-CAA-CBA
20	A	5020	CLA	CHA-CBD-CGD-O1D
20	A	5020	CLA	CHA-CBD-CGD-O2D
20	A	5023	CLA	CBD-CGD-O2D-CED
20	A	5025	CLA	CBD-CGD-O2D-CED
20	A	5026	CLA	CBD-CGD-O2D-CED
20	A	5027	CLA	CHA-CBD-CGD-O1D
20	A	5027	CLA	CHA-CBD-CGD-O2D
20	A	5027	CLA	CBD-CGD-O2D-CED
20	A	5028	CLA	C11-C10-C8-C7
20	A	5029	CLA	C1A-C2A-CAA-CBA
20	A	5029	CLA	C3A-C2A-CAA-CBA
20	A	5031	CLA	CHA-CBD-CGD-O1D
20	A	5031	CLA	CHA-CBD-CGD-O2D
20	A	5032	CLA	CBD-CGD-O2D-CED
20	A	5037	CLA	CHA-CBD-CGD-O1D
20	A	5037	CLA	CHA-CBD-CGD-O2D
20	A	5040	CLA	C1A-C2A-CAA-CBA
20	A	5041	CLA	C1A-C2A-CAA-CBA
20	A	5041	CLA	C3A-C2A-CAA-CBA
20	A	5043	CLA	CBD-CGD-O2D-CED
20	A	5044	CLA	CAD-CBD-CGD-O1D
20	A	5044	CLA	CAD-CBD-CGD-O2D
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	B	804	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C3A-C2A-CAA-CBA
20	B	805	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	806	CLA	CHA-CBD-CGD-O1D
20	B	806	CLA	CHA-CBD-CGD-O2D
20	B	808	CLA	CBD-CGD-O2D-CED
20	B	808	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	CBD-CGD-O2D-CED
20	B	814	CLA	CBD-CGD-O2D-CED
20	B	814	CLA	O1D-CGD-O2D-CED
20	B	817	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C3A-C2A-CAA-CBA
20	B	821	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	825	CLA	CHA-CBD-CGD-O1D
20	B	825	CLA	CHA-CBD-CGD-O2D
20	B	826	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	CAD-CBD-CGD-O1D
20	B	834	CLA	CAD-CBD-CGD-O2D
20	B	835	CLA	CBD-CGD-O2D-CED
20	B	839	CLA	C1A-C2A-CAA-CBA
20	B	839	CLA	C3A-C2A-CAA-CBA
20	B	840	CLA	C1A-C2A-CAA-CBA
20	F	306	CLA	CBD-CGD-O2D-CED
20	H	201	CLA	CAD-CBD-CGD-O1D
20	H	201	CLA	CAD-CBD-CGD-O2D
20	H	201	CLA	CBD-CGD-O2D-CED
20	H	201	CLA	C2-C3-C5-C6
20	H	201	CLA	C4-C3-C5-C6
20	K	4005	CLA	CAD-CBD-CGD-O1D
20	K	4005	CLA	CAD-CBD-CGD-O2D
20	L	201	CLA	CBD-CGD-O2D-CED
20	L	201	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	L	204	CLA	C1A-C2A-CAA-CBA
20	L	204	CLA	CAD-CBD-CGD-O2D
20	2	304	CLA	C1A-C2A-CAA-CBA
20	2	304	CLA	C3A-C2A-CAA-CBA
20	2	304	CLA	CBD-CGD-O2D-CED
20	2	307	CLA	CHA-CBD-CGD-O1D
20	2	307	CLA	CHA-CBD-CGD-O2D
20	2	311	CLA	C1A-C2A-CAA-CBA
20	2	311	CLA	C3A-C2A-CAA-CBA
20	2	311	CLA	CBD-CGD-O2D-CED
21	1	615	LUT	C5-C6-C7-C8
21	1	615	LUT	C21-C26-C27-C28
21	1	615	LUT	C25-C26-C27-C28
21	7	316	LUT	C21-C26-C27-C28
21	7	316	LUT	C25-C26-C27-C28
21	2	314	LUT	C21-C26-C27-C28
21	2	315	LUT	C21-C26-C27-C28
21	2	315	LUT	C25-C26-C27-C28
22	1	616	XAT	O4-C6-C7-C8
22	1	616	XAT	C6-C7-C8-C9
22	3	316	XAT	C26-C27-C28-C29
22	7	317	XAT	C25-C26-C27-C28
22	8	315	XAT	C6-C7-C8-C9
22	9	615	XAT	C6-C7-C8-C9
22	9	615	XAT	C26-C27-C28-C29
23	3	319	BCR	C6-C7-C8-C9
23	3	319	BCR	C7-C8-C9-C10
23	3	319	BCR	C7-C8-C9-C34
23	3	319	BCR	C10-C11-C12-C13
23	3	319	BCR	C11-C12-C13-C14
23	3	319	BCR	C12-C13-C14-C15
23	3	319	BCR	C35-C13-C14-C15
23	3	319	BCR	C14-C15-C16-C17
23	3	319	BCR	C17-C18-C19-C20
23	3	319	BCR	C18-C19-C20-C21
23	3	319	BCR	C20-C21-C22-C23
23	3	319	BCR	C20-C21-C22-C37
23	3	319	BCR	C22-C23-C24-C25
23	A	5049	BCR	C23-C24-C25-C26
23	A	5049	BCR	C23-C24-C25-C30
23	A	5050	BCR	C13-C14-C15-C16
23	B	842	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	B	842	BCR	C23-C24-C25-C30
23	B	844	BCR	C17-C18-C19-C20
23	B	844	BCR	C36-C18-C19-C20
23	J	102	BCR	C11-C12-C13-C14
23	J	102	BCR	C11-C12-C13-C35
23	J	102	BCR	C23-C24-C25-C26
23	J	102	BCR	C23-C24-C25-C30
23	J	105	BCR	C23-C24-C25-C26
23	K	4001	BCR	C1-C6-C7-C8
23	K	4001	BCR	C5-C6-C7-C8
23	L	206	BCR	C15-C16-C17-C18
23	L	206	BCR	C23-C24-C25-C26
24	1	618	LHG	O7-C5-C6-O8
24	1	618	LHG	O9-C7-O7-C5
24	1	618	LHG	C8-C7-O7-C5
24	1	620	LHG	C3-O3-P-O5
24	1	620	LHG	C3-O3-P-O6
24	1	620	LHG	C4-O6-P-O5
24	1	620	LHG	O6-C4-C5-O7
24	1	620	LHG	O9-C7-O7-C5
24	1	620	LHG	C8-C7-O7-C5
24	7	319	LHG	C3-O3-P-O4
24	7	319	LHG	C3-O3-P-O6
24	7	319	LHG	C4-O6-P-O3
24	7	319	LHG	C4-O6-P-O4
24	7	319	LHG	O9-C7-O7-C5
24	7	319	LHG	C8-C7-O7-C5
24	7	320	LHG	C3-O3-P-O6
24	7	320	LHG	C4-O6-P-O3
24	7	320	LHG	C4-O6-P-O4
24	8	317	LHG	C3-O3-P-O6
24	8	319	LHG	C3-O3-P-O4
24	8	319	LHG	C3-O3-P-O6
24	8	320	LHG	C3-O3-P-O4
24	8	320	LHG	C3-O3-P-O6
24	9	617	LHG	C3-O3-P-O5
24	9	617	LHG	C3-O3-P-O6
24	9	617	LHG	C4-O6-P-O4
24	9	617	LHG	O7-C5-C6-O8
24	9	617	LHG	O9-C7-O7-C5
24	9	617	LHG	C8-C7-O7-C5
24	A	5002	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
24	A	5002	LHG	C3-O3-P-O5
24	A	5002	LHG	C3-O3-P-O6
24	A	5002	LHG	C4-O6-P-O5
24	A	5002	LHG	O7-C5-C6-O8
24	A	5002	LHG	O9-C7-O7-C5
24	A	5002	LHG	C8-C7-O7-C5
24	A	5052	LHG	C3-O3-P-O4
24	A	5052	LHG	C3-O3-P-O5
24	A	5052	LHG	C3-O3-P-O6
24	A	5052	LHG	O7-C5-C6-O8
24	A	5054	LHG	C3-O3-P-O6
24	A	5054	LHG	C4-O6-P-O3
24	A	5054	LHG	C4-O6-P-O4
24	A	5054	LHG	C4-O6-P-O5
24	A	5054	LHG	O9-C7-O7-C5
24	A	5054	LHG	C8-C7-O7-C5
24	A	5054	LHG	O10-C23-O8-C6
24	A	5054	LHG	C24-C23-O8-C6
24	A	5055	LHG	O9-C7-O7-C5
24	A	5055	LHG	C8-C7-O7-C5
24	B	801	LHG	C4-O6-P-O3
24	B	801	LHG	C4-O6-P-O5
24	B	849	LHG	C3-O3-P-O6
24	B	849	LHG	O9-C7-O7-C5
24	B	849	LHG	C8-C7-O7-C5
24	B	849	LHG	O10-C23-O8-C6
24	B	849	LHG	C24-C23-O8-C6
25	1	619	SQD	O5-C1-O6-C44
25	1	619	SQD	O49-C7-O47-C45
25	1	619	SQD	C8-C7-O47-C45
25	1	619	SQD	O10-C23-O48-C46
25	1	619	SQD	C24-C23-O48-C46
25	1	619	SQD	C5-C6-S-O7
25	1	619	SQD	C5-C6-S-O8
25	1	619	SQD	C5-C6-S-O9
25	3	322	SQD	O5-C1-O6-C44
25	3	322	SQD	O49-C7-O47-C45
25	3	322	SQD	C8-C7-O47-C45
25	3	322	SQD	C5-C6-S-O8
25	3	322	SQD	C5-C6-S-O9
25	7	322	SQD	O49-C7-O47-C45
25	7	322	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
25	B	850	SQD	O5-C5-C6-S
25	F	311	SQD	O10-C23-O48-C46
25	F	311	SQD	C24-C23-O48-C46
26	3	321	PTY	C3-O11-P1-O12
26	3	321	PTY	C3-O11-P1-O14
26	3	321	PTY	C5-O14-P1-O11
26	3	321	PTY	C5-O14-P1-O12
26	3	321	PTY	C5-O14-P1-O13
26	7	302	PTY	C6-C5-O14-P1
26	7	302	PTY	O10-C8-O7-C6
26	7	302	PTY	C5-O14-P1-O11
26	7	302	PTY	C5-O14-P1-O12
26	B	802	PTY	C11-C8-O7-C6
26	B	802	PTY	C3-O11-P1-O14
26	F	301	PTY	O10-C8-O7-C6
26	F	301	PTY	C11-C8-O7-C6
26	F	301	PTY	C3-O11-P1-O13
26	F	301	PTY	C3-O11-P1-O14
26	F	301	PTY	C5-O14-P1-O12
26	F	302	PTY	N1-C2-C3-O11
26	F	302	PTY	C2-C3-O11-P1
26	F	302	PTY	C3-O11-P1-O14
26	F	302	PTY	C5-O14-P1-O11
26	F	302	PTY	C5-O14-P1-O13
26	F	310	PTY	C6-C5-O14-P1
26	F	310	PTY	C5-O14-P1-O11
26	F	310	PTY	C5-O14-P1-O12
27	7	301	LMG	O1-C7-C8-O7
27	7	324	LMG	O10-C28-O8-C9
27	7	324	LMG	C29-C28-O8-C9
27	A	5001	LMG	O6-C1-O1-C7
27	A	5001	LMG	O9-C10-O7-C8
27	A	5001	LMG	C11-C10-O7-C8
27	G	206	LMG	O7-C8-C9-O8
27	J	103	LMG	O6-C1-O1-C7
28	B	848	DGD	C2B-C1B-O2G-C2G
28	B	848	DGD	O1B-C1B-O2G-C2G
29	8	322	LMU	C2-C1-O1'-C1'
29	9	616	LMU	O5'-C1'-O1'-C1
30	A	5003	CL0	C14-C13-C15-C16
33	J	101	LMK	C2-C3-N4-C6
19	8	305	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	1	613	CLA	O1D-CGD-O2D-CED
20	3	309	CLA	O1D-CGD-O2D-CED
20	9	609	CLA	O1D-CGD-O2D-CED
20	A	5036	CLA	O1D-CGD-O2D-CED
20	B	812	CLA	O1D-CGD-O2D-CED
20	H	201	CLA	O1D-CGD-O2D-CED
20	2	311	CLA	O1D-CGD-O2D-CED
19	1	606	CHL	O1D-CGD-O2D-CED
19	7	307	CHL	O1D-CGD-O2D-CED
20	1	605	CLA	O1D-CGD-O2D-CED
20	3	302	CLA	O1D-CGD-O2D-CED
20	9	602	CLA	O1D-CGD-O2D-CED
20	B	804	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	O1D-CGD-O2D-CED
19	8	306	CHL	CBD-CGD-O2D-CED
20	1	611	CLA	CBD-CGD-O2D-CED
20	1	614	CLA	CBD-CGD-O2D-CED
20	3	308	CLA	CBD-CGD-O2D-CED
20	3	324	CLA	CBD-CGD-O2D-CED
20	7	313	CLA	CBD-CGD-O2D-CED
20	8	321	CLA	CBD-CGD-O2D-CED
20	9	602	CLA	CBD-CGD-O2D-CED
20	9	603	CLA	CBD-CGD-O2D-CED
20	9	605	CLA	CBD-CGD-O2D-CED
20	9	609	CLA	CBD-CGD-O2D-CED
20	A	5017	CLA	CBD-CGD-O2D-CED
20	A	5034	CLA	CBD-CGD-O2D-CED
20	A	5036	CLA	CBD-CGD-O2D-CED
20	B	809	CLA	CBD-CGD-O2D-CED
20	B	826	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	CBD-CGD-O2D-CED
20	F	308	CLA	CBD-CGD-O2D-CED
20	G	201	CLA	CBD-CGD-O2D-CED
20	K	4005	CLA	CBD-CGD-O2D-CED
20	3	306	CLA	O1A-CGA-O2A-C1
20	8	307	CLA	O1A-CGA-O2A-C1
20	8	309	CLA	O1A-CGA-O2A-C1
20	9	607	CLA	O1A-CGA-O2A-C1
20	B	811	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	B	834	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	F	301	PTY	O30-C30-O4-C1
20	1	611	CLA	O1A-CGA-O2A-C1
20	1	612	CLA	O1D-CGD-O2D-CED
20	F	306	CLA	O1D-CGD-O2D-CED
29	F	305	LMU	O5B-C1B-O1B-C4'
19	1	606	CHL	CBA-CGA-O2A-C1
19	8	304	CHL	CBA-CGA-O2A-C1
20	1	614	CLA	CBA-CGA-O2A-C1
20	8	313	CLA	CBA-CGA-O2A-C1
20	8	321	CLA	CBA-CGA-O2A-C1
20	2	307	CLA	CBA-CGA-O2A-C1
20	9	603	CLA	O1D-CGD-O2D-CED
20	A	5034	CLA	O1D-CGD-O2D-CED
20	G	201	CLA	O1D-CGD-O2D-CED
20	K	4005	CLA	O1D-CGD-O2D-CED
20	8	309	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	CBA-CGA-O2A-C1
26	F	301	PTY	C31-C30-O4-C1
20	A	5015	CLA	CBD-CGD-O2D-CED
20	J	104	CLA	CBD-CGD-O2D-CED
20	1	609	CLA	O1A-CGA-O2A-C1
20	1	612	CLA	O1A-CGA-O2A-C1
20	3	307	CLA	O1A-CGA-O2A-C1
20	3	311	CLA	O1A-CGA-O2A-C1
20	3	324	CLA	O1A-CGA-O2A-C1
20	3	325	CLA	O1A-CGA-O2A-C1
20	7	311	CLA	O1A-CGA-O2A-C1
20	8	311	CLA	O1A-CGA-O2A-C1
20	9	611	CLA	O1A-CGA-O2A-C1
20	A	5004	CLA	O1A-CGA-O2A-C1
20	A	5006	CLA	O1A-CGA-O2A-C1
20	A	5009	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	B	819	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	O1A-CGA-O2A-C1
20	B	830	CLA	O1A-CGA-O2A-C1
20	B	832	CLA	O1A-CGA-O2A-C1
20	F	303	CLA	O1A-CGA-O2A-C1
20	F	306	CLA	O1A-CGA-O2A-C1
20	F	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	G	202	CLA	O1A-CGA-O2A-C1
20	H	201	CLA	O1A-CGA-O2A-C1
26	3	321	PTY	O30-C30-O4-C1
26	B	802	PTY	O30-C30-O4-C1
26	F	310	PTY	O30-C30-O4-C1
19	9	606	CHL	O1A-CGA-O2A-C1
20	3	303	CLA	O1A-CGA-O2A-C1
19	1	601	CHL	O1D-CGD-O2D-CED
20	1	614	CLA	O1D-CGD-O2D-CED
20	3	312	CLA	O1D-CGD-O2D-CED
20	8	302	CLA	O1D-CGD-O2D-CED
20	A	5016	CLA	O1D-CGD-O2D-CED
20	A	5025	CLA	O1D-CGD-O2D-CED
20	B	829	CLA	O1D-CGD-O2D-CED
20	B	835	CLA	O1D-CGD-O2D-CED
29	8	318	LMU	O5B-C1B-O1B-C4'
20	1	603	CLA	O1D-CGD-O2D-CED
20	1	609	CLA	O1D-CGD-O2D-CED
20	7	323	CLA	O1D-CGD-O2D-CED
20	A	5023	CLA	O1D-CGD-O2D-CED
20	A	5027	CLA	O1D-CGD-O2D-CED
20	A	5032	CLA	O1D-CGD-O2D-CED
20	A	5043	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	O1D-CGD-O2D-CED
20	L	201	CLA	O1D-CGD-O2D-CED
20	2	304	CLA	O1D-CGD-O2D-CED
20	L	205	CLA	CBD-CGD-O2D-CED
20	3	305	CLA	O1A-CGA-O2A-C1
20	A	5015	CLA	O1A-CGA-O2A-C1
26	B	802	PTY	O10-C8-O7-C6
26	F	310	PTY	O10-C8-O7-C6
20	G	203	CLA	CBA-CGA-O2A-C1
20	3	310	CLA	O1A-CGA-O2A-C1
20	8	321	CLA	O1A-CGA-O2A-C1
20	9	601	CLA	O1A-CGA-O2A-C1
20	7	310	CLA	C3-C5-C6-C7
20	8	311	CLA	C3-C5-C6-C7
20	A	5016	CLA	C3-C5-C6-C7
20	A	5019	CLA	C3-C5-C6-C7
20	B	808	CLA	C3-C5-C6-C7
20	B	810	CLA	C3-C5-C6-C7
20	B	811	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	B	812	CLA	C3-C5-C6-C7
20	B	822	CLA	C3-C5-C6-C7
20	B	824	CLA	C3-C5-C6-C7
19	2	306	CHL	O1D-CGD-O2D-CED
20	1	609	CLA	CBA-CGA-O2A-C1
20	1	612	CLA	CBA-CGA-O2A-C1
20	1	613	CLA	CBA-CGA-O2A-C1
20	3	306	CLA	CBA-CGA-O2A-C1
20	3	311	CLA	CBA-CGA-O2A-C1
20	3	325	CLA	CBA-CGA-O2A-C1
20	7	311	CLA	CBA-CGA-O2A-C1
20	8	307	CLA	CBA-CGA-O2A-C1
20	9	607	CLA	CBA-CGA-O2A-C1
20	9	611	CLA	CBA-CGA-O2A-C1
20	A	5006	CLA	CBA-CGA-O2A-C1
20	A	5009	CLA	CBA-CGA-O2A-C1
20	B	811	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	CBA-CGA-O2A-C1
20	B	834	CLA	CBA-CGA-O2A-C1
20	G	202	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	CBA-CGA-O2A-C1
26	B	802	PTY	C31-C30-O4-C1
26	F	310	PTY	C31-C30-O4-C1
20	1	602	CLA	CBD-CGD-O2D-CED
20	3	307	CLA	CBD-CGD-O2D-CED
20	3	311	CLA	CBD-CGD-O2D-CED
20	7	305	CLA	CBD-CGD-O2D-CED
20	7	314	CLA	CBD-CGD-O2D-CED
20	7	315	CLA	CBD-CGD-O2D-CED
20	8	313	CLA	CBD-CGD-O2D-CED
20	9	608	CLA	CBD-CGD-O2D-CED
20	9	610	CLA	CBD-CGD-O2D-CED
20	A	5006	CLA	CBD-CGD-O2D-CED
20	A	5020	CLA	CBD-CGD-O2D-CED
20	A	5035	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	B	815	CLA	CBD-CGD-O2D-CED
20	B	816	CLA	CBD-CGD-O2D-CED
20	B	822	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	833	CLA	CBD-CGD-O2D-CED
20	G	203	CLA	CBD-CGD-O2D-CED
20	K	4004	CLA	CBD-CGD-O2D-CED
26	F	310	PTY	C11-C8-O7-C6
19	2	302	CHL	O1D-CGD-O2D-CED
20	3	308	CLA	O1D-CGD-O2D-CED
20	3	314	CLA	O1D-CGD-O2D-CED
20	3	324	CLA	O1D-CGD-O2D-CED
20	8	321	CLA	O1D-CGD-O2D-CED
20	A	5004	CLA	O1D-CGD-O2D-CED
20	A	5026	CLA	O1D-CGD-O2D-CED
20	B	834	CLA	O1D-CGD-O2D-CED
20	G	201	CLA	O1A-CGA-O2A-C1
19	1	606	CHL	O1A-CGA-O2A-C1
20	9	609	CLA	O1A-CGA-O2A-C1
20	9	607	CLA	C4-C3-C5-C6
20	3	310	CLA	CBA-CGA-O2A-C1
20	8	310	CLA	CBA-CGA-O2A-C1
20	8	312	CLA	CBA-CGA-O2A-C1
20	9	601	CLA	CBA-CGA-O2A-C1
20	9	609	CLA	CBA-CGA-O2A-C1
20	9	607	CLA	CBD-CGD-O2D-CED
20	A	5029	CLA	CBD-CGD-O2D-CED
20	K	4003	CLA	CBD-CGD-O2D-CED
20	9	605	CLA	O1D-CGD-O2D-CED
20	F	308	CLA	O1D-CGD-O2D-CED
20	8	308	CLA	C2A-CAA-CBA-CGA
20	8	321	CLA	C2A-CAA-CBA-CGA
20	B	815	CLA	C2A-CAA-CBA-CGA
20	B	823	CLA	C2A-CAA-CBA-CGA
20	1	603	CLA	C3-C5-C6-C7
20	B	807	CLA	C3-C5-C6-C7
20	B	816	CLA	C3-C5-C6-C7
20	B	832	CLA	C3-C5-C6-C7
20	B	840	CLA	C3-C5-C6-C7
20	F	303	CLA	C3-C5-C6-C7
20	G	201	CLA	C3-C5-C6-C7
20	L	202	CLA	C3-C5-C6-C7
20	3	305	CLA	CBA-CGA-O2A-C1
20	3	307	CLA	CBA-CGA-O2A-C1
20	3	324	CLA	CBA-CGA-O2A-C1
20	7	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	8	301	CLA	CBA-CGA-O2A-C1
20	8	311	CLA	CBA-CGA-O2A-C1
20	A	5004	CLA	CBA-CGA-O2A-C1
20	A	5013	CLA	CBA-CGA-O2A-C1
20	A	5015	CLA	CBA-CGA-O2A-C1
20	A	5025	CLA	CBA-CGA-O2A-C1
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	819	CLA	CBA-CGA-O2A-C1
20	B	825	CLA	CBA-CGA-O2A-C1
20	B	832	CLA	CBA-CGA-O2A-C1
20	B	836	CLA	CBA-CGA-O2A-C1
20	F	303	CLA	CBA-CGA-O2A-C1
20	F	306	CLA	CBA-CGA-O2A-C1
20	F	307	CLA	CBA-CGA-O2A-C1
26	3	321	PTY	C31-C30-O4-C1
30	A	5003	CL0	CBA-CGA-O2A-C1
20	8	310	CLA	O1A-CGA-O2A-C1
20	G	203	CLA	O1A-CGA-O2A-C1
20	2	307	CLA	O1A-CGA-O2A-C1
22	9	615	XAT	C33-C34-C35-C15
23	3	319	BCR	C9-C10-C11-C12
23	L	206	BCR	C13-C14-C15-C16
20	1	604	CLA	O1A-CGA-O2A-C1
20	1	613	CLA	O1A-CGA-O2A-C1
20	7	304	CLA	O1A-CGA-O2A-C1
20	7	310	CLA	O1A-CGA-O2A-C1
20	7	323	CLA	O1A-CGA-O2A-C1
20	A	5013	CLA	O1A-CGA-O2A-C1
20	A	5025	CLA	O1A-CGA-O2A-C1
20	A	5035	CLA	O1A-CGA-O2A-C1
20	A	5037	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	O1A-CGA-O2A-C1
20	2	313	CLA	O1A-CGA-O2A-C1
26	F	302	PTY	O30-C30-O4-C1
26	7	302	PTY	O30-C30-O4-C1
19	8	304	CHL	O1A-CGA-O2A-C1
20	1	614	CLA	O1A-CGA-O2A-C1
20	8	313	CLA	O1A-CGA-O2A-C1
20	B	809	CLA	O1D-CGD-O2D-CED
20	A	5029	CLA	C3-C5-C6-C7
20	B	814	CLA	C3-C5-C6-C7
20	1	608	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	7	303	CLA	CBD-CGD-O2D-CED
20	8	309	CLA	CBD-CGD-O2D-CED
20	8	312	CLA	CBD-CGD-O2D-CED
20	B	840	CLA	CBD-CGD-O2D-CED
19	8	306	CHL	O1D-CGD-O2D-CED
20	A	5017	CLA	O1D-CGD-O2D-CED
20	B	826	CLA	O1D-CGD-O2D-CED
20	A	5011	CLA	CBA-CGA-O2A-C1
20	A	5030	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	G	201	CLA	CBA-CGA-O2A-C1
30	A	5003	CL0	O1A-CGA-O2A-C1
20	1	611	CLA	O1D-CGD-O2D-CED
20	A	5037	CLA	CBD-CGD-O2D-CED
20	7	313	CLA	O1D-CGD-O2D-CED
20	A	5028	CLA	C3-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7
20	A	5010	CLA	CBD-CGD-O2D-CED
20	A	5011	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	CBA-CGA-O2A-C1
20	7	304	CLA	CBA-CGA-O2A-C1
20	7	323	CLA	CBA-CGA-O2A-C1
20	A	5035	CLA	CBA-CGA-O2A-C1
20	A	5037	CLA	CBA-CGA-O2A-C1
20	2	313	CLA	CBA-CGA-O2A-C1
26	F	302	PTY	C31-C30-O4-C1
20	A	5029	CLA	C4-C3-C5-C6
20	B	822	CLA	C4-C3-C5-C6
20	9	607	CLA	C2-C3-C5-C6
20	A	5029	CLA	C2-C3-C5-C6
20	B	822	CLA	C2-C3-C5-C6
26	7	302	PTY	C31-C30-O4-C1
20	8	301	CLA	O1A-CGA-O2A-C1
20	A	5030	CLA	O1A-CGA-O2A-C1
20	B	814	CLA	O1A-CGA-O2A-C1
20	B	836	CLA	O1A-CGA-O2A-C1
20	A	5038	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	C2A-CAA-CBA-CGA
20	A	5038	CLA	C2A-CAA-CBA-CGA
20	A	5011	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	7	324	LMG	O6-C1-O1-C7
29	F	305	LMU	O5'-C1'-O1'-C1
20	J	104	CLA	O1D-CGD-O2D-CED
20	A	5007	CLA	CBA-CGA-O2A-C1
20	B	833	CLA	CBA-CGA-O2A-C1
20	1	610	CLA	CBD-CGD-O2D-CED
20	8	301	CLA	CBD-CGD-O2D-CED
20	9	601	CLA	CBD-CGD-O2D-CED
20	9	612	CLA	CBD-CGD-O2D-CED
20	A	5009	CLA	CBD-CGD-O2D-CED
20	A	5012	CLA	CBD-CGD-O2D-CED
20	A	5042	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	CBD-CGD-O2D-CED
20	8	312	CLA	O1A-CGA-O2A-C1
20	A	5015	CLA	O1D-CGD-O2D-CED
20	A	5013	CLA	CBD-CGD-O2D-CED
20	B	828	CLA	CBD-CGD-O2D-CED
26	3	321	PTY	C11-C8-O7-C6
21	1	615	LUT	C13-C14-C15-C35
20	A	5007	CLA	O1A-CGA-O2A-C1
20	B	833	CLA	O1A-CGA-O2A-C1
26	3	321	PTY	O10-C8-O7-C6
20	3	308	CLA	CBA-CGA-O2A-C1
20	7	303	CLA	CBA-CGA-O2A-C1
20	7	313	CLA	CBA-CGA-O2A-C1
20	8	303	CLA	CBA-CGA-O2A-C1
20	9	610	CLA	CBA-CGA-O2A-C1
20	A	5016	CLA	CBA-CGA-O2A-C1
20	B	806	CLA	CBA-CGA-O2A-C1
20	B	809	CLA	CBA-CGA-O2A-C1
20	K	4003	CLA	CBA-CGA-O2A-C1
20	L	202	CLA	CBA-CGA-O2A-C1
20	2	311	CLA	CBA-CGA-O2A-C1
20	K	4002	CLA	CBD-CGD-O2D-CED
20	L	205	CLA	O1D-CGD-O2D-CED
19	3	301	CHL	C4-C3-C5-C6
19	3	301	CHL	C2-C3-C5-C6
20	A	5011	CLA	C3-C5-C6-C7
20	A	5012	CLA	C3-C5-C6-C7
20	B	804	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	B	827	CLA	C3-C5-C6-C7
19	3	301	CHL	C11-C12-C13-C14
19	3	323	CHL	C11-C10-C8-C9
20	A	5035	CLA	C6-C7-C8-C9
20	B	807	CLA	C6-C7-C8-C9
20	B	826	CLA	C11-C10-C8-C9
20	3	311	CLA	O1D-CGD-O2D-CED
20	8	313	CLA	O1D-CGD-O2D-CED
25	3	322	SQD	C2-C1-O6-C44
29	F	305	LMU	C2'-C1'-O1'-C1
29	8	322	LMU	C5'-C4'-O1B-C1B
20	B	806	CLA	O1D-CGD-O2D-CED
20	K	4003	CLA	O1A-CGA-O2A-C1
20	A	5008	CLA	CBD-CGD-O2D-CED
20	7	315	CLA	O1D-CGD-O2D-CED
20	A	5020	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	O1D-CGD-O2D-CED
20	B	822	CLA	O1D-CGD-O2D-CED
20	K	4004	CLA	O1D-CGD-O2D-CED
21	2	315	LUT	C31-C32-C33-C40
22	3	316	XAT	C27-C28-C29-C39
22	9	615	XAT	C11-C12-C13-C20
23	3	319	BCR	C11-C12-C13-C35
23	3	319	BCR	C36-C18-C19-C20
23	A	5047	BCR	C37-C22-C23-C24
23	B	803	BCR	C36-C18-C19-C20
21	2	315	LUT	C27-C28-C29-C30
21	2	315	LUT	C31-C32-C33-C34
22	3	316	XAT	C27-C28-C29-C30
22	9	615	XAT	C11-C12-C13-C14
23	A	5047	BCR	C21-C22-C23-C24
23	B	803	BCR	C17-C18-C19-C20
23	B	844	BCR	C21-C22-C23-C24
23	B	847	BCR	C7-C8-C9-C10
20	A	5004	CLA	C2A-CAA-CBA-CGA
30	A	5003	CL0	C2A-CAA-CBA-CGA
20	3	308	CLA	O1A-CGA-O2A-C1
20	7	303	CLA	O1A-CGA-O2A-C1
20	8	303	CLA	O1A-CGA-O2A-C1
20	9	610	CLA	O1A-CGA-O2A-C1
20	A	5013	CLA	C3-C5-C6-C7
20	1	608	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	8	319	LHG	O7-C5-C6-O8
24	A	5055	LHG	O7-C5-C6-O8
20	A	5018	CLA	CBA-CGA-O2A-C1
20	A	5024	CLA	CBA-CGA-O2A-C1
20	B	838	CLA	CBA-CGA-O2A-C1
20	A	5013	CLA	C15-C16-C17-C18
20	F	303	CLA	C2-C1-O2A-CGA
20	7	314	CLA	O1D-CGD-O2D-CED
20	A	5035	CLA	O1D-CGD-O2D-CED
20	B	816	CLA	O1D-CGD-O2D-CED
20	A	5011	CLA	C5-C6-C7-C8
20	A	5035	CLA	C8-C10-C11-C12
20	B	804	CLA	C13-C15-C16-C17
20	B	809	CLA	C15-C16-C17-C18
20	L	201	CLA	C5-C6-C7-C8
20	A	5006	CLA	O1D-CGD-O2D-CED
20	B	831	CLA	C3-C5-C6-C7
20	B	833	CLA	O1D-CGD-O2D-CED
20	A	5016	CLA	O1A-CGA-O2A-C1
29	8	322	LMU	C3'-C4'-O1B-C1B
20	B	825	CLA	CBD-CGD-O2D-CED
19	2	302	CHL	C11-C10-C8-C7
30	A	5003	CL0	C11-C12-C13-C15
20	8	302	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
19	1	606	CHL	C2C-C3C-CAC-CBC
20	3	307	CLA	O1D-CGD-O2D-CED
20	7	305	CLA	O1D-CGD-O2D-CED
20	G	204	CLA	C2C-C3C-CAC-CBC
20	1	602	CLA	O1D-CGD-O2D-CED
20	A	5014	CLA	C15-C16-C17-C18
20	B	806	CLA	O1A-CGA-O2A-C1
20	B	809	CLA	O1A-CGA-O2A-C1
20	L	202	CLA	O1A-CGA-O2A-C1
20	A	5024	CLA	CBD-CGD-O2D-CED
20	G	202	CLA	C2-C1-O2A-CGA
20	G	203	CLA	O1D-CGD-O2D-CED
19	3	301	CHL	C8-C10-C11-C12
20	B	815	CLA	C15-C16-C17-C18
19	3	301	CHL	C2A-CAA-CBA-CGA
19	8	306	CHL	C2A-CAA-CBA-CGA
19	2	306	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	3	308	CLA	C2A-CAA-CBA-CGA
20	3	312	CLA	C2A-CAA-CBA-CGA
20	A	5012	CLA	C2A-CAA-CBA-CGA
20	A	5023	CLA	C2A-CAA-CBA-CGA
20	B	838	CLA	C2A-CAA-CBA-CGA
19	3	323	CHL	C8-C10-C11-C12
20	9	607	CLA	C10-C11-C12-C13
20	A	5026	CLA	C5-C6-C7-C8
20	B	822	CLA	C10-C11-C12-C13
20	B	830	CLA	C15-C16-C17-C18
20	L	201	CLA	C10-C11-C12-C13
20	9	610	CLA	O1D-CGD-O2D-CED
19	8	305	CHL	CBA-CGA-O2A-C1
20	1	610	CLA	CBA-CGA-O2A-C1
23	B	847	BCR	C6-C7-C8-C9
23	J	102	BCR	C22-C23-C24-C25
25	7	322	SQD	O5-C1-O6-C44
28	7	321	DGD	O6D-C1D-O3G-C3G
28	B	848	DGD	O6D-C1D-O3G-C3G
20	8	303	CLA	C10-C11-C12-C13
20	A	5031	CLA	C8-C10-C11-C12
20	A	5044	CLA	C5-C6-C7-C8
20	B	820	CLA	C15-C16-C17-C18
20	B	822	CLA	C8-C10-C11-C12
20	B	825	CLA	C8-C10-C11-C12
20	B	839	CLA	C5-C6-C7-C8
20	L	202	CLA	C10-C11-C12-C13
30	A	5003	CL0	C15-C16-C17-C18
20	7	313	CLA	O1A-CGA-O2A-C1
20	2	311	CLA	O1A-CGA-O2A-C1
20	A	5025	CLA	C10-C11-C12-C13
20	A	5029	CLA	C5-C6-C7-C8
20	B	822	CLA	C13-C15-C16-C17
20	B	828	CLA	C13-C15-C16-C17
29	8	318	LMU	O1'-C1-C2-C3
20	1	608	CLA	O1D-CGD-O2D-CED
20	9	608	CLA	O1D-CGD-O2D-CED
20	A	5029	CLA	O1D-CGD-O2D-CED
20	B	823	CLA	O1D-CGD-O2D-CED
20	B	826	CLA	C5-C6-C7-C8
20	8	307	CLA	CBD-CGD-O2D-CED
20	B	820	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	2	305	CLA	CBD-CGD-O2D-CED
20	7	303	CLA	O1D-CGD-O2D-CED
20	K	4003	CLA	O1D-CGD-O2D-CED
20	7	305	CLA	CBA-CGA-O2A-C1
20	7	312	CLA	CBA-CGA-O2A-C1
20	8	308	CLA	CBA-CGA-O2A-C1
20	8	302	CLA	O1A-CGA-O2A-C1
20	A	5024	CLA	O1A-CGA-O2A-C1
20	B	823	CLA	O1A-CGA-O2A-C1
20	B	838	CLA	O1A-CGA-O2A-C1
20	8	309	CLA	O1D-CGD-O2D-CED
20	8	312	CLA	O1D-CGD-O2D-CED
20	9	607	CLA	O1D-CGD-O2D-CED
20	7	309	CLA	CBA-CGA-O2A-C1
20	B	816	CLA	C5-C6-C7-C8
20	9	607	CLA	C3-C5-C6-C7
20	B	820	CLA	C8-C10-C11-C12
20	B	829	CLA	C8-C10-C11-C12
20	B	830	CLA	C13-C15-C16-C17
20	L	202	CLA	C8-C10-C11-C12
20	3	309	CLA	C2A-CAA-CBA-CGA
20	A	5030	CLA	C2A-CAA-CBA-CGA
20	B	819	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
20	H	201	CLA	C2A-CAA-CBA-CGA
20	L	202	CLA	C2A-CAA-CBA-CGA
20	2	313	CLA	C2A-CAA-CBA-CGA
20	A	5017	CLA	CBA-CGA-O2A-C1
20	A	5019	CLA	CBA-CGA-O2A-C1
20	2	304	CLA	CBA-CGA-O2A-C1
19	2	302	CHL	C5-C6-C7-C8
20	A	5024	CLA	C8-C10-C11-C12
20	A	5028	CLA	C10-C11-C12-C13
20	B	824	CLA	C15-C16-C17-C18
20	B	840	CLA	C15-C16-C17-C18
20	A	5037	CLA	O1D-CGD-O2D-CED
20	8	308	CLA	CBD-CGD-O2D-CED
20	B	818	CLA	CBD-CGD-O2D-CED
20	B	840	CLA	O1D-CGD-O2D-CED
19	2	302	CHL	C8-C10-C11-C12
20	A	5017	CLA	C5-C6-C7-C8
20	B	828	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	832	CLA	C10-C11-C12-C13
20	3	307	CLA	C10-C11-C12-C13
20	9	607	CLA	C5-C6-C7-C8
20	A	5020	CLA	C8-C10-C11-C12
20	B	829	CLA	C10-C11-C12-C13
20	A	5013	CLA	C4-C3-C5-C6
20	A	5035	CLA	C4-C3-C5-C6
20	B	831	CLA	C4-C3-C5-C6
20	A	5036	CLA	C13-C15-C16-C17
20	9	611	CLA	C3-C5-C6-C7
20	A	5011	CLA	O1D-CGD-O2D-CED
25	7	322	SQD	C2-C1-O6-C44
28	B	848	DGD	C2D-C1D-O3G-C3G
29	9	616	LMU	C2'-C1'-O1'-C1
20	A	5014	CLA	CBA-CGA-O2A-C1
30	A	5003	CL0	C16-C17-C18-C19
20	A	5018	CLA	O1A-CGA-O2A-C1
25	B	850	SQD	C24-C23-O48-C46
20	A	5013	CLA	C13-C15-C16-C17
21	2	315	LUT	C27-C28-C29-C39
23	3	319	BCR	C37-C22-C23-C24
23	A	5047	BCR	C11-C12-C13-C35
23	B	844	BCR	C7-C8-C9-C34
23	B	844	BCR	C37-C22-C23-C24
23	B	847	BCR	C7-C8-C9-C34
24	9	617	LHG	C5-C4-O6-P
29	9	616	LMU	O1'-C1-C2-C3
23	A	5047	BCR	C11-C12-C13-C14
23	B	844	BCR	C7-C8-C9-C10
23	K	4001	BCR	C21-C22-C23-C24
23	L	206	BCR	C21-C22-C23-C24
20	A	5019	CLA	O1A-CGA-O2A-C1
20	A	5019	CLA	C2A-CAA-CBA-CGA
20	B	821	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
20	K	4005	CLA	C2A-CAA-CBA-CGA
20	1	603	CLA	C6-C7-C8-C9
20	3	311	CLA	C6-C7-C8-C10
20	B	839	CLA	C16-C17-C18-C19
20	7	305	CLA	O1A-CGA-O2A-C1
29	7	325	LMU	O5'-C5'-C6'-O6'
21	1	615	LUT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	A	5009	CLA	C15-C16-C17-C18
20	A	5010	CLA	O1D-CGD-O2D-CED
28	B	848	DGD	CAB-CBB-CCB-CDB
20	2	313	CLA	CBD-CGD-O2D-CED
20	A	5040	CLA	C3-C5-C6-C7
20	7	311	CLA	C2-C1-O2A-CGA
20	7	312	CLA	C2-C1-O2A-CGA
20	8	309	CLA	C2-C1-O2A-CGA
20	B	830	CLA	C2-C1-O2A-CGA
19	2	302	CHL	C11-C12-C13-C15
20	1	603	CLA	C6-C7-C8-C10
20	3	311	CLA	C6-C7-C8-C9
20	7	303	CLA	C11-C12-C13-C15
20	A	5014	CLA	C16-C17-C18-C20
20	A	5015	CLA	C6-C7-C8-C9
20	A	5017	CLA	C6-C7-C8-C10
20	A	5018	CLA	C11-C12-C13-C14
20	B	839	CLA	C16-C17-C18-C20
20	8	308	CLA	O1A-CGA-O2A-C1
20	2	304	CLA	O1A-CGA-O2A-C1
20	B	826	CLA	C10-C11-C12-C13
20	A	5038	CLA	O1D-CGD-O2D-CED
20	9	612	CLA	O1D-CGD-O2D-CED
20	B	824	CLA	C13-C15-C16-C17
20	7	312	CLA	O1A-CGA-O2A-C1
24	A	5052	LHG	C9-C10-C11-C12
29	F	305	LMU	C2-C1-O1'-C1'
20	1	610	CLA	O1D-CGD-O2D-CED
20	2	312	CLA	O1D-CGD-O2D-CED
20	A	5004	CLA	C5-C6-C7-C8
20	A	5006	CLA	C8-C10-C11-C12
24	1	620	LHG	C7-C8-C9-C10
24	8	317	LHG	C7-C8-C9-C10
25	1	619	SQD	C25-C26-C27-C28
20	8	308	CLA	C11-C12-C13-C14
20	A	5015	CLA	C6-C7-C8-C10
20	A	5024	CLA	C11-C12-C13-C14
20	A	5024	CLA	C11-C12-C13-C15
20	A	5042	CLA	C11-C12-C13-C14
20	B	828	CLA	C16-C17-C18-C19
20	B	828	CLA	C16-C17-C18-C20
20	A	5012	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	5042	CLA	O1D-CGD-O2D-CED
20	3	303	CLA	C2A-CAA-CBA-CGA
20	3	311	CLA	C2A-CAA-CBA-CGA
20	8	312	CLA	C2A-CAA-CBA-CGA
20	B	813	CLA	C2A-CAA-CBA-CGA
20	J	104	CLA	C2A-CAA-CBA-CGA
20	A	5028	CLA	C8-C10-C11-C12
20	B	808	CLA	C10-C11-C12-C13
20	A	5009	CLA	O1D-CGD-O2D-CED
20	3	302	CLA	C12-C13-C15-C16
20	A	5016	CLA	C12-C13-C15-C16
20	B	832	CLA	C11-C12-C13-C15
31	B	841	PQN	C22-C23-C25-C26
24	7	320	LHG	C23-C24-C25-C26
20	B	814	CLA	C5-C6-C7-C8
24	8	320	LHG	C14-C15-C16-C17
20	A	5017	CLA	O1A-CGA-O2A-C1
19	7	307	CHL	C3A-C2A-CAA-CBA
19	9	606	CHL	C3A-C2A-CAA-CBA
19	2	306	CHL	C3A-C2A-CAA-CBA
20	1	611	CLA	C3A-C2A-CAA-CBA
20	3	304	CLA	C3A-C2A-CAA-CBA
20	3	325	CLA	C3A-C2A-CAA-CBA
20	8	302	CLA	C3A-C2A-CAA-CBA
20	8	308	CLA	C3A-C2A-CAA-CBA
20	9	610	CLA	C3A-C2A-CAA-CBA
20	A	5006	CLA	C3A-C2A-CAA-CBA
20	A	5009	CLA	C3A-C2A-CAA-CBA
20	A	5019	CLA	C4-C3-C5-C6
20	A	5024	CLA	C3A-C2A-CAA-CBA
20	A	5038	CLA	C3A-C2A-CAA-CBA
20	A	5040	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	835	CLA	C3A-C2A-CAA-CBA
20	B	840	CLA	C3A-C2A-CAA-CBA
20	G	203	CLA	C3A-C2A-CAA-CBA
20	H	201	CLA	C3A-C2A-CAA-CBA
20	K	4003	CLA	C3A-C2A-CAA-CBA
20	K	4005	CLA	C3A-C2A-CAA-CBA
20	L	201	CLA	C3A-C2A-CAA-CBA
20	2	305	CLA	C3A-C2A-CAA-CBA
20	2	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	A	5003	CL0	C3A-C2A-CAA-CBA
19	2	302	CHL	C10-C11-C12-C13
20	A	5020	CLA	C15-C16-C17-C18
20	7	303	CLA	C11-C12-C13-C14
20	8	308	CLA	C11-C12-C13-C15
20	A	5018	CLA	C11-C12-C13-C15
20	A	5042	CLA	C11-C12-C13-C15
20	2	303	CLA	CBD-CGD-O2D-CED
19	3	323	CHL	CBA-CGA-O2A-C1
20	9	601	CLA	O1D-CGD-O2D-CED
20	A	5014	CLA	O1A-CGA-O2A-C1
24	A	5002	LHG	C26-C27-C28-C29
27	7	301	LMG	C19-C20-C21-C22
20	8	301	CLA	O1D-CGD-O2D-CED
20	9	603	CLA	C6-C7-C8-C9
20	A	5017	CLA	C6-C7-C8-C9
20	K	4003	CLA	C6-C7-C8-C9
21	1	615	LUT	C1-C6-C7-C8
21	9	613	LUT	C1-C6-C7-C8
21	9	613	LUT	C5-C6-C7-C8
21	2	314	LUT	C1-C6-C7-C8
21	2	314	LUT	C5-C6-C7-C8
23	3	317	BCR	C1-C6-C7-C8
23	3	317	BCR	C5-C6-C7-C8
23	3	317	BCR	C23-C24-C25-C30
23	7	318	BCR	C23-C24-C25-C26
23	7	318	BCR	C23-C24-C25-C30
23	8	316	BCR	C1-C6-C7-C8
23	8	316	BCR	C5-C6-C7-C8
23	B	845	BCR	C23-C24-C25-C30
23	B	847	BCR	C1-C6-C7-C8
23	B	847	BCR	C5-C6-C7-C8
23	J	105	BCR	C1-C6-C7-C8
23	J	105	BCR	C23-C24-C25-C30
23	L	206	BCR	C23-C24-C25-C30
20	B	823	CLA	C5-C6-C7-C8
20	9	611	CLA	C2A-CAA-CBA-CGA
20	A	5044	CLA	C2A-CAA-CBA-CGA
20	2	304	CLA	C2A-CAA-CBA-CGA
26	3	321	PTY	C30-C31-C32-C33
26	F	302	PTY	C12-C13-C14-C15
20	A	5027	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	2	315	LUT	C30-C31-C32-C33
20	A	5013	CLA	C2-C3-C5-C6
20	A	5035	CLA	C2-C3-C5-C6
20	B	831	CLA	C2-C3-C5-C6
20	B	840	CLA	CBA-CGA-O2A-C1
20	L	204	CLA	CBA-CGA-O2A-C1
20	2	303	CLA	CBA-CGA-O2A-C1
20	8	303	CLA	C11-C12-C13-C14
20	B	818	CLA	C6-C7-C8-C9
25	1	619	SQD	C2-C1-O6-C44
29	A	5053	LMU	C2'-C1'-O1'-C1
23	A	5047	BCR	C9-C10-C11-C12
23	A	5049	BCR	C13-C14-C15-C16
20	A	5025	CLA	C5-C6-C7-C8
20	1	608	CLA	O1A-CGA-O2A-C1
20	1	602	CLA	C3-C5-C6-C7
20	L	205	CLA	CBA-CGA-O2A-C1
20	1	610	CLA	O1A-CGA-O2A-C1
20	3	306	CLA	C2A-CAA-CBA-CGA
20	B	805	CLA	C2A-CAA-CBA-CGA
20	B	834	CLA	C2A-CAA-CBA-CGA
20	F	307	CLA	C2A-CAA-CBA-CGA
20	9	603	CLA	C6-C7-C8-C10
20	A	5014	CLA	C16-C17-C18-C19
20	K	4003	CLA	C6-C7-C8-C10
30	A	5003	CL0	C16-C17-C18-C20
20	2	307	CLA	CBD-CGD-O2D-CED
20	A	5005	CLA	C10-C11-C12-C13
26	3	321	PTY	C17-C18-C19-C20
20	A	5022	CLA	C3-C5-C6-C7
20	K	4003	CLA	C3-C5-C6-C7
25	B	850	SQD	O10-C23-O48-C46
27	7	301	LMG	O6-C5-C6-O5
29	A	5053	LMU	O5B-C5B-C6B-O6B
20	A	5044	CLA	CBD-CGD-O2D-CED
20	A	5040	CLA	C5-C6-C7-C8
20	B	808	CLA	C15-C16-C17-C18
26	3	321	PTY	C13-C14-C15-C16
19	3	323	CHL	O1A-CGA-O2A-C1
20	B	822	CLA	C15-C16-C17-C18
20	A	5013	CLA	O1D-CGD-O2D-CED
29	8	322	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
24	B	849	LHG	O7-C5-C6-O8
20	A	5023	CLA	CBA-CGA-O2A-C1
20	B	831	CLA	CBA-CGA-O2A-C1
19	3	301	CHL	C5-C6-C7-C8
20	A	5008	CLA	C5-C6-C7-C8
20	B	828	CLA	O1D-CGD-O2D-CED
20	2	301	CLA	CBA-CGA-O2A-C1
19	8	305	CHL	O1A-CGA-O2A-C1
20	B	831	CLA	C2-C1-O2A-CGA
20	L	202	CLA	C2-C1-O2A-CGA
20	2	304	CLA	C2-C1-O2A-CGA
20	G	201	CLA	C8-C10-C11-C12
26	3	321	PTY	C32-C33-C34-C35
20	G	204	CLA	C4C-C3C-CAC-CBC
20	9	603	CLA	C4-C3-C5-C6
20	7	313	CLA	C2A-CAA-CBA-CGA
20	A	5041	CLA	C2A-CAA-CBA-CGA
20	2	301	CLA	C2A-CAA-CBA-CGA
20	A	5007	CLA	CBD-CGD-O2D-CED
20	A	5021	CLA	CBD-CGD-O2D-CED
20	K	4002	CLA	O1D-CGD-O2D-CED
20	3	309	CLA	CBA-CGA-O2A-C1
19	7	308	CHL	C2C-C3C-CAC-CBC
20	B	825	CLA	O1D-CGD-O2D-CED
20	3	307	CLA	C3-C5-C6-C7
19	1	601	CHL	C1A-C2A-CAA-CBA
19	3	301	CHL	C1A-C2A-CAA-CBA
19	7	308	CHL	C1A-C2A-CAA-CBA
19	9	606	CHL	C1A-C2A-CAA-CBA
19	2	306	CHL	C1A-C2A-CAA-CBA
20	1	604	CLA	C1A-C2A-CAA-CBA
20	1	607	CLA	C1A-C2A-CAA-CBA
20	1	609	CLA	C1A-C2A-CAA-CBA
20	1	610	CLA	C1A-C2A-CAA-CBA
20	3	303	CLA	C1A-C2A-CAA-CBA
20	3	304	CLA	C1A-C2A-CAA-CBA
20	3	307	CLA	C1A-C2A-CAA-CBA
20	3	308	CLA	C1A-C2A-CAA-CBA
20	3	314	CLA	C1A-C2A-CAA-CBA
20	8	301	CLA	C1A-C2A-CAA-CBA
20	8	302	CLA	C1A-C2A-CAA-CBA
20	9	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	5006	CLA	C1A-C2A-CAA-CBA
20	A	5007	CLA	C1A-C2A-CAA-CBA
20	A	5009	CLA	C1A-C2A-CAA-CBA
20	A	5013	CLA	C1A-C2A-CAA-CBA
20	A	5021	CLA	C1A-C2A-CAA-CBA
20	A	5031	CLA	C1A-C2A-CAA-CBA
20	A	5036	CLA	C1A-C2A-CAA-CBA
20	A	5037	CLA	C1A-C2A-CAA-CBA
20	A	5038	CLA	C1A-C2A-CAA-CBA
20	A	5042	CLA	C1A-C2A-CAA-CBA
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	819	CLA	C1A-C2A-CAA-CBA
20	B	822	CLA	C1A-C2A-CAA-CBA
20	B	835	CLA	C1A-C2A-CAA-CBA
20	F	303	CLA	C1A-C2A-CAA-CBA
20	G	203	CLA	C1A-C2A-CAA-CBA
20	G	204	CLA	C1A-C2A-CAA-CBA
20	K	4003	CLA	C1A-C2A-CAA-CBA
20	K	4005	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	C1A-C2A-CAA-CBA
20	2	301	CLA	C1A-C2A-CAA-CBA
20	2	305	CLA	C1A-C2A-CAA-CBA
20	2	307	CLA	C1A-C2A-CAA-CBA
20	2	310	CLA	C1A-C2A-CAA-CBA
30	A	5003	CL0	C1A-C2A-CAA-CBA
20	A	5030	CLA	C15-C16-C17-C18
20	B	840	CLA	O1A-CGA-O2A-C1
20	L	204	CLA	O1A-CGA-O2A-C1
26	F	310	PTY	O14-C5-C6-C1
20	1	607	CLA	CBD-CGD-O2D-CED
19	3	323	CHL	C11-C10-C8-C7
20	7	313	CLA	C6-C7-C8-C10
20	8	302	CLA	C11-C10-C8-C7
20	8	311	CLA	C11-C12-C13-C15
20	8	311	CLA	C12-C13-C15-C16
20	A	5006	CLA	C6-C7-C8-C10
20	A	5006	CLA	C12-C13-C15-C16
20	A	5031	CLA	C11-C12-C13-C15
20	A	5035	CLA	C11-C12-C13-C15
20	A	5041	CLA	C11-C10-C8-C7
20	B	807	CLA	C11-C10-C8-C7
20	B	810	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	B	817	CLA	C11-C10-C8-C7
20	B	818	CLA	C12-C13-C15-C16
20	B	830	CLA	C6-C7-C8-C10
20	H	201	CLA	C6-C7-C8-C10
20	L	201	CLA	C11-C10-C8-C7
30	A	5003	CL0	C11-C10-C8-C7
20	B	833	CLA	C11-C12-C13-C15
20	2	303	CLA	O1A-CGA-O2A-C1
20	3	307	CLA	C4-C3-C5-C6
20	B	804	CLA	C2-C3-C5-C6
20	F	303	CLA	C2-C3-C5-C6
20	7	310	CLA	C10-C11-C12-C13
19	3	301	CHL	C6-C7-C8-C9
19	2	302	CHL	C11-C10-C8-C9
20	8	302	CLA	C11-C10-C8-C9
20	8	303	CLA	C6-C7-C8-C9
20	8	311	CLA	C11-C12-C13-C14
20	A	5004	CLA	C6-C7-C8-C9
20	A	5006	CLA	C14-C13-C15-C16
20	A	5016	CLA	C11-C12-C13-C14
20	A	5016	CLA	C14-C13-C15-C16
20	A	5020	CLA	C11-C12-C13-C14
20	A	5030	CLA	C14-C13-C15-C16
20	A	5041	CLA	C11-C10-C8-C9
20	B	804	CLA	C6-C7-C8-C9
20	B	817	CLA	C11-C10-C8-C9
20	B	818	CLA	C11-C12-C13-C14
20	B	827	CLA	C11-C10-C8-C9
20	1	603	CLA	CBA-CGA-O2A-C1
24	1	618	LHG	C4-C5-C6-O8
24	8	319	LHG	C4-C5-C6-O8
24	9	617	LHG	C4-C5-C6-O8
24	A	5055	LHG	C4-C5-C6-O8
24	B	849	LHG	C4-C5-C6-O8
24	I	4002	LHG	C4-C5-C6-O8
24	2	316	LHG	C4-C5-C6-O8
25	B	850	SQD	C44-C45-C46-O48
27	7	301	LMG	O1-C7-C8-C9
27	G	206	LMG	C7-C8-C9-O8
20	7	314	CLA	CBA-CGA-O2A-C1
20	B	838	CLA	C6-C7-C8-C9
20	L	205	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	5008	CLA	O1D-CGD-O2D-CED
20	7	309	CLA	O1A-CGA-O2A-C1
19	9	606	CHL	C2C-C3C-CAC-CBC
19	3	323	CHL	C10-C11-C12-C13
20	B	804	CLA	C4-C3-C5-C6
20	F	303	CLA	C4-C3-C5-C6
20	9	603	CLA	C2-C3-C5-C6
20	A	5019	CLA	C2-C3-C5-C6
20	A	5012	CLA	C10-C11-C12-C13
20	A	5035	CLA	C5-C6-C7-C8
20	A	5023	CLA	O1A-CGA-O2A-C1
20	B	831	CLA	O1A-CGA-O2A-C1
26	3	321	PTY	C22-C23-C24-C25
20	1	602	CLA	C2A-CAA-CBA-CGA
20	8	311	CLA	C2A-CAA-CBA-CGA
24	A	5052	LHG	C30-C31-C32-C33
20	B	806	CLA	O2A-C1-C2-C3
26	3	321	PTY	C5-C6-O7-C8
26	F	310	PTY	C5-C6-O7-C8
19	3	301	CHL	C3C-C2C-CMC-OMC
19	8	306	CHL	C3C-C2C-CMC-OMC
19	2	302	CHL	C3C-C2C-CMC-OMC
19	1	606	CHL	C4C-C3C-CAC-CBC
20	B	833	CLA	C11-C12-C13-C14
20	B	838	CLA	C6-C7-C8-C10
20	A	5027	CLA	CBA-CGA-O2A-C1
20	A	5029	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	CBA-CGA-O2A-C1
19	9	606	CHL	CBD-CGD-O2D-CED
20	A	5040	CLA	C4-C3-C5-C6
20	3	307	CLA	C2-C3-C5-C6
24	I	4002	LHG	O7-C5-C6-O8
27	J	103	LMG	O1-C7-C8-O7
24	B	801	LHG	O2-C2-C3-O3
20	A	5024	CLA	O1D-CGD-O2D-CED
19	3	301	CHL	C3-C5-C6-C7
20	1	612	CLA	C3-C5-C6-C7
20	B	811	CLA	C2-C1-O2A-CGA
26	F	302	PTY	C14-C15-C16-C17
20	1	603	CLA	O1A-CGA-O2A-C1
20	3	307	CLA	C8-C10-C11-C12
20	L	201	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	2	305	CLA	O1D-CGD-O2D-CED
19	3	301	CHL	C14-C13-C15-C16
20	B	819	CLA	C16-C17-C18-C20
20	B	810	CLA	C4-C3-C5-C6
20	B	815	CLA	C4-C3-C5-C6
20	B	832	CLA	C4-C3-C5-C6
30	A	5003	CL0	C4-C3-C5-C6
20	3	312	CLA	CAA-CBA-CGA-O2A
20	8	309	CLA	C2-C3-C5-C6
20	A	5008	CLA	CBA-CGA-O2A-C1
20	B	839	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	C8-C10-C11-C12
20	F	306	CLA	C5-C6-C7-C8
29	7	325	LMU	C2-C1-O1'-C1'
20	3	302	CLA	C14-C13-C15-C16
20	7	313	CLA	C6-C7-C8-C9
20	8	308	CLA	C6-C7-C8-C9
20	8	309	CLA	C11-C10-C8-C9
20	9	607	CLA	C11-C10-C8-C9
20	A	5009	CLA	C11-C12-C13-C14
20	A	5028	CLA	C6-C7-C8-C9
20	A	5031	CLA	C11-C12-C13-C14
20	A	5035	CLA	C11-C12-C13-C14
20	B	807	CLA	C11-C10-C8-C9
20	B	809	CLA	C11-C10-C8-C9
20	B	810	CLA	C11-C12-C13-C14
20	B	818	CLA	C11-C10-C8-C9
20	B	818	CLA	C14-C13-C15-C16
20	B	830	CLA	C6-C7-C8-C9
20	B	830	CLA	C11-C10-C8-C9
20	H	201	CLA	C6-C7-C8-C9
20	L	201	CLA	C6-C7-C8-C9
20	L	201	CLA	C11-C10-C8-C9
20	L	202	CLA	C6-C7-C8-C9
30	A	5003	CL0	C11-C10-C8-C9
20	B	820	CLA	O1D-CGD-O2D-CED
24	8	317	LHG	C5-C4-O6-P
20	A	5028	CLA	CBA-CGA-O2A-C1
20	B	817	CLA	CBA-CGA-O2A-C1
20	A	5014	CLA	C2A-CAA-CBA-CGA
27	7	301	LMG	C2-C1-O1-C7
20	A	5004	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	1	620	LHG	O6-C4-C5-C6
26	B	802	PTY	O14-C5-C6-C1
19	3	301	CHL	C6-C7-C8-C10
20	7	313	CLA	C12-C13-C15-C16
20	8	303	CLA	C6-C7-C8-C10
20	8	308	CLA	C6-C7-C8-C10
20	8	309	CLA	C11-C10-C8-C7
20	9	602	CLA	C11-C10-C8-C7
20	A	5004	CLA	C6-C7-C8-C10
20	A	5009	CLA	C11-C12-C13-C15
20	A	5009	CLA	C12-C13-C15-C16
20	A	5016	CLA	C11-C12-C13-C15
20	A	5020	CLA	C11-C12-C13-C15
20	A	5022	CLA	C12-C13-C15-C16
20	A	5028	CLA	C6-C7-C8-C10
20	A	5029	CLA	C11-C12-C13-C15
20	A	5030	CLA	C12-C13-C15-C16
20	B	804	CLA	C6-C7-C8-C10
20	B	808	CLA	C12-C13-C15-C16
20	B	818	CLA	C11-C10-C8-C7
20	B	818	CLA	C11-C12-C13-C15
20	B	827	CLA	C11-C10-C8-C7
20	B	828	CLA	C6-C7-C8-C10
20	B	830	CLA	C11-C10-C8-C7
20	L	201	CLA	C11-C12-C13-C15
20	L	202	CLA	C6-C7-C8-C10
31	A	5045	PQN	C22-C23-C25-C26
20	2	310	CLA	CBA-CGA-O2A-C1
20	7	314	CLA	O1A-CGA-O2A-C1
19	7	308	CHL	C3A-C2A-CAA-CBA
20	1	607	CLA	C3A-C2A-CAA-CBA
20	8	309	CLA	C4-C3-C5-C6
20	A	5043	CLA	C3A-C2A-CAA-CBA
20	B	807	CLA	C4-C3-C5-C6
20	B	818	CLA	C3A-C2A-CAA-CBA
20	F	307	CLA	C3A-C2A-CAA-CBA
20	2	307	CLA	C3A-C2A-CAA-CBA
20	3	302	CLA	C15-C16-C17-C18
20	8	308	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	C2-C3-C5-C6
19	2	302	CHL	CBA-CGA-O2A-C1
23	3	319	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	803	BCR	C15-C16-C17-C18
23	B	844	BCR	C9-C10-C11-C12
20	A	5044	CLA	C3-C5-C6-C7
20	8	307	CLA	O1D-CGD-O2D-CED
23	3	319	BCR	C21-C22-C23-C24
19	7	307	CHL	C2C-C3C-CAC-CBC
20	J	104	CLA	O2A-C1-C2-C3
24	A	5052	LHG	C4-C5-C6-O8
25	3	322	SQD	O6-C44-C45-C46
27	G	206	LMG	O1-C7-C8-C9
28	B	848	DGD	O1G-C1G-C2G-C3G
26	3	321	PTY	C31-C32-C33-C34
19	3	323	CHL	C11-C12-C13-C14
20	A	5028	CLA	C5-C6-C7-C8
20	B	818	CLA	O1D-CGD-O2D-CED
19	3	323	CHL	C1-C2-C3-C4
20	1	610	CLA	CAA-CBA-CGA-O2A
20	B	807	CLA	C2-C3-C5-C6
20	B	815	CLA	C2-C3-C5-C6
20	8	302	CLA	C16-C17-C18-C20
20	B	819	CLA	C16-C17-C18-C19
26	B	802	PTY	O14-C5-C6-O7
29	9	616	LMU	C5'-C4'-O1B-C1B
21	8	314	LUT	C1-C6-C7-C8
21	2	315	LUT	C1-C6-C7-C8
23	3	318	BCR	C1-C6-C7-C8
23	3	319	BCR	C23-C24-C25-C30
23	A	5050	BCR	C1-C6-C7-C8
23	B	845	BCR	C23-C24-C25-C26
23	J	105	BCR	C5-C6-C7-C8
23	J	106	BCR	C23-C24-C25-C30
23	K	4006	BCR	C1-C6-C7-C8
20	8	303	CLA	C13-C15-C16-C17
20	B	832	CLA	C8-C10-C11-C12
24	7	319	LHG	C2-C3-O3-P
24	A	5002	LHG	C2-C3-O3-P
20	A	5027	CLA	C11-C10-C8-C9
20	A	5022	CLA	C13-C15-C16-C17
20	B	840	CLA	C13-C15-C16-C17
20	A	5024	CLA	CAA-CBA-CGA-O2A
20	A	5016	CLA	C5-C6-C7-C8
25	3	322	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
25	B	850	SQD	O47-C45-C46-O48
27	7	301	LMG	O7-C8-C9-O8
28	B	848	DGD	O2G-C2G-C3G-O3G
20	2	313	CLA	O1D-CGD-O2D-CED
20	A	5027	CLA	O1A-CGA-O2A-C1
20	A	5028	CLA	C4-C3-C5-C6
20	A	5028	CLA	C2-C3-C5-C6
30	A	5003	CL0	C2-C3-C5-C6
19	3	323	CHL	C1-C2-C3-C5
20	A	5026	CLA	C10-C11-C12-C13
20	A	5021	CLA	CBA-CGA-O2A-C1
20	7	311	CLA	C3-C5-C6-C7
20	7	313	CLA	C14-C13-C15-C16
20	8	311	CLA	C14-C13-C15-C16
20	A	5006	CLA	C6-C7-C8-C9
20	A	5012	CLA	C11-C12-C13-C14
20	A	5022	CLA	C14-C13-C15-C16
31	A	5045	PQN	C24-C23-C25-C26
24	A	5052	LHG	C26-C27-C28-C29
29	A	5053	LMU	O5'-C1'-O1'-C1
20	A	5029	CLA	O1A-CGA-O2A-C1
19	3	323	CHL	C11-C12-C13-C15
19	2	302	CHL	C11-C12-C13-C14
20	K	4003	CLA	C2A-CAA-CBA-CGA
29	9	616	LMU	C3'-C4'-O1B-C1B
33	J	101	LMK	C2-C3-N4-C5
20	B	818	CLA	C10-C11-C12-C13
20	B	829	CLA	C3-C5-C6-C7
20	7	311	CLA	C5-C6-C7-C8
19	3	301	CHL	C11-C10-C8-C7
20	7	310	CLA	C12-C13-C15-C16
20	A	5006	CLA	C11-C10-C8-C7
20	A	5012	CLA	C11-C12-C13-C15
20	A	5014	CLA	C11-C10-C8-C7
20	A	5036	CLA	C12-C13-C15-C16
20	A	5044	CLA	C12-C13-C15-C16
20	B	804	CLA	C12-C13-C15-C16
20	B	805	CLA	C6-C7-C8-C10
20	B	808	CLA	C6-C7-C8-C10
20	B	809	CLA	C11-C10-C8-C7
20	B	820	CLA	C6-C7-C8-C10
20	B	824	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	829	CLA	C6-C7-C8-C10
20	L	201	CLA	C6-C7-C8-C10
20	L	202	CLA	C11-C10-C8-C7
30	A	5003	CL0	C6-C7-C8-C10
30	A	5003	CL0	C12-C13-C15-C16
31	B	841	PQN	C21-C22-C23-C25
20	B	805	CLA	C13-C15-C16-C17
20	B	817	CLA	O1A-CGA-O2A-C1
25	3	322	SQD	C45-C44-O6-C1
28	7	321	DGD	C2G-C3G-O3G-C1D
28	7	321	DGD	C5D-C6D-O5D-C1E
24	2	316	LHG	C7-C8-C9-C10
20	2	307	CLA	O1D-CGD-O2D-CED
20	2	308	CLA	C2A-CAA-CBA-CGA
19	2	302	CHL	O1A-CGA-O2A-C1
20	A	5008	CLA	O1A-CGA-O2A-C1
20	A	5021	CLA	O1A-CGA-O2A-C1
20	B	820	CLA	O1A-CGA-O2A-C1
20	9	602	CLA	C3-C5-C6-C7
20	B	839	CLA	O1A-CGA-O2A-C1
20	3	312	CLA	CBA-CGA-O2A-C1
20	8	302	CLA	C16-C17-C18-C19
20	A	5028	CLA	O1A-CGA-O2A-C1
24	I	4002	LHG	O6-C4-C5-O7
26	3	321	PTY	O14-C5-C6-O7
26	F	310	PTY	O14-C5-C6-O7
24	B	801	LHG	C4-C5-C6-O8
25	1	619	SQD	O6-C44-C45-C46
25	3	322	SQD	C44-C45-C46-O48
26	7	302	PTY	O4-C1-C6-C5
26	F	301	PTY	O4-C1-C6-C5
26	F	310	PTY	O4-C1-C6-C5
27	7	301	LMG	C7-C8-C9-O8
20	A	5007	CLA	O1D-CGD-O2D-CED
20	7	313	CLA	C3-C5-C6-C7
30	A	5003	CL0	C3-C5-C6-C7
20	A	5030	CLA	C4-C3-C5-C6
20	1	609	CLA	C2A-CAA-CBA-CGA
20	9	602	CLA	C2A-CAA-CBA-CGA
26	3	321	PTY	C2-C3-O11-P1
20	B	808	CLA	C8-C10-C11-C12
20	A	5021	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	2	316	LHG	O7-C5-C6-O8
25	F	311	SQD	O47-C45-C46-O48
26	F	302	PTY	O4-C1-C6-O7
26	F	310	PTY	O4-C1-C6-O7
27	7	324	LMG	O1-C7-C8-O7
27	G	206	LMG	O1-C7-C8-O7
19	3	301	CHL	C11-C10-C8-C9
20	A	5008	CLA	C11-C12-C13-C14
20	A	5014	CLA	C11-C10-C8-C9
20	B	820	CLA	C6-C7-C8-C9
20	B	829	CLA	C6-C7-C8-C9
30	A	5003	CL0	C6-C7-C8-C9
31	B	841	PQN	C21-C22-C23-C24
20	B	836	CLA	C5-C6-C7-C8
21	2	314	LUT	C26-C27-C28-C29
20	3	302	CLA	C5-C6-C7-C8
20	B	818	CLA	C2-C1-O2A-CGA
20	K	4005	CLA	O2A-C1-C2-C3
28	7	321	DGD	C2E-C1E-O5D-C6D
20	B	821	CLA	C5-C6-C7-C8
20	1	602	CLA	C4-C3-C5-C6
20	A	5025	CLA	C4-C3-C5-C6
20	H	201	CLA	C3-C5-C6-C7
20	G	201	CLA	C10-C11-C12-C13
20	1	612	CLA	C11-C12-C13-C15
20	1	603	CLA	C5-C6-C7-C8
20	A	5009	CLA	C13-C15-C16-C17
26	B	802	PTY	C11-C12-C13-C14
20	B	809	CLA	C8-C10-C11-C12
20	A	5029	CLA	CAA-CBA-CGA-O2A
20	1	607	CLA	O1D-CGD-O2D-CED
20	3	311	CLA	C3-C5-C6-C7
19	8	304	CHL	C1A-C2A-CAA-CBA
20	7	314	CLA	C1A-C2A-CAA-CBA
20	9	609	CLA	C1A-C2A-CAA-CBA
20	A	5024	CLA	C1A-C2A-CAA-CBA
20	A	5025	CLA	C1A-C2A-CAA-CBA
20	A	5035	CLA	C1A-C2A-CAA-CBA
20	B	806	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	F	307	CLA	C1A-C2A-CAA-CBA
20	H	201	CLA	C1A-C2A-CAA-CBA
20	L	202	CLA	C1A-C2A-CAA-CBA
20	L	205	CLA	C1A-C2A-CAA-CBA
20	A	5044	CLA	O1D-CGD-O2D-CED
20	3	324	CLA	C4-C3-C5-C6
28	7	321	DGD	O6E-C1E-O5D-C6D
22	7	317	XAT	C27-C28-C29-C30
20	A	5016	CLA	C2A-CAA-CBA-CGA
19	9	606	CHL	O1D-CGD-O2D-CED
24	I	4002	LHG	O6-C4-C5-C6
20	A	5014	CLA	C10-C11-C12-C13
20	8	311	CLA	C11-C10-C8-C7
20	A	5008	CLA	C11-C12-C13-C15
20	A	5026	CLA	C11-C12-C13-C15
20	B	811	CLA	C11-C12-C13-C15
20	F	303	CLA	C11-C10-C8-C7
20	9	603	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	C8-C10-C11-C12
19	8	304	CHL	C3A-C2A-CAA-CBA
20	B	819	CLA	C4-C3-C5-C6
20	7	310	CLA	C16-C17-C18-C20
20	A	5018	CLA	C2A-CAA-CBA-CGA
20	7	310	CLA	C14-C13-C15-C16
20	A	5006	CLA	C11-C10-C8-C9
20	A	5009	CLA	C14-C13-C15-C16
20	A	5028	CLA	C11-C12-C13-C14
20	A	5044	CLA	C14-C13-C15-C16
20	B	808	CLA	C6-C7-C8-C9
20	B	824	CLA	C14-C13-C15-C16
20	B	828	CLA	C6-C7-C8-C9
20	L	202	CLA	C11-C10-C8-C9
20	2	301	CLA	O1A-CGA-O2A-C1
23	3	319	BCR	C15-C16-C17-C18
20	B	809	CLA	C16-C17-C18-C20
20	7	310	CLA	C8-C10-C11-C12
19	3	323	CHL	C1C-C2C-CMC-OMC
19	2	302	CHL	C1C-C2C-CMC-OMC
25	1	619	SQD	O5-C5-C6-S
20	2	303	CLA	O1D-CGD-O2D-CED
24	B	801	LHG	O7-C5-C6-O8
25	1	619	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
25	3	322	SQD	O6-C44-C45-O47
26	7	302	PTY	O4-C1-C6-O7
26	F	301	PTY	O4-C1-C6-O7
28	B	848	DGD	O1G-C1G-C2G-O2G
20	A	5007	CLA	C8-C10-C11-C12
24	A	5002	LHG	C4-C5-C6-O8
25	F	311	SQD	C44-C45-C46-O48
27	7	324	LMG	O1-C7-C8-C9
20	A	5012	CLA	C5-C6-C7-C8
20	3	309	CLA	O1A-CGA-O2A-C1
20	7	323	CLA	CAD-CBD-CGD-O2D
20	9	609	CLA	CAD-CBD-CGD-O2D
20	B	807	CLA	CAD-CBD-CGD-O2D
20	G	201	CLA	CAD-CBD-CGD-O2D
20	K	4002	CLA	CAD-CBD-CGD-O2D
20	K	4004	CLA	CAD-CBD-CGD-O2D
24	A	5052	LHG	C10-C11-C12-C13
20	9	603	CLA	O1A-CGA-O2A-C1
20	B	827	CLA	C8-C10-C11-C12
20	A	5015	CLA	C3-C5-C6-C7
19	8	304	CHL	CAD-CBD-CGD-O1D
20	1	603	CLA	CAD-CBD-CGD-O1D
20	7	323	CLA	CAD-CBD-CGD-O1D
20	9	602	CLA	CAD-CBD-CGD-O1D
20	9	608	CLA	CHA-CBD-CGD-O2D
20	9	609	CLA	CAD-CBD-CGD-O1D
20	A	5017	CLA	CHA-CBD-CGD-O1D
20	A	5017	CLA	CHA-CBD-CGD-O2D
20	A	5018	CLA	CHA-CBD-CGD-O1D
20	A	5018	CLA	CHA-CBD-CGD-O2D
20	A	5026	CLA	CHA-CBD-CGD-O1D
20	A	5026	CLA	CHA-CBD-CGD-O2D
20	A	5035	CLA	CHA-CBD-CGD-O2D
20	B	807	CLA	CAD-CBD-CGD-O1D
20	B	809	CLA	CHA-CBD-CGD-O2D
20	B	816	CLA	CHA-CBD-CGD-O1D
20	B	816	CLA	CHA-CBD-CGD-O2D
20	B	826	CLA	CHA-CBD-CGD-O1D
20	B	826	CLA	CHA-CBD-CGD-O2D
20	G	201	CLA	CAD-CBD-CGD-O1D
20	K	4002	CLA	CAD-CBD-CGD-O1D
20	K	4004	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	L	204	CLA	CAD-CBD-CGD-O1D
21	2	315	LUT	C29-C30-C31-C32
24	1	618	LHG	C4-O6-P-O5
24	7	320	LHG	C3-O3-P-O5
24	7	320	LHG	C4-O6-P-O5
24	8	317	LHG	C4-O6-P-O5
24	8	319	LHG	C4-O6-P-O3
24	8	319	LHG	C4-O6-P-O4
24	8	319	LHG	C4-O6-P-O5
24	8	320	LHG	C3-O3-P-O5
24	8	320	LHG	C4-O6-P-O5
24	9	617	LHG	C3-O3-P-O4
24	9	617	LHG	C4-O6-P-O3
24	9	617	LHG	C4-O6-P-O5
24	A	5054	LHG	C3-O3-P-O5
24	B	801	LHG	C4-O6-P-O4
24	B	849	LHG	C3-O3-P-O5
26	B	802	PTY	C3-O11-P1-O13
26	B	802	PTY	C5-O14-P1-O13
26	F	301	PTY	C3-O11-P1-O12
26	F	302	PTY	C3-O11-P1-O13
26	F	302	PTY	C5-O14-P1-O12
20	8	309	CLA	C3-C5-C6-C7
33	J	101	LMK	C8-C7-O1-C1
20	A	5013	CLA	C10-C11-C12-C13
21	3	315	LUT	C1-C6-C7-C8
20	A	5041	CLA	CAA-CBA-CGA-O2A
20	A	5030	CLA	C2-C3-C5-C6
20	A	5040	CLA	C2-C3-C5-C6
23	K	4001	BCR	C37-C22-C23-C24
24	1	620	LHG	C5-C4-O6-P
24	9	617	LHG	C2-C3-O3-P
24	I	4002	LHG	C5-C4-O6-P
24	9	617	LHG	C25-C26-C27-C28
26	F	302	PTY	C30-C31-C32-C33
20	A	5019	CLA	CAA-CBA-CGA-O2A
19	3	301	CHL	C12-C13-C15-C16
23	A	5049	BCR	C18-C19-C20-C21
23	B	844	BCR	C18-C19-C20-C21
23	J	102	BCR	C10-C11-C12-C13
26	3	321	PTY	O14-C5-C6-C1
19	2	302	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	9	602	CLA	C11-C10-C8-C9
20	A	5016	CLA	C6-C7-C8-C9
20	A	5029	CLA	C11-C12-C13-C14
20	A	5036	CLA	C14-C13-C15-C16
20	B	805	CLA	C6-C7-C8-C9
20	B	808	CLA	C14-C13-C15-C16
20	F	303	CLA	C11-C10-C8-C9
20	B	807	CLA	C6-C7-C8-C10
20	B	832	CLA	CBD-CGD-O2D-CED
20	1	612	CLA	C11-C12-C13-C14
20	7	310	CLA	C16-C17-C18-C19
19	9	606	CHL	C4C-C3C-CAC-CBC
20	2	307	CLA	CAA-CBA-CGA-O2A
19	3	323	CHL	C4-C3-C5-C6
24	7	320	LHG	O8-C23-C24-C25
20	9	602	CLA	CAA-CBA-CGA-O2A
20	A	5042	CLA	C5-C6-C7-C8
20	B	809	CLA	C16-C17-C18-C19
31	B	841	PQN	C23-C25-C26-C27
20	8	303	CLA	CAA-CBA-CGA-O2A
20	B	827	CLA	CAA-CBA-CGA-O2A
20	B	839	CLA	CAA-CBA-CGA-O2A
24	8	319	LHG	C23-C24-C25-C26
20	B	805	CLA	C16-C17-C18-C20
24	9	617	LHG	O8-C23-C24-C25
20	8	301	CLA	C2A-CAA-CBA-CGA
20	B	809	CLA	C2A-CAA-CBA-CGA
20	B	829	CLA	C2A-CAA-CBA-CGA
20	B	836	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C16-C17-C18-C20
20	B	830	CLA	C5-C6-C7-C8
20	8	301	CLA	C11-C12-C13-C15
20	A	5026	CLA	C11-C12-C13-C14
20	B	811	CLA	C11-C12-C13-C14
31	B	841	PQN	C24-C23-C25-C26
26	F	301	PTY	C8-C11-C12-C13
20	2	309	CLA	CAA-CBA-CGA-O2A
20	B	820	CLA	C16-C17-C18-C20
20	G	201	CLA	C16-C17-C18-C20
20	1	607	CLA	CBA-CGA-O2A-C1
20	G	204	CLA	CAA-CBA-CGA-O2A
20	A	5011	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	3	323	CHL	C2-C3-C5-C6
20	B	832	CLA	C2-C3-C5-C6
20	K	4003	CLA	C5-C6-C7-C8
19	3	301	CHL	C11-C12-C13-C15
20	3	302	CLA	C11-C12-C13-C15
20	A	5005	CLA	C11-C10-C8-C7
20	B	814	CLA	C6-C7-C8-C10
20	F	303	CLA	C6-C7-C8-C10
20	G	201	CLA	C11-C10-C8-C7
20	1	607	CLA	O1A-CGA-O2A-C1
20	A	5030	CLA	O1D-CGD-O2D-CED
20	B	832	CLA	O1D-CGD-O2D-CED
20	2	310	CLA	O1A-CGA-O2A-C1
20	B	804	CLA	C8-C10-C11-C12
25	B	850	SQD	O6-C44-C45-O47
19	8	306	CHL	C3A-C2A-CAA-CBA
20	1	612	CLA	C3A-C2A-CAA-CBA
20	A	5005	CLA	C3A-C2A-CAA-CBA
20	B	807	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C2-C3-C5-C6
21	1	615	LUT	C40-C33-C34-C35
21	2	315	LUT	C40-C33-C34-C35
23	A	5051	BCR	C11-C10-C9-C34
23	A	5051	BCR	C16-C17-C18-C36
23	F	309	BCR	C16-C17-C18-C36
23	G	205	BCR	C35-C13-C14-C15
23	G	205	BCR	C16-C17-C18-C36
23	I	4001	BCR	C35-C13-C14-C15
23	J	102	BCR	C11-C10-C9-C34
23	L	203	BCR	C11-C10-C9-C34
20	2	312	CLA	CAA-CBA-CGA-O1A
20	A	5030	CLA	CBD-CGD-O2D-CED
20	B	822	CLA	C2-C1-O2A-CGA
30	A	5003	CL0	C5-C6-C7-C8
24	8	317	LHG	C2-C3-O3-P
20	2	309	CLA	CAA-CBA-CGA-O1A
29	F	305	LMU	C2B-C1B-O1B-C4'
26	3	321	PTY	C8-C11-C12-C13
20	G	204	CLA	CAA-CBA-CGA-O1A
20	7	311	CLA	C4-C3-C5-C6
20	A	5039	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	5024	CLA	C5-C6-C7-C8
20	B	833	CLA	C8-C10-C11-C12
24	1	620	LHG	C4-C5-C6-O8
20	3	312	CLA	CAA-CBA-CGA-O1A
20	3	302	CLA	C6-C7-C8-C9
20	8	311	CLA	C6-C7-C8-C9
20	8	311	CLA	C11-C10-C8-C9
20	A	5005	CLA	C11-C10-C8-C9
20	B	814	CLA	C6-C7-C8-C9
20	B	833	CLA	C11-C10-C8-C9
20	F	303	CLA	C6-C7-C8-C9
20	G	201	CLA	C11-C10-C8-C9
30	A	5003	CL0	C11-C12-C13-C14
20	F	306	CLA	C11-C12-C13-C14
26	F	301	PTY	C1-C6-O7-C8
20	B	827	CLA	C13-C15-C16-C17
26	F	302	PTY	C11-C8-O7-C6
20	L	204	CLA	CBD-CGD-O2D-CED
20	B	807	CLA	C8-C10-C11-C12
20	1	605	CLA	CAA-CBA-CGA-O1A
20	A	5020	CLA	C2A-CAA-CBA-CGA
19	8	306	CHL	C1A-C2A-CAA-CBA
20	7	311	CLA	C1A-C2A-CAA-CBA
20	A	5005	CLA	C1A-C2A-CAA-CBA
20	A	5028	CLA	C1A-C2A-CAA-CBA
20	A	5033	CLA	C1A-C2A-CAA-CBA
20	A	5043	CLA	C1A-C2A-CAA-CBA
20	B	807	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C1A-C2A-CAA-CBA
20	F	308	CLA	C1A-C2A-CAA-CBA
21	1	615	LUT	C32-C33-C34-C35
23	A	5051	BCR	C11-C10-C9-C8
23	A	5051	BCR	C16-C17-C18-C19
23	F	309	BCR	C16-C17-C18-C19
23	G	205	BCR	C12-C13-C14-C15
23	G	205	BCR	C16-C17-C18-C19
23	I	4001	BCR	C12-C13-C14-C15
23	J	102	BCR	C11-C10-C9-C8
23	L	203	BCR	C11-C10-C9-C8
26	F	302	PTY	O10-C8-O7-C6
20	2	305	CLA	CAA-CBA-CGA-O2A
26	F	301	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
29	F	305	LMU	C5'-C4'-O1B-C1B
28	B	848	DGD	O6D-C5D-C6D-O5D
21	3	315	LUT	C5-C6-C7-C8
21	8	314	LUT	C5-C6-C7-C8
21	2	315	LUT	C5-C6-C7-C8
23	3	317	BCR	C23-C24-C25-C26
23	3	318	BCR	C5-C6-C7-C8
23	3	319	BCR	C23-C24-C25-C26
23	A	5050	BCR	C5-C6-C7-C8
23	B	844	BCR	C1-C6-C7-C8
23	F	309	BCR	C23-C24-C25-C26
23	F	309	BCR	C23-C24-C25-C30
23	J	106	BCR	C23-C24-C25-C26
23	K	4006	BCR	C5-C6-C7-C8
20	F	303	CLA	C5-C6-C7-C8
24	8	320	LHG	C2-C3-O3-P
24	2	316	LHG	C5-C4-O6-P
26	B	802	PTY	C6-C5-O14-P1
26	3	321	PTY	C39-C40-C41-C42
20	7	313	CLA	C5-C6-C7-C8
20	2	305	CLA	CAA-CBA-CGA-O1A
20	2	312	CLA	CAA-CBA-CGA-O2A
20	8	311	CLA	C6-C7-C8-C10
20	A	5004	CLA	C11-C12-C13-C15
20	A	5014	CLA	C6-C7-C8-C10
20	A	5024	CLA	C11-C10-C8-C7
20	B	805	CLA	C12-C13-C15-C16
20	B	808	CLA	C11-C12-C13-C15
20	B	829	CLA	C11-C12-C13-C15
20	B	833	CLA	C11-C10-C8-C7
20	B	805	CLA	C16-C17-C18-C19
20	3	305	CLA	C2A-CAA-CBA-CGA
20	A	5005	CLA	C2A-CAA-CBA-CGA
24	1	620	LHG	O7-C5-C6-O8
25	3	320	SQD	O6-C44-C45-O47
27	7	324	LMG	O7-C8-C9-O8
20	1	605	CLA	CAA-CBA-CGA-O2A
27	7	301	LMG	C33-C34-C35-C36
23	L	206	BCR	C37-C22-C23-C24
20	3	312	CLA	O1A-CGA-O2A-C1
19	3	301	CHL	C1-C2-C3-C5
20	B	829	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	8	311	CLA	O1D-CGD-O2D-CED
20	A	5028	CLA	C11-C10-C8-C9
20	A	5030	CLA	C11-C12-C13-C14
20	B	828	CLA	C15-C16-C17-C18
20	L	202	CLA	C5-C6-C7-C8
20	8	303	CLA	C8-C10-C11-C12
28	B	848	DGD	C4D-C5D-C6D-O5D
24	B	801	LHG	C2-C3-O3-P
20	1	602	CLA	C2-C3-C5-C6
20	3	324	CLA	C2-C3-C5-C6
20	A	5025	CLA	C2-C3-C5-C6
20	K	4002	CLA	CAA-CBA-CGA-O2A
20	K	4004	CLA	CAA-CBA-CGA-O2A
27	J	103	LMG	O1-C7-C8-C9
20	7	315	CLA	CAA-CBA-CGA-O2A
20	A	5035	CLA	C10-C11-C12-C13
33	J	101	LMK	O9-C10-C11-C12
20	A	5022	CLA	C5-C6-C7-C8
26	F	310	PTY	C31-C32-C33-C34
20	9	602	CLA	C4-C3-C5-C6
20	A	5022	CLA	C4-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
20	9	605	CLA	CAA-CBA-CGA-O2A
20	8	313	CLA	CAA-CBA-CGA-O2A
20	A	5039	CLA	C2-C3-C5-C6
20	B	810	CLA	C16-C17-C18-C19
20	A	5006	CLA	C15-C16-C17-C18
20	2	308	CLA	CAA-CBA-CGA-O2A
29	F	305	LMU	C3'-C4'-O1B-C1B
20	1	602	CLA	C6-C7-C8-C10
20	B	820	CLA	C16-C17-C18-C19
20	G	201	CLA	C16-C17-C18-C19
20	L	204	CLA	O1D-CGD-O2D-CED
20	1	607	CLA	CAA-CBA-CGA-O2A
20	8	311	CLA	CBD-CGD-O2D-CED
20	1	610	CLA	CAA-CBA-CGA-O1A
20	7	311	CLA	C2-C3-C5-C6
27	7	301	LMG	C13-C14-C15-C16
20	B	804	CLA	C15-C16-C17-C18
20	3	302	CLA	C6-C7-C8-C10
20	8	301	CLA	C11-C12-C13-C14
20	8	303	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	9	607	CLA	C6-C7-C8-C9
20	B	804	CLA	C11-C12-C13-C14
20	B	814	CLA	C14-C13-C15-C16
20	B	830	CLA	C14-C13-C15-C16
20	H	201	CLA	C11-C10-C8-C9
27	7	324	LMG	C8-C7-O1-C1
20	9	608	CLA	C2A-CAA-CBA-CGA
19	3	323	CHL	C2-C1-O2A-CGA
20	3	306	CLA	C2-C1-O2A-CGA
20	A	5007	CLA	C2-C1-O2A-CGA
20	B	825	CLA	C2-C1-O2A-CGA
20	H	201	CLA	C2-C1-O2A-CGA
20	A	5016	CLA	C15-C16-C17-C18
19	2	302	CHL	C3A-C2A-CAA-CBA
20	8	312	CLA	C3A-C2A-CAA-CBA
20	9	604	CLA	C3A-C2A-CAA-CBA
20	A	5015	CLA	C3A-C2A-CAA-CBA
20	A	5017	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA
20	7	315	CLA	CAA-CBA-CGA-O1A
20	2	308	CLA	CAA-CBA-CGA-O1A
19	9	606	CHL	CAA-CBA-CGA-O2A
27	G	206	LMG	O7-C10-C11-C12
20	8	311	CLA	C16-C17-C18-C20
26	F	301	PTY	C5-C6-O7-C8
20	A	5024	CLA	CAA-CBA-CGA-O1A
20	K	4002	CLA	CAA-CBA-CGA-O1A
20	K	4004	CLA	CAA-CBA-CGA-O1A
20	7	310	CLA	C2A-CAA-CBA-CGA
21	2	315	LUT	C32-C33-C34-C35
22	7	317	XAT	O24-C26-C27-C28
20	9	605	CLA	CAA-CBA-CGA-O1A
25	B	850	SQD	O6-C44-C45-C46
26	F	302	PTY	O4-C1-C6-C5
20	3	302	CLA	C3-C5-C6-C7
20	A	5018	CLA	O1D-CGD-O2D-CED
19	7	308	CHL	C4C-C3C-CAC-CBC
20	1	603	CLA	CAA-CBA-CGA-O2A
20	1	614	CLA	CAA-CBA-CGA-O2A
24	7	320	LHG	C26-C27-C28-C29
20	A	5031	CLA	C14-C13-C15-C16
20	B	832	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	A	5020	CLA	C16-C17-C18-C20
20	9	604	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	CAA-CBA-CGA-O2A
27	7	324	LMG	O7-C10-C11-C12
20	B	832	CLA	C5-C6-C7-C8
20	A	5020	CLA	C4-C3-C5-C6
20	3	310	CLA	CAA-CBA-CGA-O2A
20	9	603	CLA	CAA-CBA-CGA-O2A
25	B	850	SQD	O47-C7-C8-C9
20	3	324	CLA	C6-C7-C8-C9
20	A	5025	CLA	C2A-CAA-CBA-CGA
20	B	811	CLA	C2A-CAA-CBA-CGA
20	A	5030	CLA	C11-C12-C13-C15
20	B	804	CLA	C11-C12-C13-C15
20	B	830	CLA	C12-C13-C15-C16
20	B	833	CLA	C6-C7-C8-C10
20	H	201	CLA	C11-C10-C8-C7
24	9	617	LHG	C33-C34-C35-C36
26	3	321	PTY	C14-C15-C16-C17
23	3	318	BCR	C23-C24-C25-C30
23	B	844	BCR	C5-C6-C7-C8
23	G	205	BCR	C23-C24-C25-C26
23	G	205	BCR	C23-C24-C25-C30
23	I	4001	BCR	C23-C24-C25-C26
23	I	4001	BCR	C23-C24-C25-C30
23	K	4006	BCR	C23-C24-C25-C26
23	K	4006	BCR	C23-C24-C25-C30
23	L	203	BCR	C1-C6-C7-C8
23	L	203	BCR	C5-C6-C7-C8
20	9	601	CLA	CAA-CBA-CGA-O2A
20	B	804	CLA	CAA-CBA-CGA-O2A
20	9	611	CLA	C2-C1-O2A-CGA
20	B	806	CLA	C2-C1-O2A-CGA
33	J	101	LMK	N4-C3-C4-O2
20	B	834	CLA	CAA-CBA-CGA-O2A
20	A	5020	CLA	C2-C3-C5-C6
24	B	801	LHG	C1-C2-C3-O3
20	2	311	CLA	C2A-CAA-CBA-CGA
20	8	310	CLA	CAA-CBA-CGA-O2A
20	L	204	CLA	CAA-CBA-CGA-O2A
20	F	306	CLA	C11-C12-C13-C15
20	3	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	9	610	CLA	CAA-CBA-CGA-O2A
20	B	821	CLA	CAA-CBA-CGA-O2A
24	A	5052	LHG	O8-C23-C24-C25
25	3	322	SQD	O48-C23-C24-C25
25	1	619	SQD	C4-C5-C6-S
26	3	321	PTY	C20-C21-C22-C23
19	8	306	CHL	CAA-CBA-CGA-O2A
20	F	306	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	O1A-CGA-O2A-C1
20	B	835	CLA	C2A-CAA-CBA-CGA
20	8	321	CLA	CAA-CBA-CGA-O2A
20	A	5026	CLA	CAA-CBA-CGA-O2A
24	1	620	LHG	O8-C23-C24-C25
20	A	5018	CLA	CBD-CGD-O2D-CED
20	A	5024	CLA	C11-C10-C8-C9
20	9	612	CLA	CAA-CBA-CGA-O2A
20	B	819	CLA	CAA-CBA-CGA-O2A
28	7	321	DGD	O2G-C1B-C2B-C3B
26	3	321	PTY	O4-C1-C6-C5
28	B	848	DGD	C1G-C2G-C3G-O3G
20	1	602	CLA	C6-C7-C8-C9
20	1	613	CLA	C1A-C2A-CAA-CBA
20	3	310	CLA	C1A-C2A-CAA-CBA
20	8	310	CLA	C1A-C2A-CAA-CBA
20	8	312	CLA	C1A-C2A-CAA-CBA
20	A	5017	CLA	C1A-C2A-CAA-CBA
20	A	5044	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	2	312	CLA	C1A-C2A-CAA-CBA
25	B	850	SQD	O5-C1-O6-C44
29	7	325	LMU	O5'-C1'-O1'-C1
29	8	322	LMU	O5'-C1'-O1'-C1
20	3	304	CLA	CAA-CBA-CGA-O2A
20	3	308	CLA	CAA-CBA-CGA-O2A
20	B	824	CLA	CAA-CBA-CGA-O2A
20	2	310	CLA	CAA-CBA-CGA-O2A
25	3	320	SQD	O47-C7-C8-C9
28	7	321	DGD	O1G-C1G-C2G-O2G
23	3	319	BCR	C19-C20-C21-C22
20	7	310	CLA	CAA-CBA-CGA-O2A
20	G	202	CLA	CAA-CBA-CGA-O2A
20	A	5029	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	2	310	CLA	C2A-CAA-CBA-CGA
20	B	831	CLA	C5-C6-C7-C8
27	7	301	LMG	C28-C29-C30-C31
19	1	606	CHL	CAA-CBA-CGA-O2A
20	3	309	CLA	CAA-CBA-CGA-O2A
20	B	829	CLA	CAA-CBA-CGA-O2A
25	3	322	SQD	C5-C6-S-O7
20	8	311	CLA	C2-C1-O2A-CGA
20	B	824	CLA	C2-C1-O2A-CGA
19	3	323	CHL	C6-C7-C8-C10
20	7	303	CLA	C11-C10-C8-C7
20	8	303	CLA	C12-C13-C15-C16
20	A	5035	CLA	C6-C7-C8-C10
20	B	809	CLA	C6-C7-C8-C10
20	B	814	CLA	C12-C13-C15-C16
20	B	828	CLA	C12-C13-C15-C16
20	B	830	CLA	C11-C12-C13-C15
20	B	816	CLA	CBA-CGA-O2A-C1
20	A	5009	CLA	C10-C11-C12-C13
20	B	827	CLA	C15-C16-C17-C18
20	8	311	CLA	C16-C17-C18-C19
25	3	320	SQD	C44-C45-O47-C7
27	A	5001	LMG	C12-C13-C14-C15
20	B	816	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	C10-C11-C12-C13
20	B	812	CLA	C2A-CAA-CBA-CGA
20	B	814	CLA	C10-C11-C12-C13
20	B	810	CLA	C10-C11-C12-C13
20	A	5028	CLA	C3A-C2A-CAA-CBA
20	L	204	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	CAA-CBA-CGA-O1A
20	1	603	CLA	CAA-CBA-CGA-O1A
20	8	310	CLA	CAA-CBA-CGA-O1A
20	9	603	CLA	CAA-CBA-CGA-O1A
24	7	320	LHG	C24-C25-C26-C27
20	B	828	CLA	CBA-CGA-O2A-C1
28	B	848	DGD	C5B-C6B-C7B-C8B
19	8	304	CHL	CAA-CBA-CGA-O2A
20	A	5040	CLA	CAA-CBA-CGA-O2A
20	1	614	CLA	CAA-CBA-CGA-O1A
20	3	305	CLA	CAA-CBA-CGA-O1A
20	3	310	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	9	612	CLA	CAA-CBA-CGA-O1A
20	B	829	CLA	CAA-CBA-CGA-O1A
20	A	5009	CLA	C2A-CAA-CBA-CGA
20	A	5004	CLA	C11-C12-C13-C14
20	A	5014	CLA	C6-C7-C8-C9
20	B	805	CLA	C14-C13-C15-C16
20	L	202	CLA	CAA-CBA-CGA-O2A
20	9	604	CLA	CAA-CBA-CGA-O1A
20	L	204	CLA	CAA-CBA-CGA-O1A
20	2	310	CLA	CAA-CBA-CGA-O1A
27	7	324	LMG	O9-C10-C11-C12
27	G	206	LMG	C35-C36-C37-C38
20	A	5020	CLA	C16-C17-C18-C19
20	9	610	CLA	CAA-CBA-CGA-O1A
25	F	311	SQD	O5-C5-C6-S
20	B	804	CLA	CAA-CBA-CGA-O1A
24	1	620	LHG	O10-C23-C24-C25
20	B	819	CLA	CAA-CBA-CGA-O1A
20	F	306	CLA	CAA-CBA-CGA-O1A
25	B	850	SQD	O49-C7-C8-C9
29	7	325	LMU	C2'-C1'-O1'-C1
29	8	322	LMU	C2'-C1'-O1'-C1
20	7	303	CLA	CAA-CBA-CGA-O2A
20	B	817	CLA	CAA-CBA-CGA-O2A
25	3	320	SQD	O48-C23-C24-C25
20	A	5039	CLA	C2A-CAA-CBA-CGA
27	A	5001	LMG	C13-C14-C15-C16
20	8	321	CLA	CAA-CBA-CGA-O1A
20	A	5026	CLA	CAA-CBA-CGA-O1A
20	A	5029	CLA	CAA-CBA-CGA-O1A
20	B	814	CLA	CAA-CBA-CGA-O1A
20	B	821	CLA	CAA-CBA-CGA-O1A
28	7	321	DGD	O1B-C1B-C2B-C3B
20	3	309	CLA	CAA-CBA-CGA-O1A
20	7	310	CLA	CAA-CBA-CGA-O1A
20	3	309	CLA	CAD-CBD-CGD-O2D
20	8	302	CLA	CAD-CBD-CGD-O2D
20	A	5021	CLA	CAD-CBD-CGD-O2D
20	B	815	CLA	CAD-CBD-CGD-O2D
20	2	310	CLA	CAD-CBD-CGD-O2D
30	A	5003	CL0	CAD-CBD-CGD-O2D
20	A	5025	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A	5052	LHG	O7-C7-C8-C9
19	1	606	CHL	CAA-CBA-CGA-O1A
20	G	202	CLA	CAA-CBA-CGA-O1A
24	A	5052	LHG	O10-C23-C24-C25
20	B	831	CLA	O1D-CGD-O2D-CED
20	A	5029	CLA	C2-C1-O2A-CGA
20	F	306	CLA	C2-C1-O2A-CGA
20	L	205	CLA	C2-C1-O2A-CGA
20	2	311	CLA	C2-C1-O2A-CGA
20	3	308	CLA	CAA-CBA-CGA-O1A
25	3	322	SQD	O10-C23-C24-C25
20	B	805	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	CAA-CBA-CGA-O2A
20	3	324	CLA	C6-C7-C8-C10
20	A	5043	CLA	CBA-CGA-O2A-C1
20	7	303	CLA	C2A-CAA-CBA-CGA
19	8	306	CHL	CAA-CBA-CGA-O1A
20	B	824	CLA	CAA-CBA-CGA-O1A
20	9	609	CLA	CAA-CBA-CGA-O2A
20	K	4005	CLA	CAA-CBA-CGA-O2A
24	I	4002	LHG	O7-C7-C8-C9
27	A	5001	LMG	O7-C10-C11-C12
20	1	602	CLA	CAA-CBA-CGA-O2A
20	7	312	CLA	CAA-CBA-CGA-O2A
20	B	837	CLA	CAA-CBA-CGA-O2A
25	F	311	SQD	O48-C23-C24-C25
26	B	802	PTY	C12-C11-C8-O7
27	7	324	LMG	O8-C28-C29-C30
20	3	304	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

229 monomers are involved in 645 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	819	CLA	6	0
20	3	305	CLA	4	0
20	A	5035	CLA	6	0
32	C	102	SF4	1	0
29	8	322	LMU	4	0
31	B	841	PQN	8	0
20	B	837	CLA	1	0
21	1	615	LUT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	5045	PQN	3	0
22	8	315	XAT	1	0
23	L	203	BCR	2	0
20	B	810	CLA	6	0
20	A	5040	CLA	5	0
27	7	324	LMG	2	0
20	B	829	CLA	5	0
20	K	4005	CLA	4	0
20	K	4002	CLA	2	0
20	F	303	CLA	3	0
20	A	5017	CLA	2	0
20	8	308	CLA	3	0
25	3	322	SQD	2	0
20	1	614	CLA	1	0
20	A	5014	CLA	4	0
20	7	314	CLA	2	0
23	A	5049	BCR	5	0
23	3	319	BCR	10	0
27	G	206	LMG	6	0
23	L	206	BCR	3	0
20	1	607	CLA	3	0
20	3	325	CLA	2	0
19	1	601	CHL	4	0
26	3	321	PTY	1	0
23	K	4006	BCR	3	0
23	A	5051	BCR	4	0
23	J	106	BCR	3	0
20	7	303	CLA	5	0
20	3	311	CLA	4	0
20	8	307	CLA	3	0
19	1	606	CHL	3	0
20	2	313	CLA	1	0
20	1	603	CLA	1	0
20	B	833	CLA	2	0
20	B	815	CLA	3	0
23	J	105	BCR	3	0
24	A	5052	LHG	2	0
20	B	821	CLA	2	0
20	B	840	CLA	4	0
22	9	614	XAT	1	0
20	A	5025	CLA	5	0
24	7	319	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	F	302	PTY	1	0
20	H	201	CLA	2	0
20	L	204	CLA	4	0
29	8	318	LMU	1	0
20	1	604	CLA	1	0
19	2	306	CHL	5	0
20	8	310	CLA	2	0
20	8	301	CLA	6	0
24	2	316	LHG	1	0
20	A	5021	CLA	3	0
20	B	825	CLA	5	0
20	7	323	CLA	2	0
23	B	847	BCR	4	0
20	A	5034	CLA	1	0
20	1	612	CLA	5	0
21	2	315	LUT	2	0
20	G	204	CLA	5	0
20	B	832	CLA	8	0
20	A	5019	CLA	2	0
20	B	818	CLA	1	0
20	A	5033	CLA	5	0
23	B	846	BCR	3	0
20	B	823	CLA	3	0
20	2	301	CLA	1	0
20	8	303	CLA	6	0
20	A	5007	CLA	2	0
20	3	314	CLA	2	0
20	7	313	CLA	5	0
20	B	812	CLA	3	0
20	A	5042	CLA	6	0
20	1	605	CLA	7	0
19	3	301	CHL	13	0
19	7	307	CHL	7	0
20	A	5008	CLA	1	0
20	3	324	CLA	2	0
20	F	307	CLA	6	0
23	3	318	BCR	7	0
23	A	5047	BCR	5	0
24	I	4002	LHG	2	0
25	7	322	SQD	1	0
20	B	811	CLA	4	0
20	A	5028	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	202	CLA	2	0
28	B	848	DGD	9	0
20	L	201	CLA	4	0
20	B	809	CLA	4	0
22	3	316	XAT	7	0
20	8	311	CLA	1	0
20	G	203	CLA	8	0
24	A	5055	LHG	2	0
20	F	306	CLA	2	0
19	2	302	CHL	5	0
20	A	5032	CLA	3	0
20	B	836	CLA	5	0
23	A	5050	BCR	4	0
24	8	319	LHG	2	0
20	7	304	CLA	1	0
23	J	102	BCR	9	0
19	8	306	CHL	5	0
20	7	310	CLA	3	0
20	B	824	CLA	5	0
30	A	5003	CL0	10	0
24	1	620	LHG	3	0
20	A	5010	CLA	4	0
20	2	308	CLA	5	0
19	3	323	CHL	9	0
19	7	306	CHL	5	0
20	A	5018	CLA	5	0
20	A	5023	CLA	3	0
23	K	4001	BCR	3	0
26	F	301	PTY	2	0
20	A	5020	CLA	6	0
20	8	309	CLA	4	0
20	A	5027	CLA	2	0
20	B	830	CLA	2	0
20	1	602	CLA	1	0
24	1	618	LHG	3	0
25	3	320	SQD	1	0
20	8	312	CLA	1	0
20	8	321	CLA	2	0
20	B	827	CLA	6	0
23	F	304	BCR	4	0
20	9	602	CLA	2	0
25	1	619	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5016	CLA	7	0
20	B	820	CLA	4	0
20	A	5005	CLA	13	0
19	8	305	CHL	7	0
20	G	201	CLA	4	0
20	2	303	CLA	3	0
20	J	104	CLA	2	0
20	9	611	CLA	3	0
24	7	320	LHG	5	0
20	2	305	CLA	1	0
32	A	5046	SF4	1	0
20	7	312	CLA	1	0
20	A	5041	CLA	7	0
23	B	845	BCR	2	0
20	B	839	CLA	9	0
20	B	805	CLA	12	0
23	7	318	BCR	3	0
23	B	844	BCR	5	0
20	L	205	CLA	1	0
21	9	613	LUT	2	0
26	7	302	PTY	1	0
20	7	305	CLA	2	0
23	F	309	BCR	6	0
20	B	816	CLA	3	0
20	B	828	CLA	5	0
20	B	834	CLA	2	0
24	A	5054	LHG	2	0
23	B	803	BCR	4	0
22	9	615	XAT	1	0
20	A	5036	CLA	3	0
21	7	316	LUT	2	0
20	B	838	CLA	2	0
25	F	311	SQD	3	0
20	8	302	CLA	2	0
20	1	611	CLA	3	0
27	A	5001	LMG	2	0
20	9	604	CLA	1	0
20	1	610	CLA	3	0
29	A	5053	LMU	2	0
20	9	603	CLA	4	0
20	B	817	CLA	2	0
20	1	609	CLA	2	0

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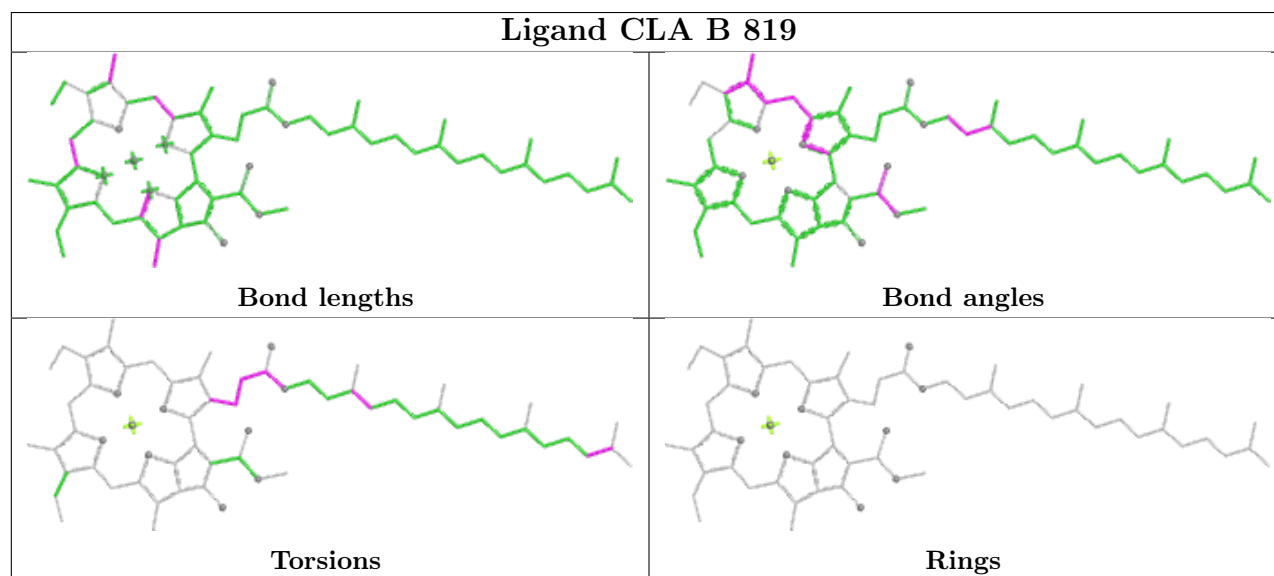
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	314	LUT	4	0
20	A	5043	CLA	3	0
23	A	5048	BCR	4	0
20	9	608	CLA	1	0
20	A	5012	CLA	5	0
24	8	317	LHG	1	0
19	7	308	CHL	3	0
20	A	5029	CLA	8	0
20	A	5006	CLA	3	0
19	8	304	CHL	9	0
23	G	205	BCR	1	0
23	B	843	BCR	4	0
20	B	814	CLA	8	0
20	K	4004	CLA	3	0
22	7	317	XAT	4	0
20	A	5013	CLA	3	0
23	1	617	BCR	5	0
20	B	826	CLA	8	0
20	3	302	CLA	6	0
24	A	5002	LHG	2	0
20	3	308	CLA	1	0
20	A	5009	CLA	1	0
24	B	849	LHG	1	0
20	A	5011	CLA	6	0
20	A	5031	CLA	3	0
23	3	317	BCR	1	0
27	7	301	LMG	5	0
20	3	313	CLA	2	0
20	3	304	CLA	1	0
23	8	316	BCR	10	0
20	A	5030	CLA	4	0
20	2	307	CLA	1	0
20	7	311	CLA	1	0
20	3	306	CLA	5	0
20	9	607	CLA	19	0
20	A	5004	CLA	7	0
23	B	842	BCR	1	0
20	B	835	CLA	1	0
20	B	807	CLA	8	0
20	A	5022	CLA	1	0
20	2	311	CLA	8	0
20	B	808	CLA	5	0

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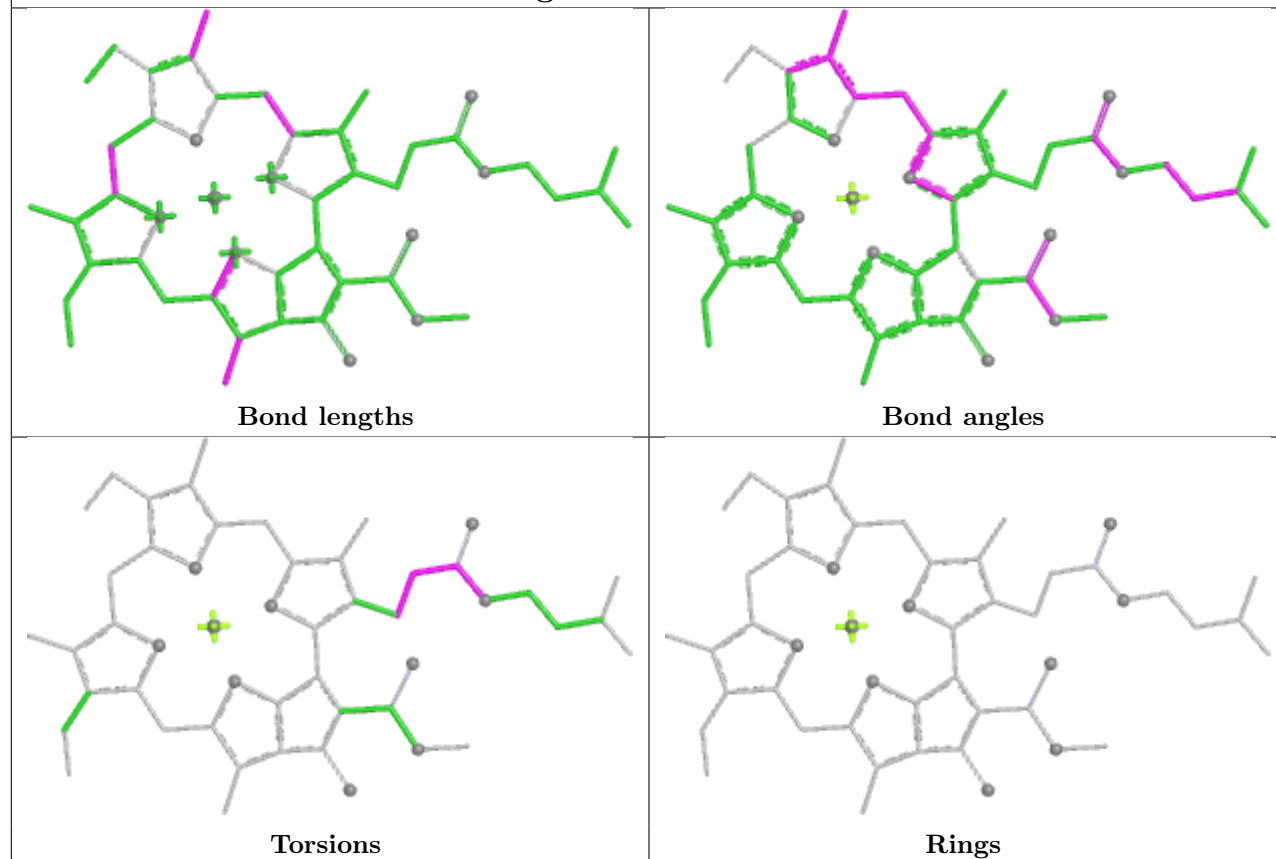
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	1	608	CLA	4	0
19	9	606	CHL	2	0
20	A	5044	CLA	7	0
20	B	806	CLA	2	0
20	3	307	CLA	8	0
20	A	5026	CLA	4	0
20	B	822	CLA	4	0
20	B	831	CLA	6	0
21	3	315	LUT	2	0
23	I	4001	BCR	1	0

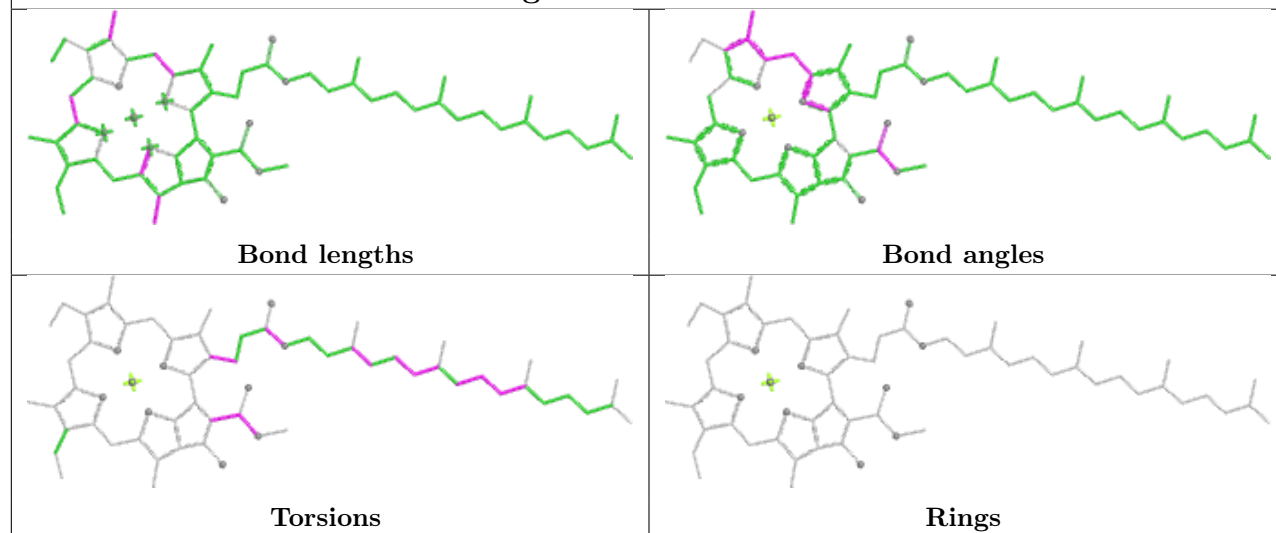
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



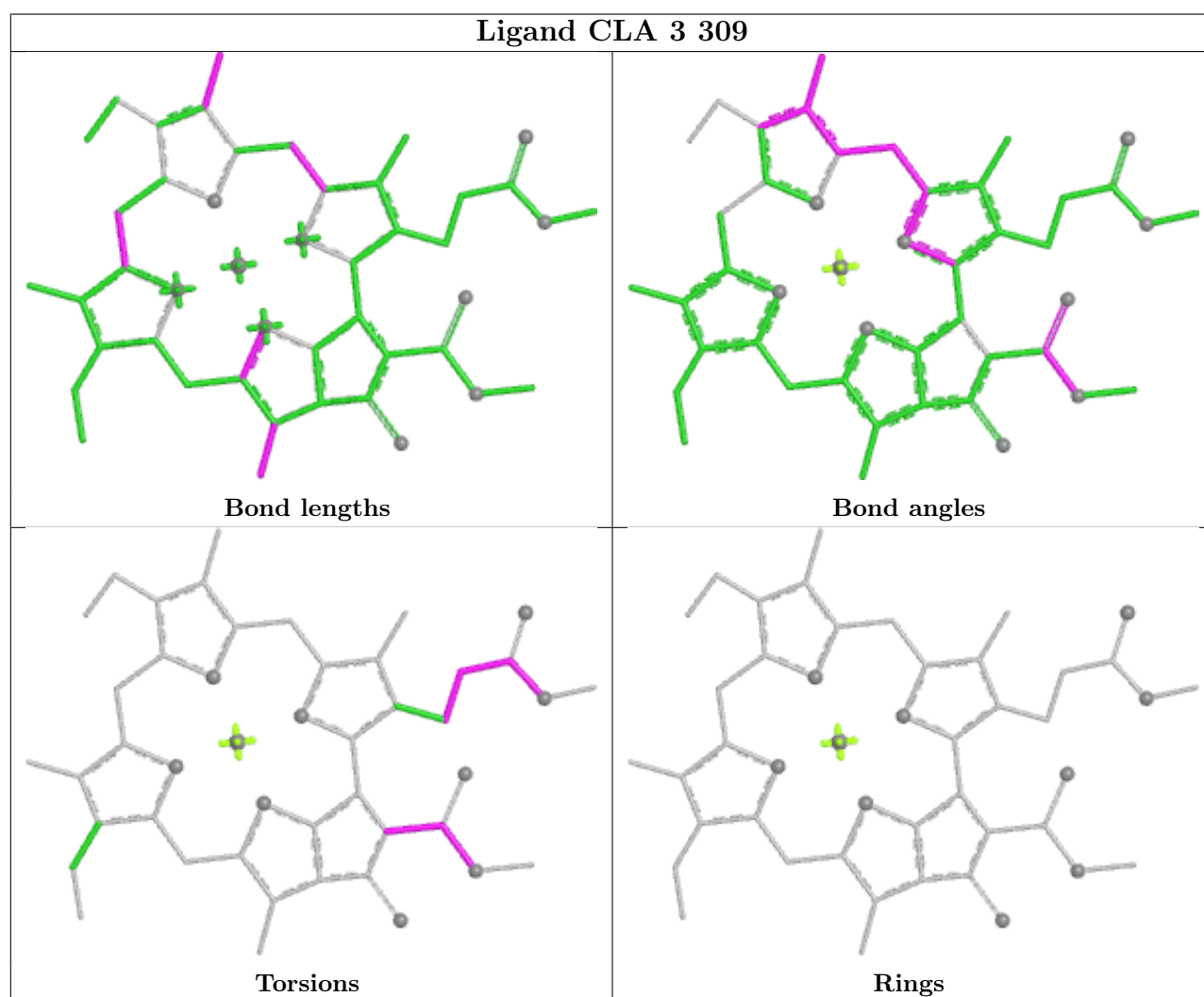
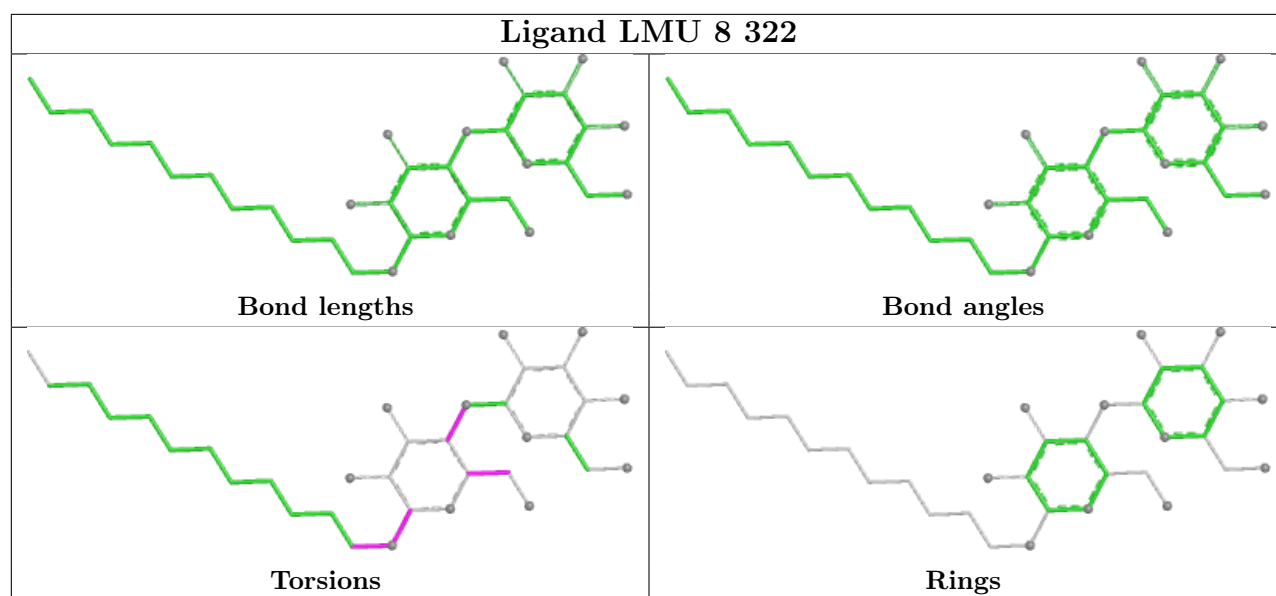
## Ligand CLA 3 305

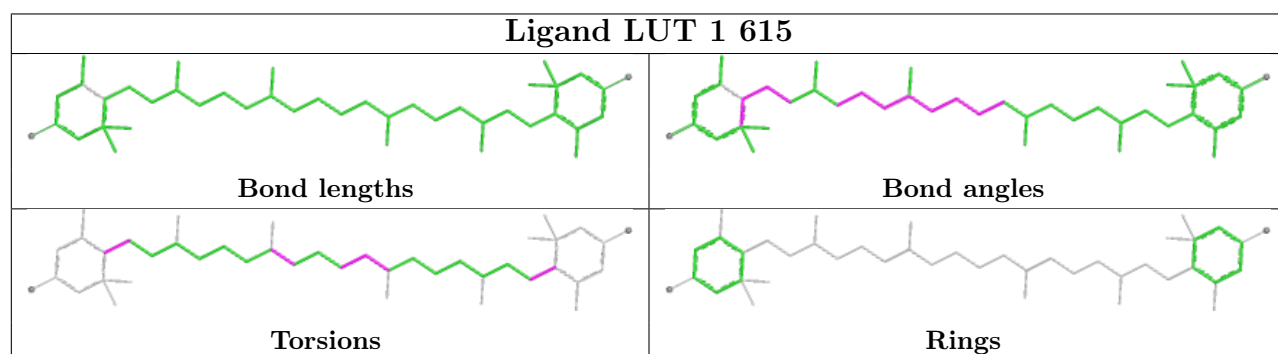
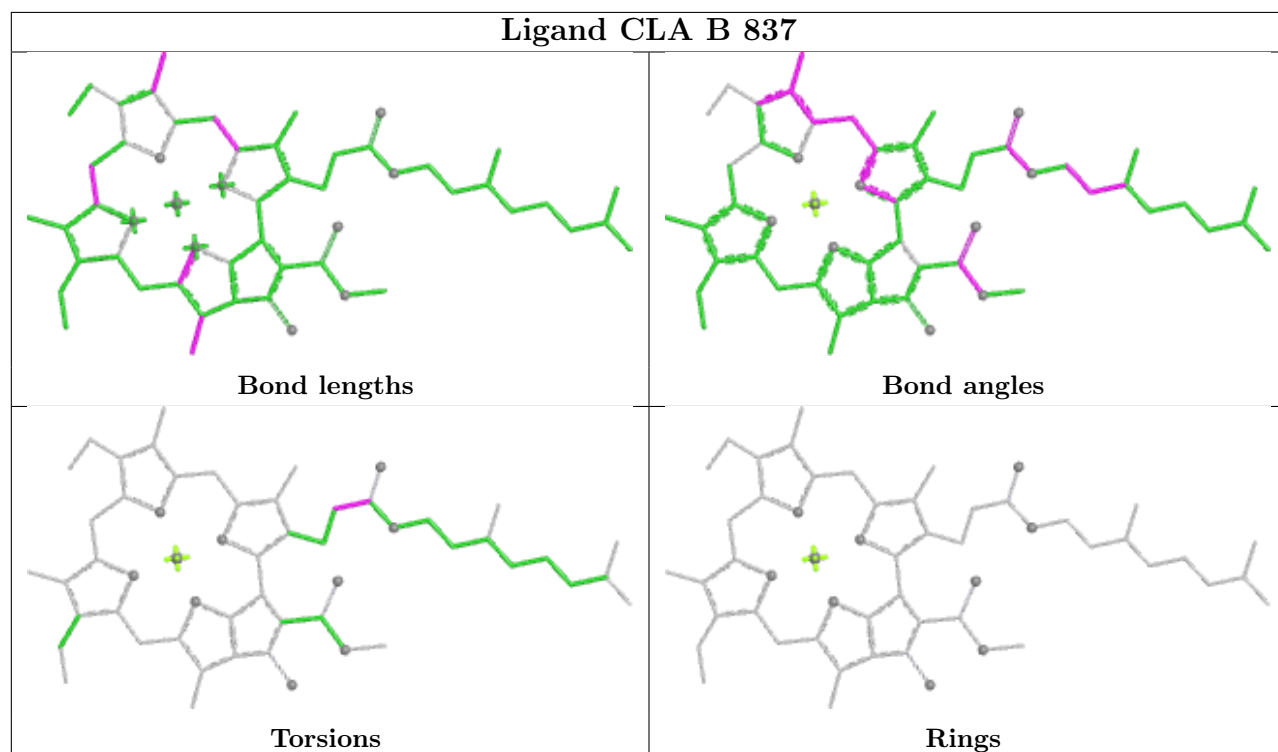
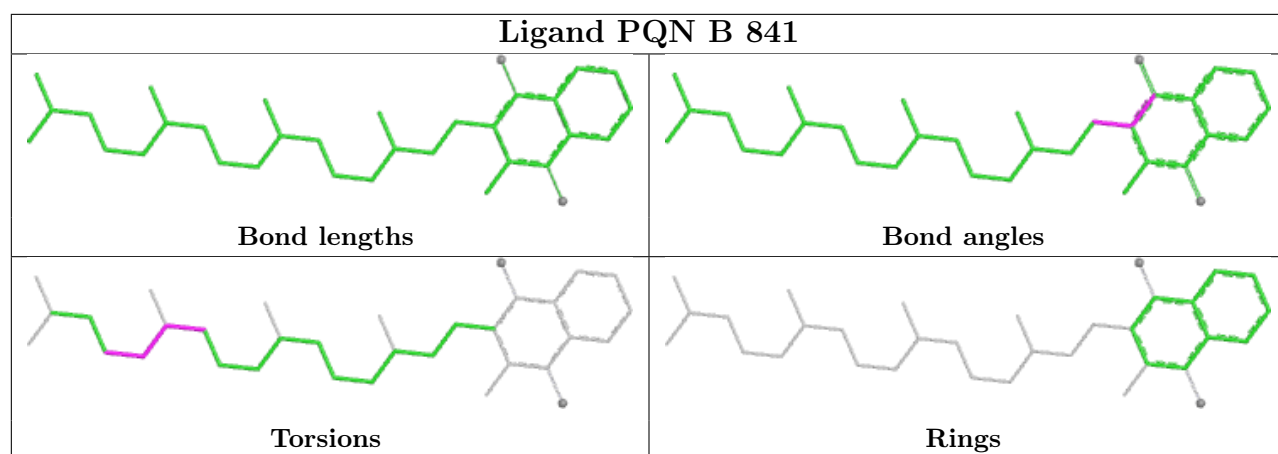


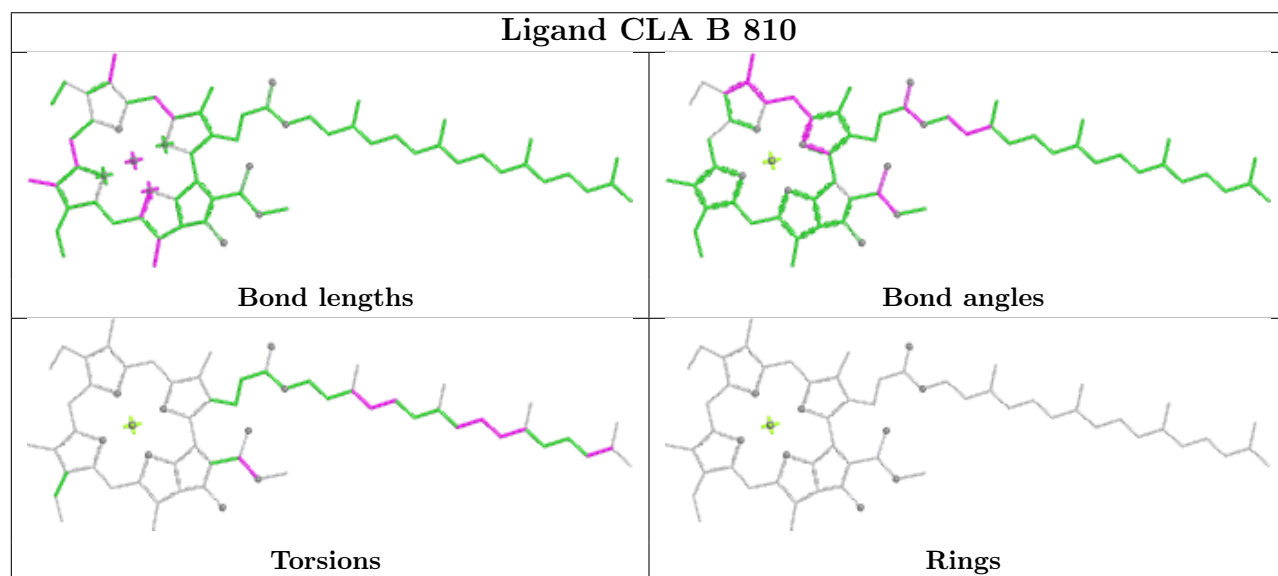
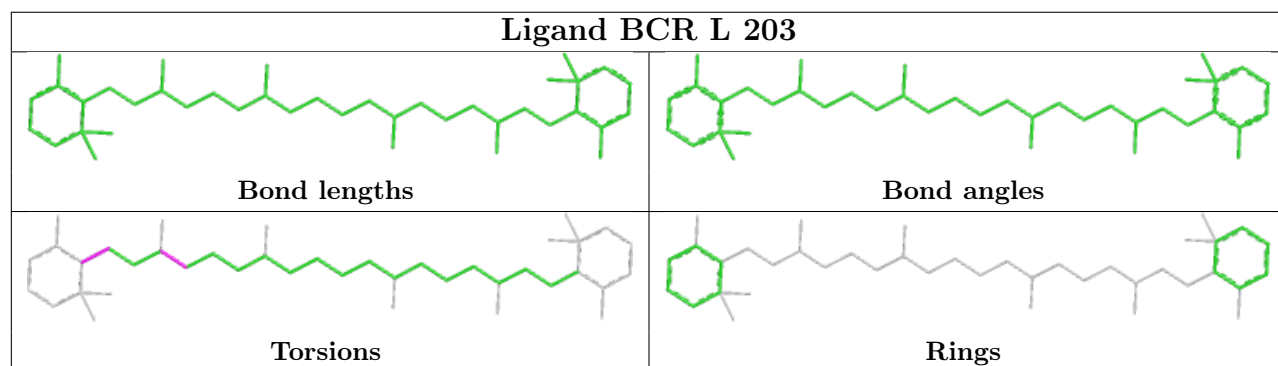
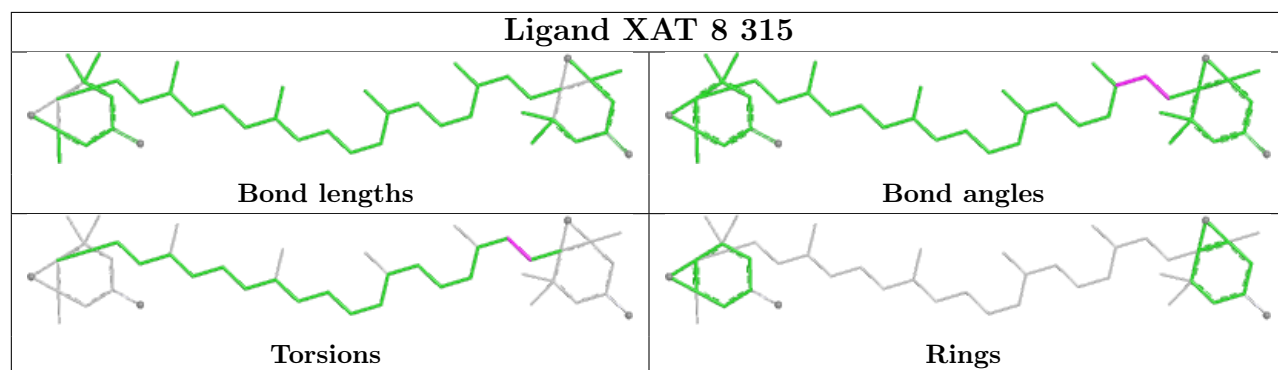
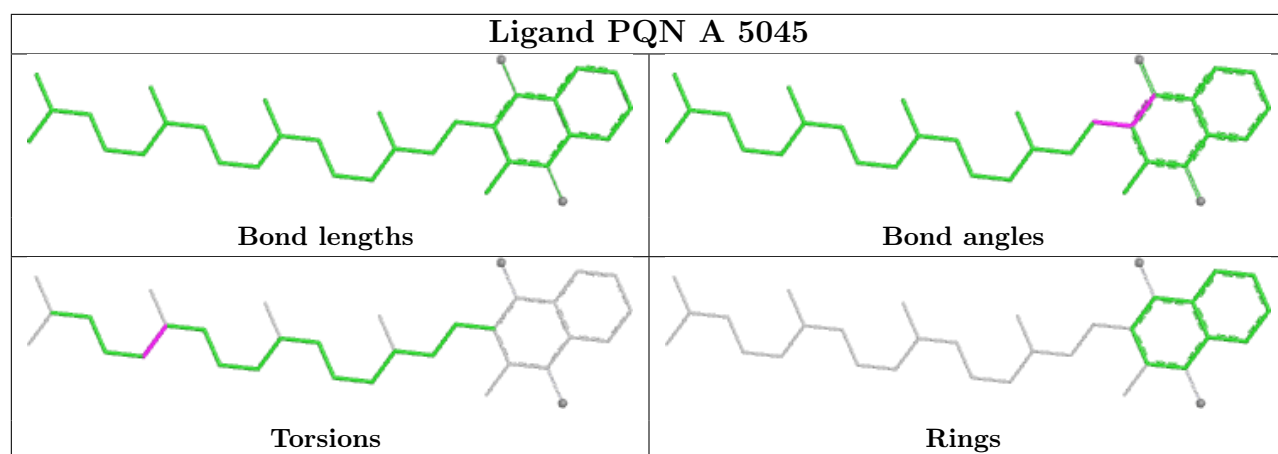
## Ligand CLA A 5035



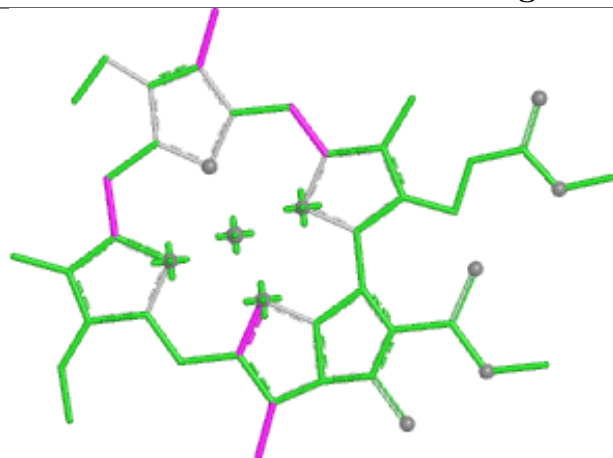




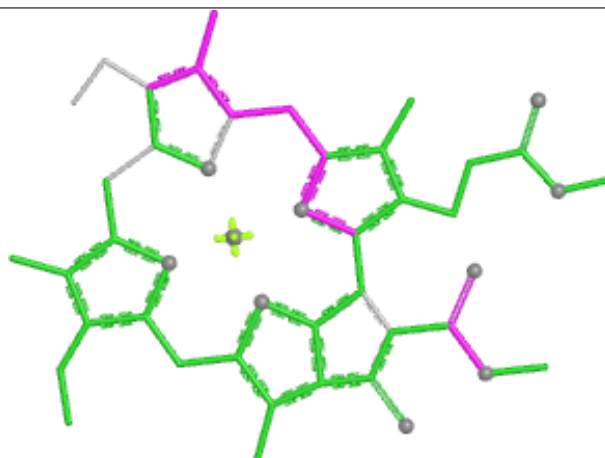




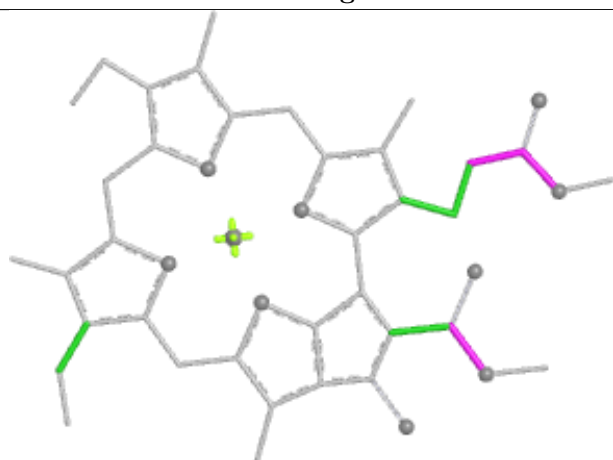
## Ligand CLA 9 612



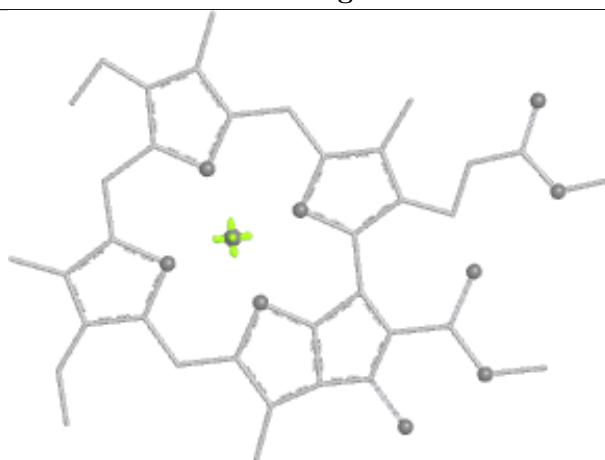
Bond lengths



Bond angles

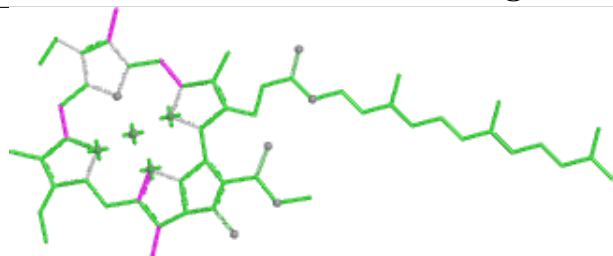


Torsions

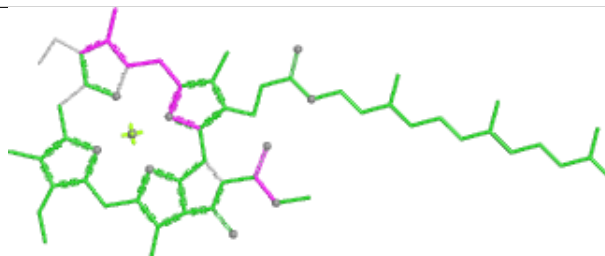


Rings

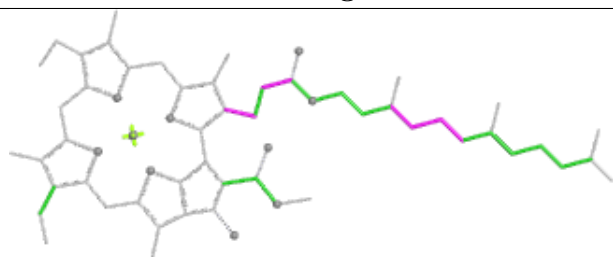
## Ligand CLA A 5040



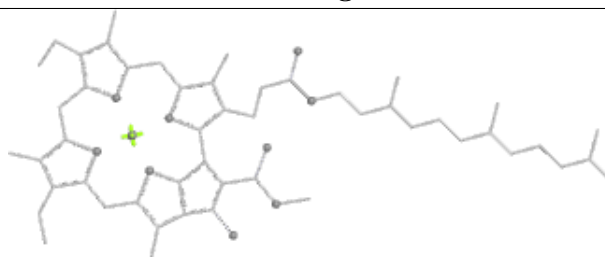
Bond lengths



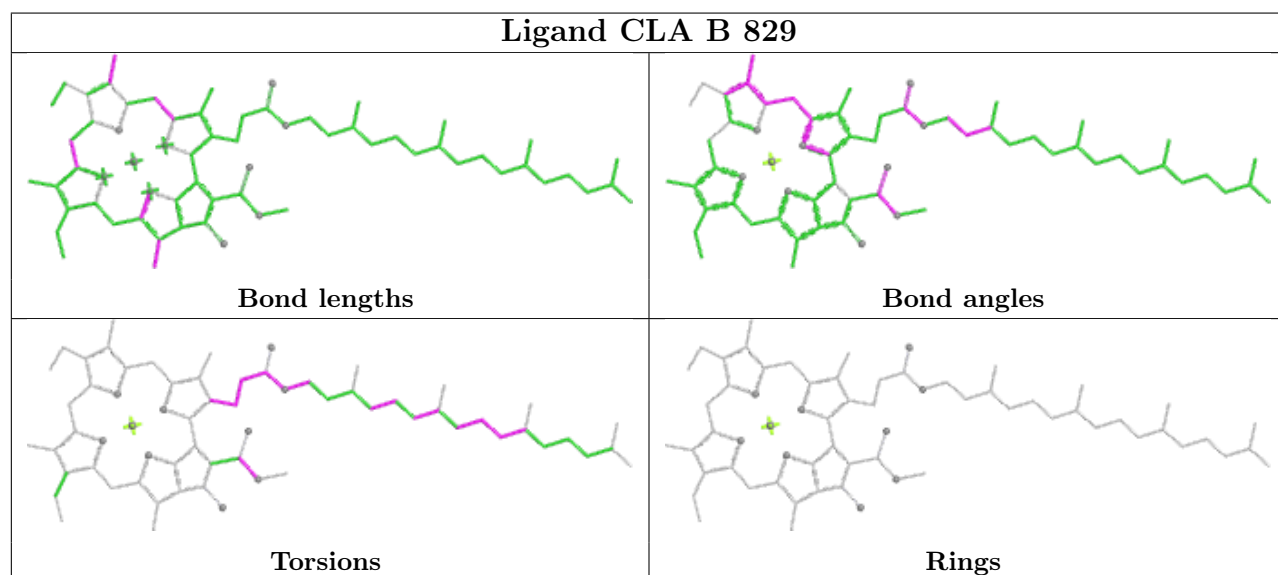
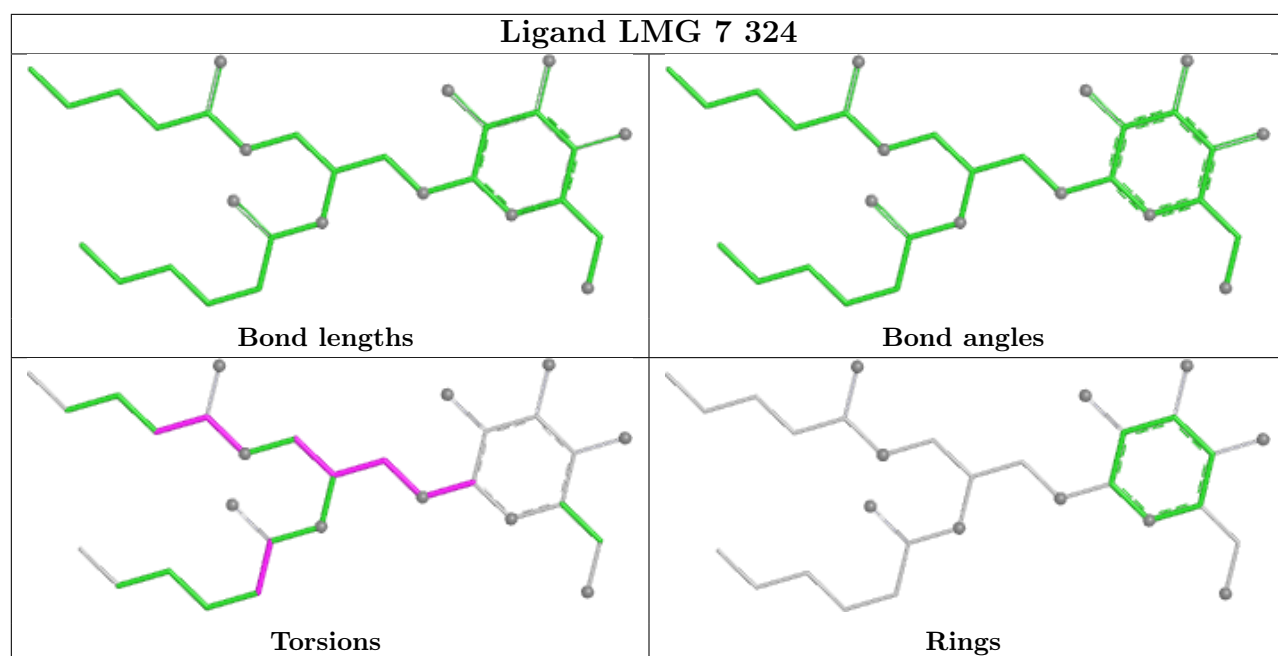
Bond angles

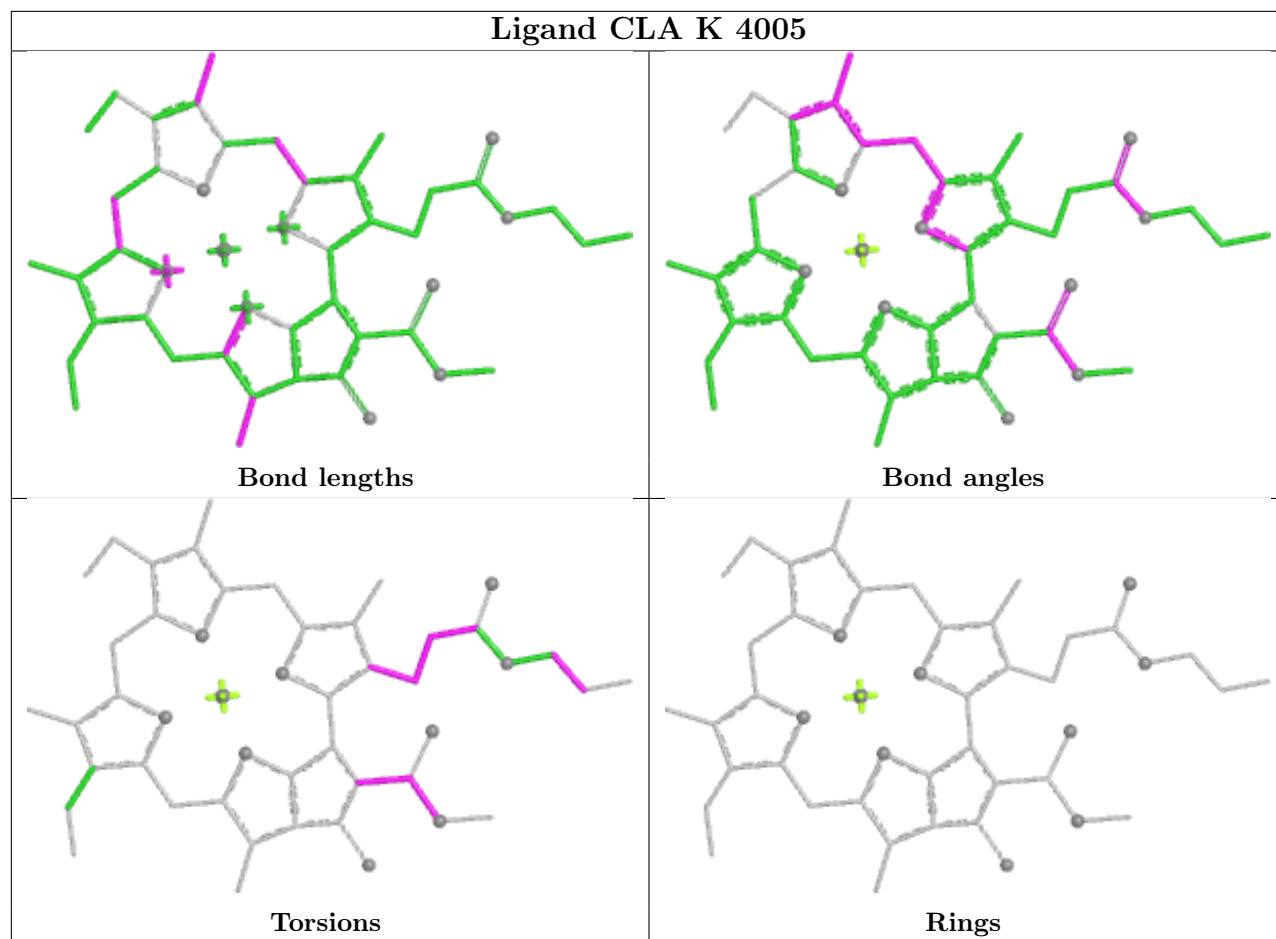


Torsions

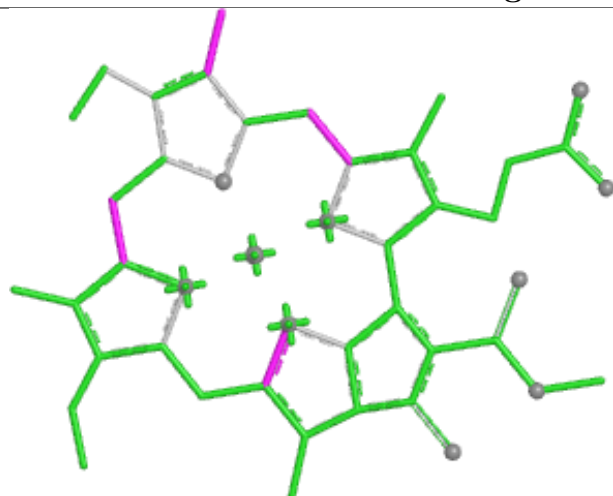


Rings

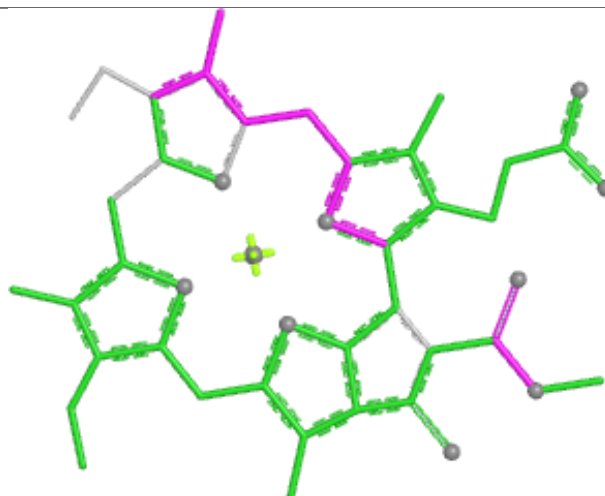




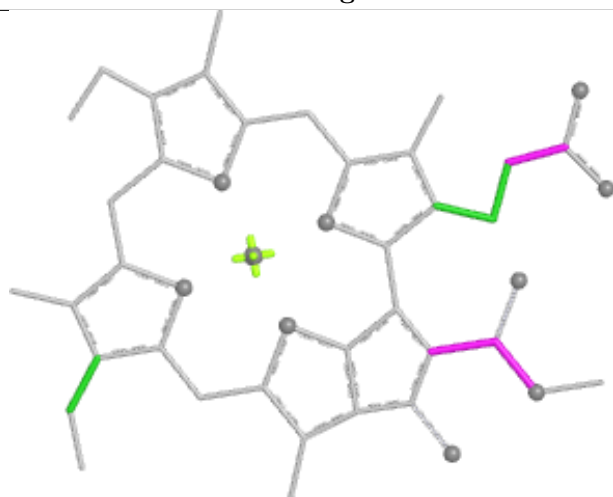
## Ligand CLA K 4002



Bond lengths



Bond angles

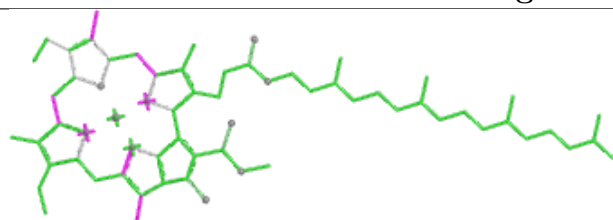


Torsions

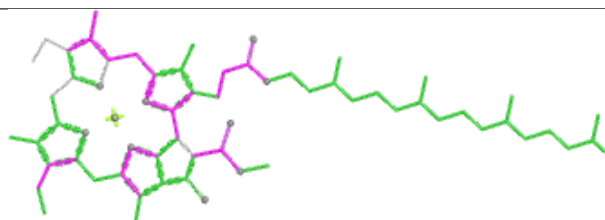


Rings

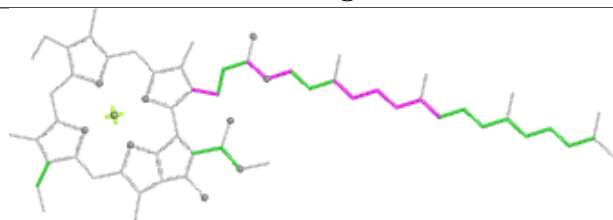
## Ligand CLA F 303



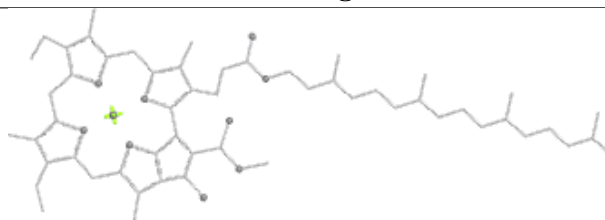
Bond lengths



Bond angles

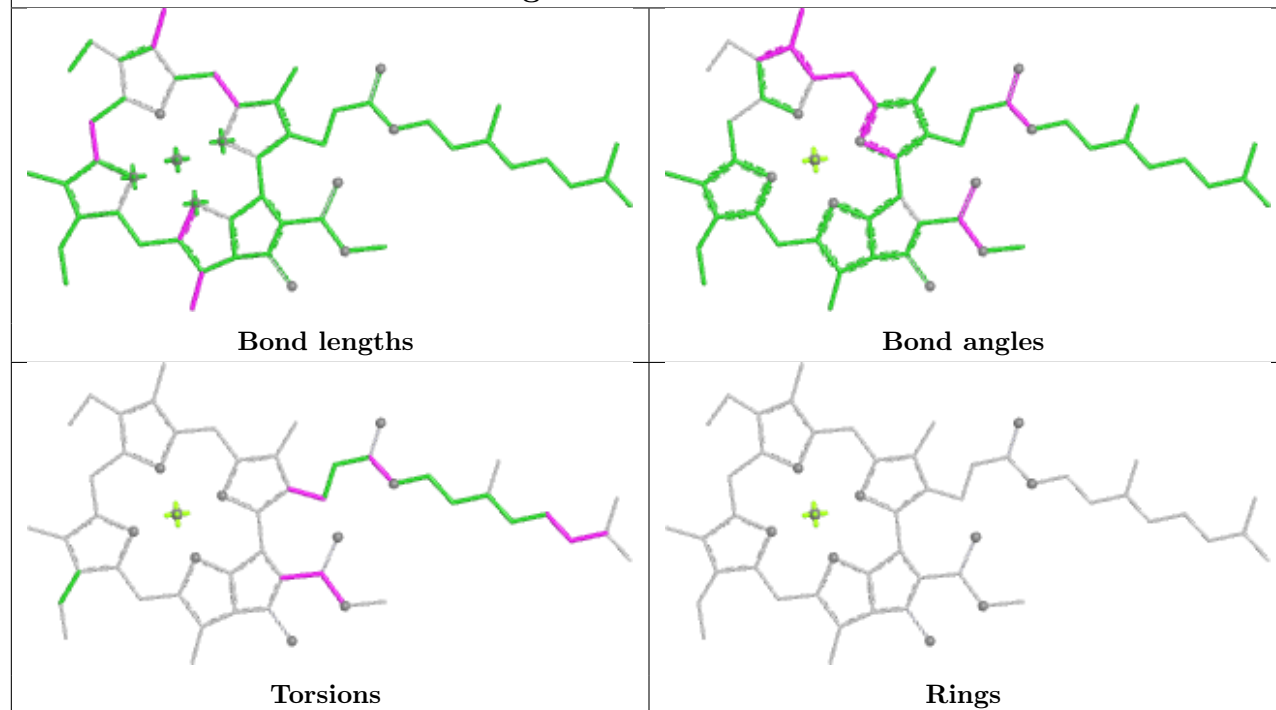


Torsions

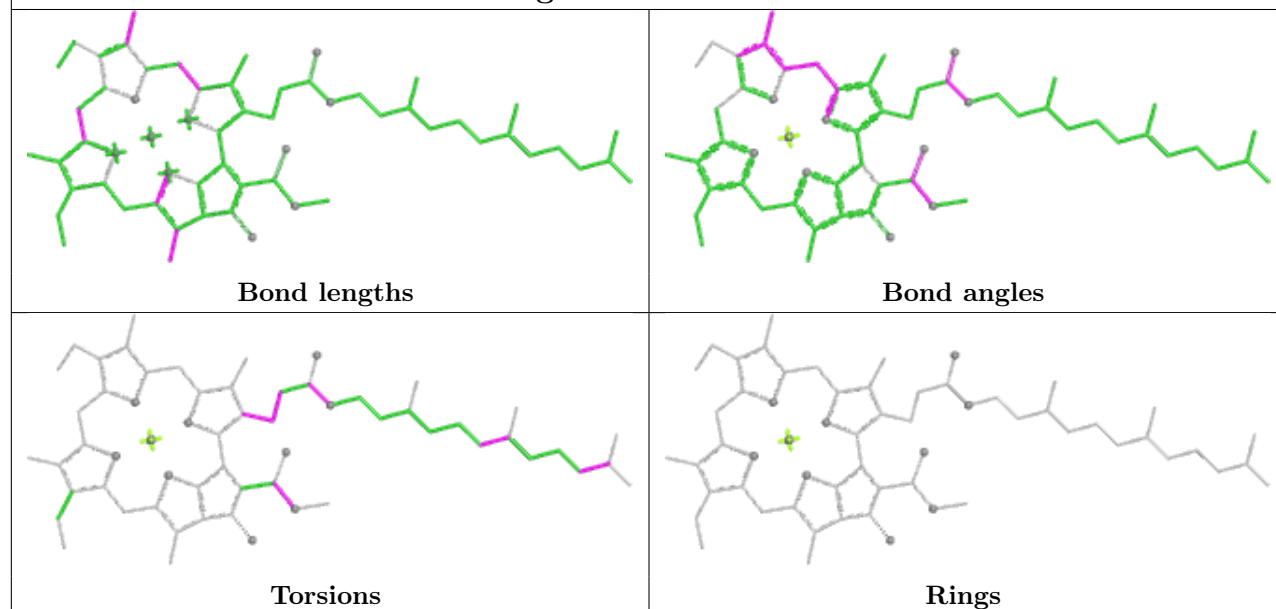


Rings

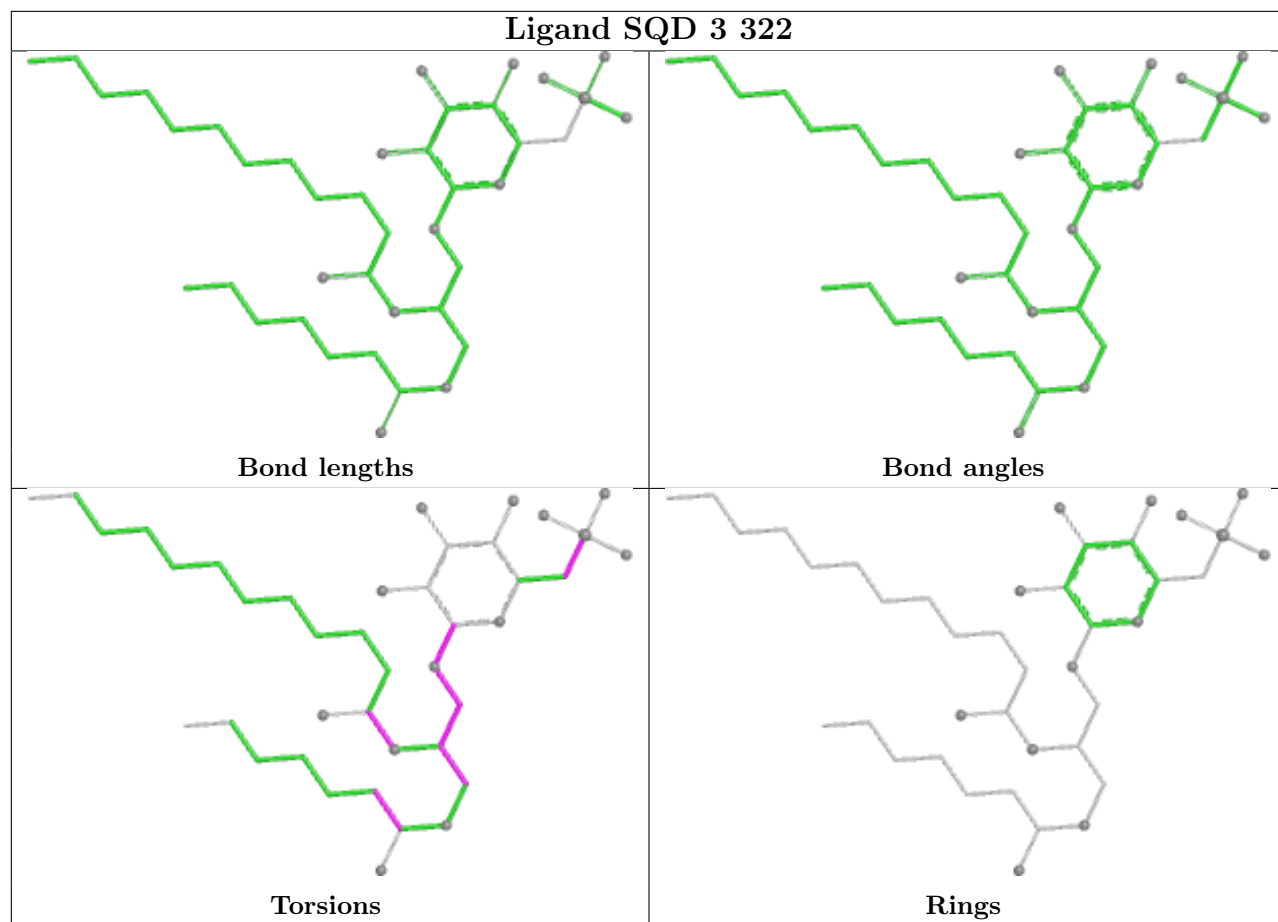
## Ligand CLA A 5017



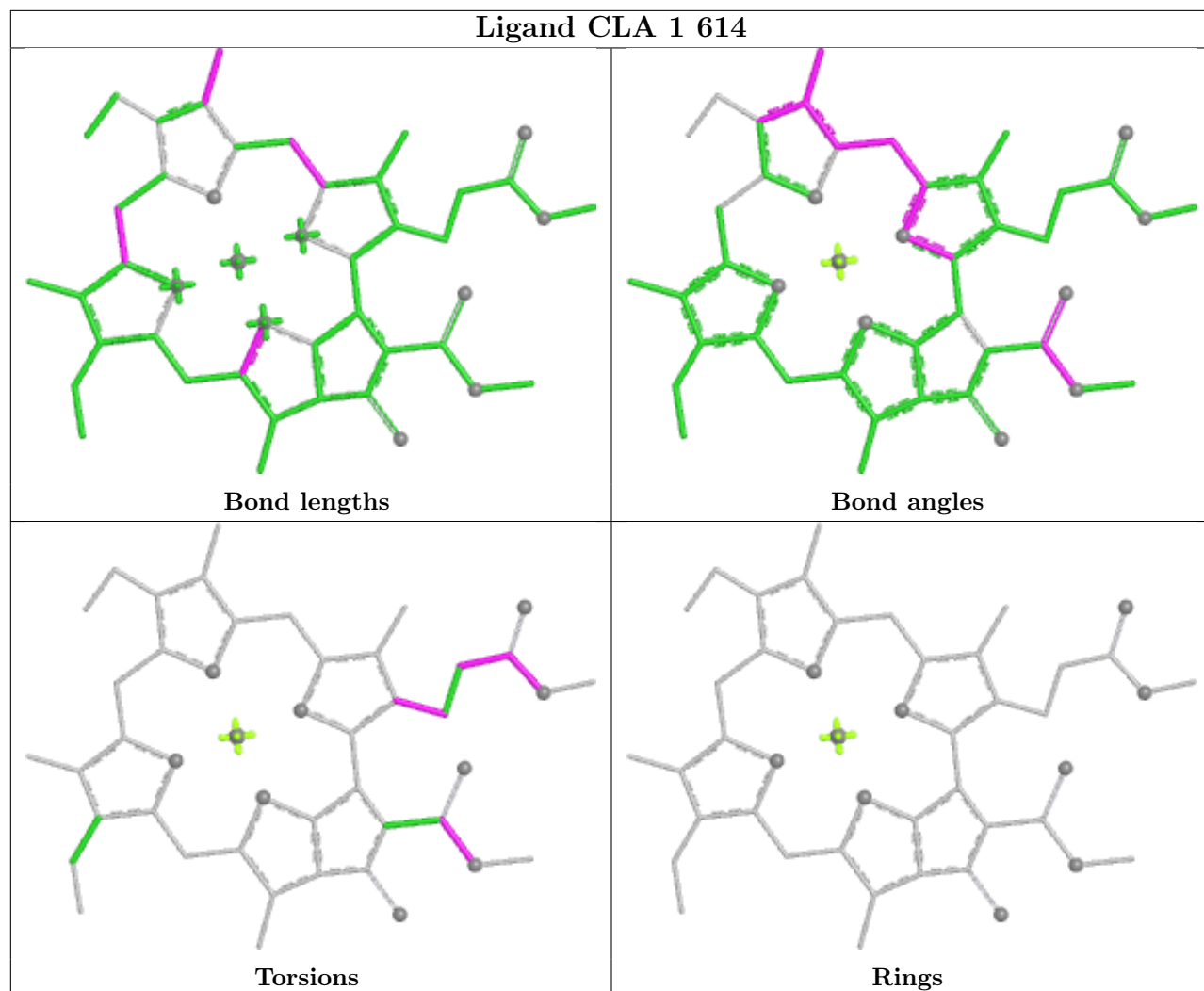
## Ligand CLA 8 308



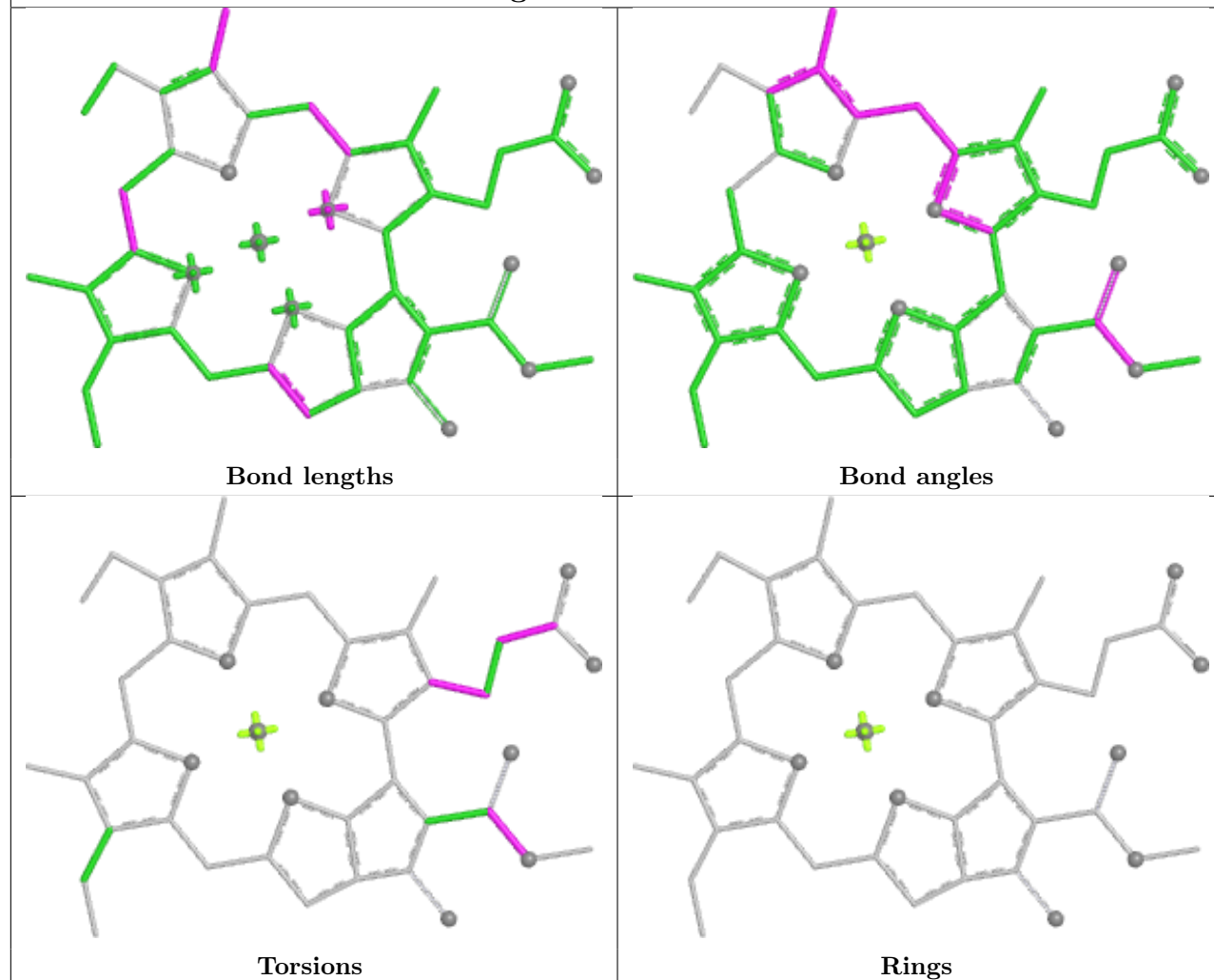




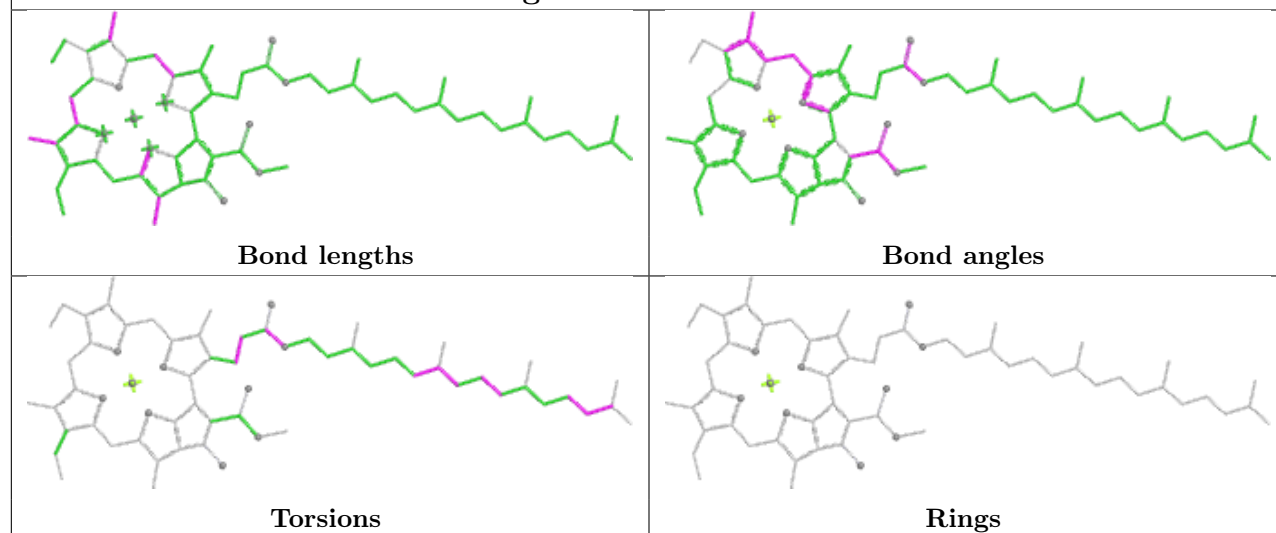
## Ligand CLA 1 614



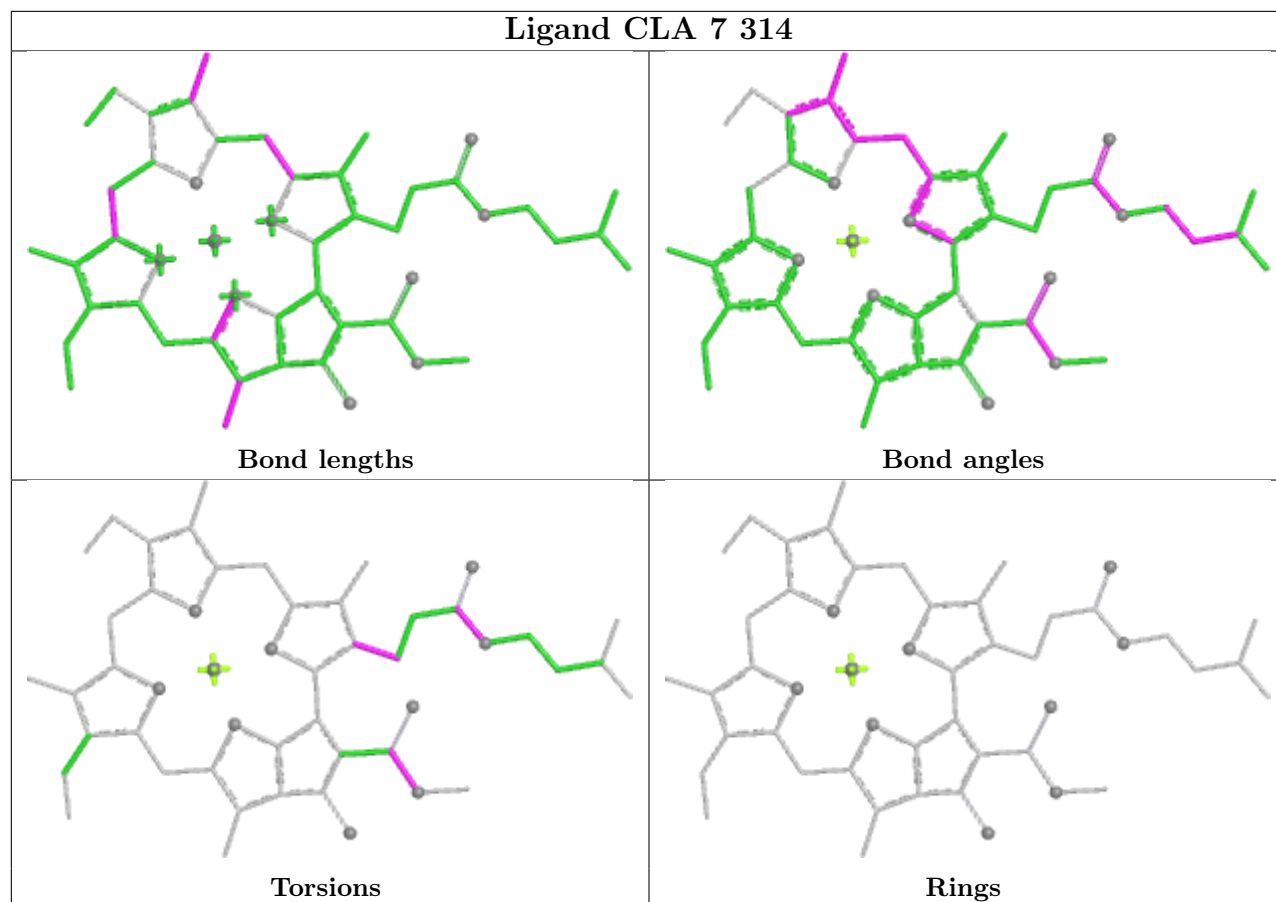
## Ligand CLA 2 312



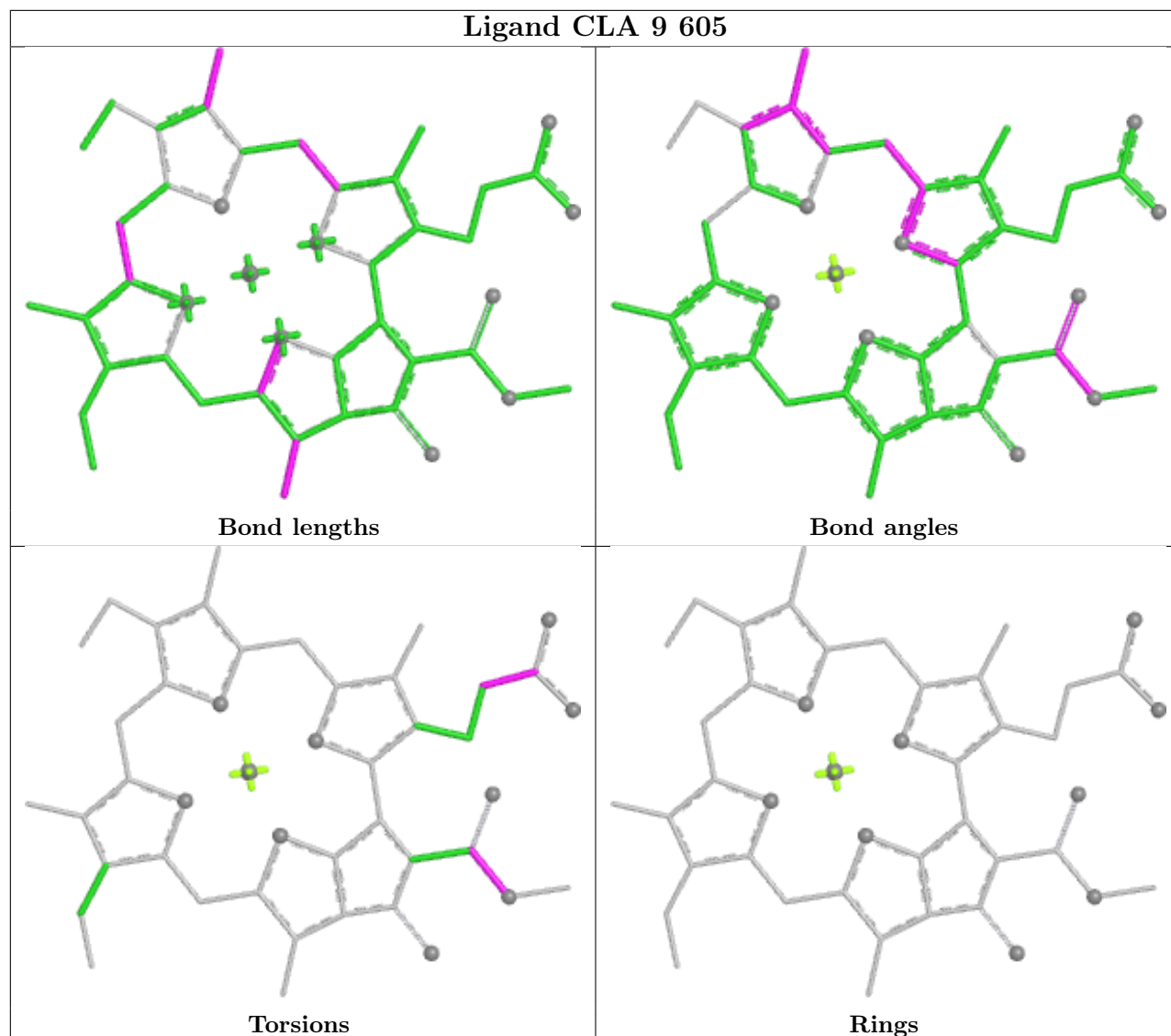
## Ligand CLA A 5014



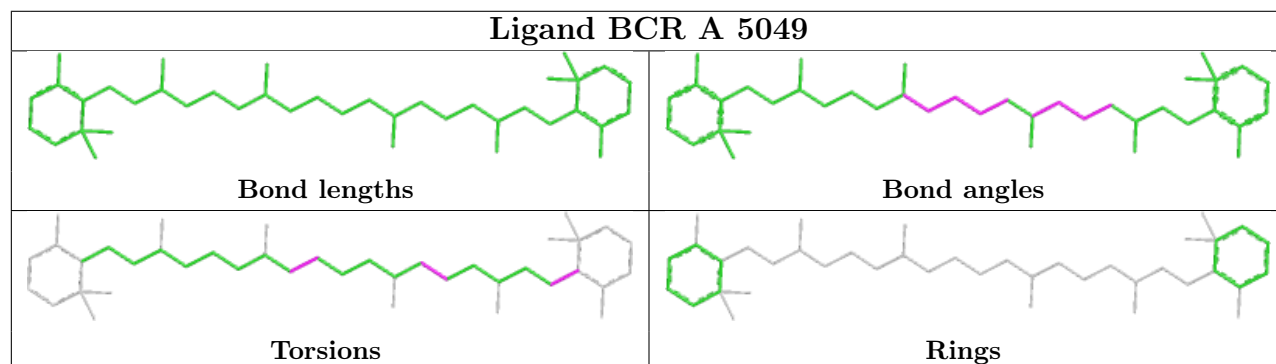
## Ligand CLA 7 314

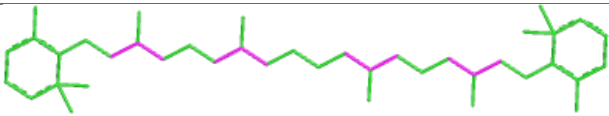
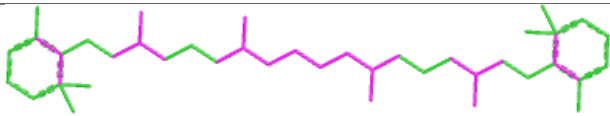
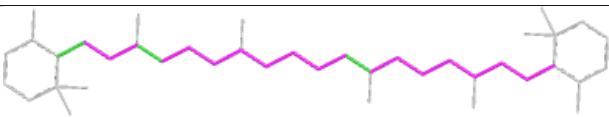
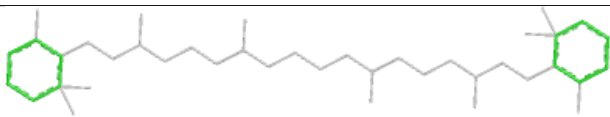



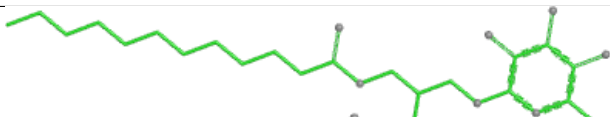
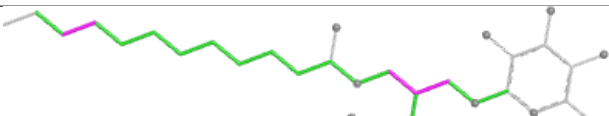
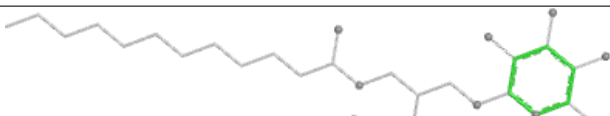
## Ligand CLA 9 605

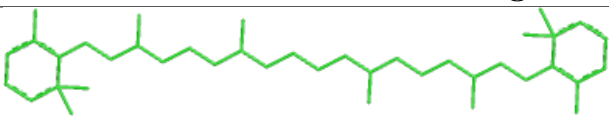
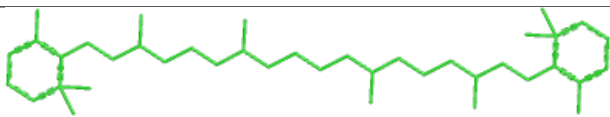
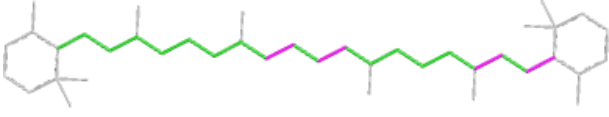
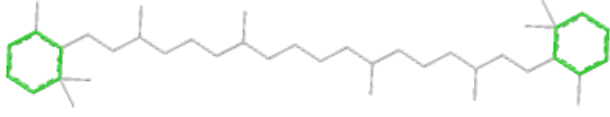


## Ligand BCR A 5049

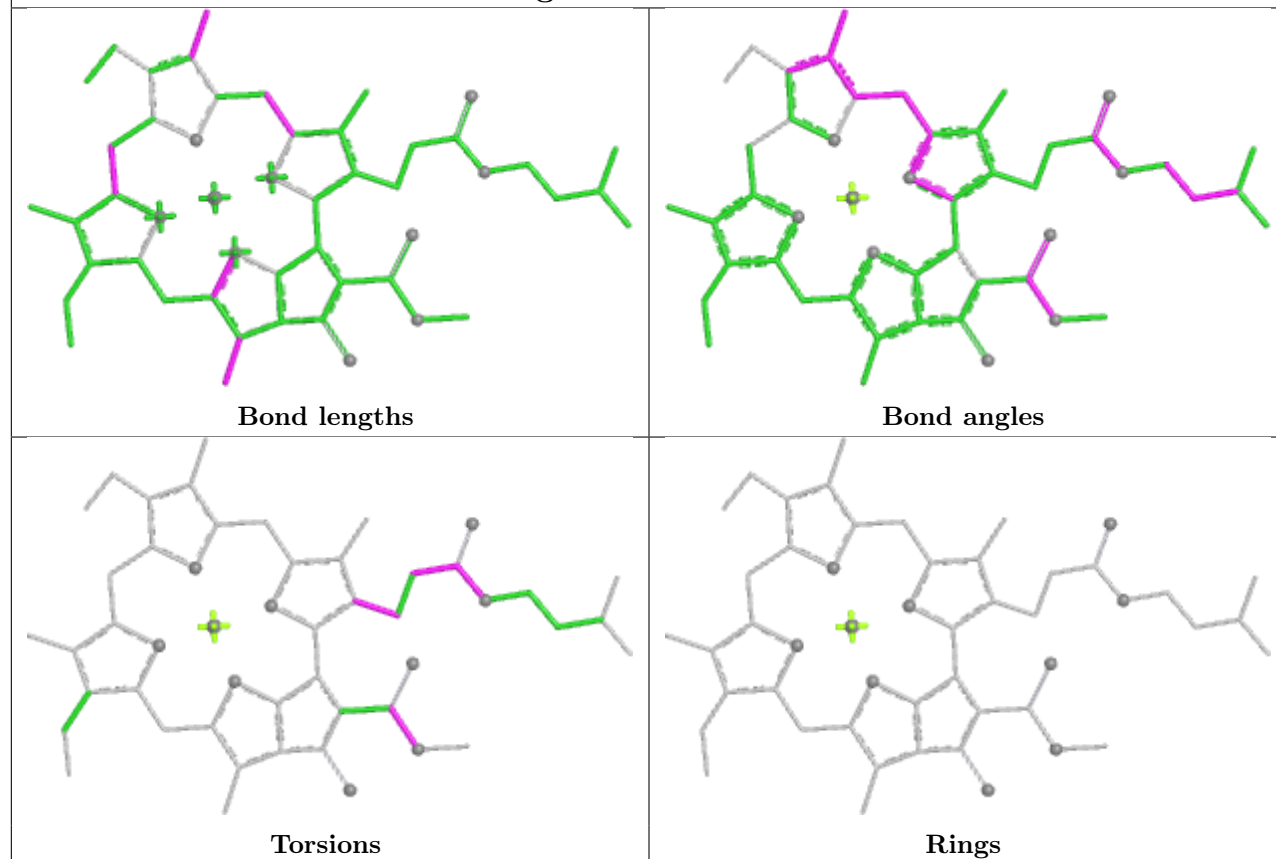


Ligand BCR 3 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

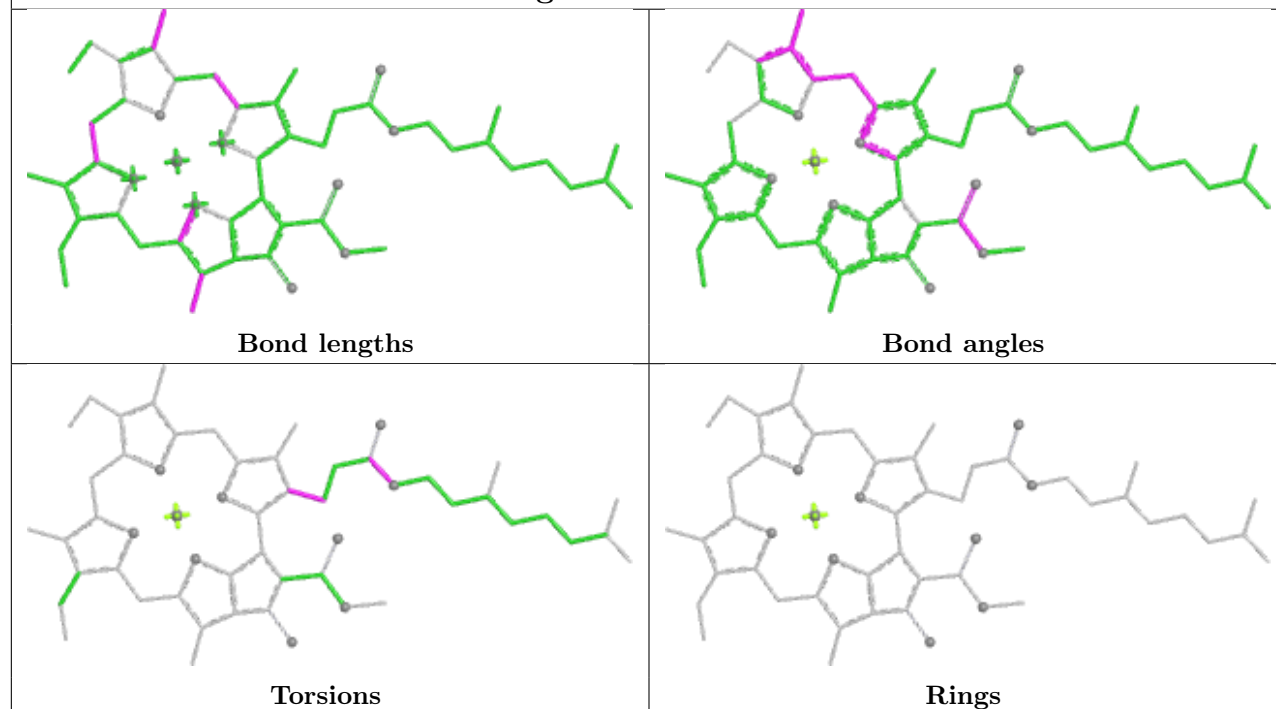
Ligand LMG G 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

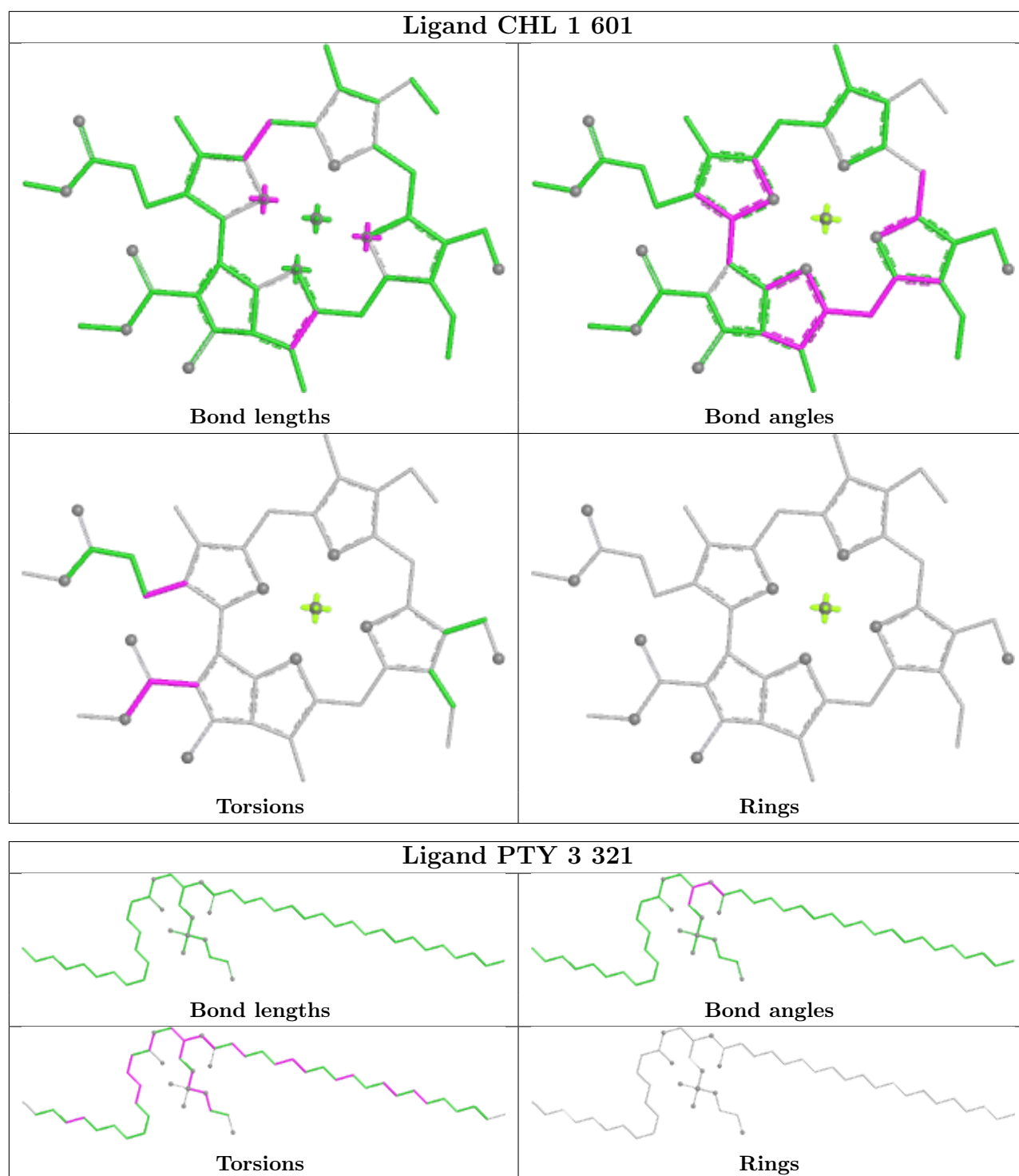
Ligand BCR L 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA 1 607

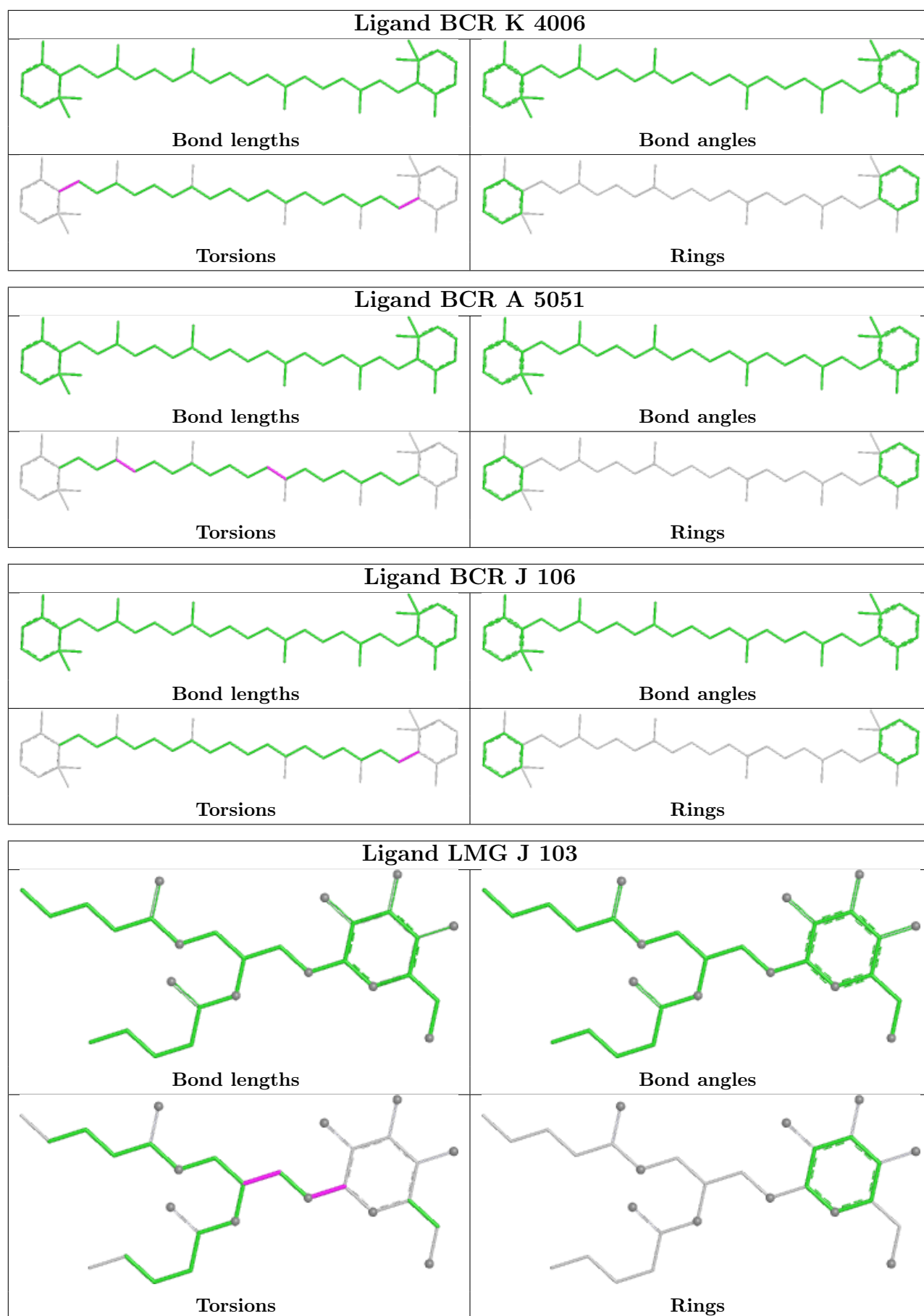


## Ligand CLA 3 325

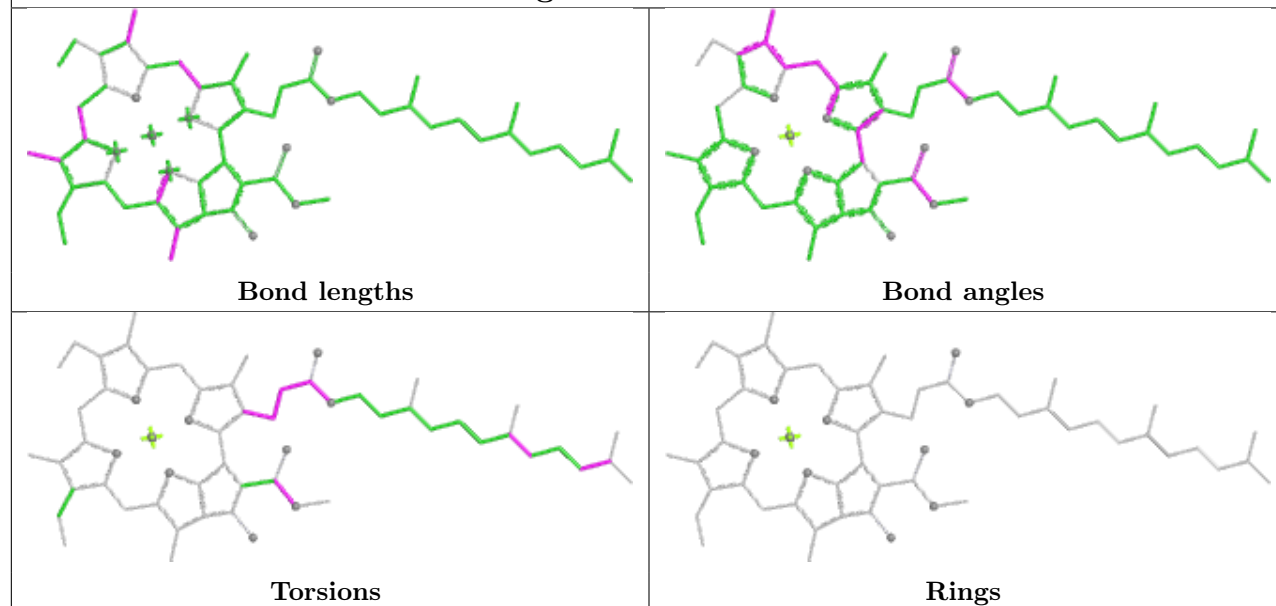




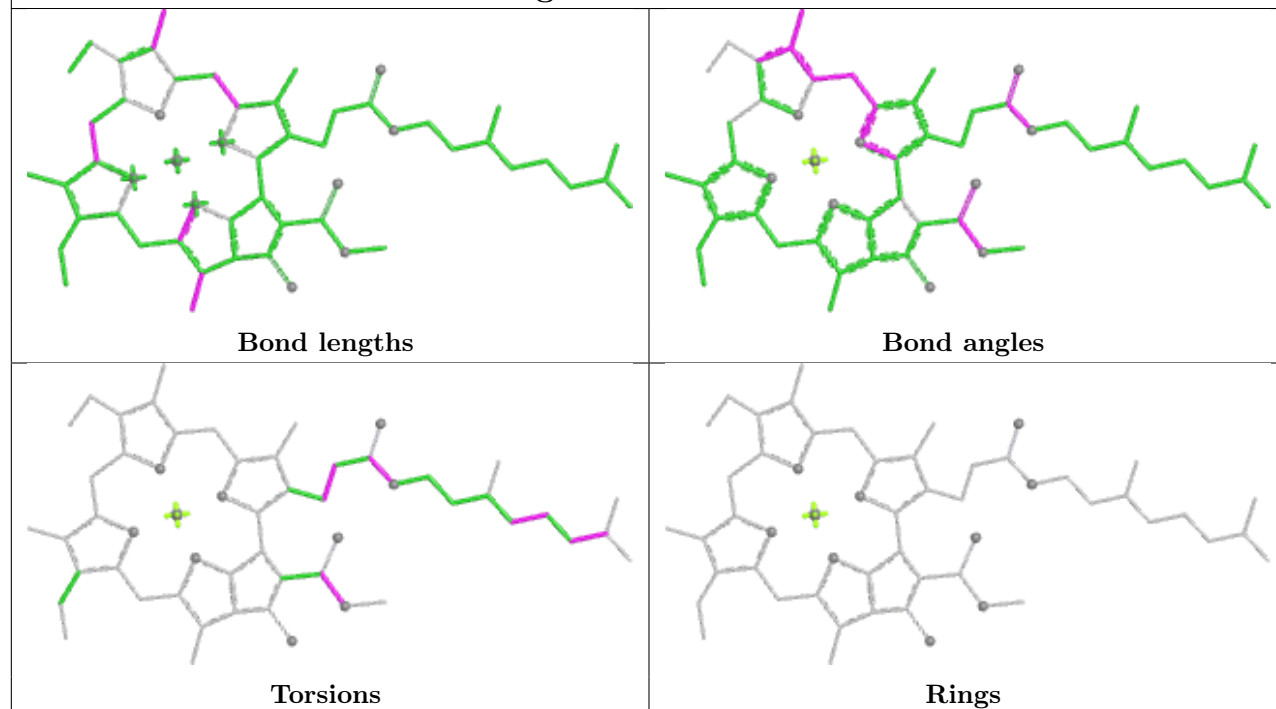


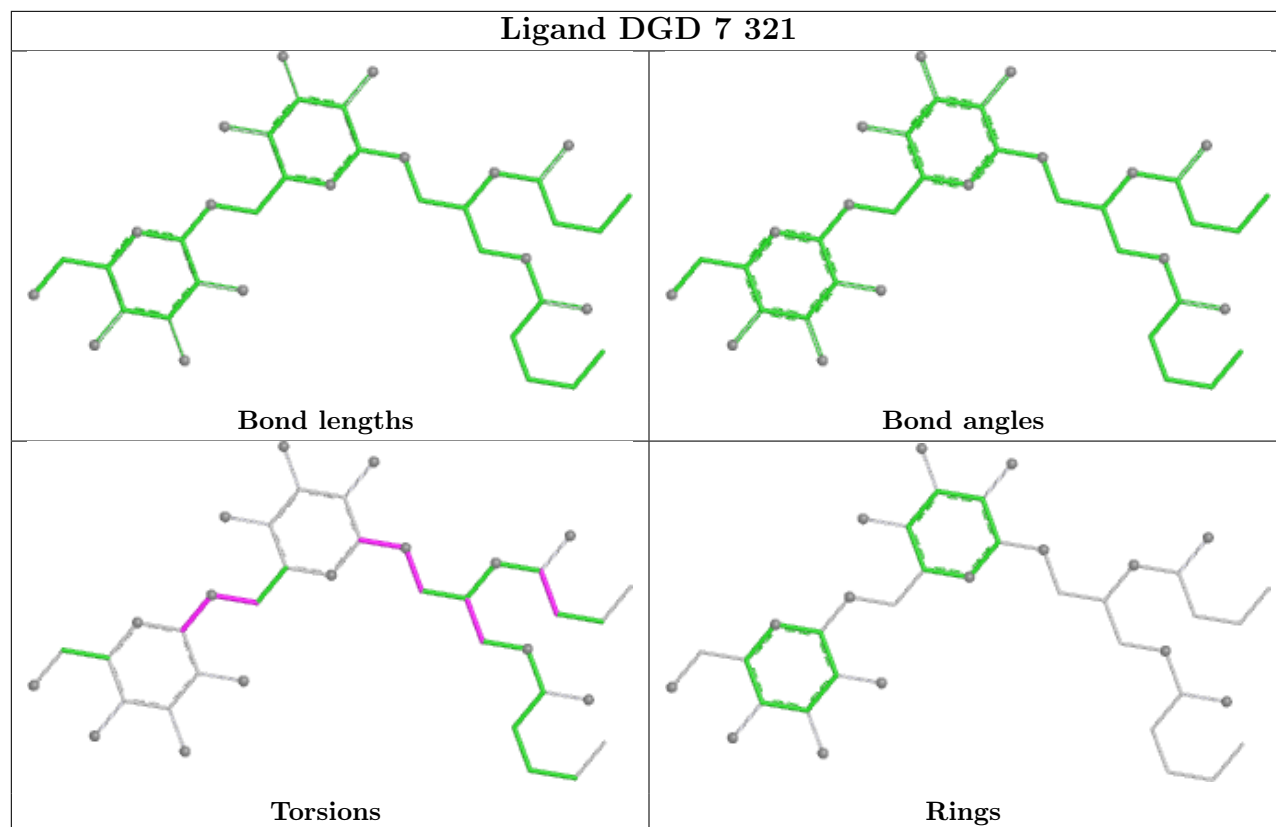


## Ligand CLA 7 303

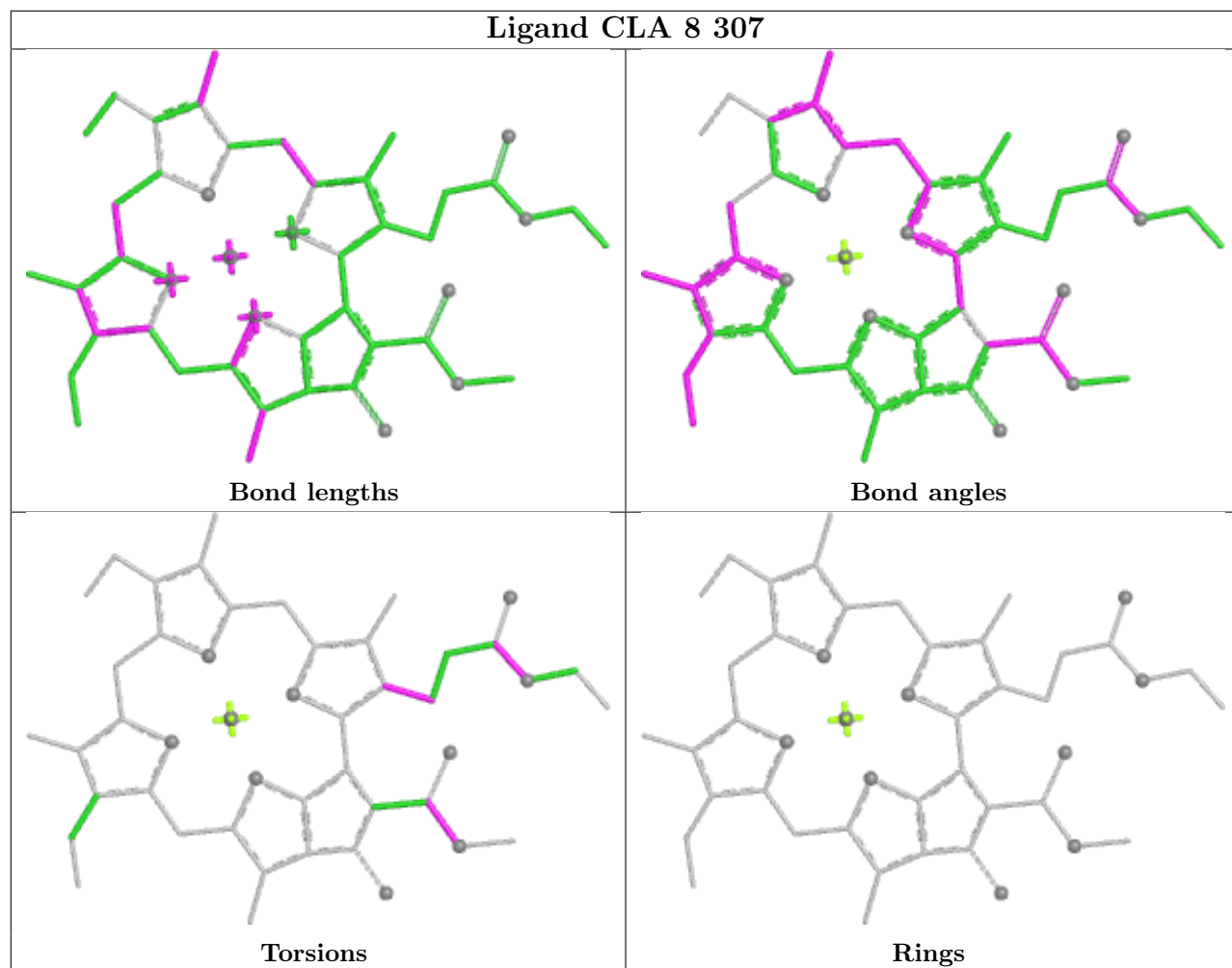


## Ligand CLA 3 311

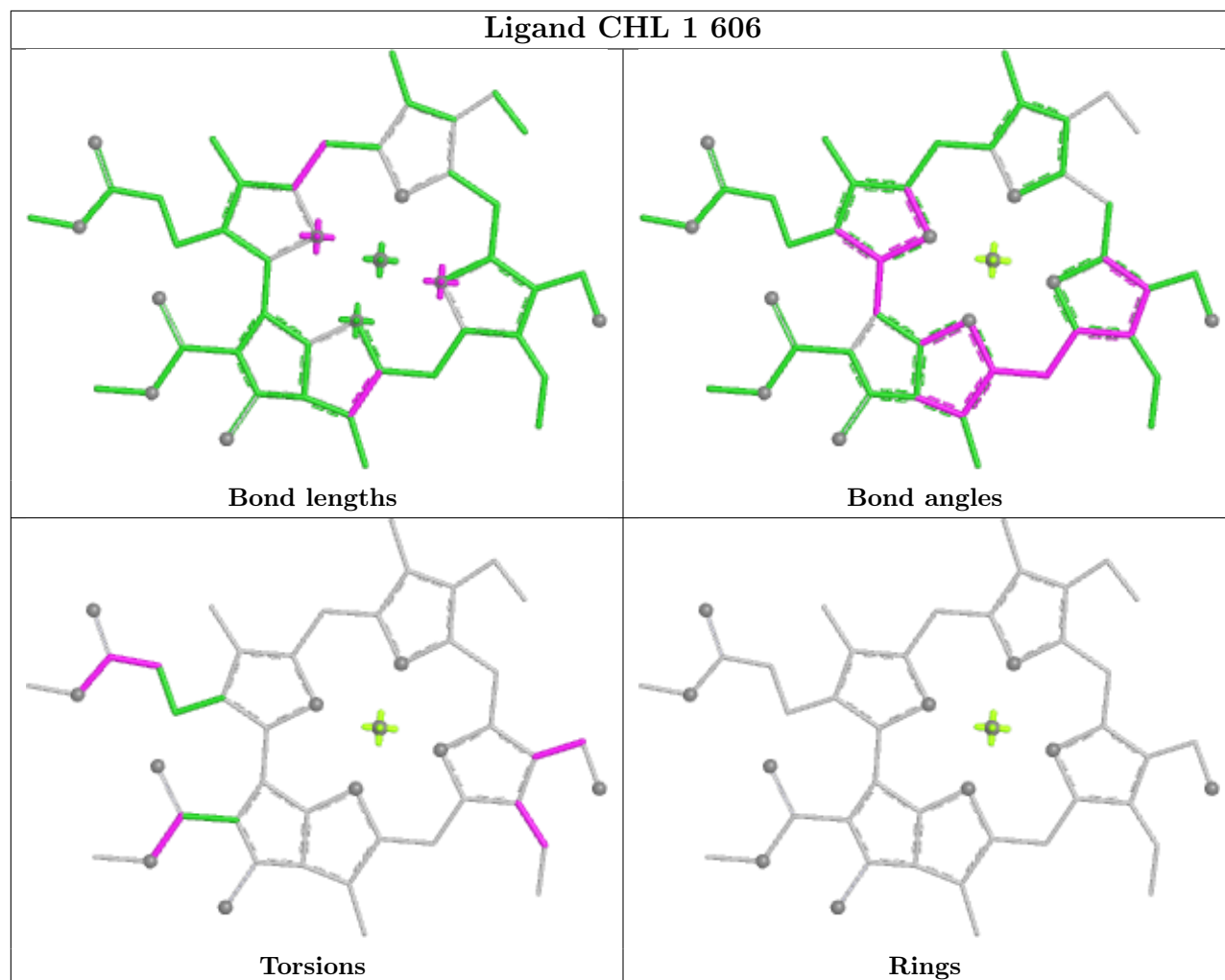




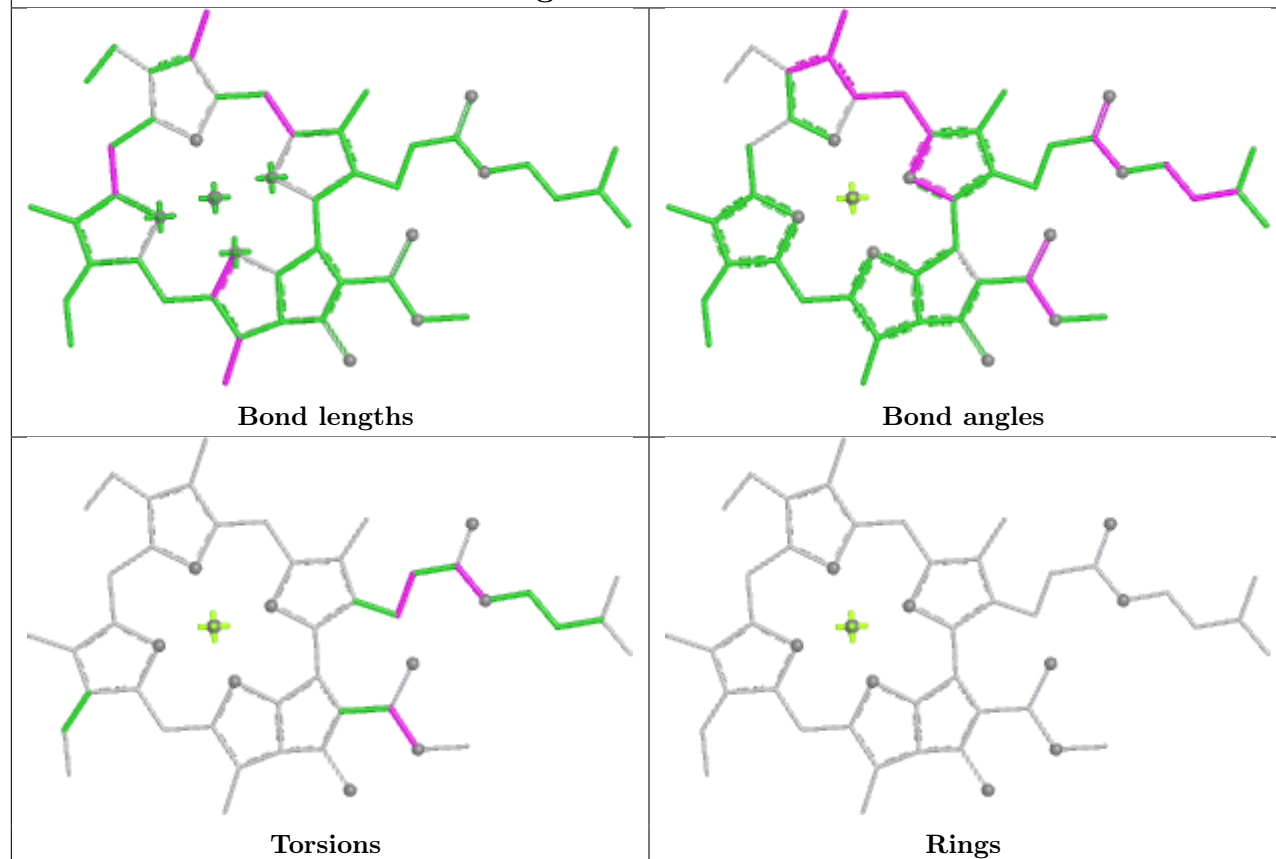
## Ligand CLA 8 307



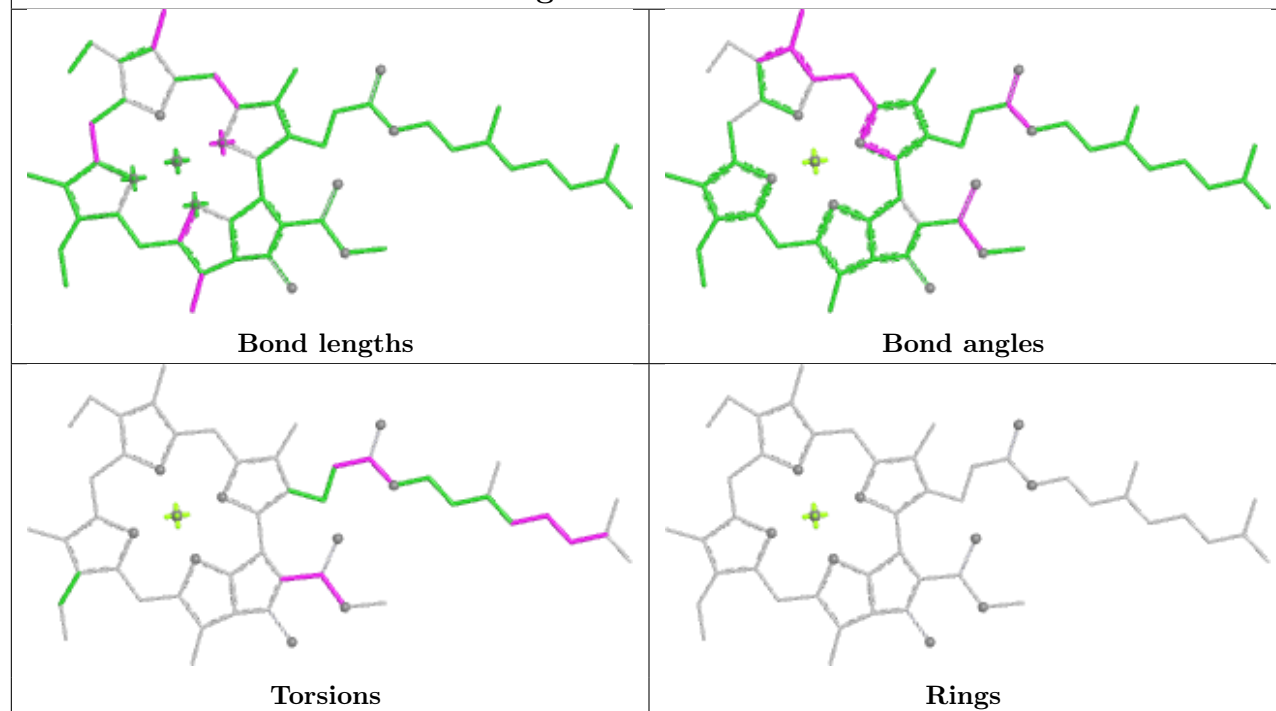
## Ligand CHL 1 606

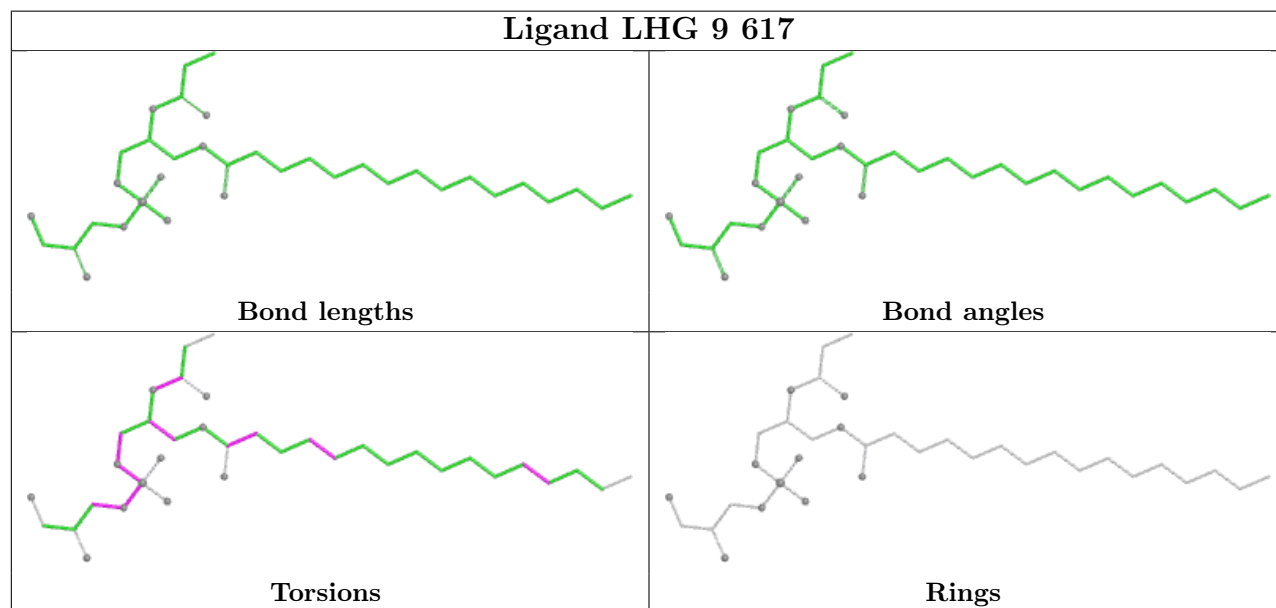
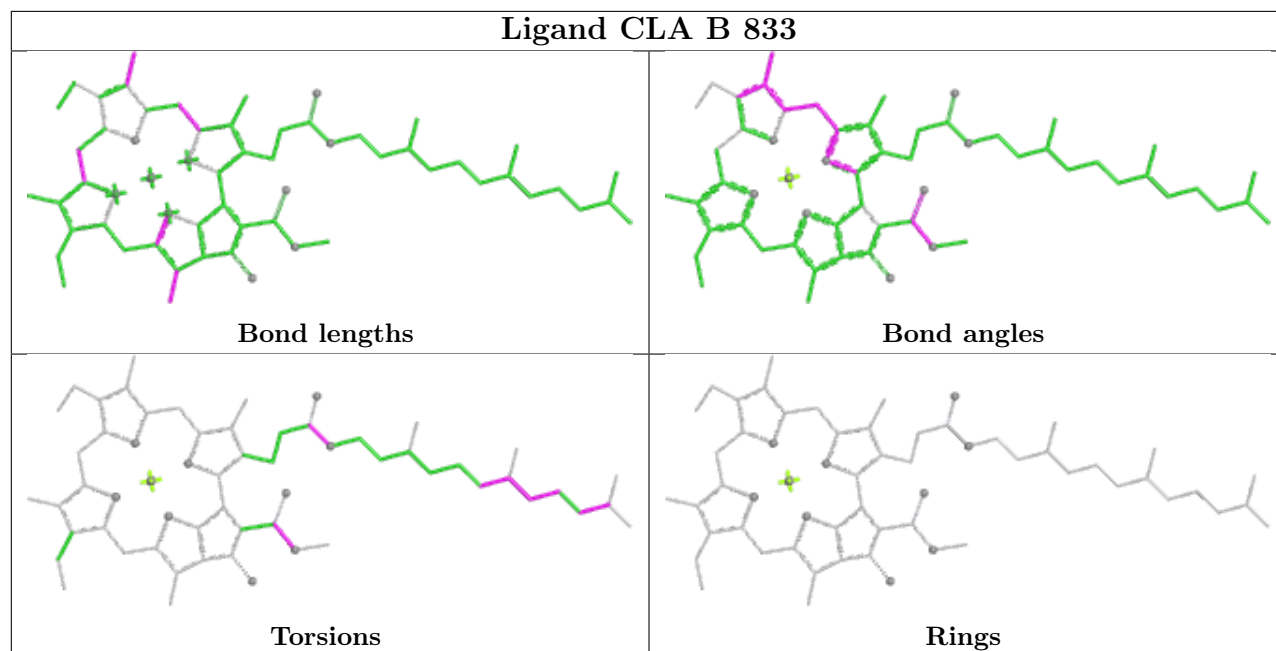


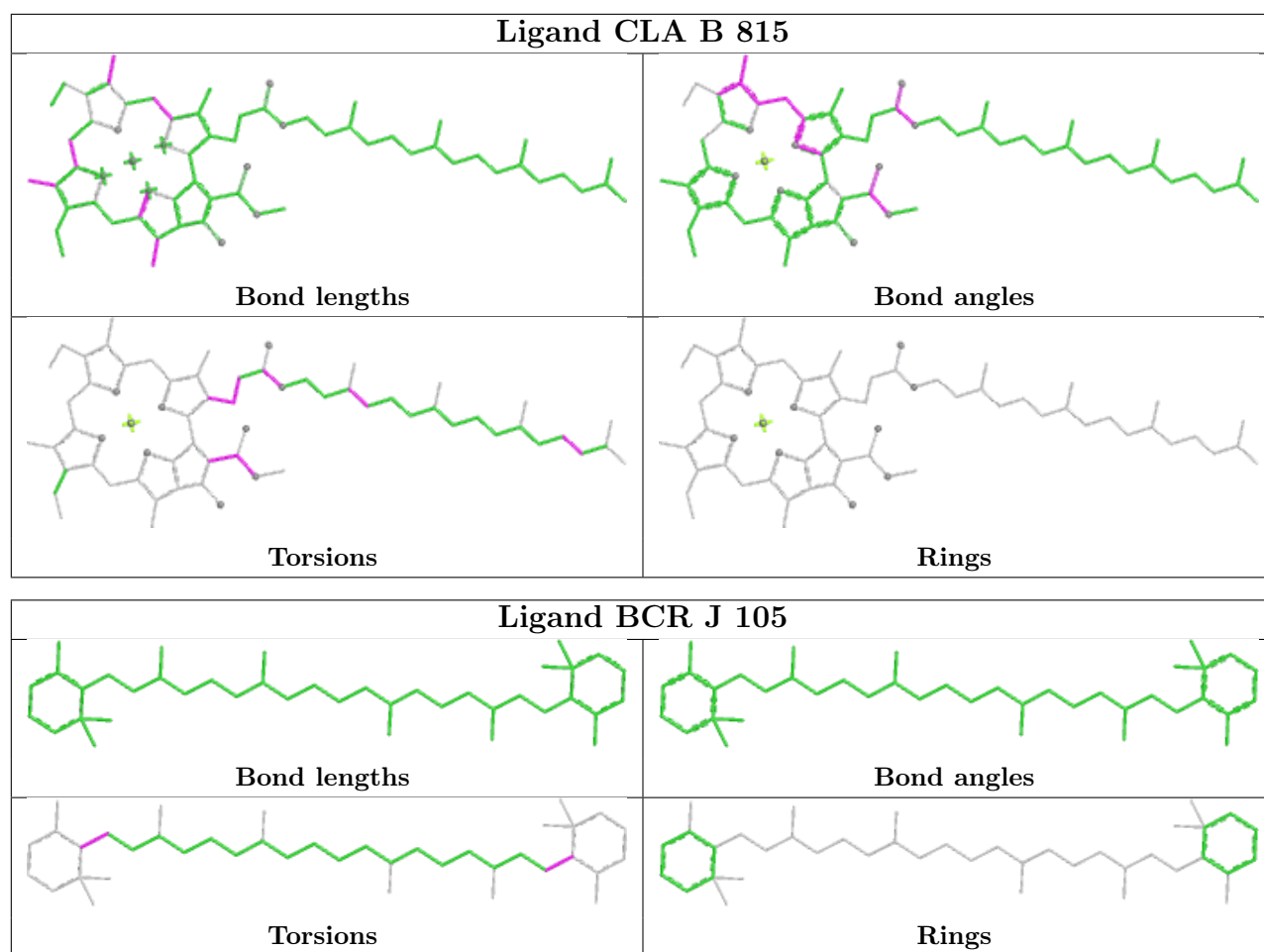
## Ligand CLA 2 313



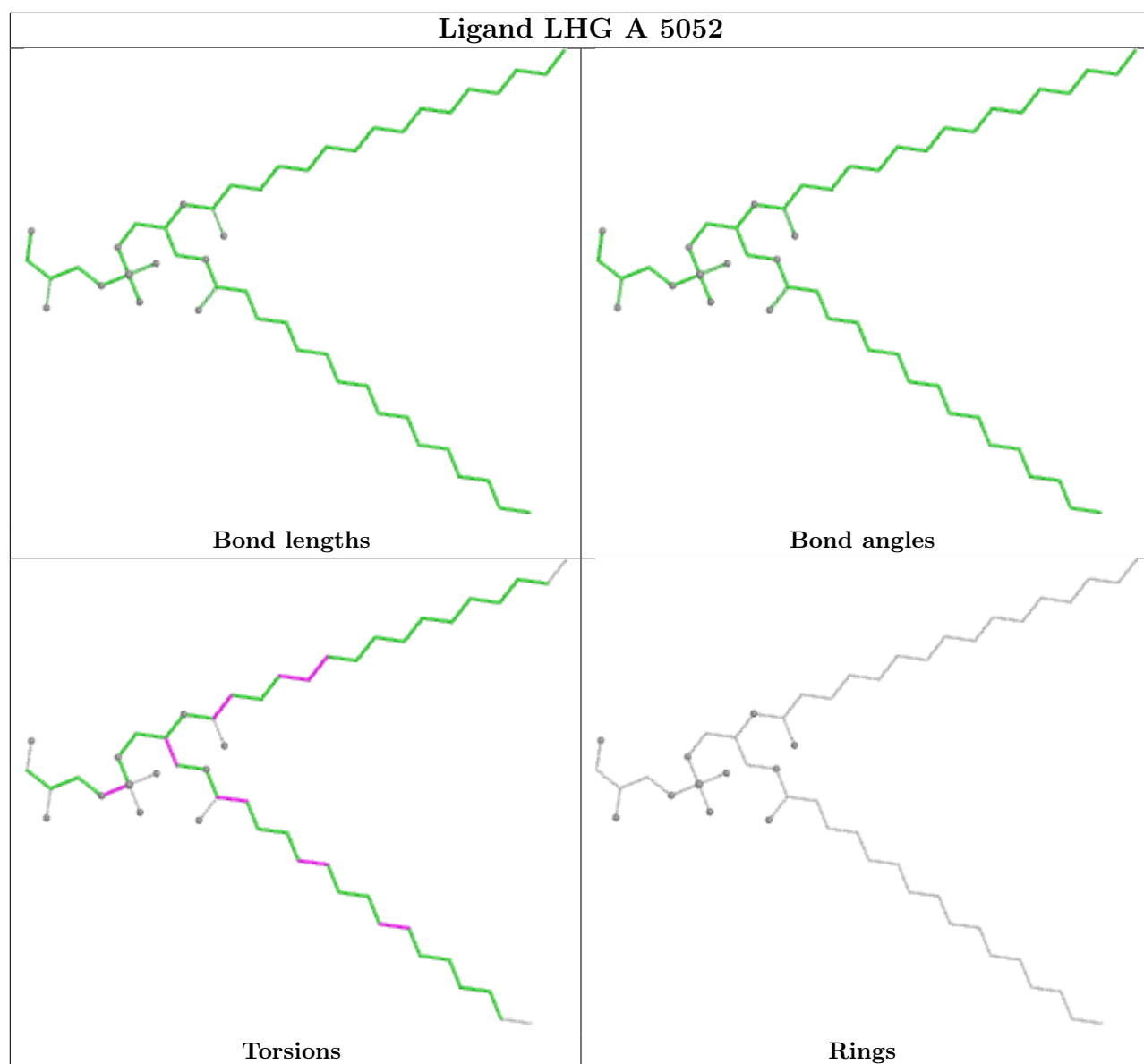
## Ligand CLA 1 603



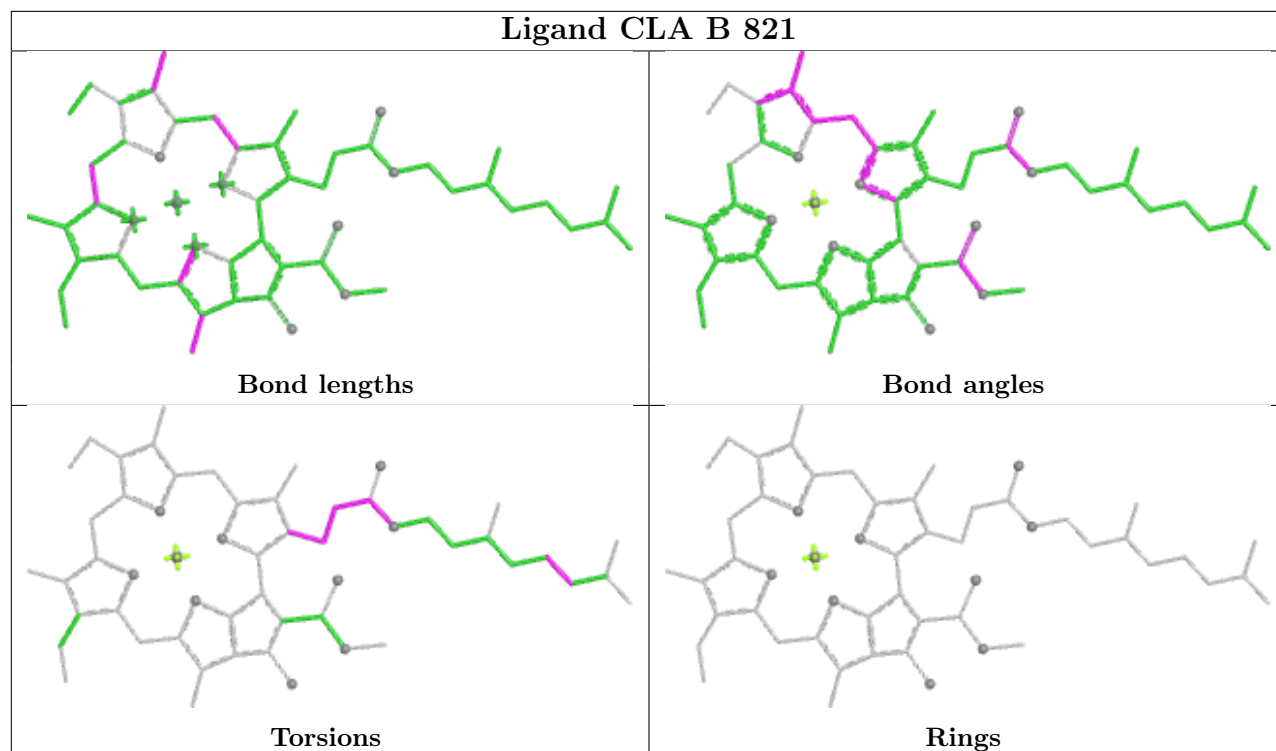




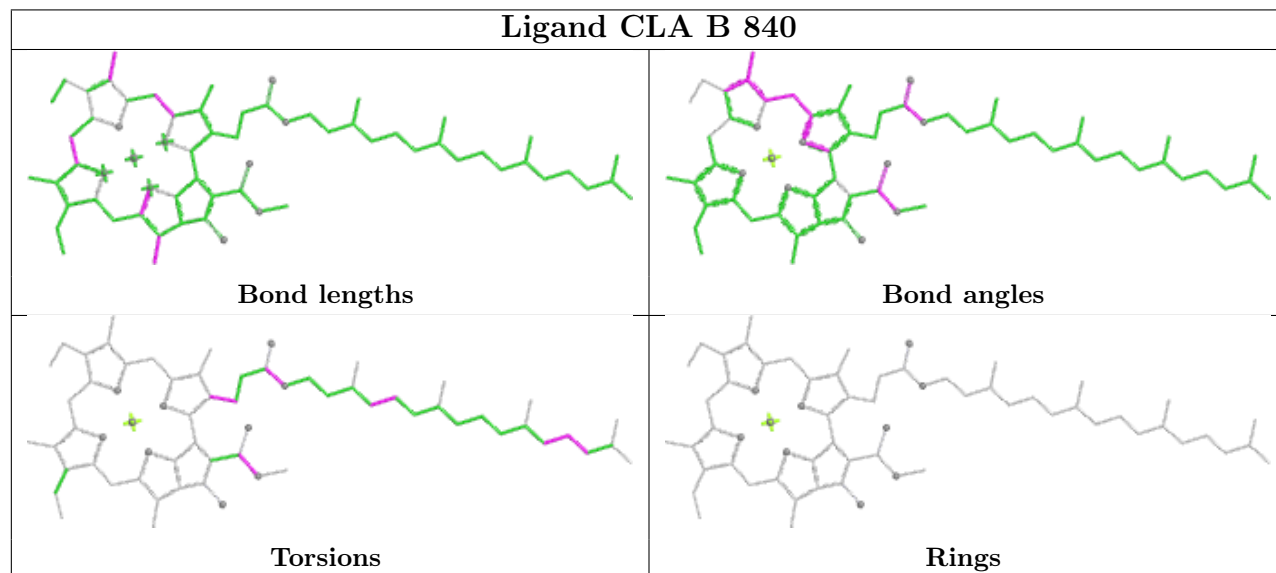




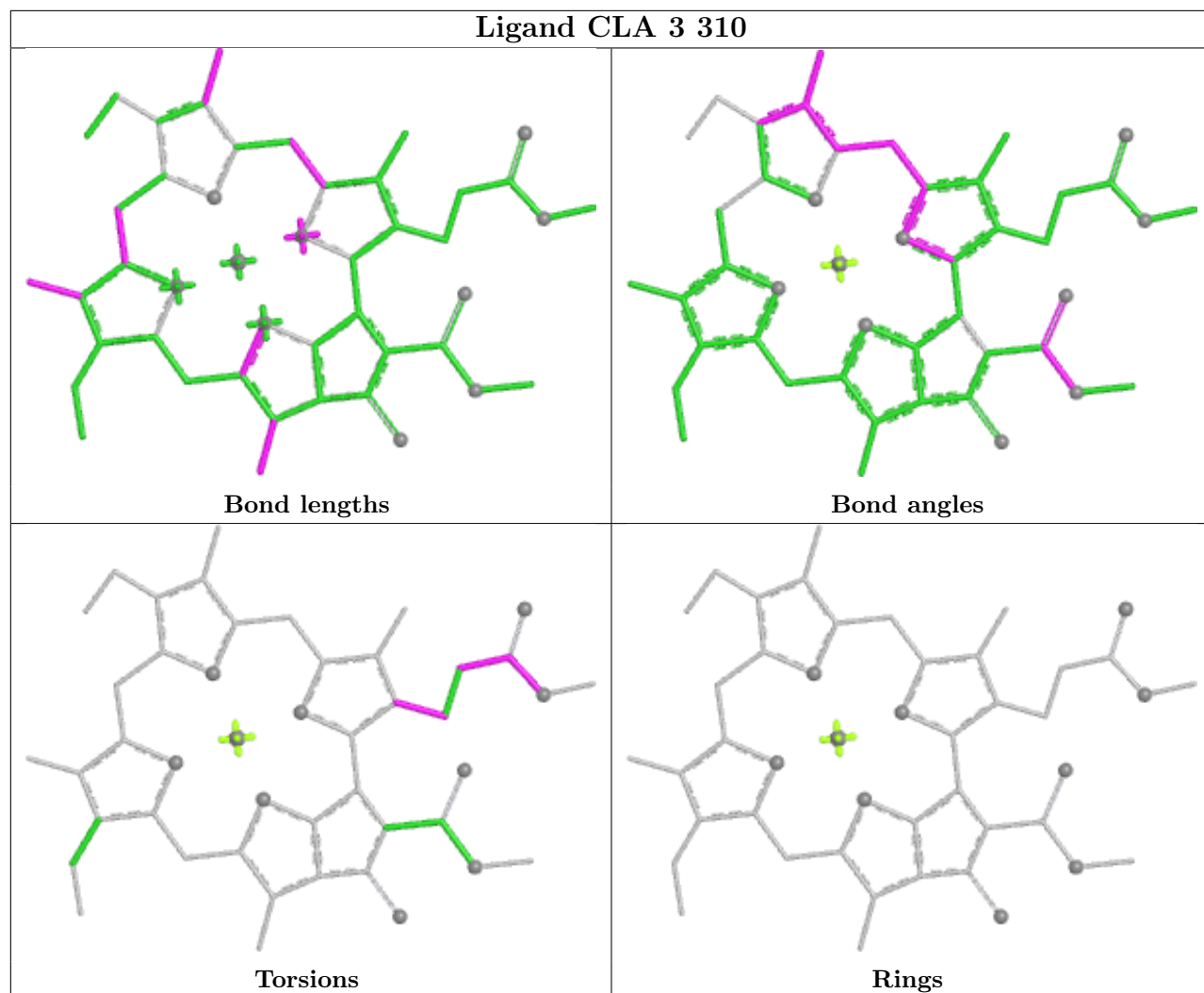
## Ligand CLA B 821



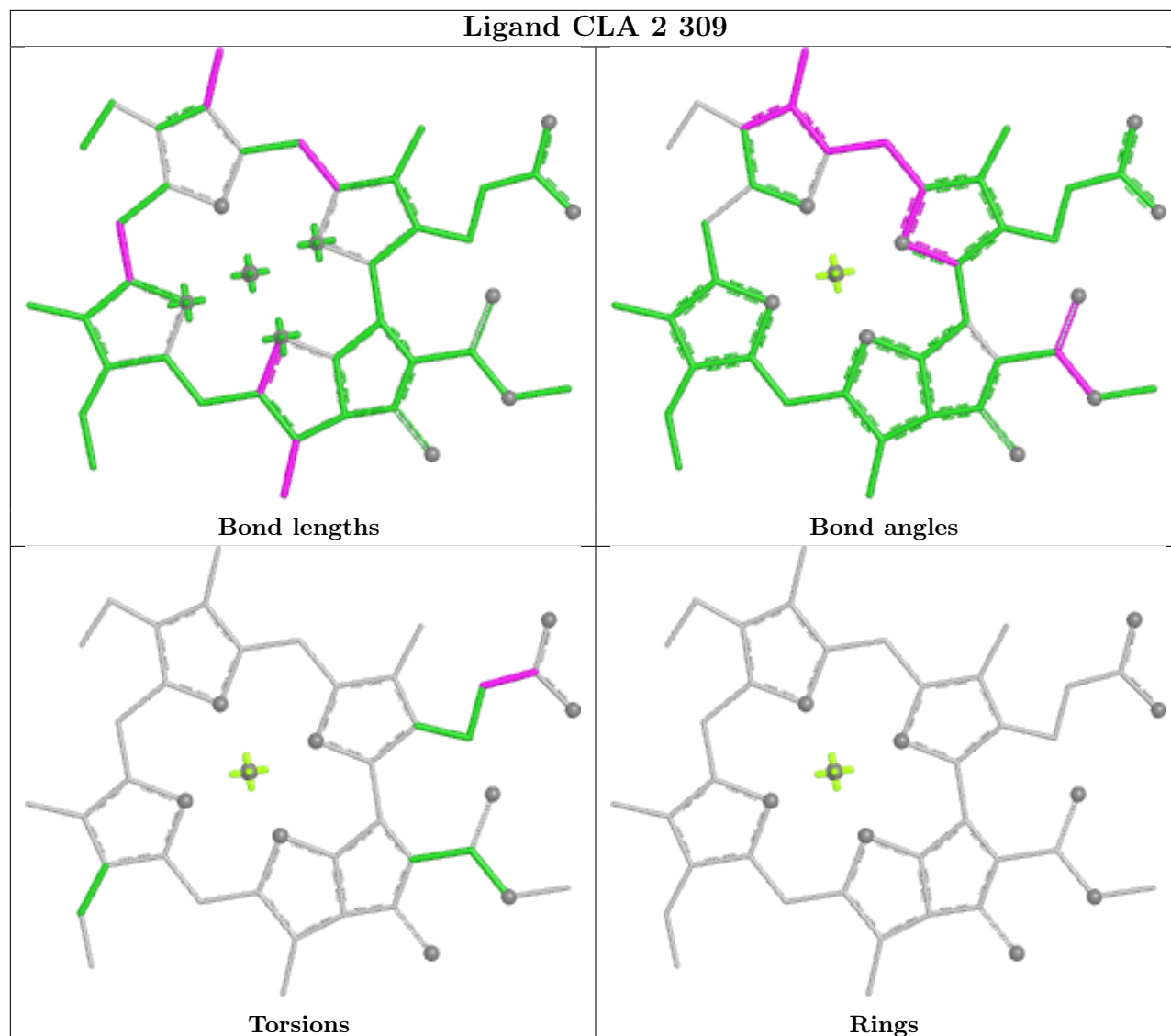
## Ligand CLA B 840



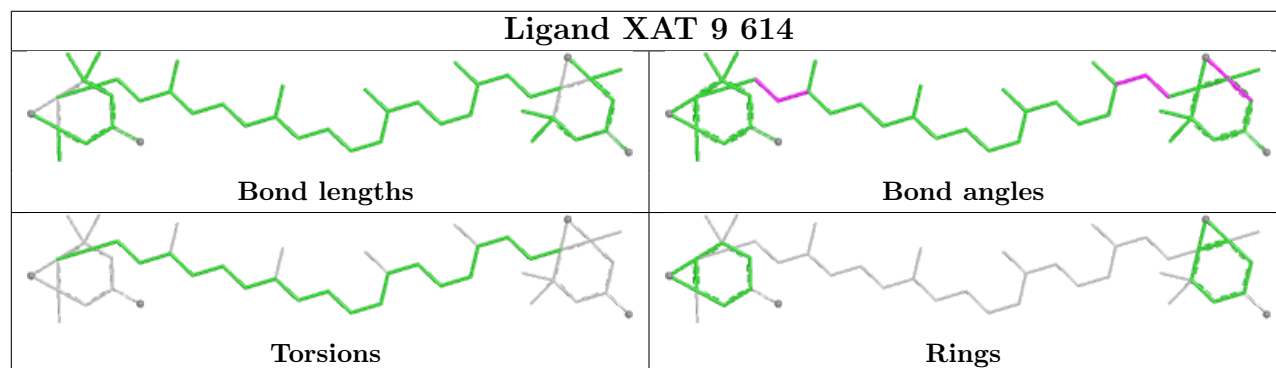
## Ligand CLA 3 310



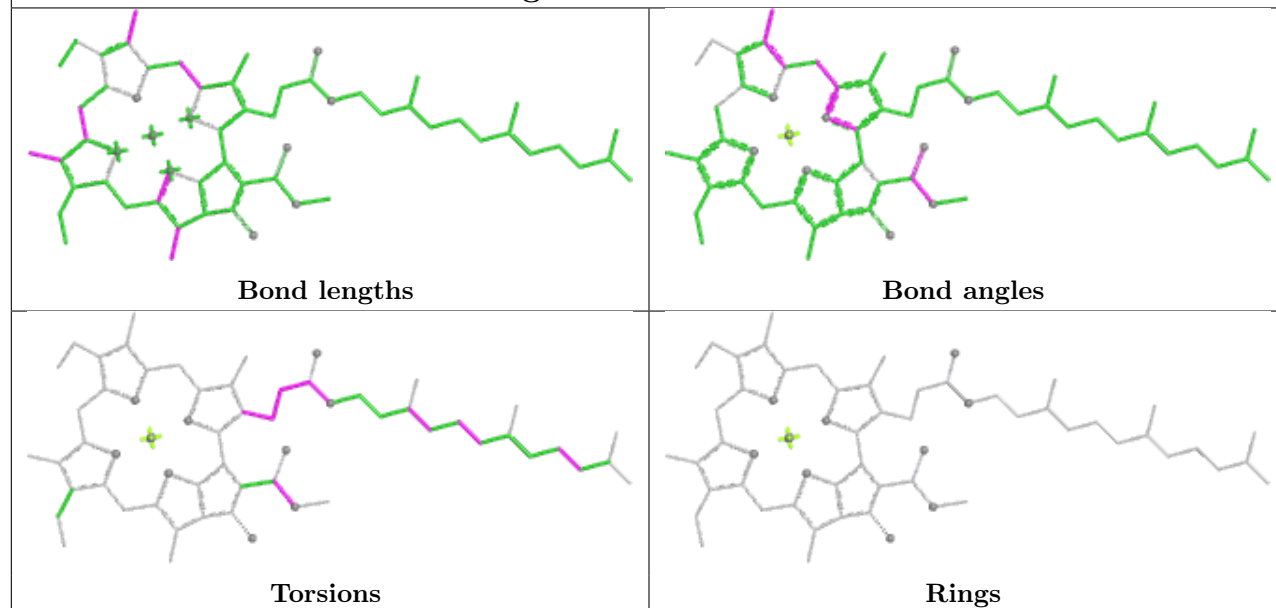
## Ligand CLA 2 309



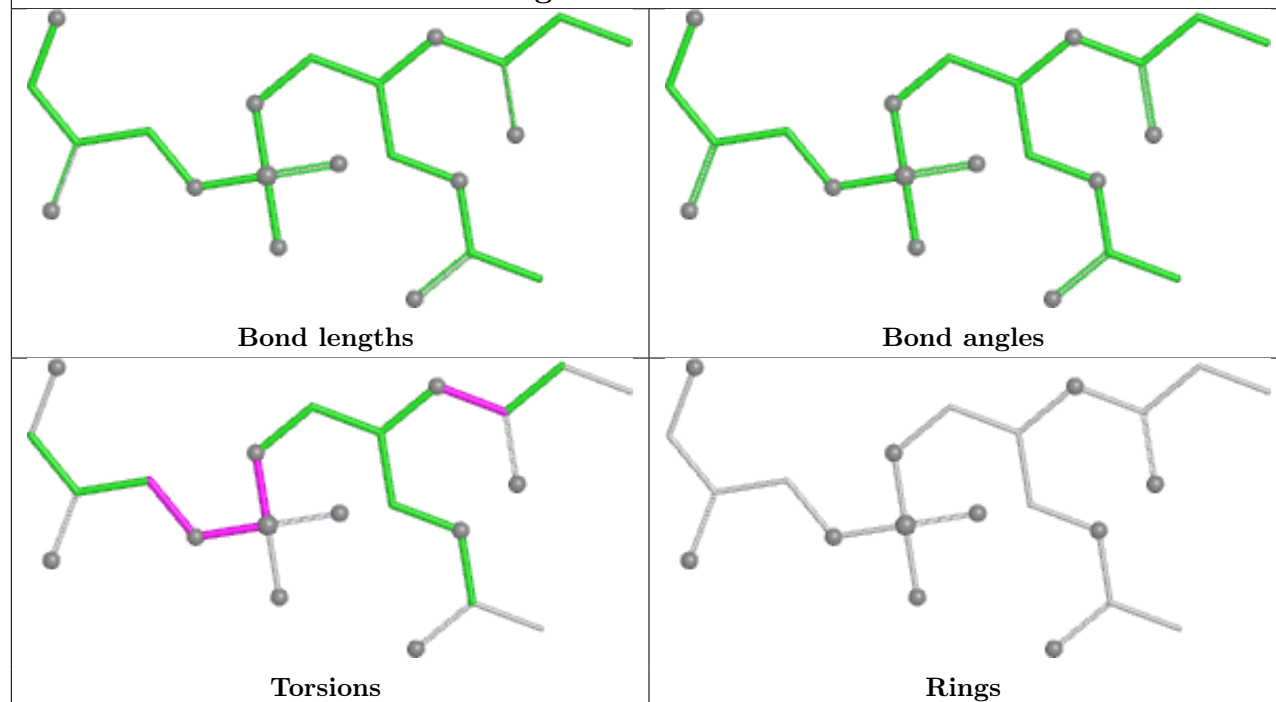
## Ligand XAT 9 614

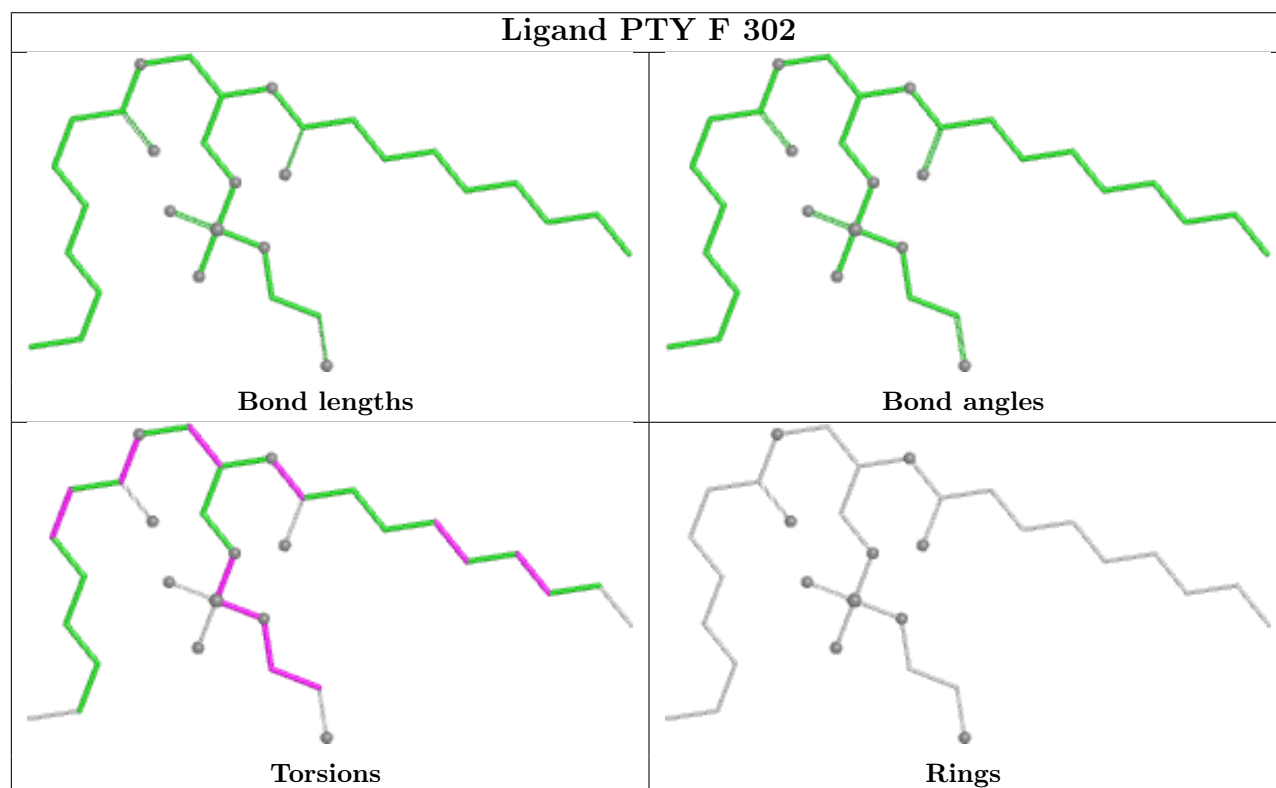
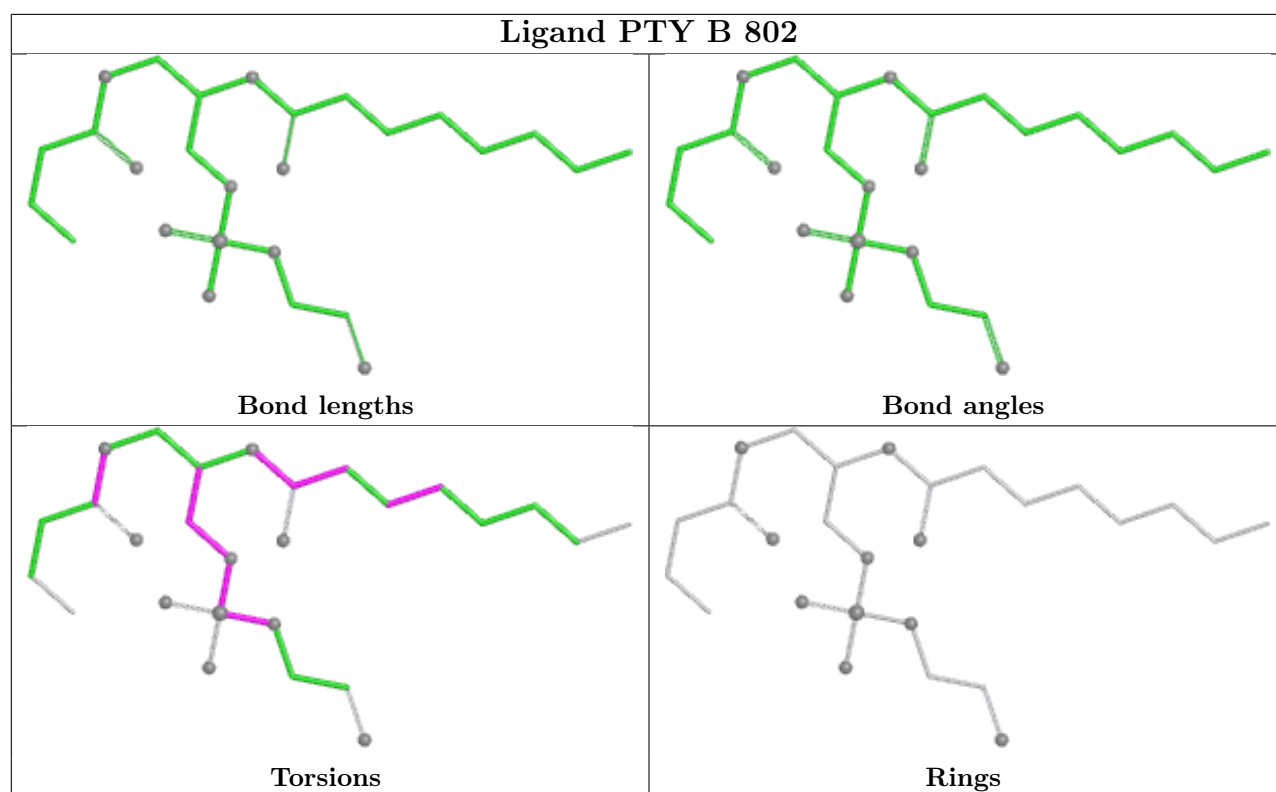


## Ligand CLA A 5025

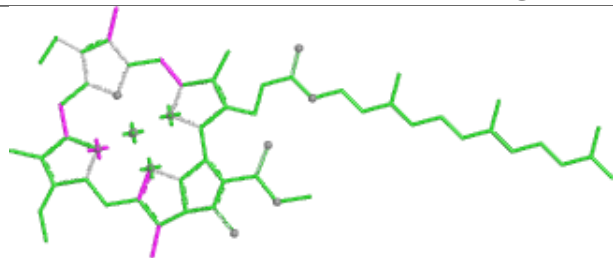


## Ligand LHG 7 319

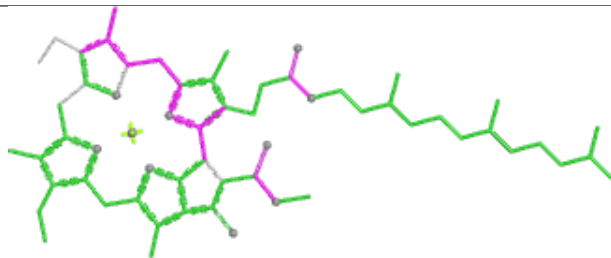




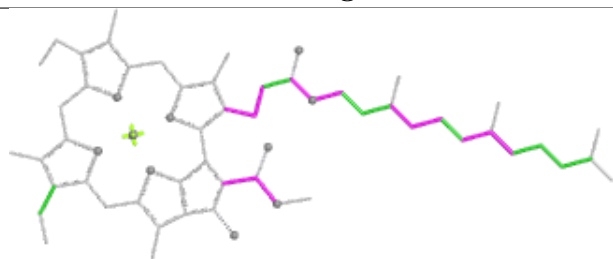
## Ligand CLA H 201



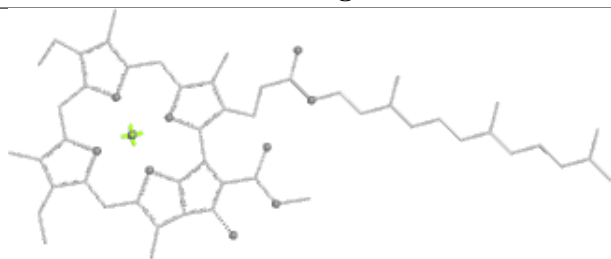
Bond lengths



Bond angles

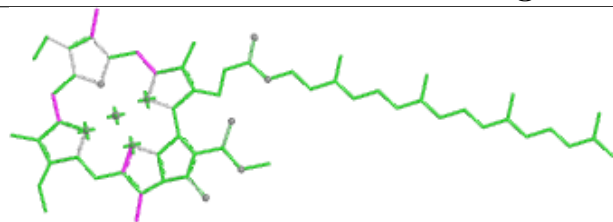


Torsions

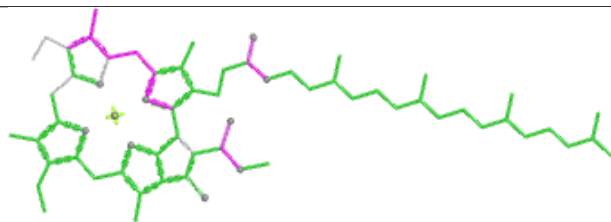


Rings

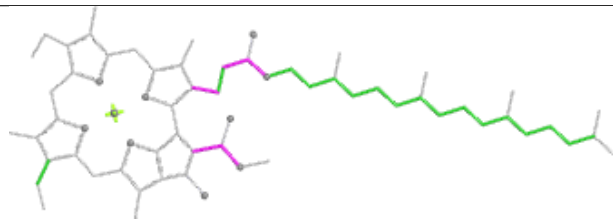
## Ligand CLA L 204



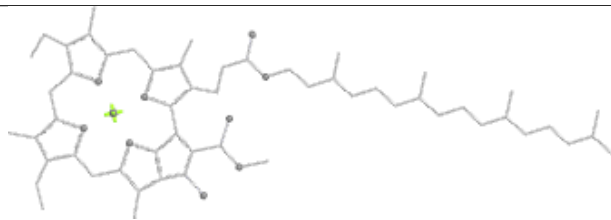
Bond lengths



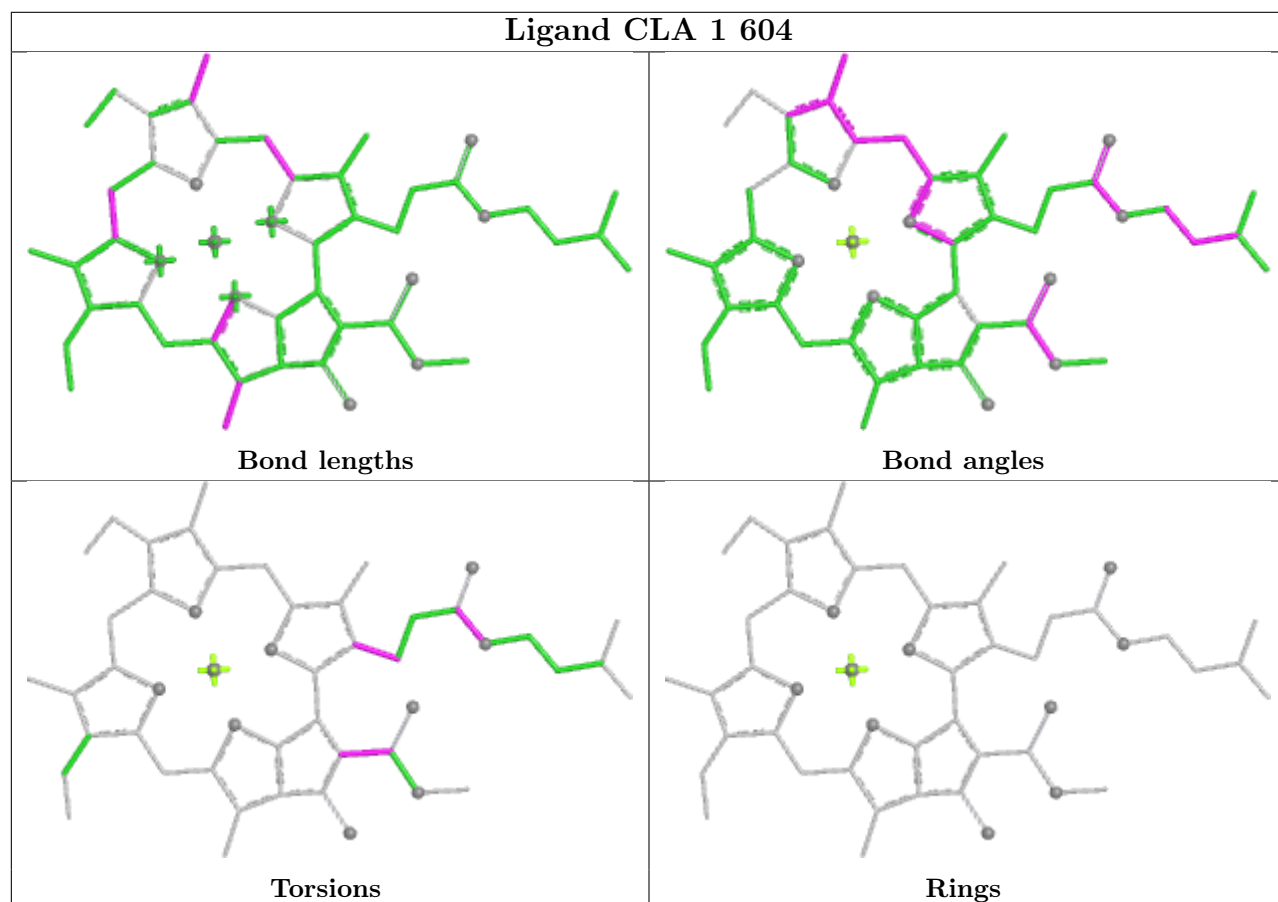
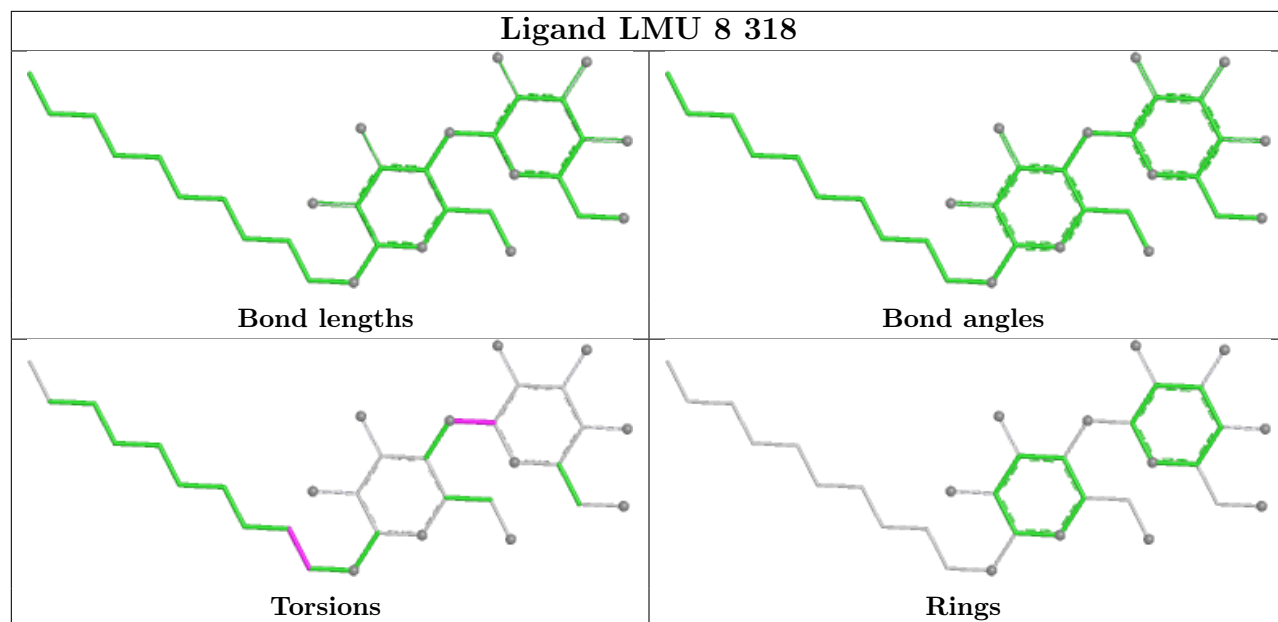
Bond angles



Torsions

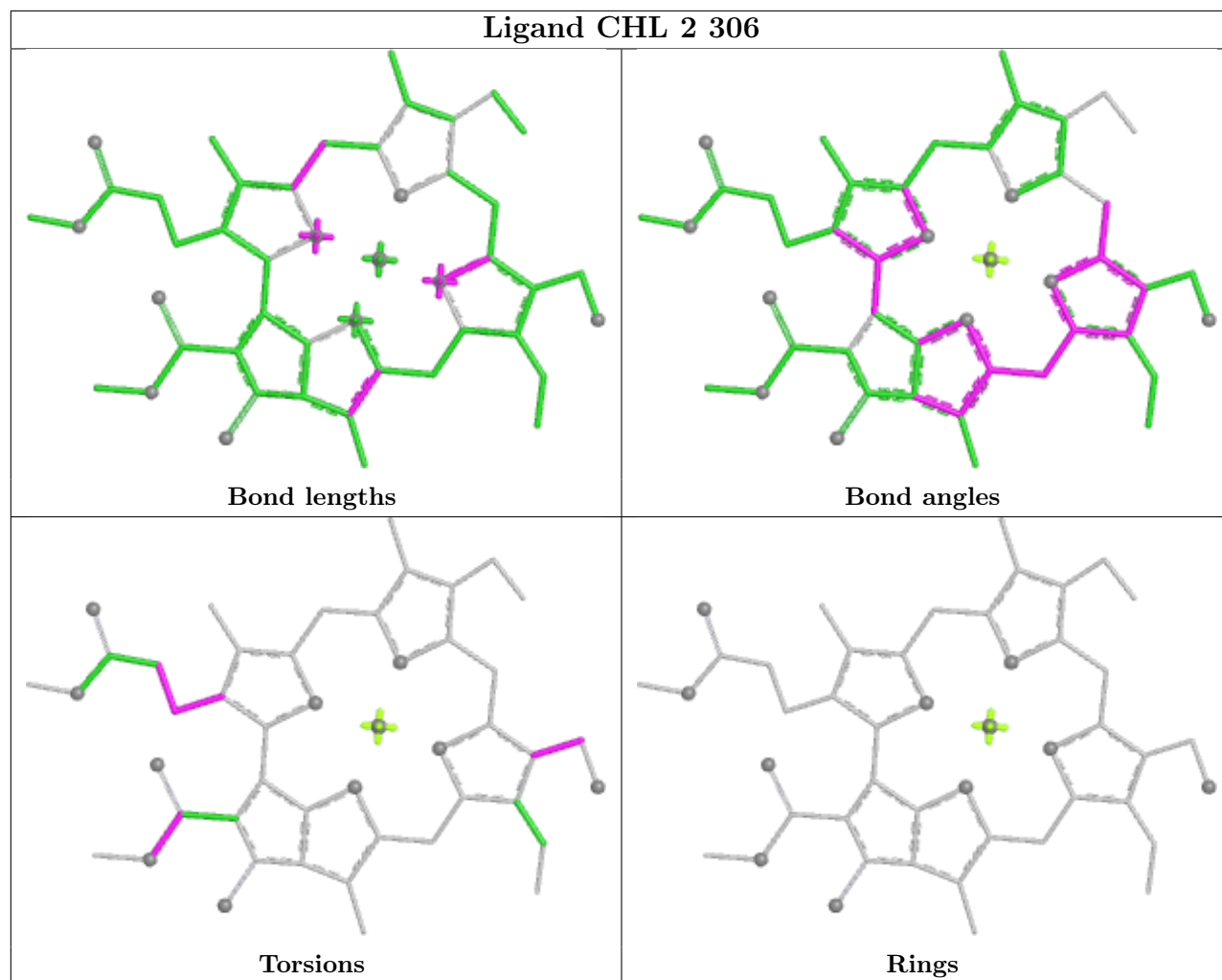


Rings

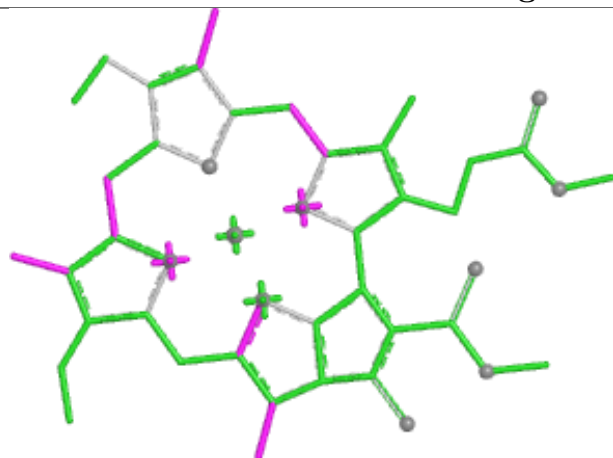




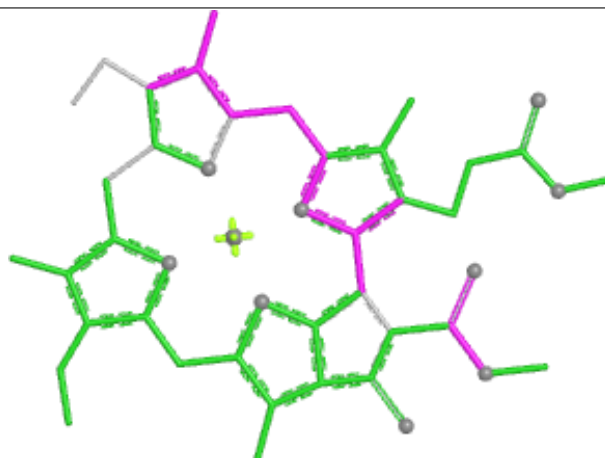
## Ligand CHL 2 306



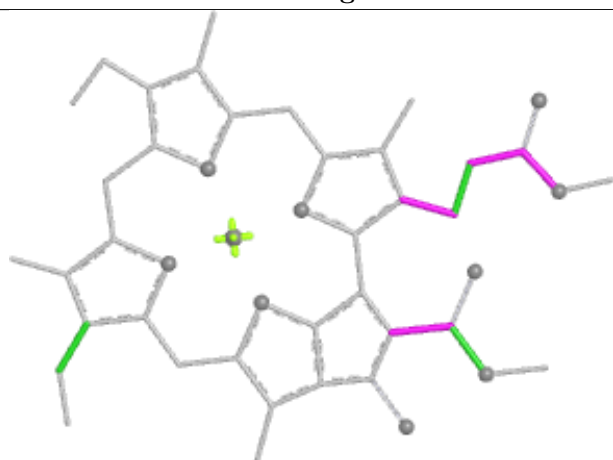
## Ligand CLA 8 310



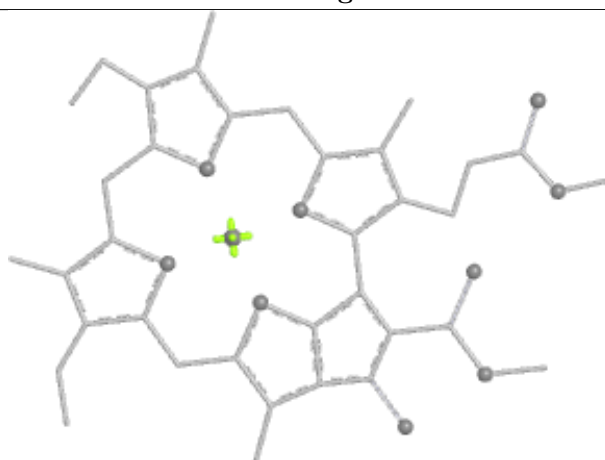
Bond lengths



Bond angles

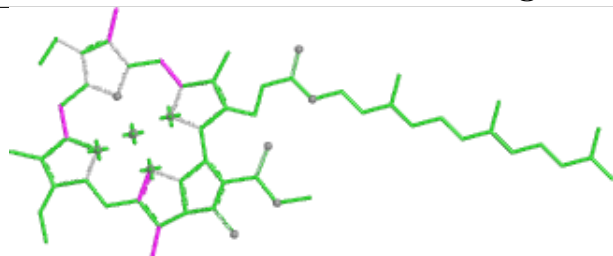


Torsions

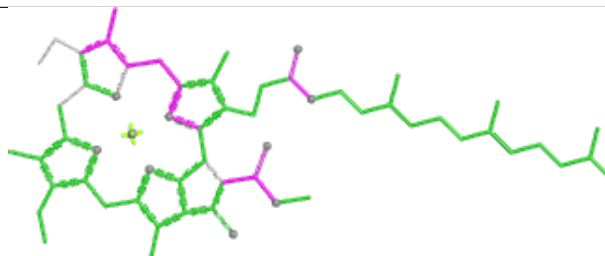


Rings

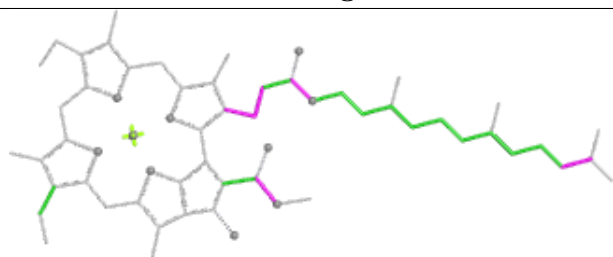
## Ligand CLA 8 301



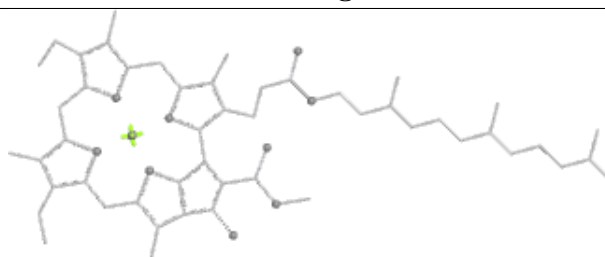
Bond lengths



Bond angles

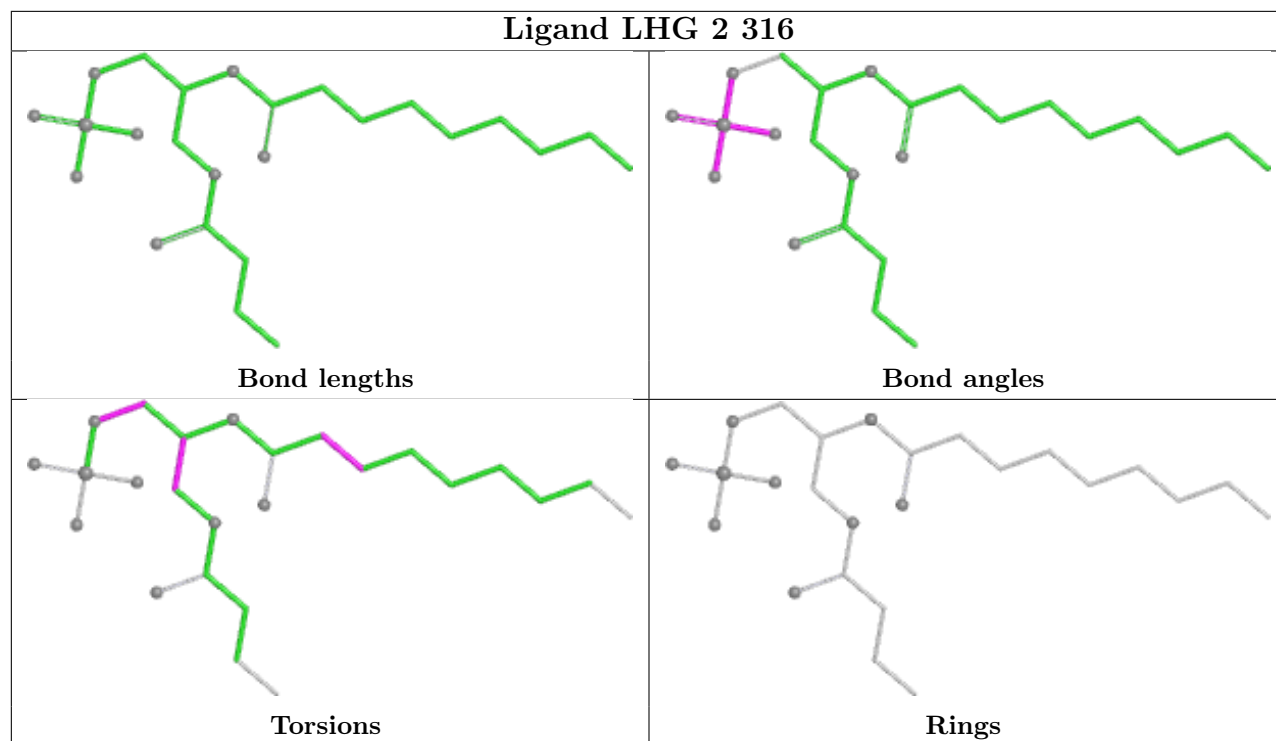


Torsions

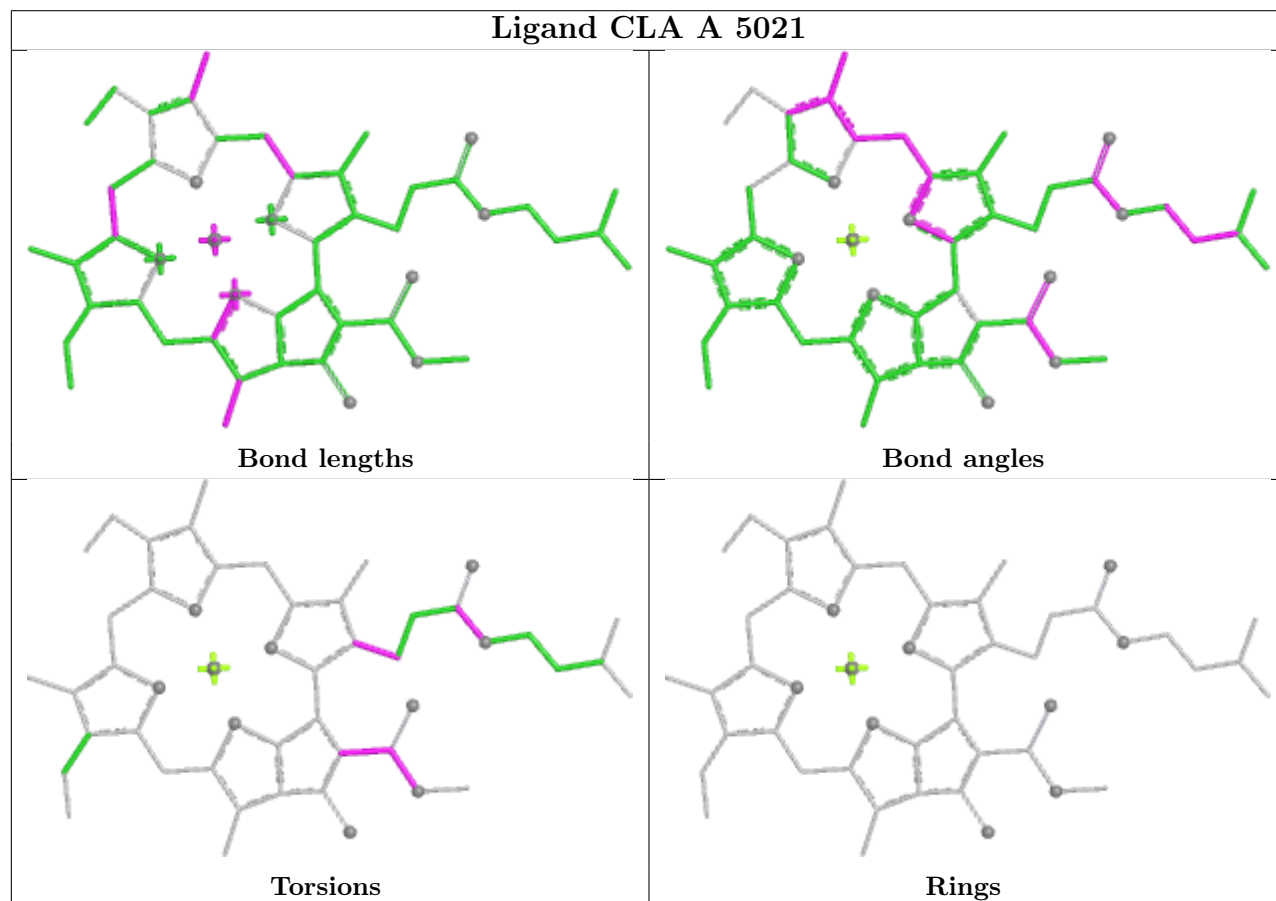


Rings

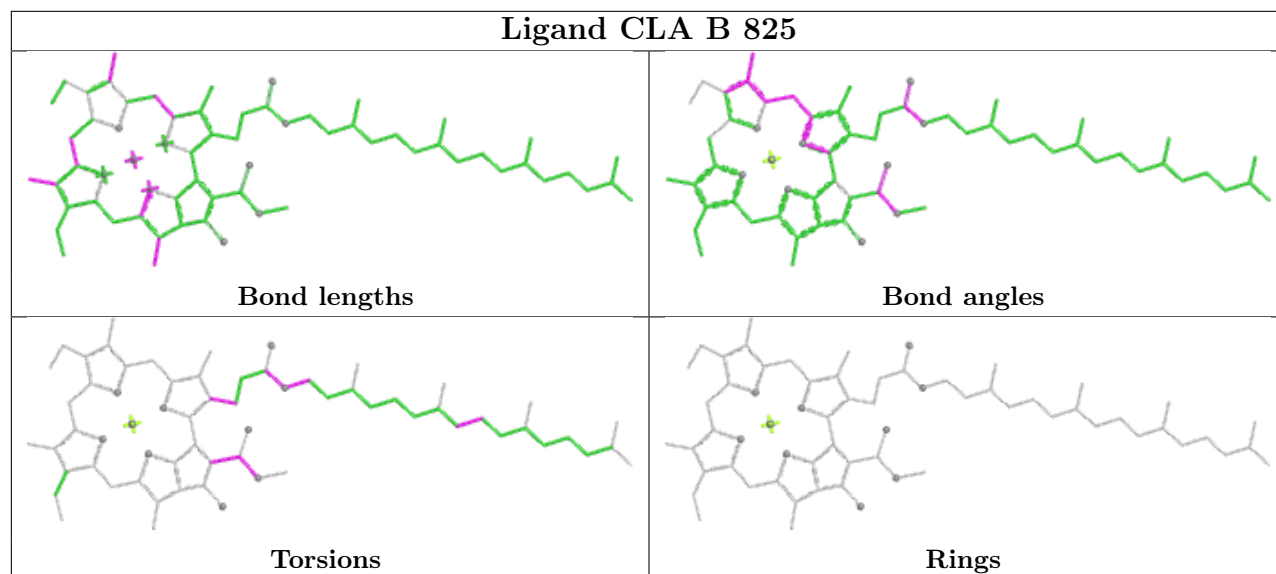
## Ligand LHG 2 316



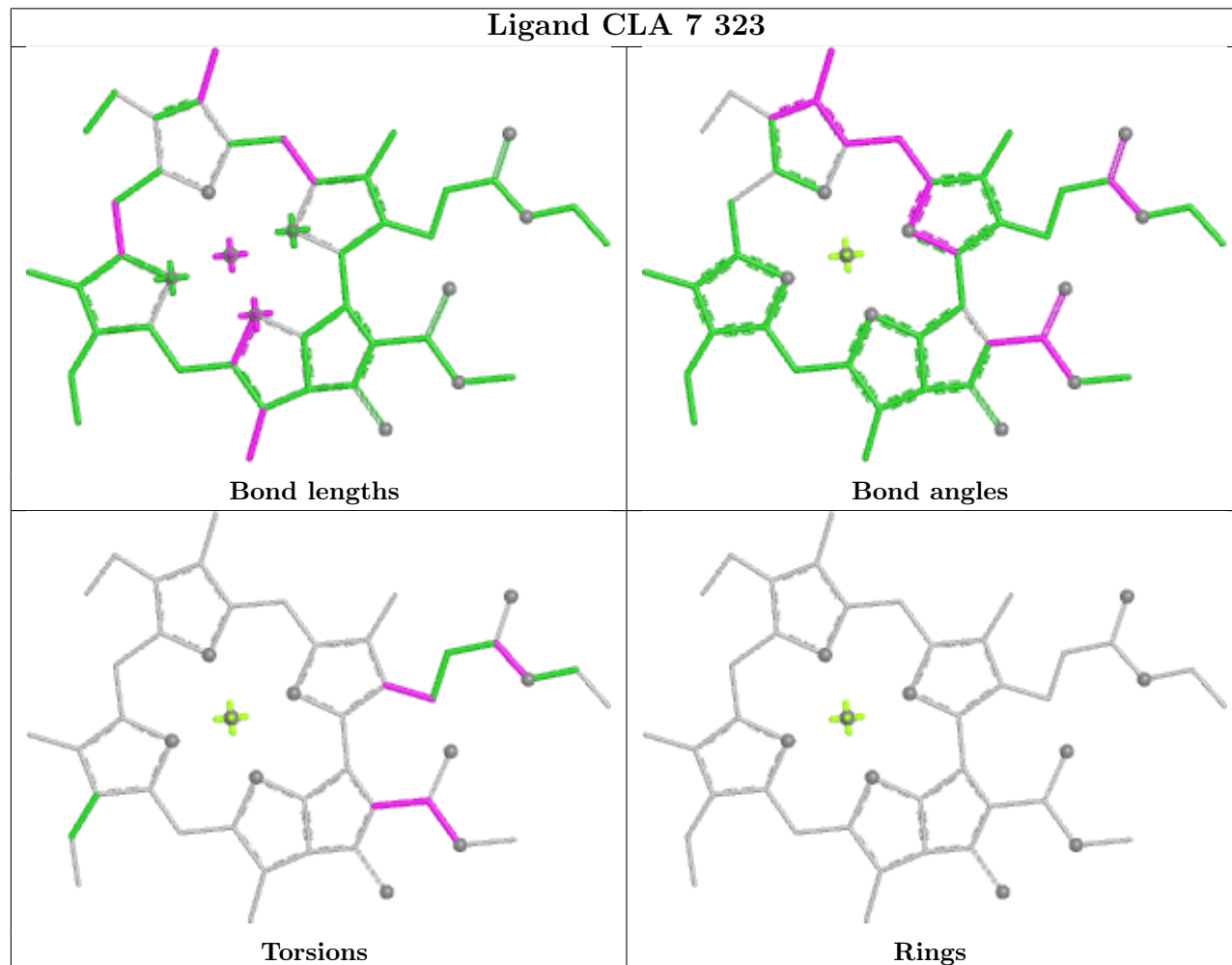
## Ligand CLA A 5021

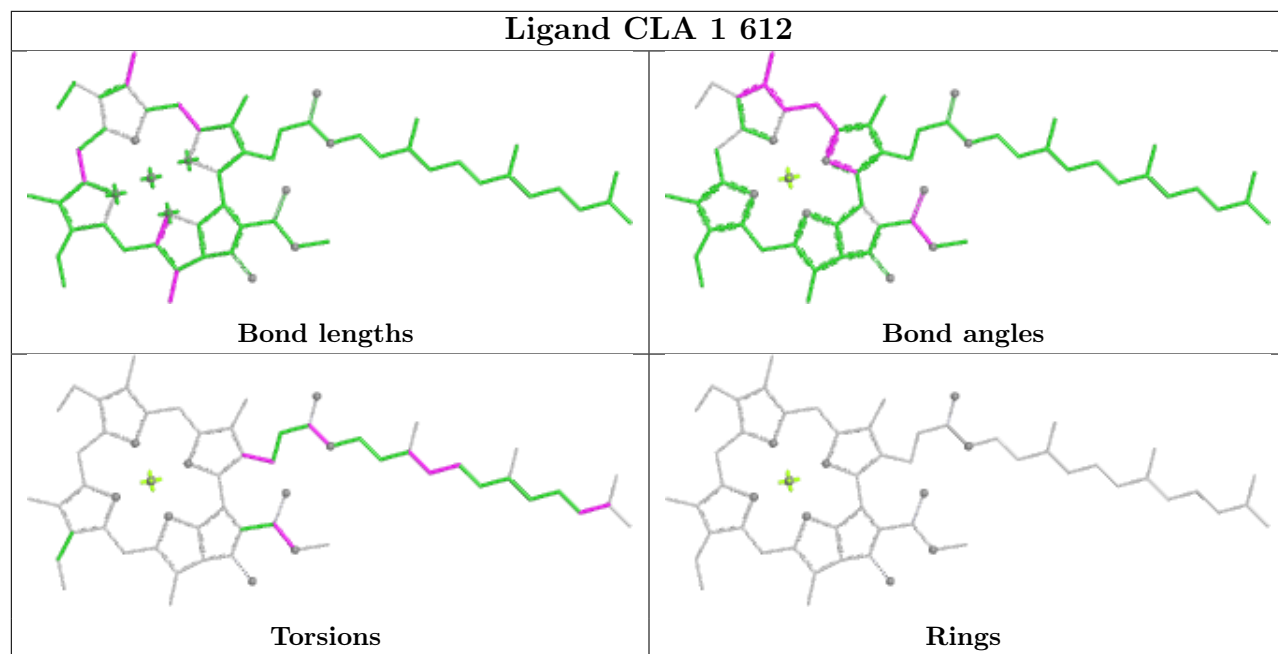
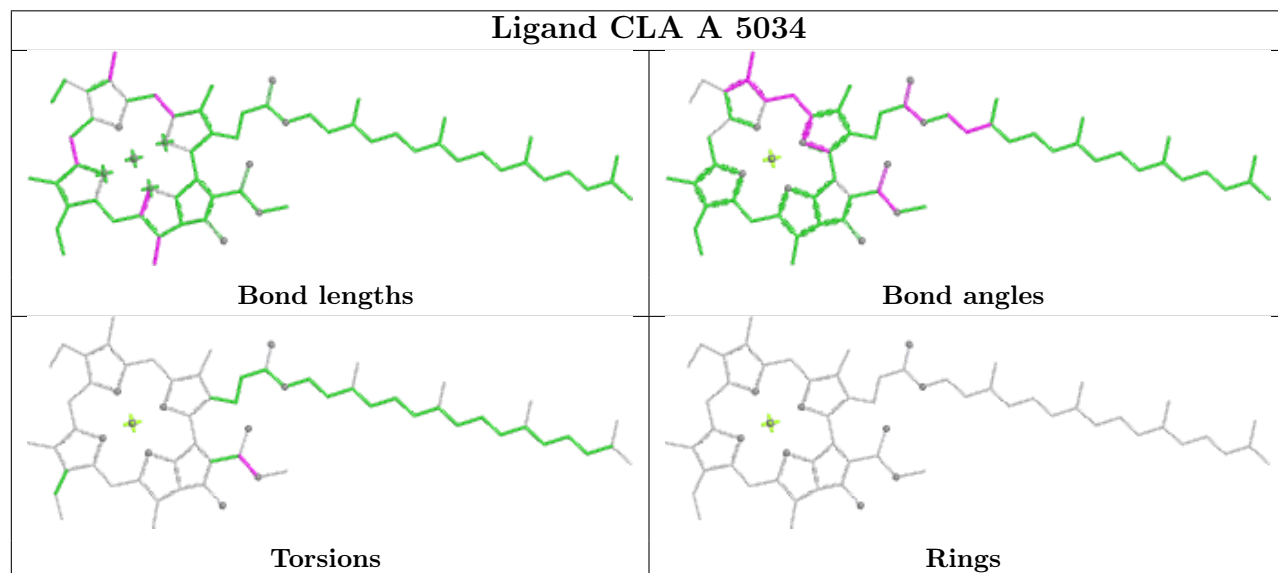
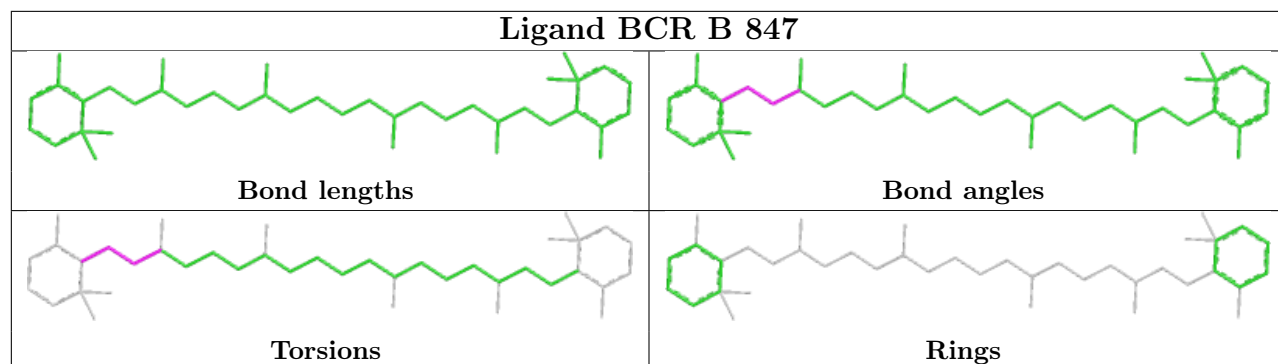


## Ligand CLA B 825

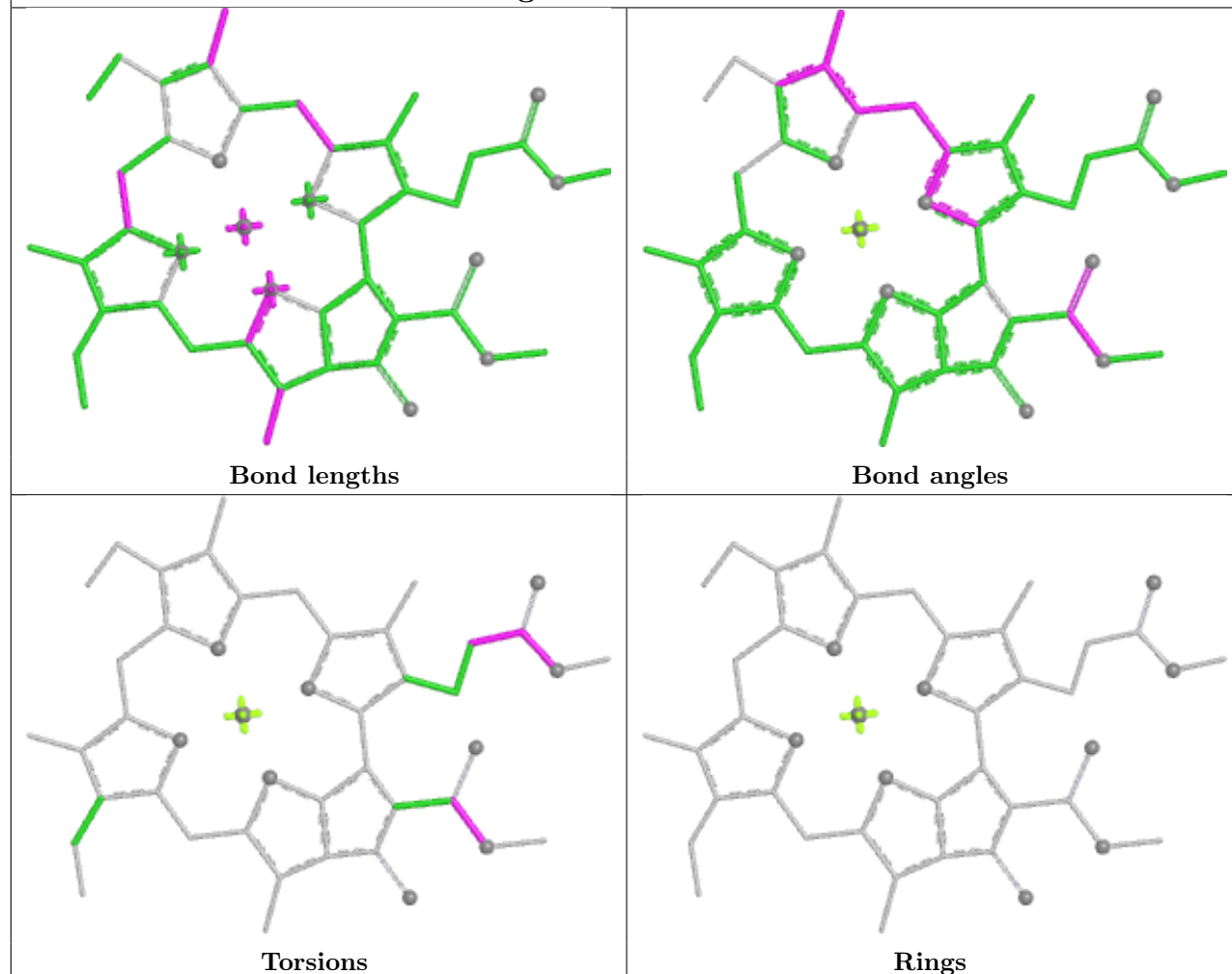


## Ligand CLA 7 323

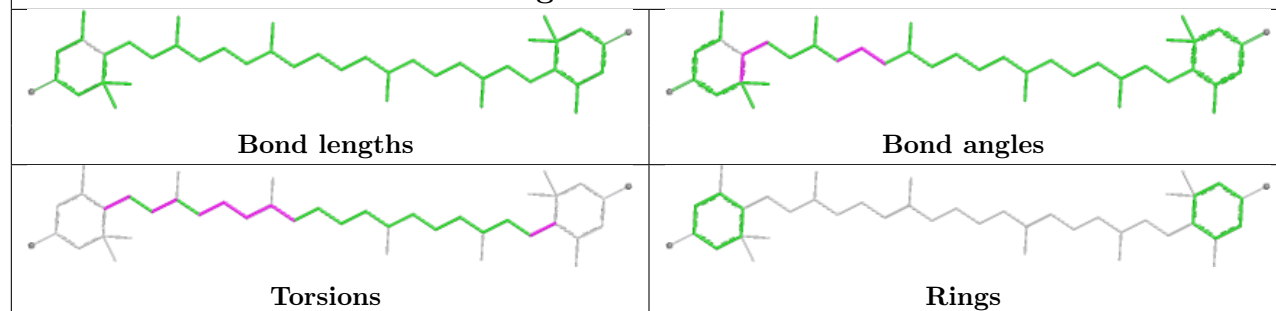




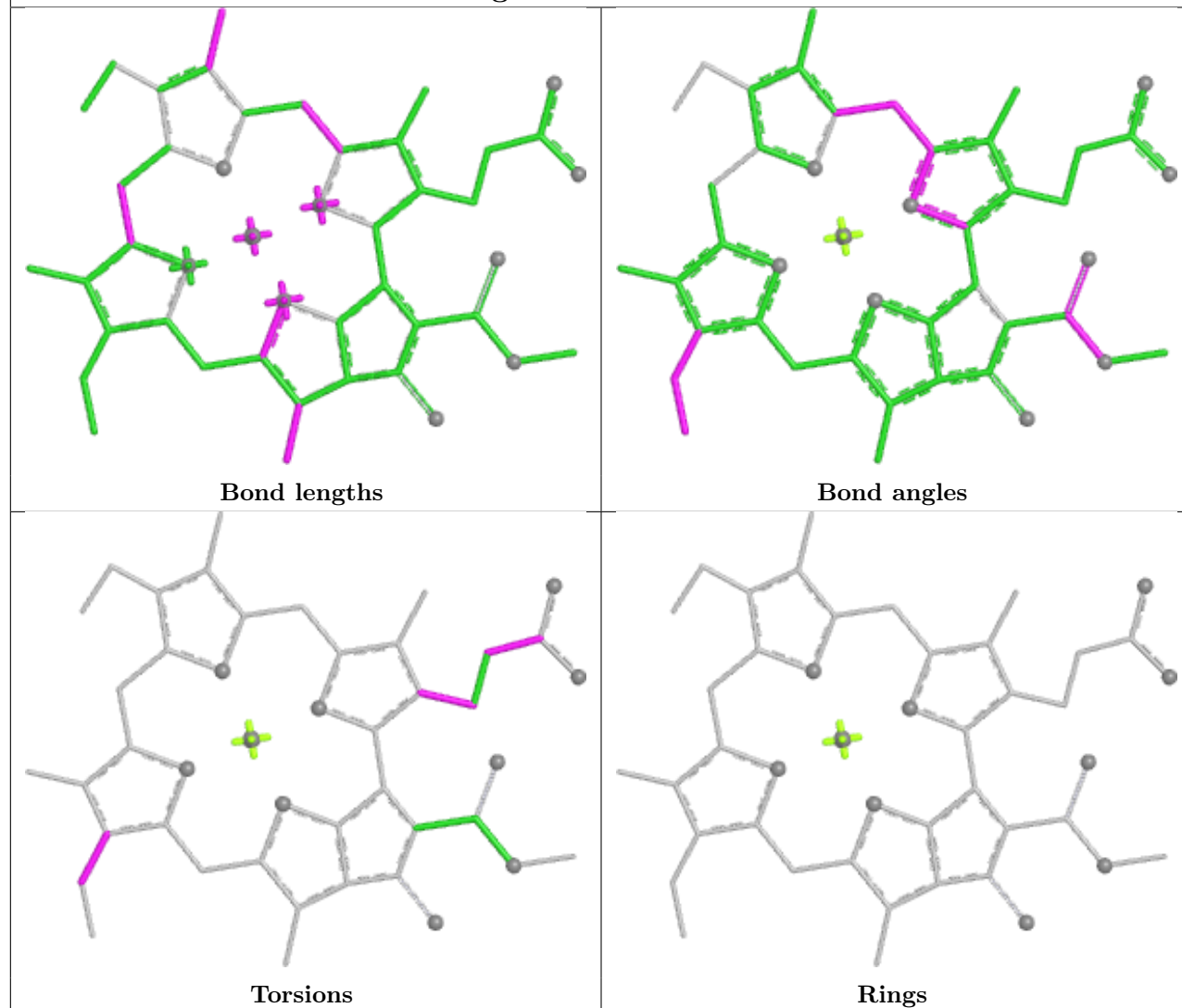
## Ligand CLA 8 313



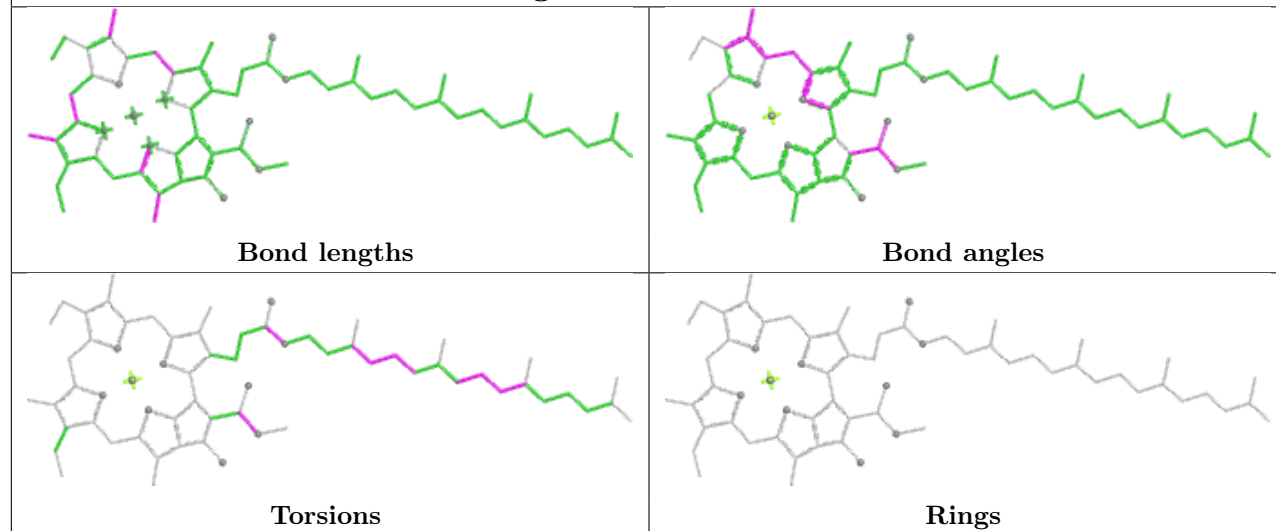
## Ligand LUT 2 315



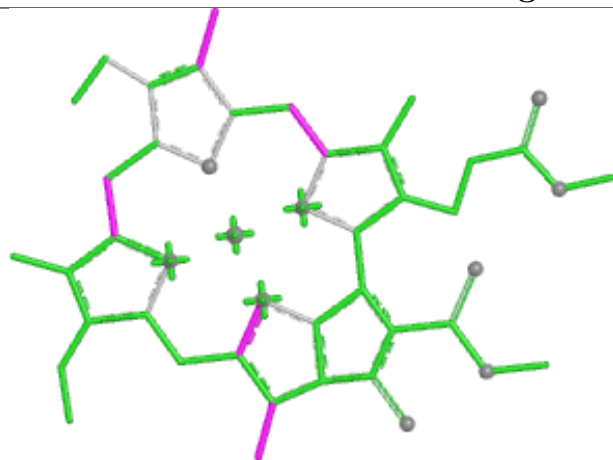
## Ligand CLA G 204



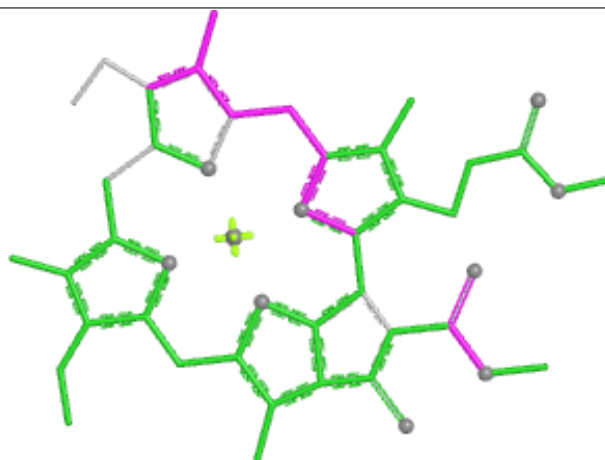
## Ligand CLA B 832



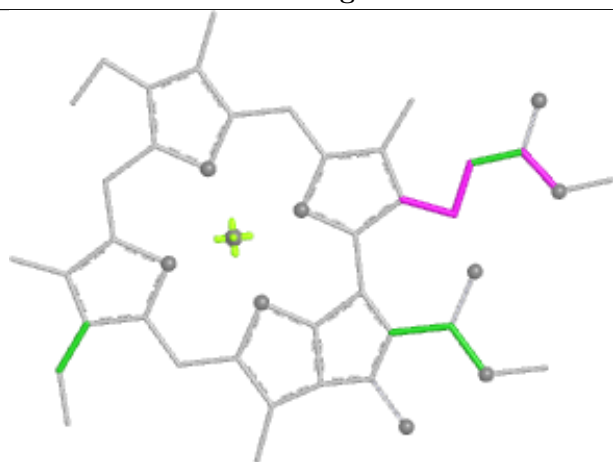
## Ligand CLA 3 303



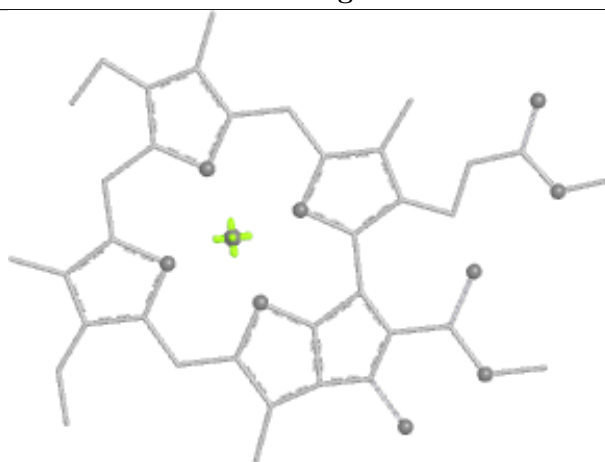
Bond lengths



Bond angles

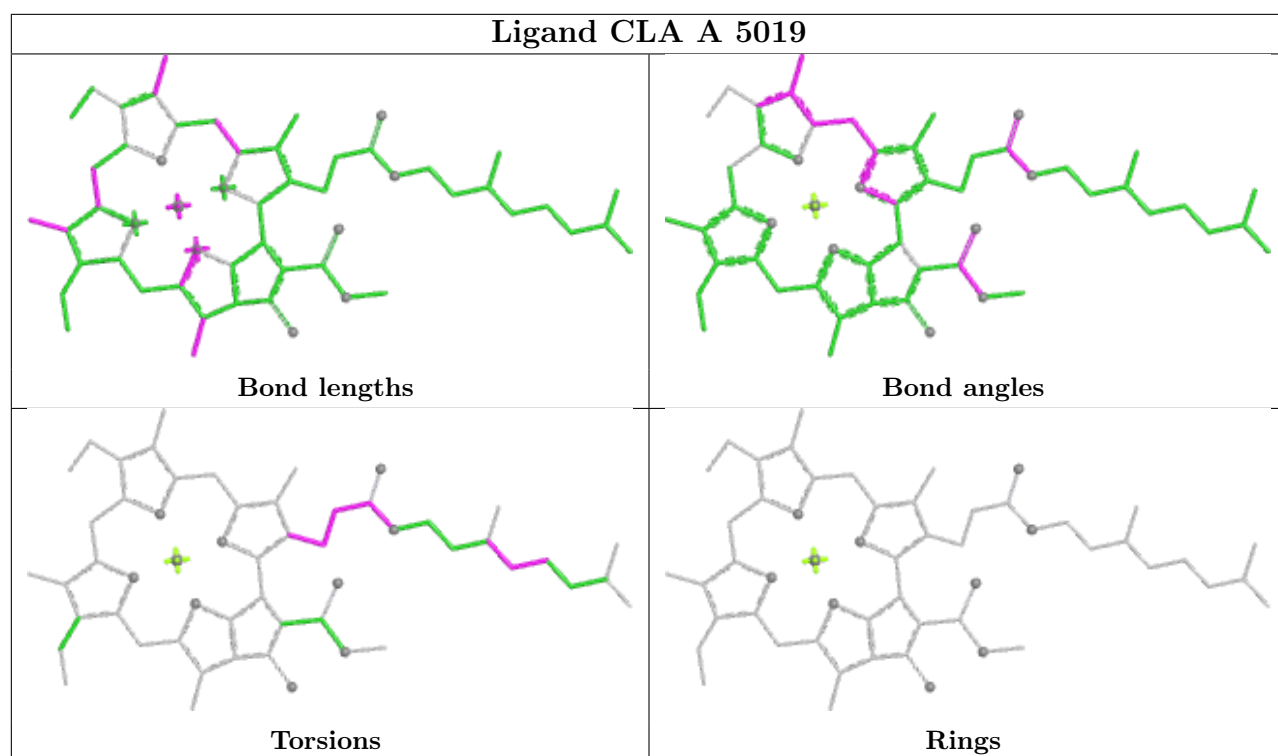


Torsions

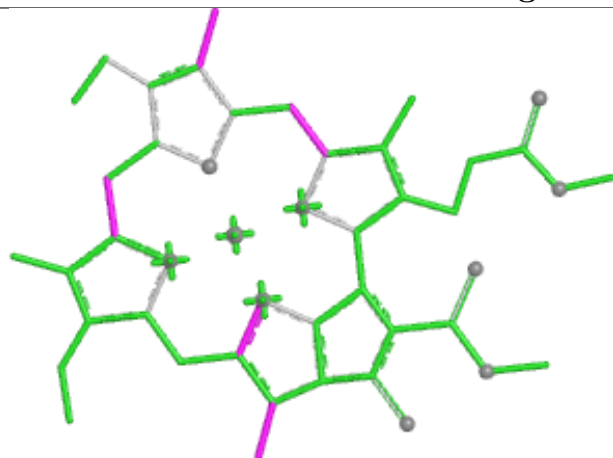


Rings

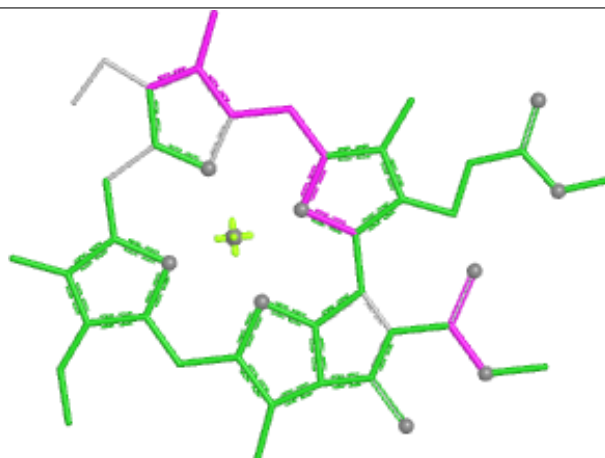




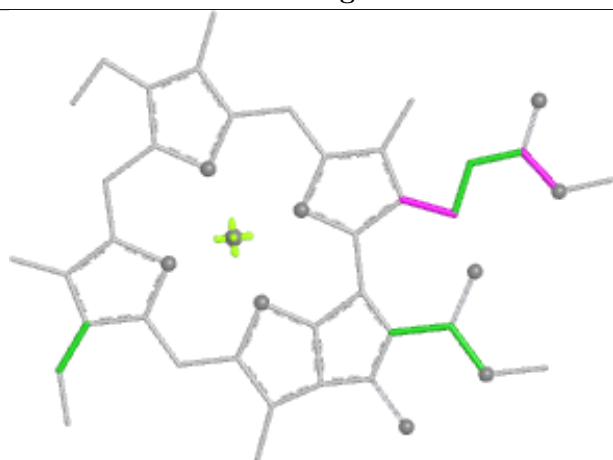
## Ligand CLA 7 309



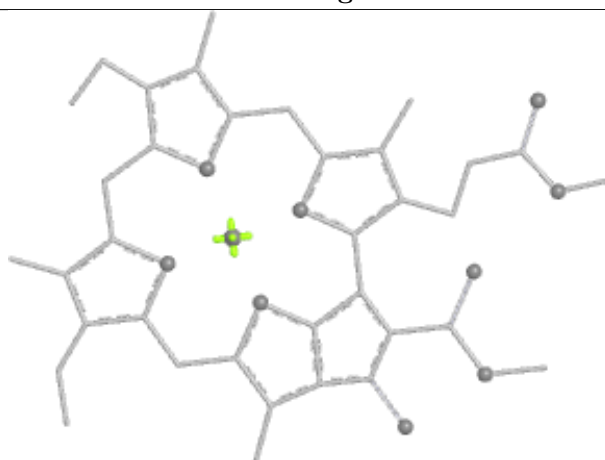
Bond lengths



Bond angles

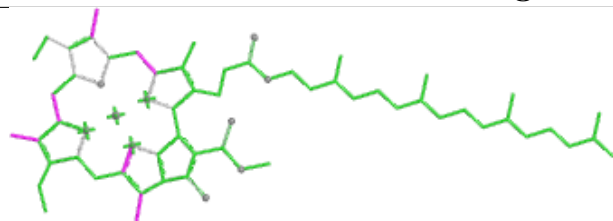


Torsions

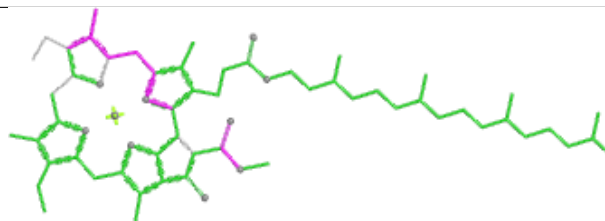


Rings

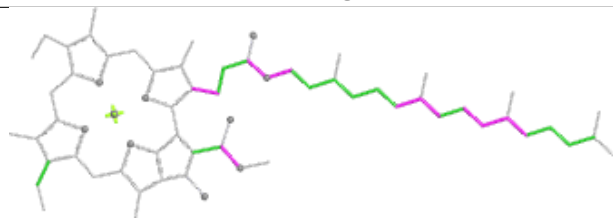
## Ligand CLA B 818



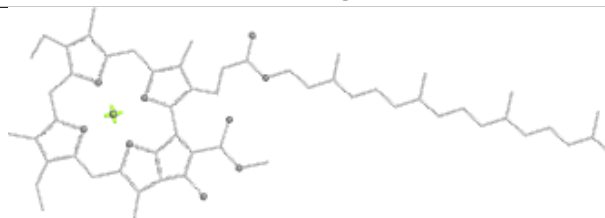
Bond lengths



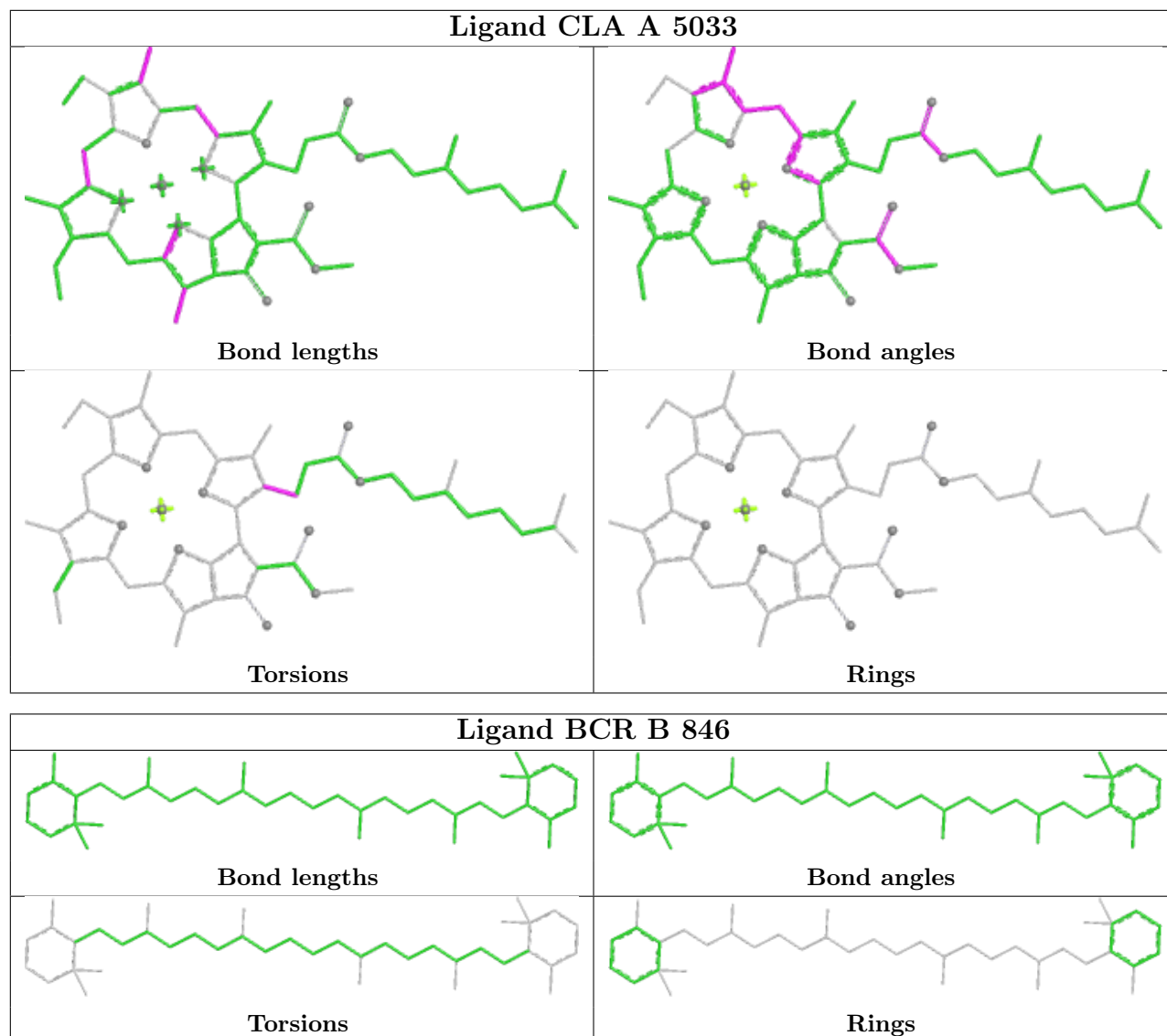
Bond angles



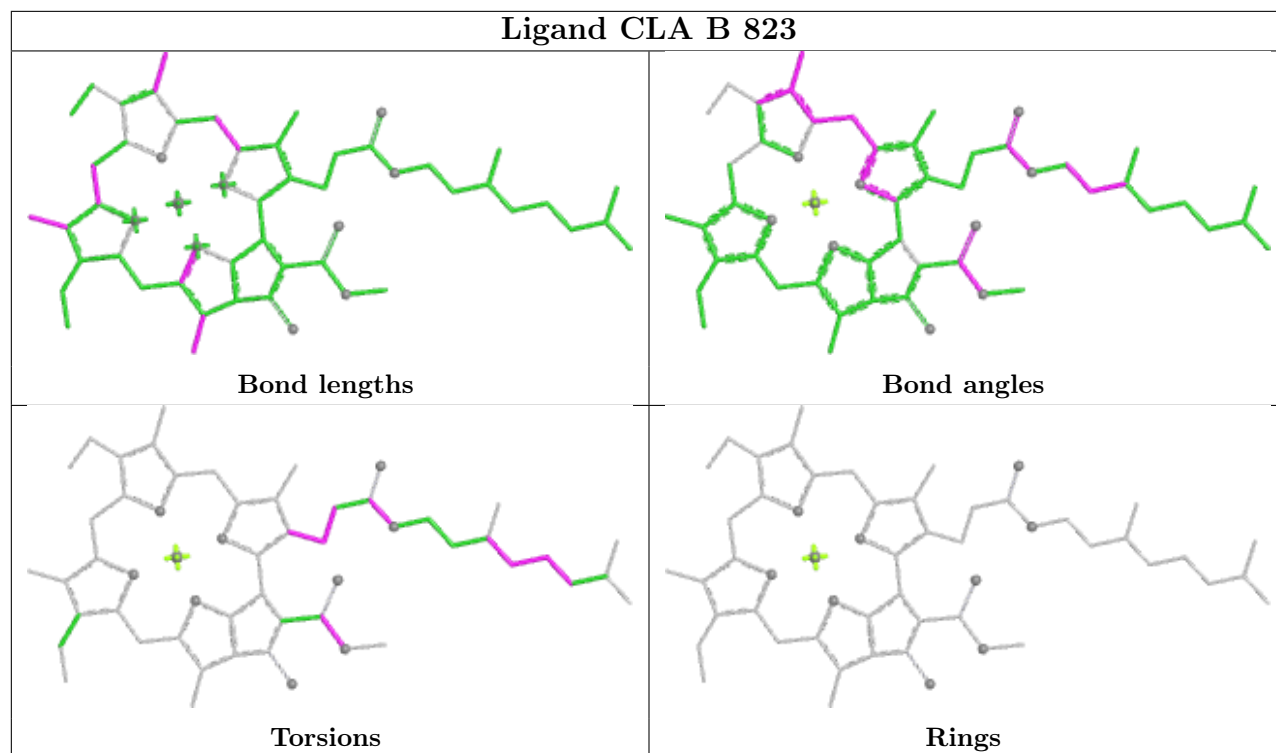
Torsions



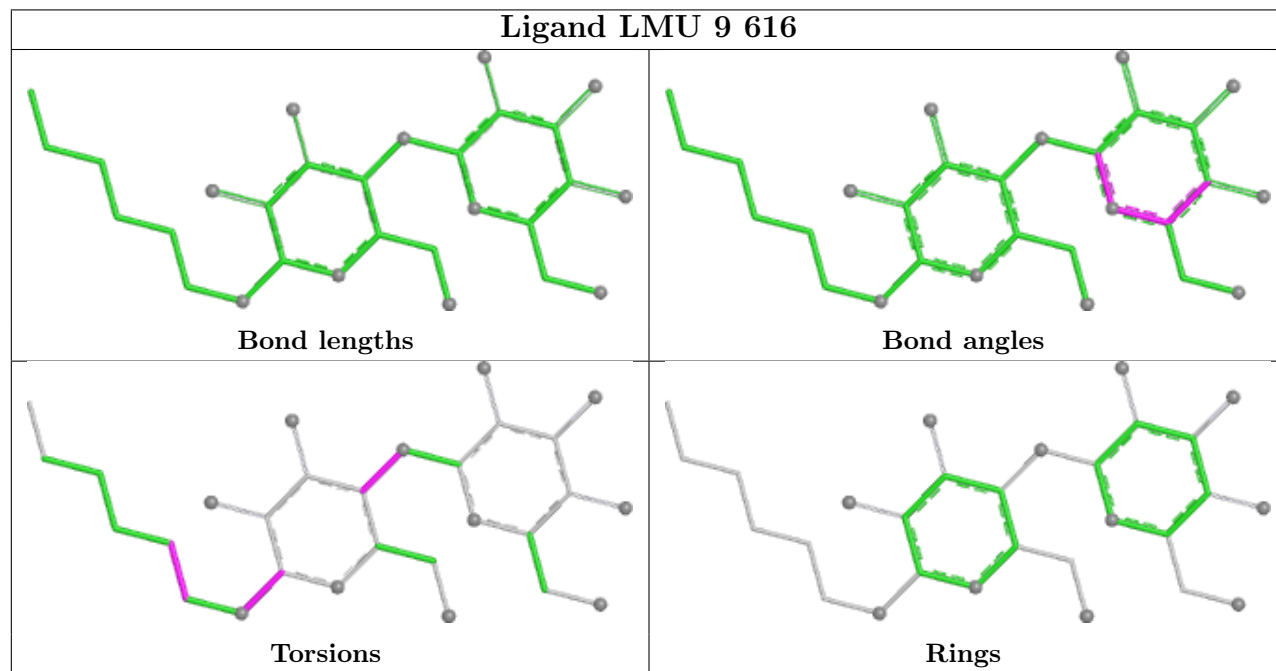
Rings



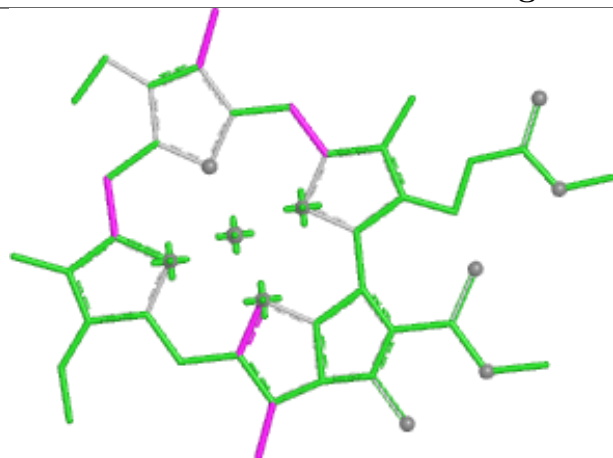
## Ligand CLA B 823



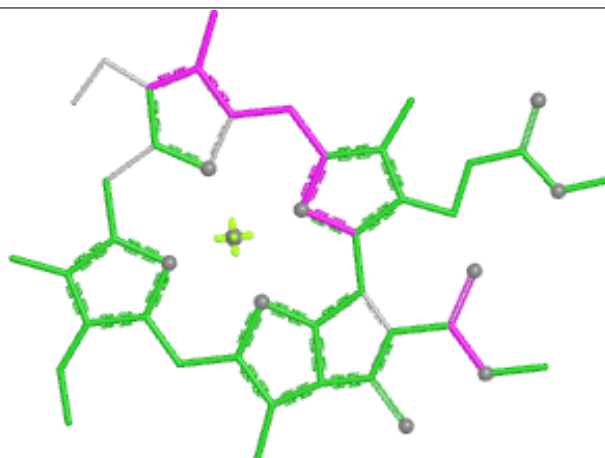
## Ligand LMU 9 616



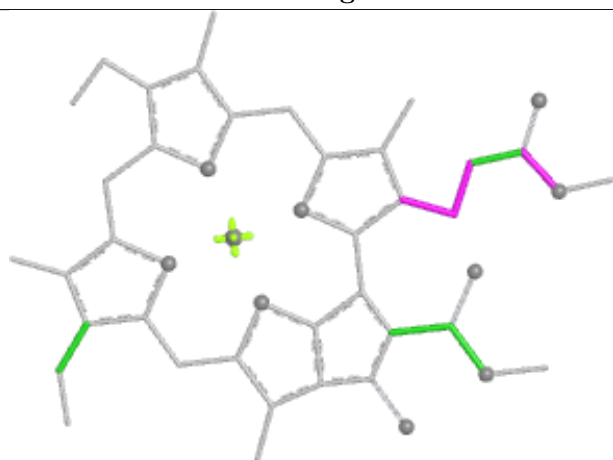
## Ligand CLA 2 301



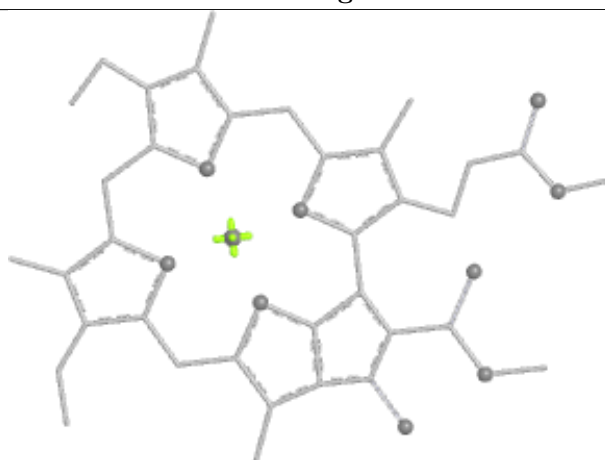
Bond lengths



Bond angles

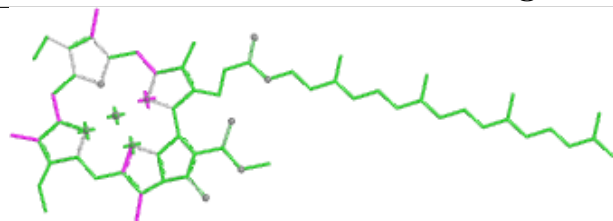


Torsions



Rings

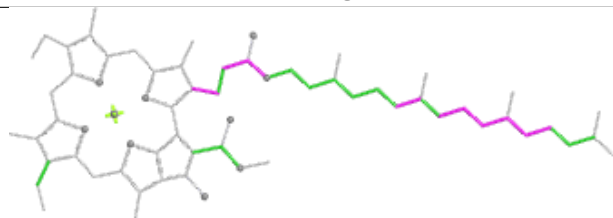
## Ligand CLA 8 303



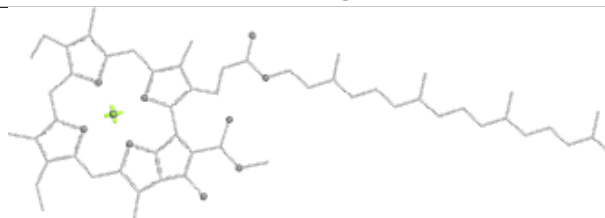
Bond lengths



Bond angles

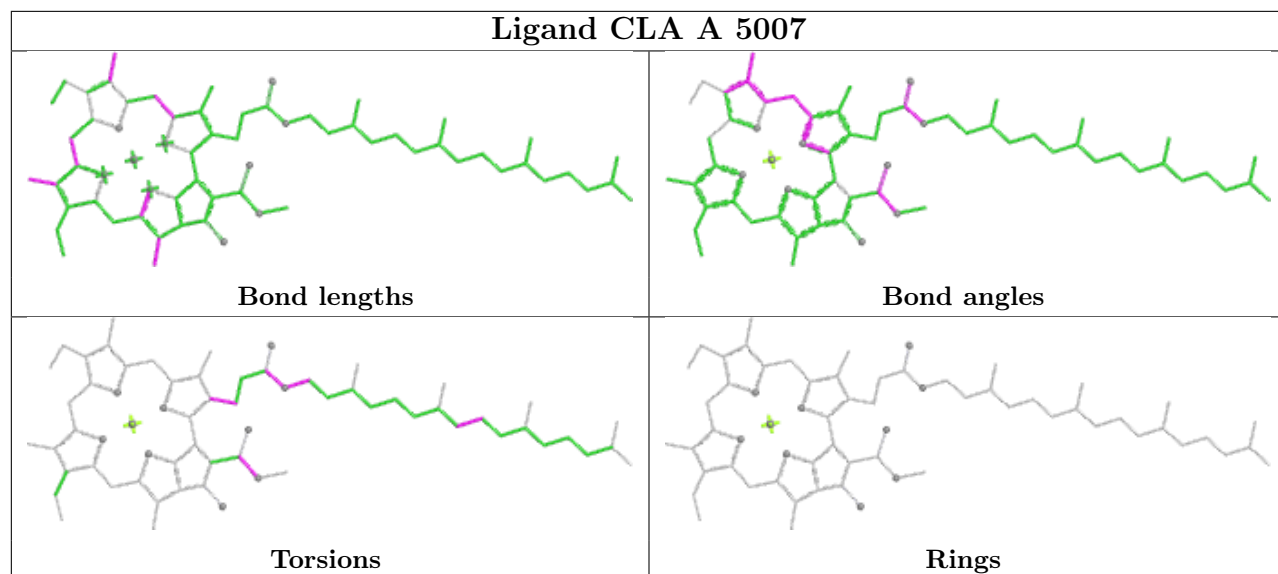


Torsions

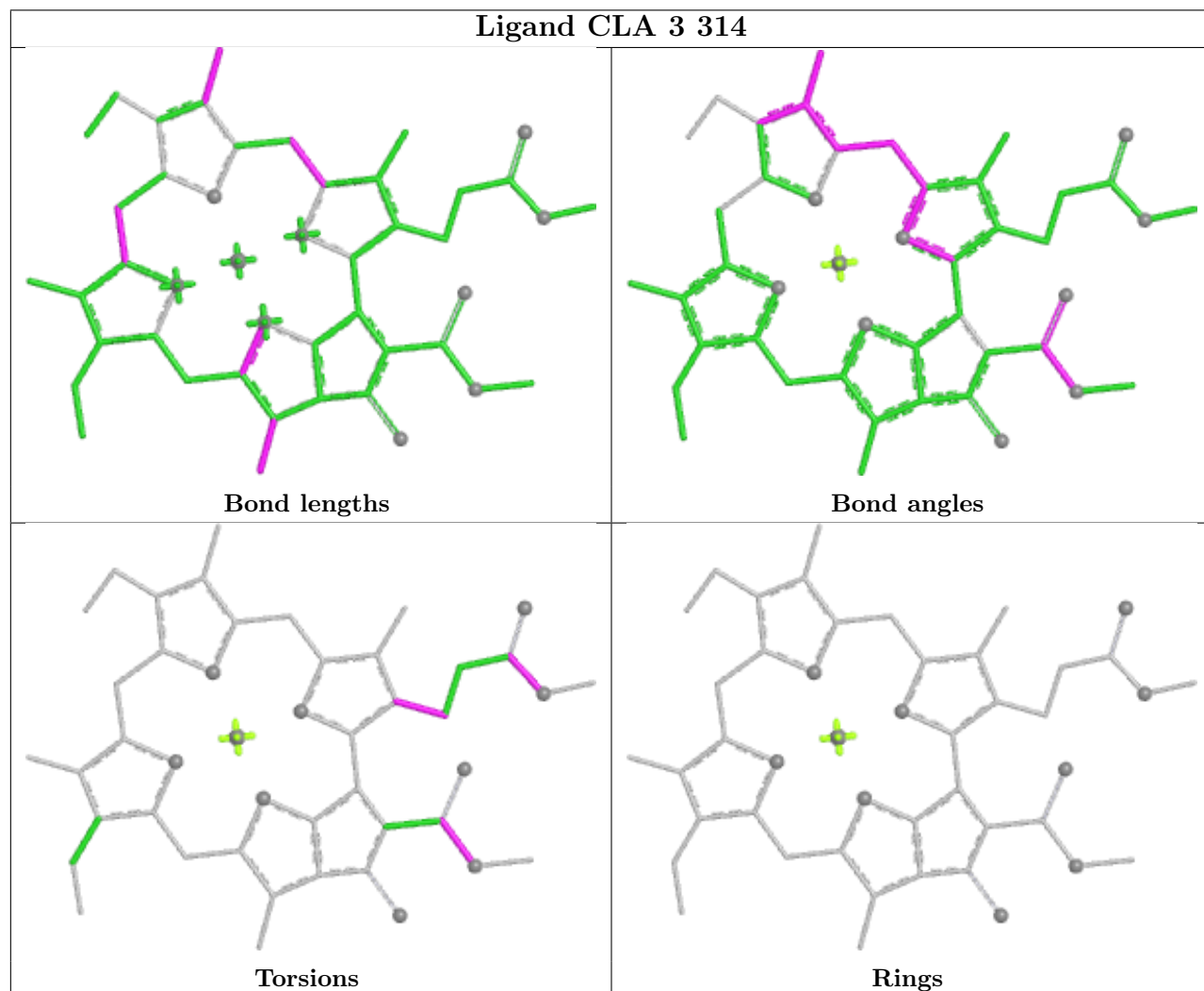


Rings

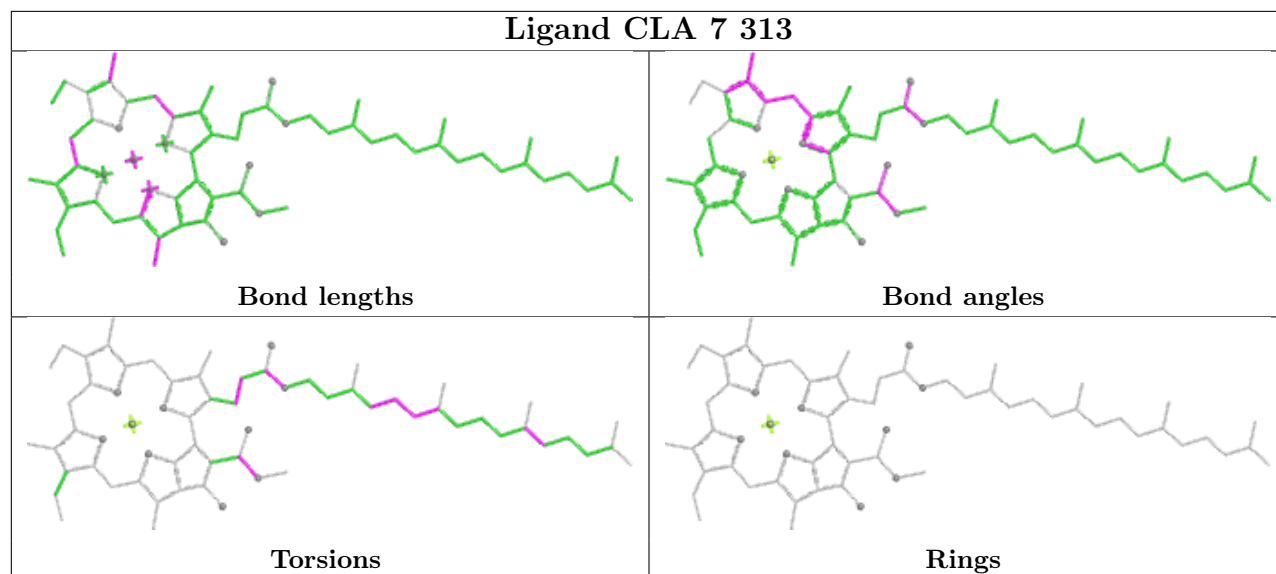
## Ligand CLA A 5007



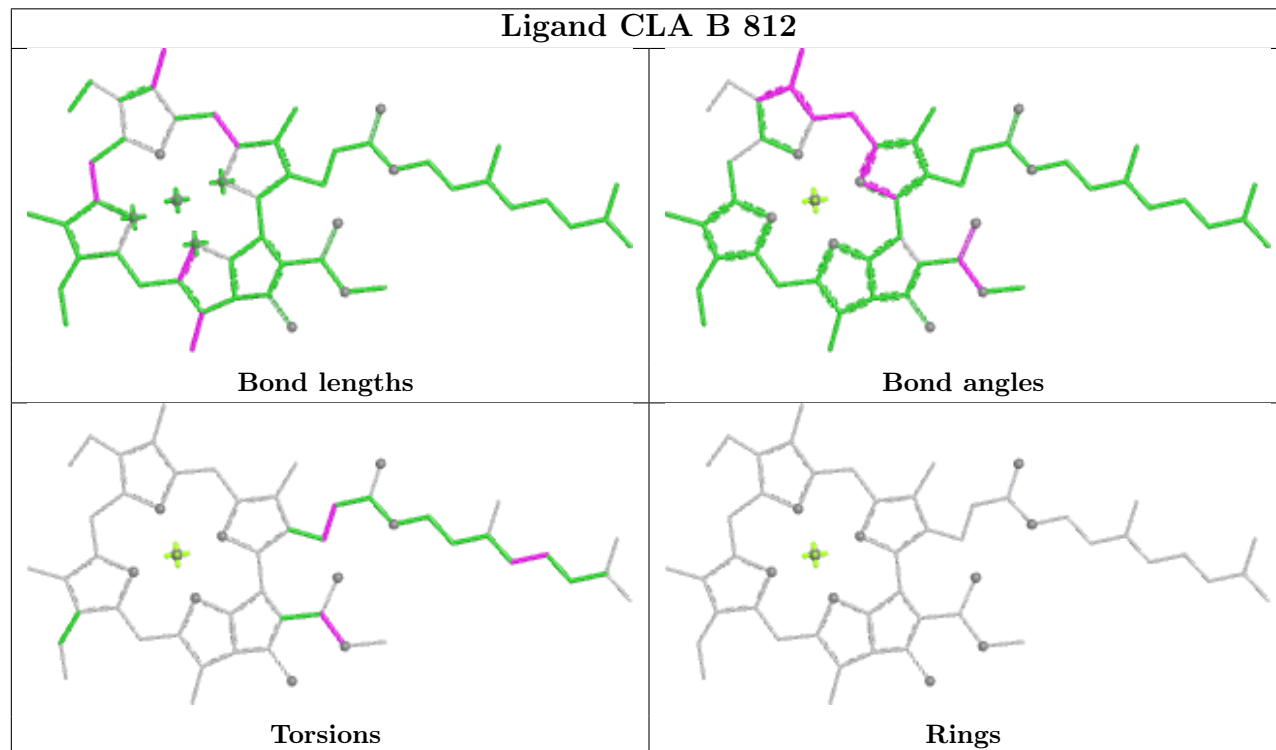
## Ligand CLA 3 314



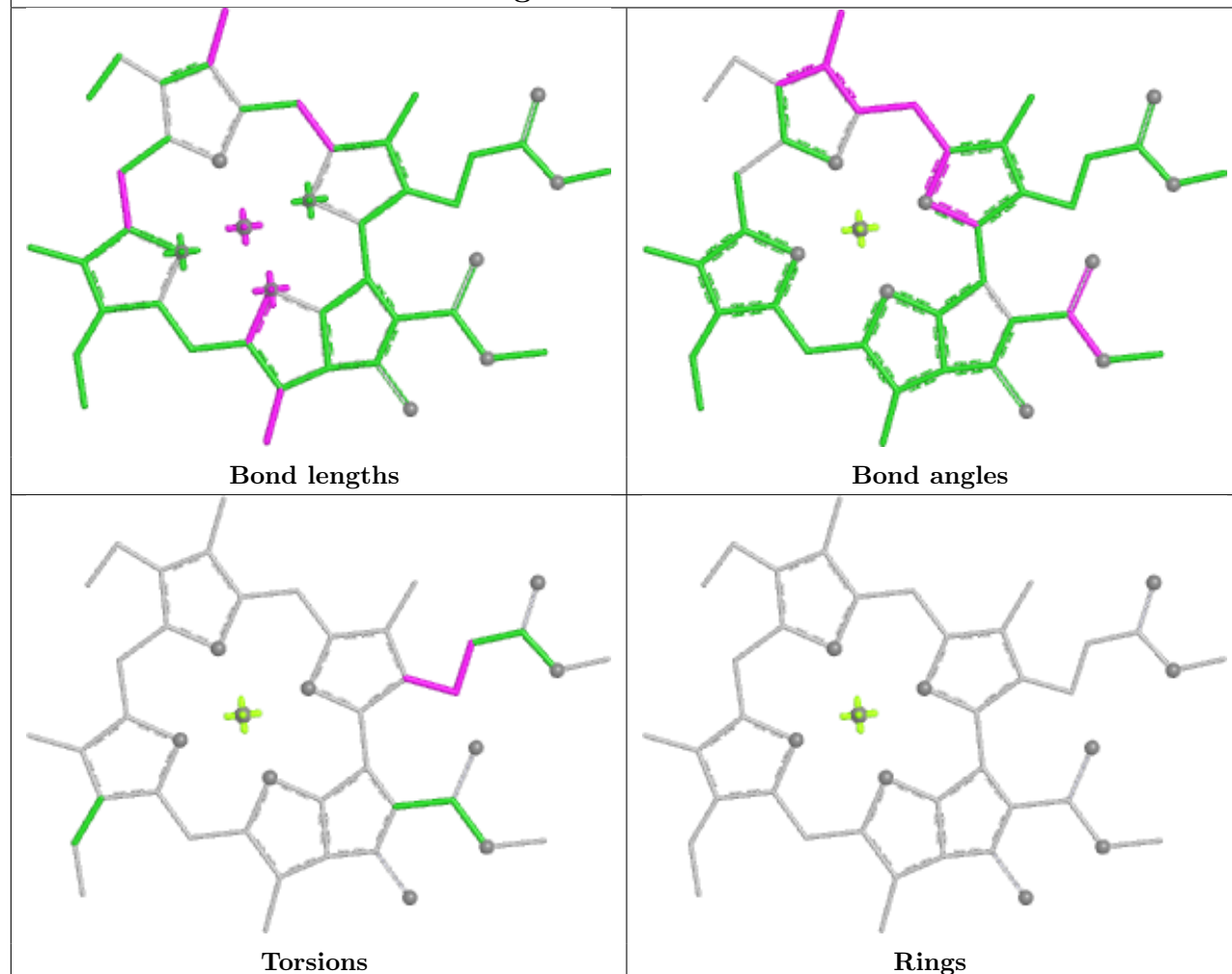
## Ligand CLA 7 313



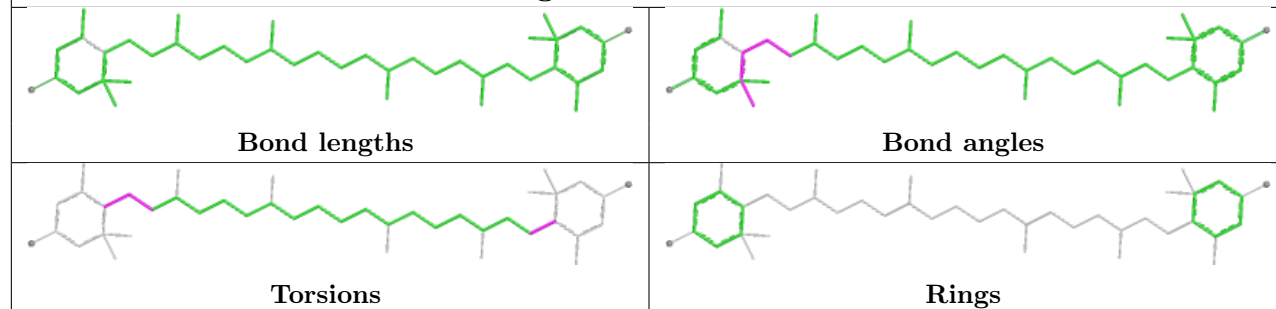
## Ligand CLA B 812



## Ligand CLA B 813

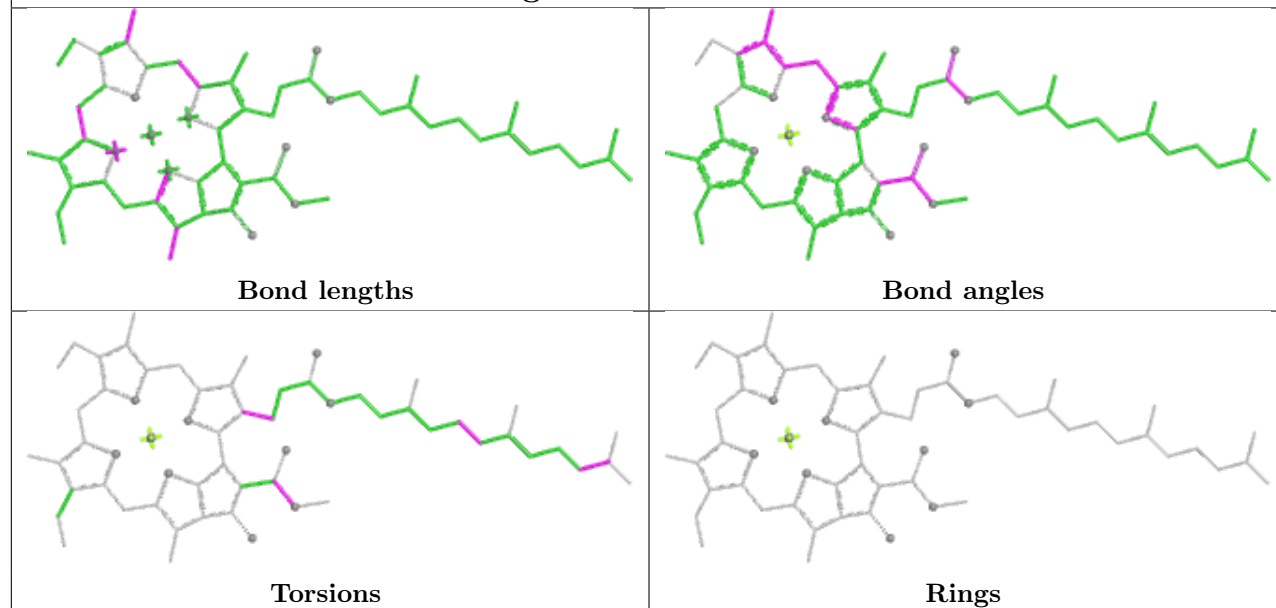


## Ligand LUT 2 314

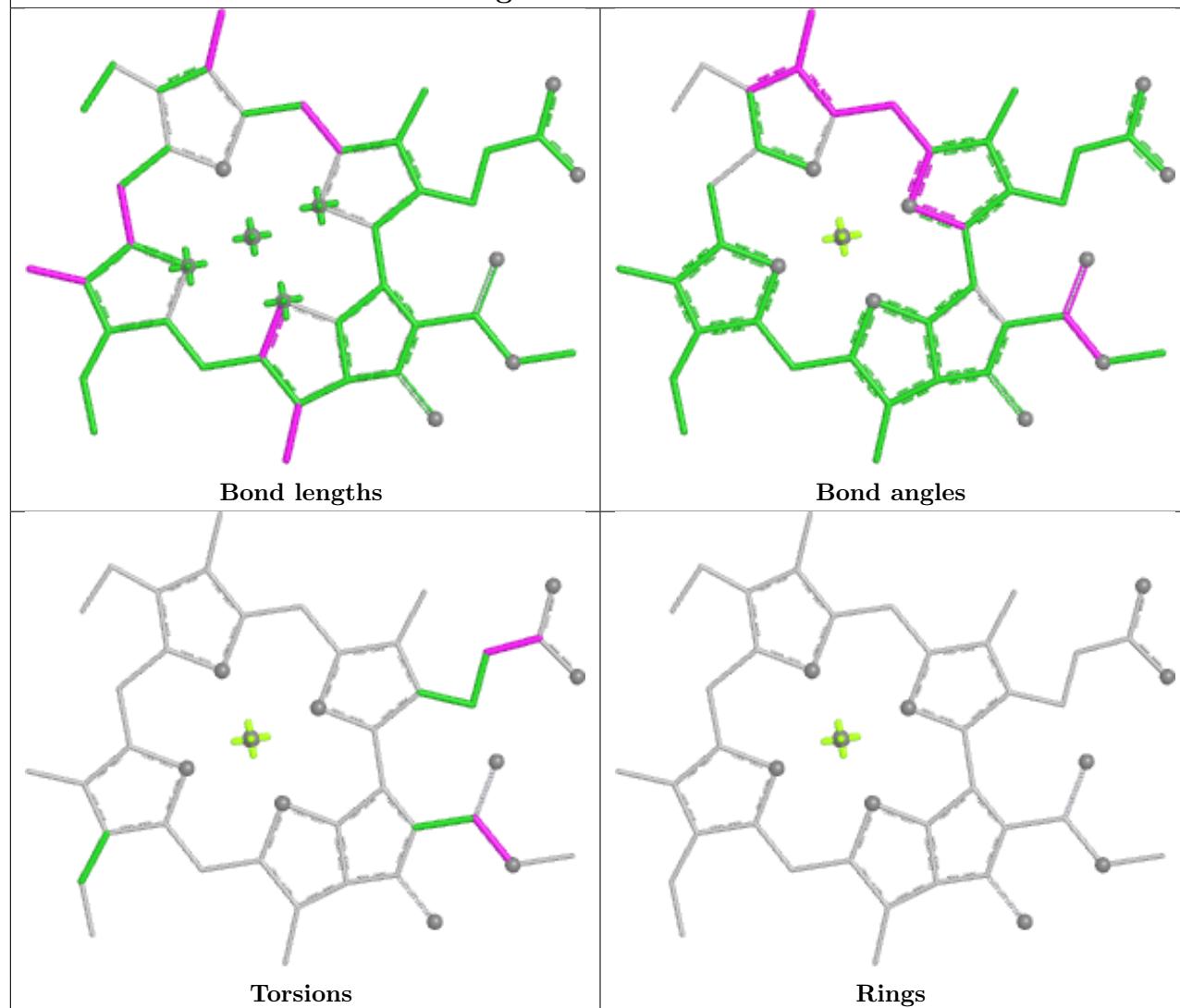


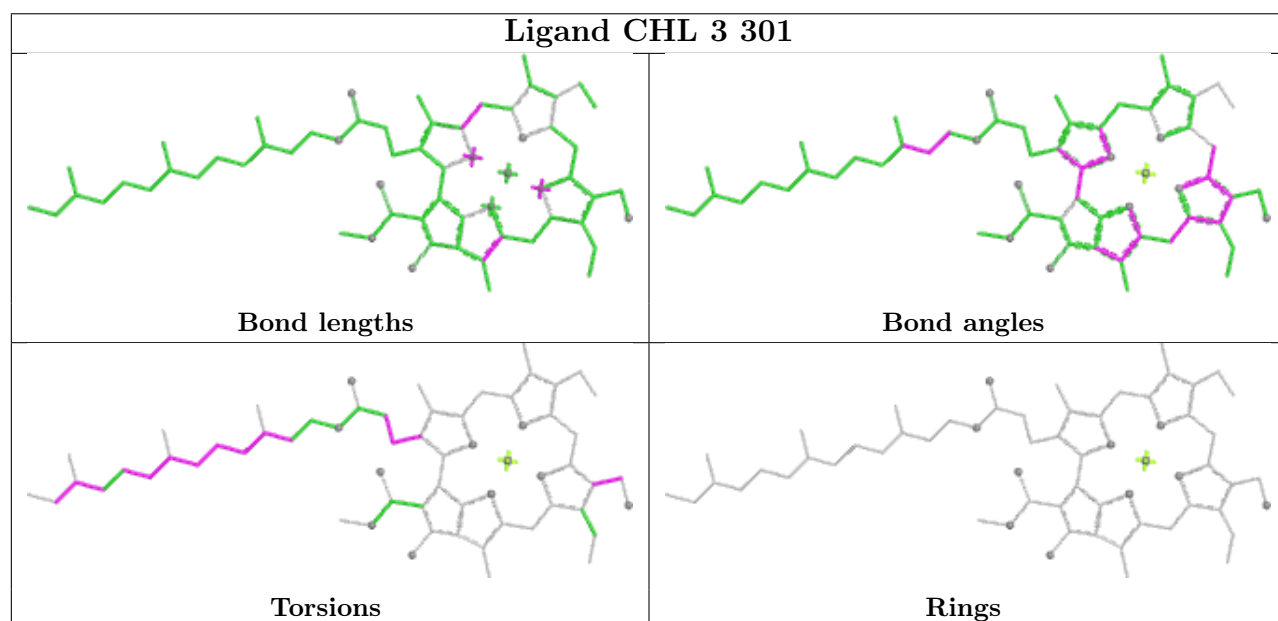
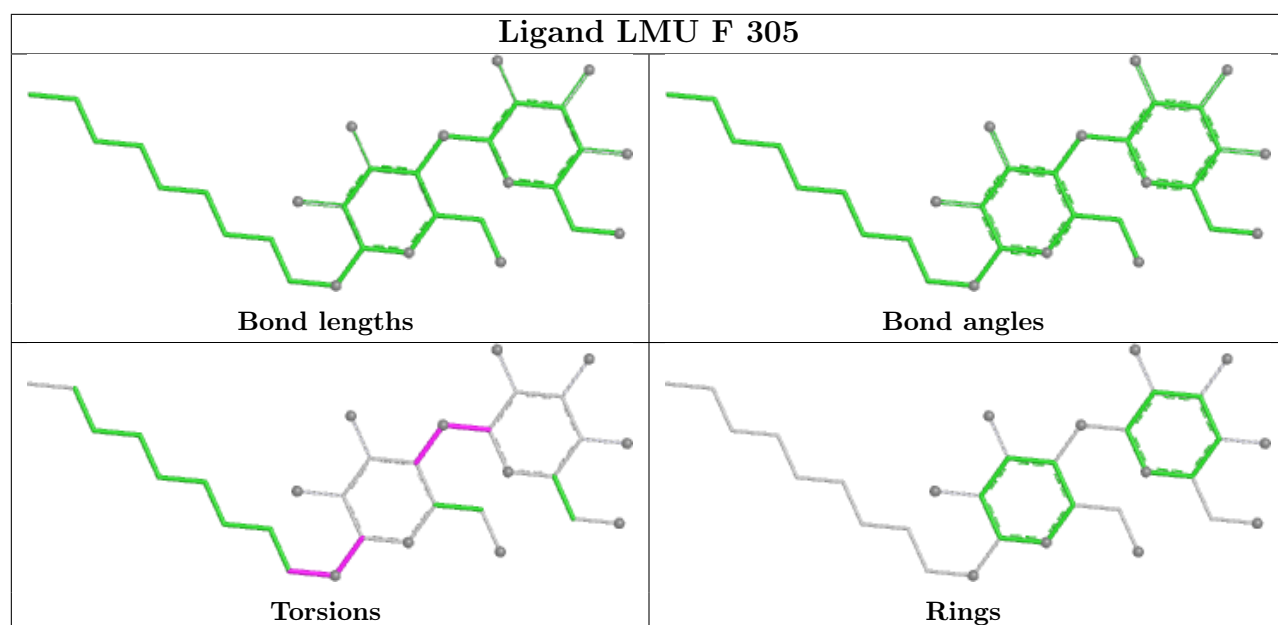


## Ligand CLA A 5042

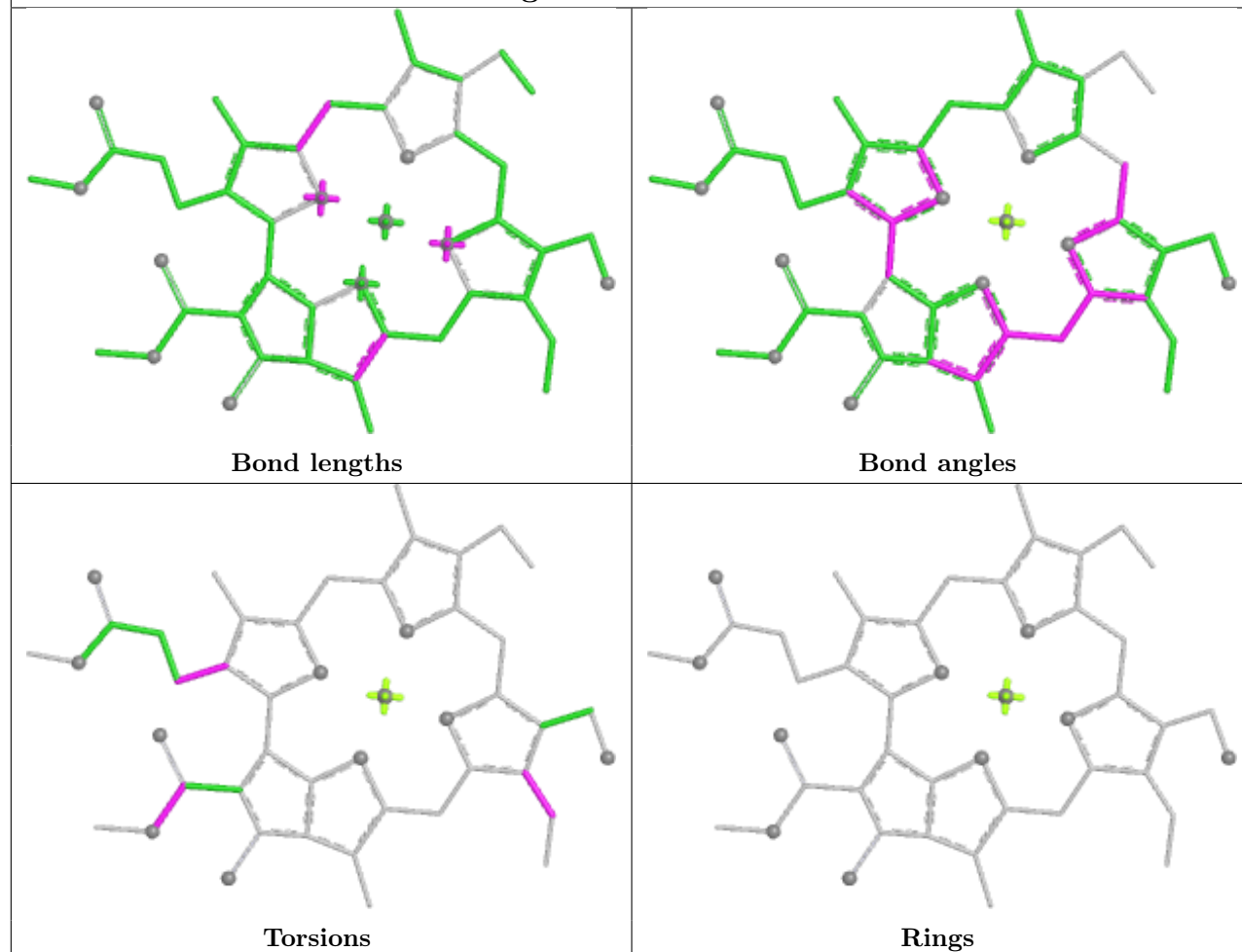


## Ligand CLA 1 605

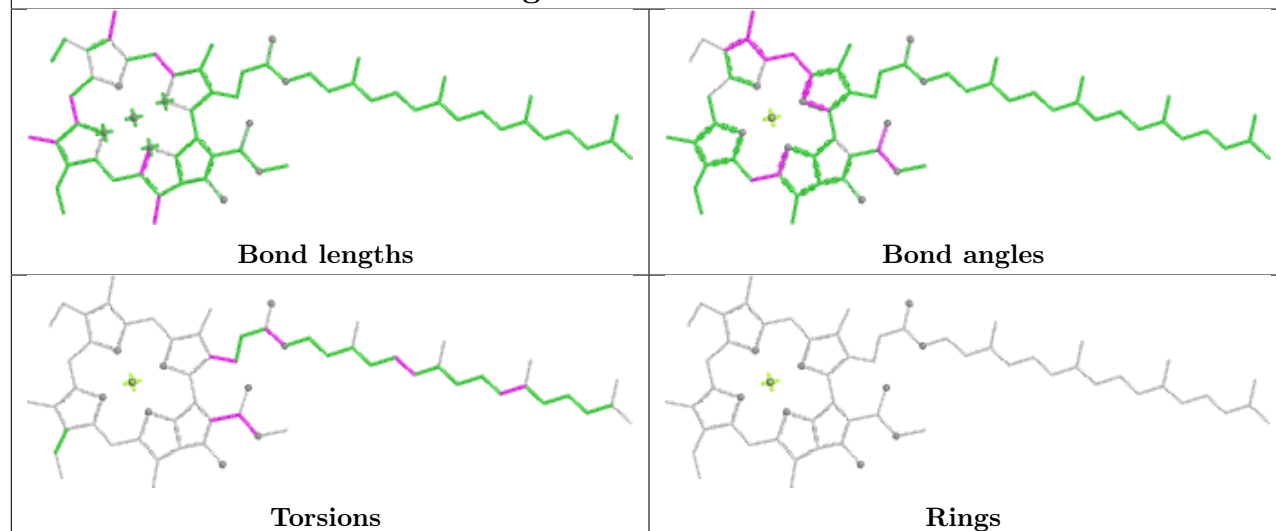




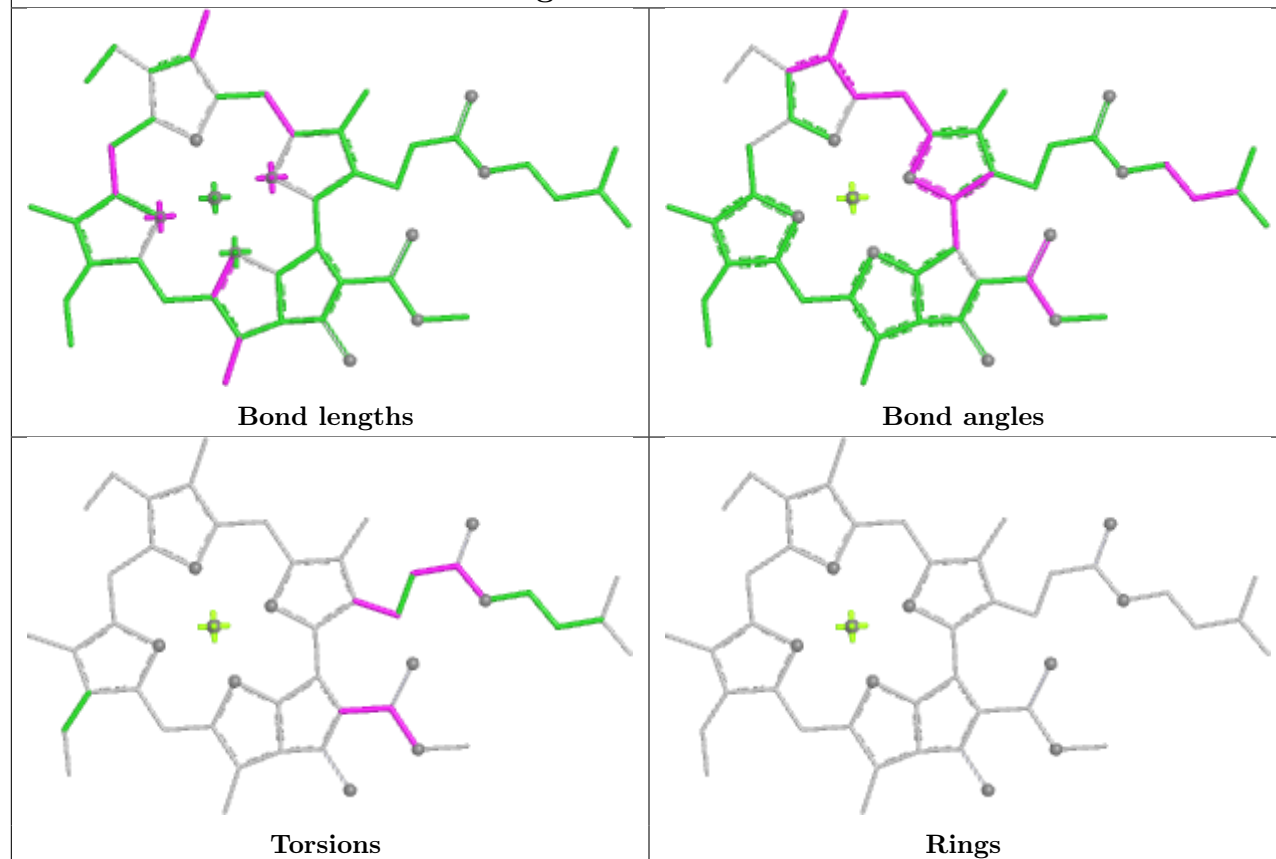
## Ligand CHL 7 307



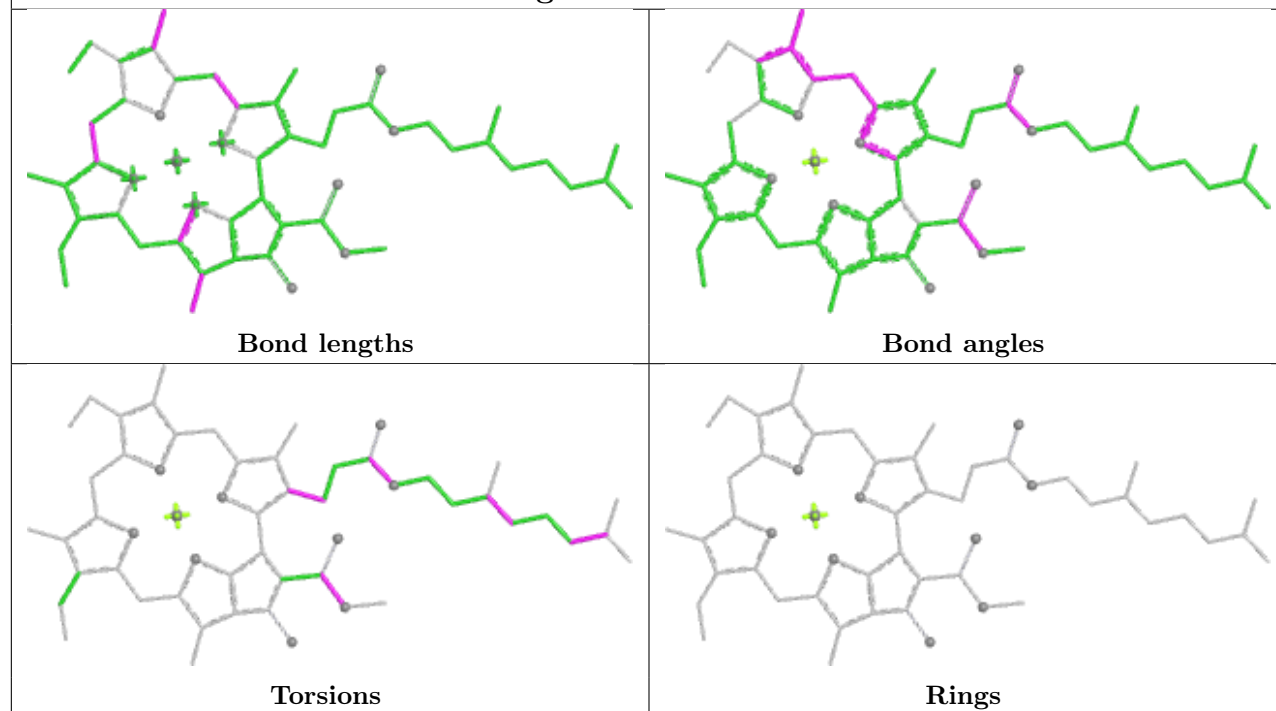
## Ligand CLA A 5008

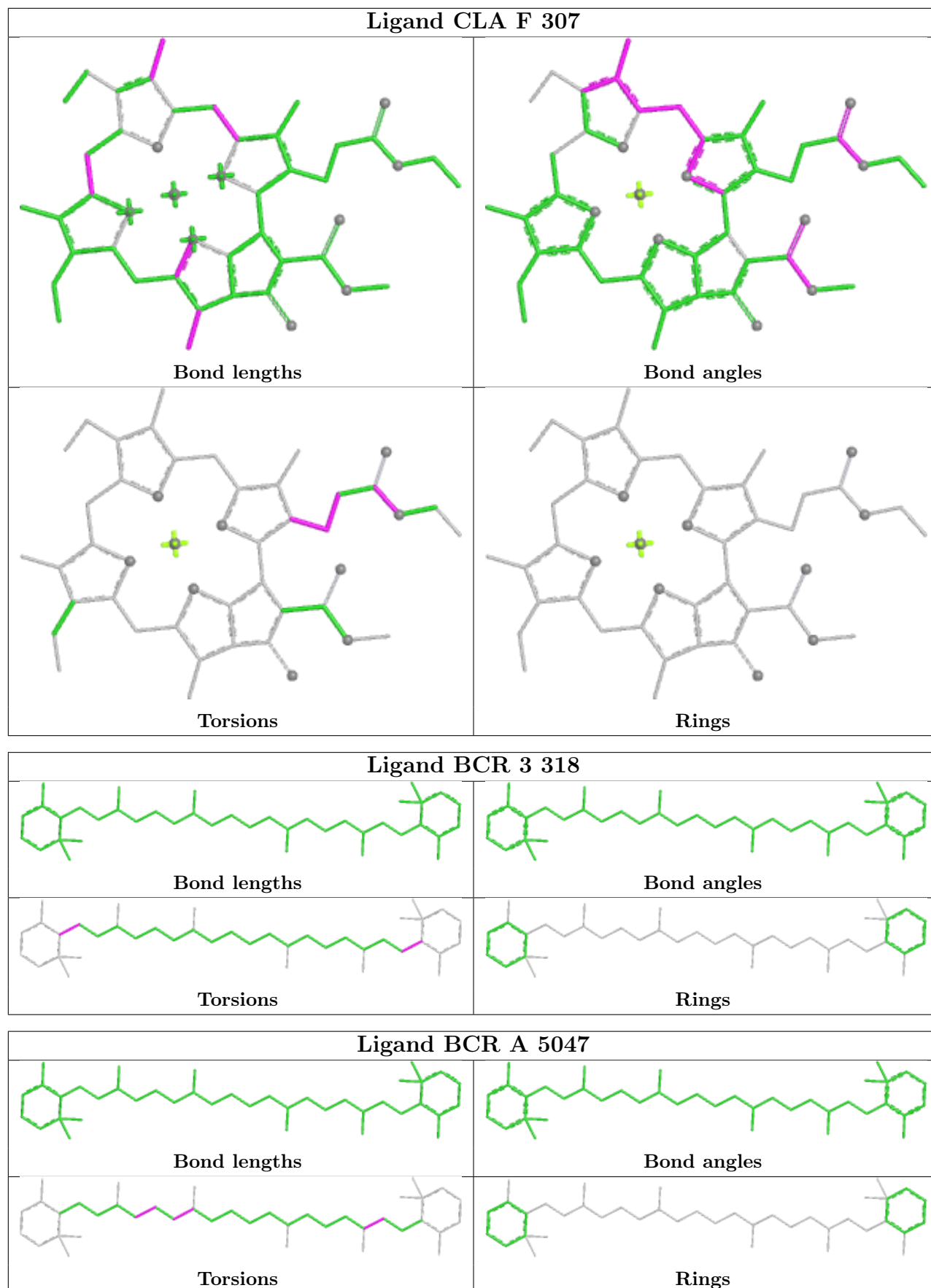


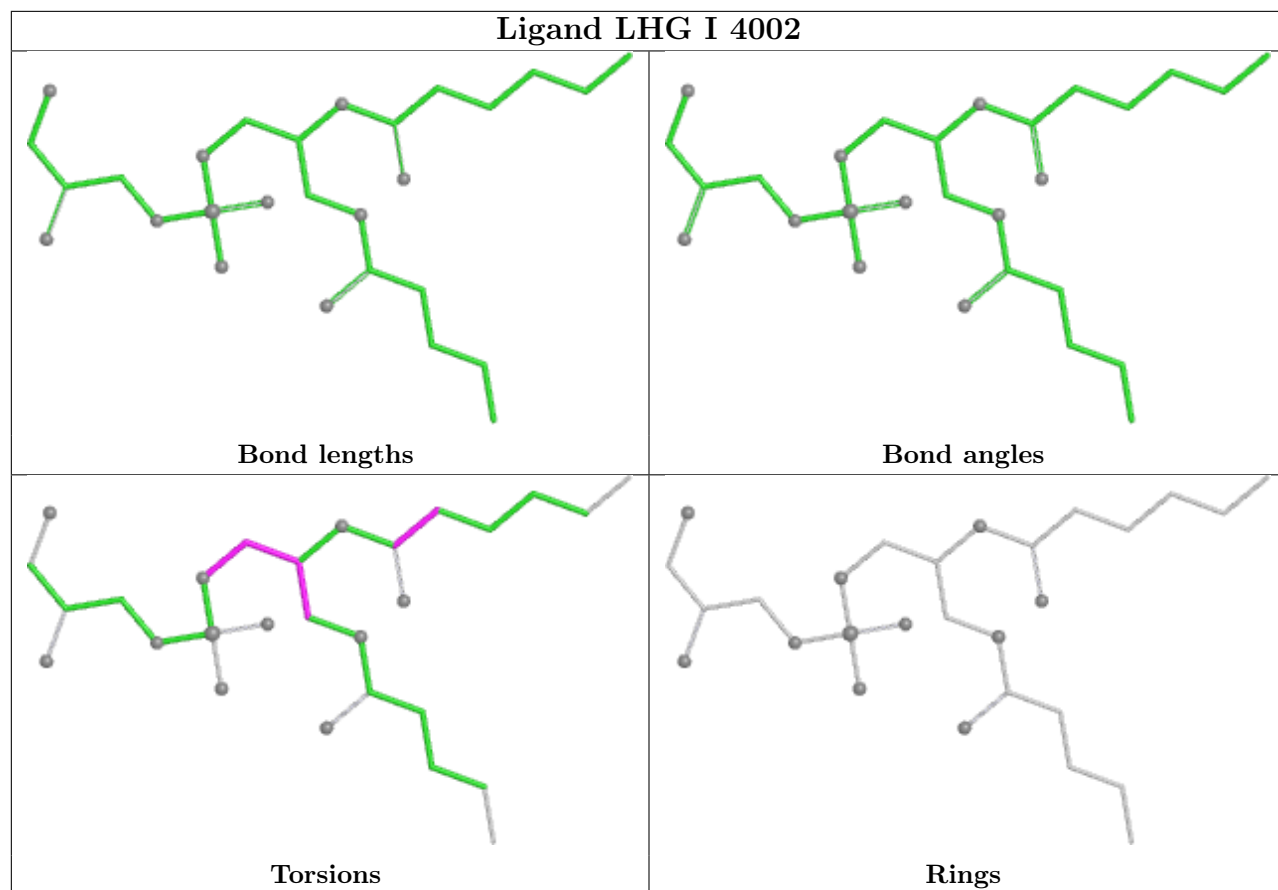
## Ligand CLA 9 610

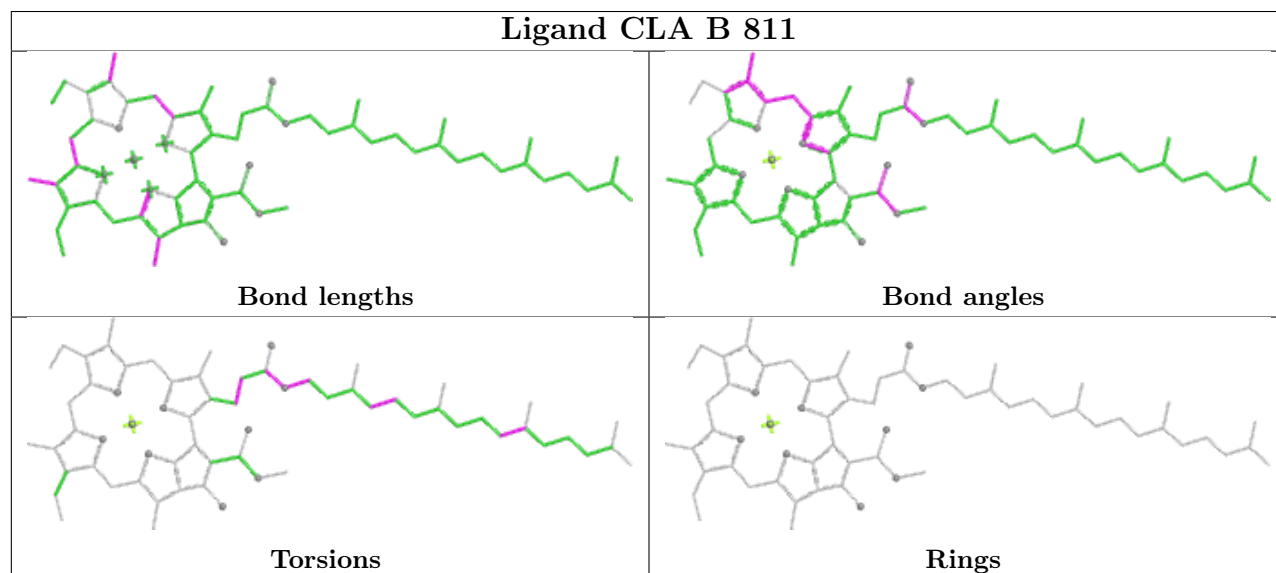
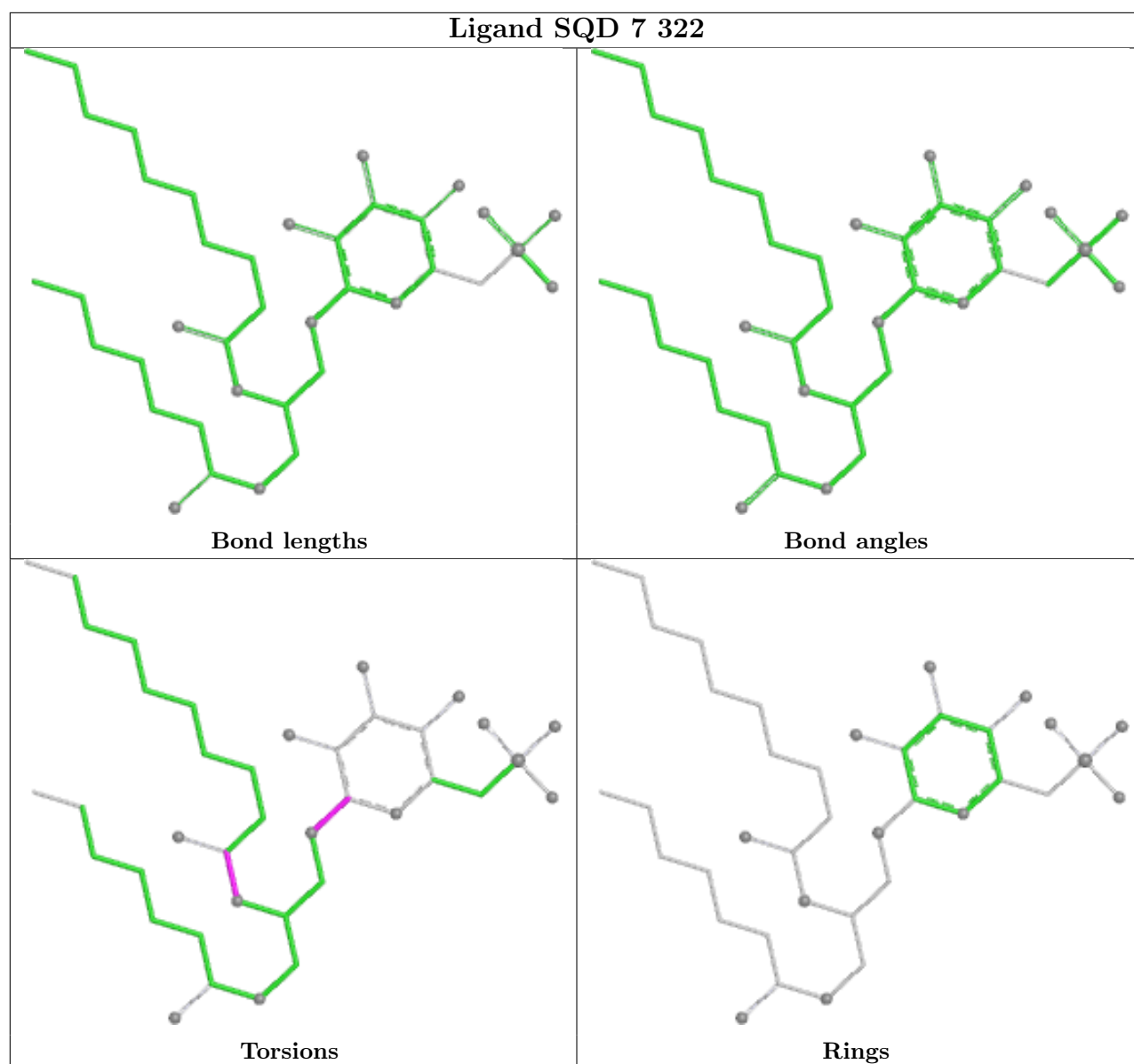


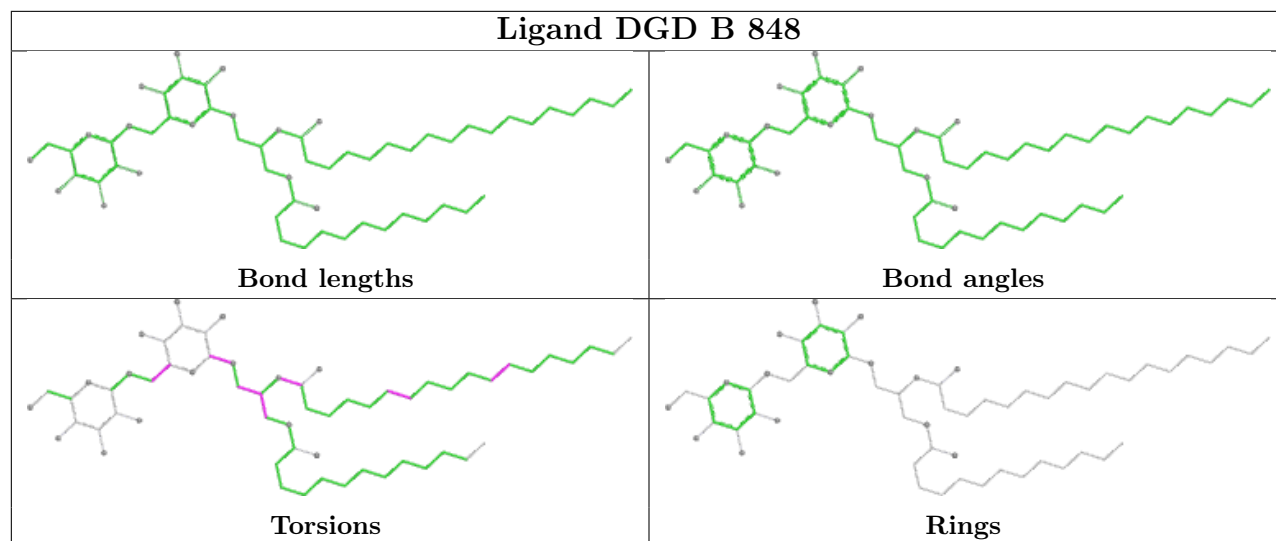
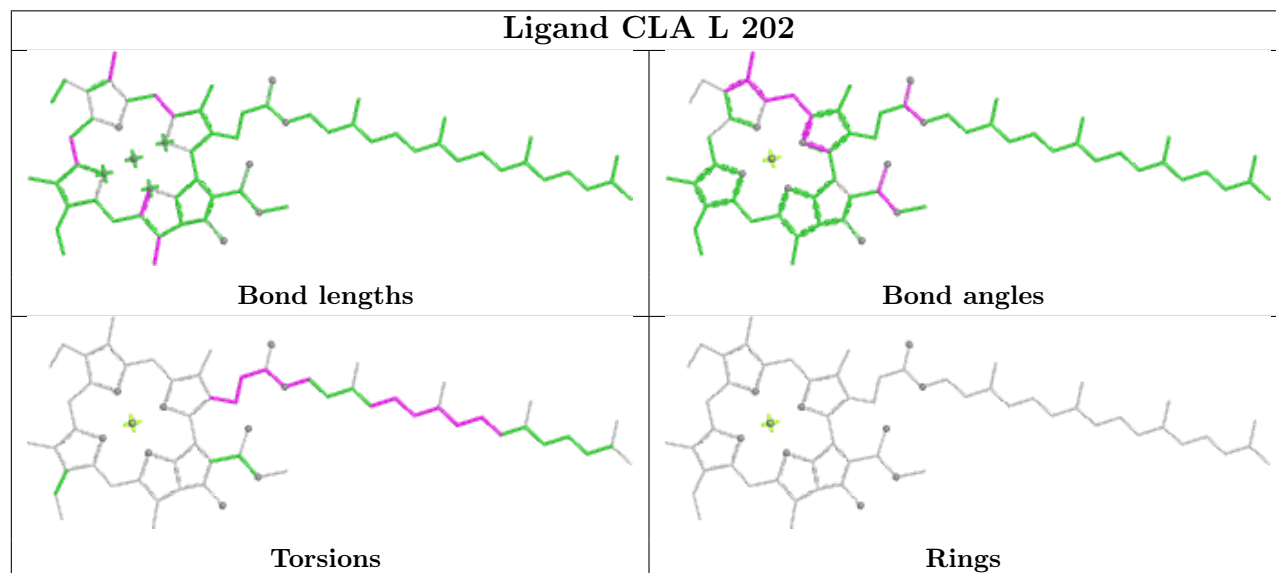
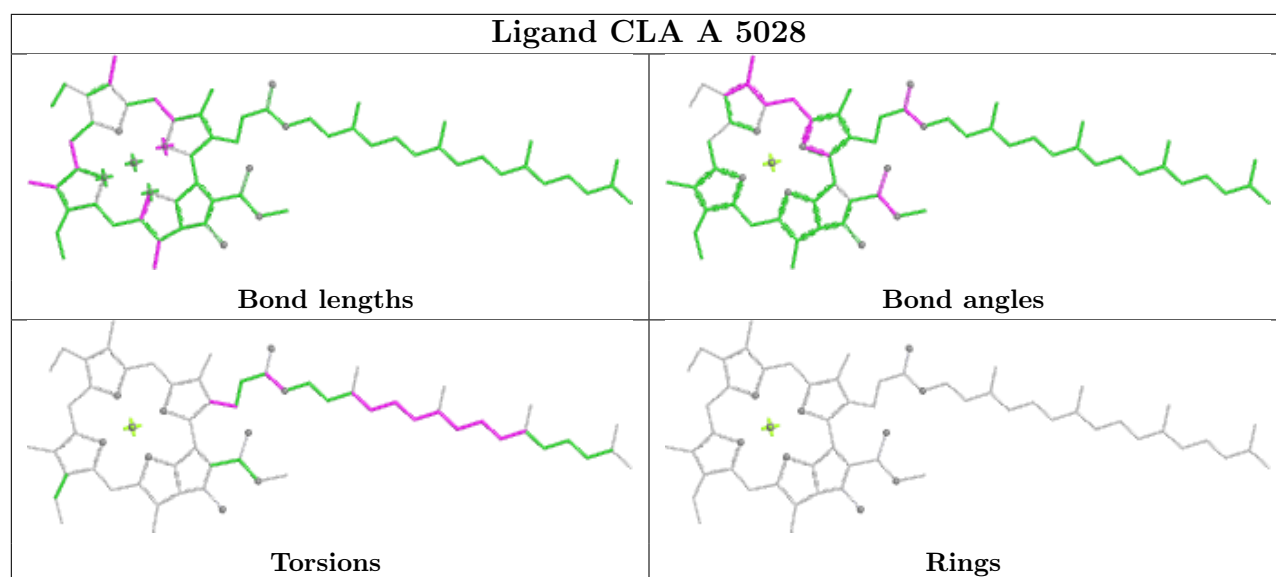
## Ligand CLA 3 324





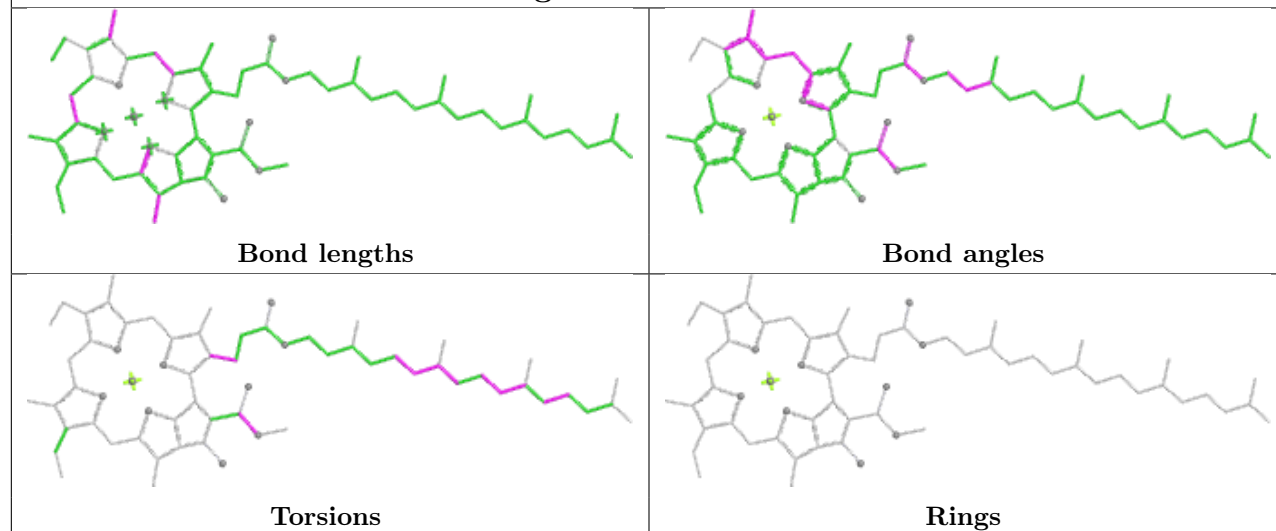




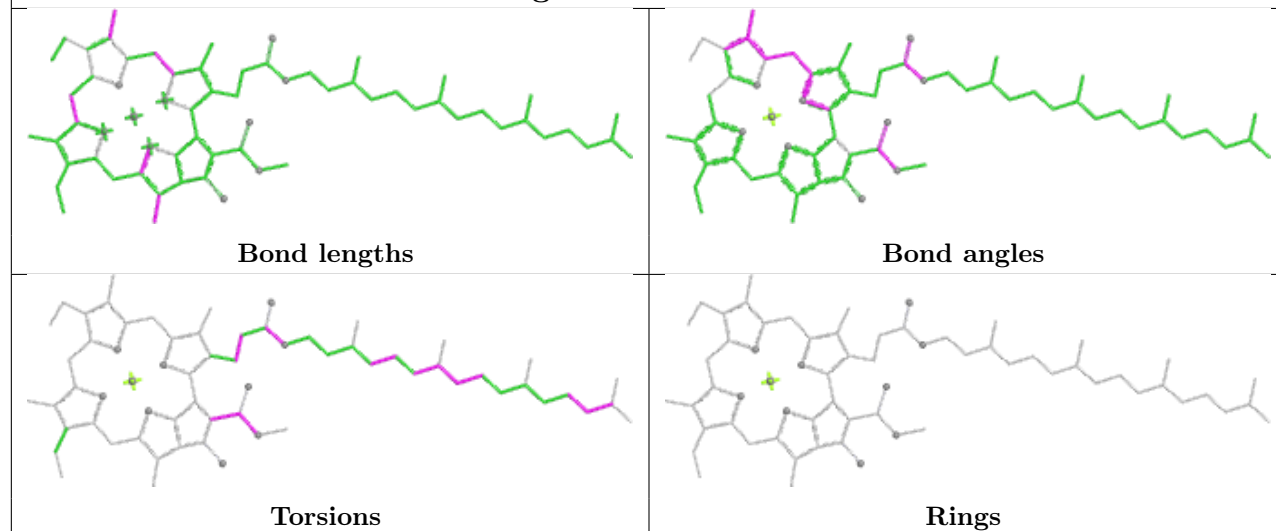




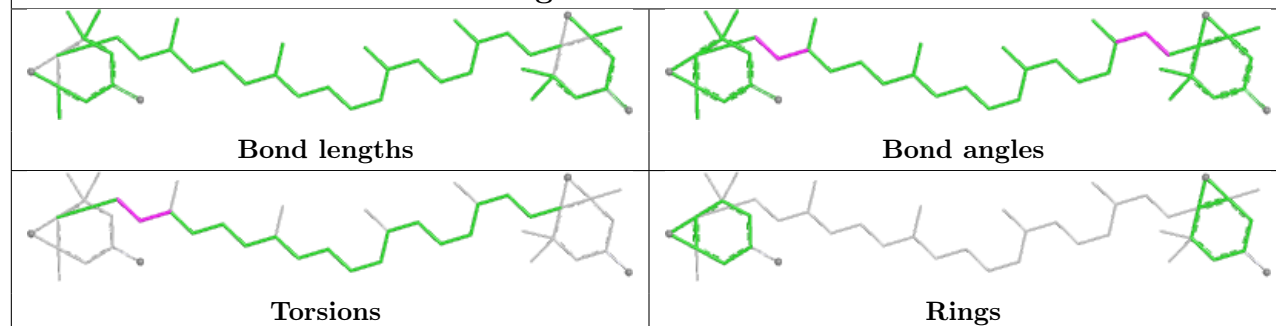
## Ligand CLA L 201



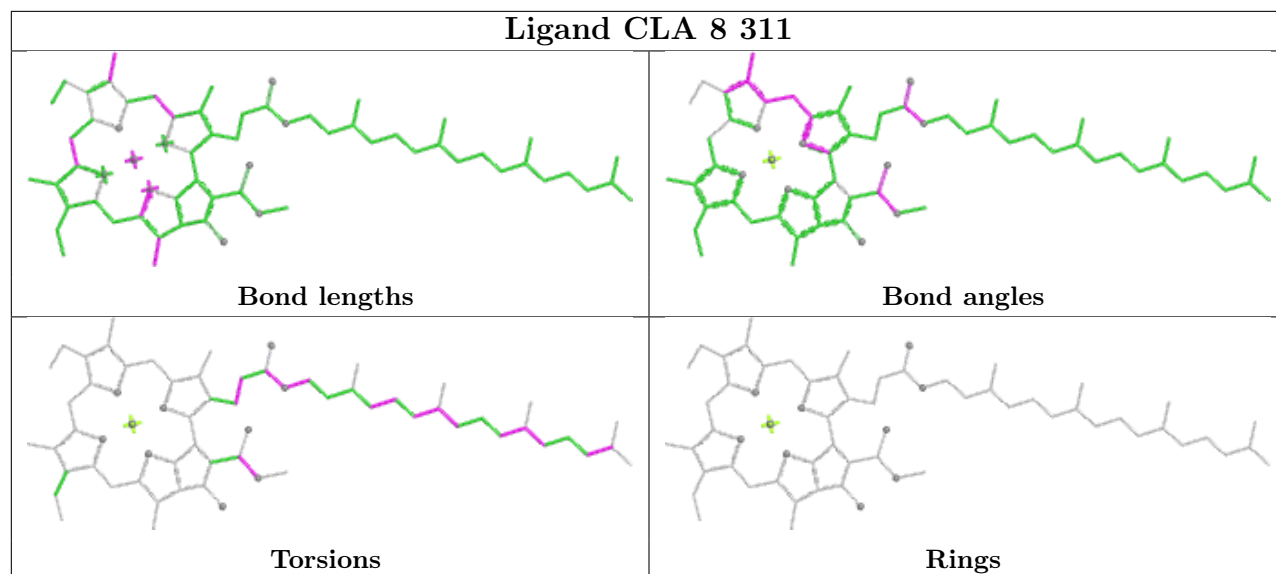
## Ligand CLA B 809



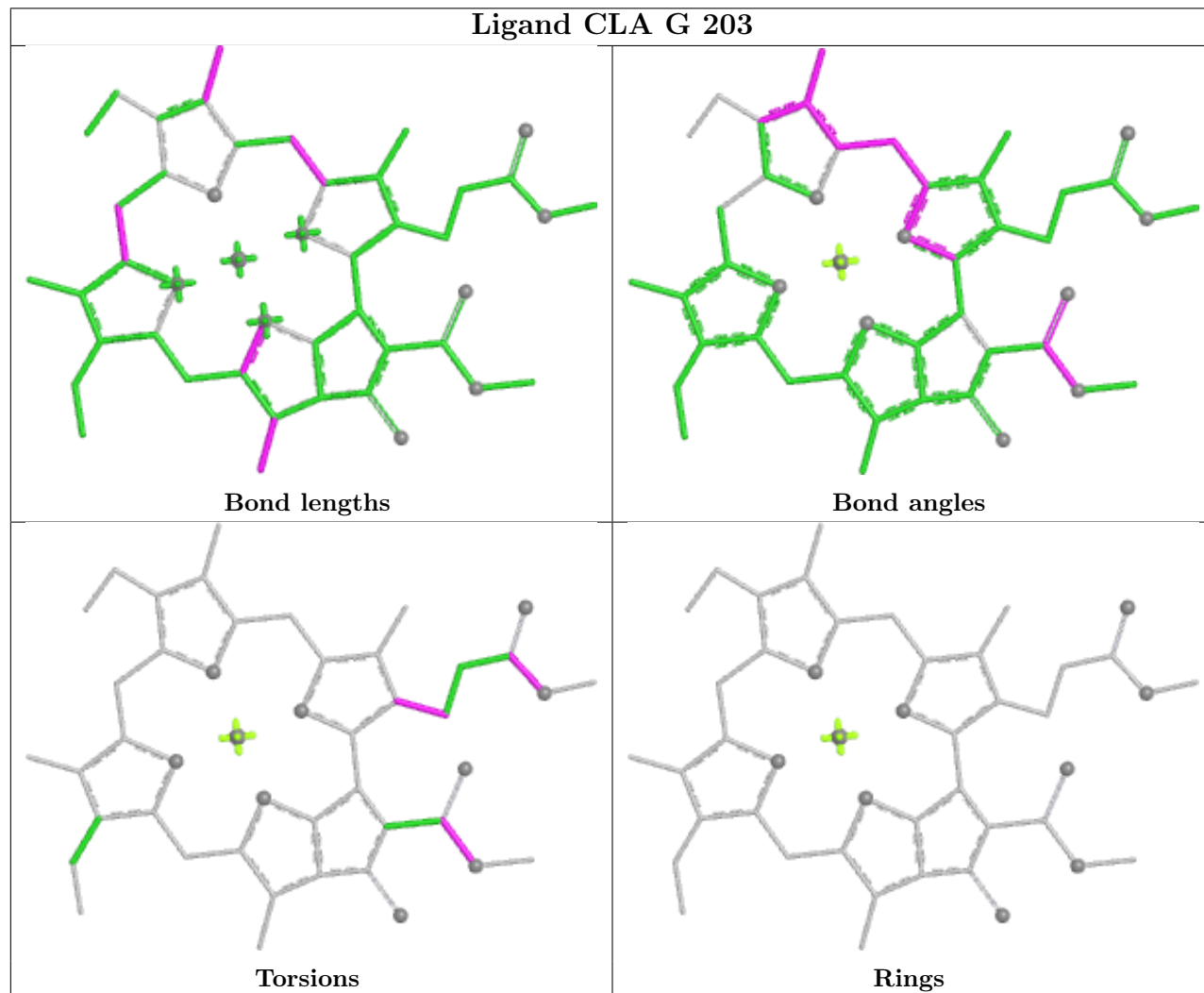
## Ligand XAT 3 316

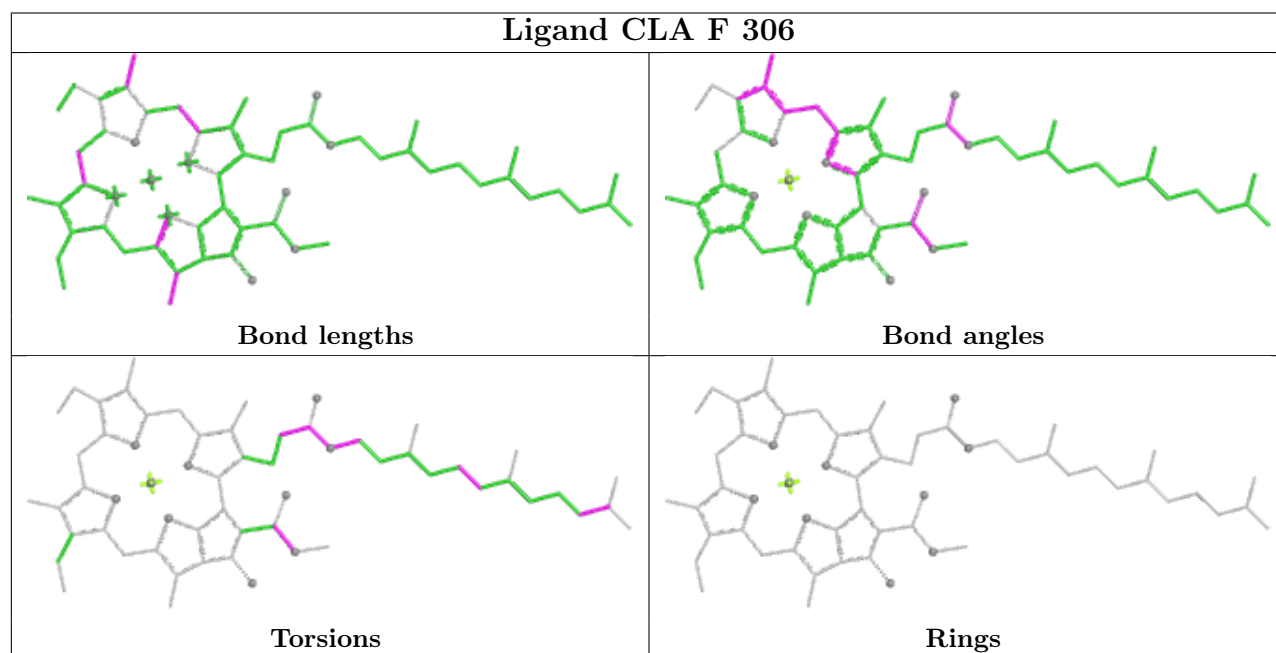
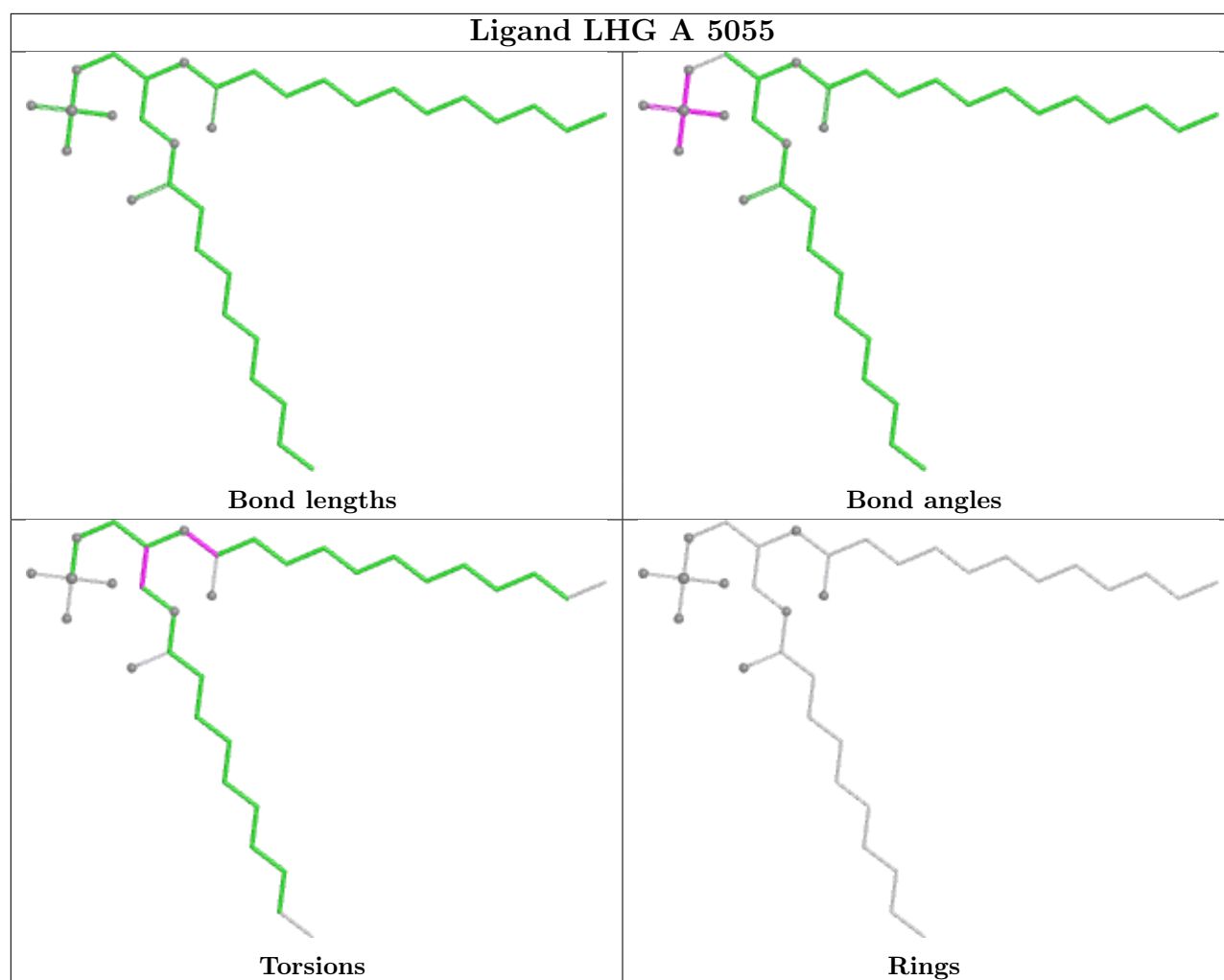


## Ligand CLA 8 311

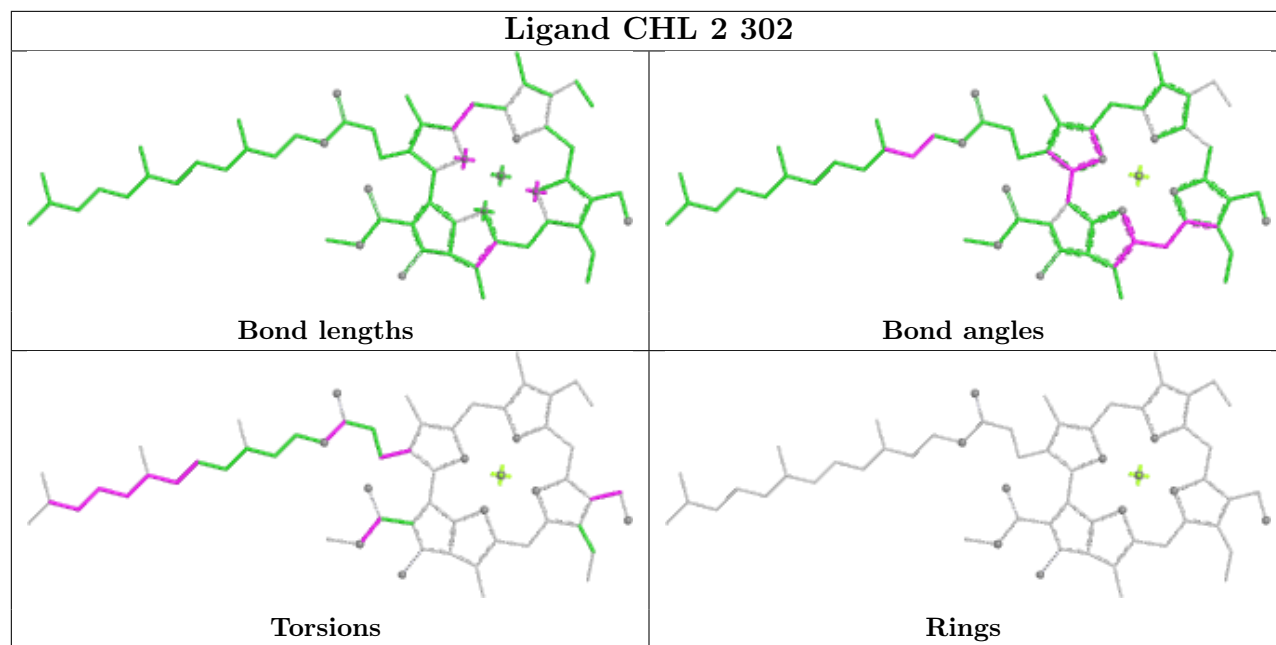


## Ligand CLA G 203

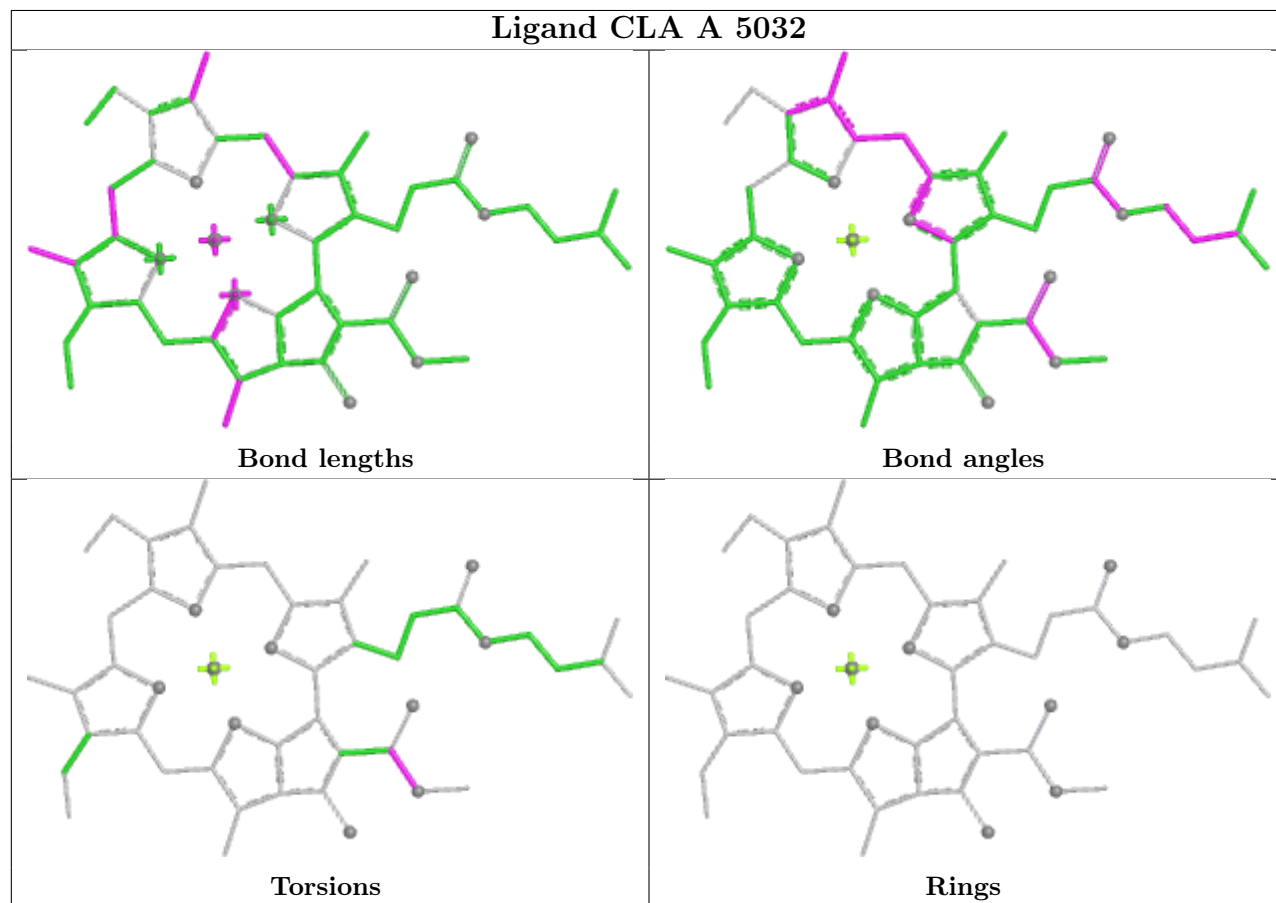


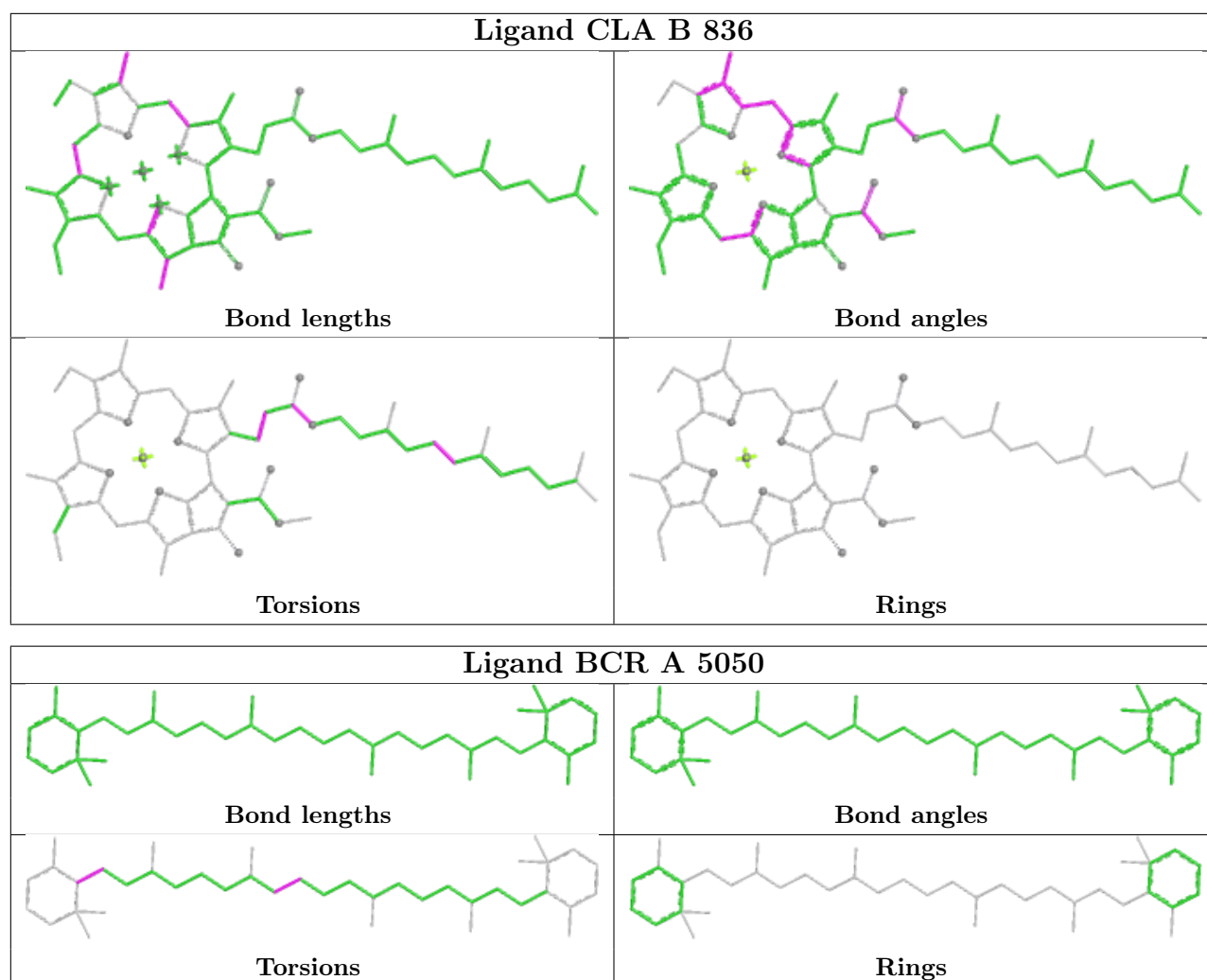


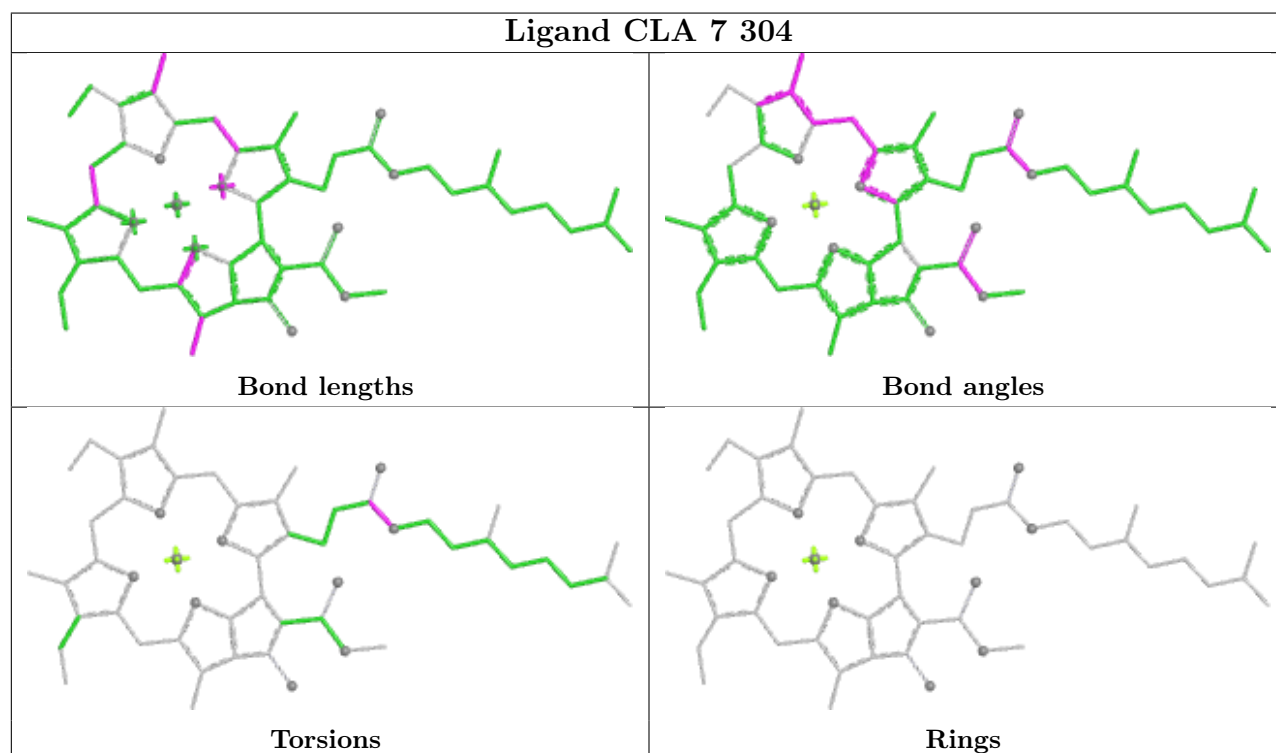
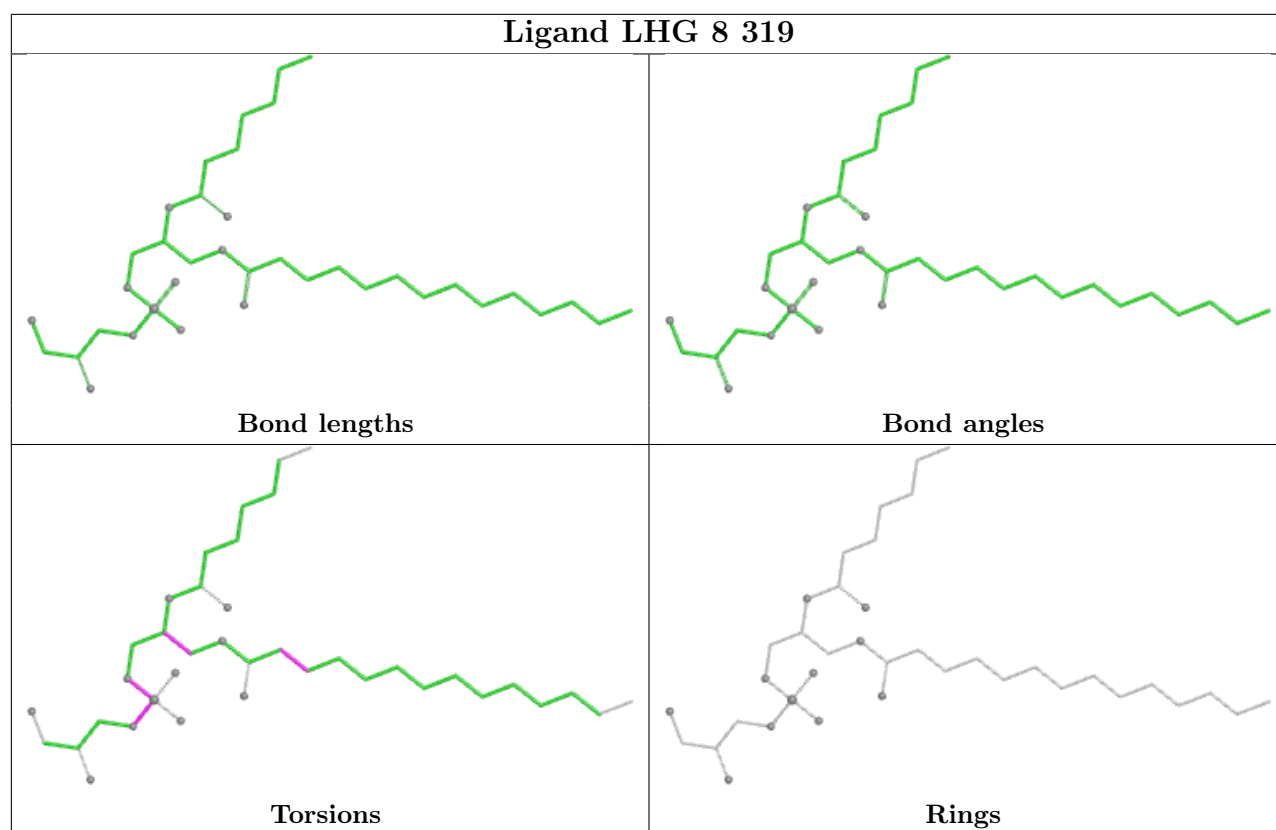
## Ligand CHL 2 302

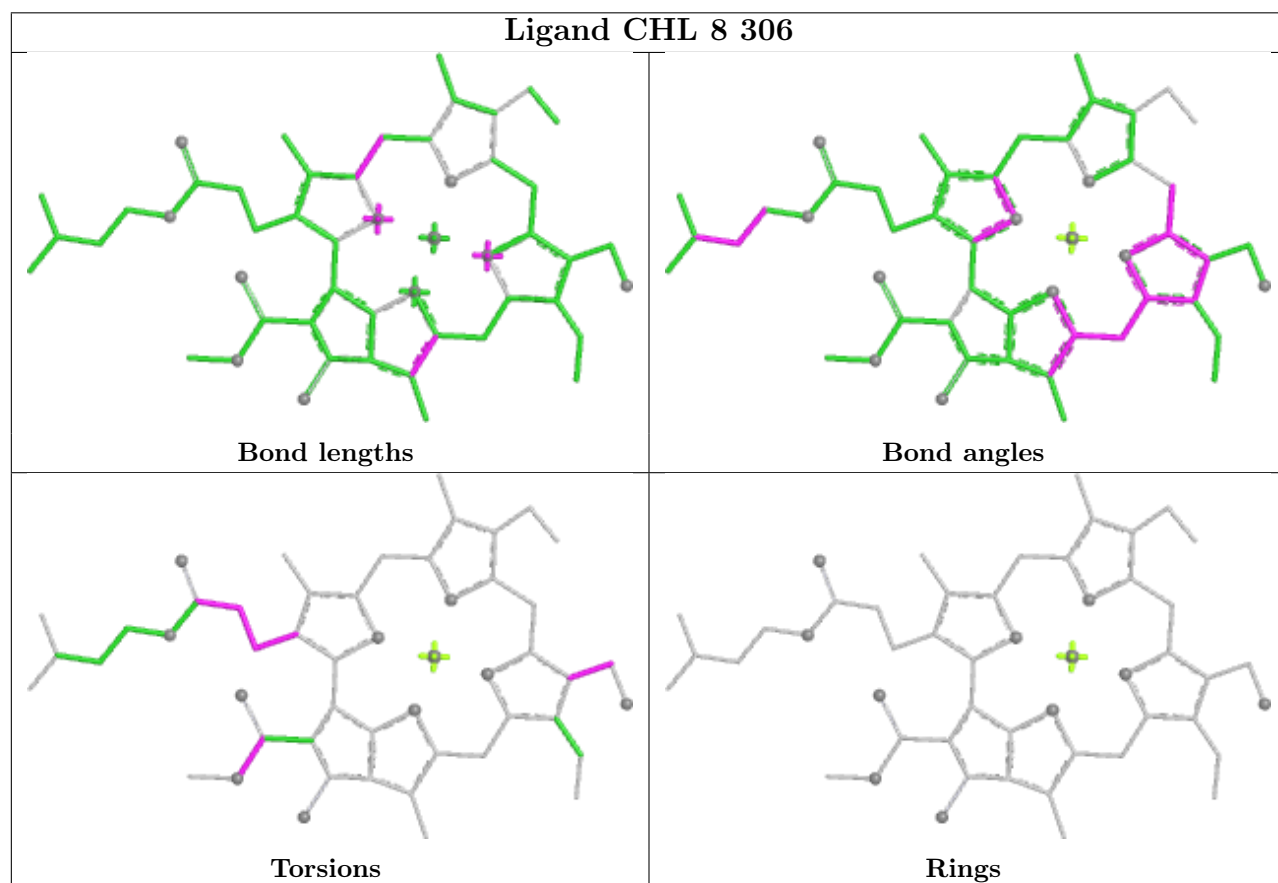
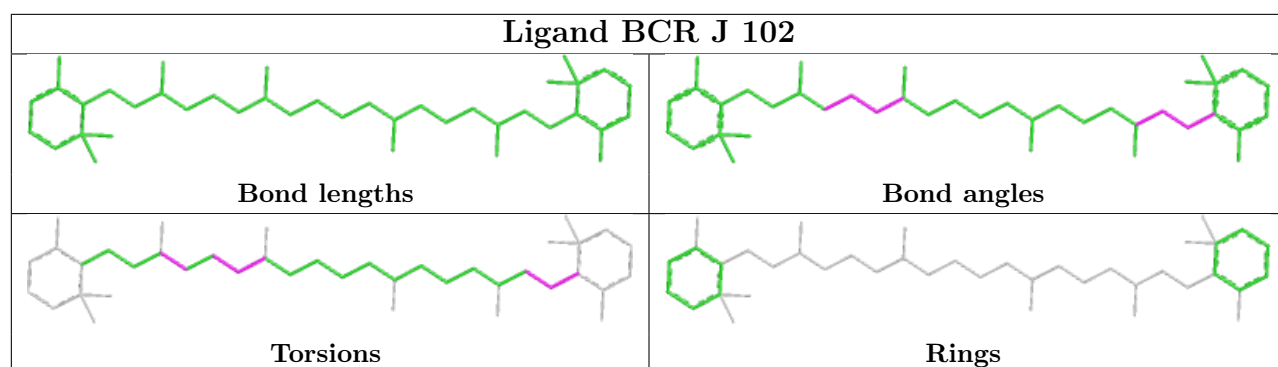


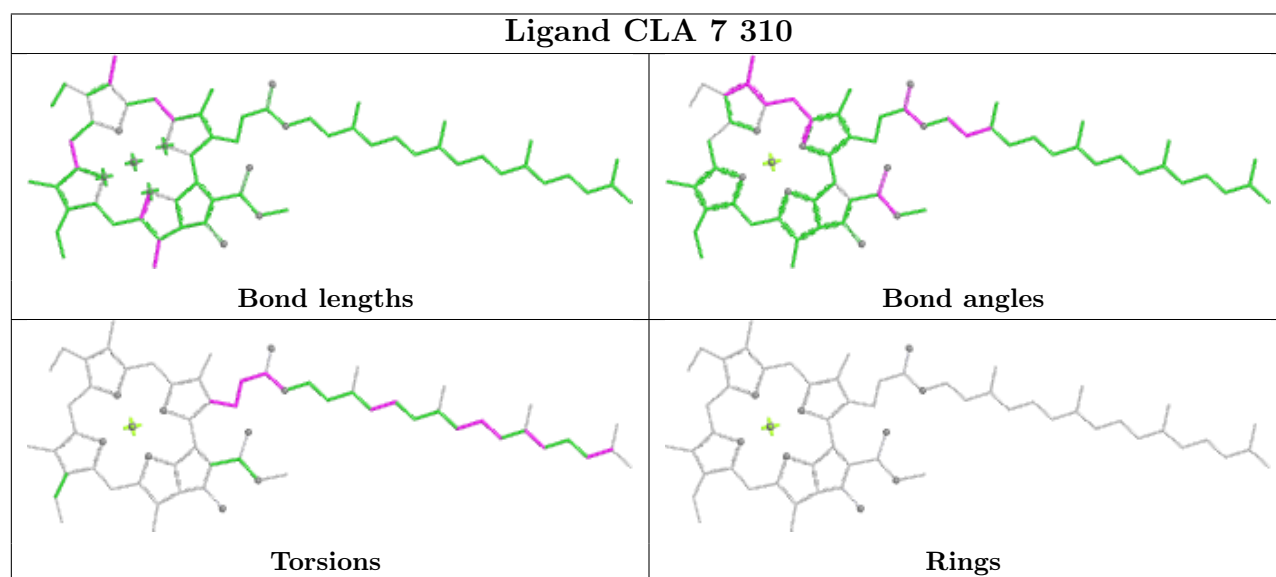
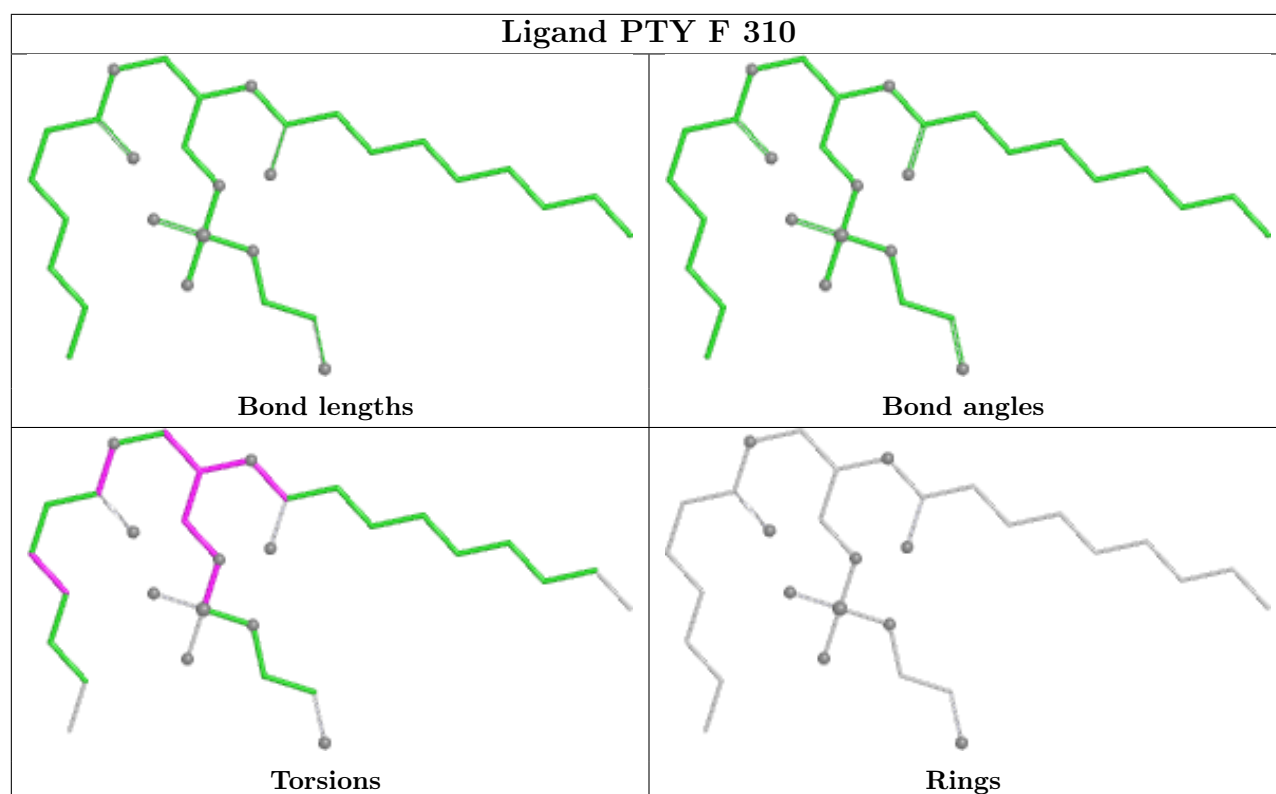
## Ligand CLA A 5032



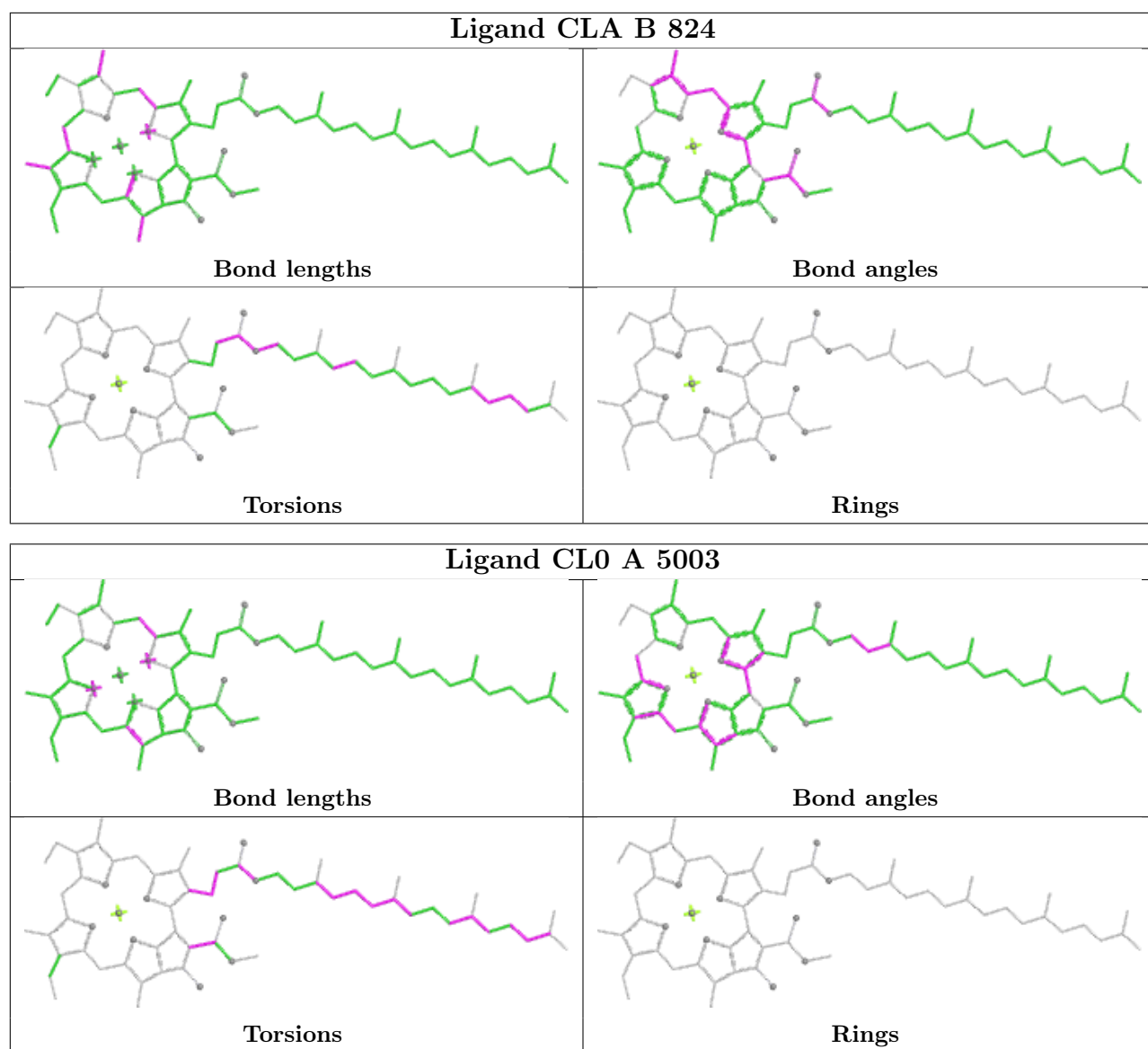


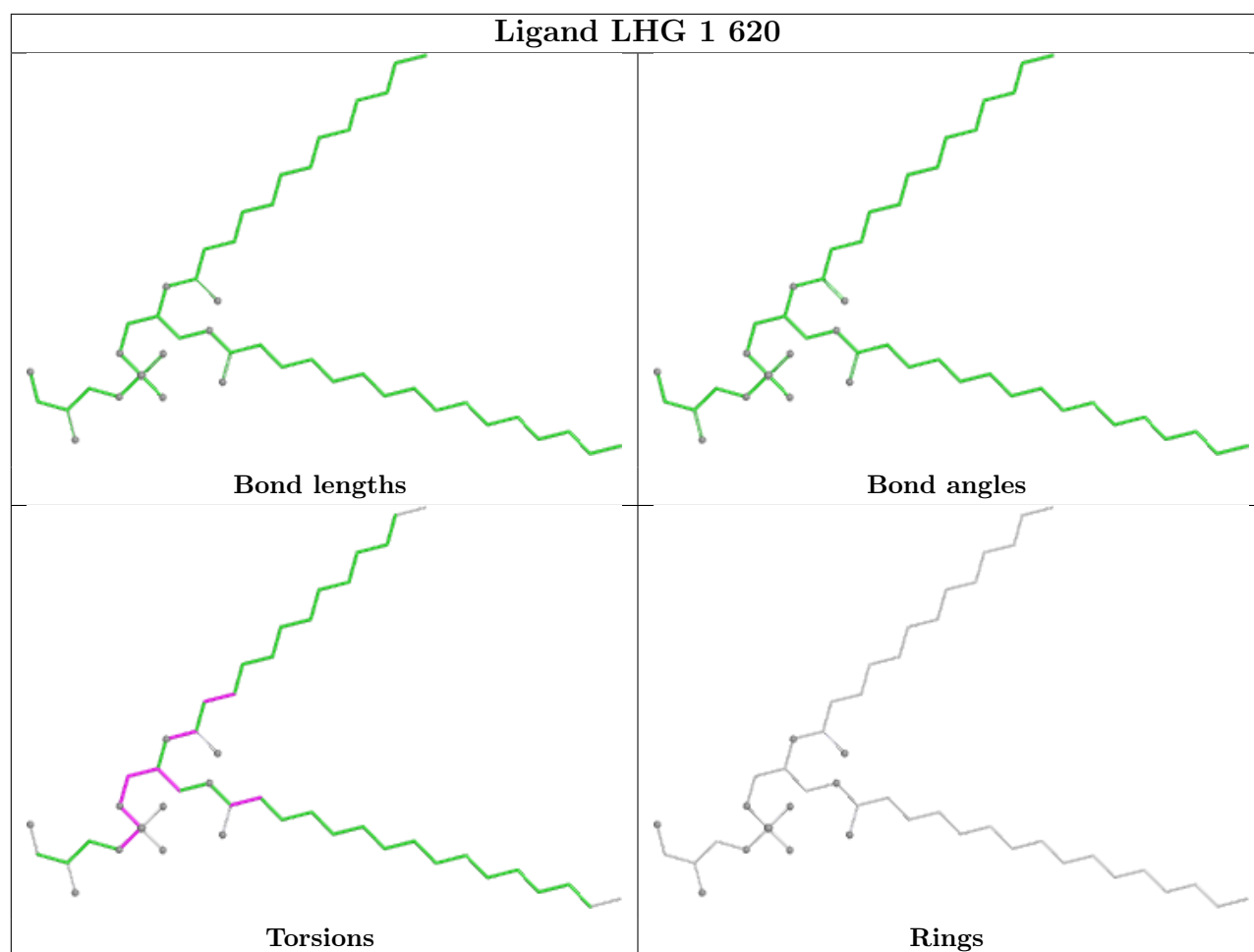


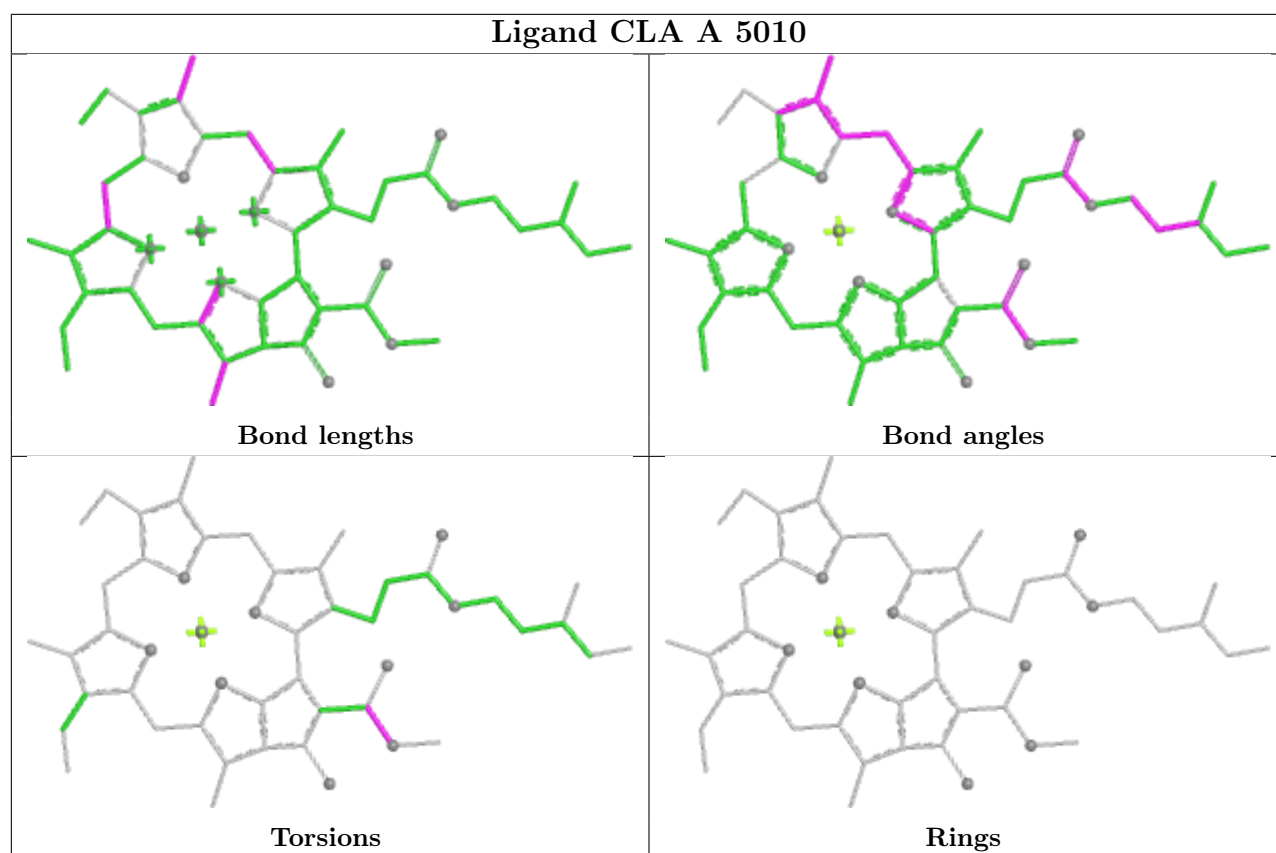




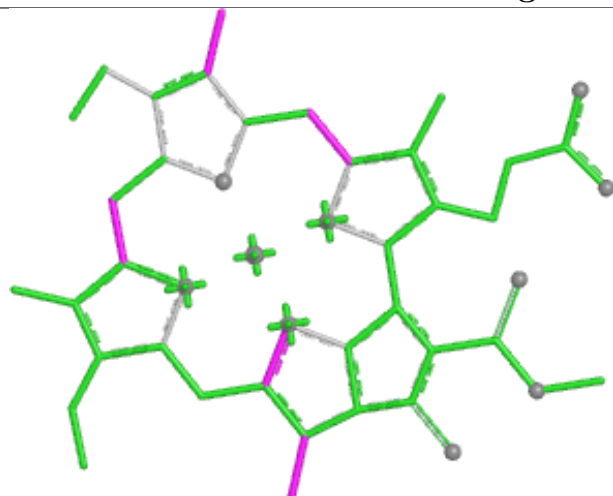




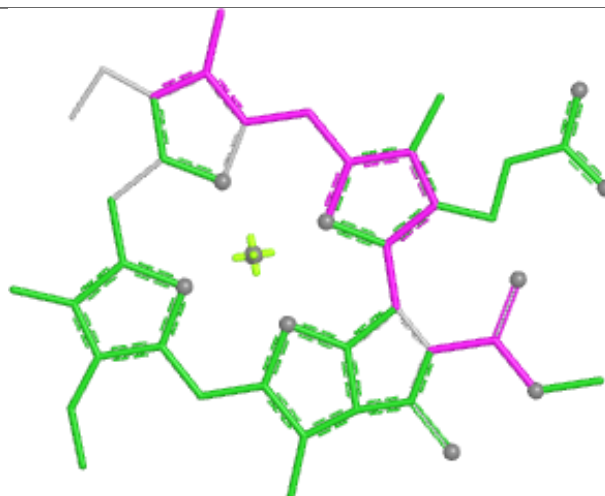




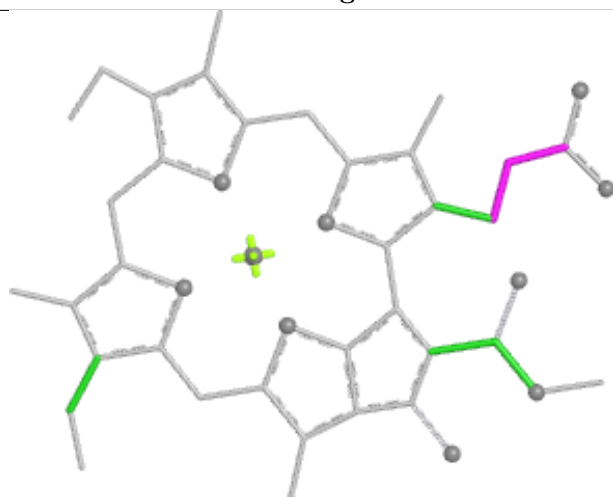
## Ligand CLA 2 308



Bond lengths



Bond angles

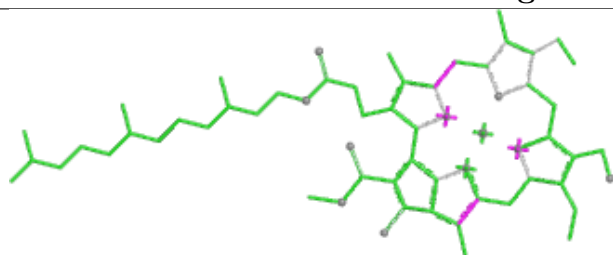


Torsions

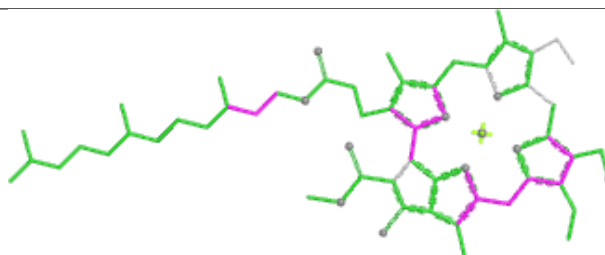


Rings

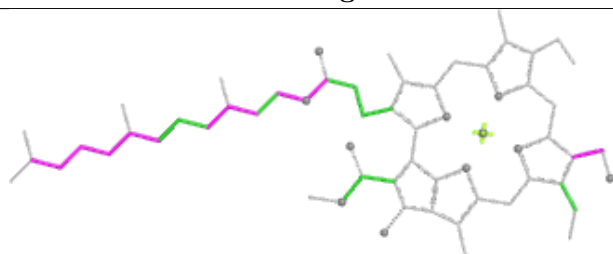
## Ligand CHL 3 323



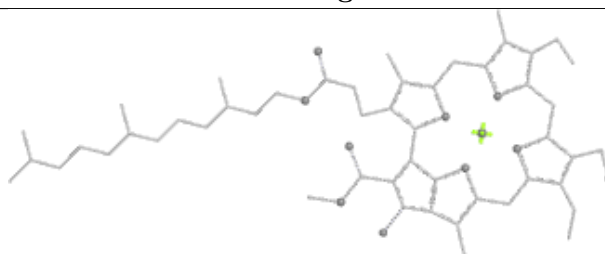
Bond lengths



Bond angles

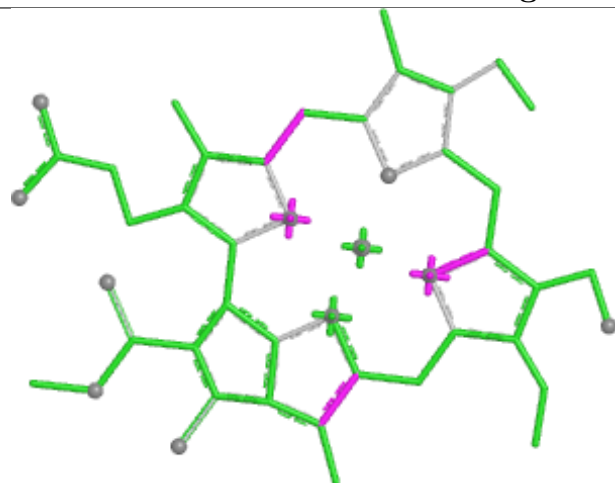


Torsions

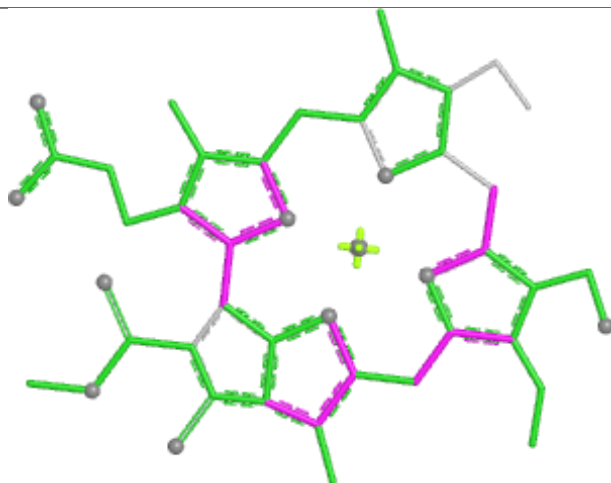


Rings

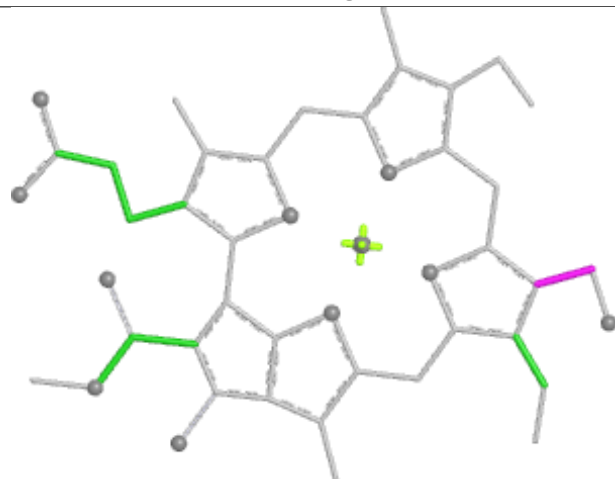
## Ligand CHL 7 306



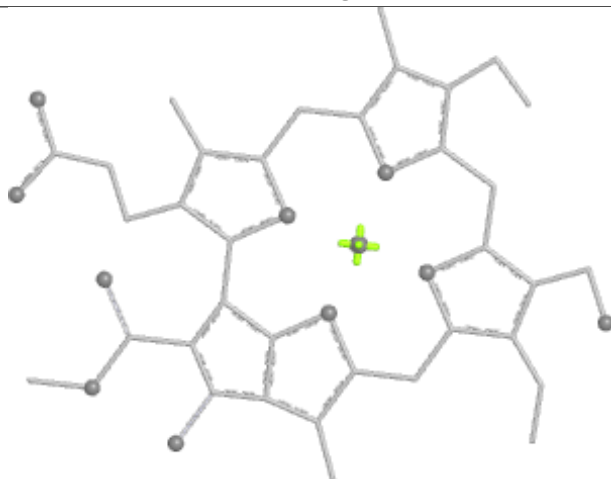
Bond lengths



Bond angles

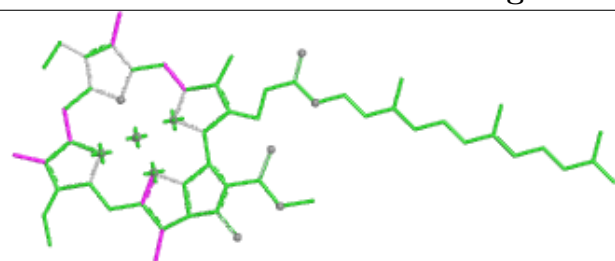


Torsions

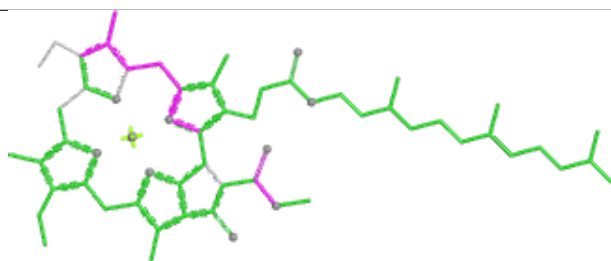


Rings

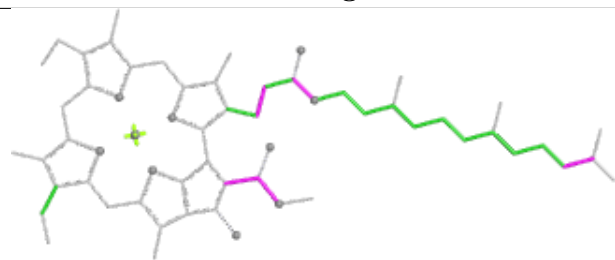
## Ligand CLA A 5018



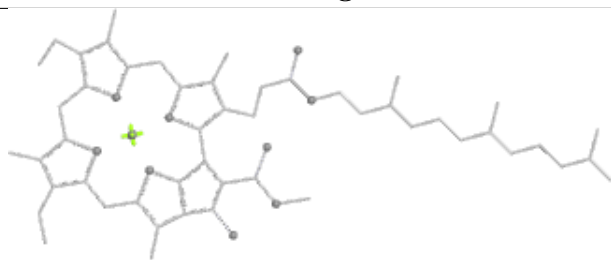
Bond lengths



Bond angles

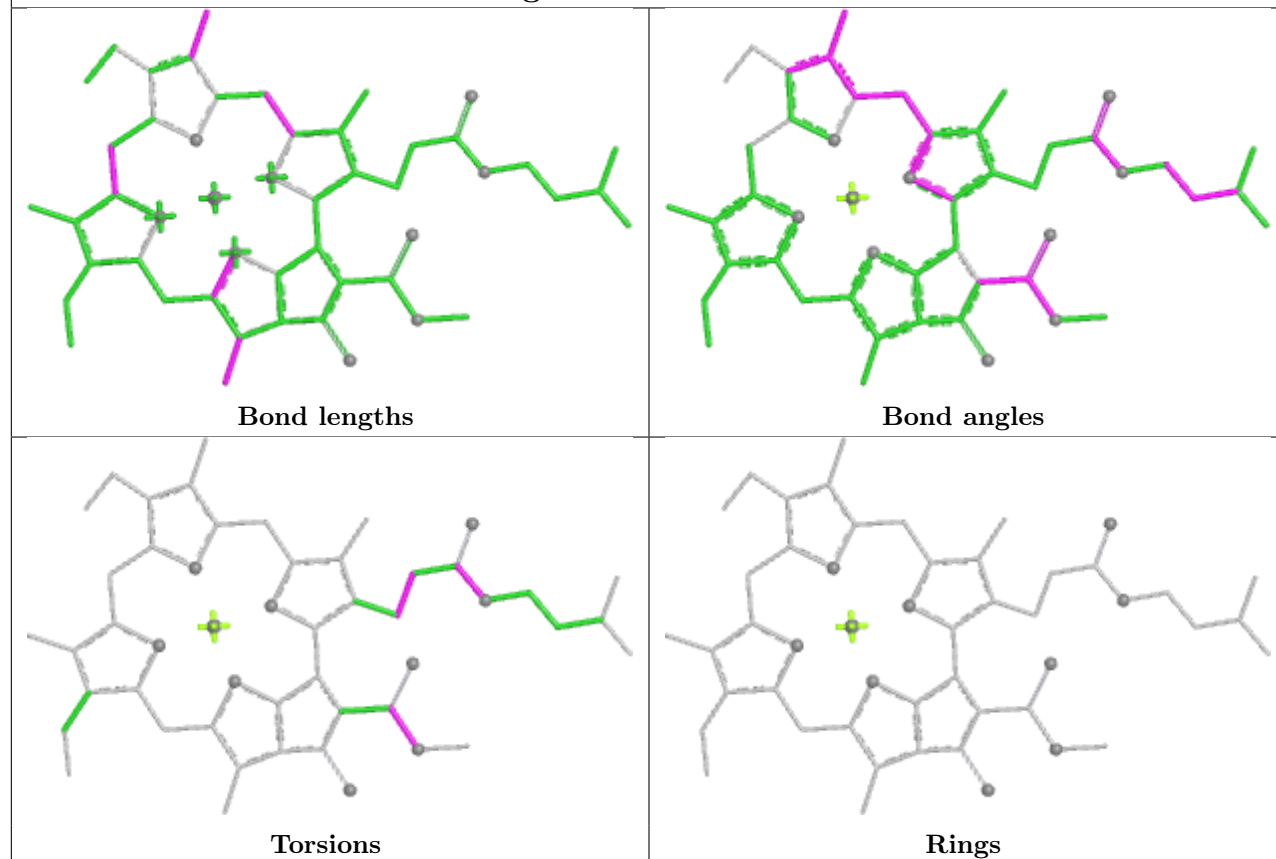


Torsions

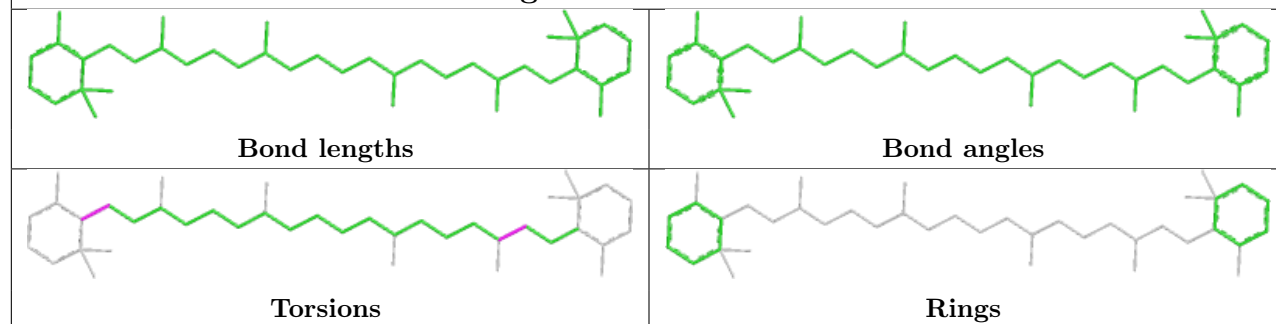


Rings

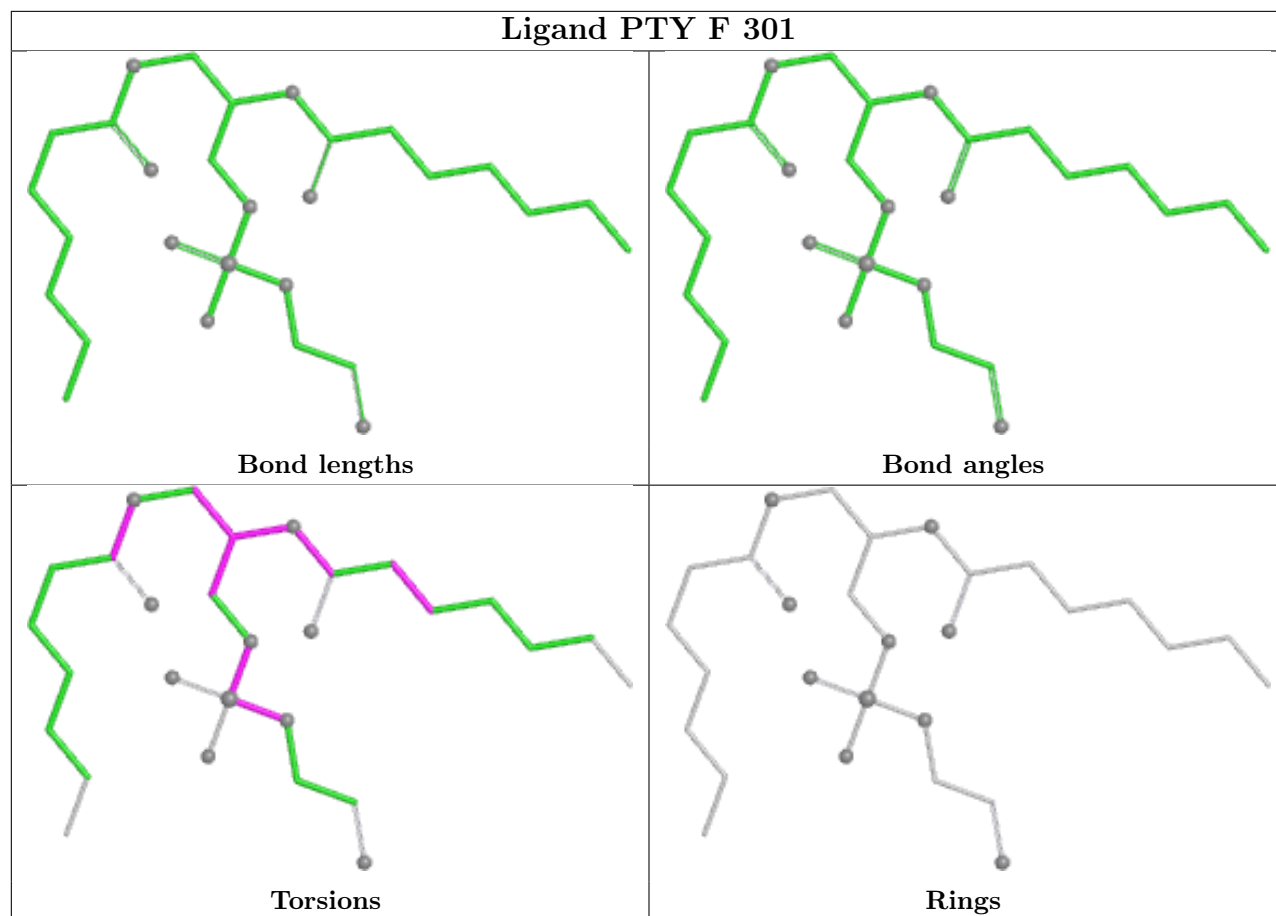
## Ligand CLA A 5023



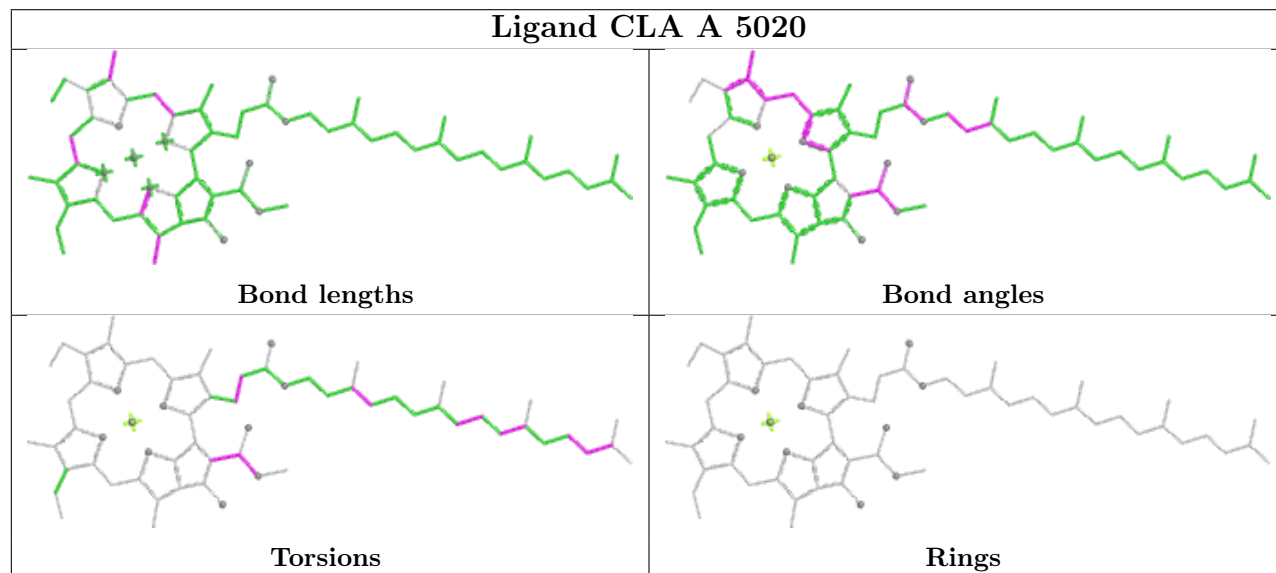
## Ligand BCR K 4001



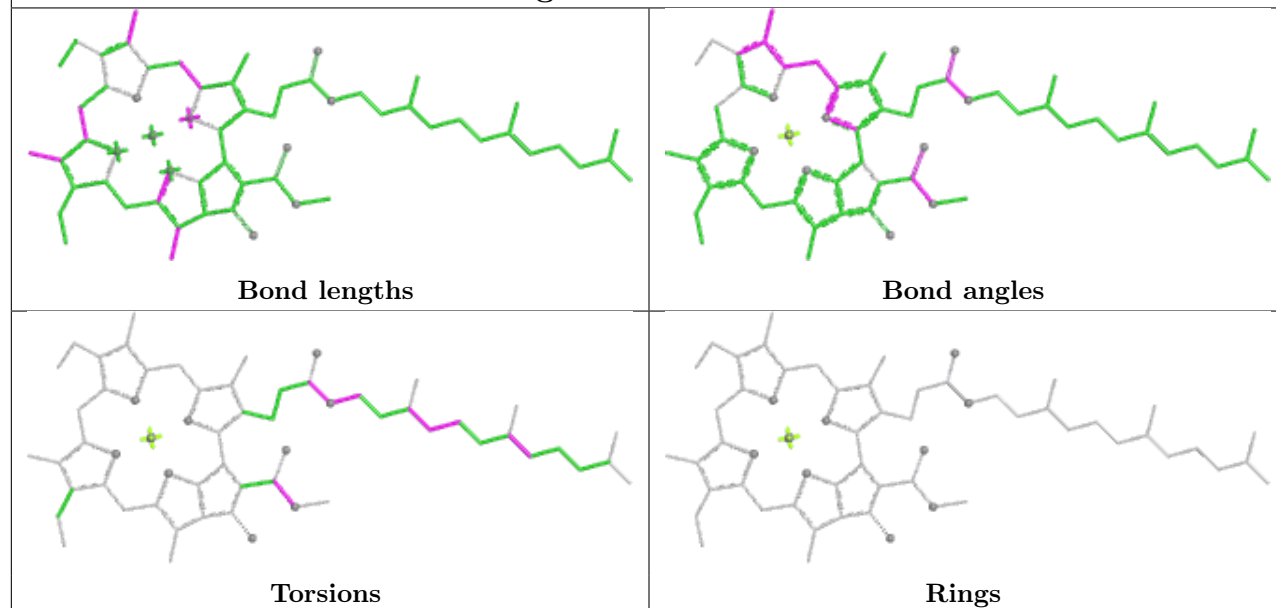
## Ligand PTY F 301



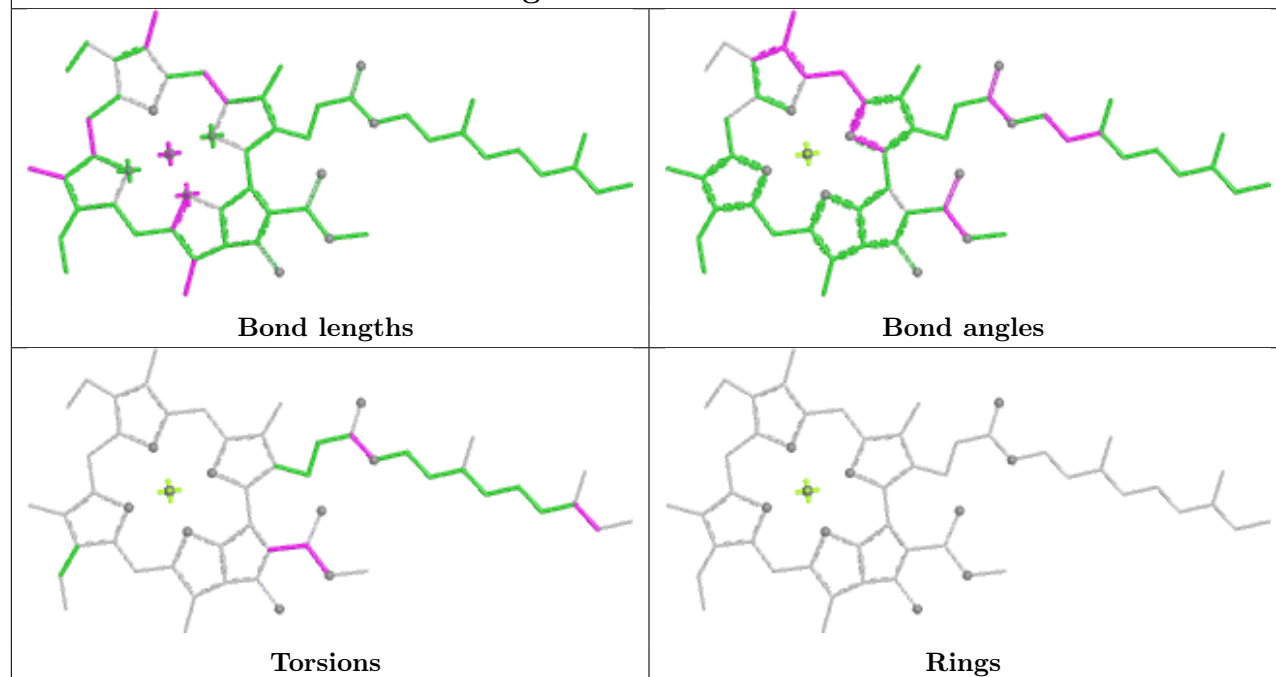
## Ligand CLA A 5020



## Ligand CLA 8 309

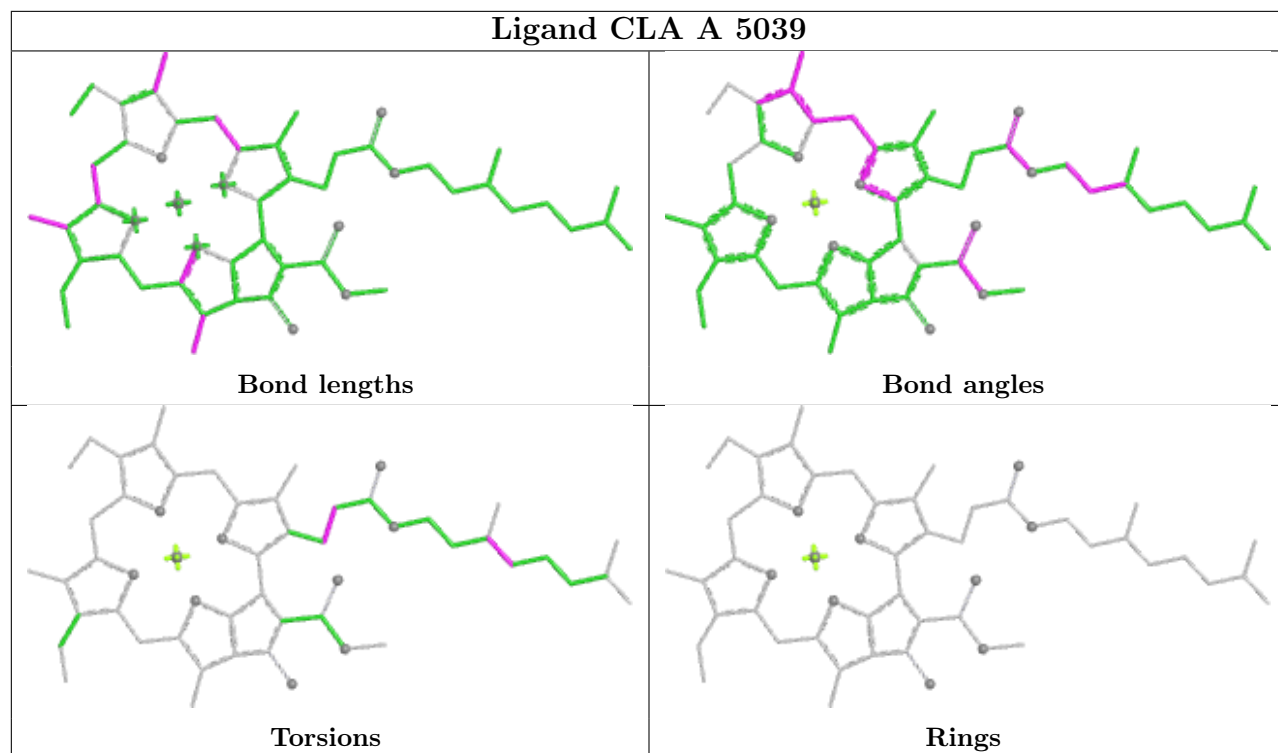


## Ligand CLA A 5027

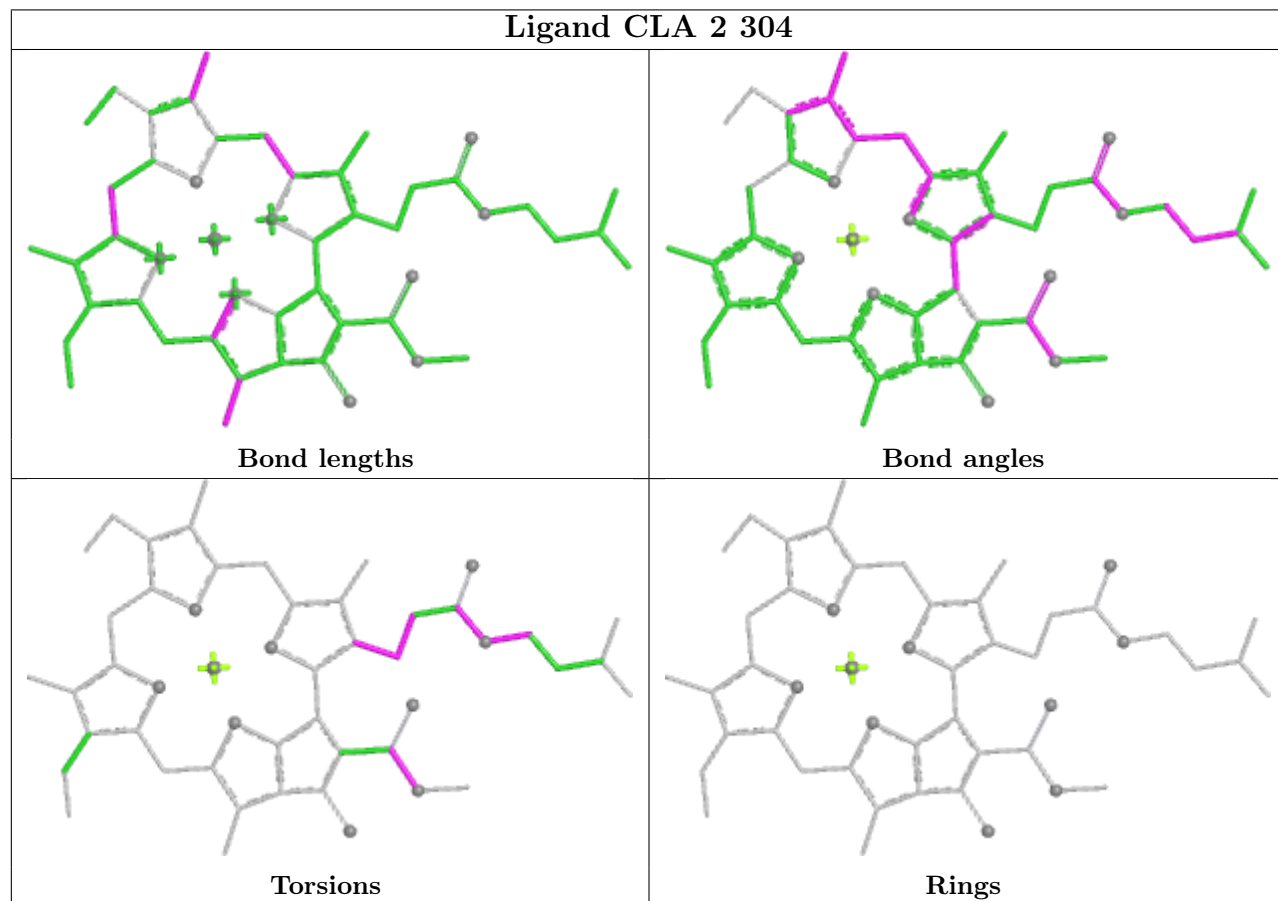


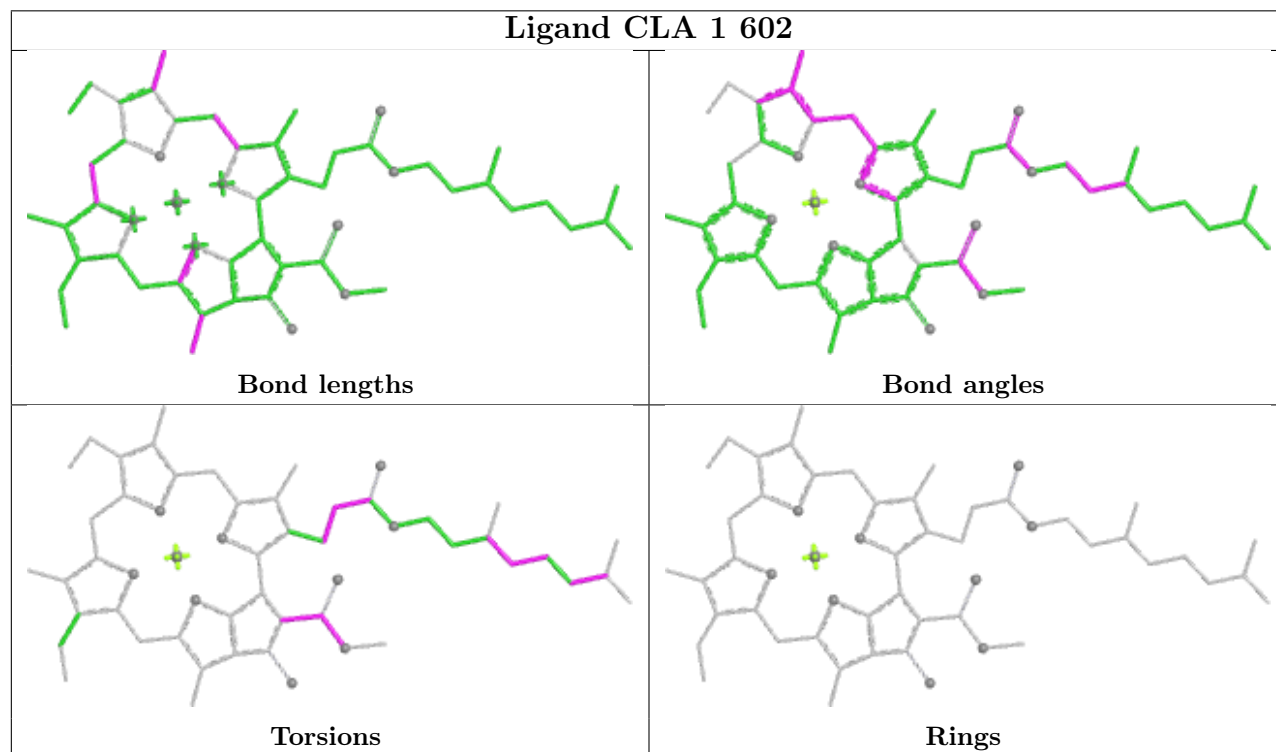
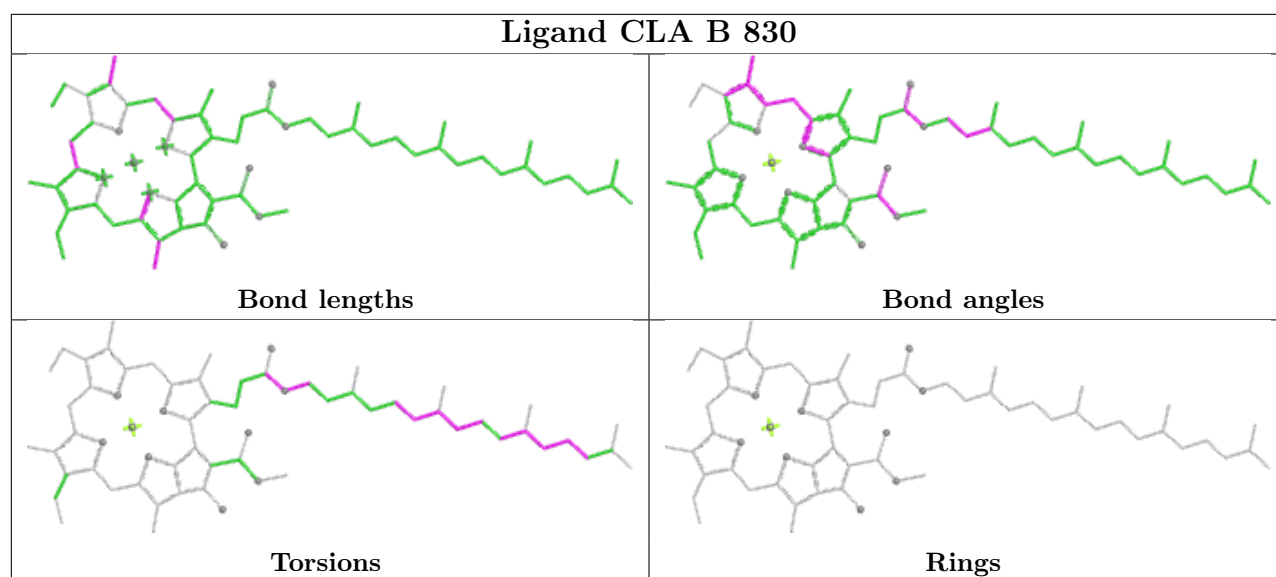


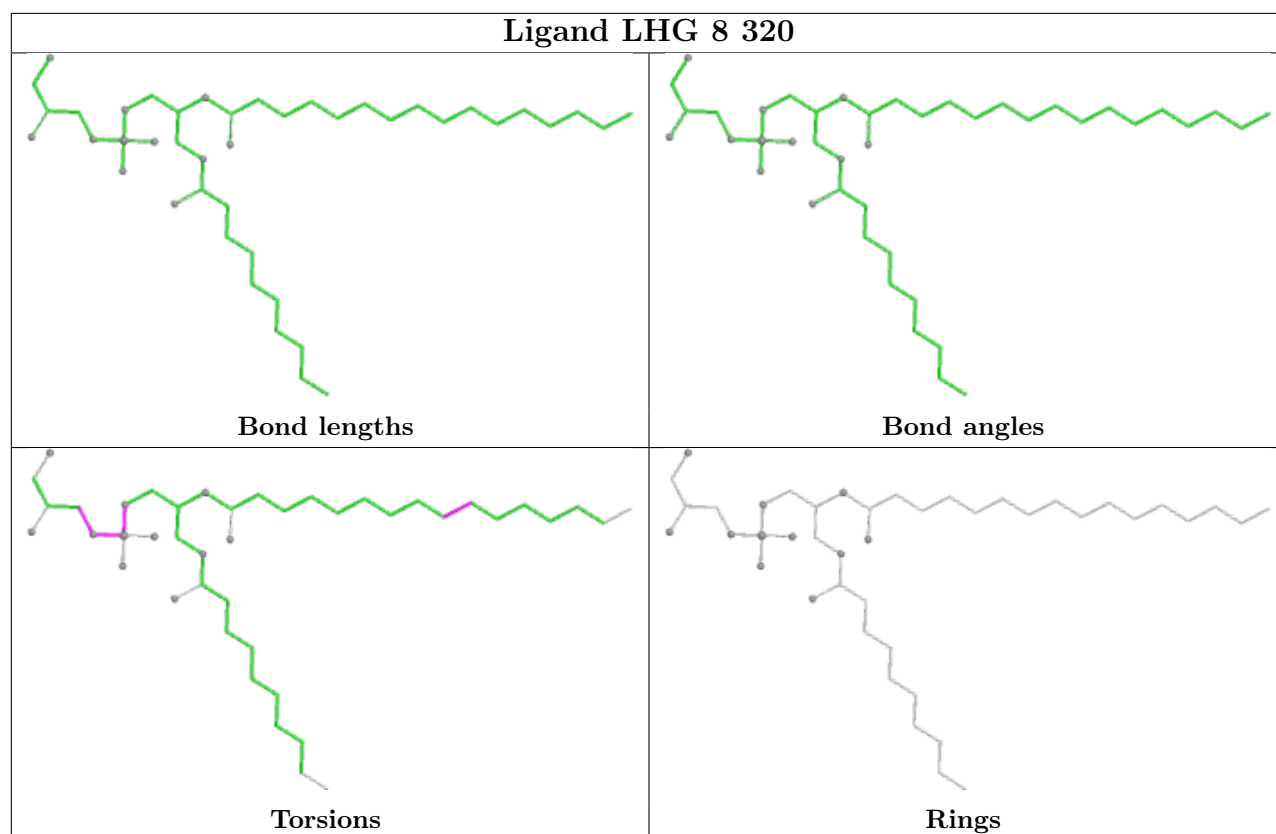
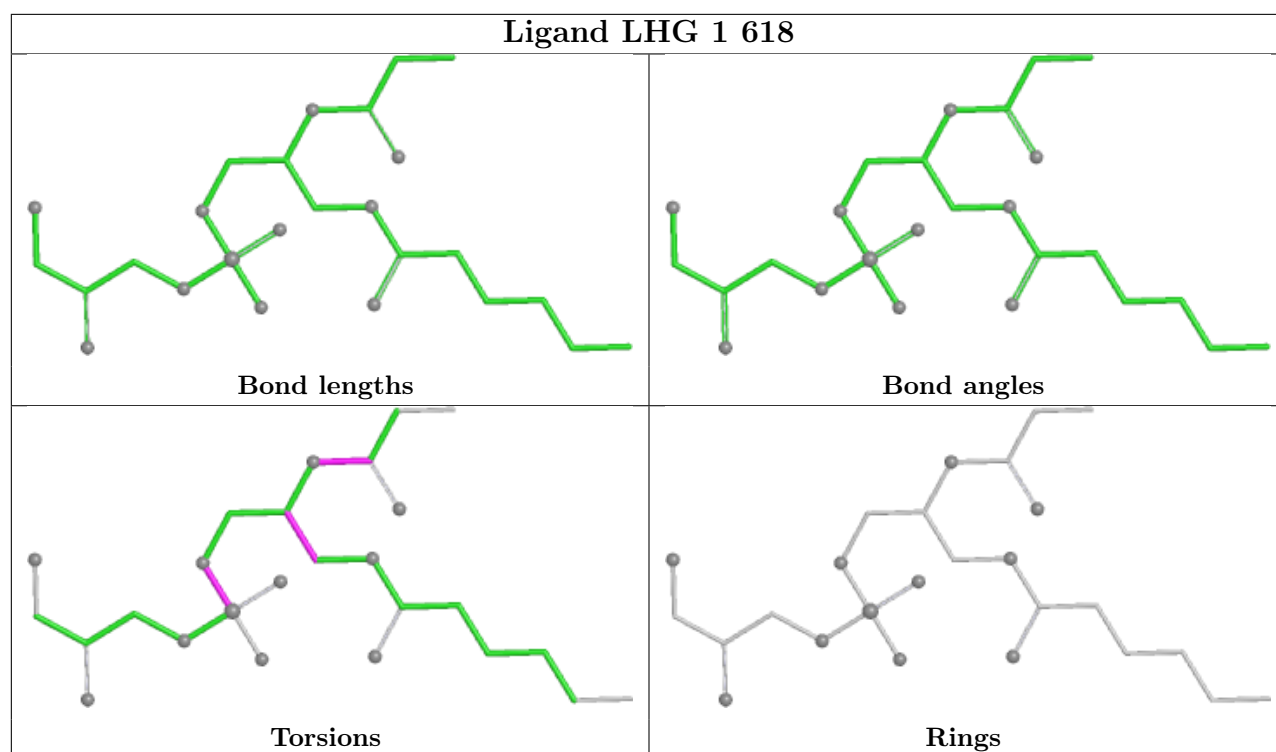
## Ligand CLA A 5039

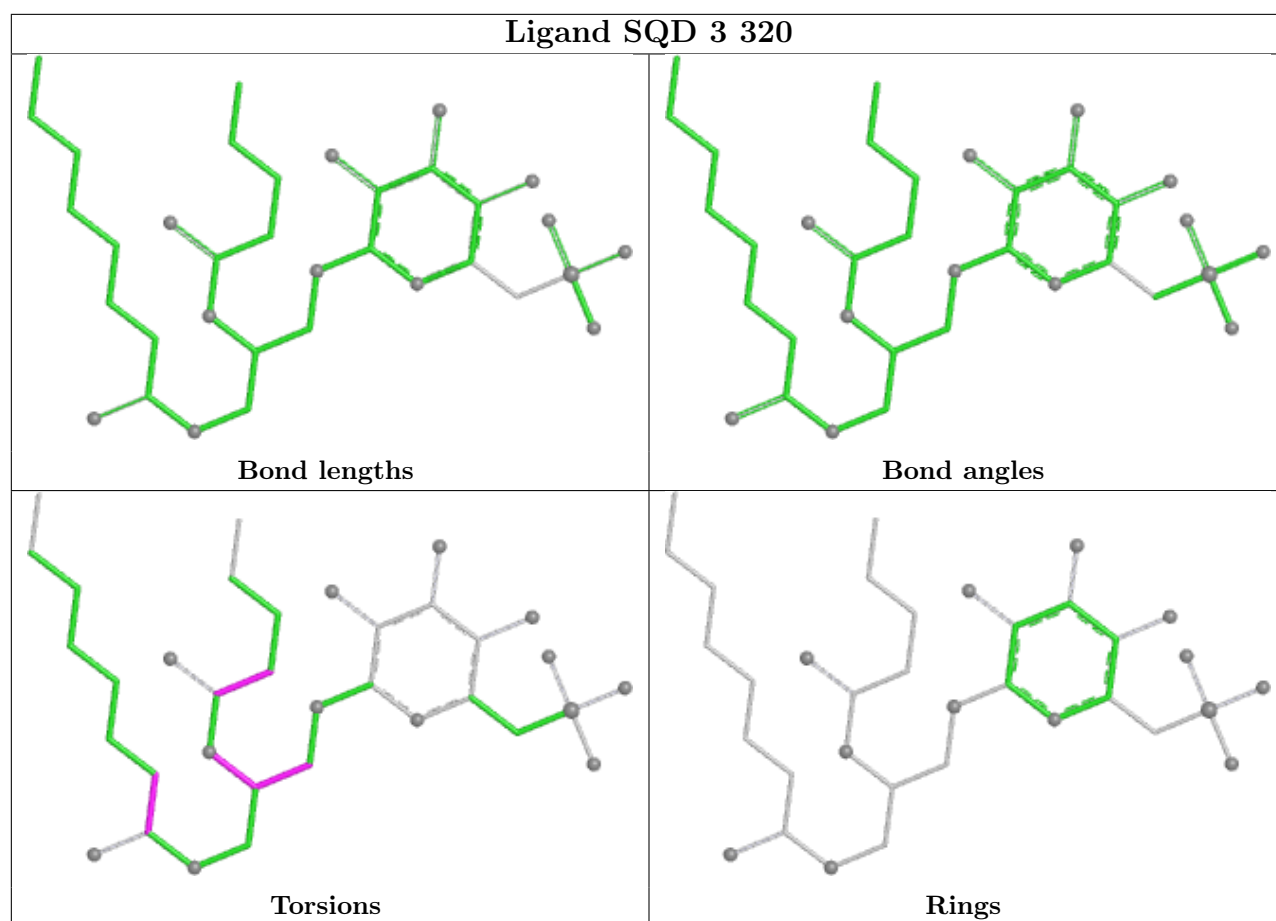


## Ligand CLA 2 304

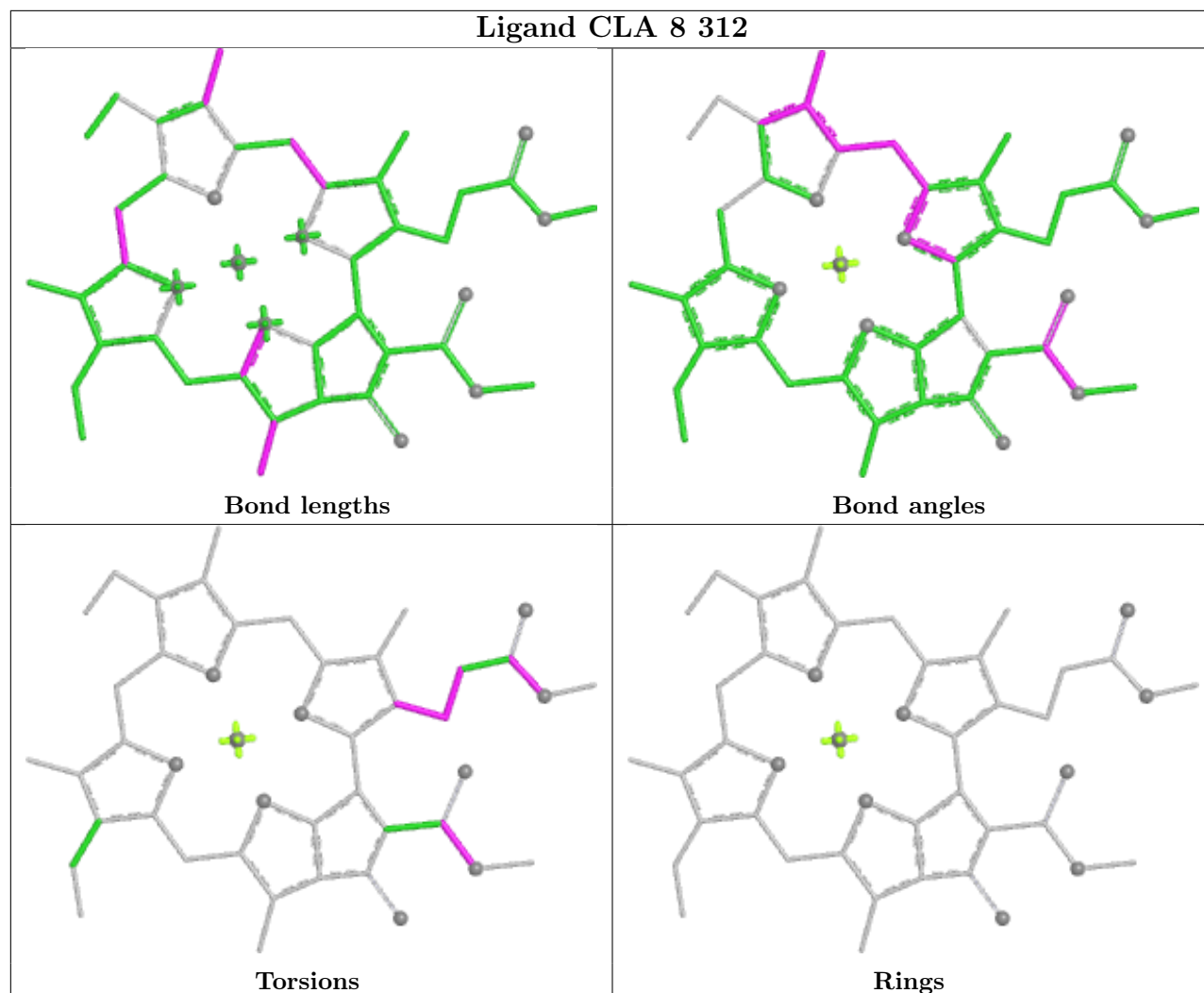




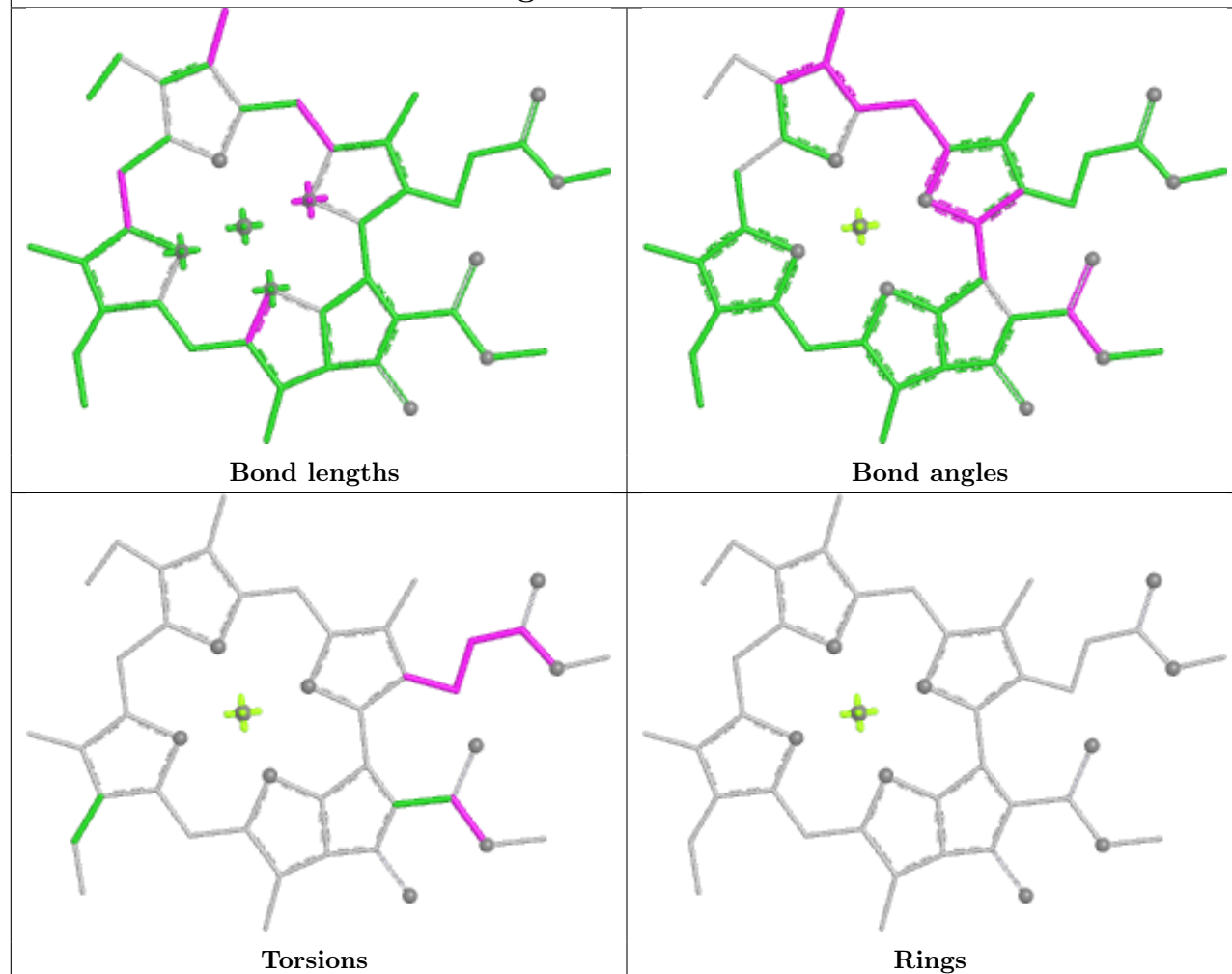




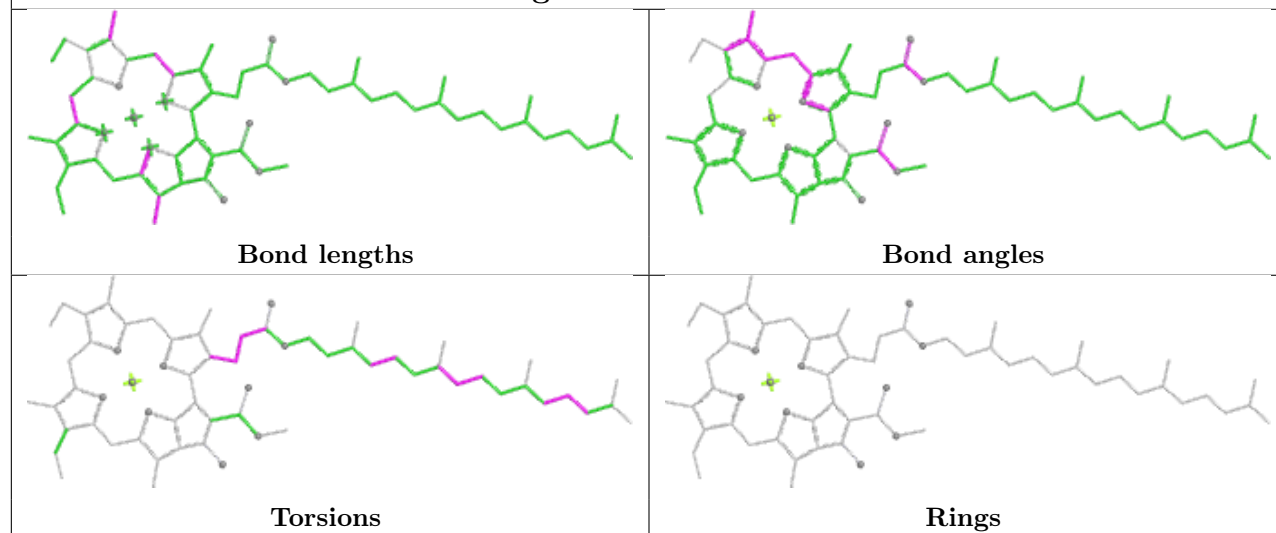
## Ligand CLA 8 312

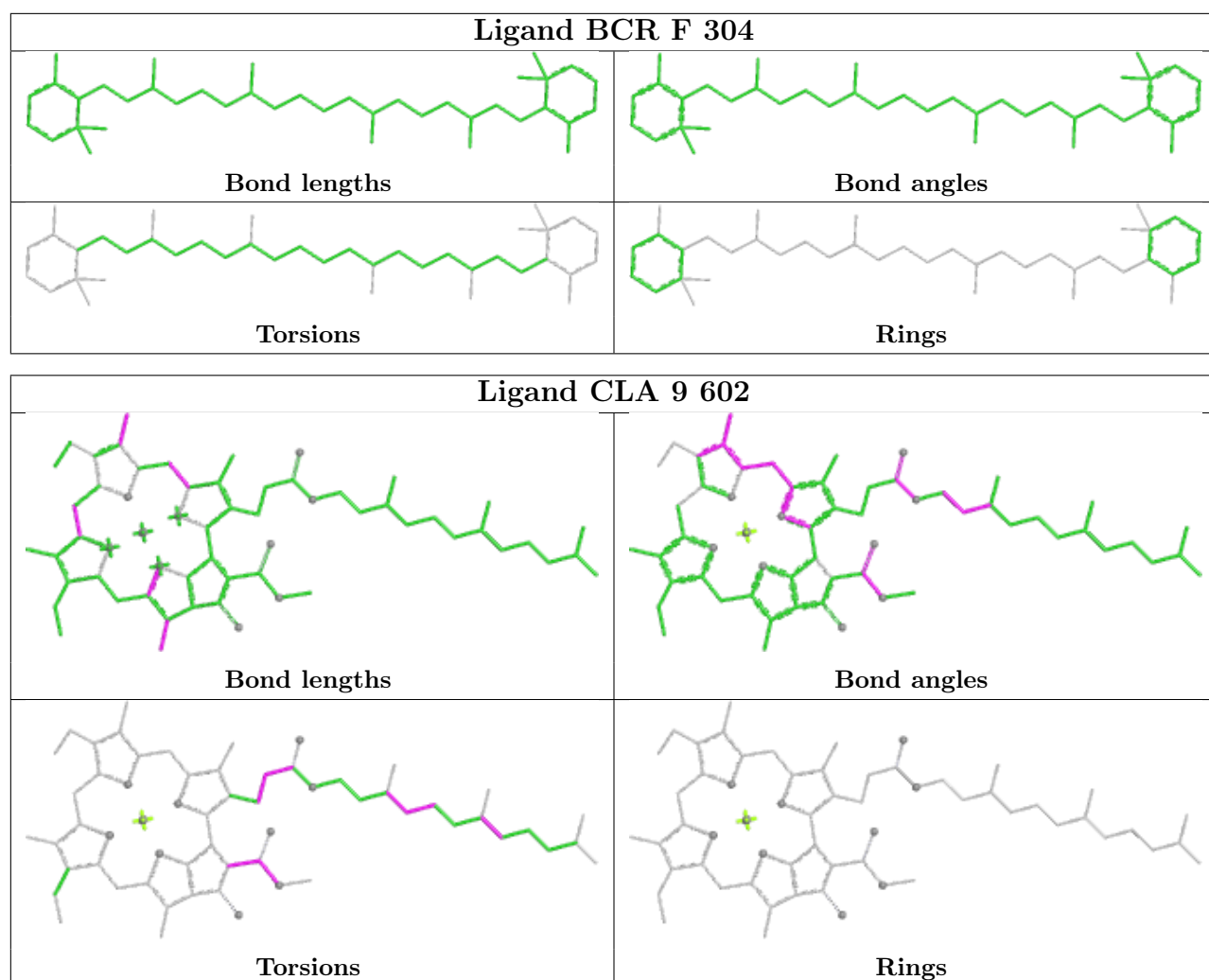


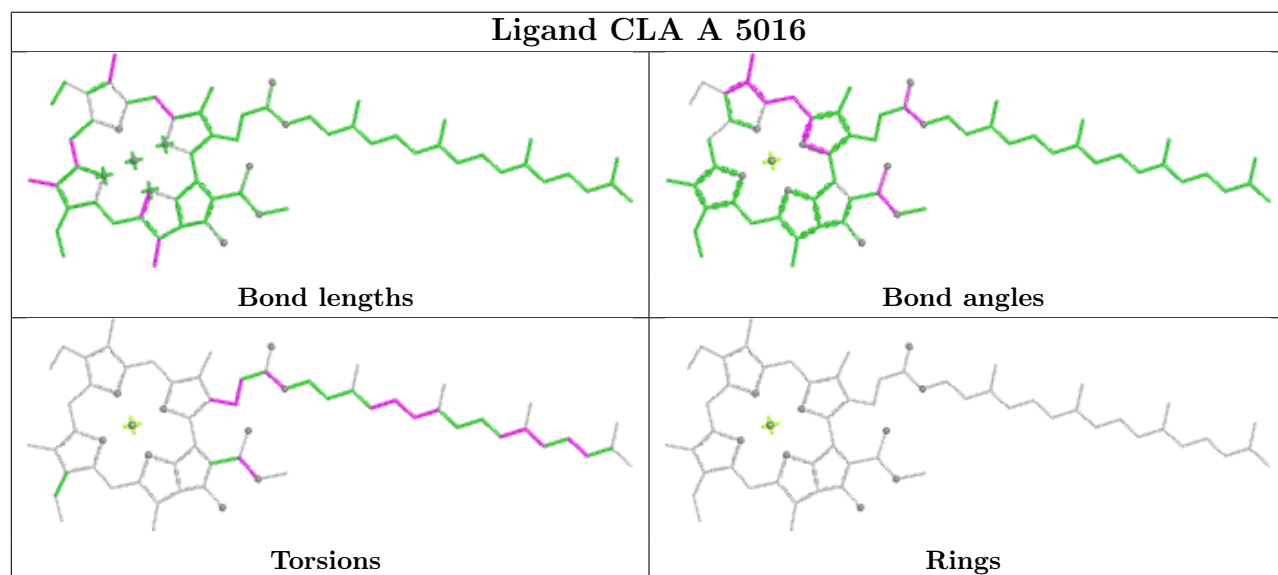
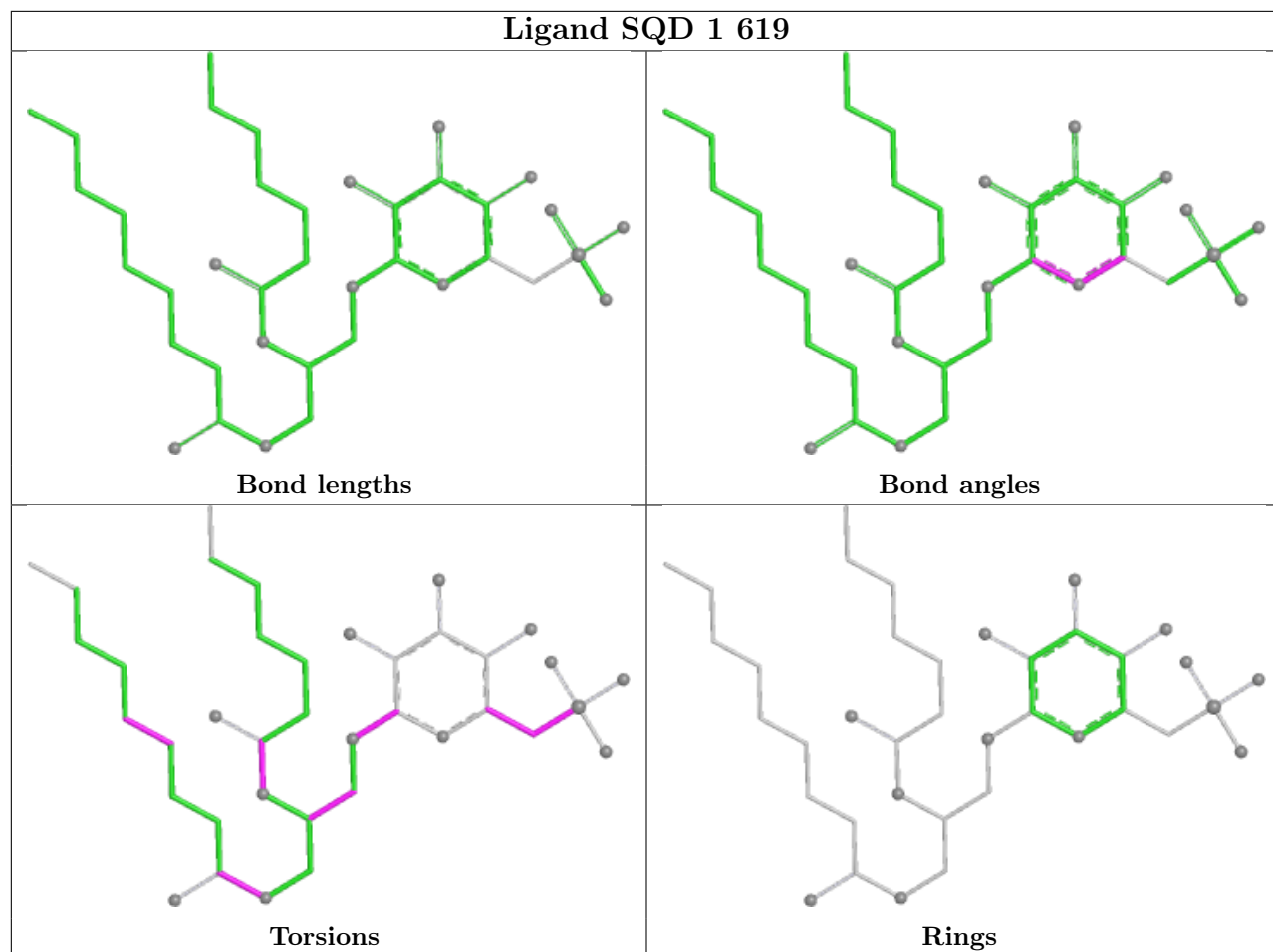
## Ligand CLA 8 321



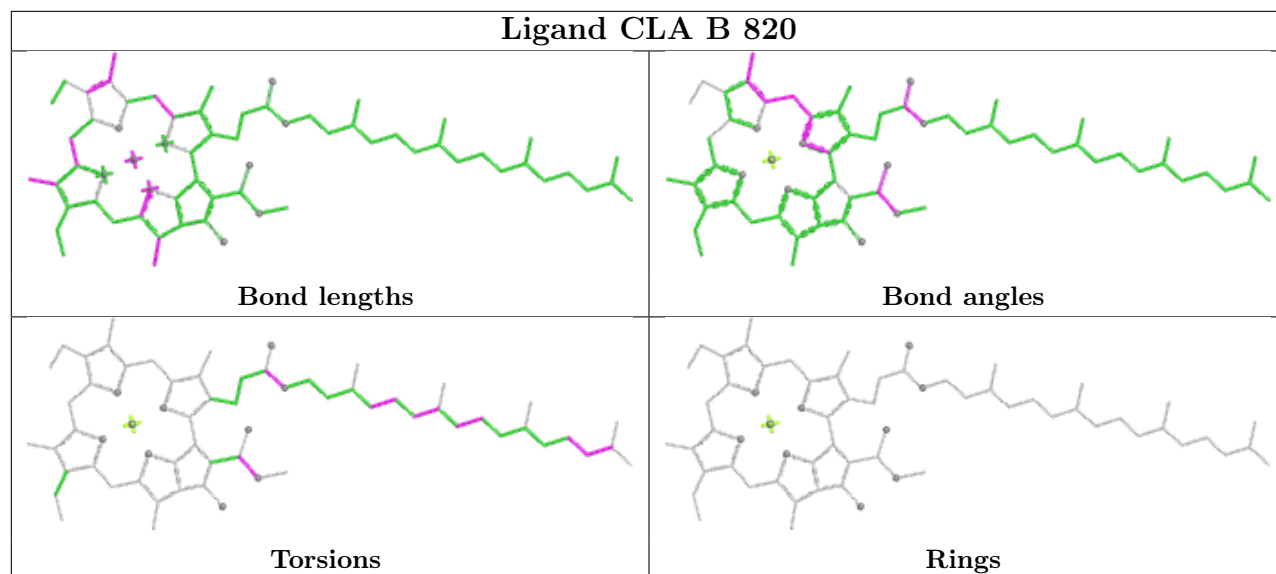
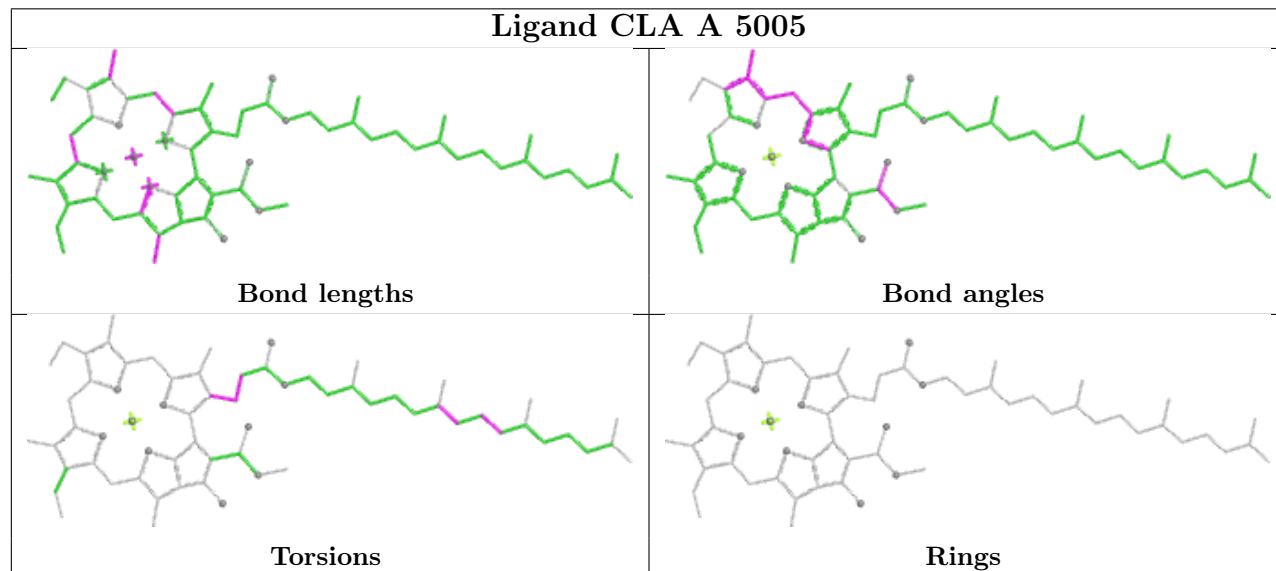
## Ligand CLA B 827



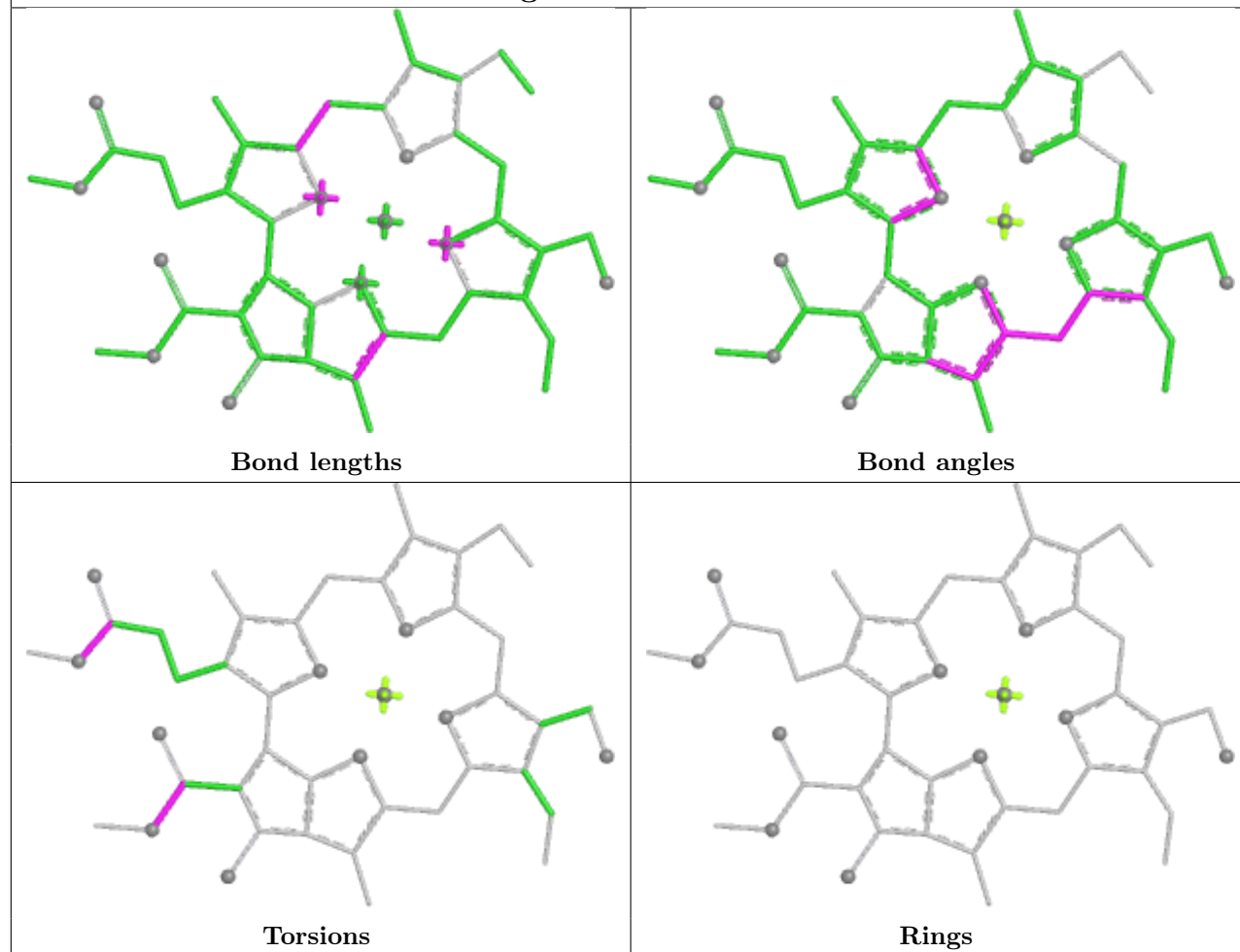




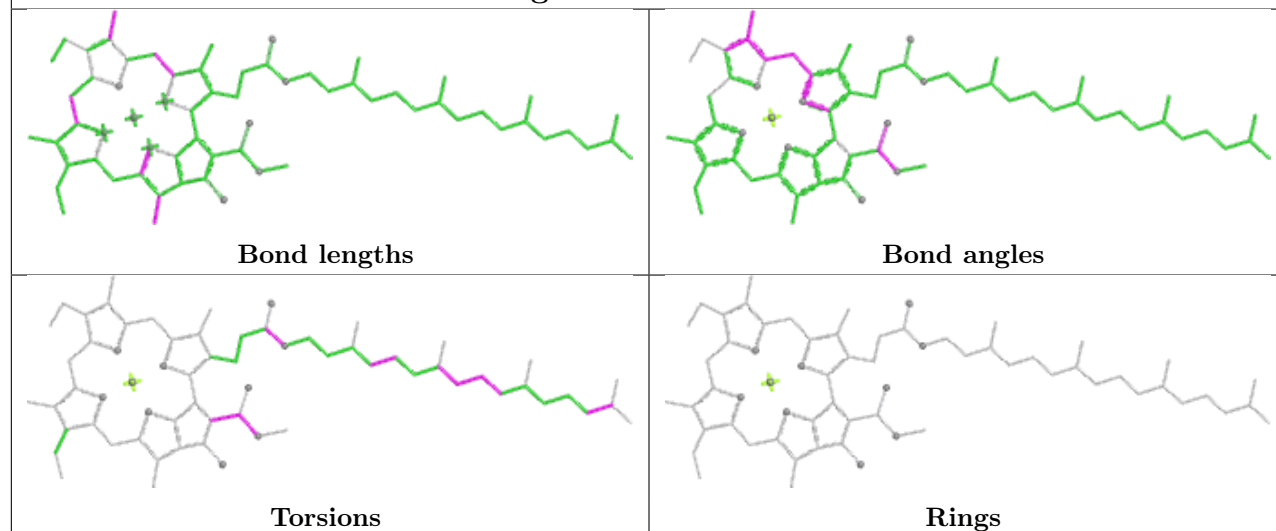


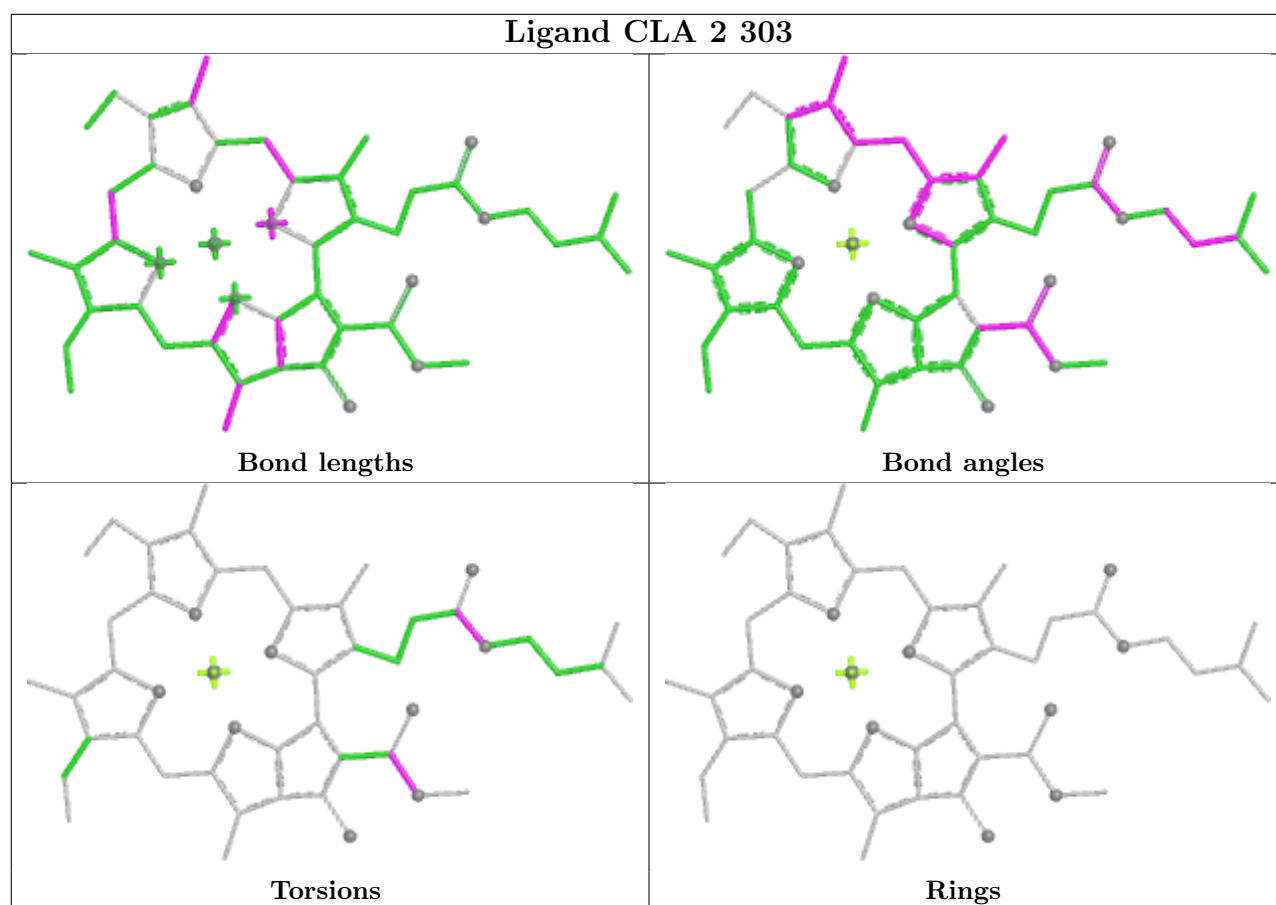
**Ligand CLA B 820****Ligand CLA A 5005**

## Ligand CHL 8 305

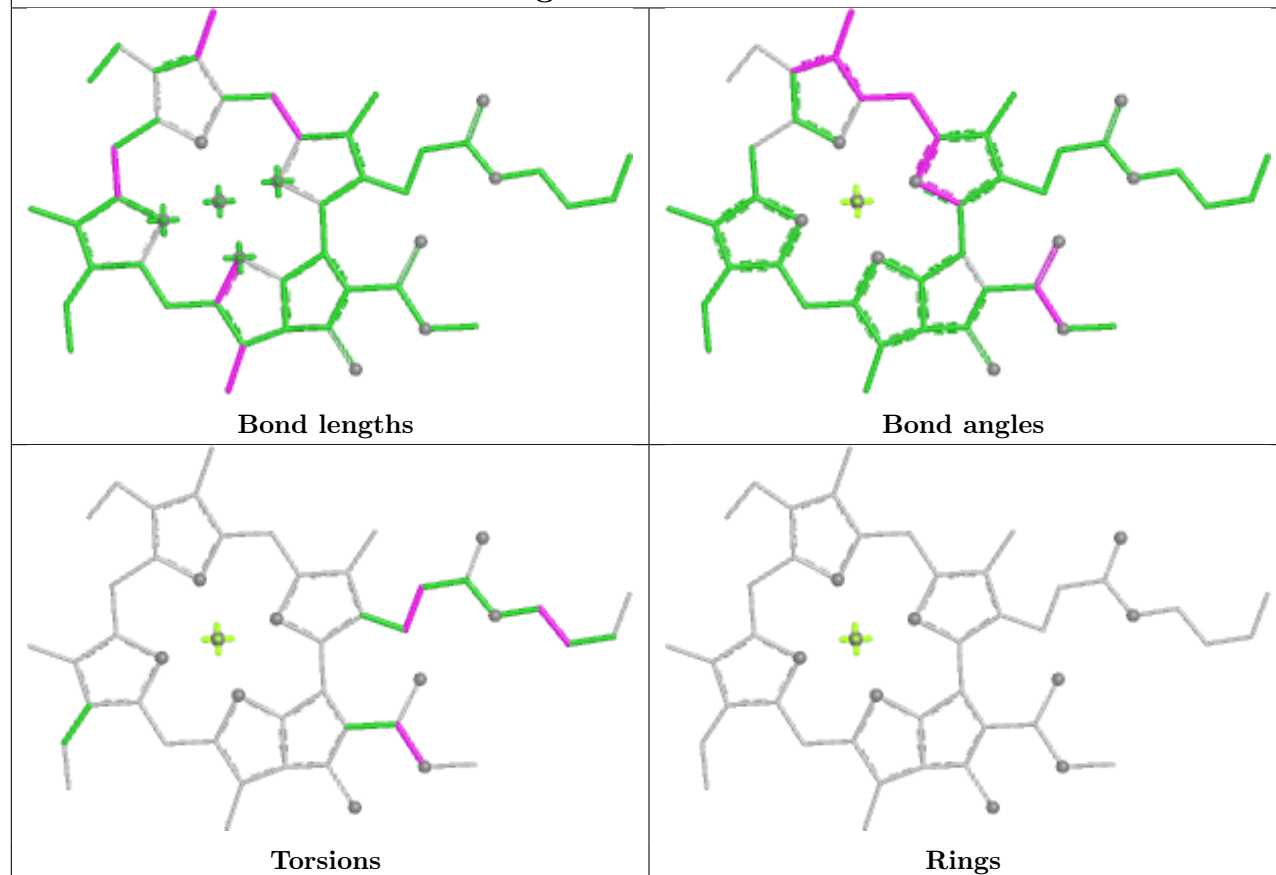


## Ligand CLA G 201

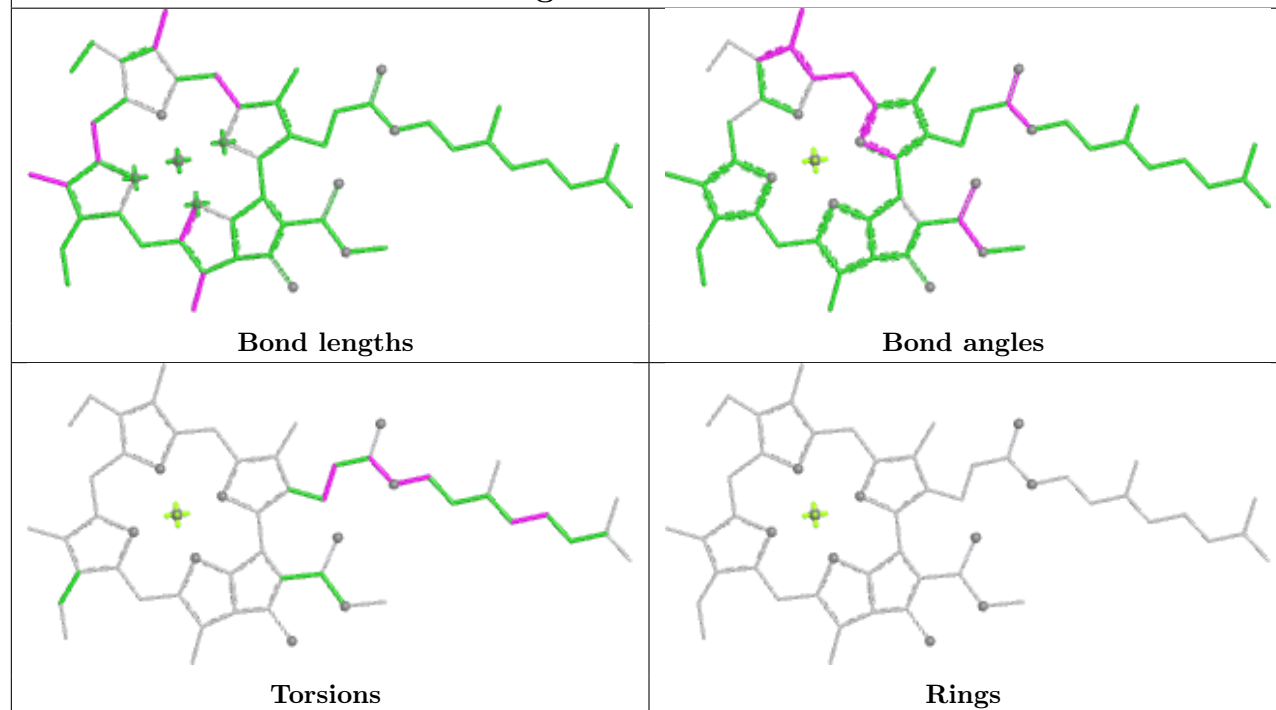


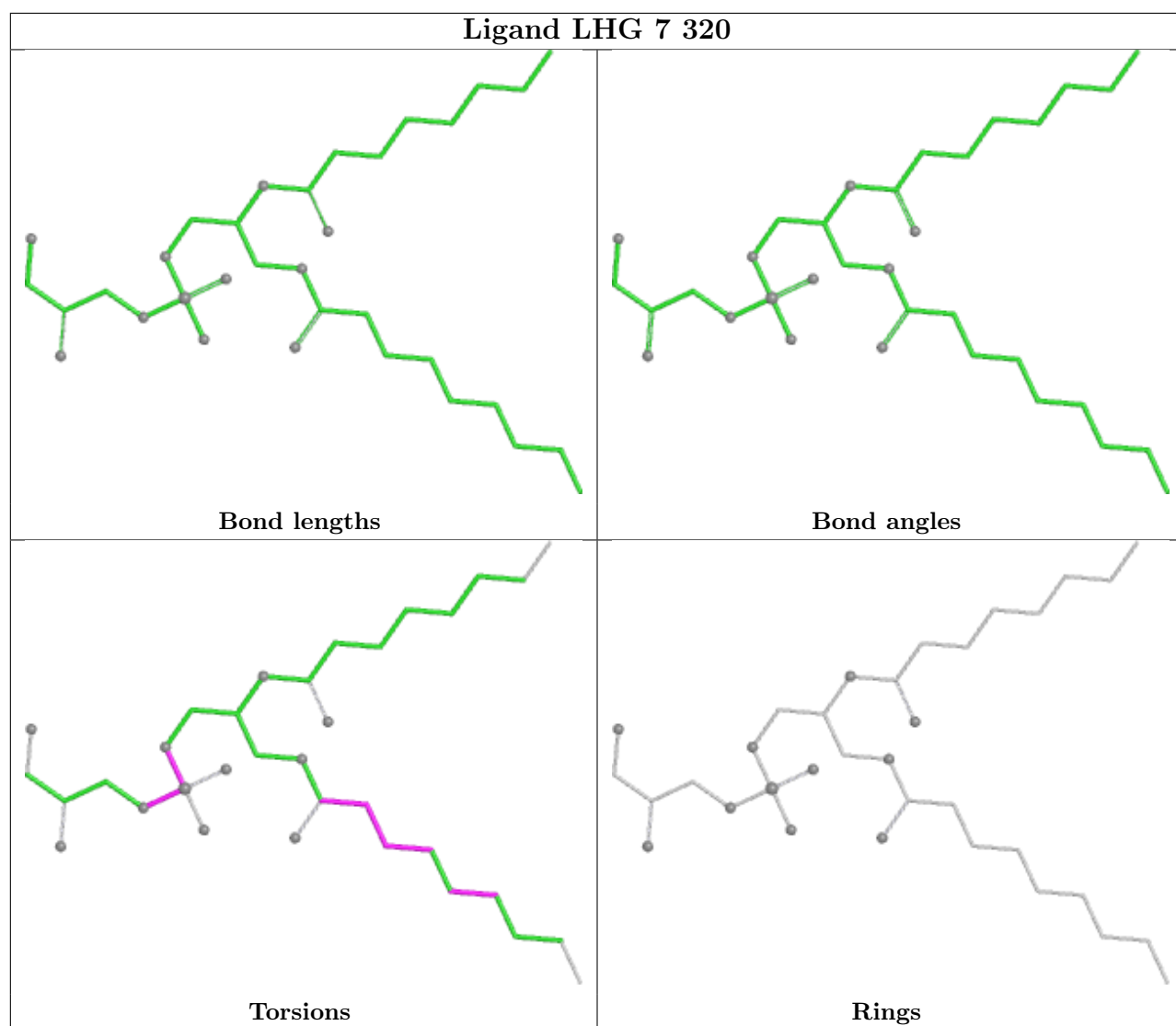


## Ligand CLA J 104

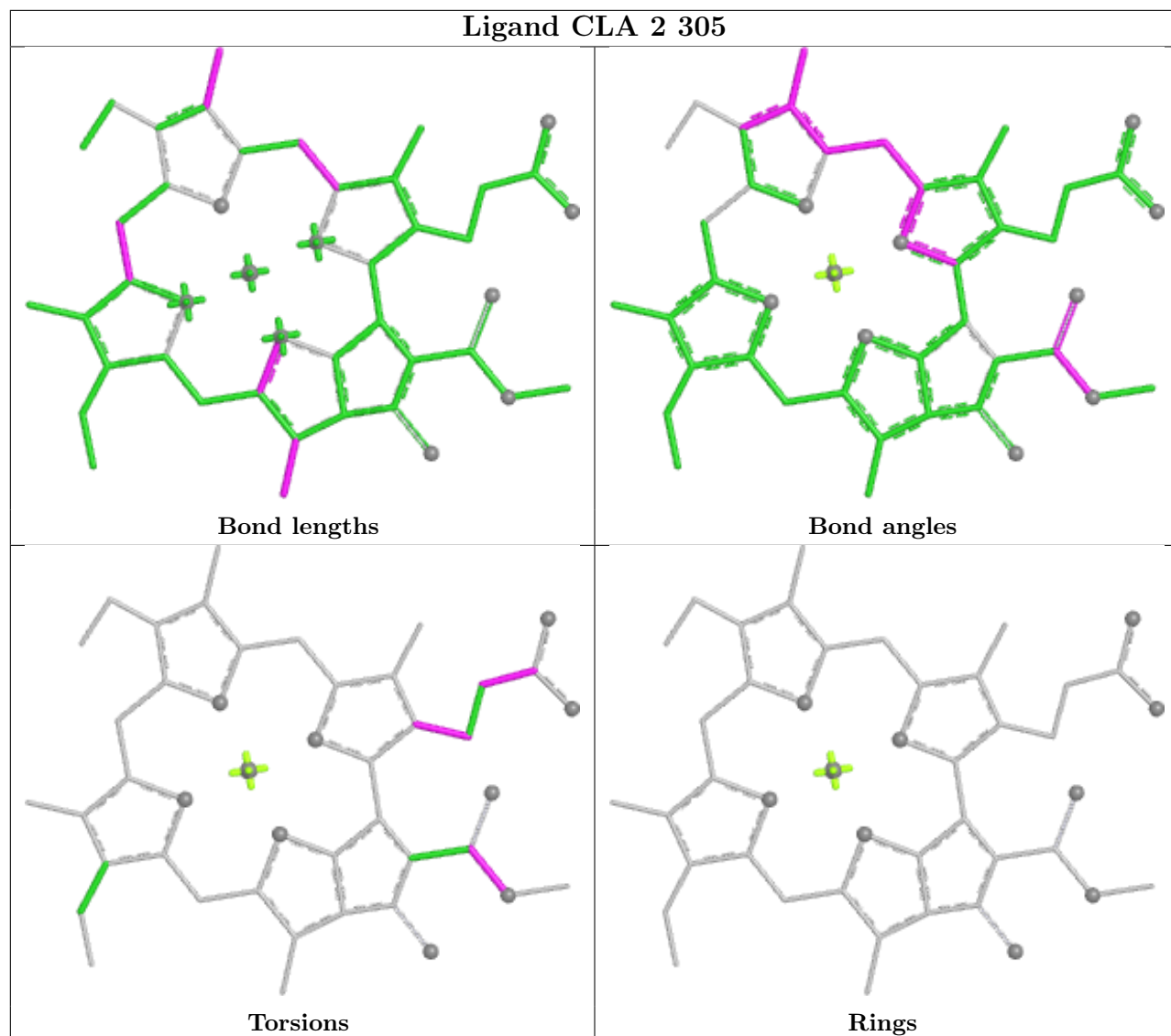


## Ligand CLA 9 611

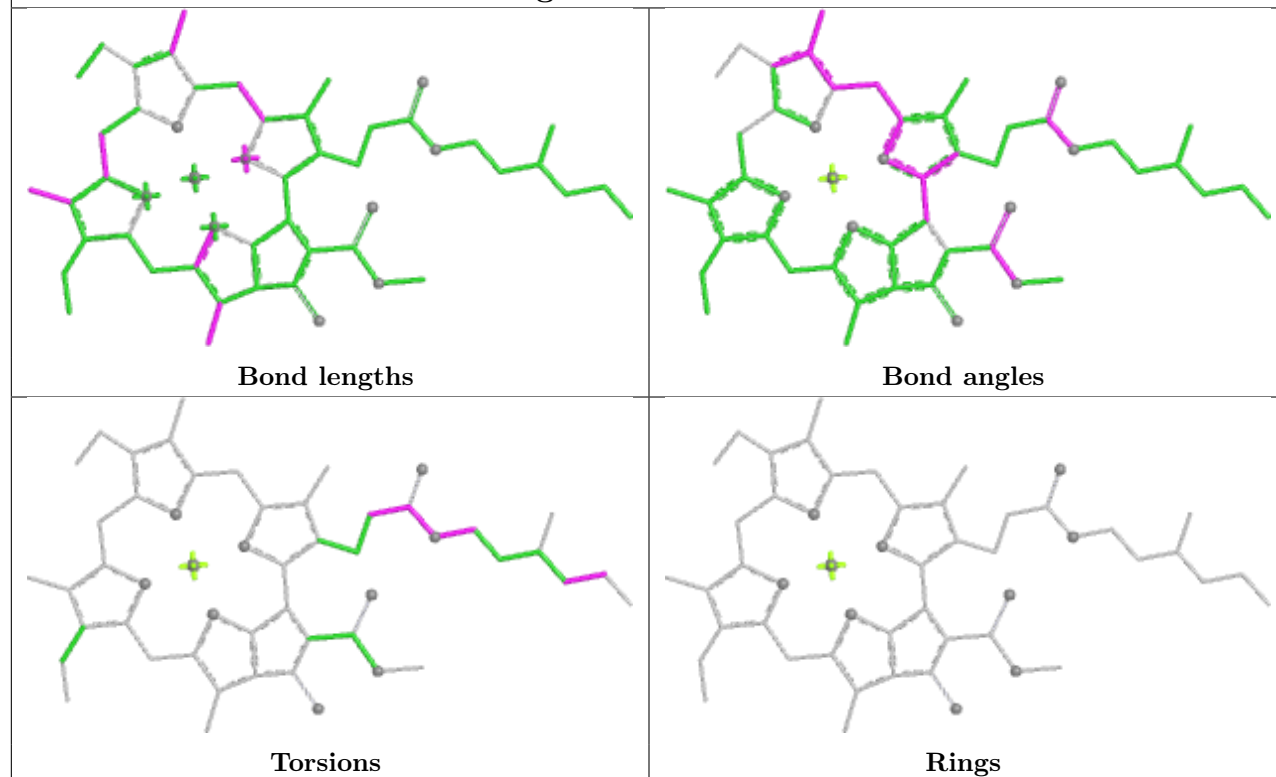




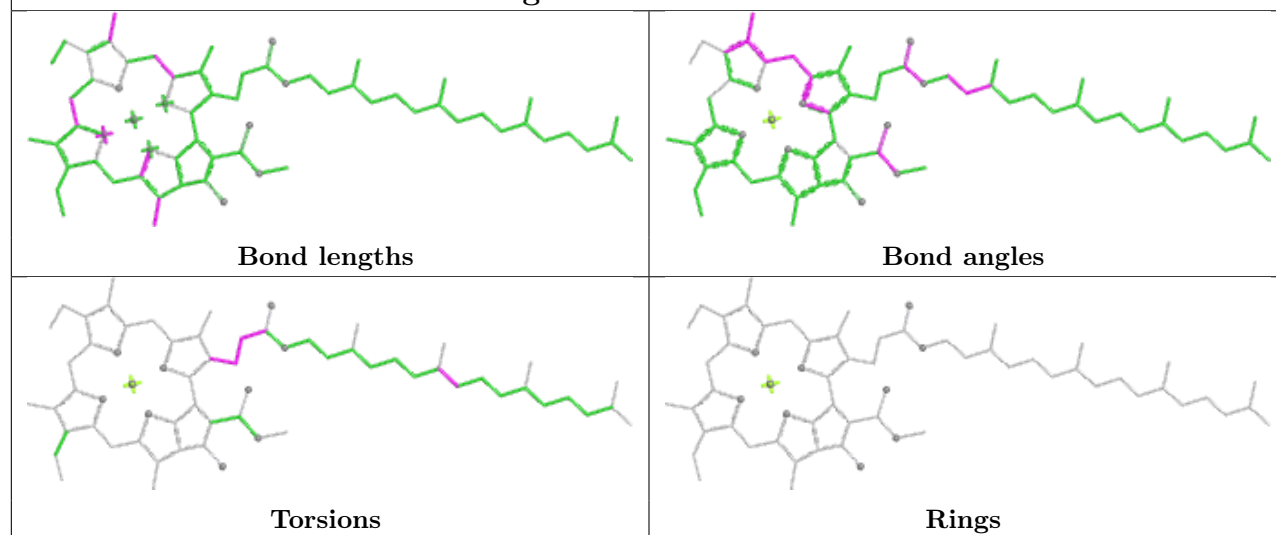
## Ligand CLA 2 305

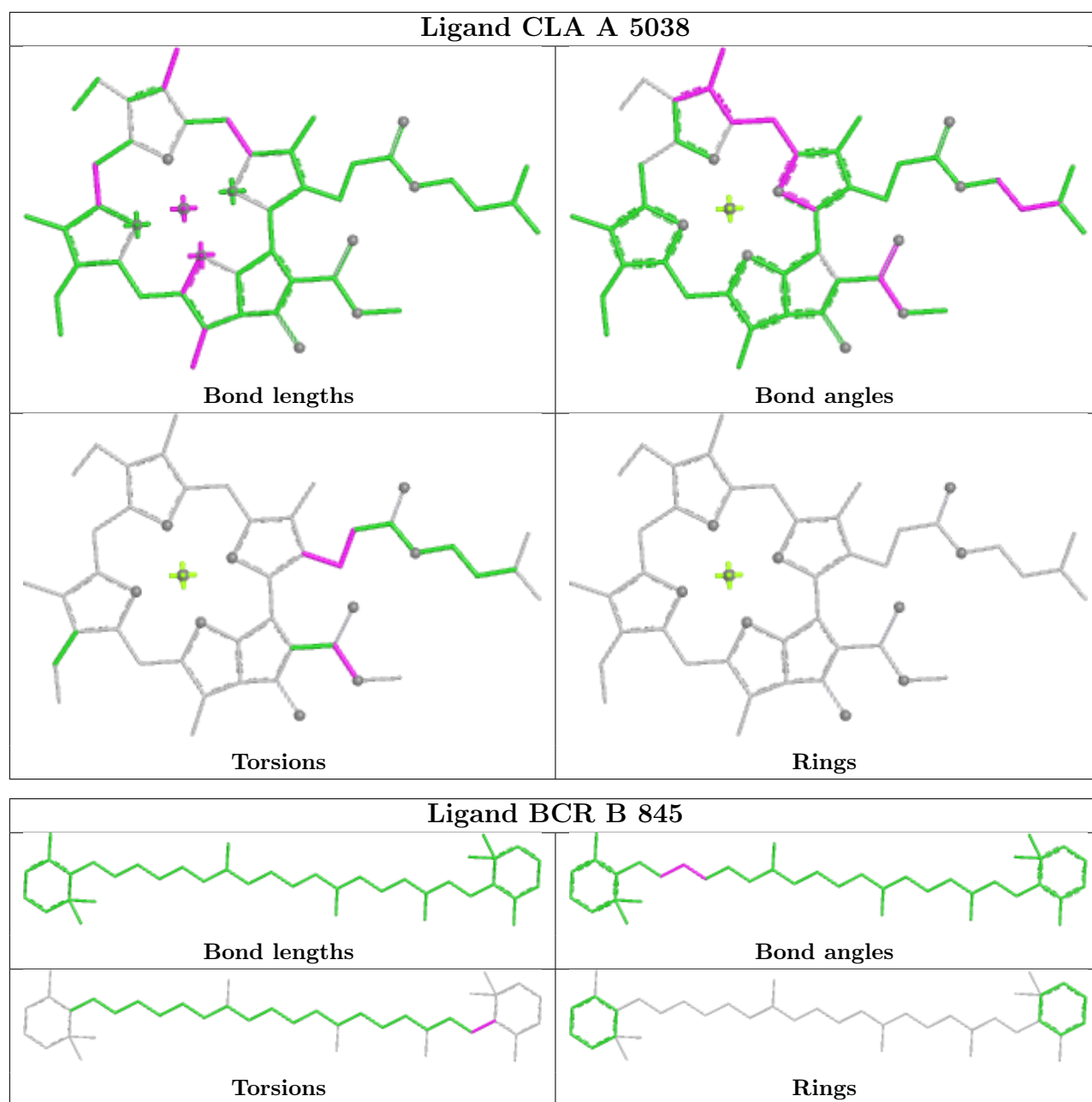


## Ligand CLA 7 312

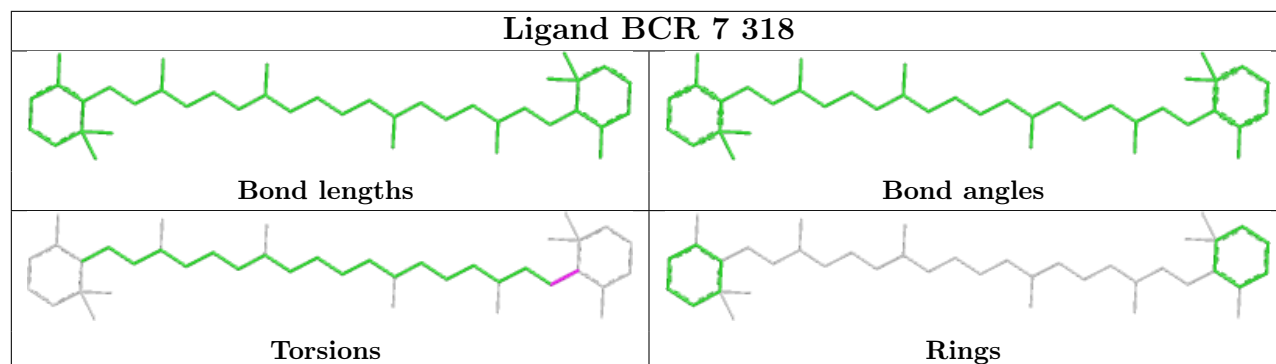
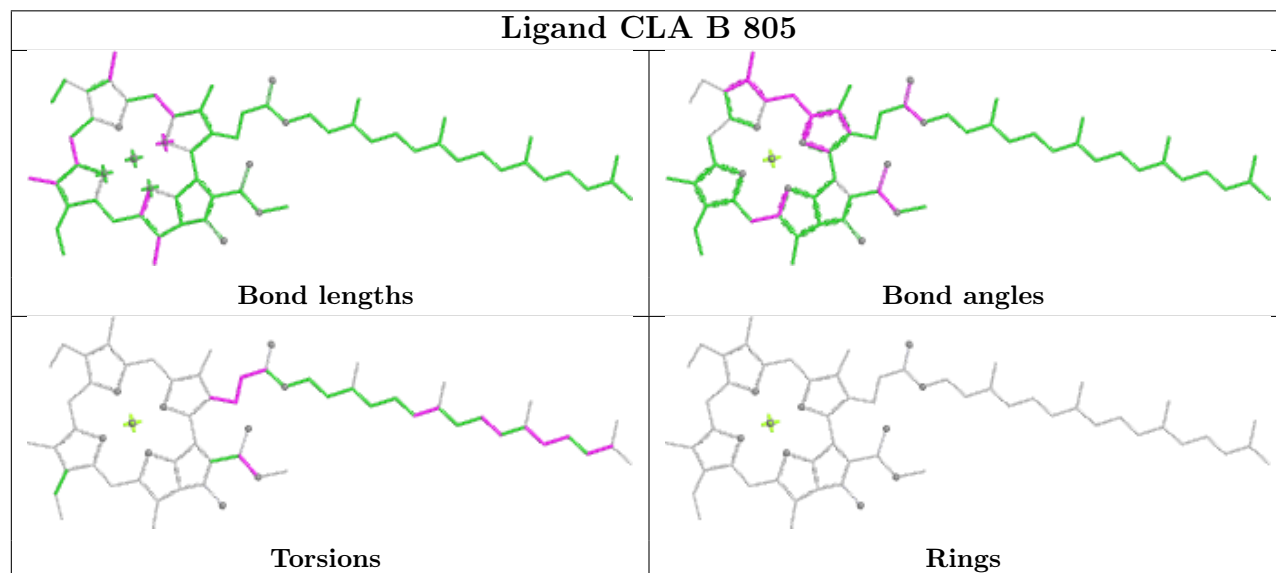
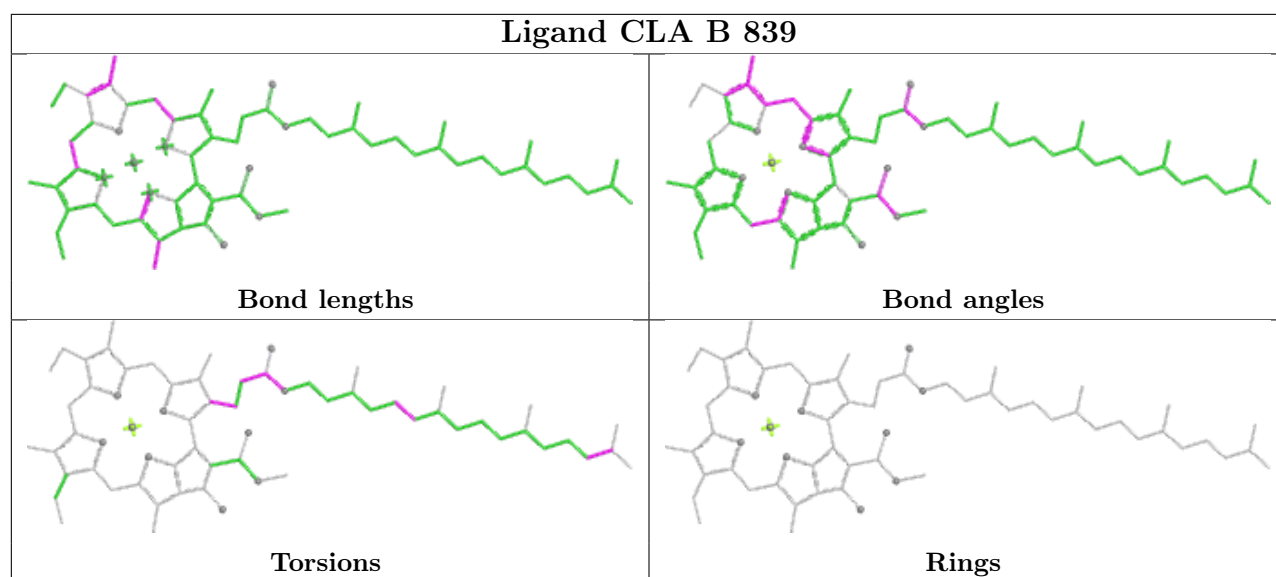


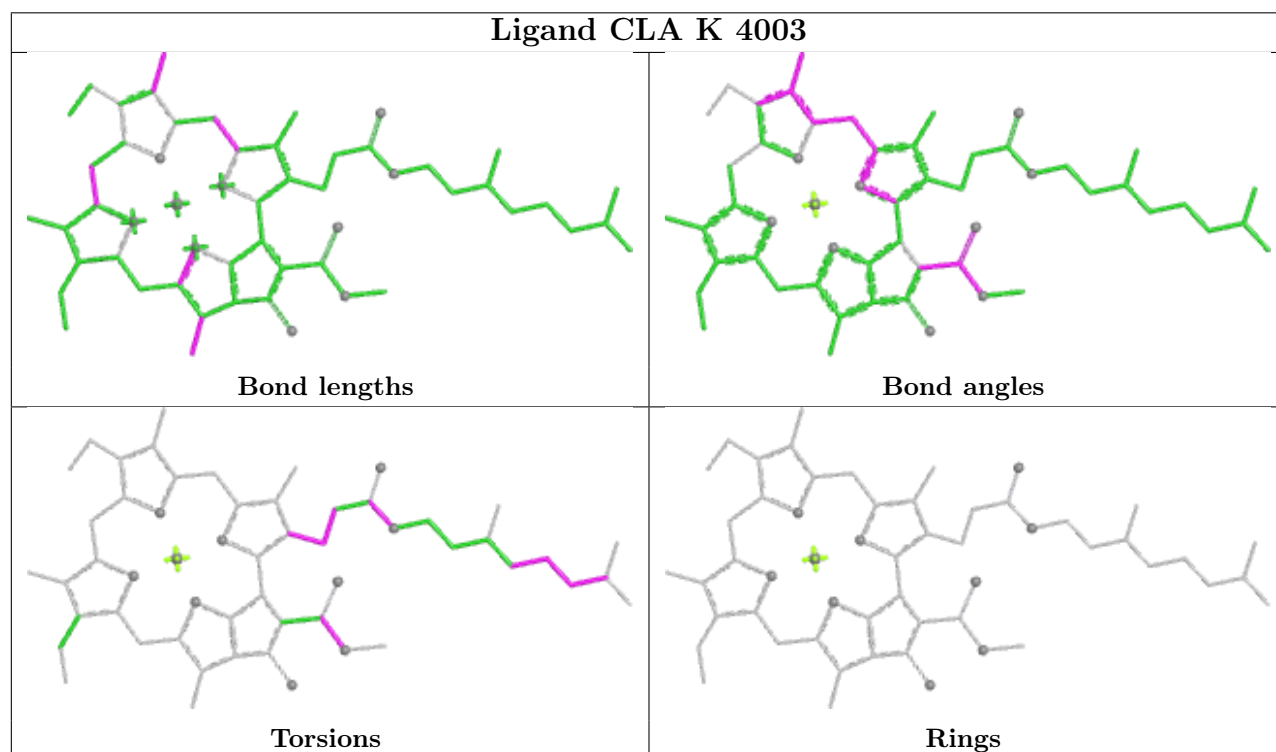
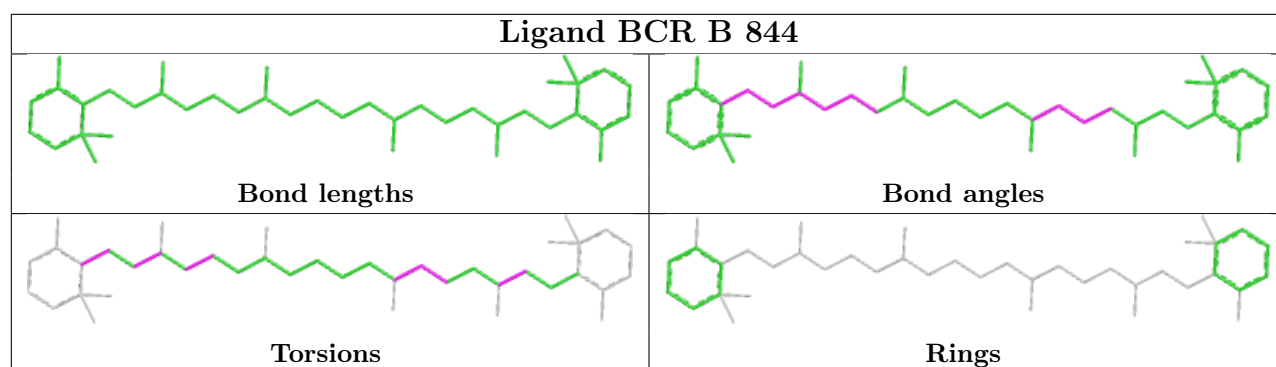
## Ligand CLA A 5041



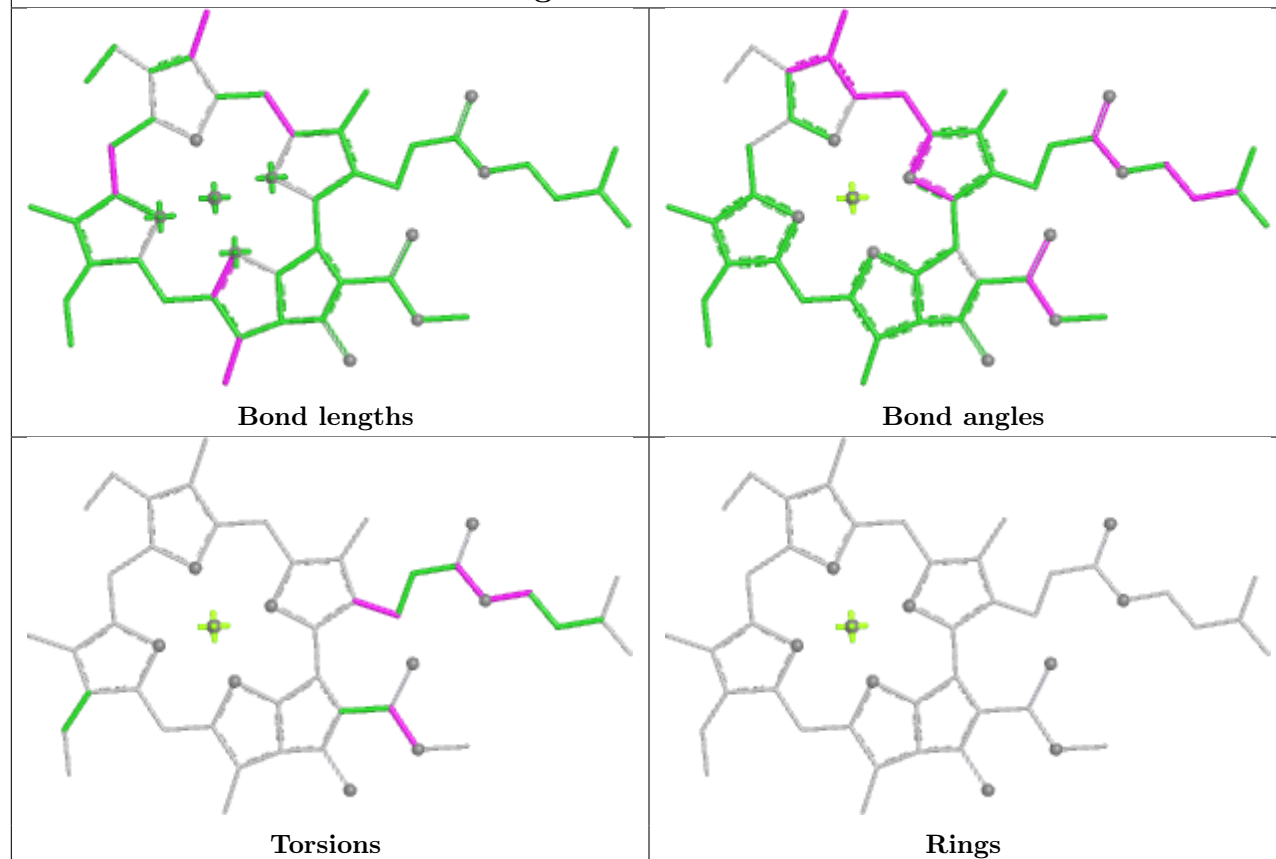




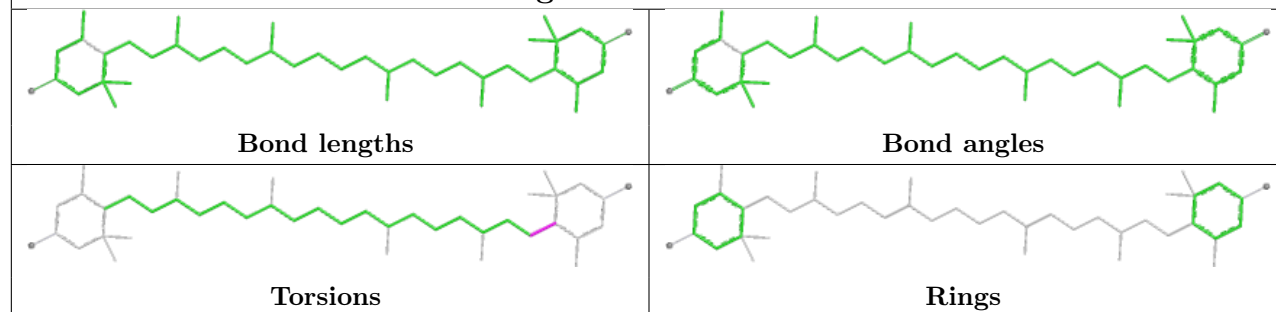


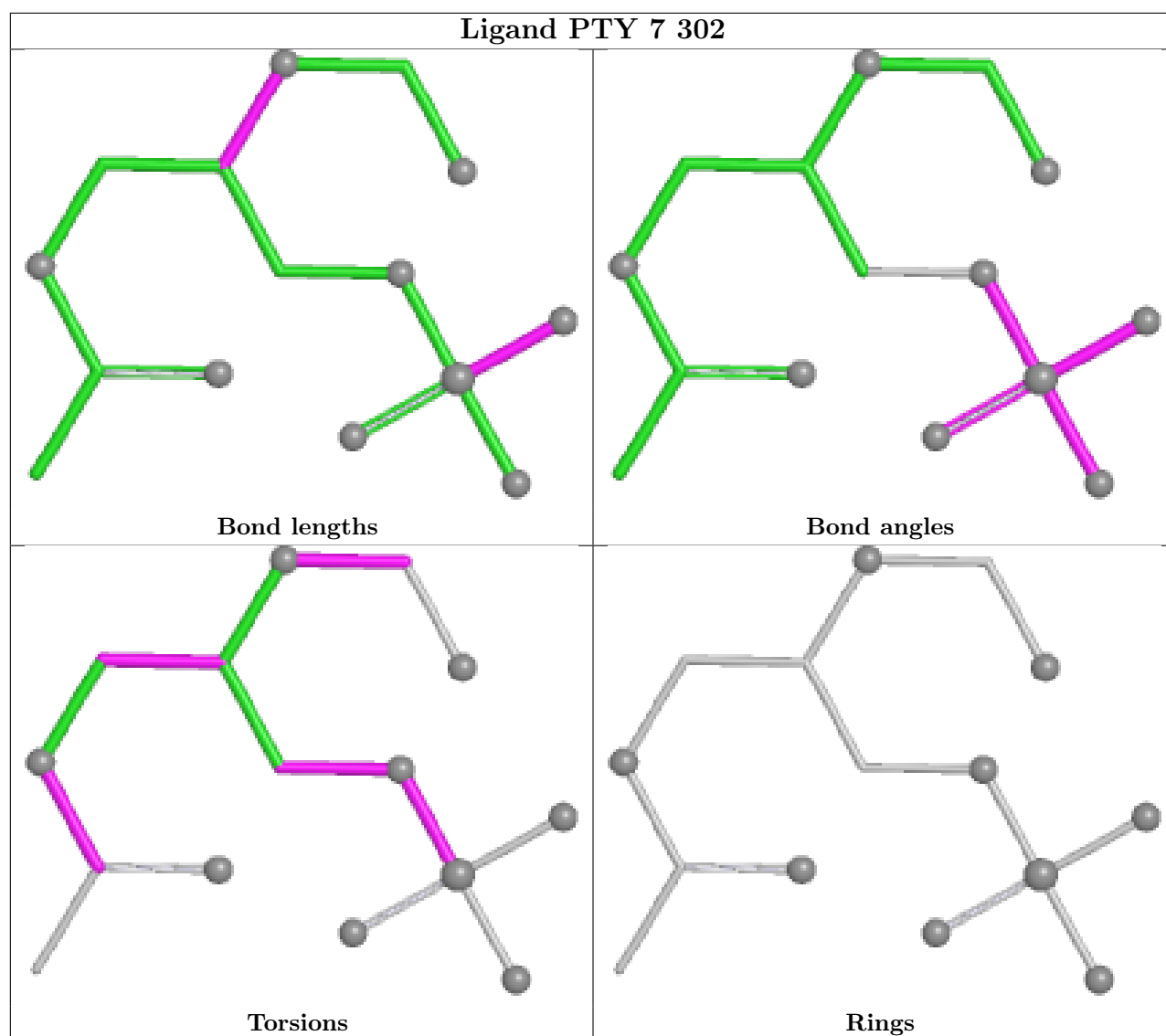


## Ligand CLA L 205

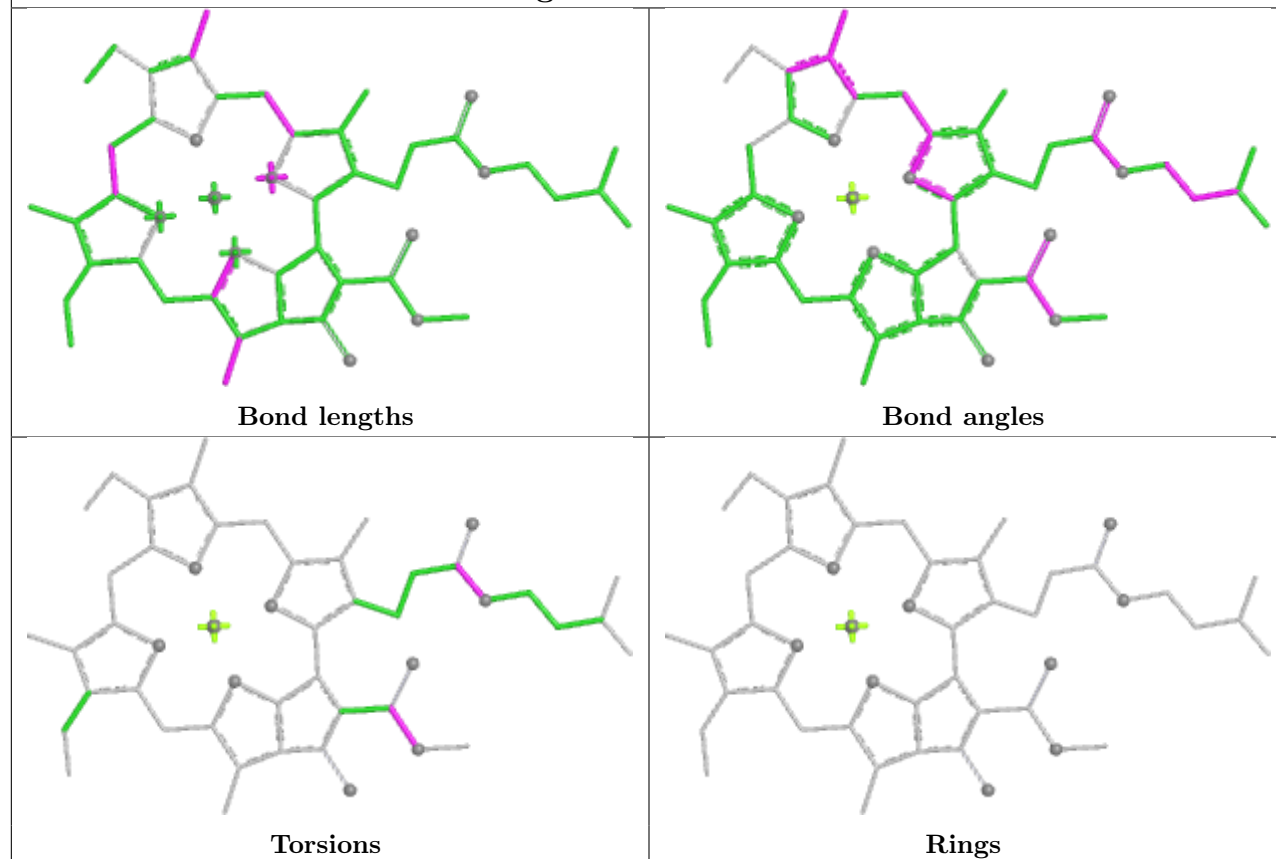


## Ligand LUT 9 613

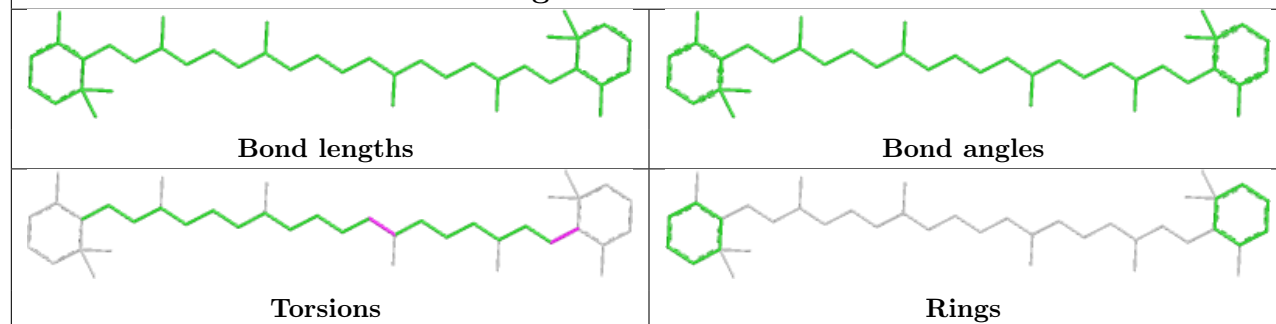


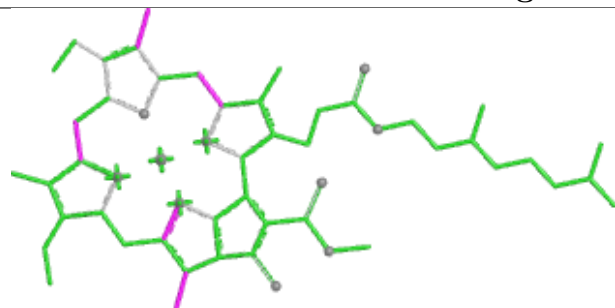
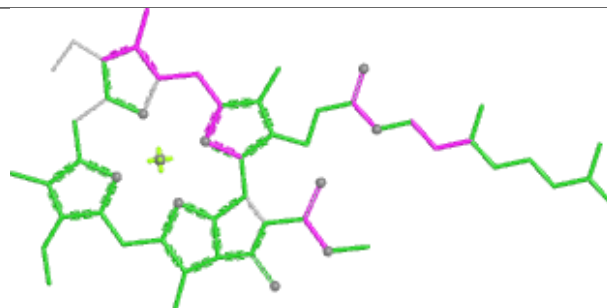
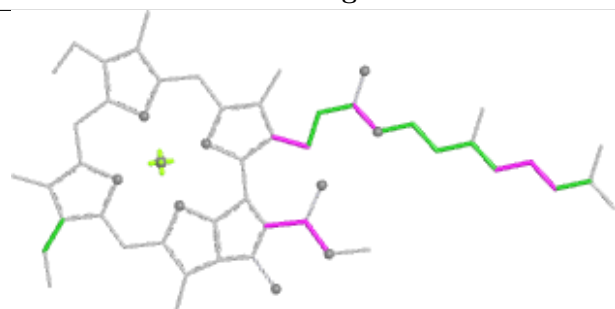
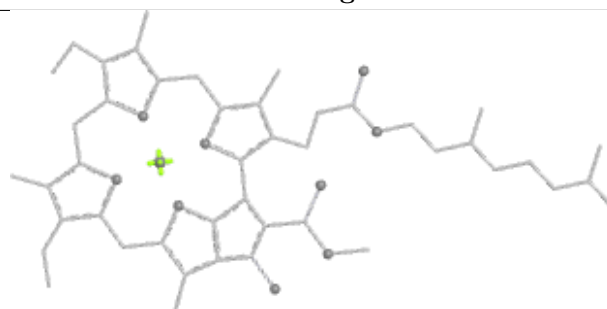
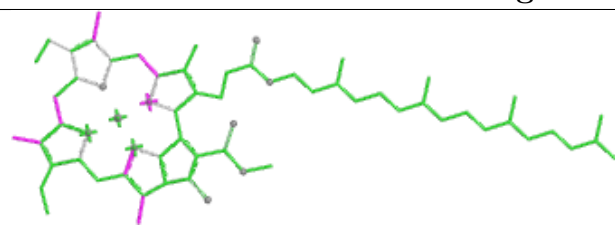
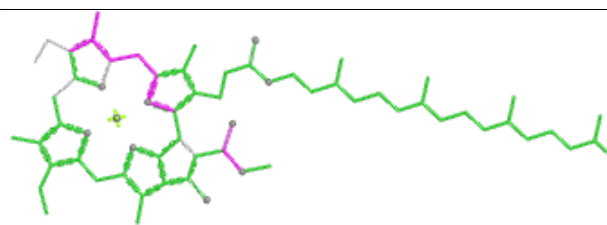
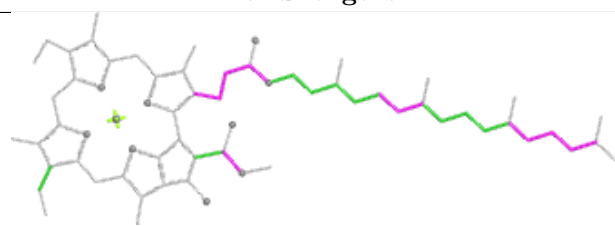
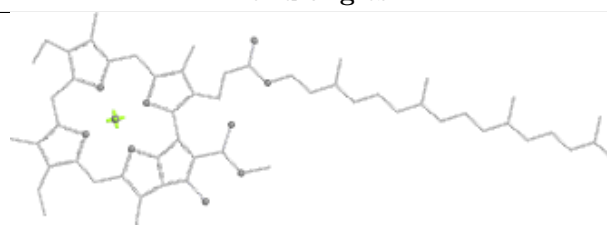


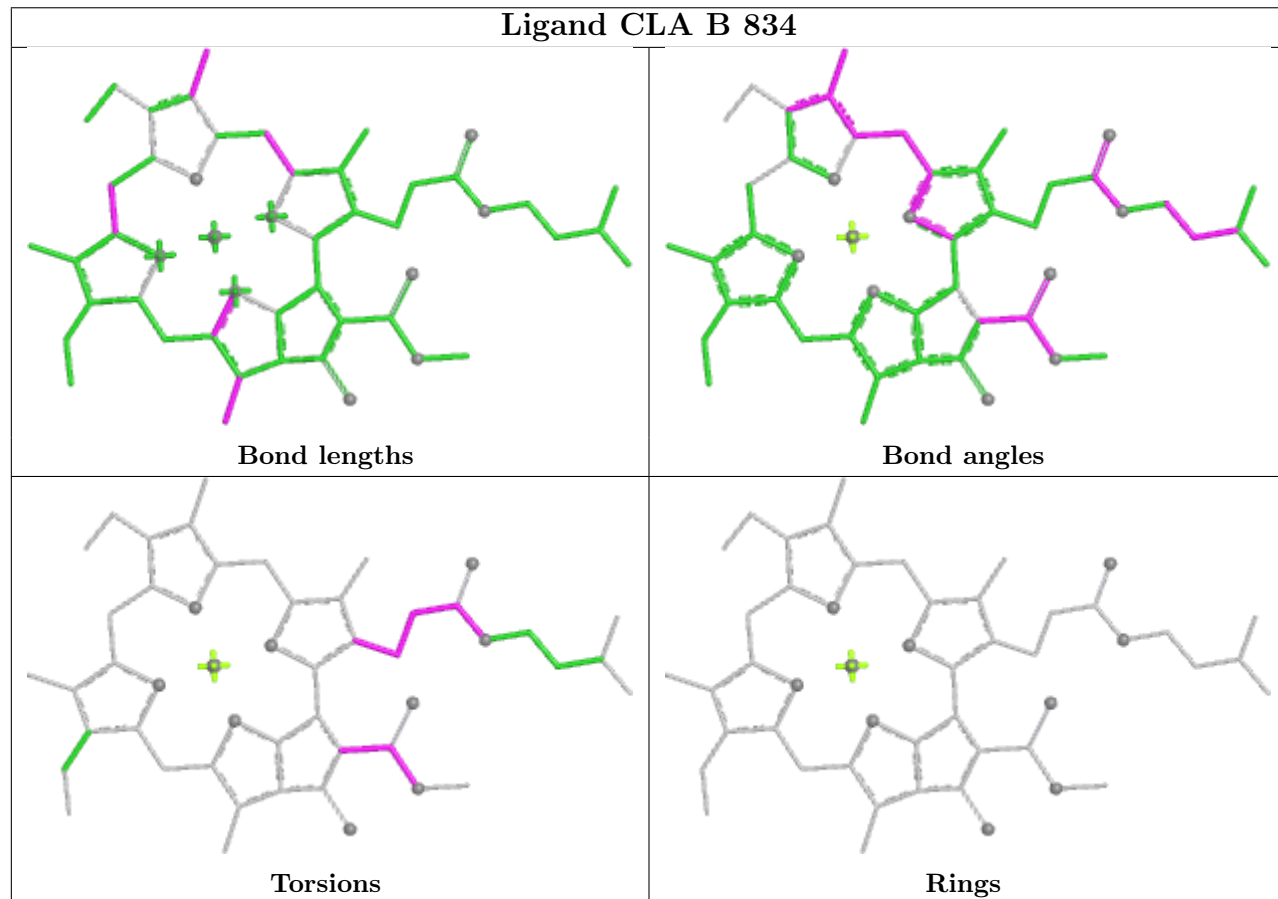
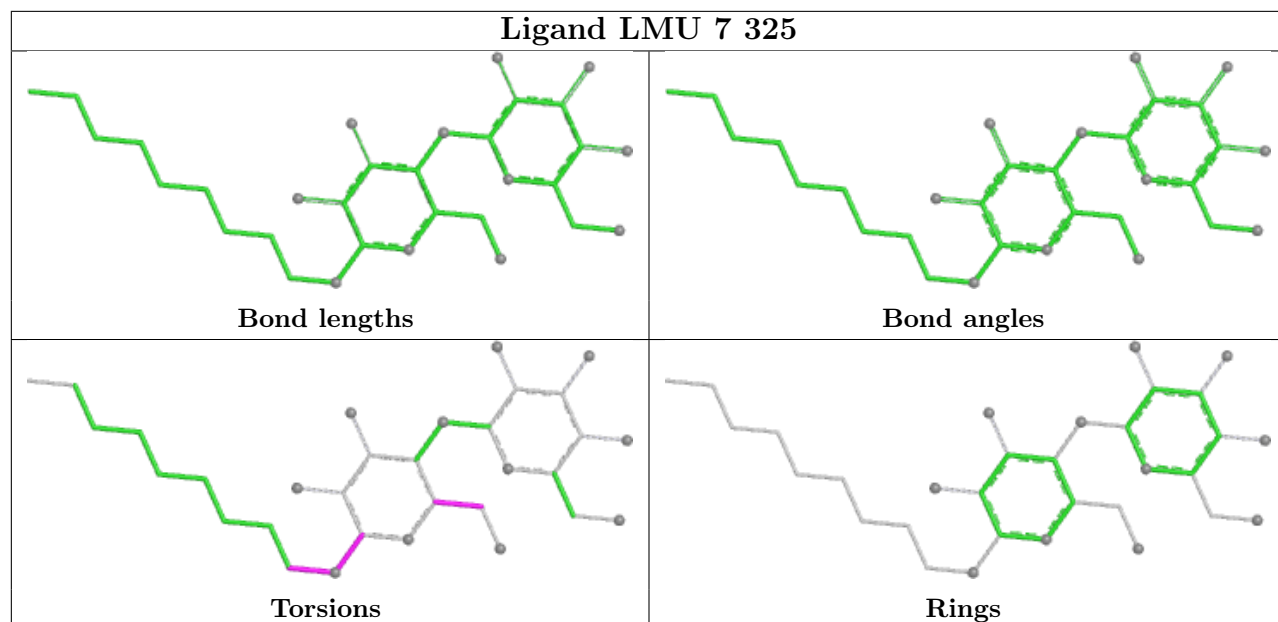
## Ligand CLA 7 305

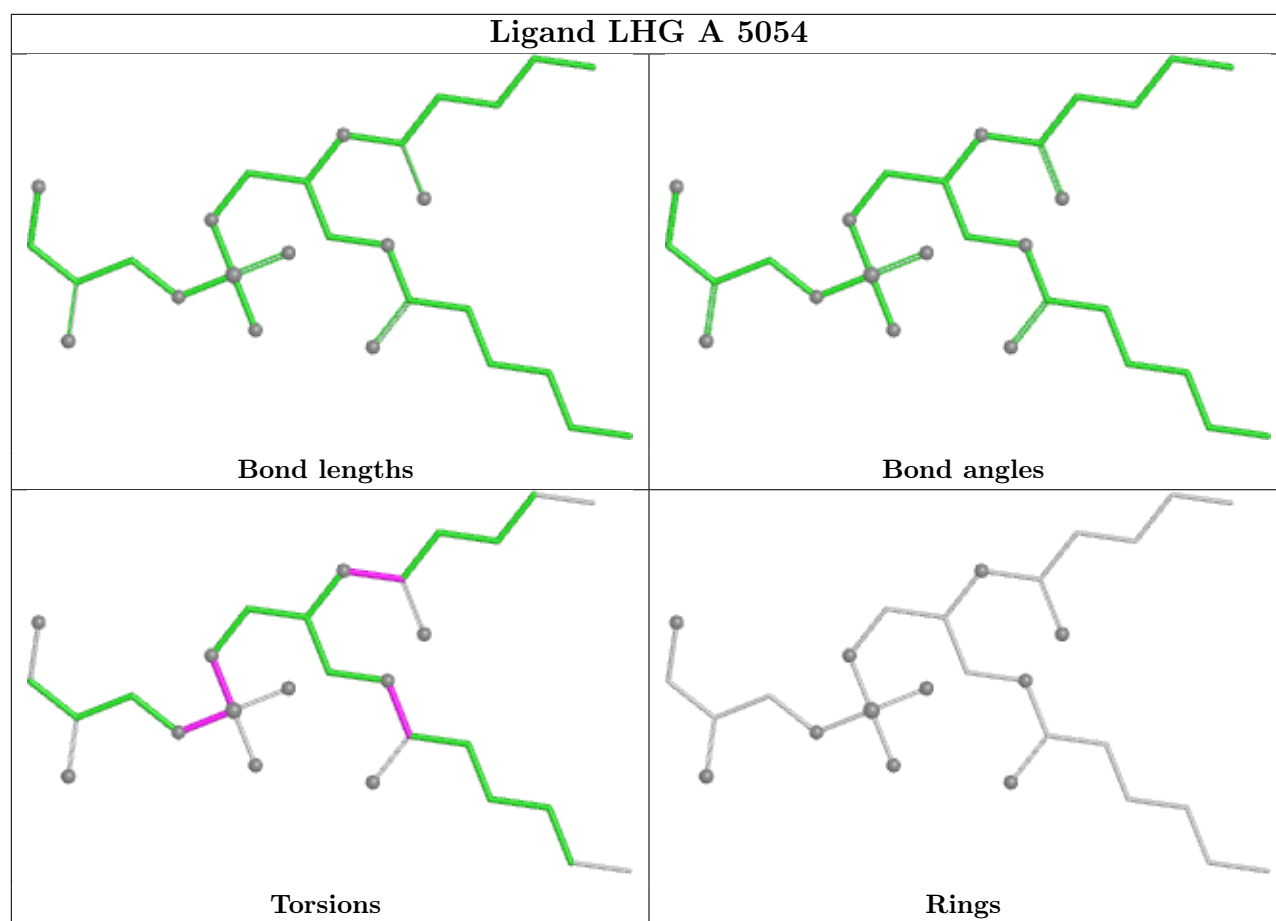


## Ligand BCR F 309



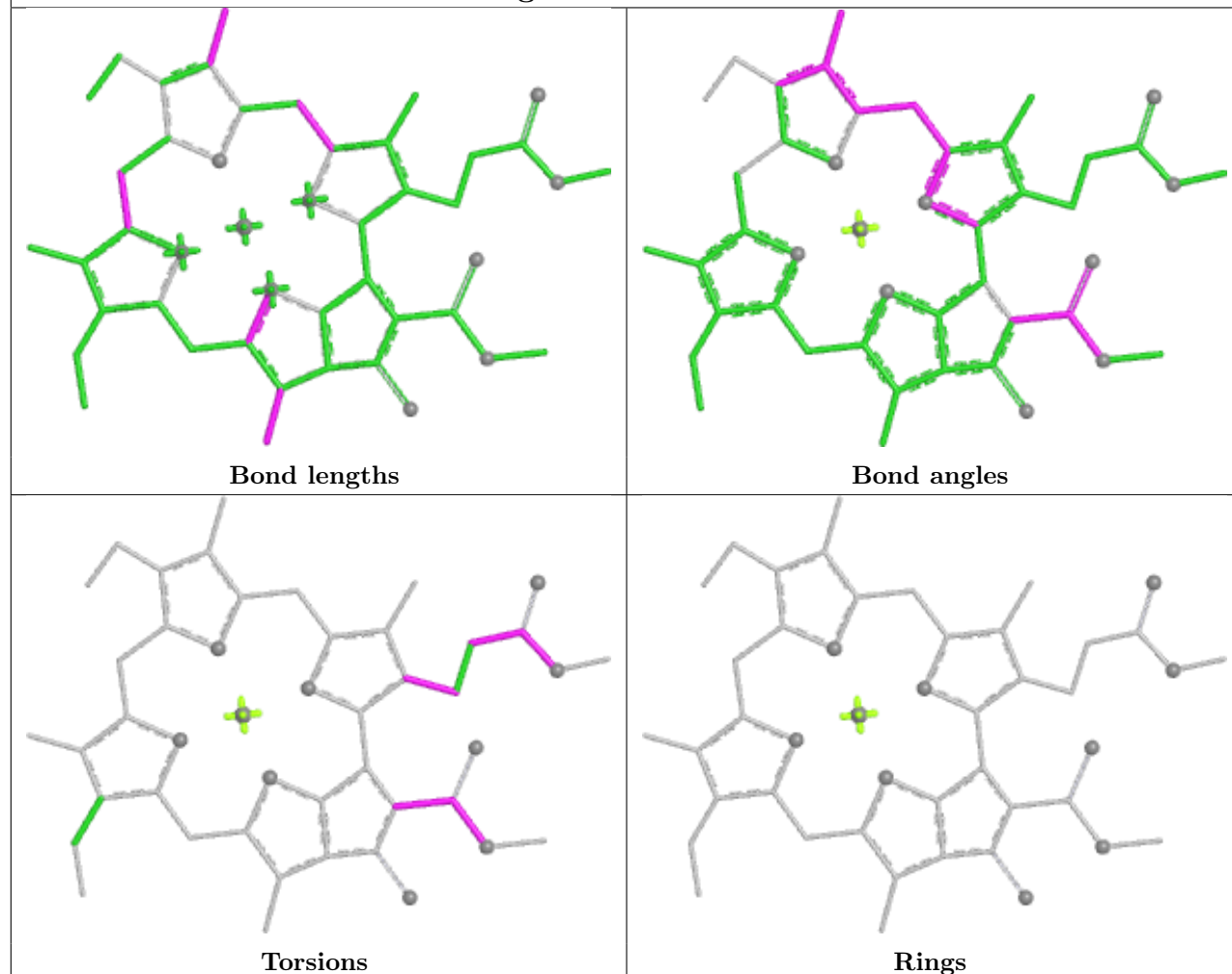
**Ligand CLA B 816****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 828****Bond lengths****Bond angles****Torsions****Rings**



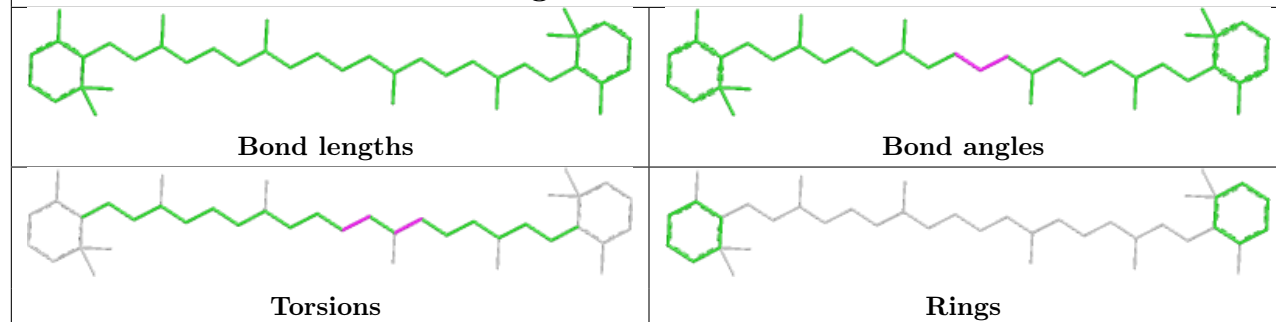


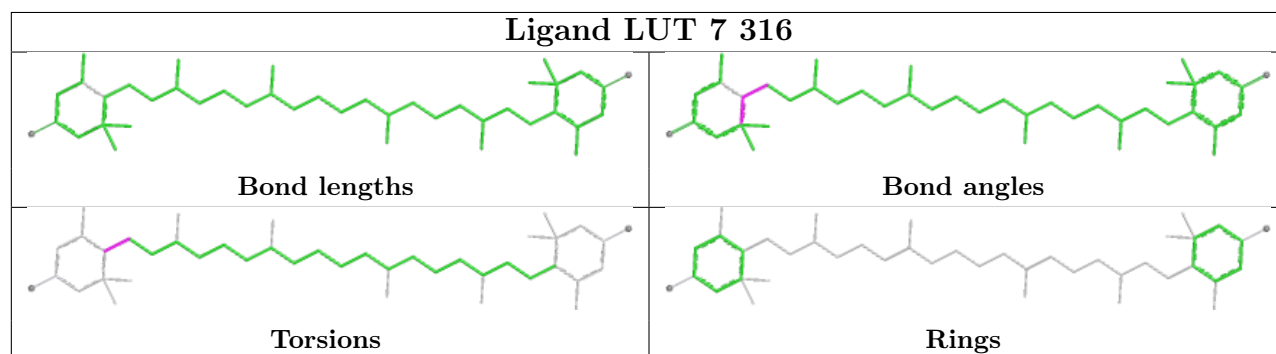
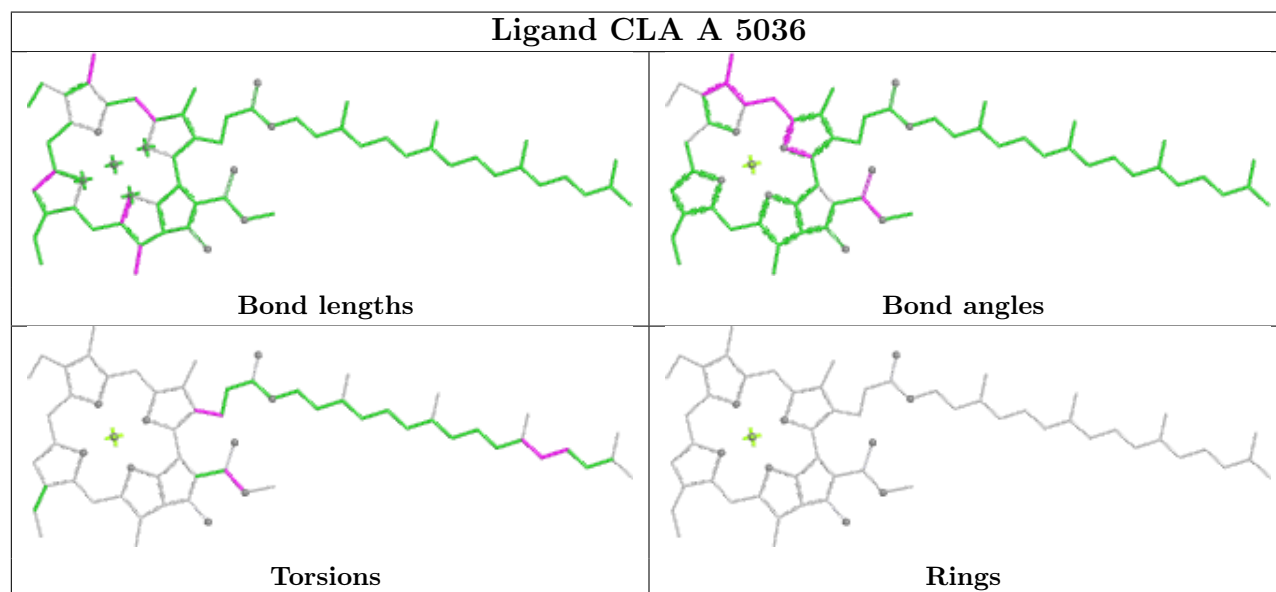
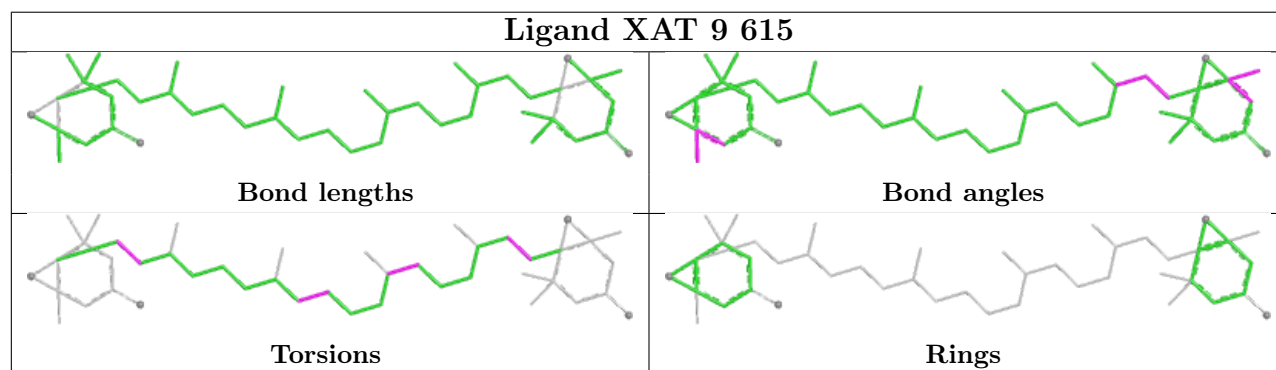
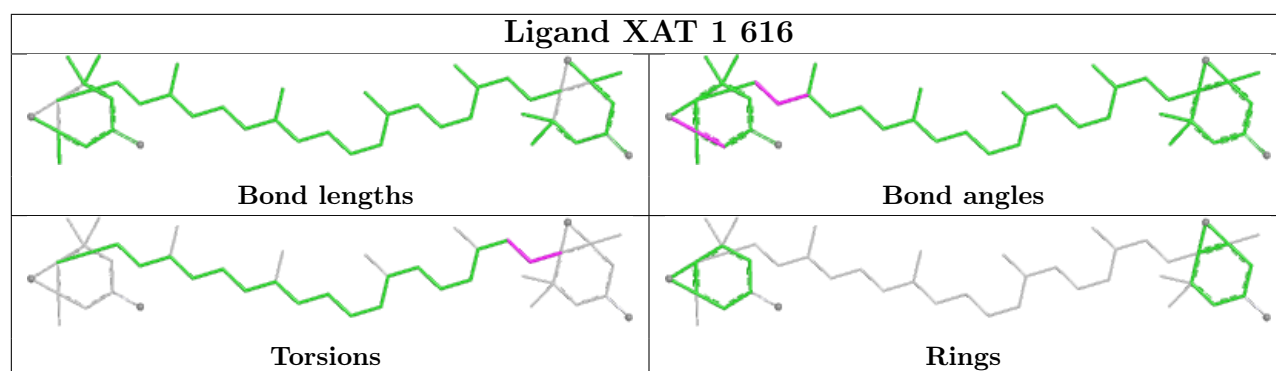


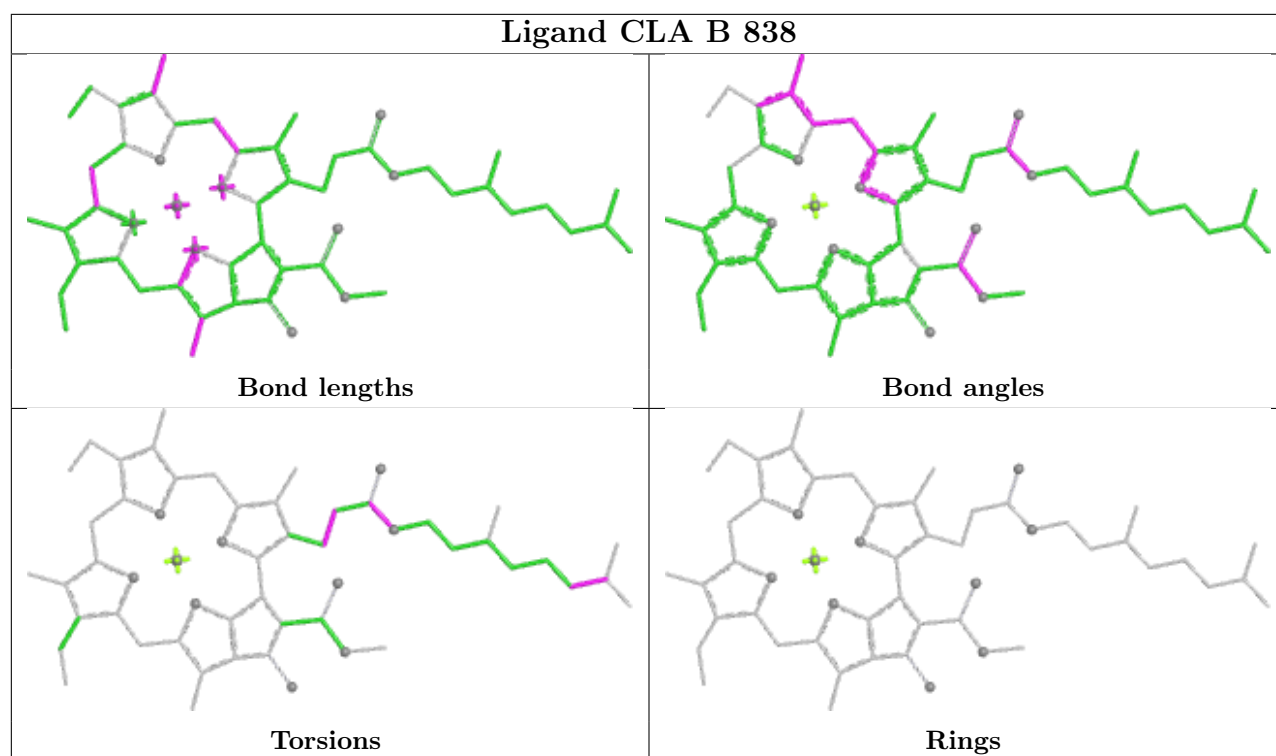
## Ligand CLA 9 601



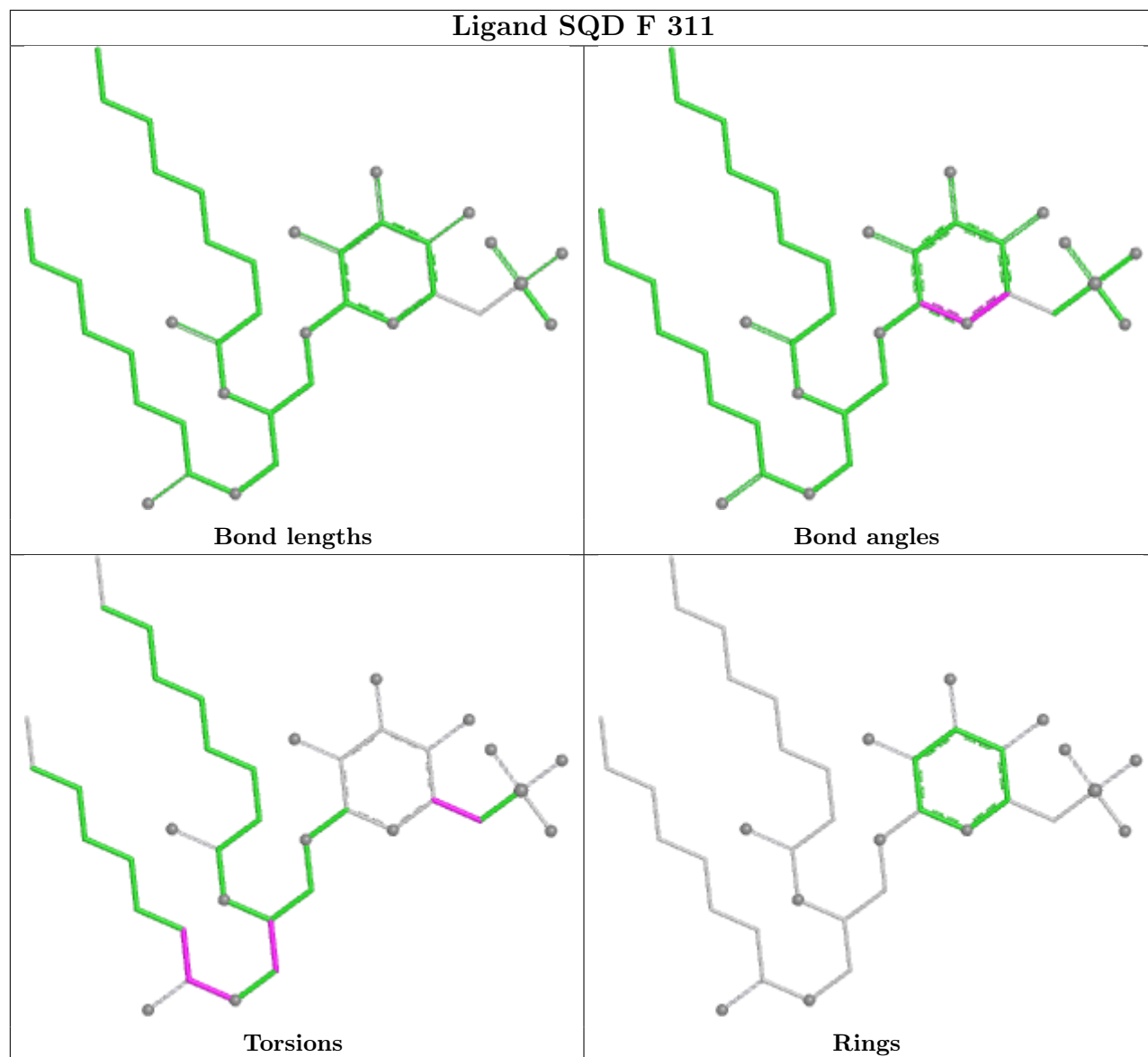
## Ligand BCR B 803



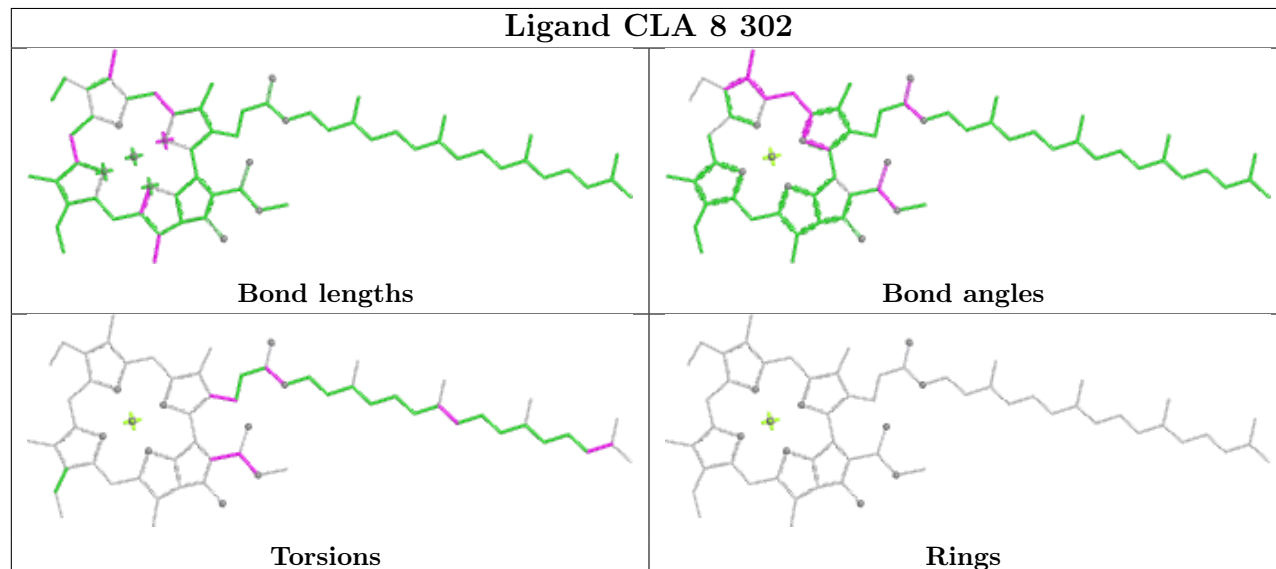




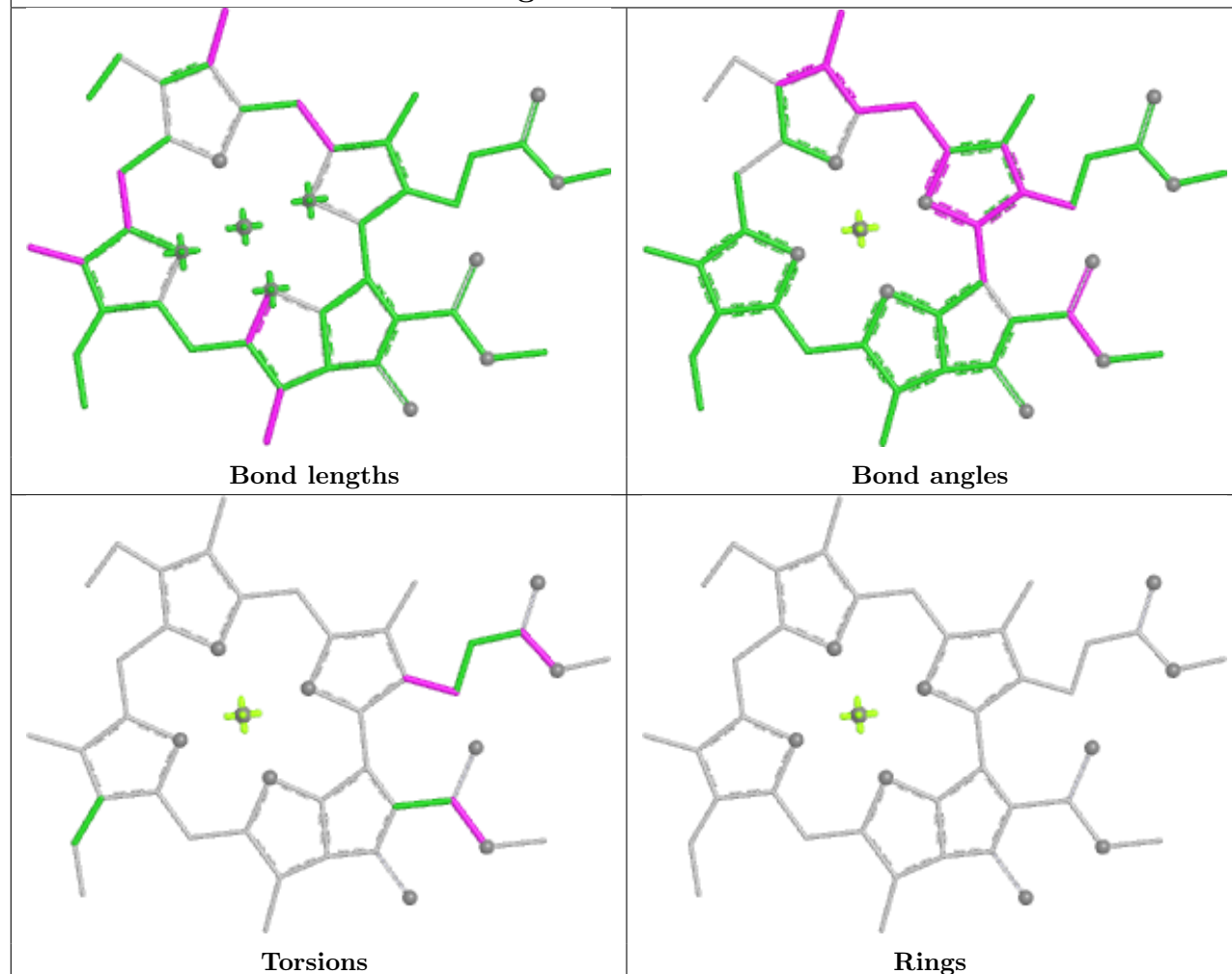
## Ligand SQD F 311



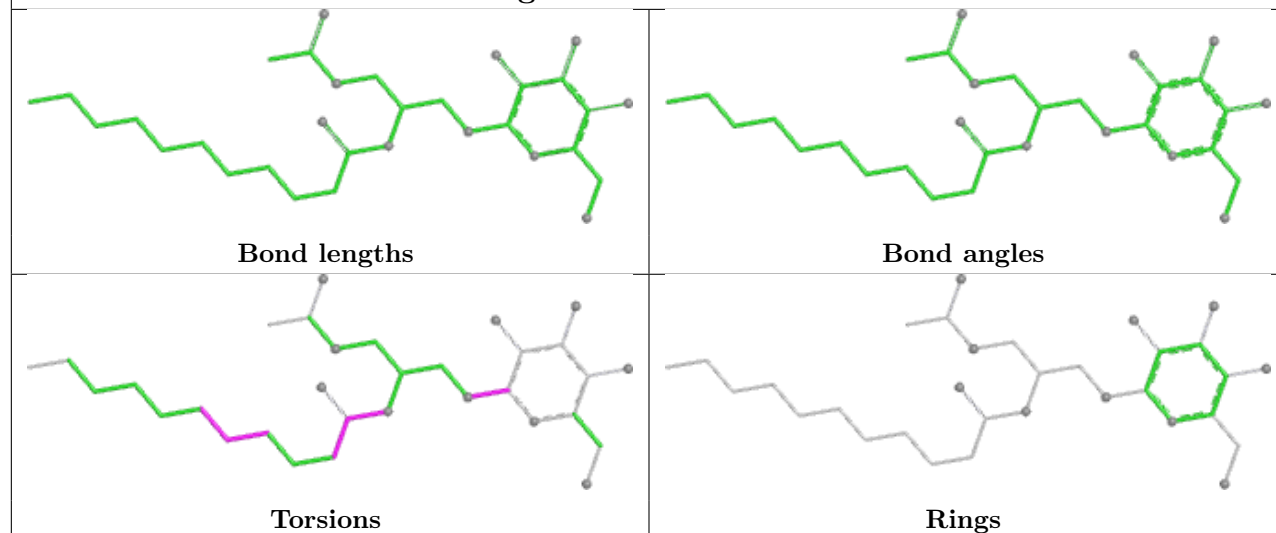
## Ligand CLA 8 302



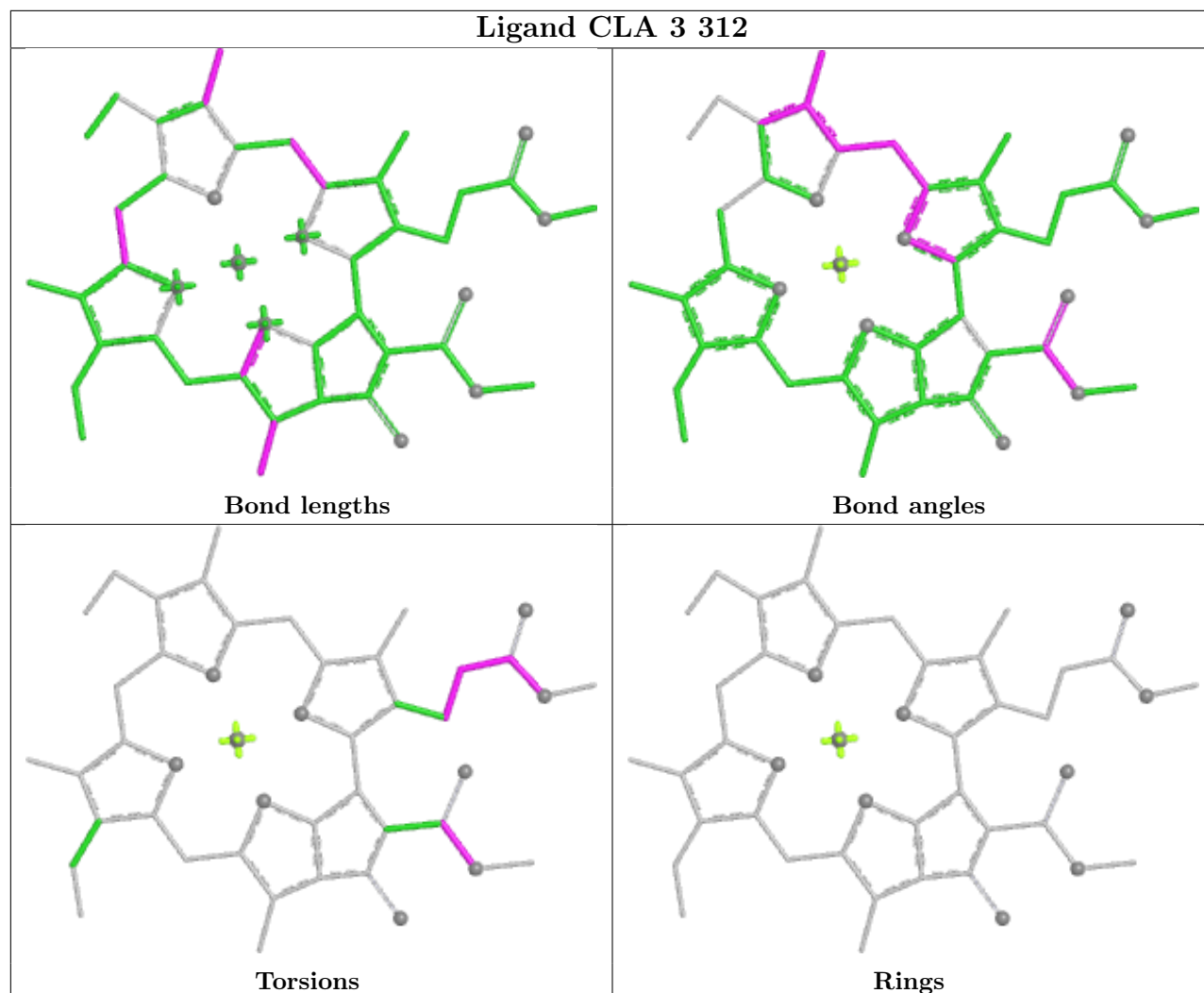
## Ligand CLA 1 611



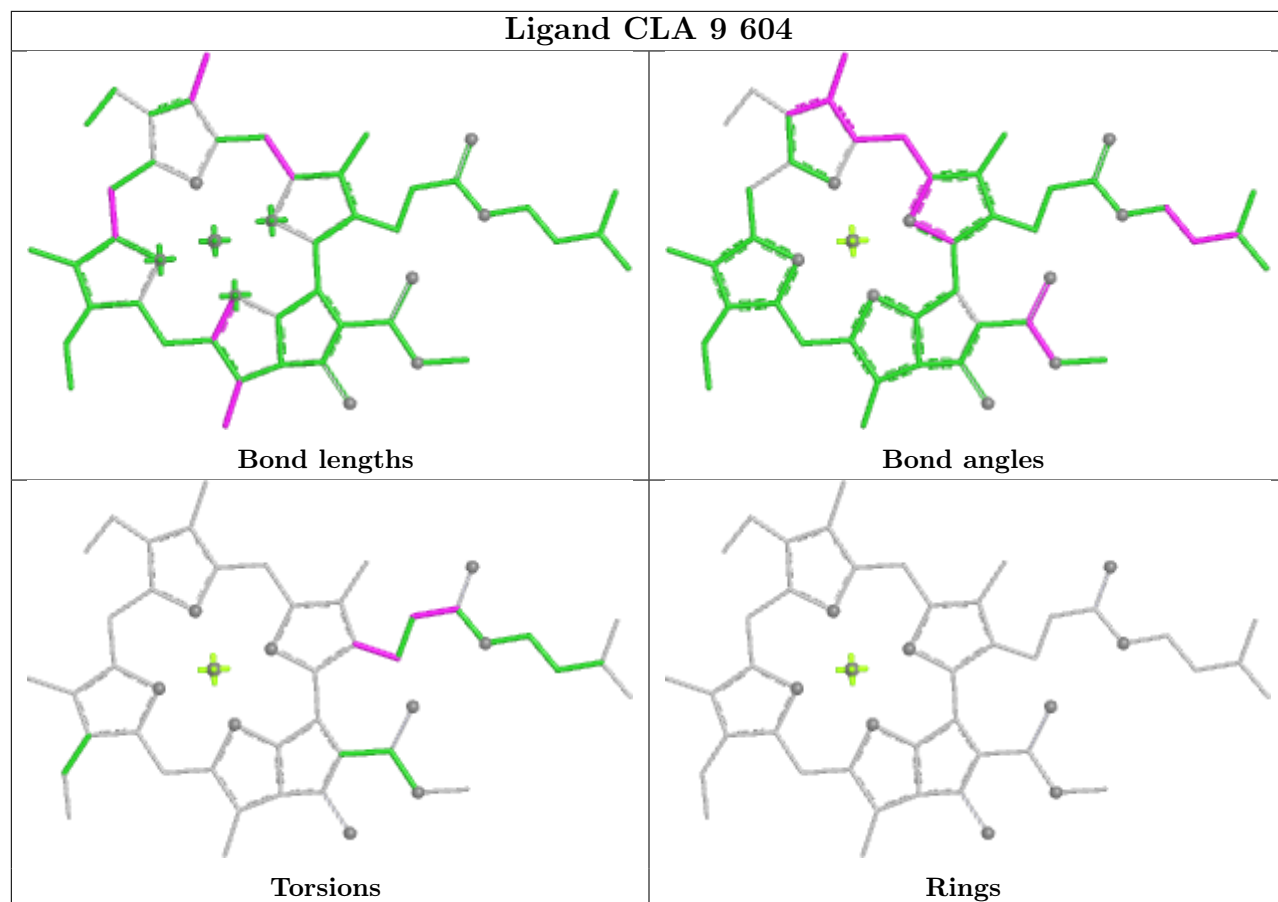
## Ligand LMG A 5001



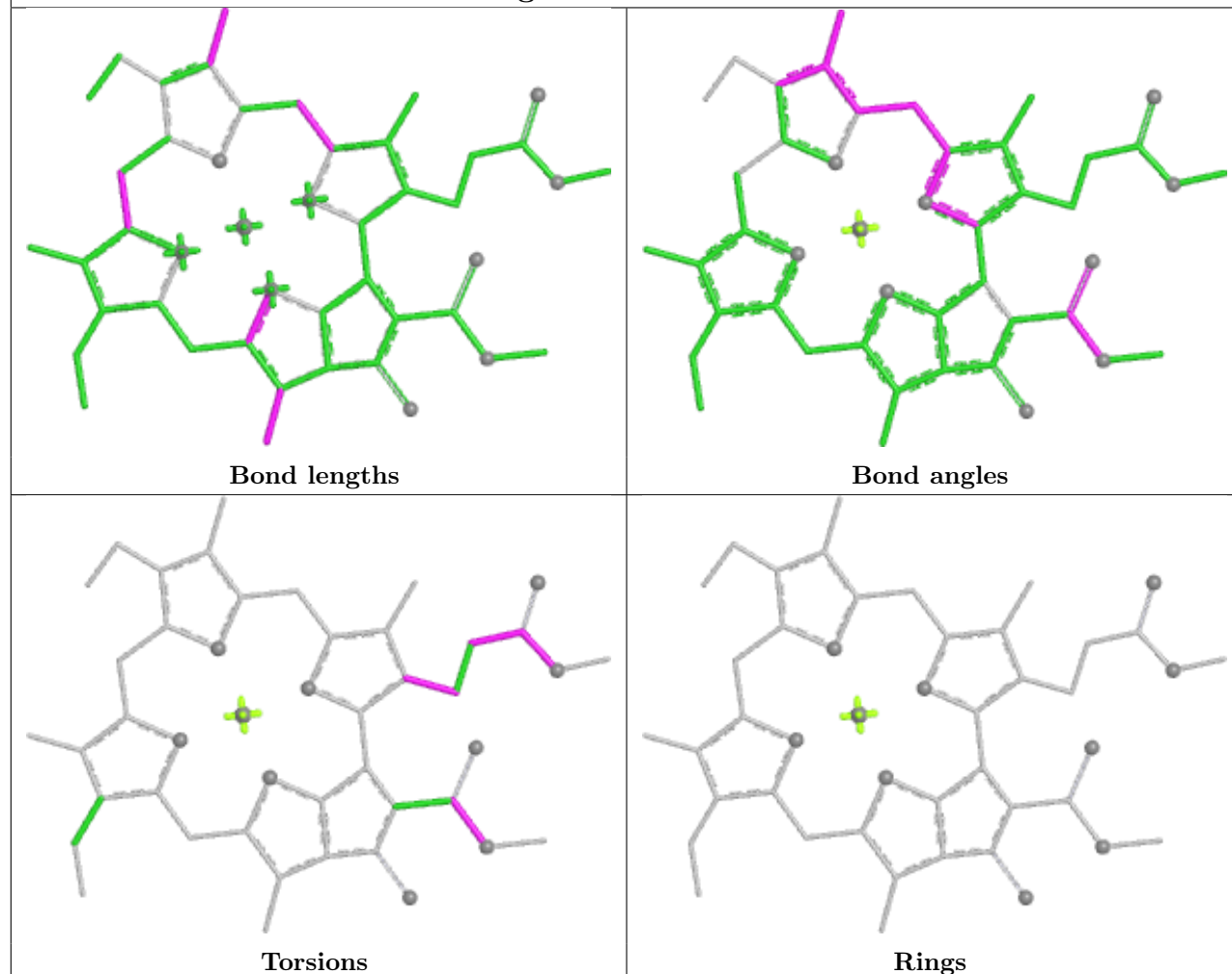
## Ligand CLA 3 312



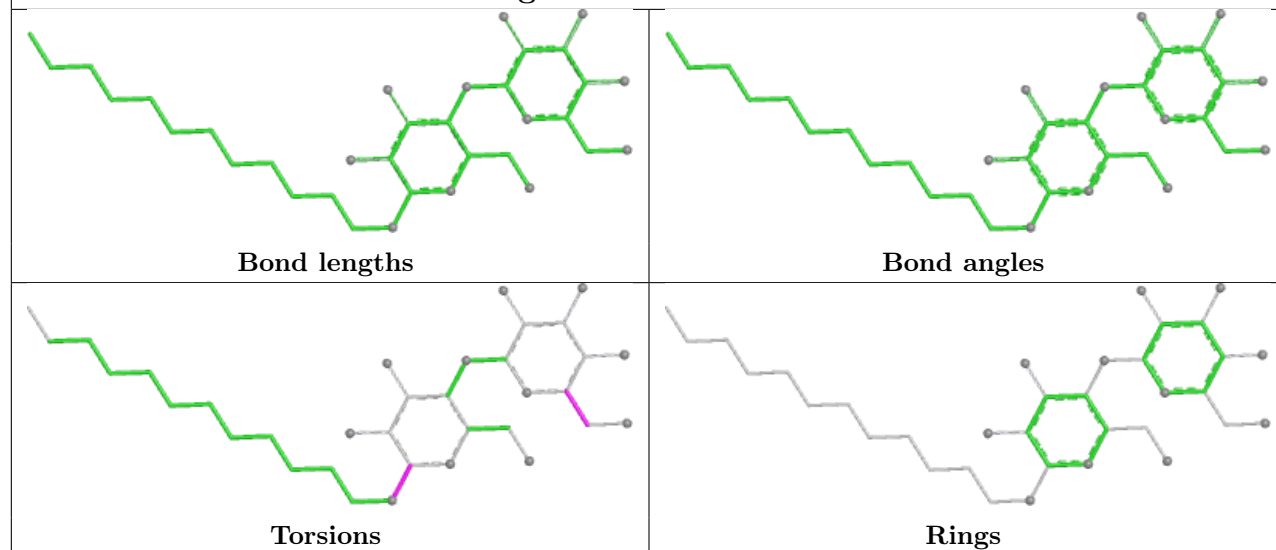
## Ligand CLA 9 604



## Ligand CLA 1 610

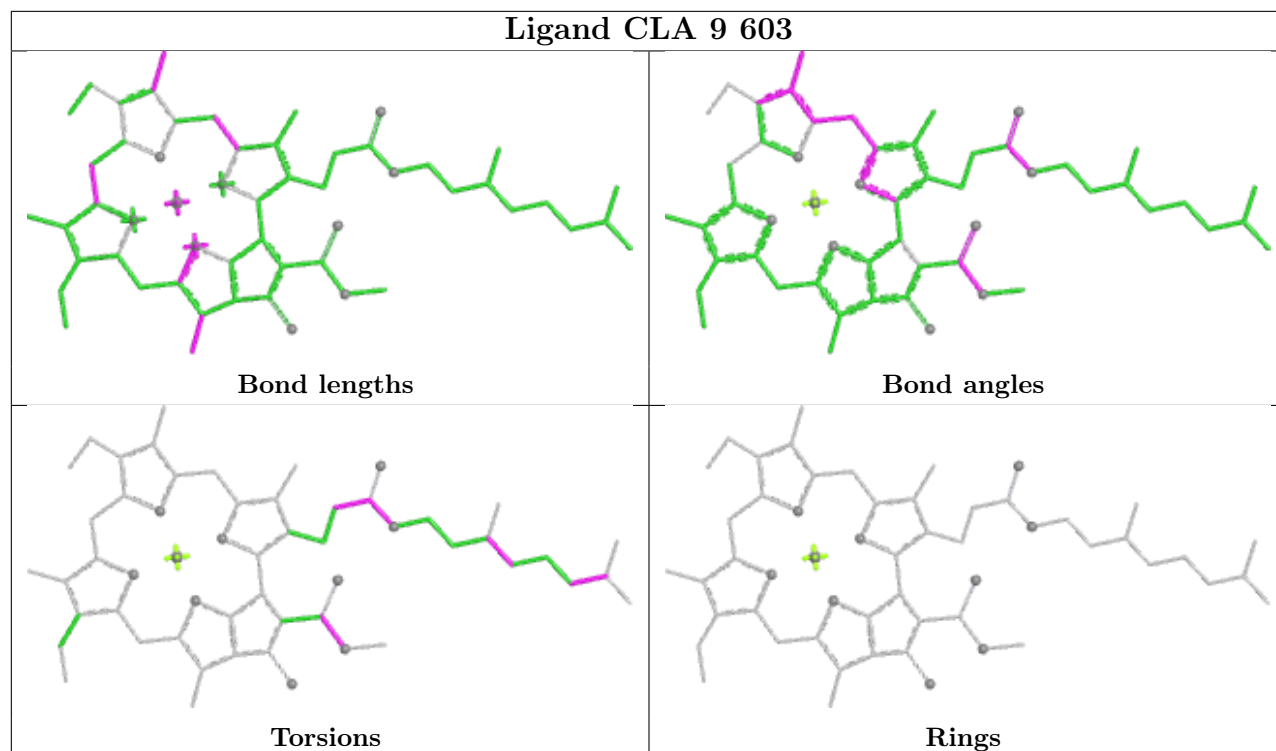


## Ligand LMU A 5053

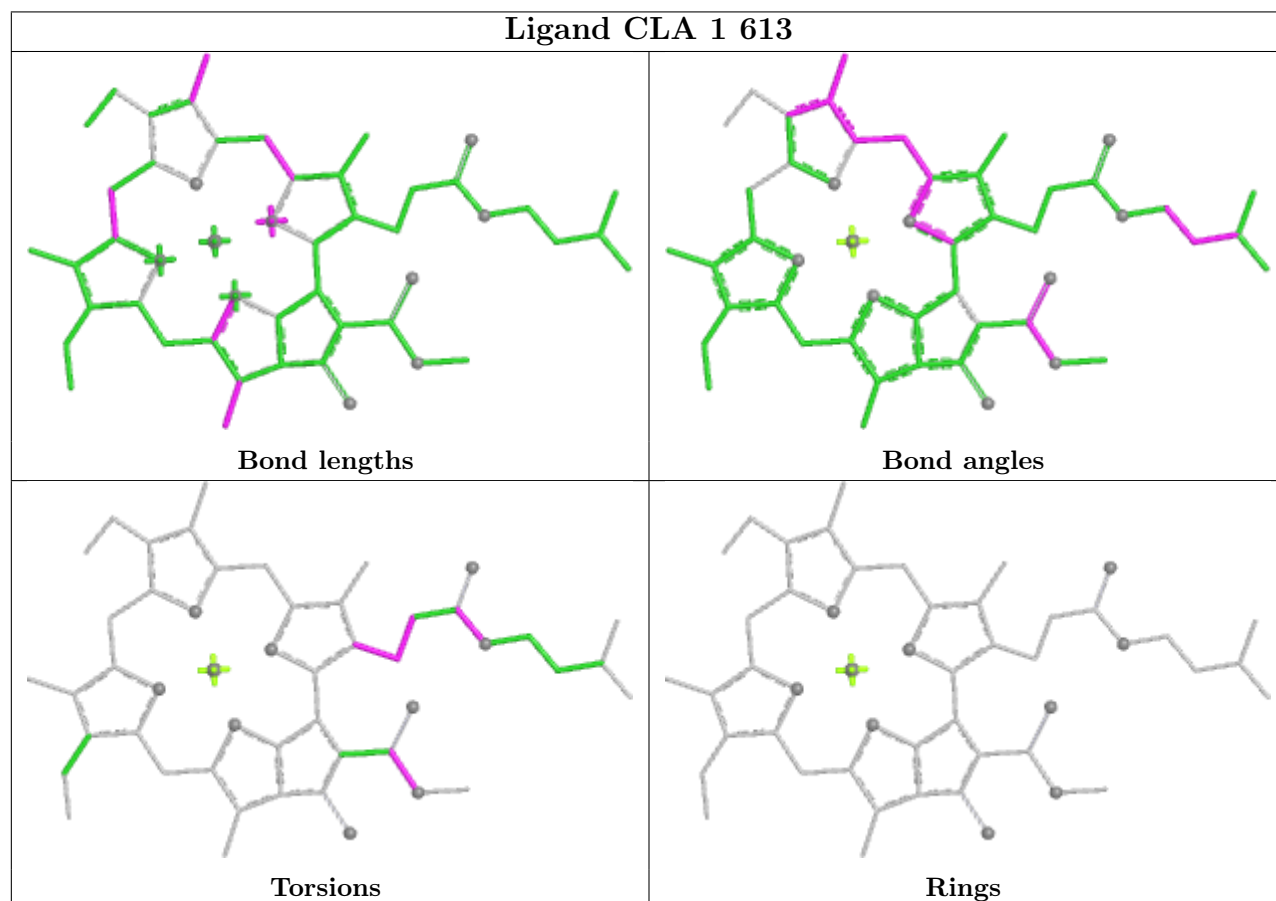




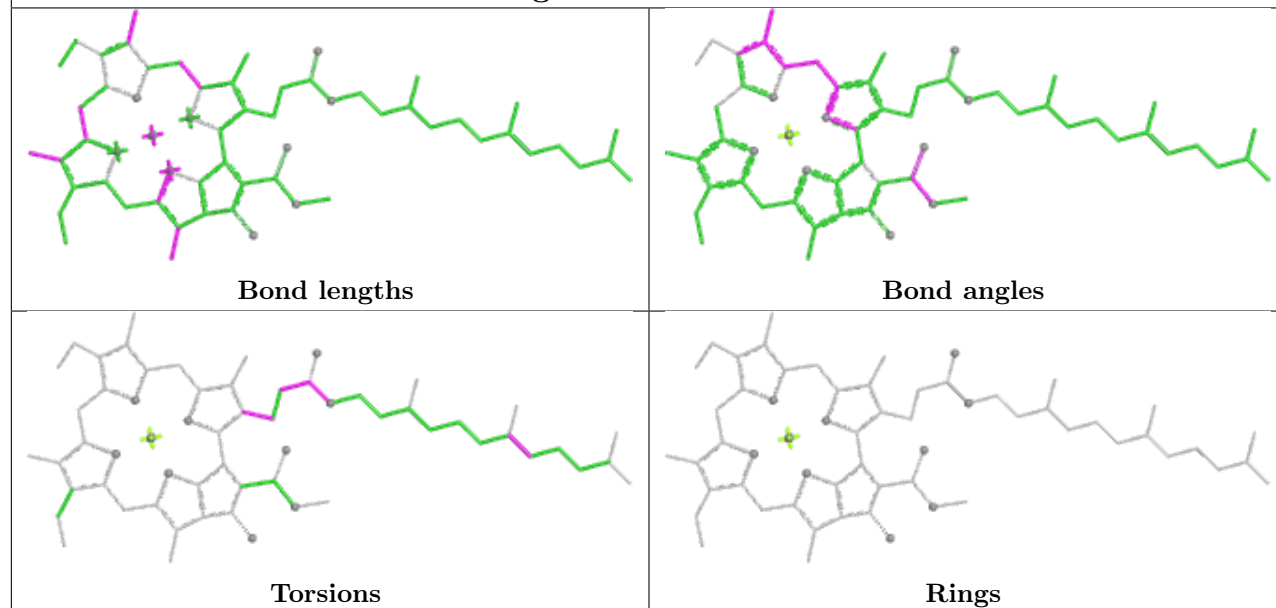
## Ligand CLA 9 603



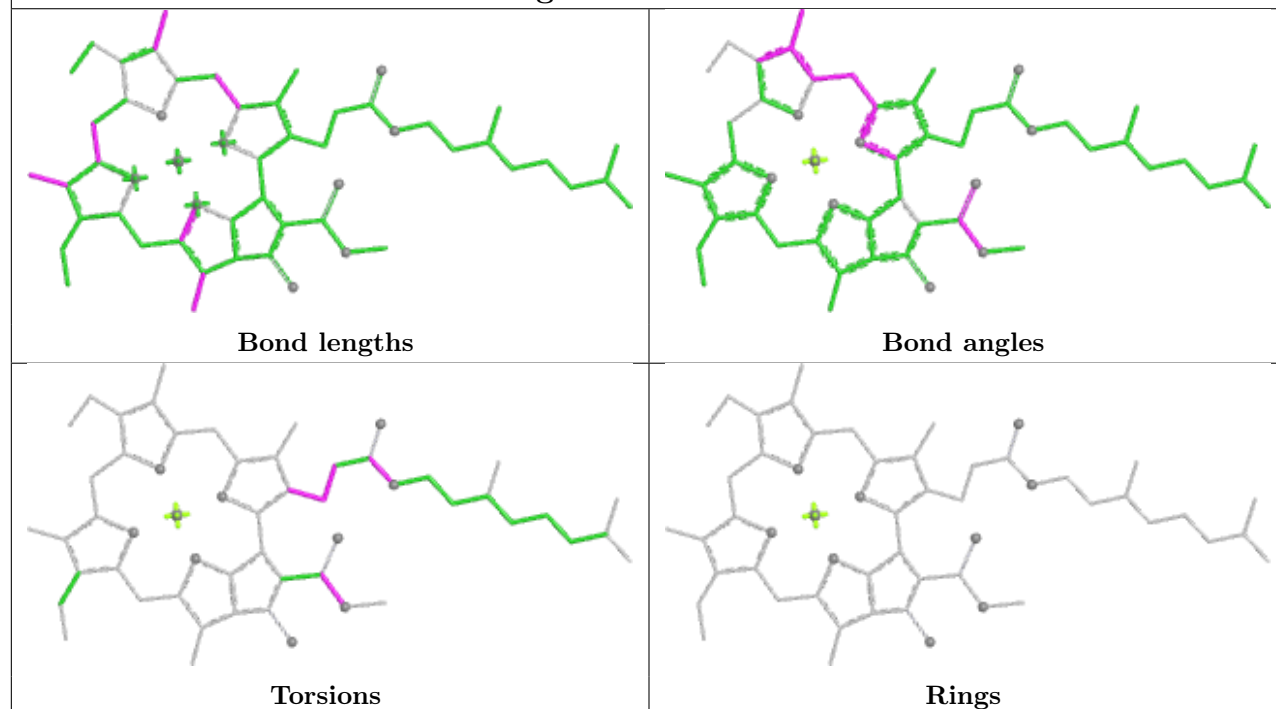
## Ligand CLA 1 613



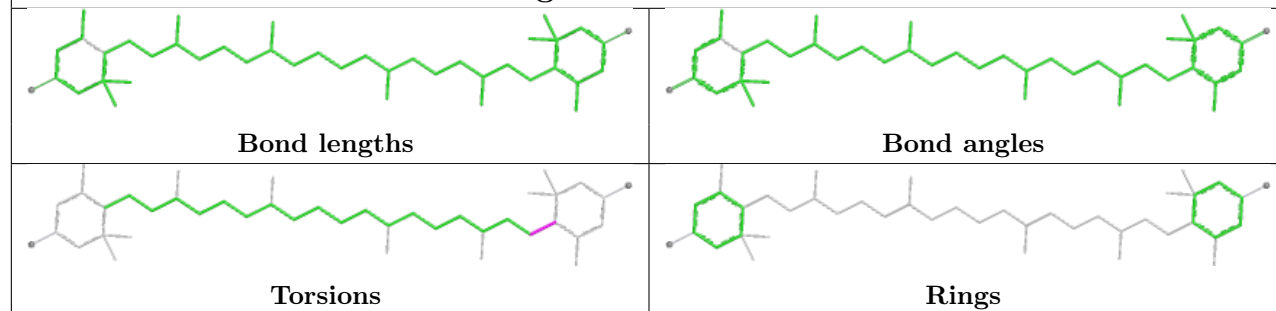
## Ligand CLA B 817



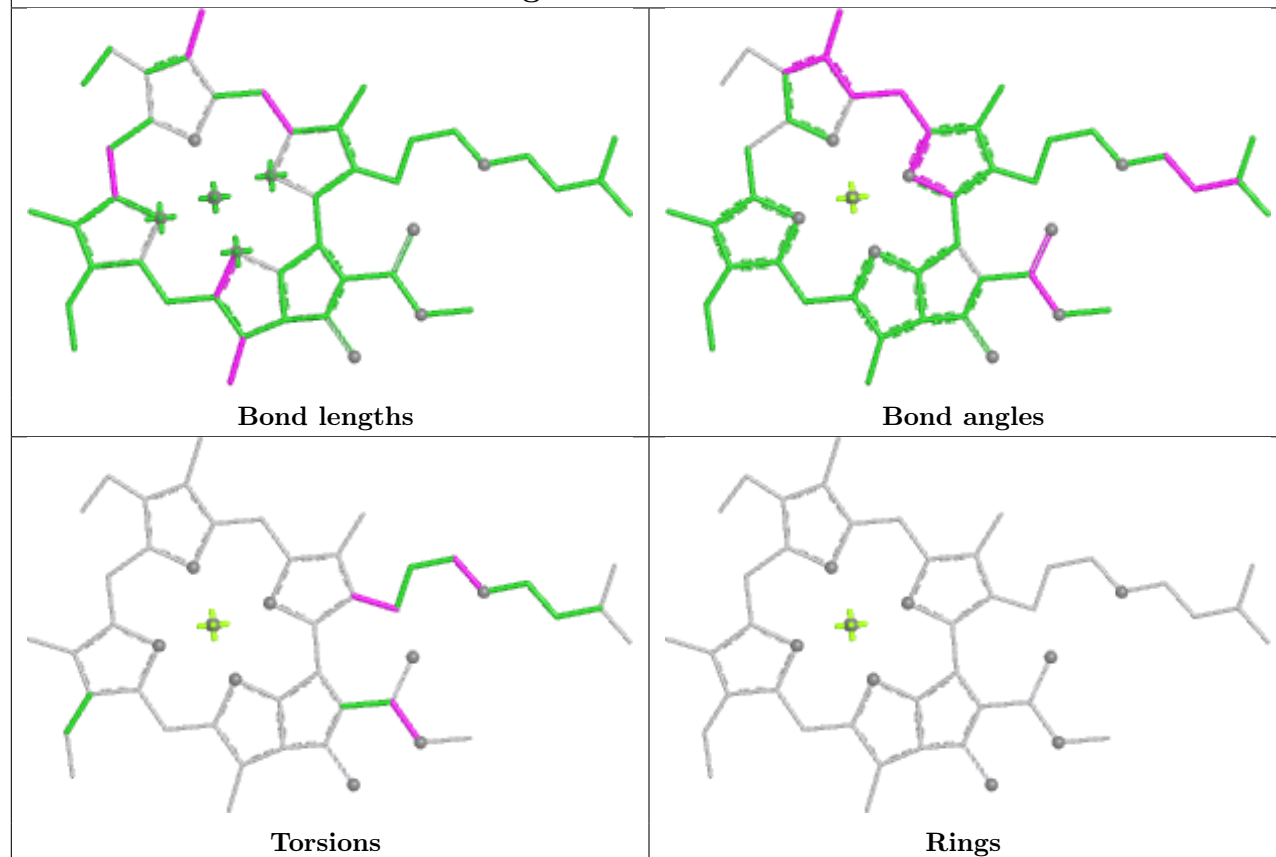
## Ligand CLA 1 609



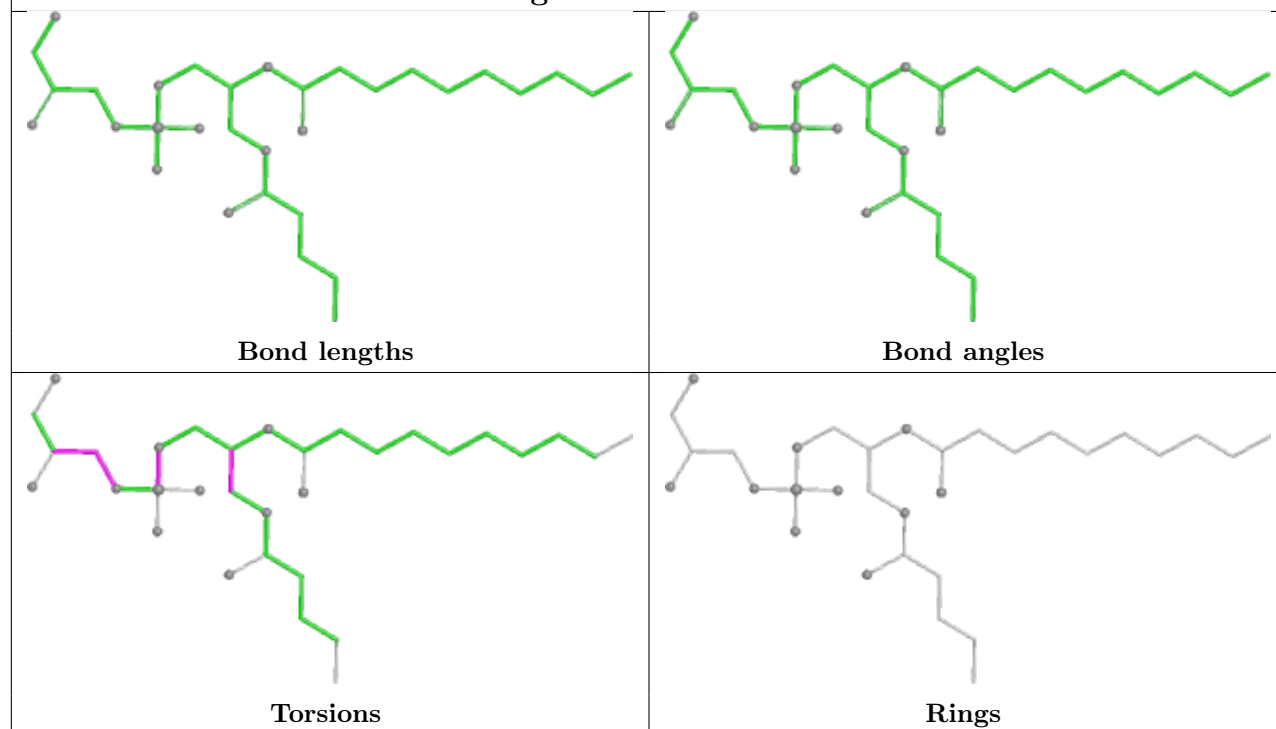
## Ligand LUT 8 314

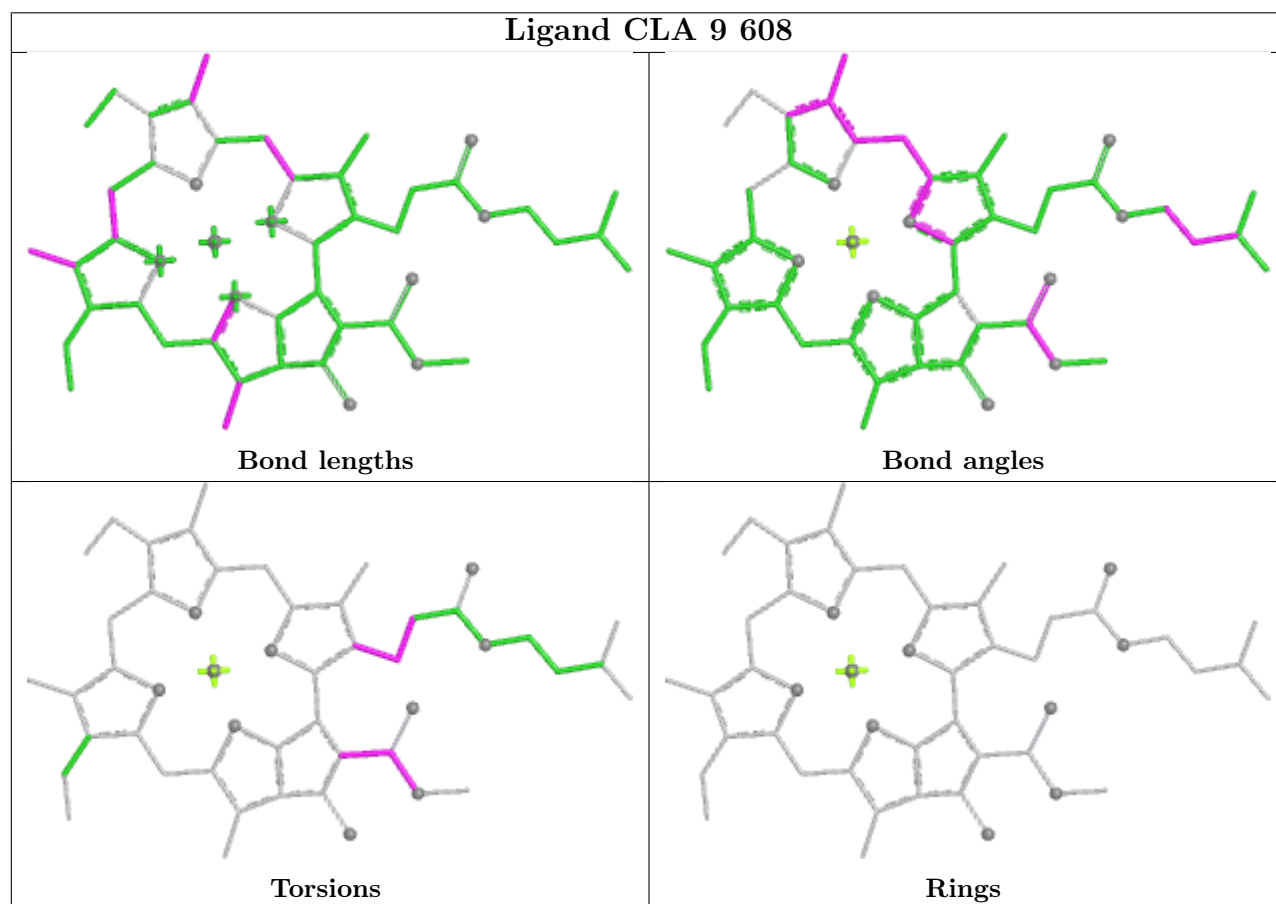
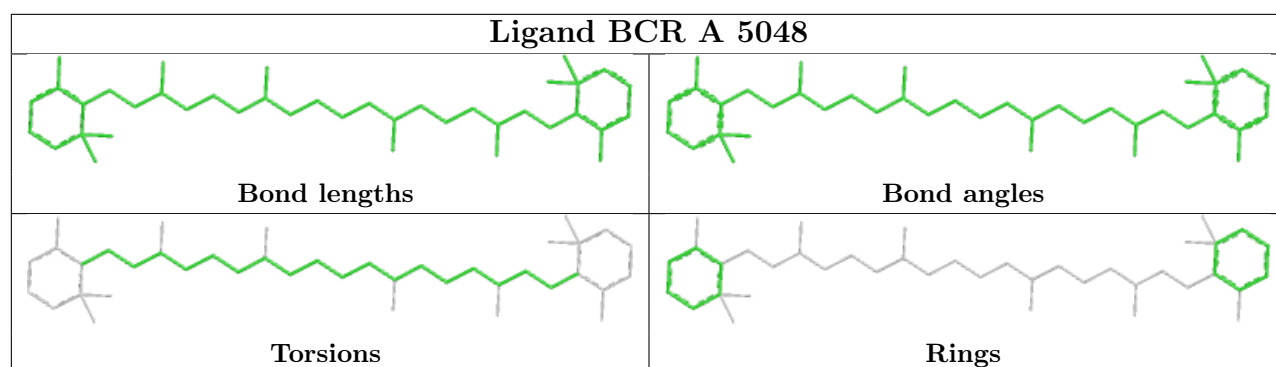


## Ligand CLA A 5043

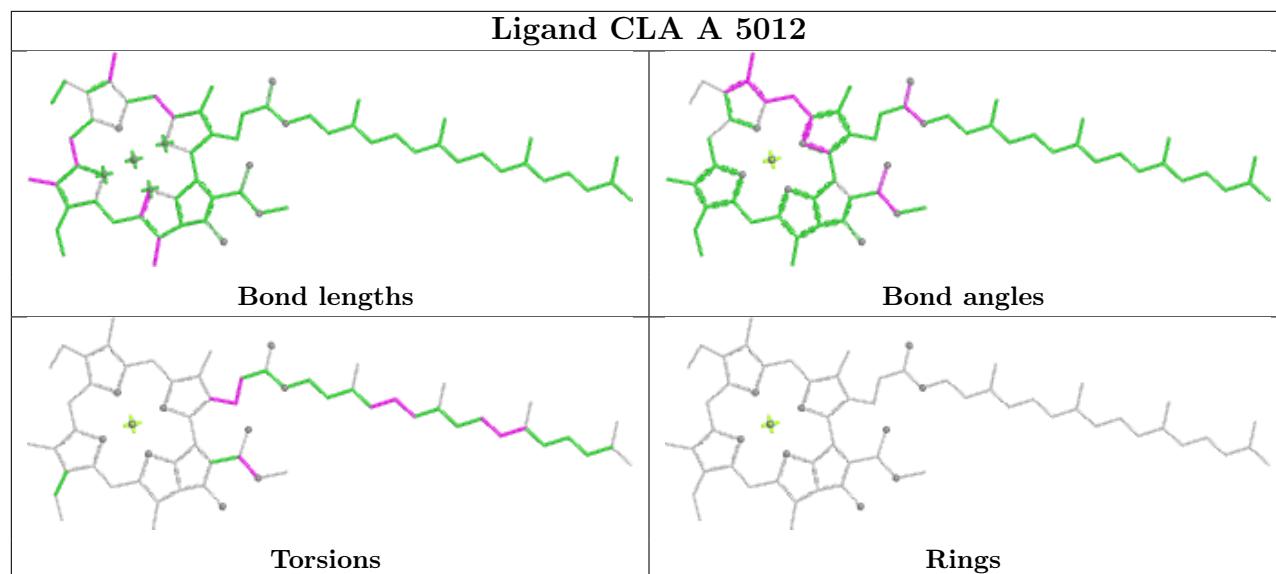


## Ligand LHG B 801

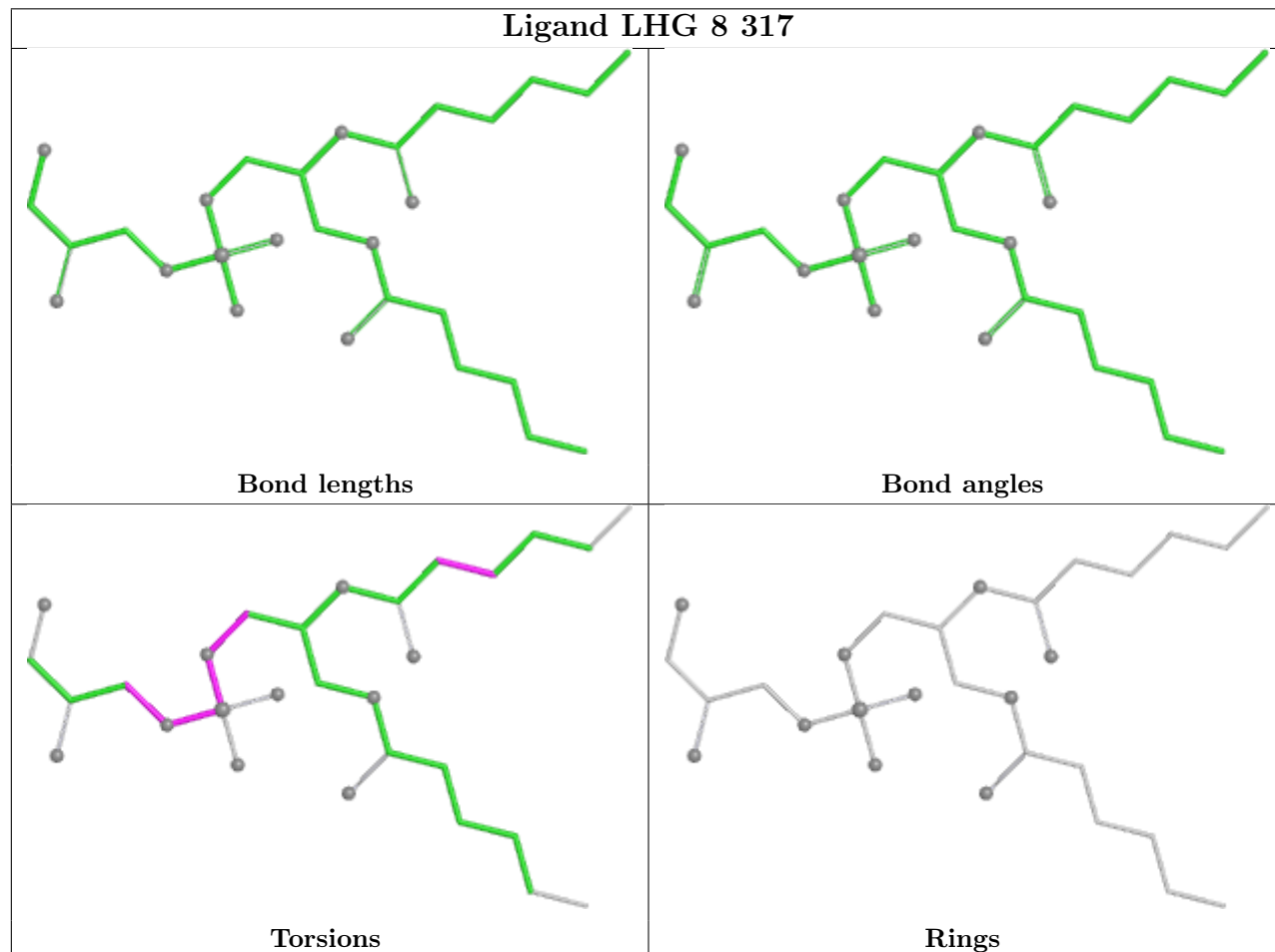




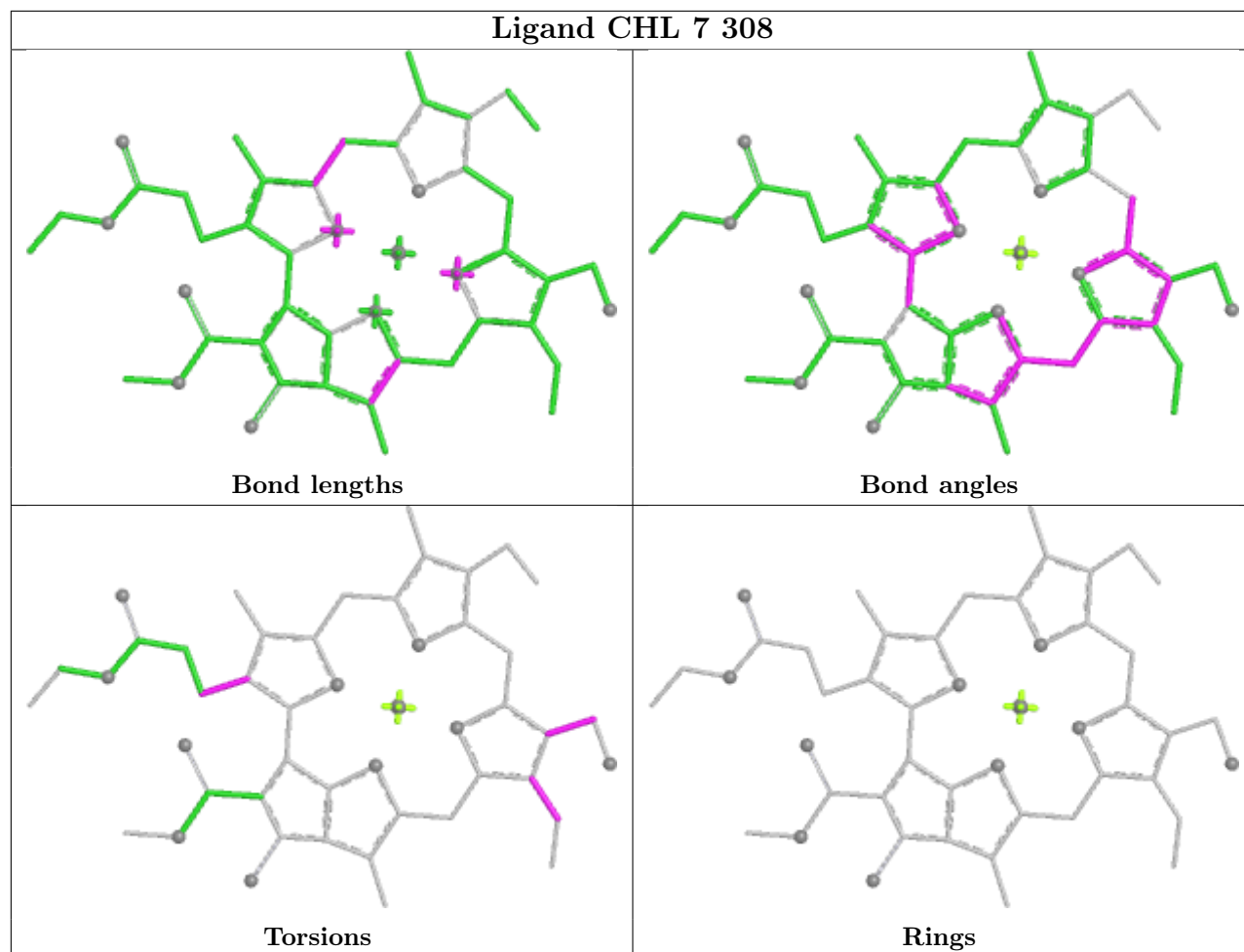
## Ligand CLA A 5012



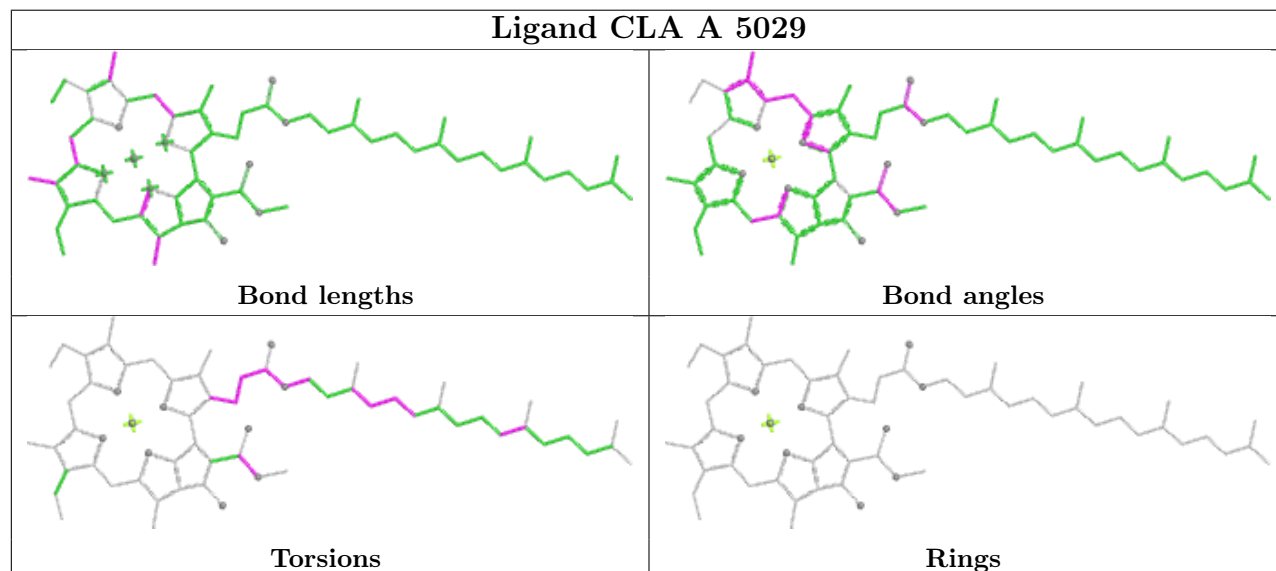
## Ligand LHG 8 317



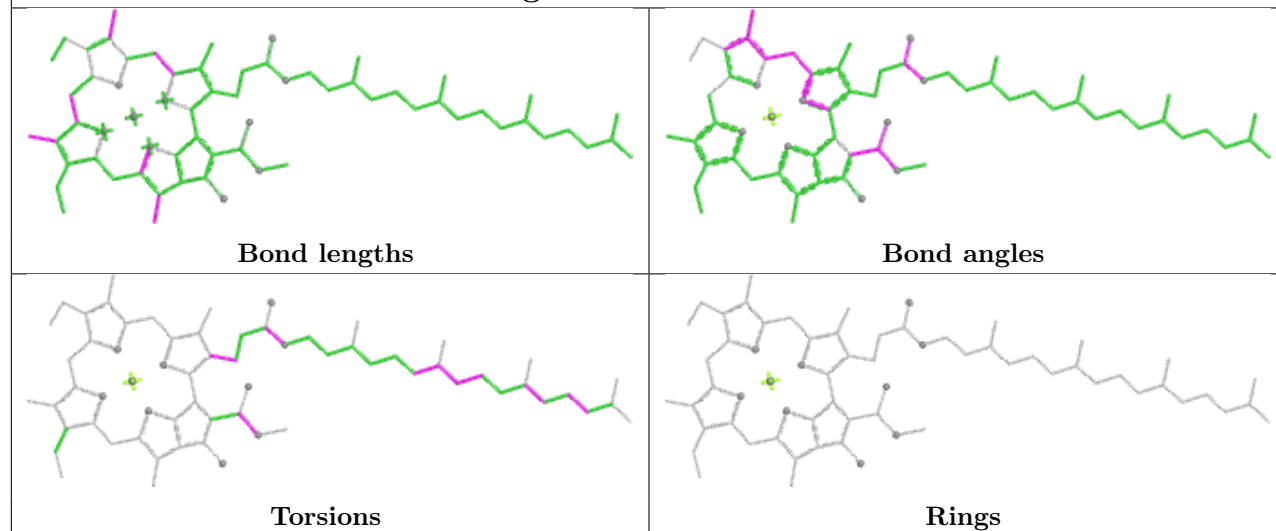
## Ligand CHL 7 308



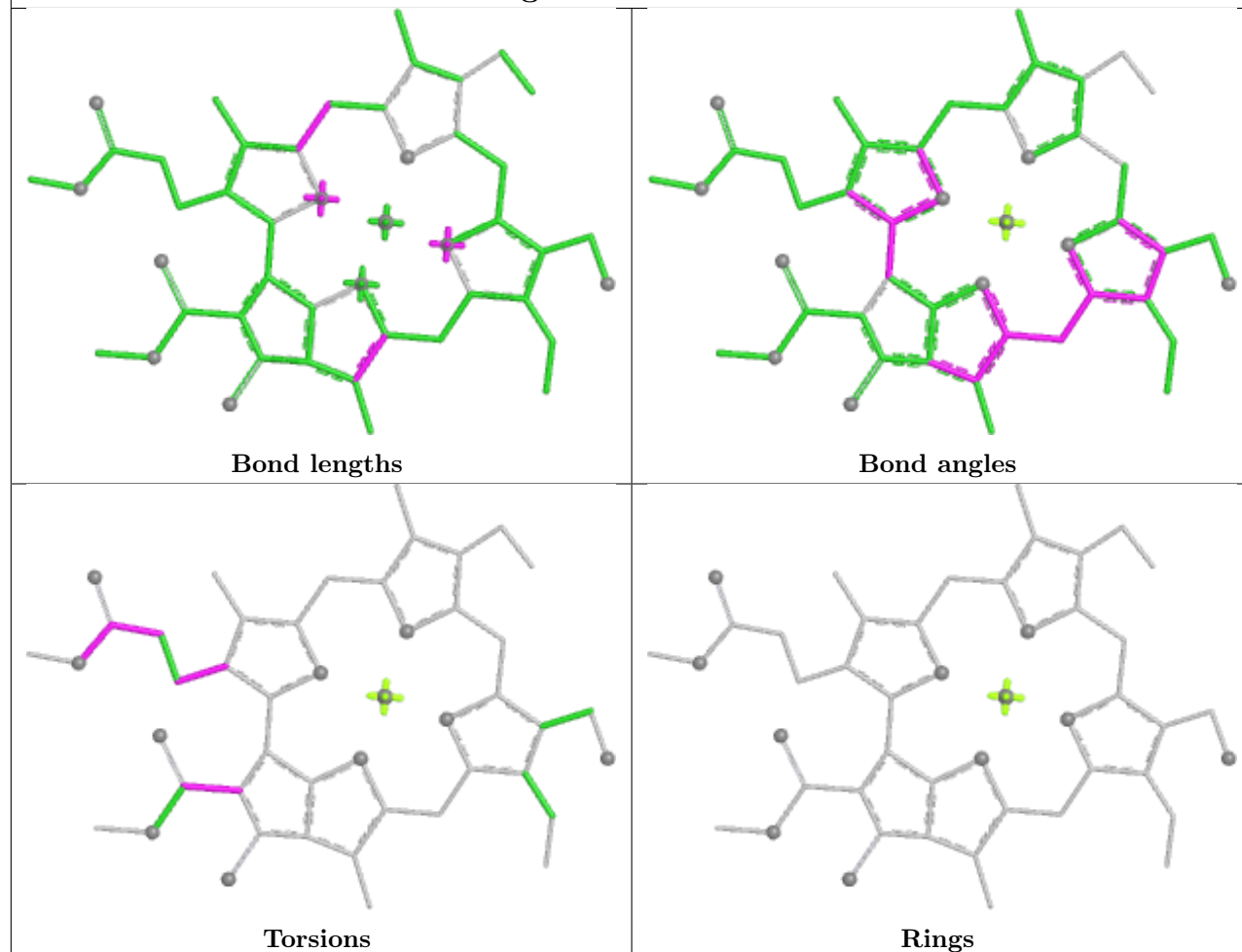
## Ligand CLA A 5029

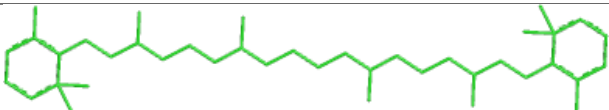
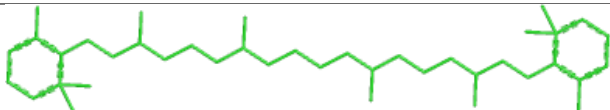
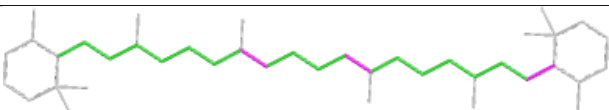
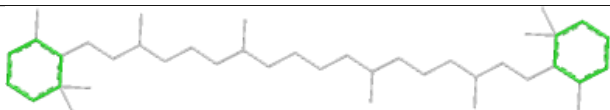




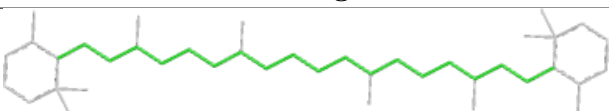
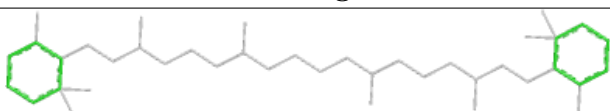
## Ligand CLA A 5006

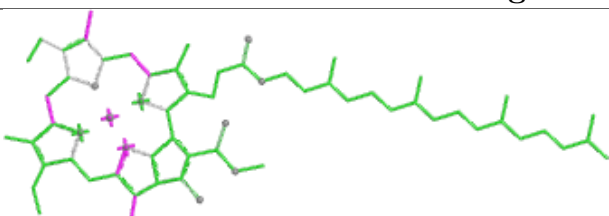
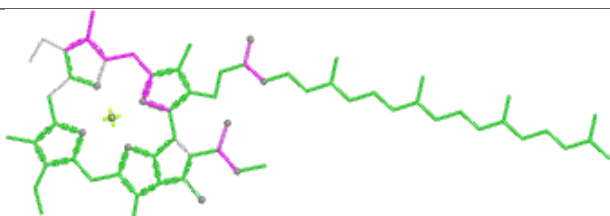
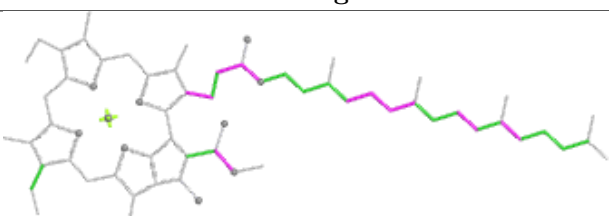
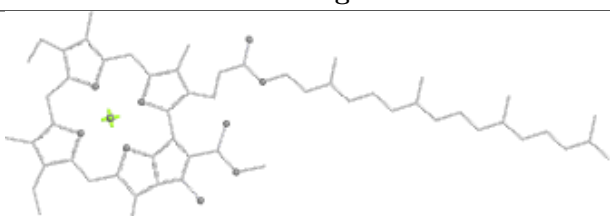


## Ligand CHL 8 304



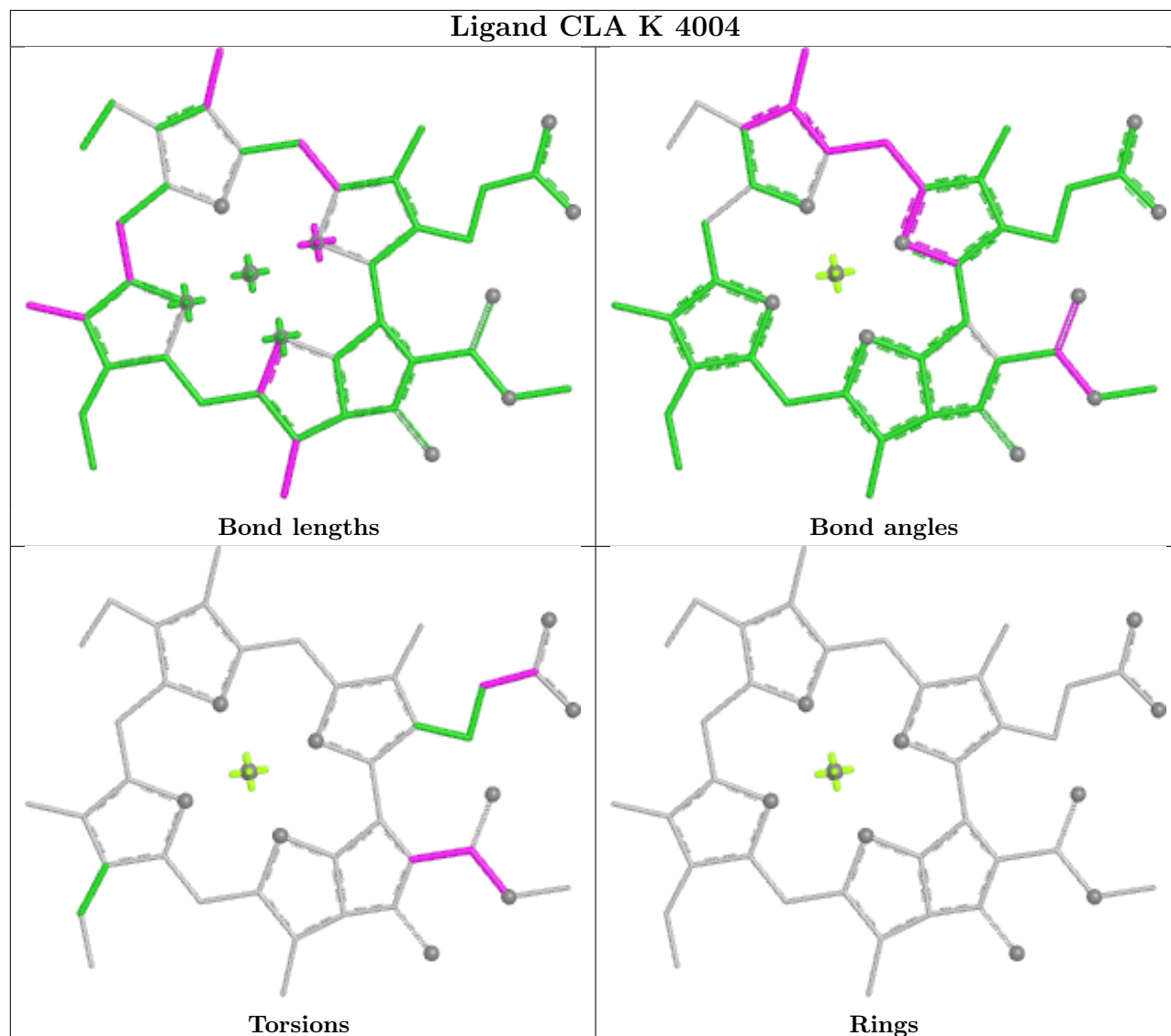
Ligand BCR G 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

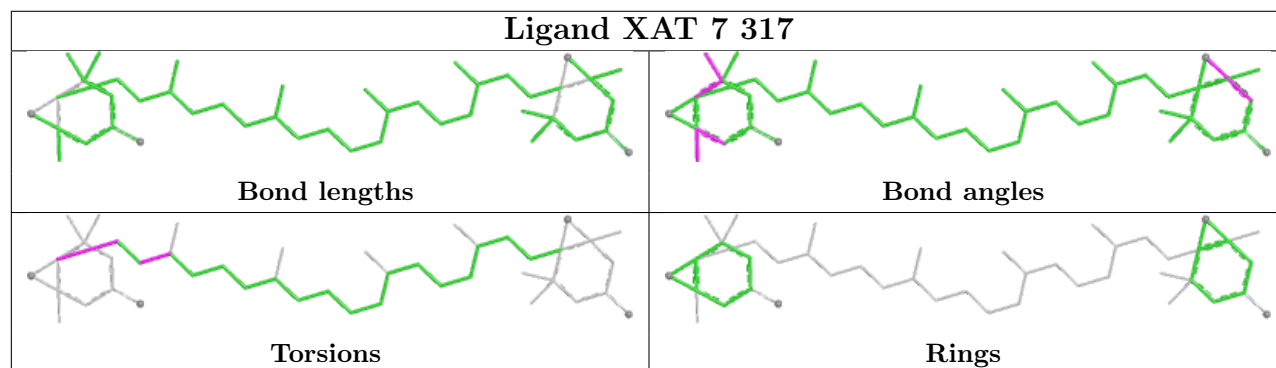
Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

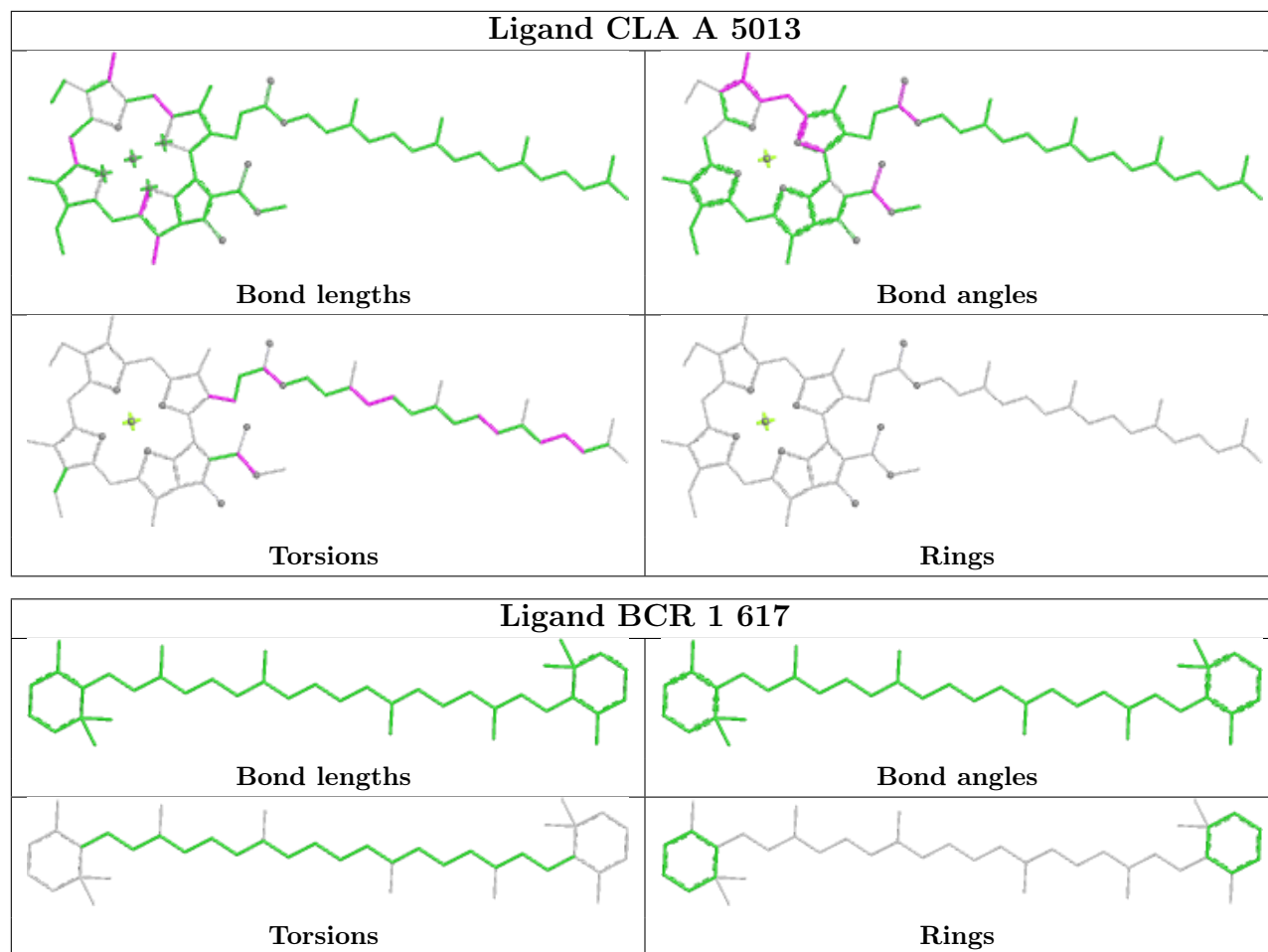


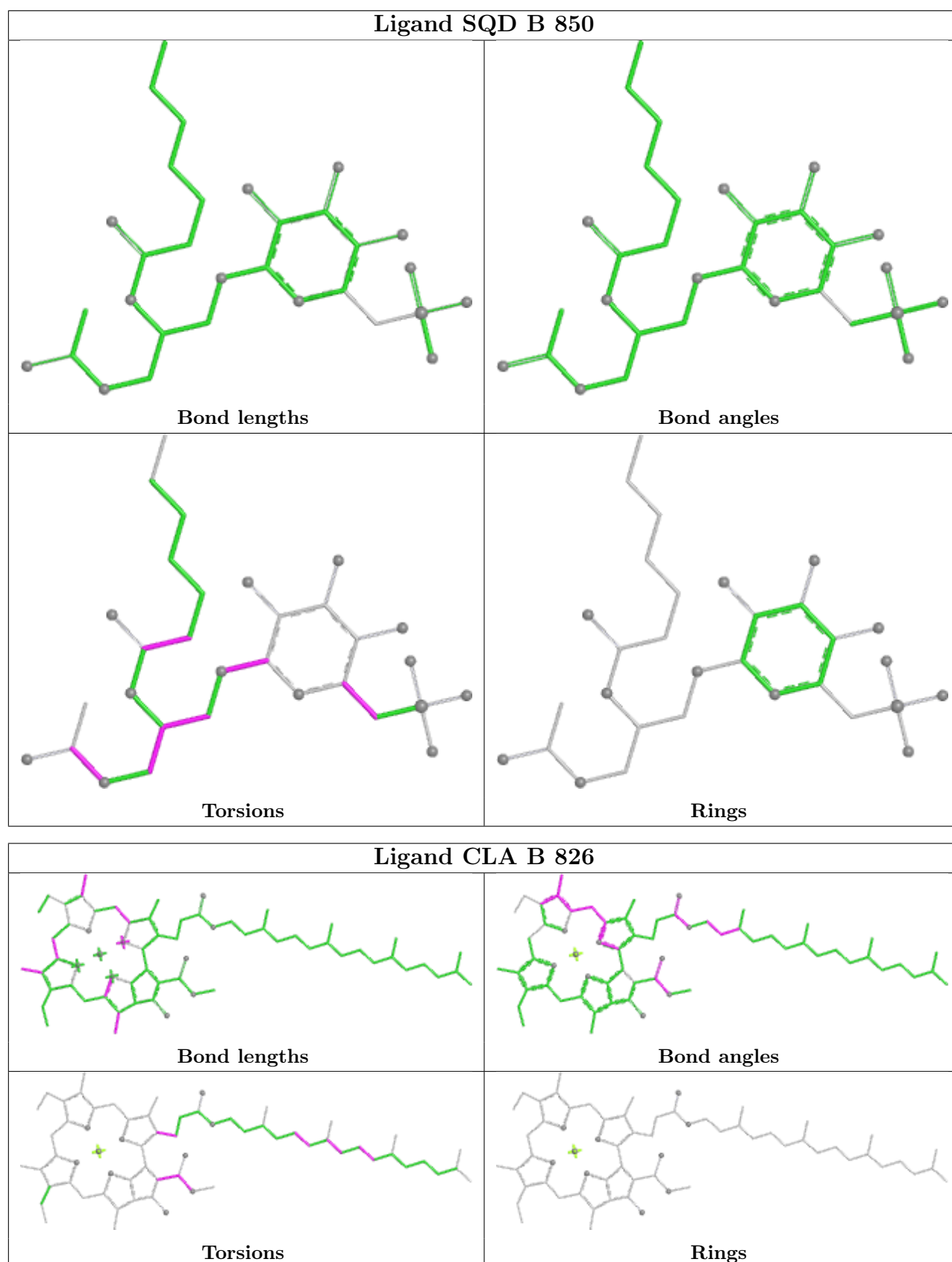
## Ligand CLA K 4004

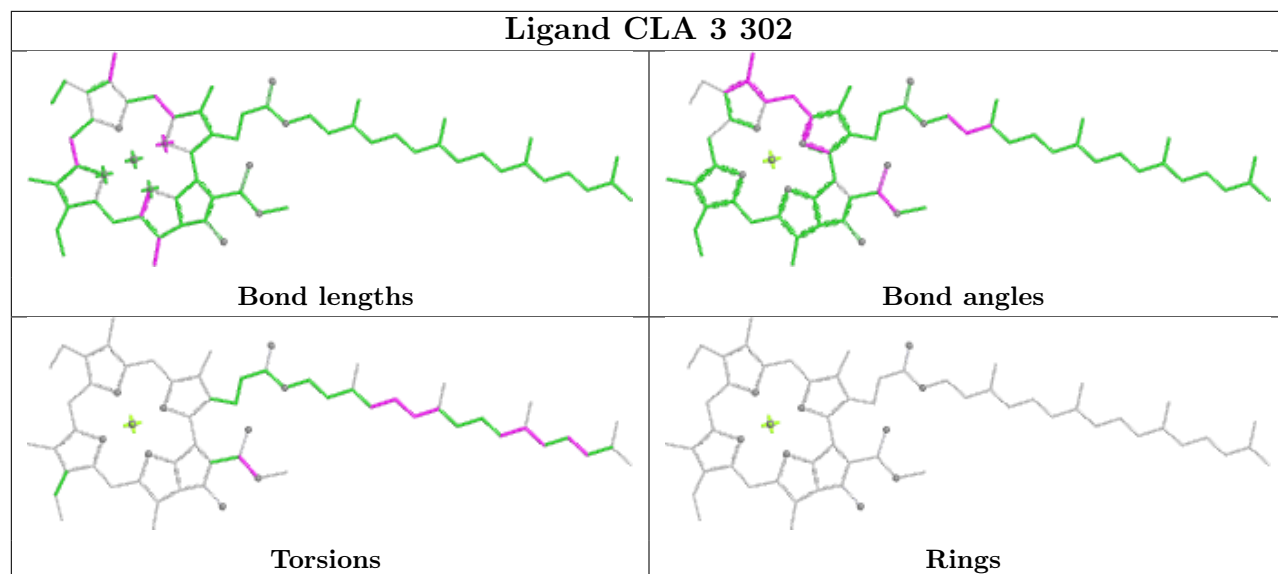
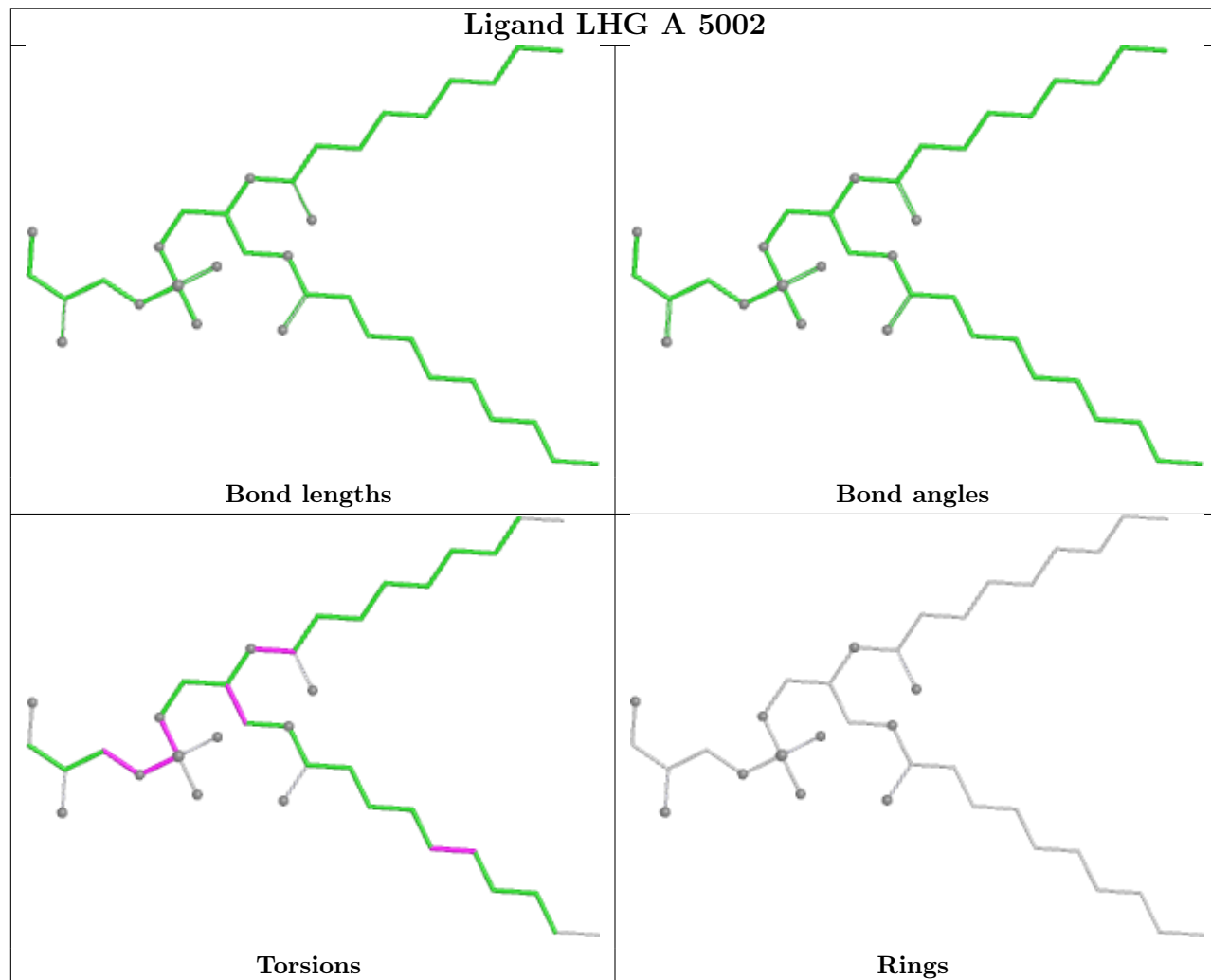


## Ligand XAT 7 317

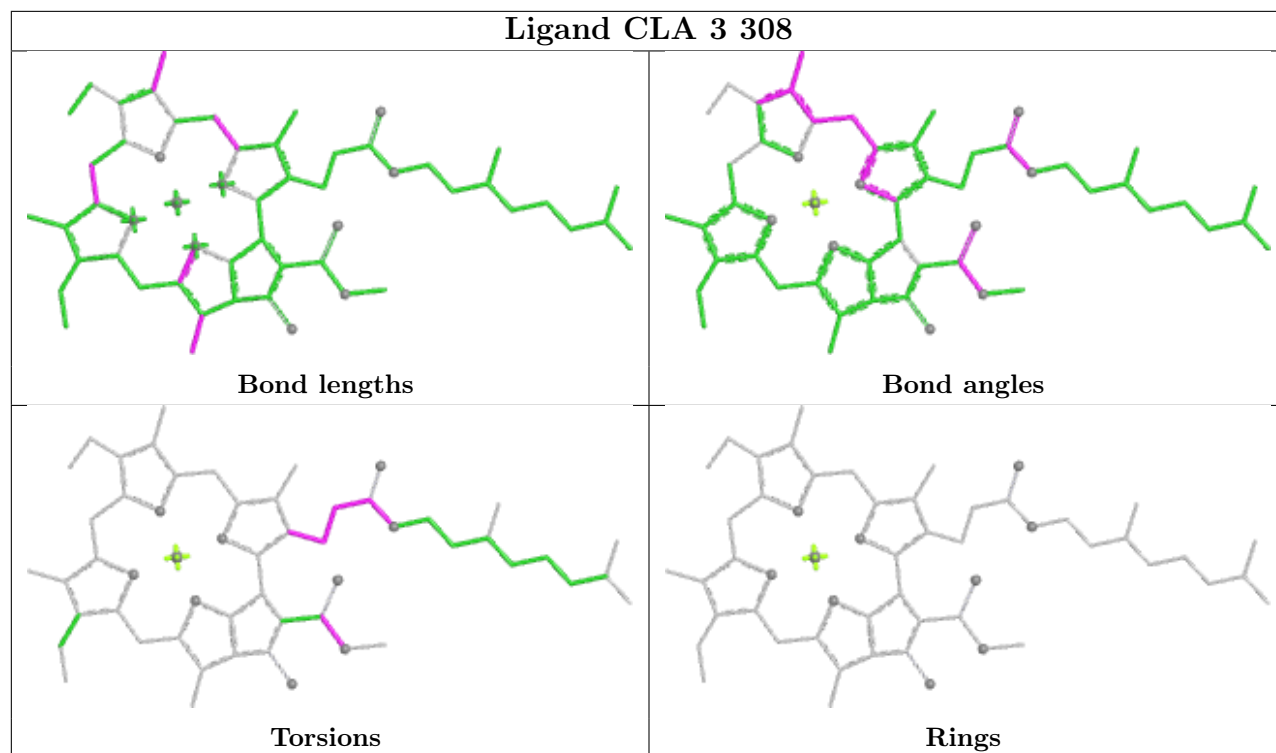




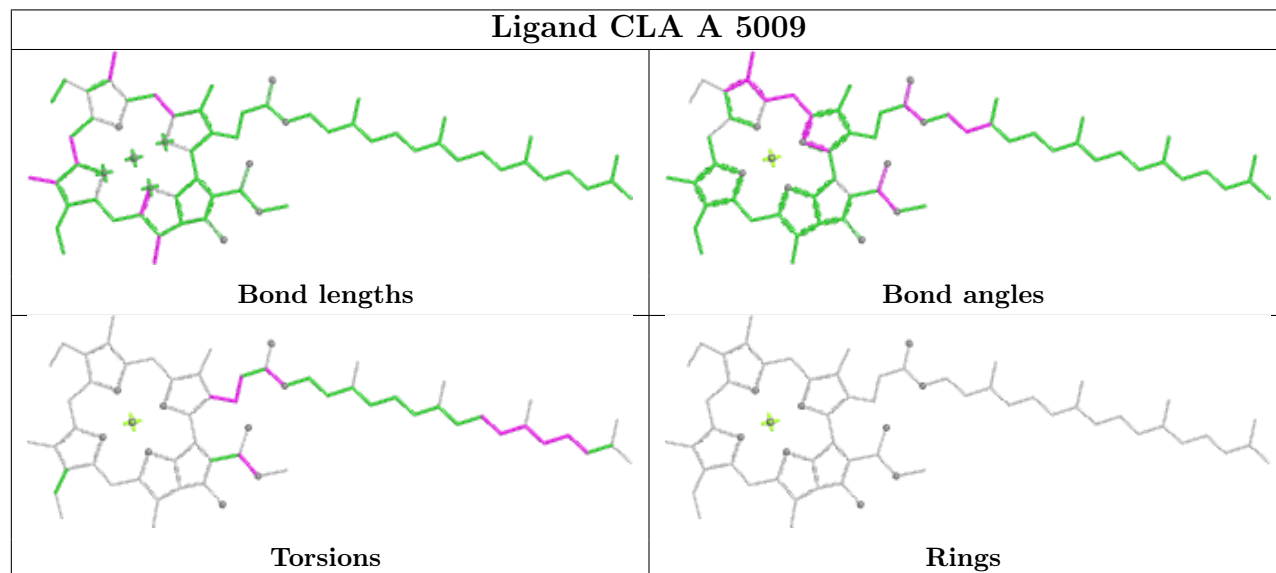


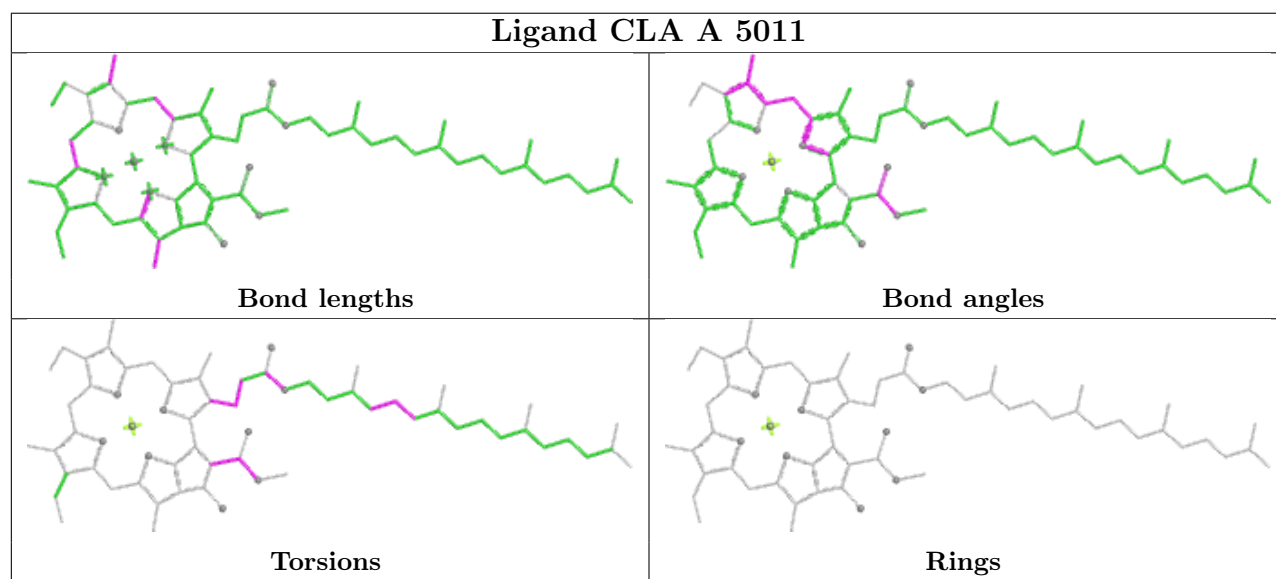
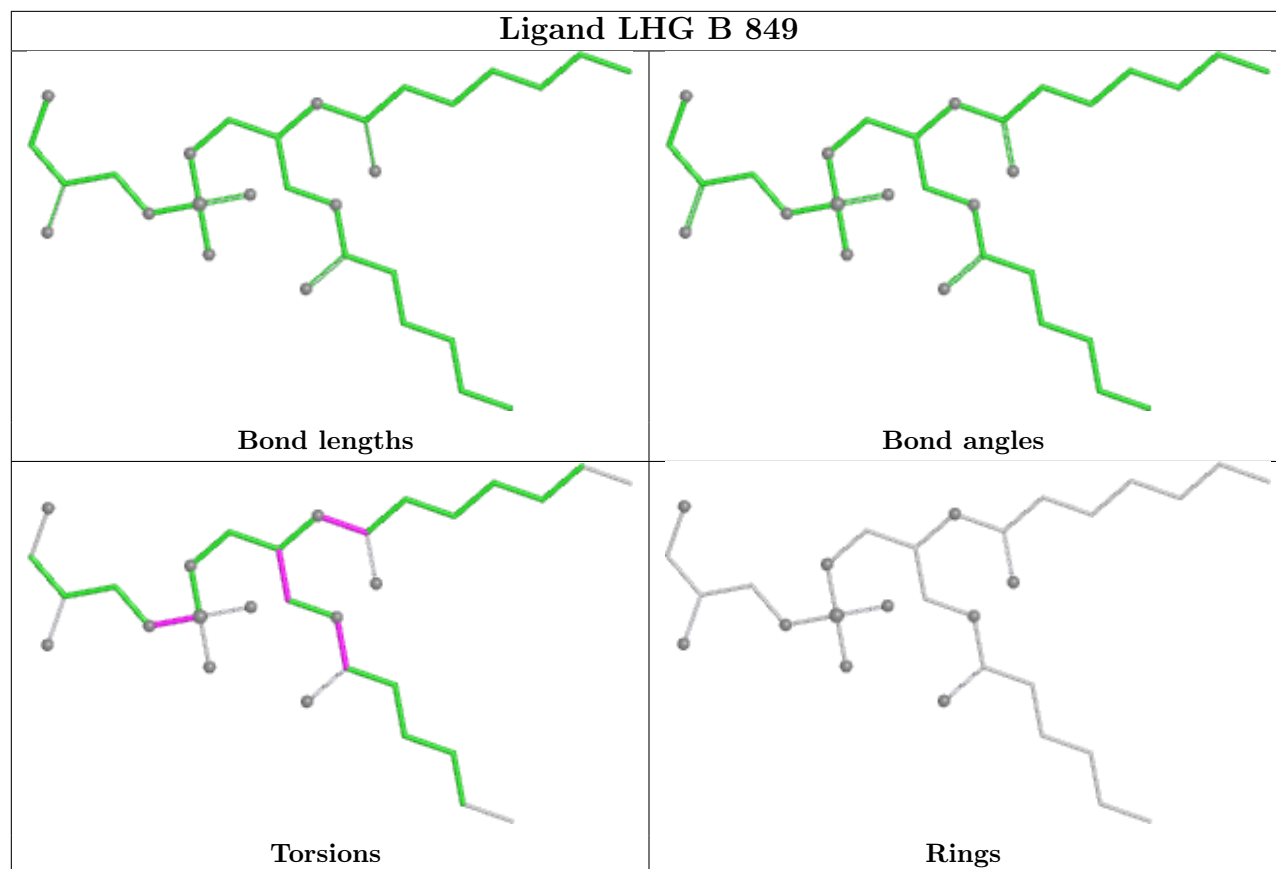
**Ligand CLA 3 302****Ligand LHG A 5002**

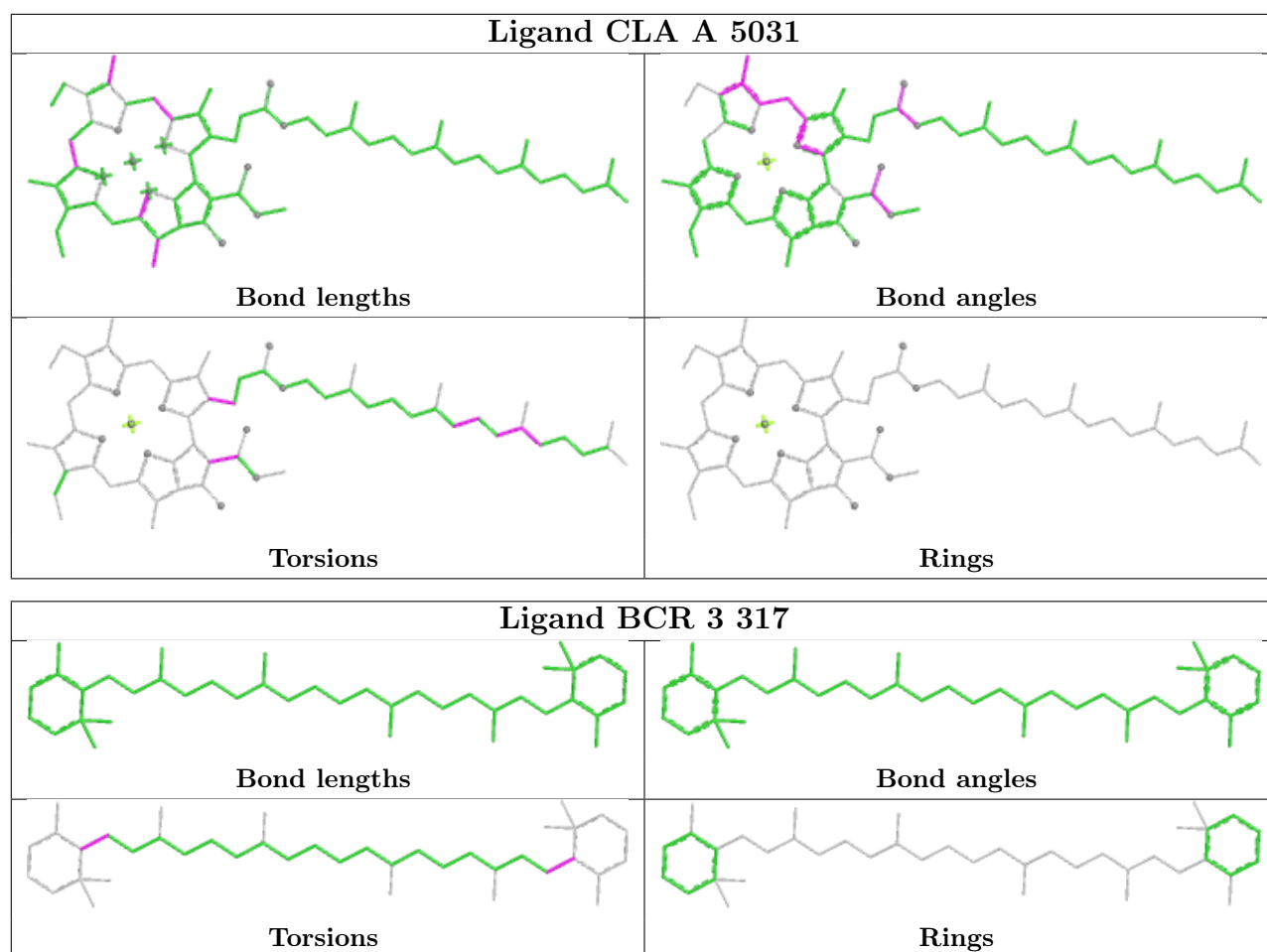
## Ligand CLA 3 308



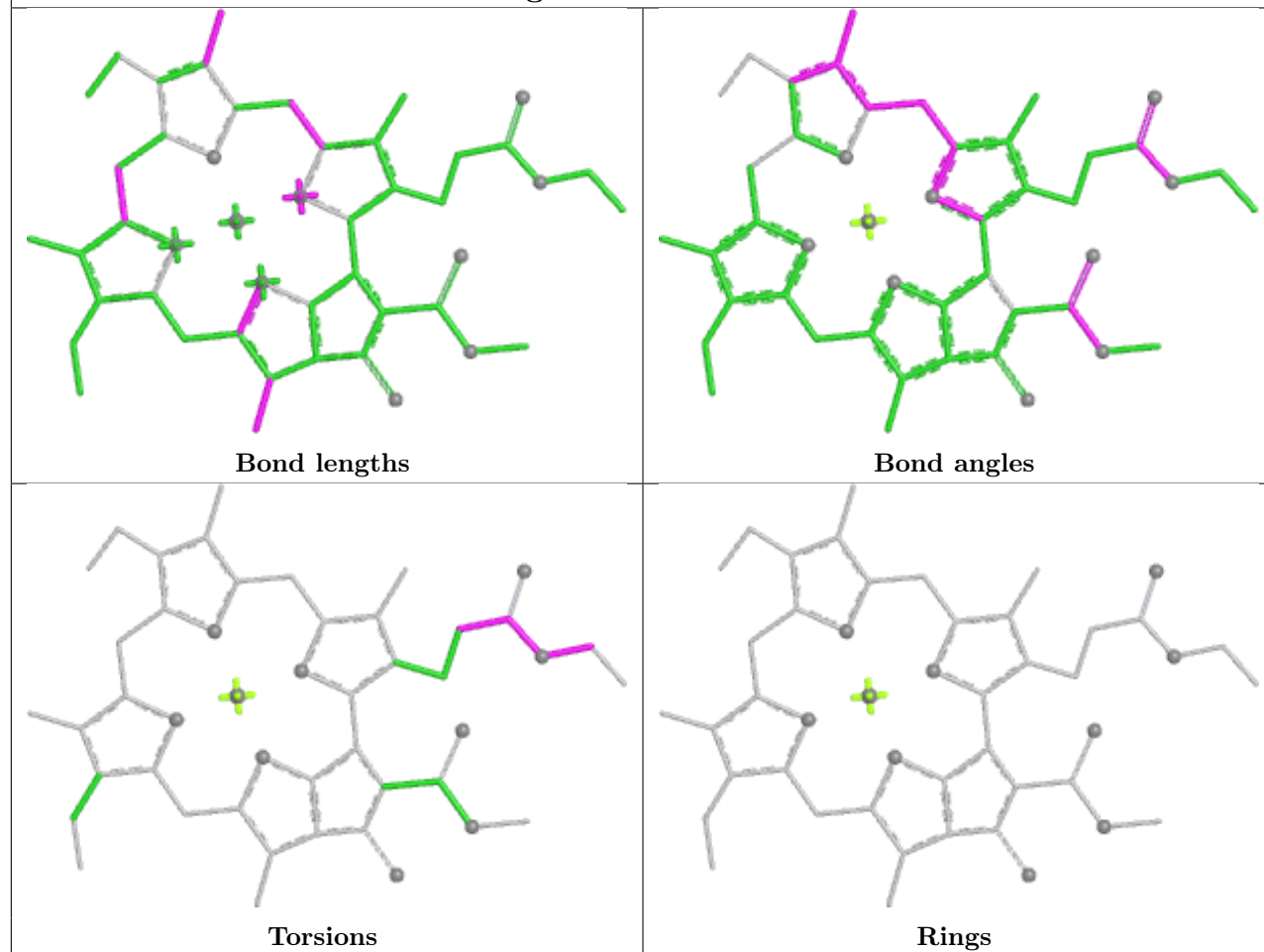
## Ligand CLA A 5009



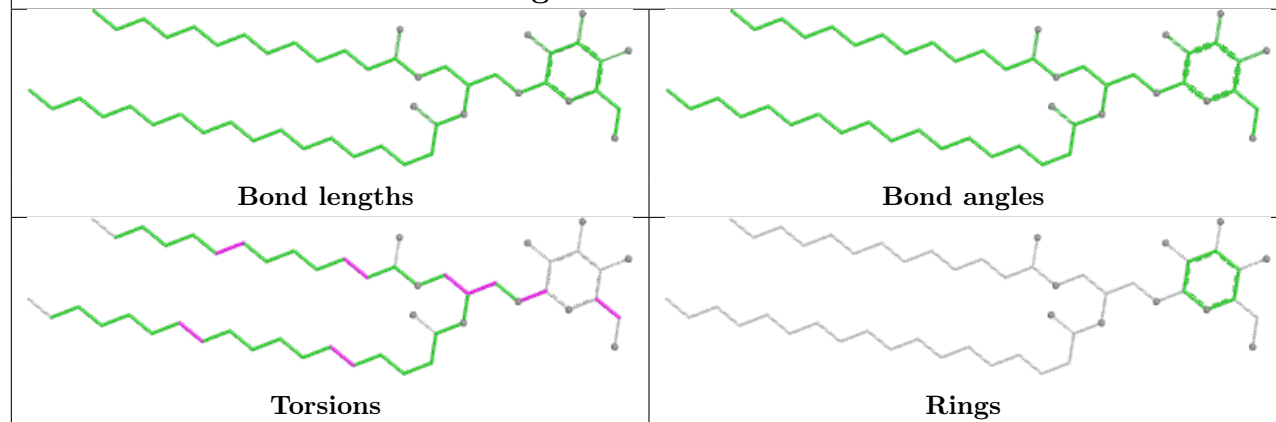




## Ligand CLA G 202

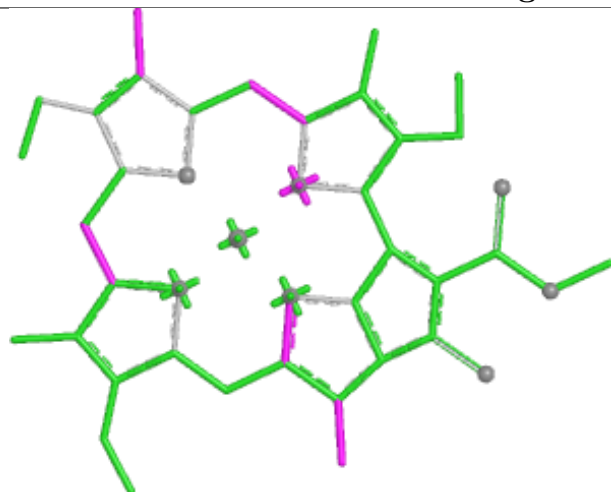


## Ligand LMG 7 301





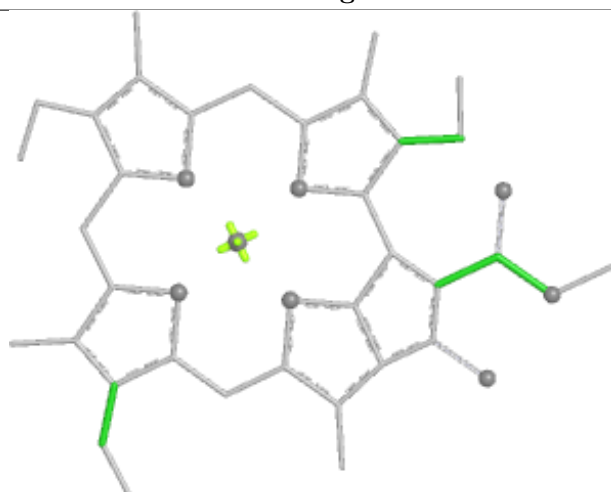
## Ligand CLA 3 313



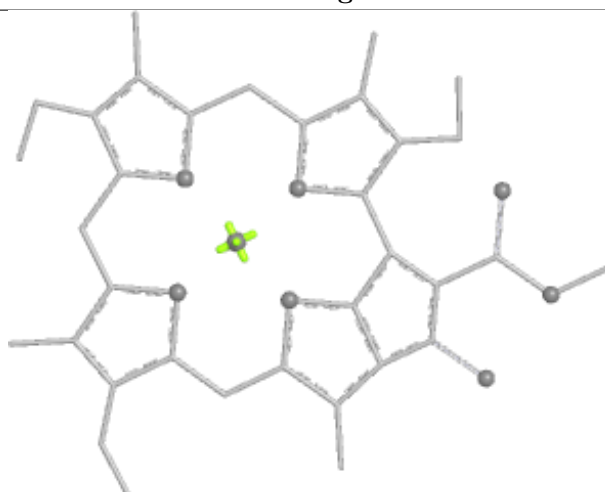
Bond lengths



Bond angles

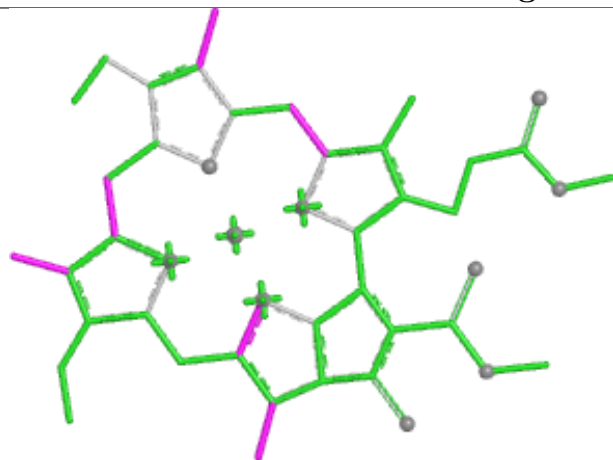


Torsions

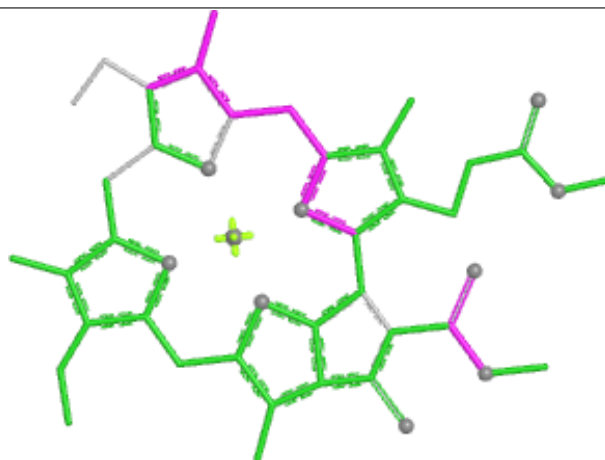


Rings

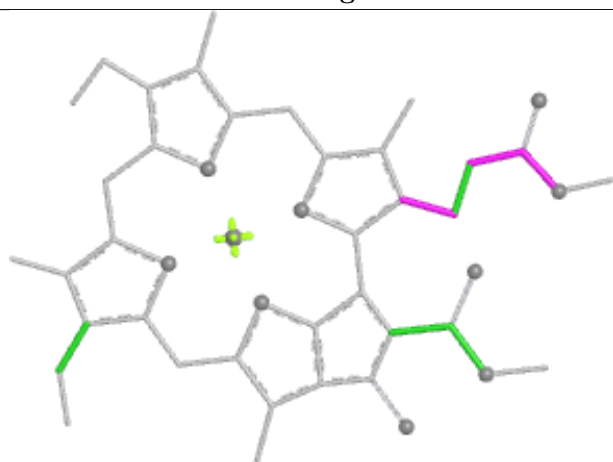
## Ligand CLA 3 304



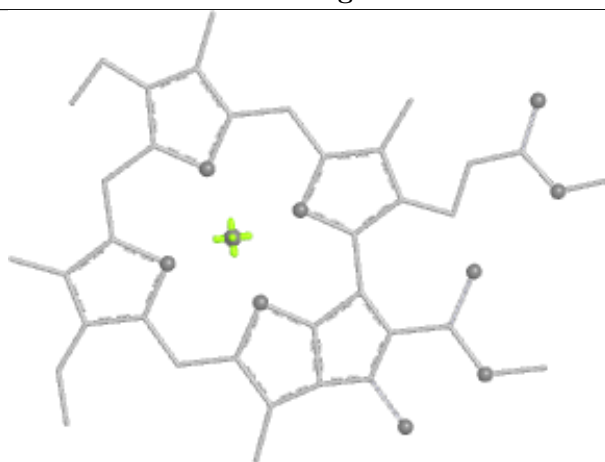
Bond lengths



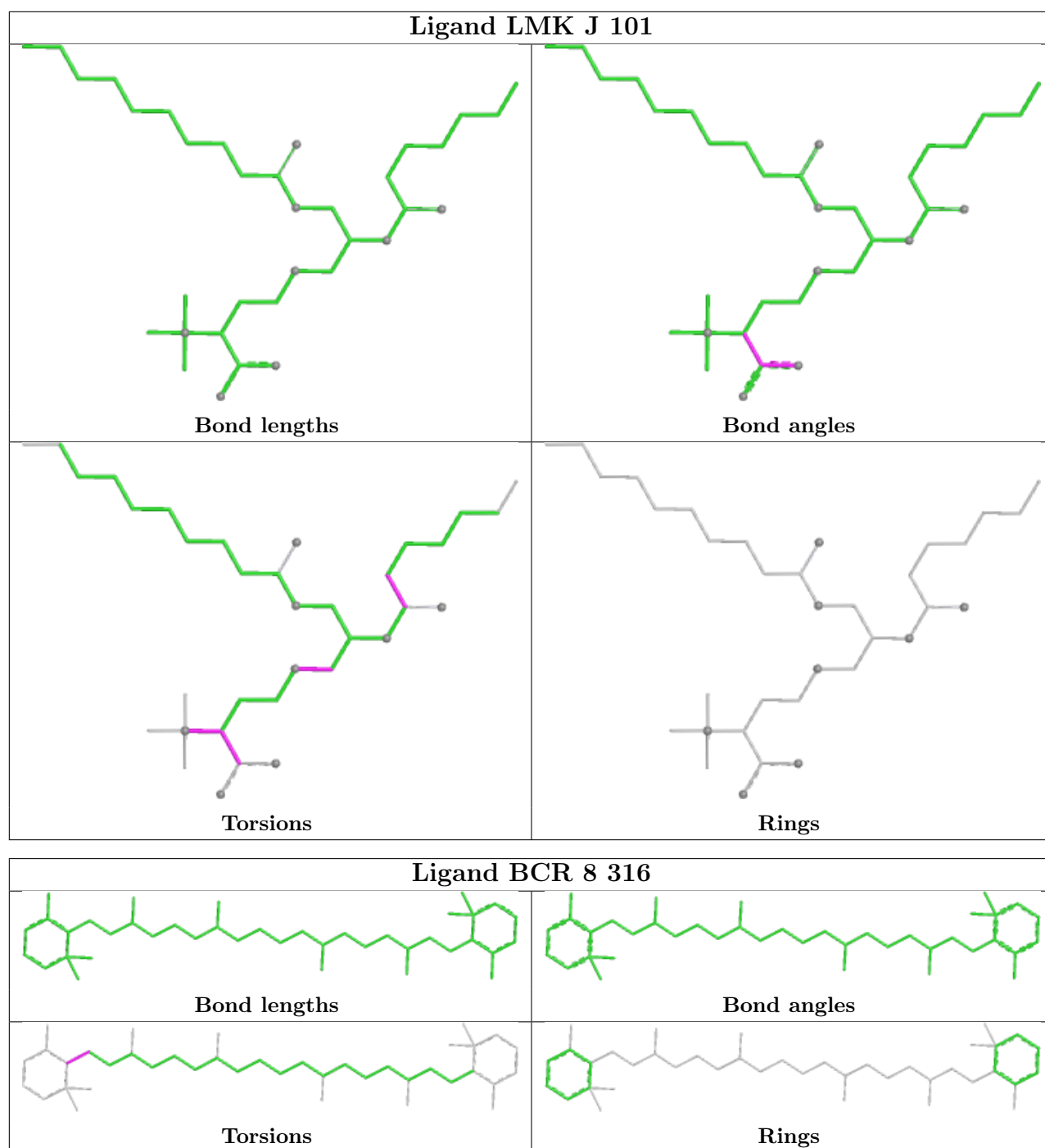
Bond angles



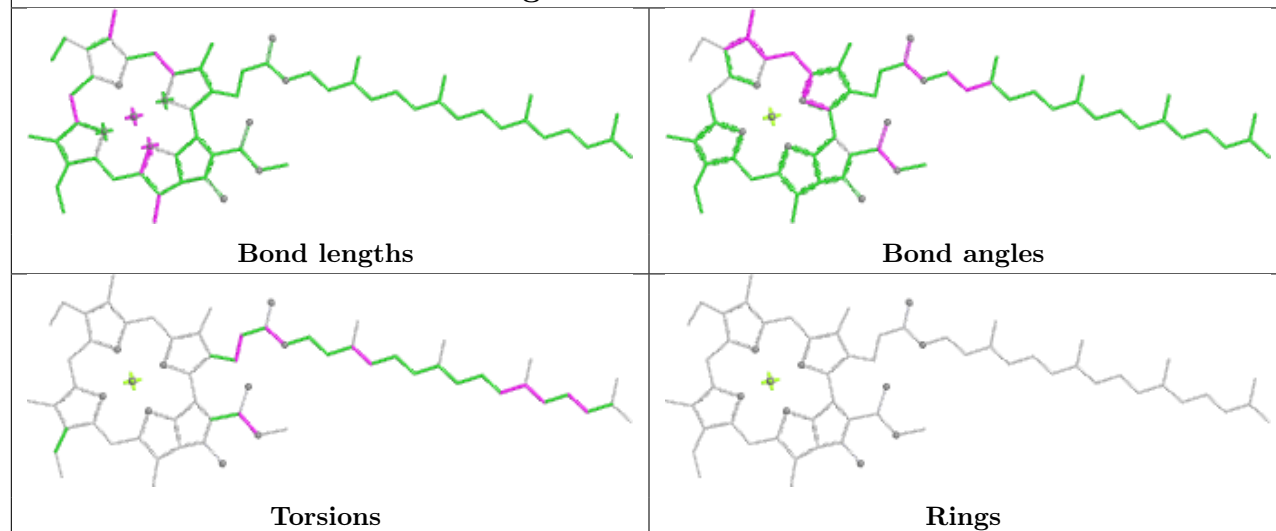
Torsions



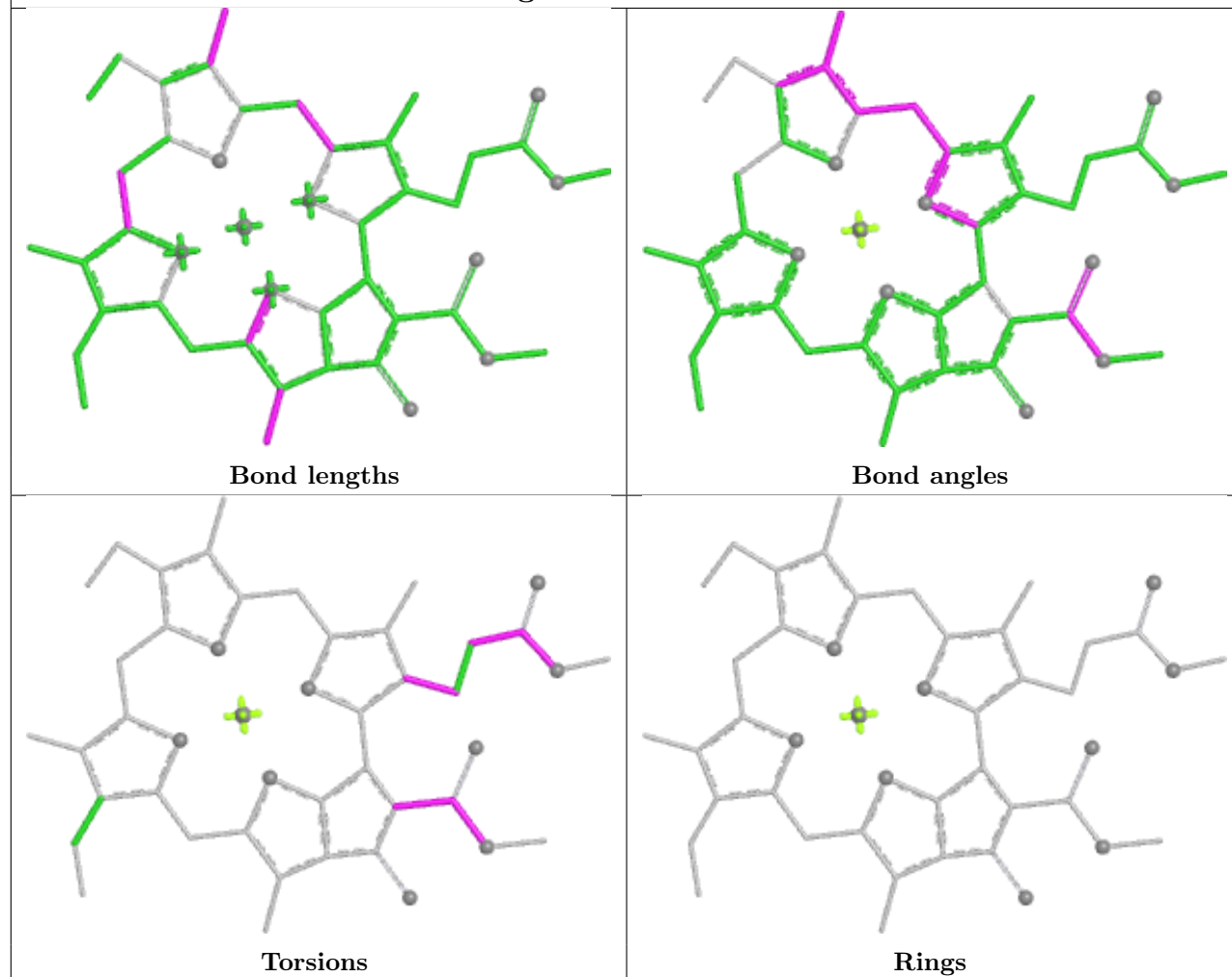
Rings



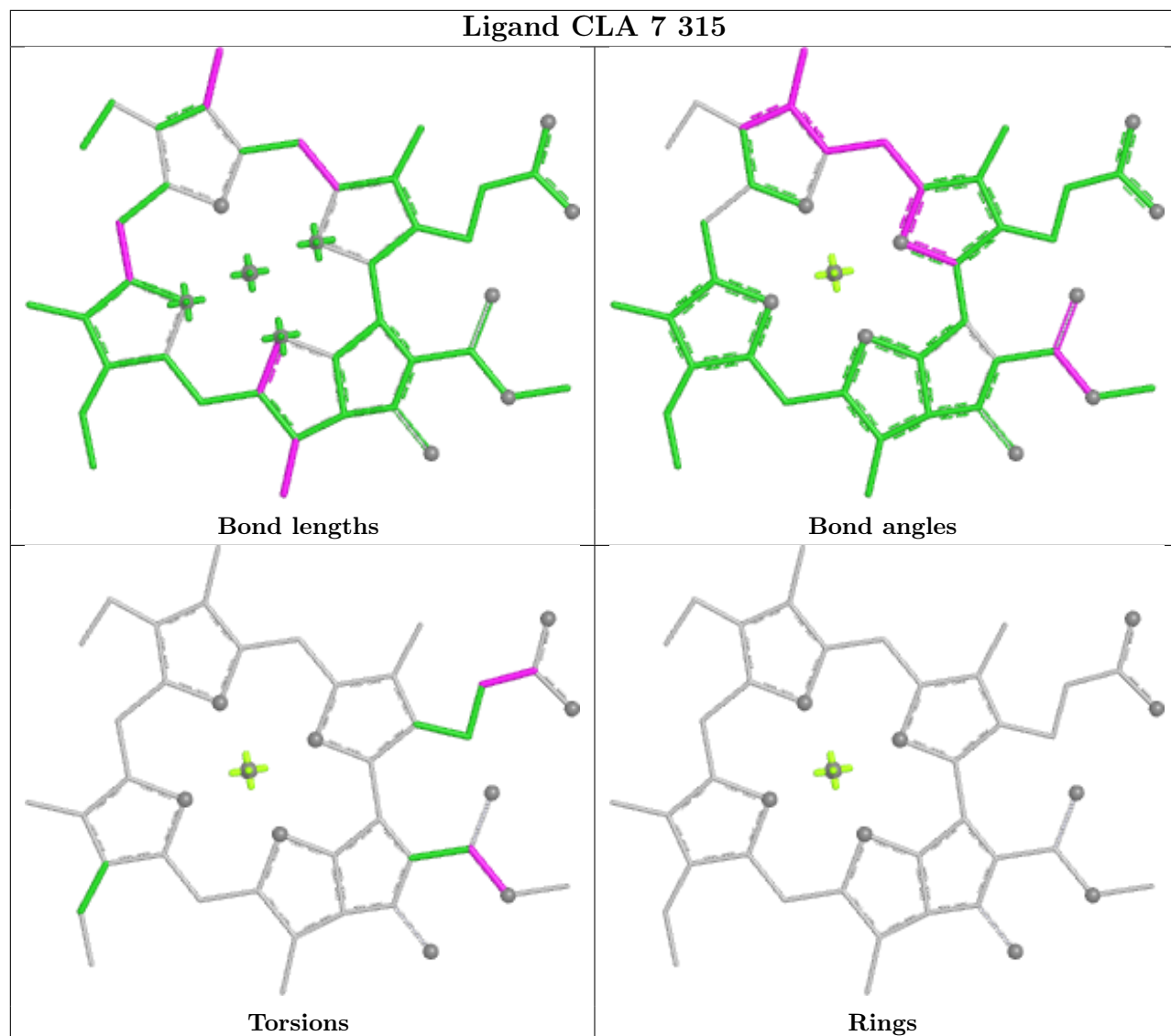
## Ligand CLA A 5030



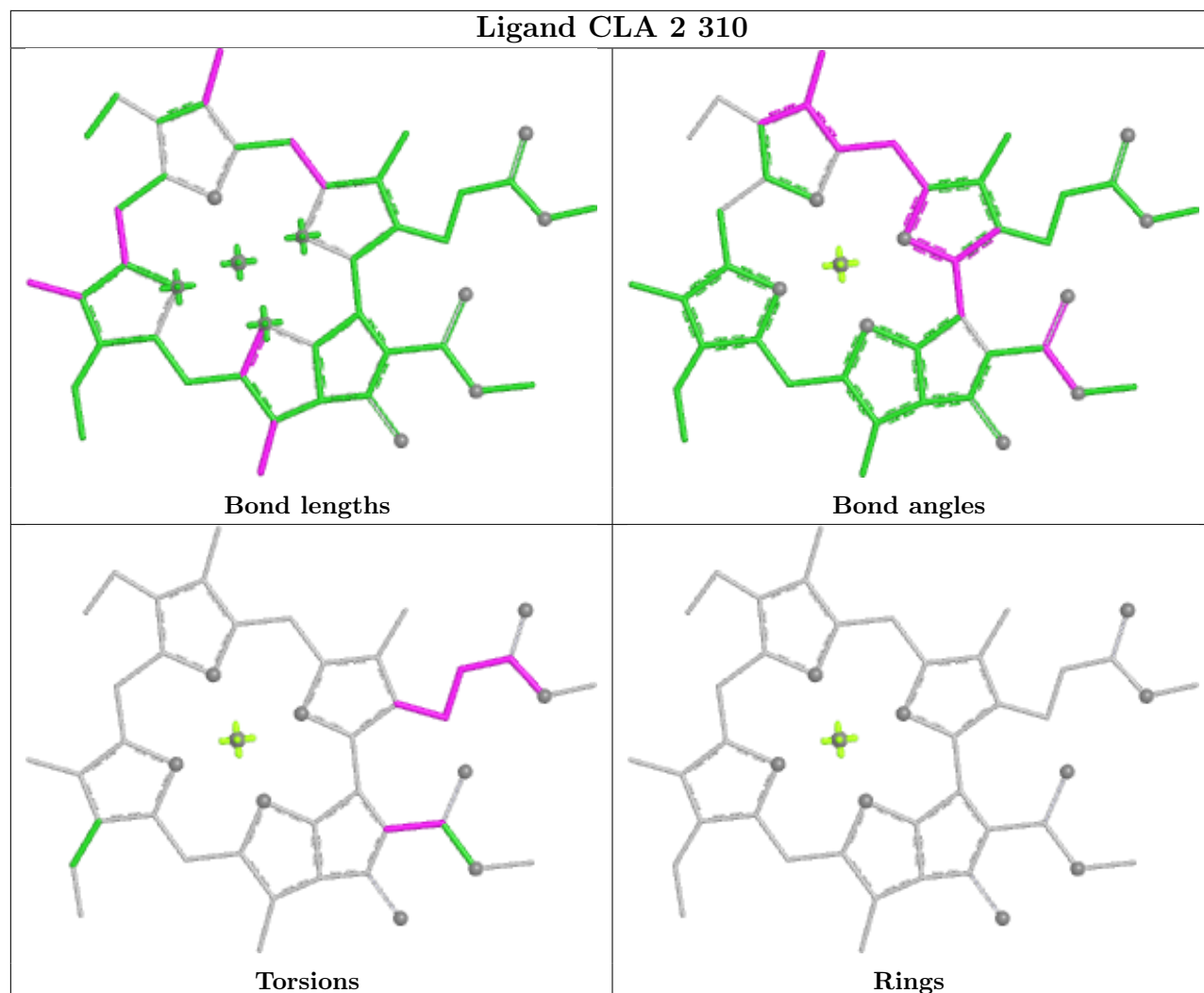
## Ligand CLA 2 307



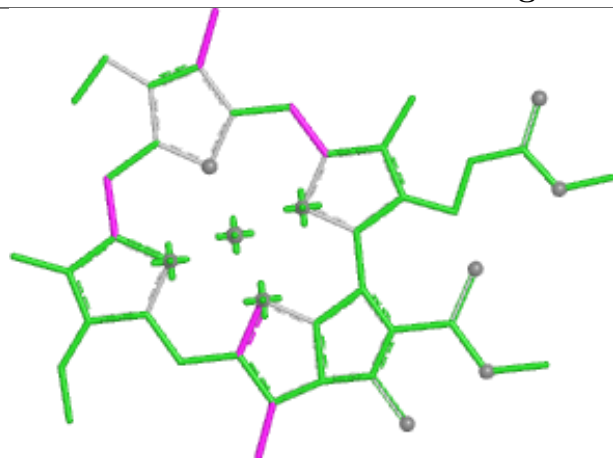
## Ligand CLA 7 315



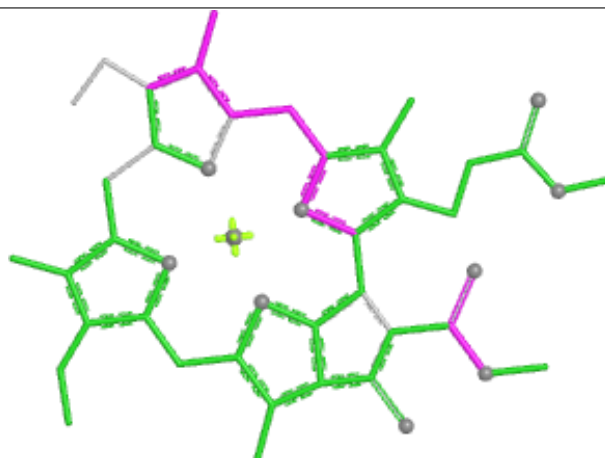
## Ligand CLA 2 310



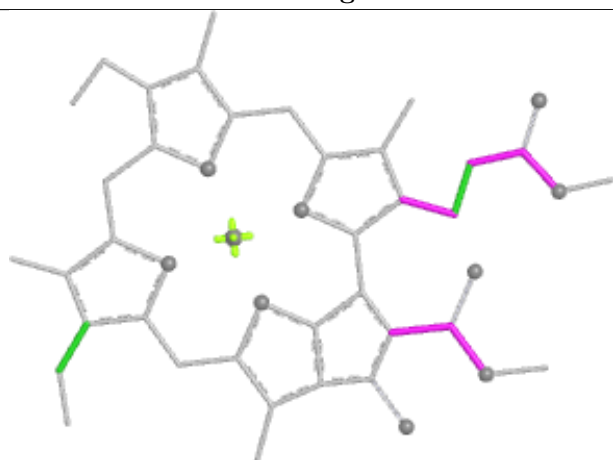
## Ligand CLA 9 609



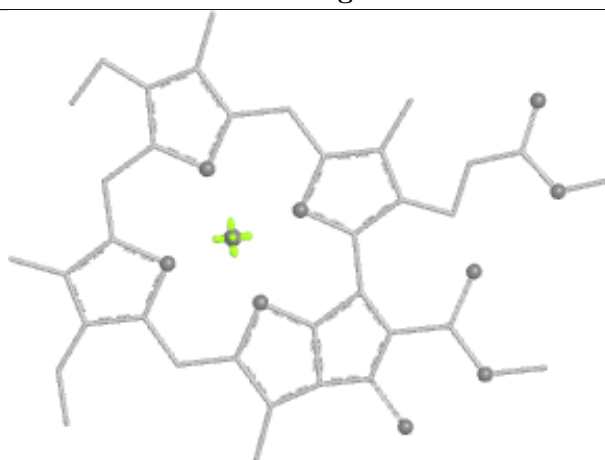
Bond lengths



Bond angles

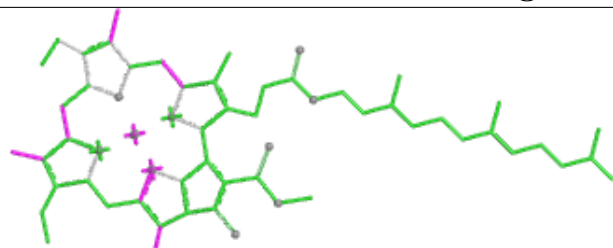


Torsions

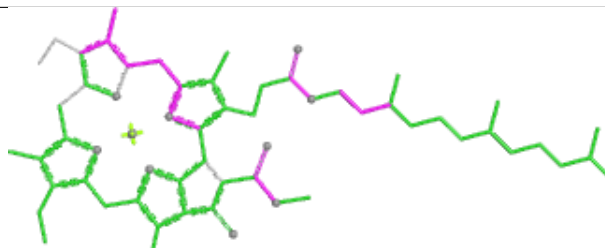


Rings

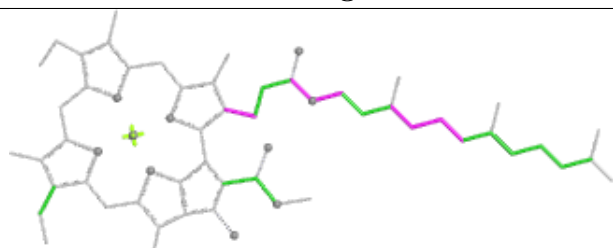
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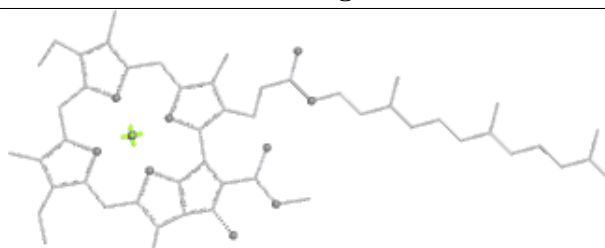
Bond lengths



Bond angles

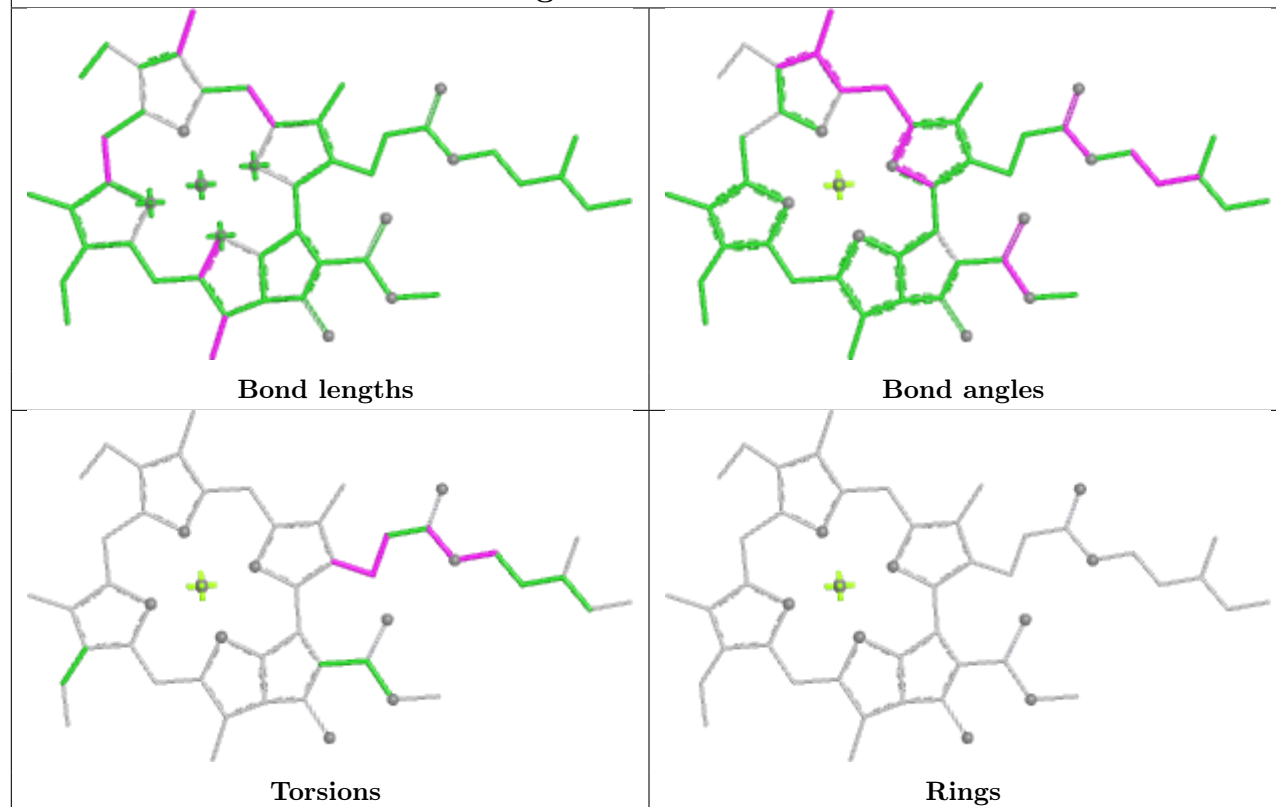


Torsions

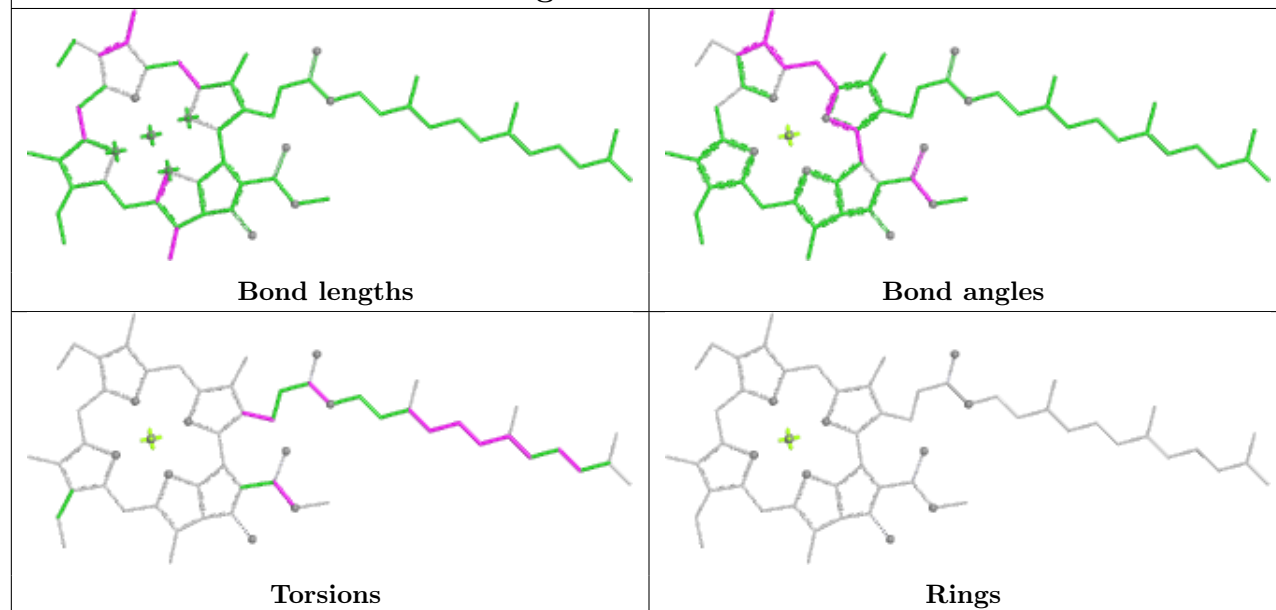


Rings

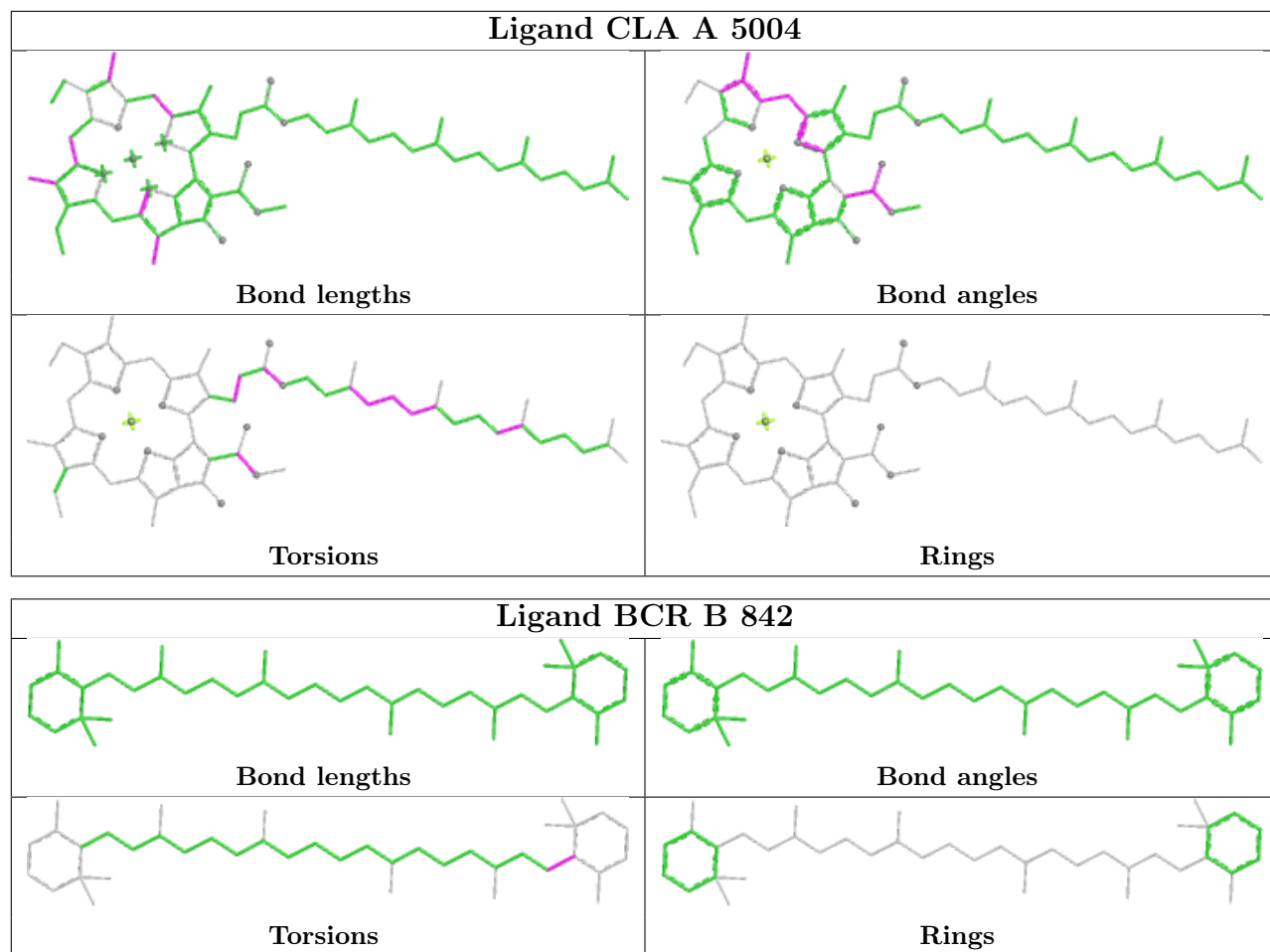
## Ligand CLA 3 306



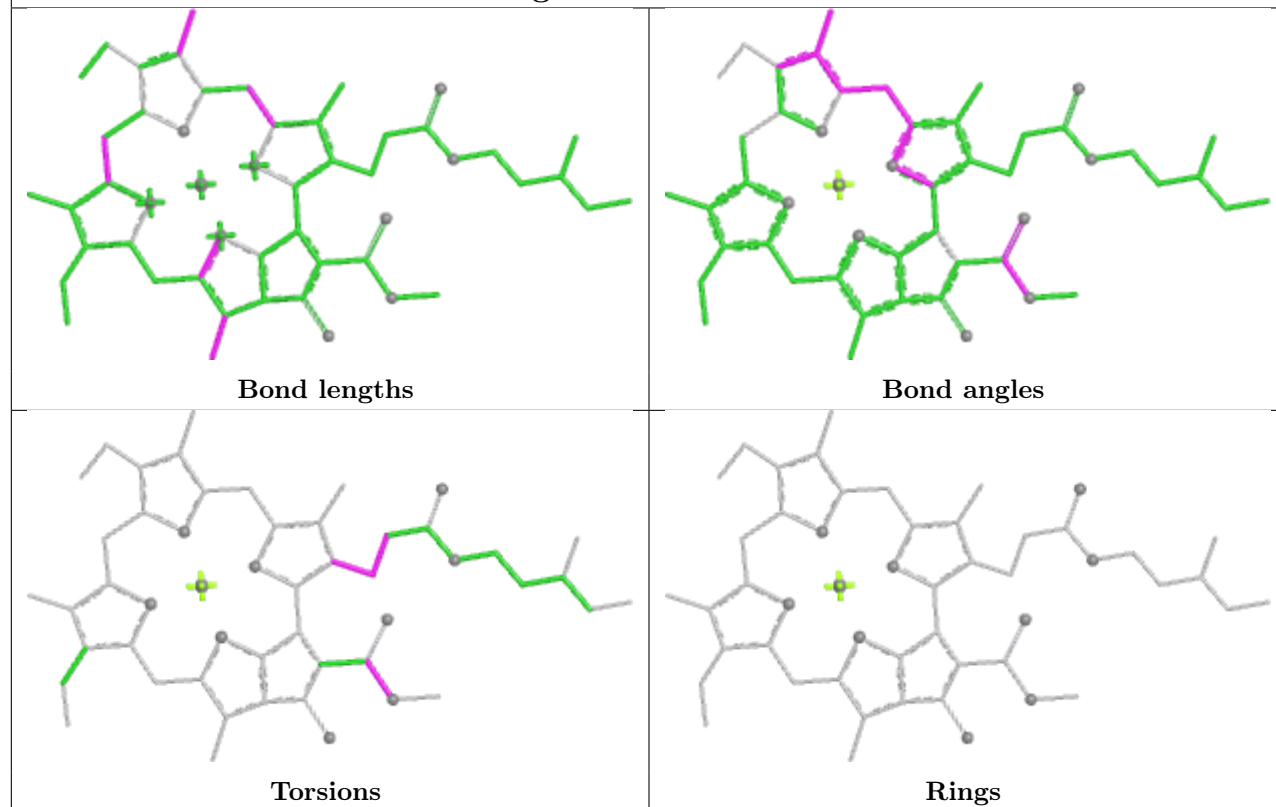
## Ligand CLA 9 607



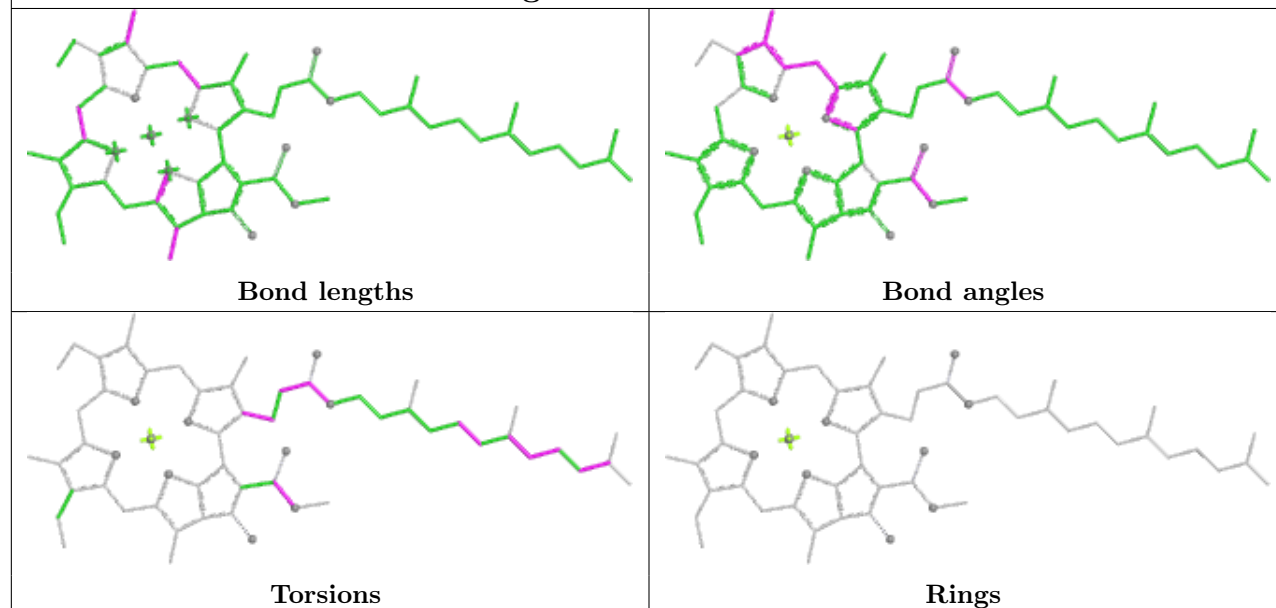




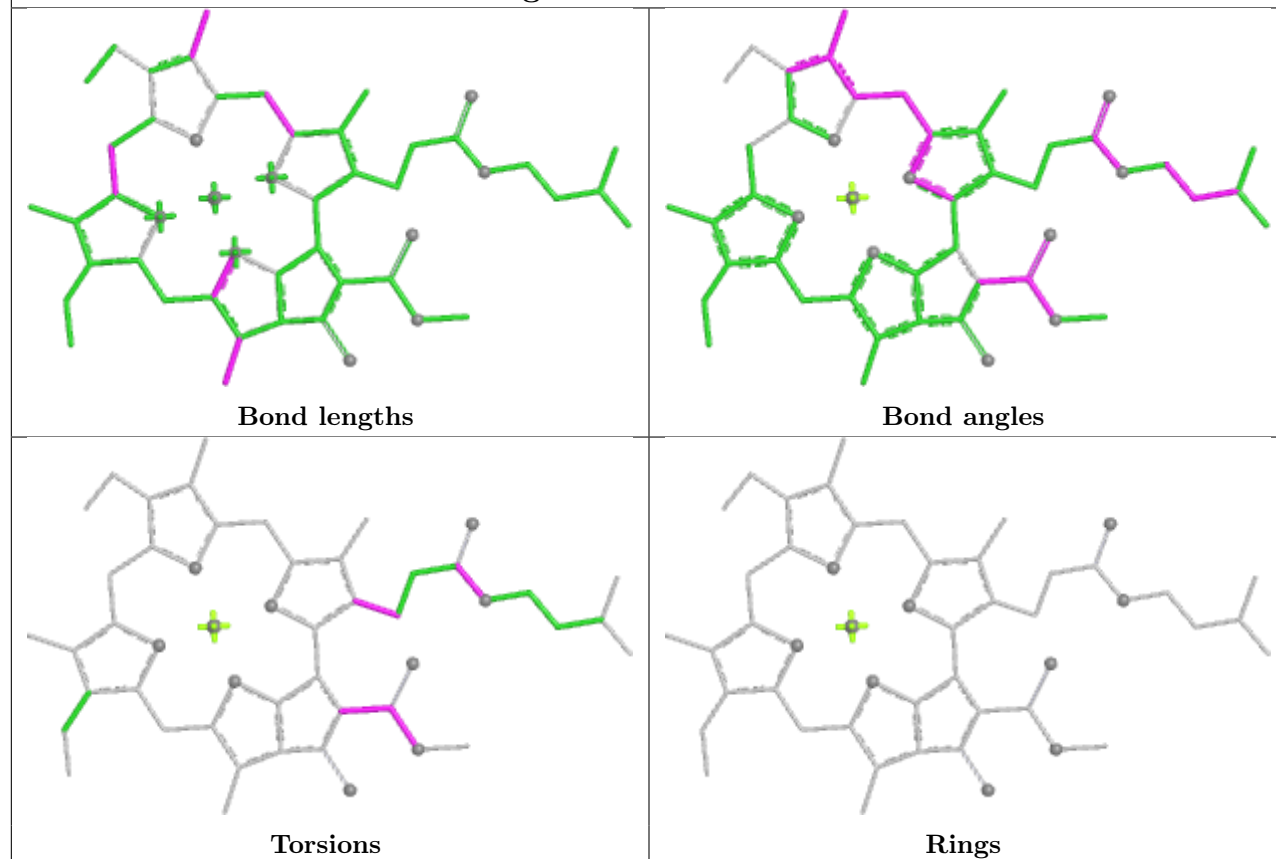
## Ligand CLA B 835



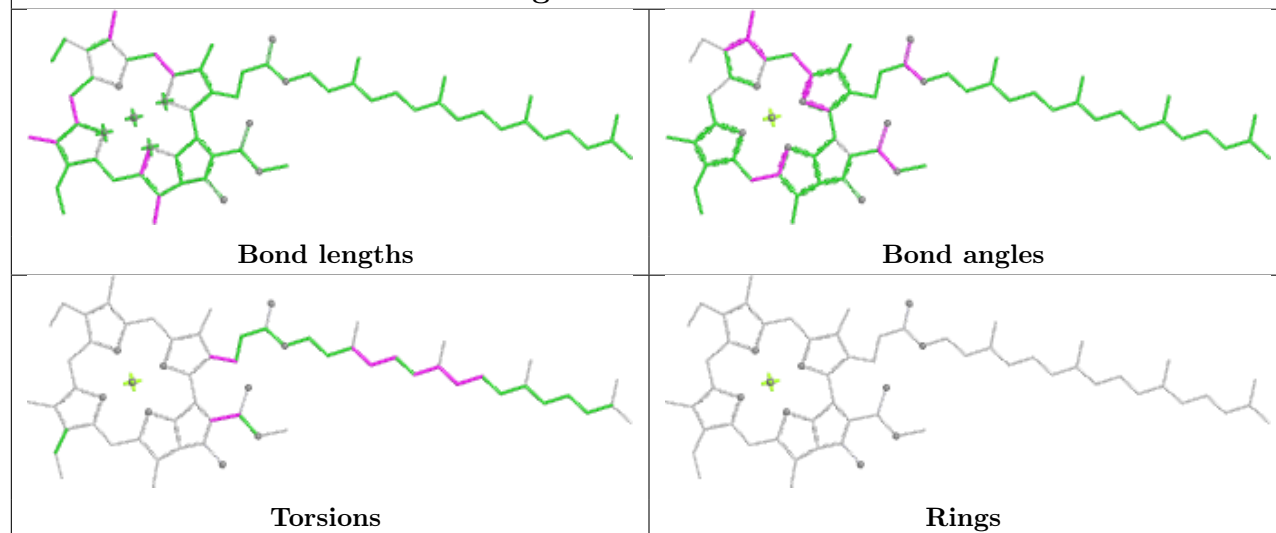
## Ligand CLA A 5024



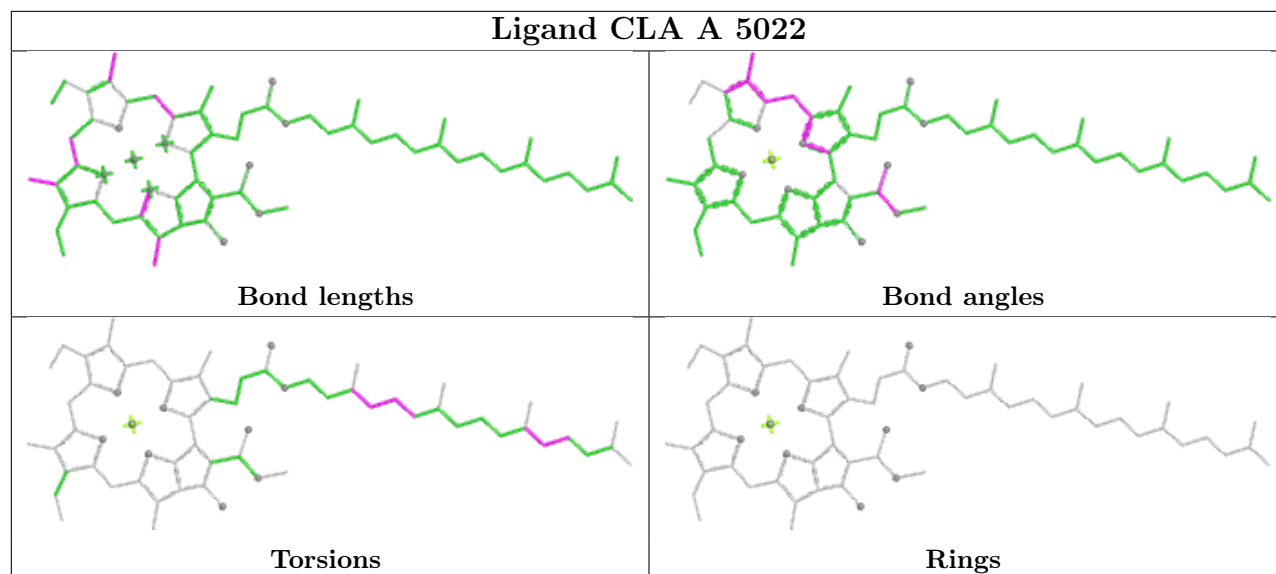
## Ligand CLA A 5037



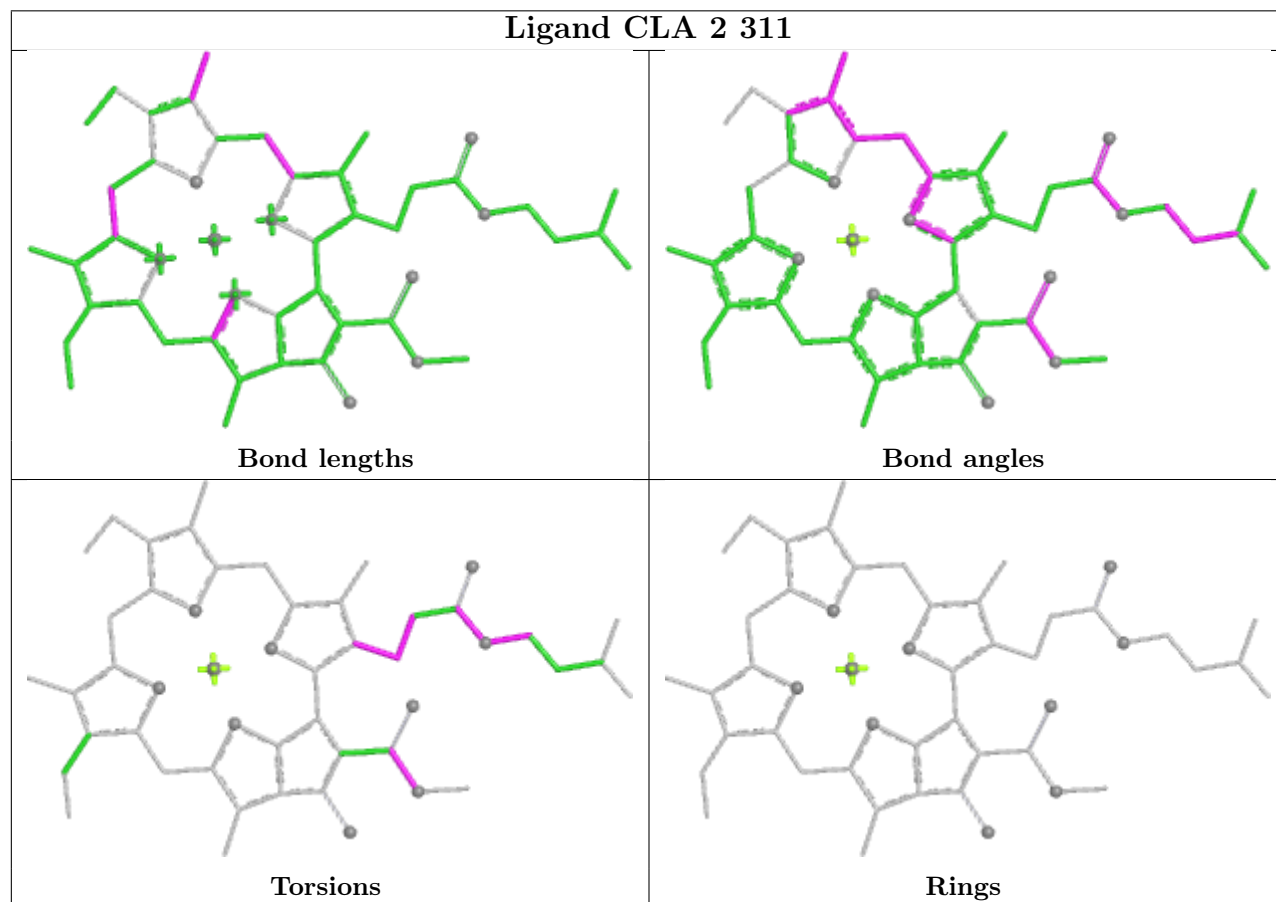
## Ligand CLA B 807

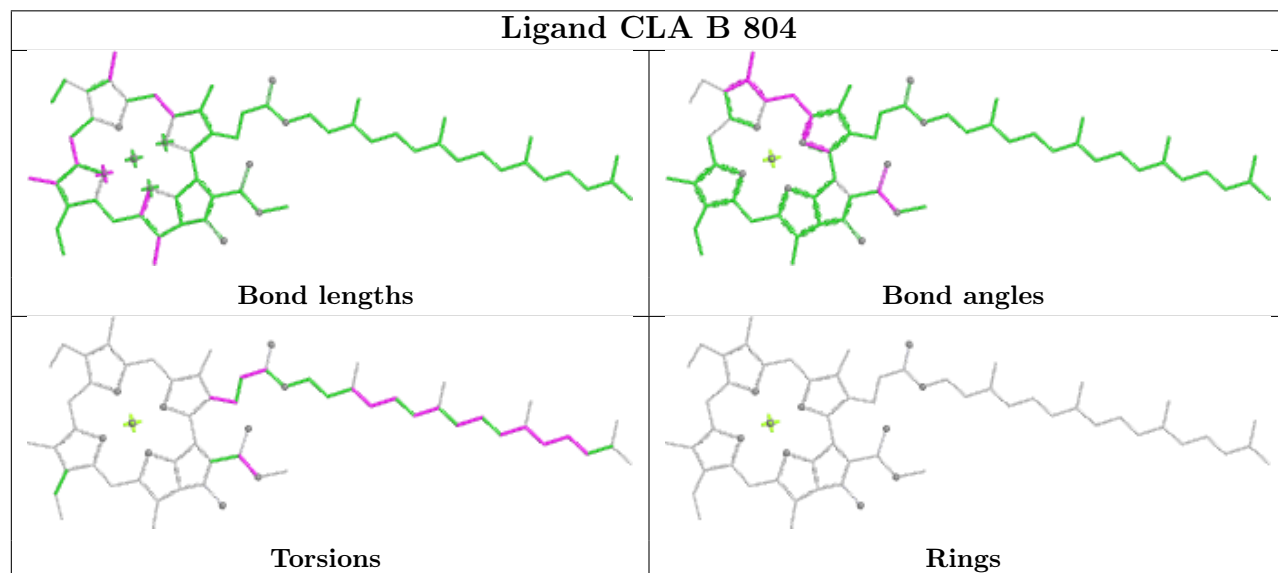
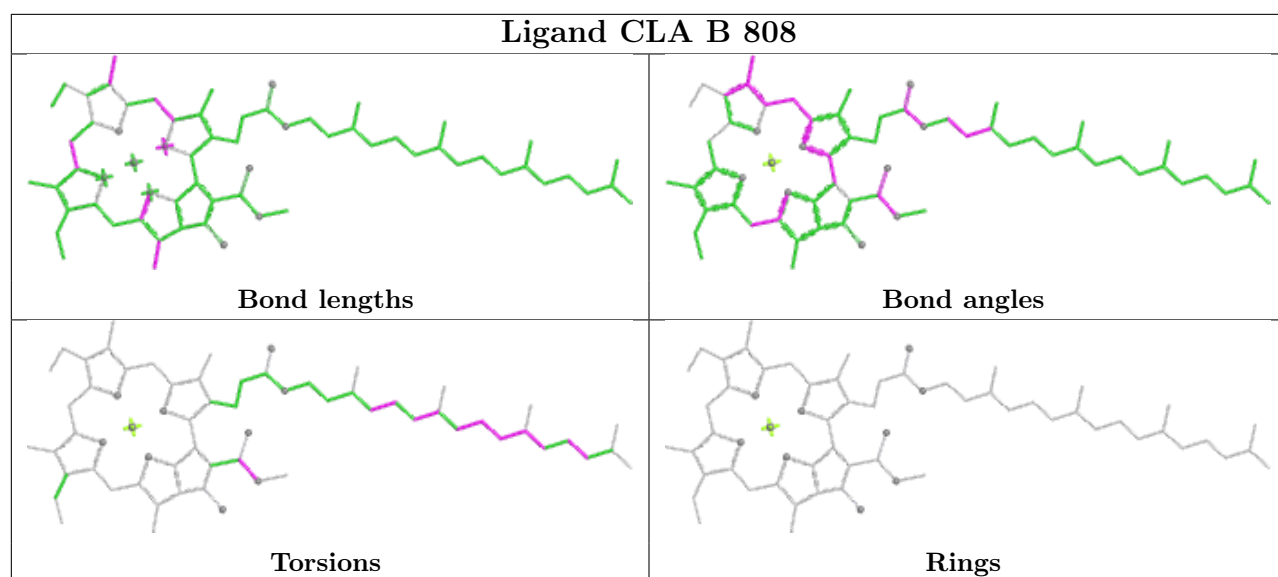


## Ligand CLA A 5022

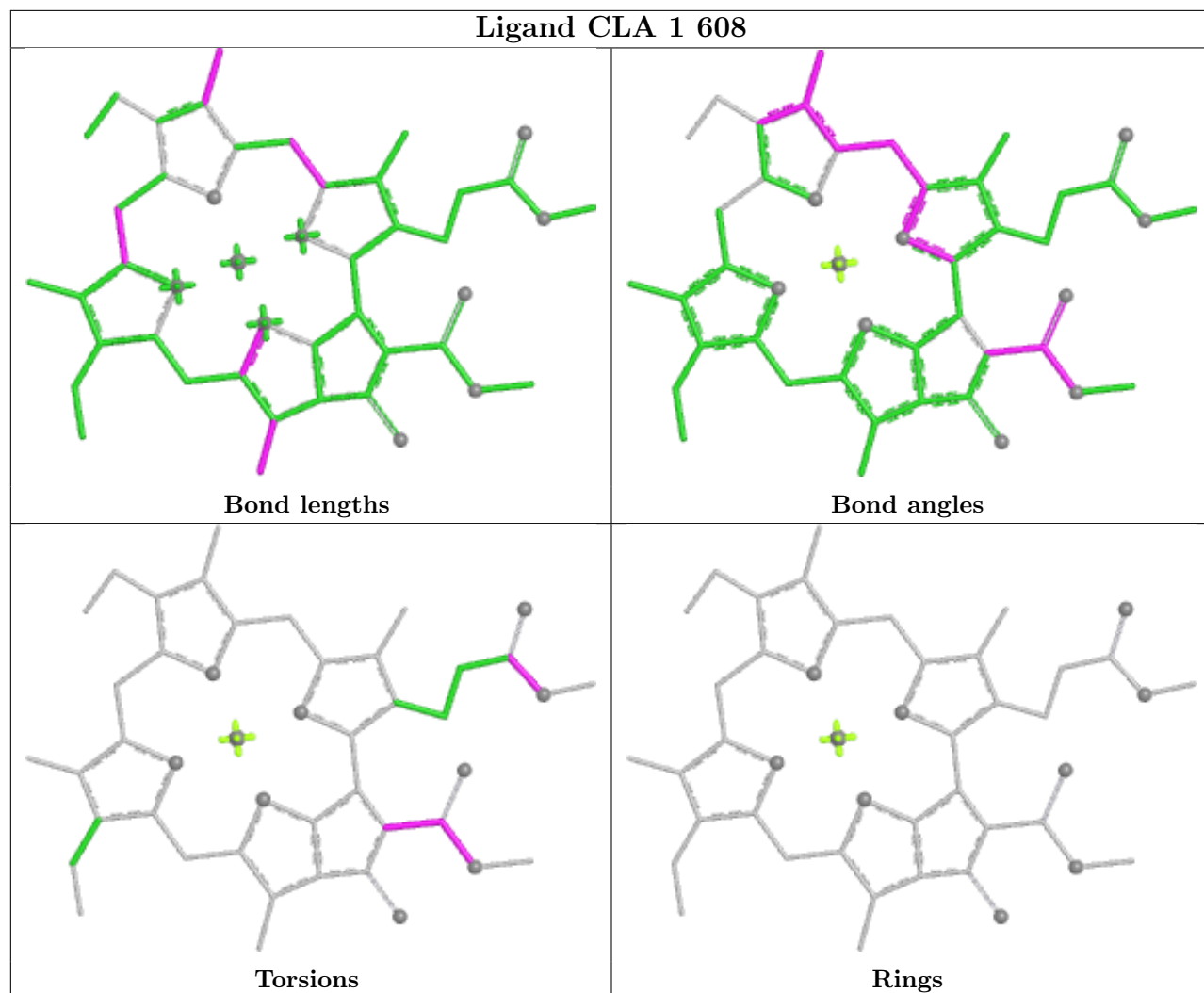


## Ligand CLA 2 311

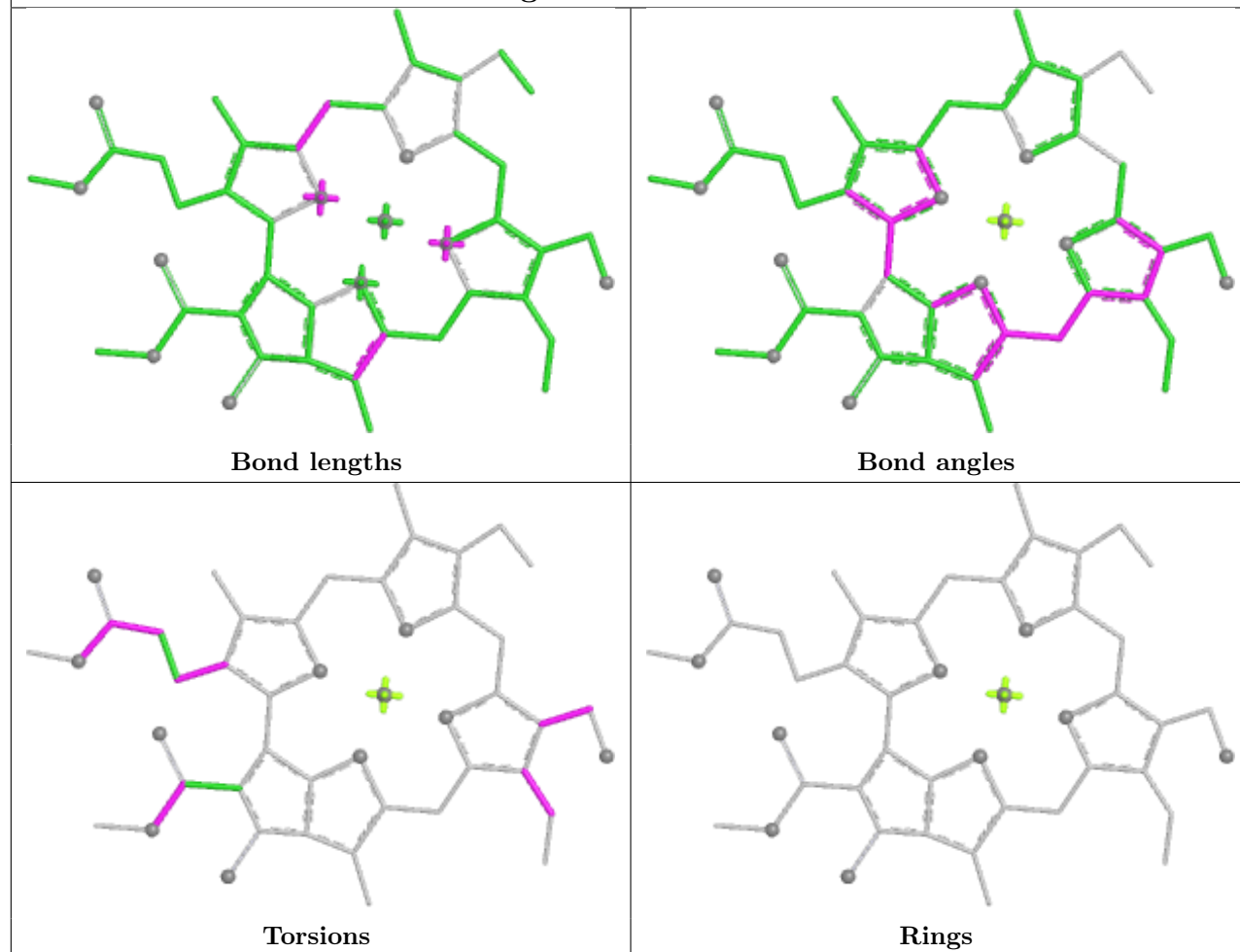




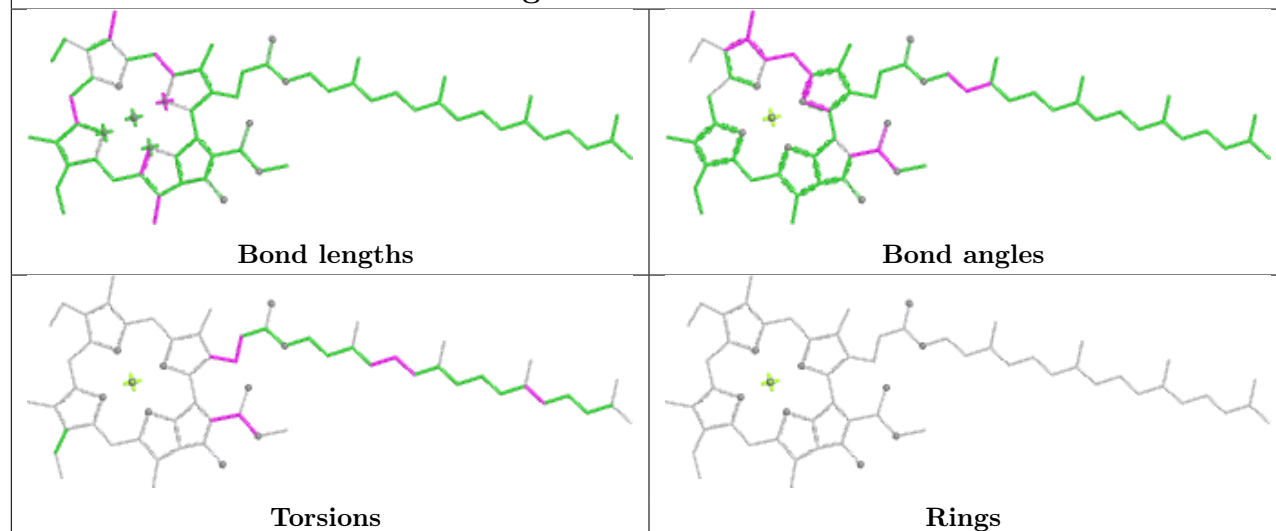
## Ligand CLA 1 608



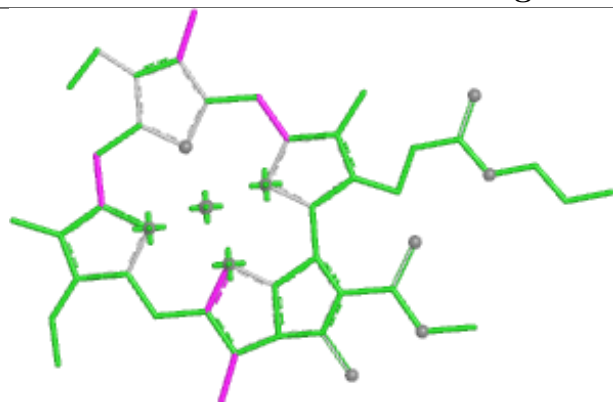
## Ligand CHL 9 606



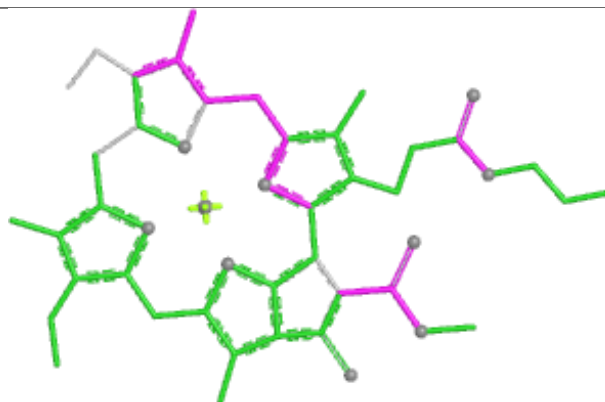
## Ligand CLA A 5044



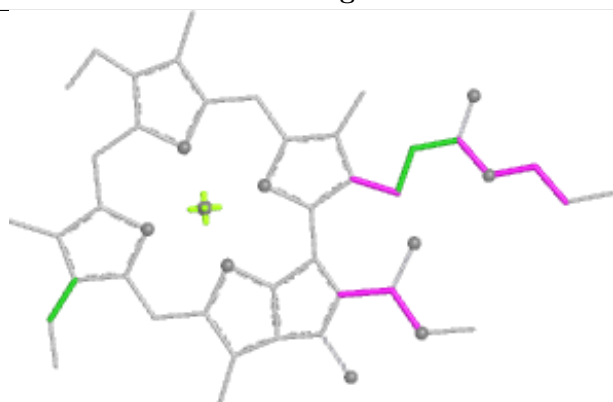
## Ligand CLA B 806



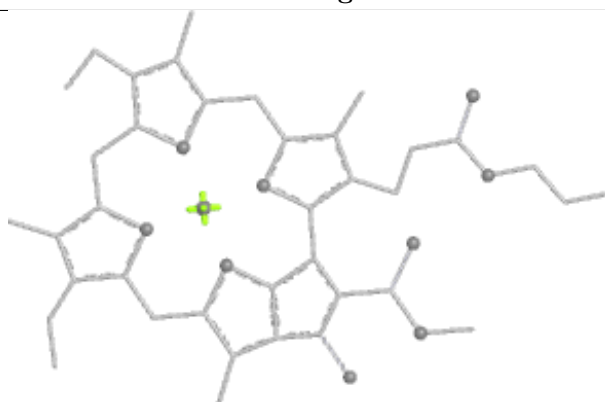
Bond lengths



Bond angles

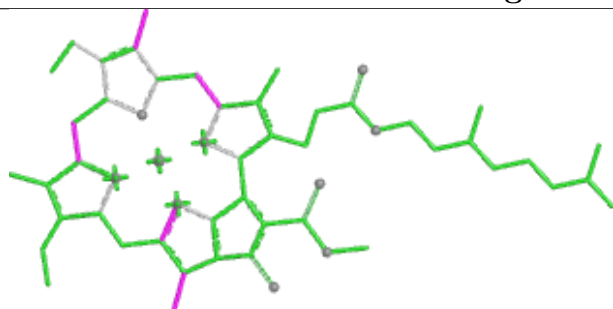


Torsions

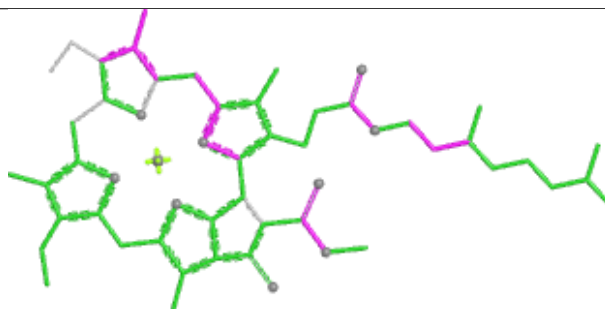


Rings

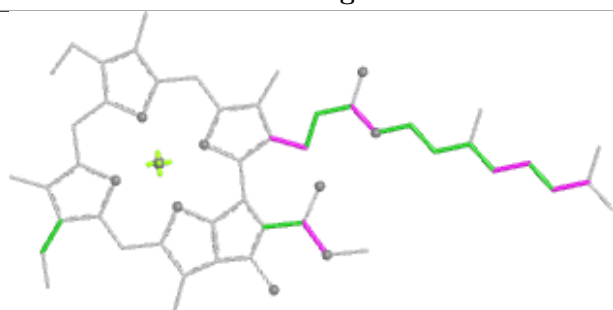
## Ligand CLA A 5015



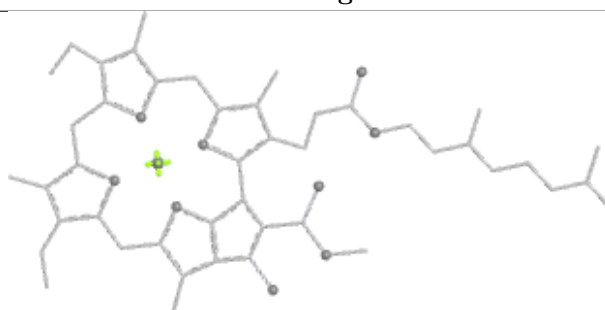
Bond lengths



Bond angles

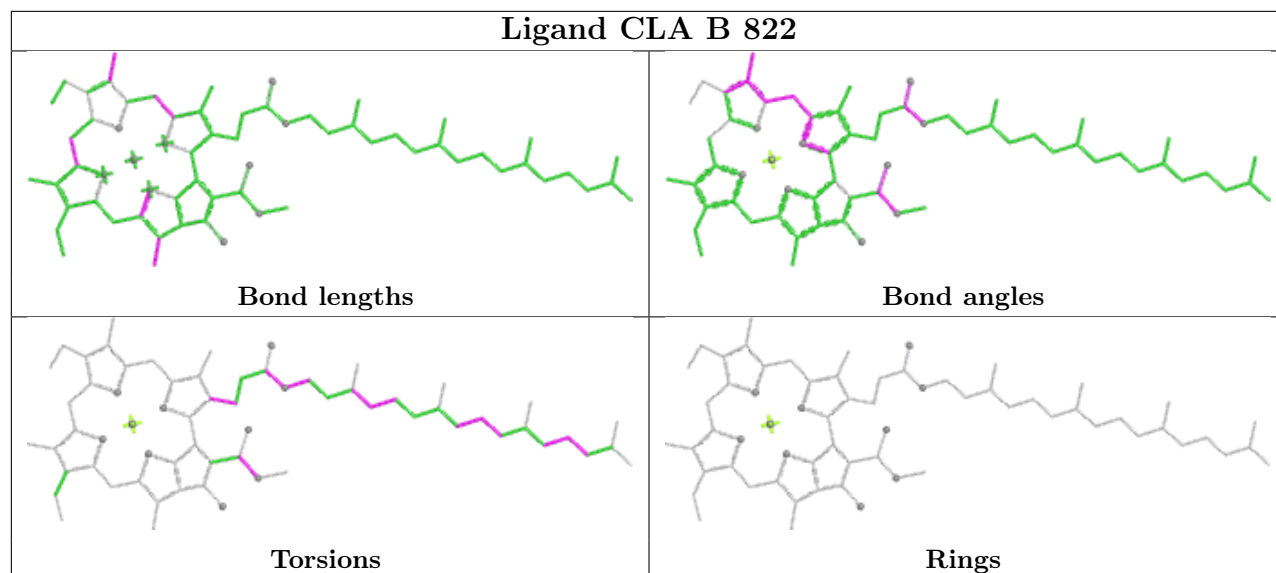
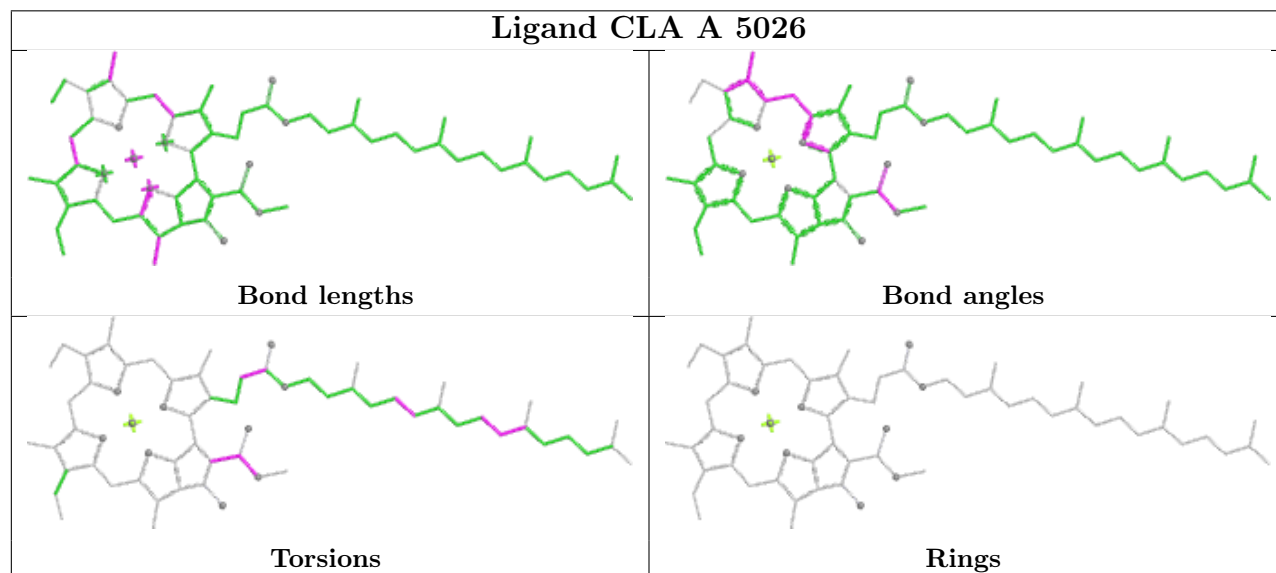
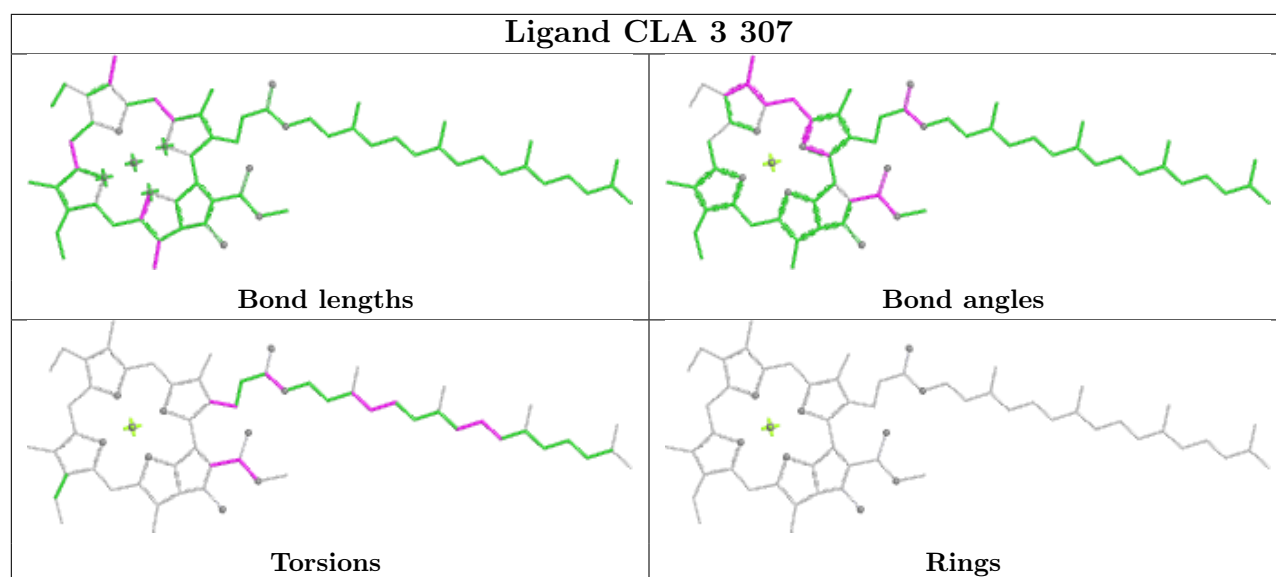


Torsions

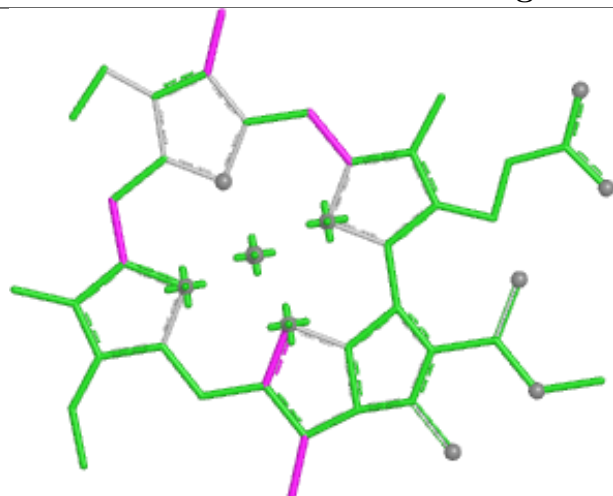


Rings

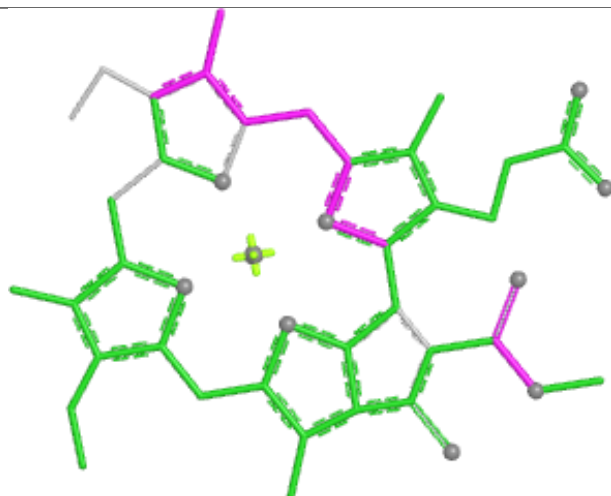




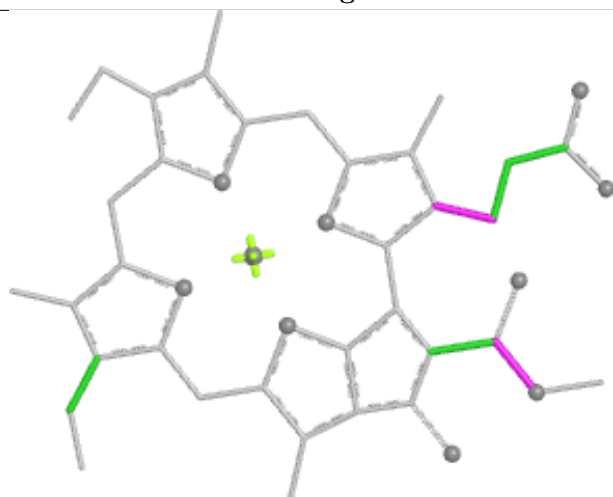
## Ligand CLA F 308



Bond lengths



Bond angles

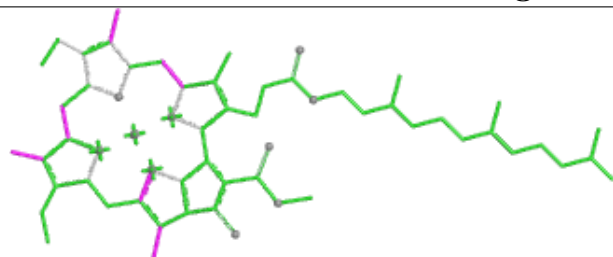


Torsions

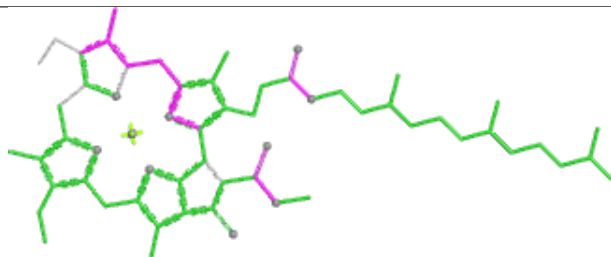


Rings

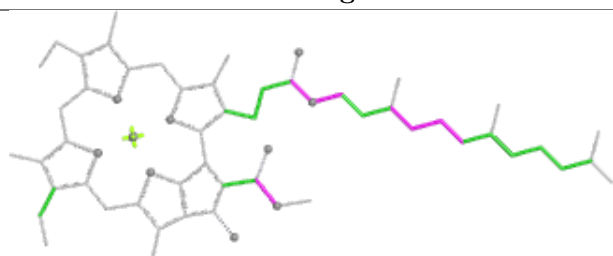
## Ligand CLA B 831



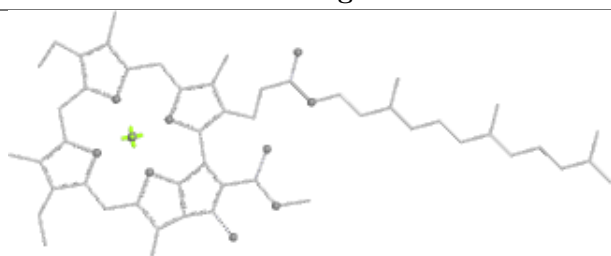
Bond lengths



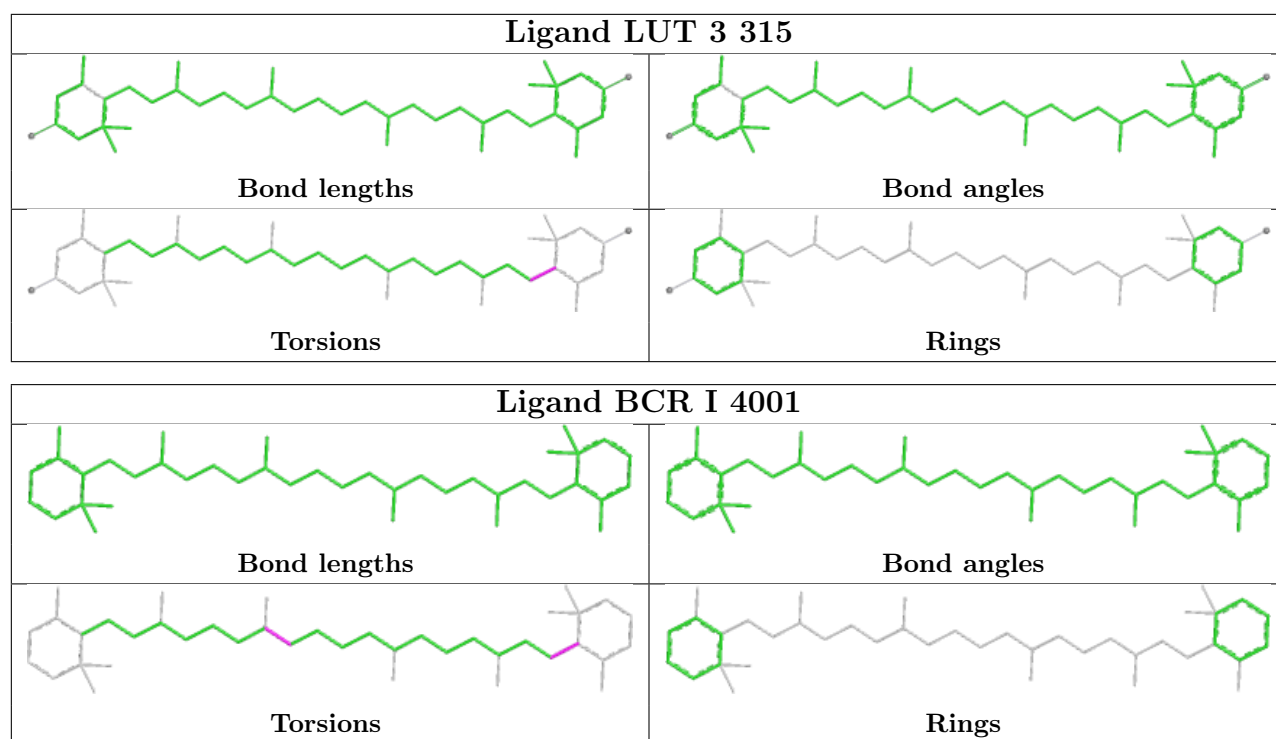
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

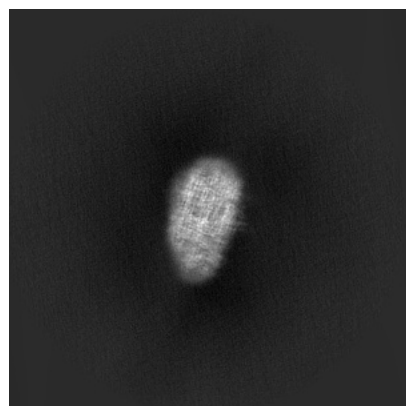
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48266. These allow visual inspection of the internal detail of the map and identification of artifacts.

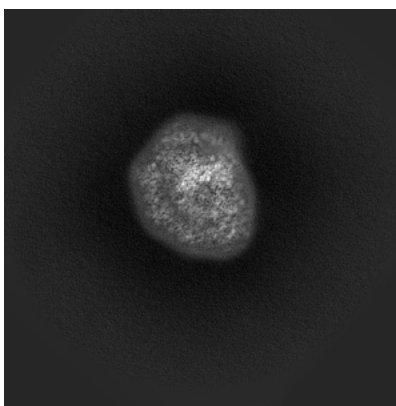
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

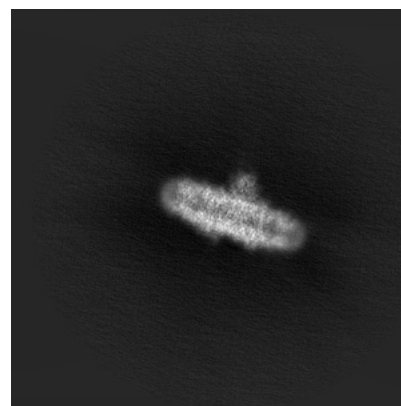
#### 6.1.1 Primary map



X

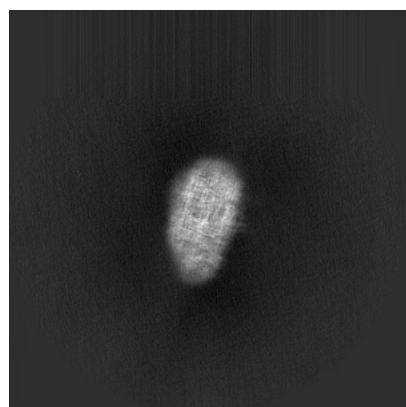


Y

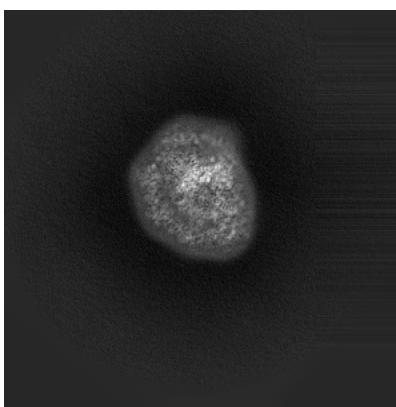


Z

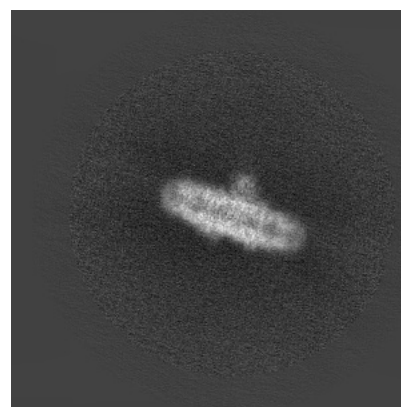
#### 6.1.2 Raw map



X



Y

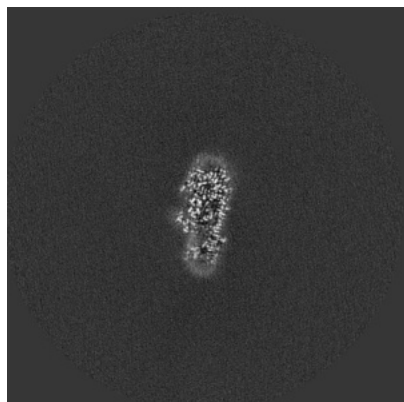


Z

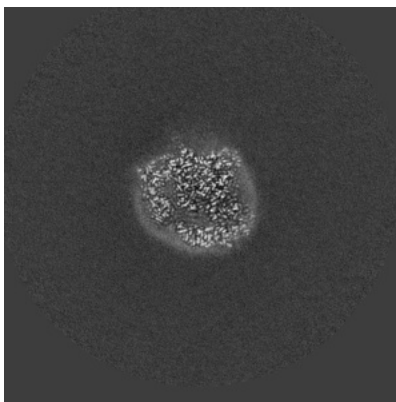
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 240

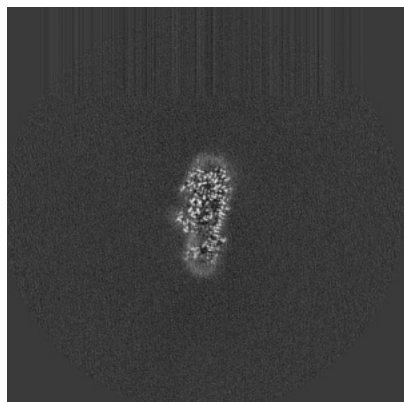


Y Index: 240

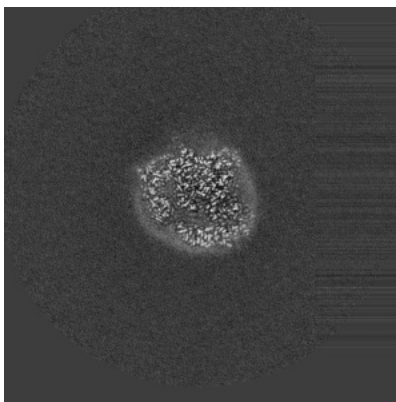


Z Index: 240

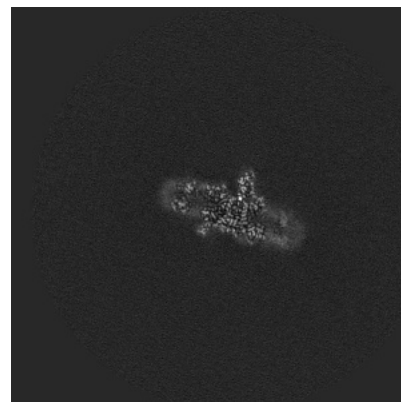
### 6.2.2 Raw map



X Index: 240



Y Index: 240

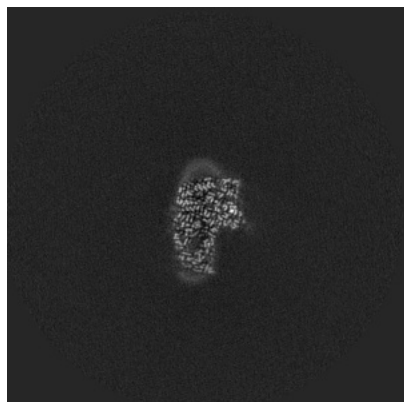


Z Index: 240

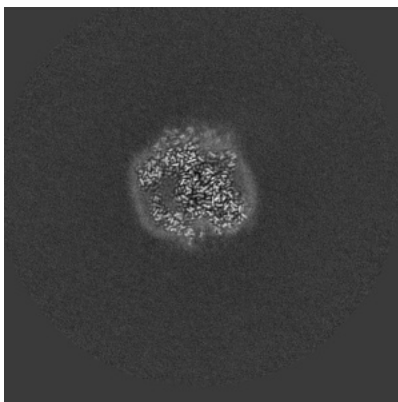
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

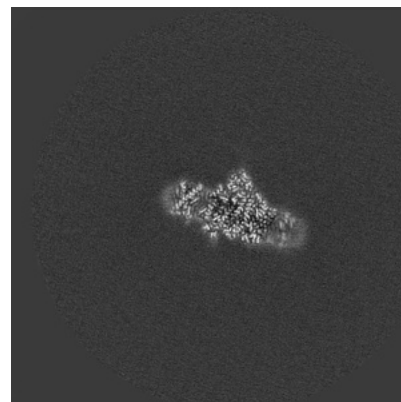
### 6.3.1 Primary map



X Index: 277

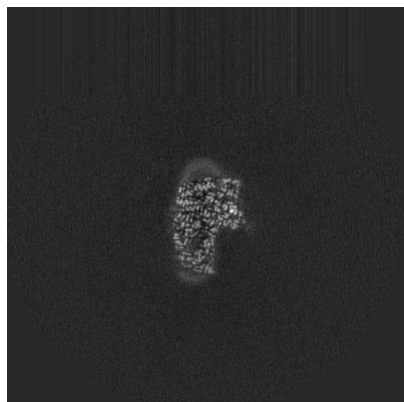


Y Index: 231

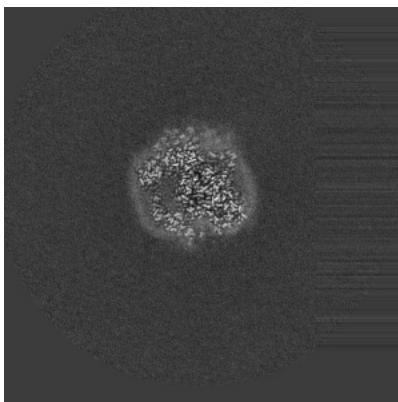


Z Index: 224

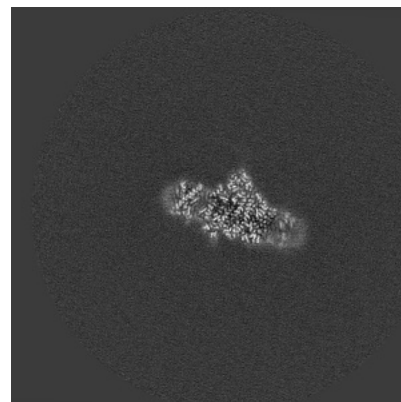
### 6.3.2 Raw map



X Index: 277



Y Index: 231



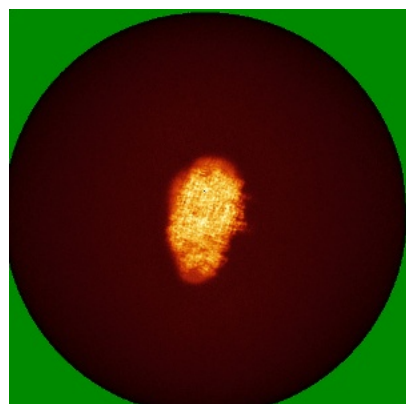
Z Index: 224

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

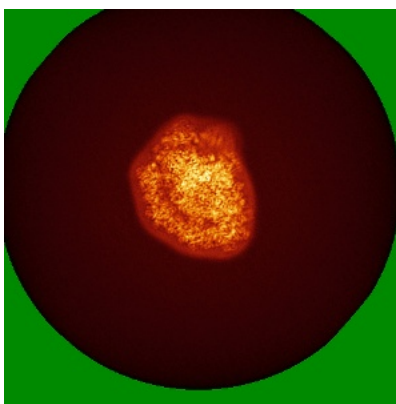


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

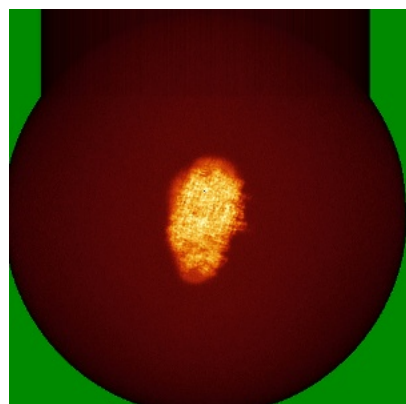


Y

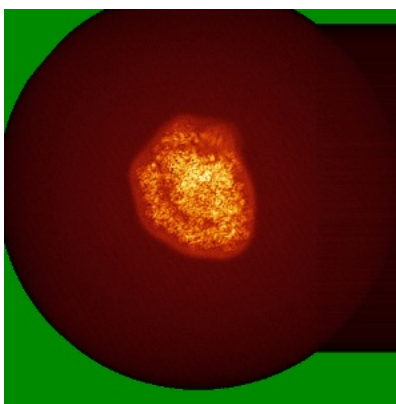


Z

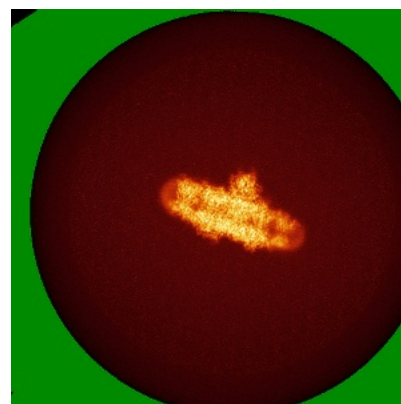
### 6.4.2 Raw map



X



Y

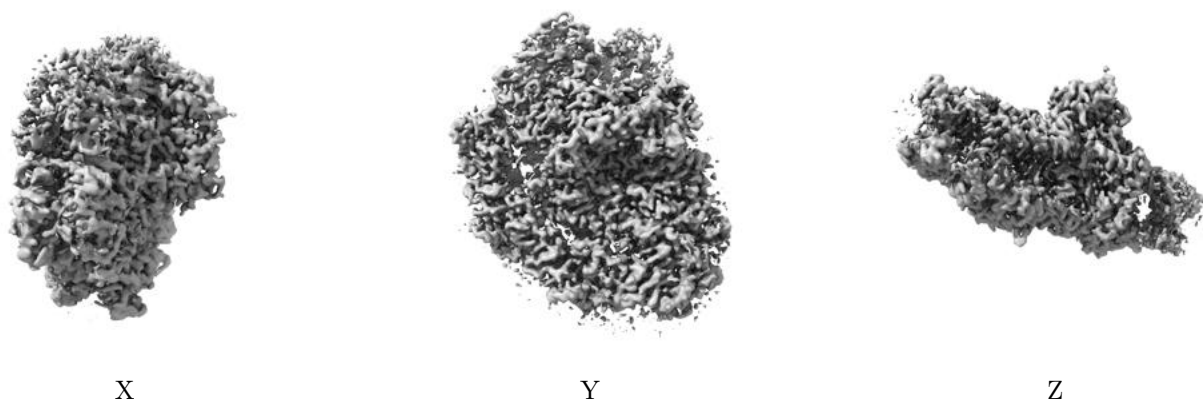


Z

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

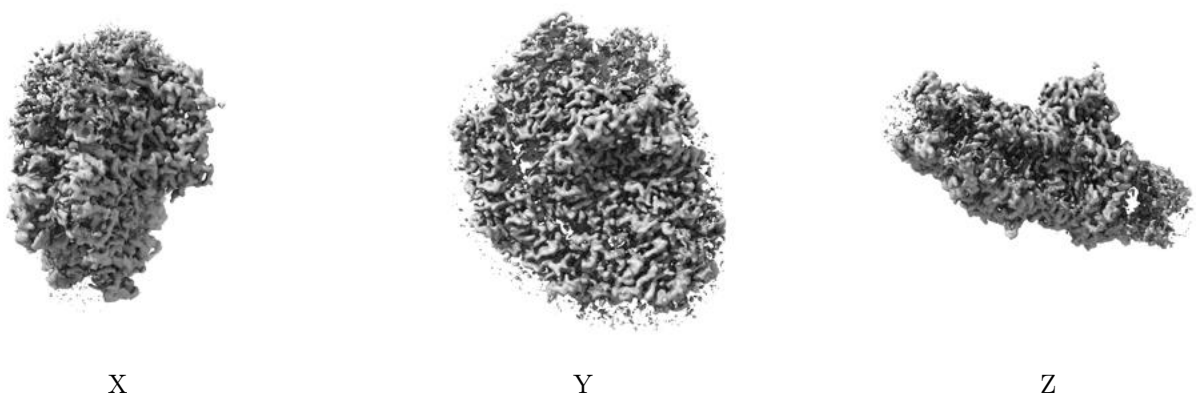
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0172. 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.



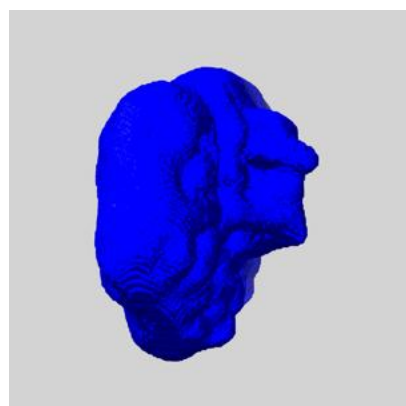
## 6.6 Mask visualisation [i](#)

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

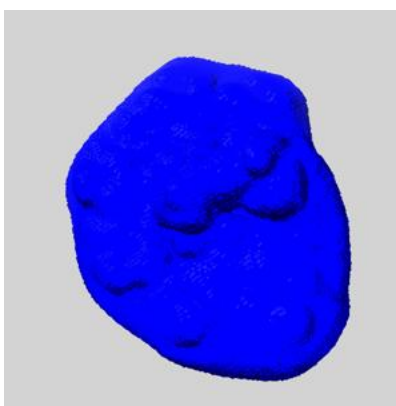
A mask typically either:

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

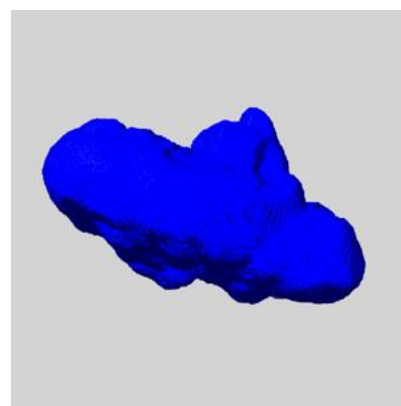
### 6.6.1 emd\_48266\_msk\_1.map [i](#)



X



Y

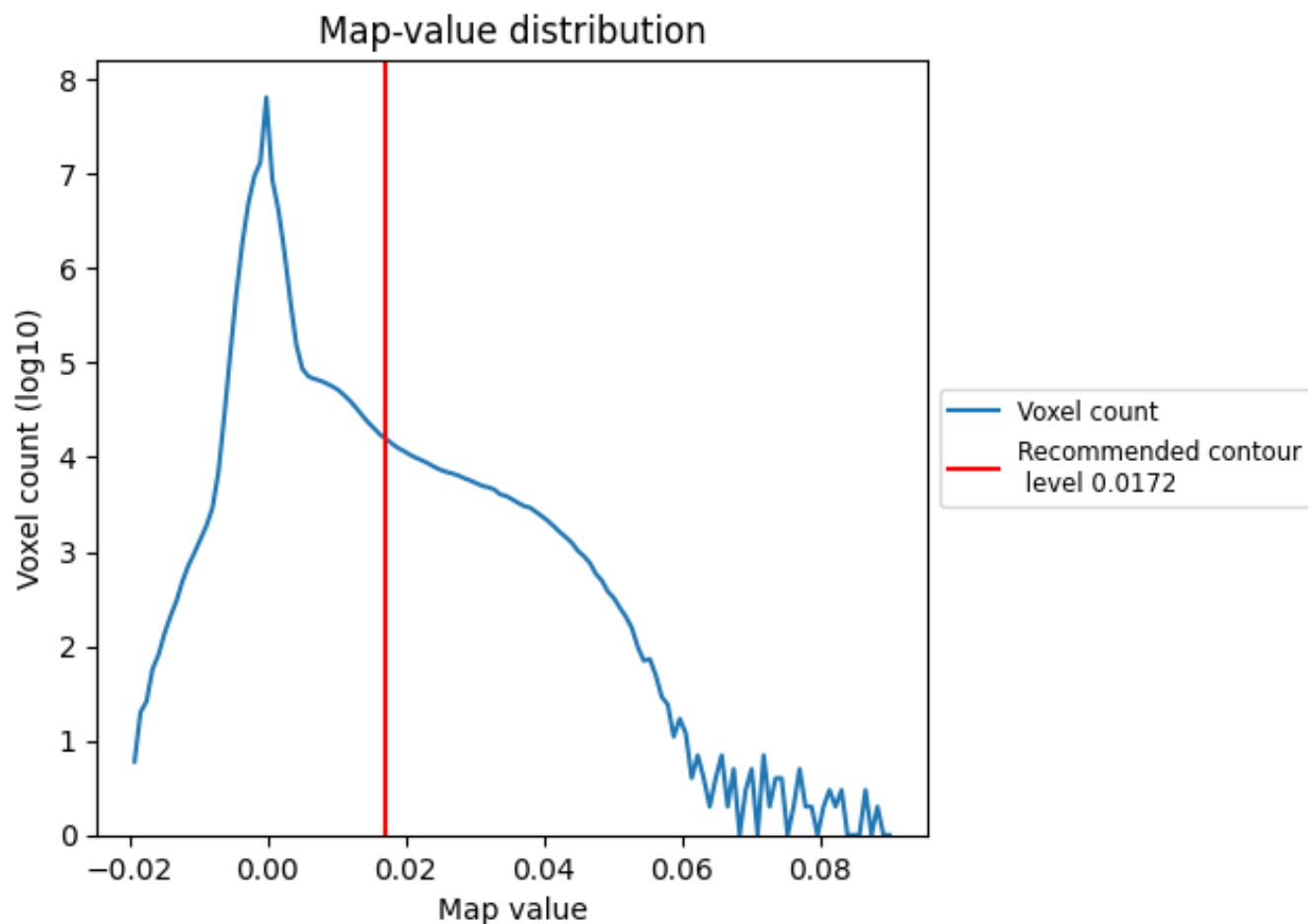


Z

## 7 Map analysis [i](#)

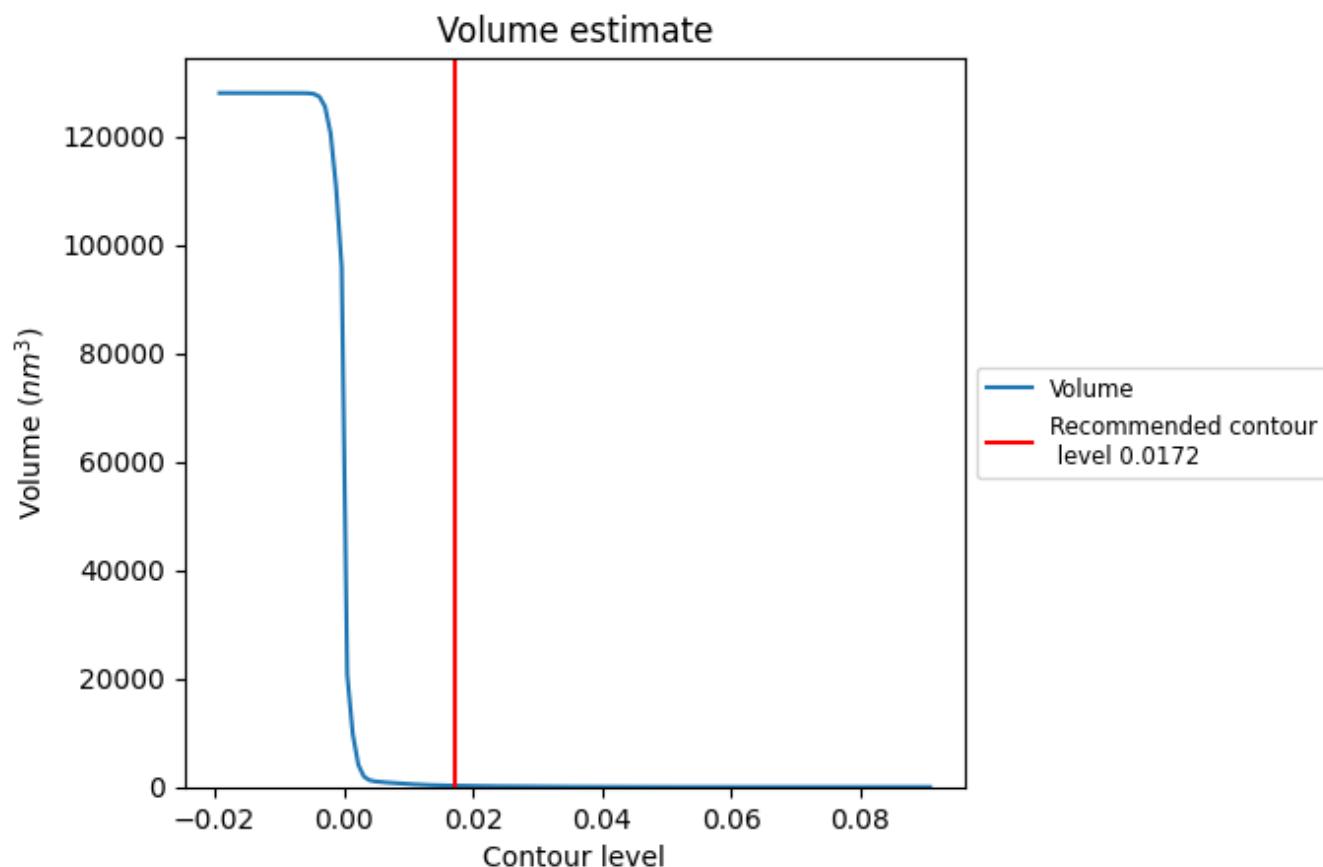
This section contains the results of statistical analysis of the map.

### 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.

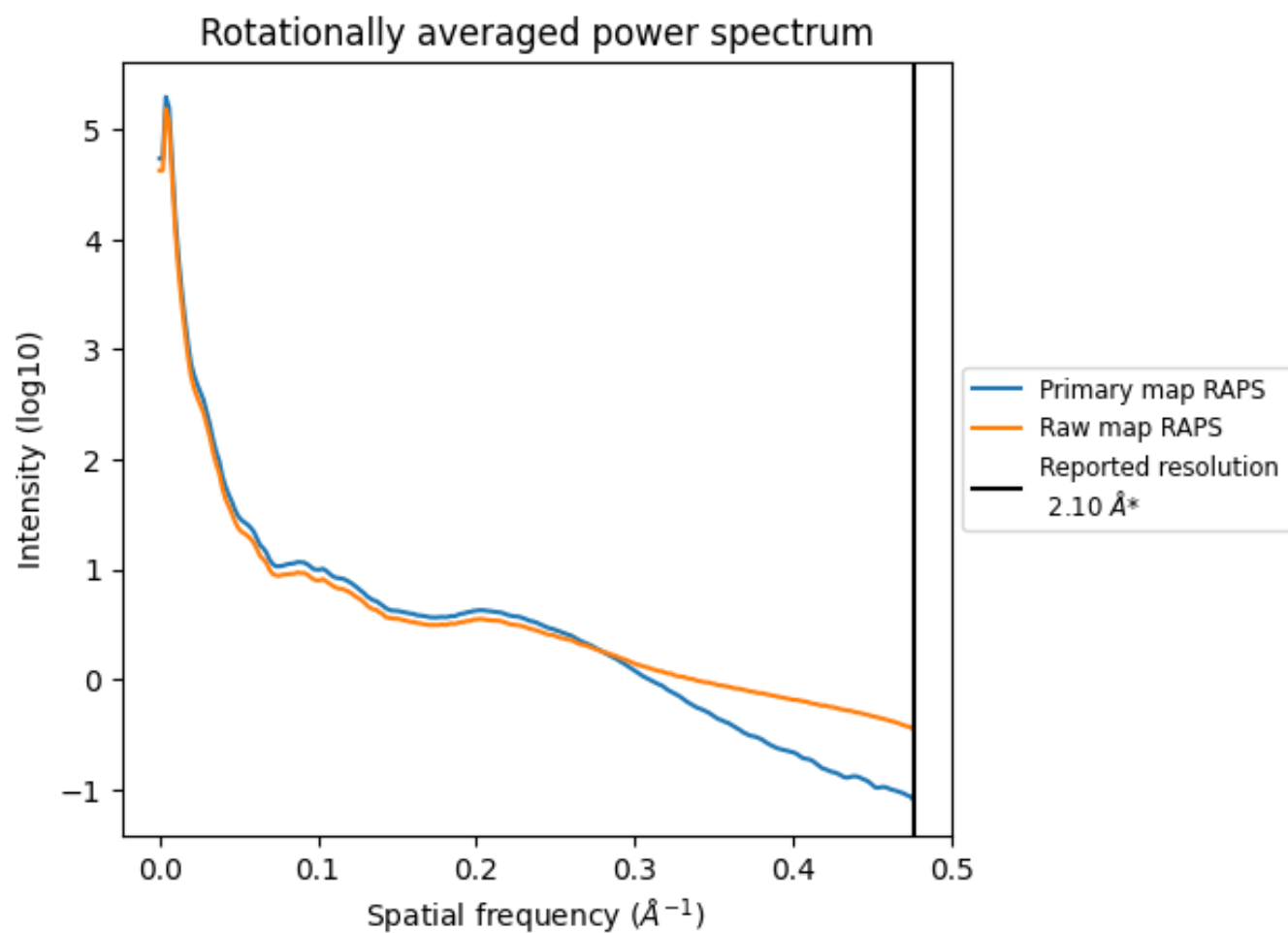
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229  $\text{nm}^3$ ; this corresponds to an approximate mass of 207 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 ⓘ

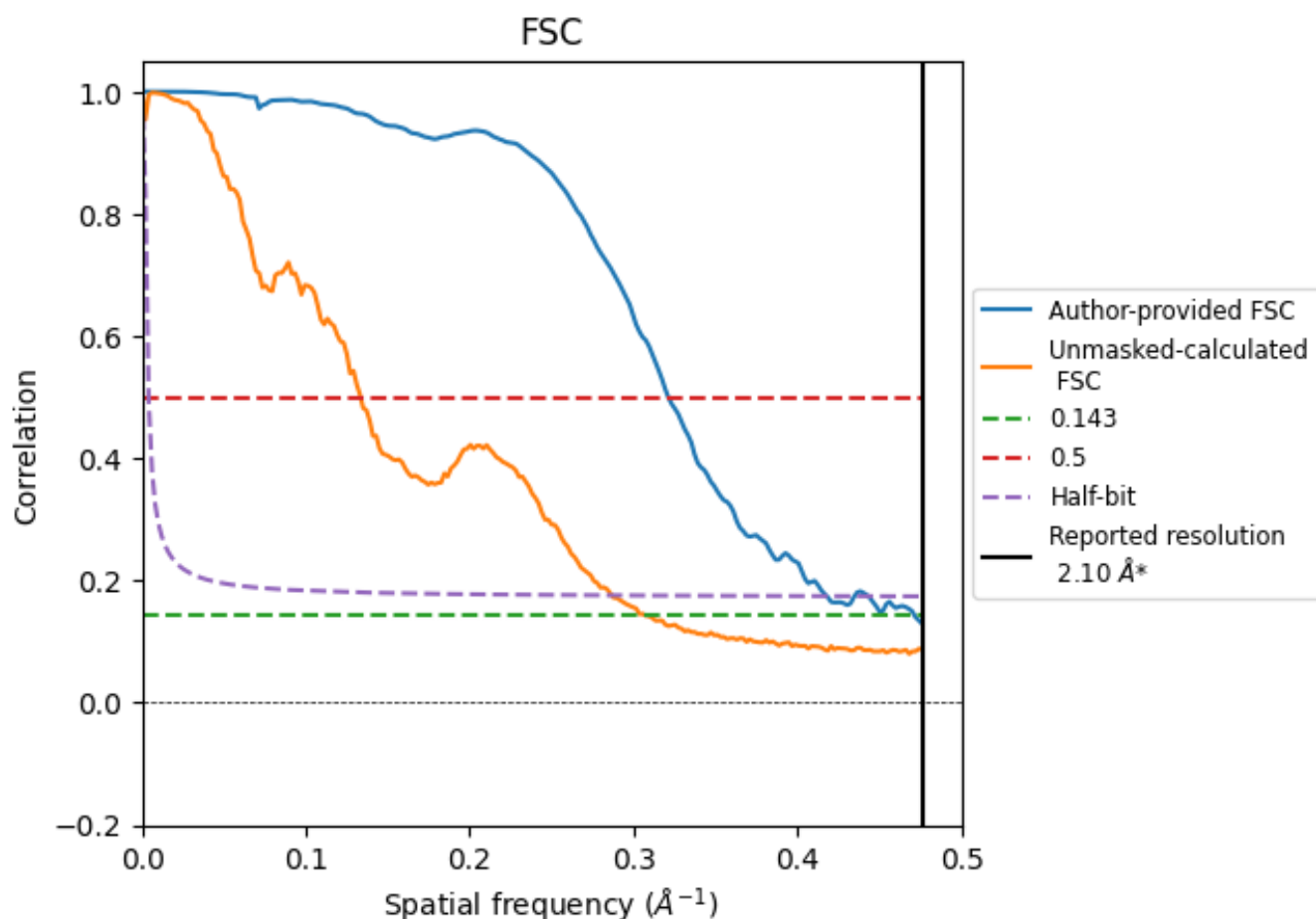


\*Reported resolution corresponds to spatial frequency of 0.476 Å<sup>-1</sup>

## 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 0.476  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

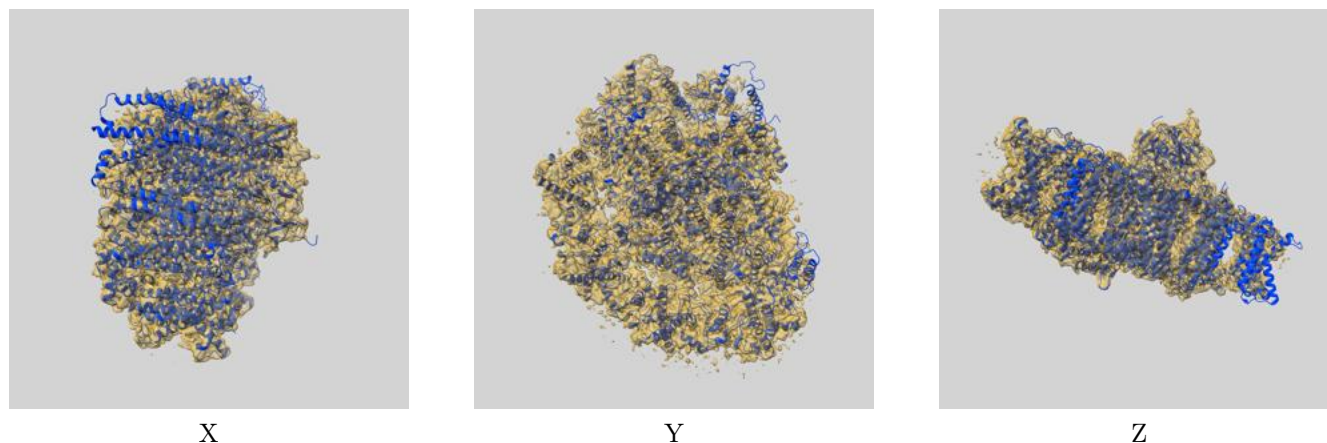
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	3.11	2.39
Unmasked-calculated*	3.26	7.50	3.49

\*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 3.26 differs from the reported value 2.1 by more than 10 %

## 9 Map-model fit [i](#)

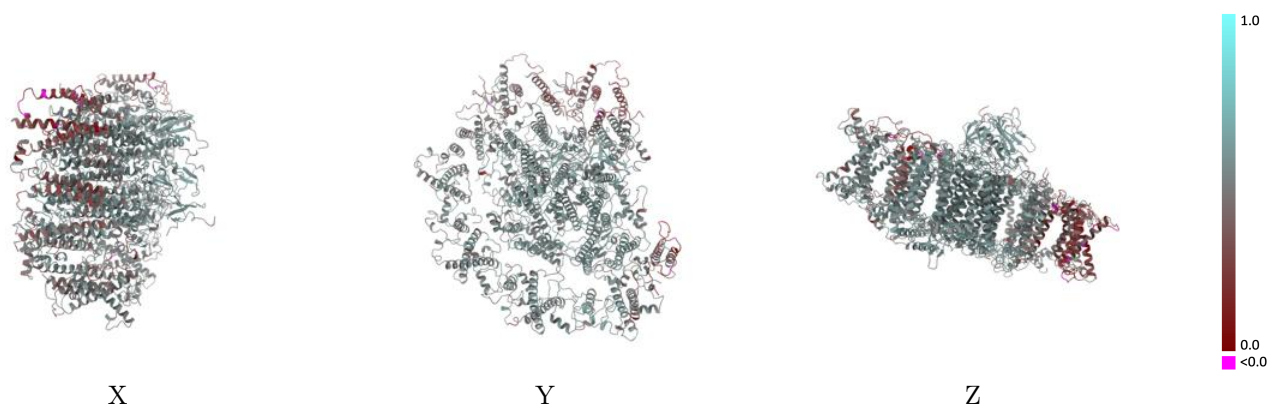
This section contains information regarding the fit between EMDB map EMD-48266 and PDB model 9MH1. Per-residue inclusion information can be found in section 3 on page 32.

### 9.1 Map-model overlay [i](#)



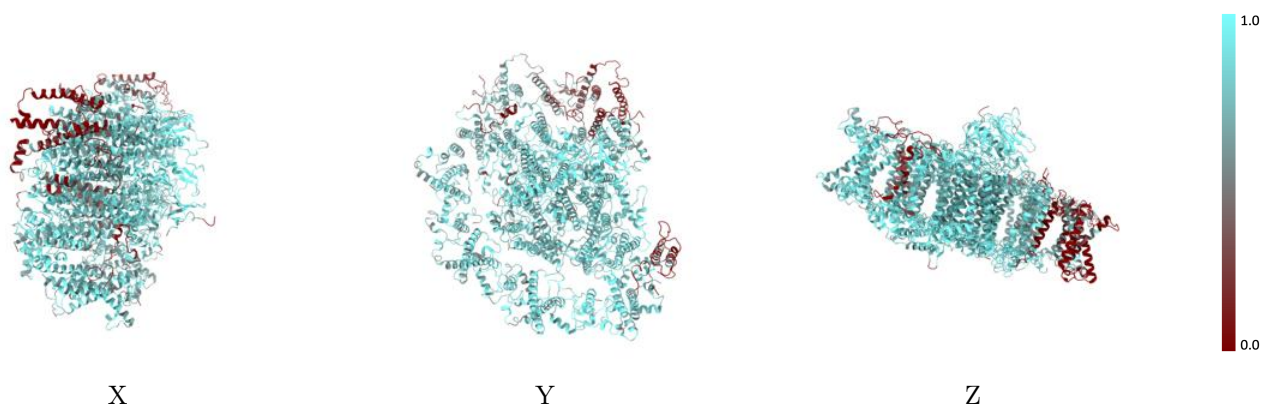
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

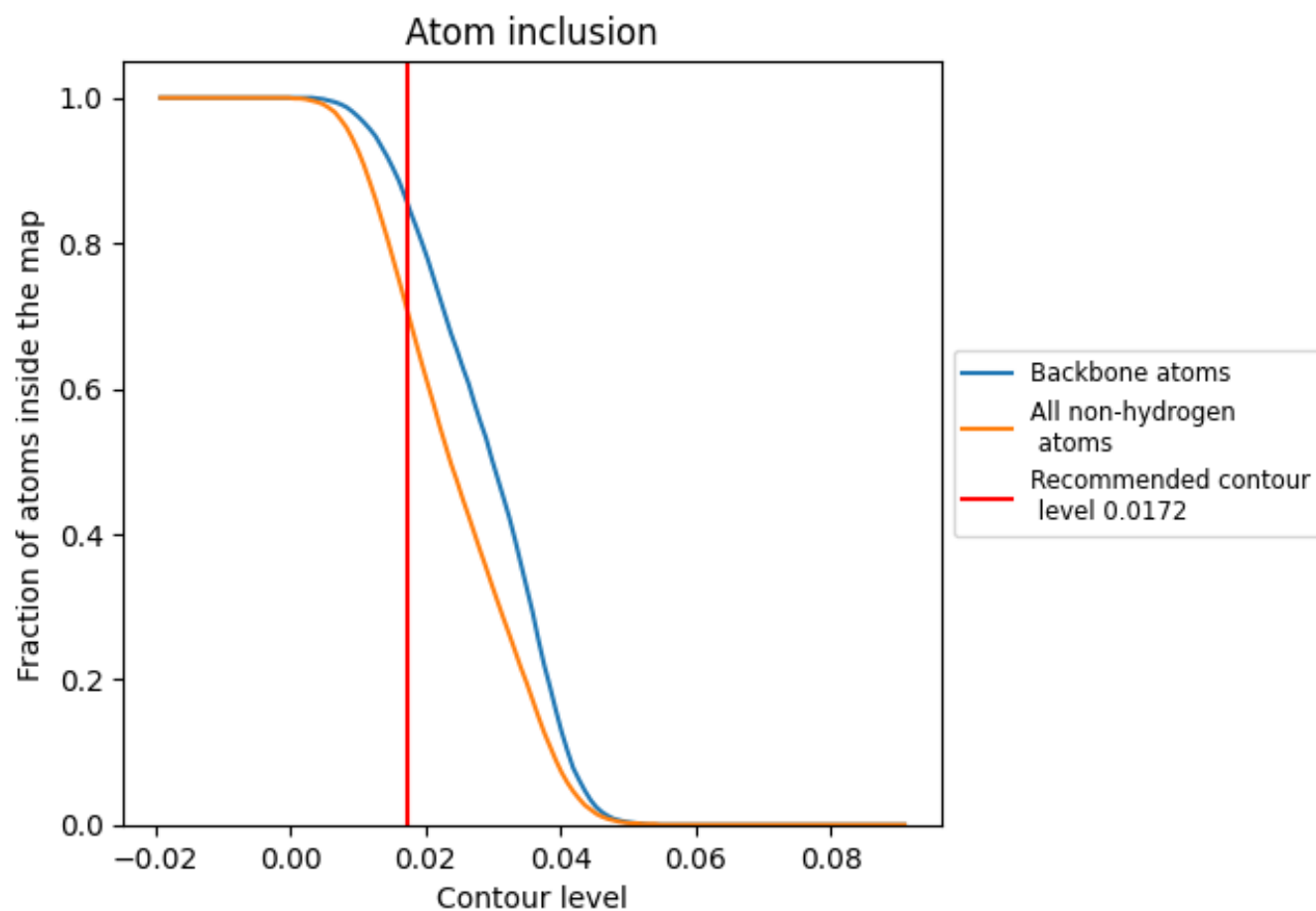
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0172).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7100	 0.4980
1	 0.7310	 0.4860
2	 0.2090	 0.2700
3	 0.7210	 0.5040
7	 0.7580	 0.5100
8	 0.7130	 0.4890
9	 0.5830	 0.4050
A	 0.8190	 0.5560
B	 0.8060	 0.5480
C	 0.9350	 0.5560
D	 0.8560	 0.5350
E	 0.7870	 0.5370
F	 0.7380	 0.5230
G	 0.5650	 0.4550
H	 0.0980	 0.2690
I	 0.7050	 0.4850
J	 0.7390	 0.5190
K	 0.2050	 0.3020
L	 0.6460	 0.4800

