



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 9MH0 / pdb_00009mh0
EMDB ID : EMD-48265
Title : Dunaliella salina PSI-LHCI supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 2.90 Å(reported)
Based on initial model : 6SL5

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

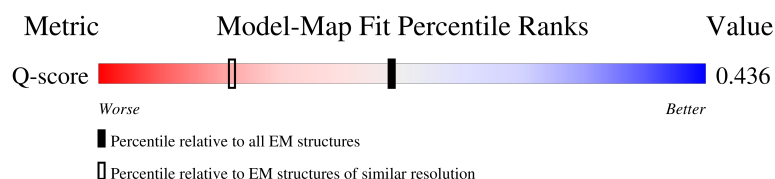
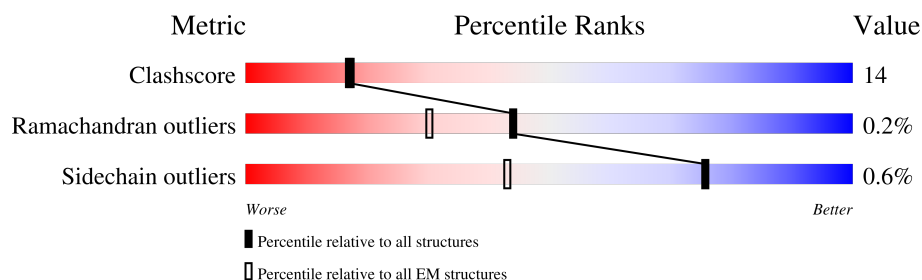
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	228	13% 63% 24% 14%
2	2	263	41% 65% 19% 16%
3	3	320	8% 48% 17% 35%
4	7	256	7% 65% 17% 18%

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Mol	Chain	Length	Quality of chain
5	8	254	
6	9	222	
7	A	751	
8	B	735	
9	C	81	
10	D	202	
11	E	125	
12	F	232	
13	G	141	
14	H	135	
15	I	109	
16	J	41	
17	K	123	
18	L	202	

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	601	X	-	-	-
19	CHL	2	606	X	-	-	-
19	CHL	3	401	X	-	-	-
19	CHL	7	302	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	602	X	-	-	-
20	CLA	2	603	X	-	-	-
20	CLA	2	604	X	-	-	-
20	CLA	2	605	X	-	-	-
20	CLA	2	607	X	-	-	-
20	CLA	2	608	X	-	-	-
20	CLA	2	609	X	-	-	-
20	CLA	2	610	X	-	-	-
20	CLA	2	611	X	-	-	-
20	CLA	2	612	X	-	-	-
20	CLA	2	613	X	-	-	-
20	CLA	2	622	X	-	-	-
20	CLA	3	402	X	-	-	-
20	CLA	3	403	X	-	-	-
20	CLA	3	404	X	-	-	-
20	CLA	3	405	X	-	-	-
20	CLA	3	406	X	-	-	-
20	CLA	3	407	X	-	-	-
20	CLA	3	408	X	-	-	-
20	CLA	3	409	X	-	-	-
20	CLA	3	410	X	-	-	-
20	CLA	3	411	X	-	-	-
20	CLA	3	412	X	-	-	-
20	CLA	3	413	X	-	-	-
20	CLA	3	414	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	324	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	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	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	844	X	-	-	-
20	CLA	B	803	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
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	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	842	X	-	-	-
20	CLA	B	843	X	-	-	-
20	CLA	F	5003	X	-	-	-
20	CLA	F	5005	X	-	-	-
20	CLA	F	5006	X	-	-	-
20	CLA	F	5007	X	-	-	-
20	CLA	G	4002	X	-	-	-
20	CLA	G	4003	X	-	-	-
20	CLA	G	4004	X	-	-	-
20	CLA	H	204	X	-	-	-
20	CLA	J	4002	X	-	-	-
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	204	X	-	-	-
20	CLA	L	301	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	305	X	-	-	-
20	CLA	L	306	X	-	-	-
20	CLA	L	307	X	-	-	-
21	LUT	1	615	X	-	-	-
21	LUT	2	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LUT	2	615	X	-	-	-
21	LUT	2	616	X	-	-	-
21	LUT	2	617	X	-	-	-
21	LUT	3	415	X	-	-	-
21	LUT	7	316	X	-	-	-
21	LUT	8	314	X	-	-	-
21	LUT	9	613	X	-	-	-
34	SF4	A	846	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 43016 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
			1498	962	253	276	7		

- Molecule 2 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1736	1128	286	313	9		

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	208	Total	C	N	O	S	0	0
			1597	1042	264	286	5		

- Molecule 4 is a protein called LHCA7.

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

- Molecule 5 is a protein called LHCA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	226	Total	C	N	O	S	0	0
			1726	1113	288	319	6		

- Molecule 6 is a protein called LHCA9.

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

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

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

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

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

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

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

- Molecule 10 is a protein called PSAD1.

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

- Molecule 11 is a protein called PSAE1.

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

- Molecule 12 is a protein called PSAF1.

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

- Molecule 13 is a protein called PSAG1.

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

- Molecule 14 is a protein called PSAH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	65	Total	C	N	O	S	0	0
			488	307	88	92	1		

- Molecule 15 is a protein called PSAI1.

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

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

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

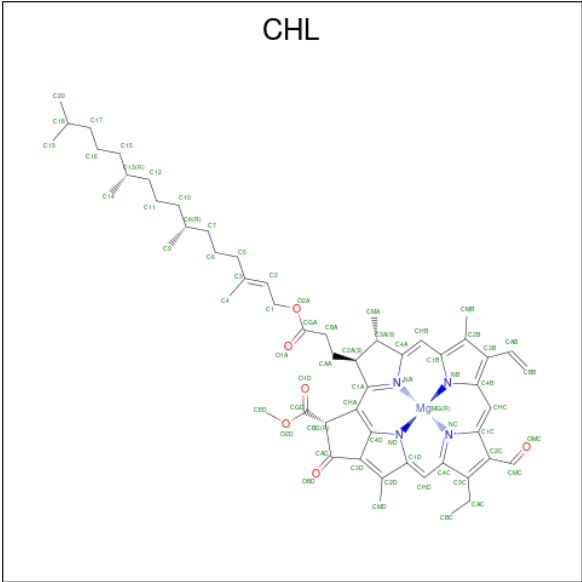
- Molecule 17 is a protein called PSAK1.

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

- Molecule 18 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	156	Total	C	N	O	S	0	0
			1149	749	188	206	6		

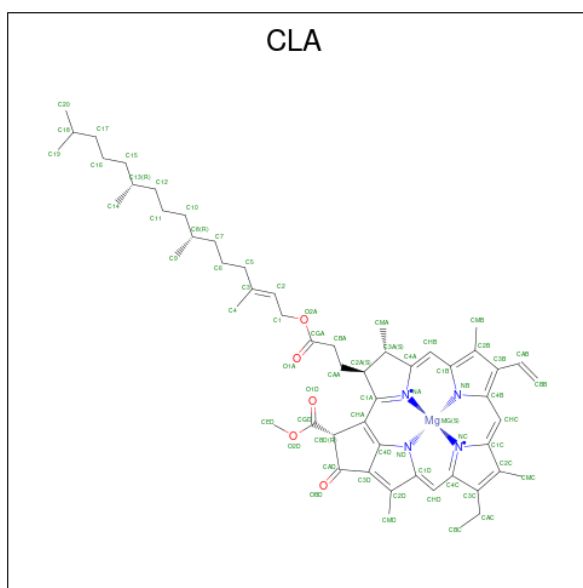
- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	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 65	C 55	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 65	C 55	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 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 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	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
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	3	1	Total 57	C 47	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
			65	55	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	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
			65	55	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	
20	7	1	Total	C	Mg	N	O	0
			65	55	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
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 51	C 41	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 65	C 55	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 60	C 50	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 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
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 65	C 55	Mg 1	N 4	O 5	0

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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 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	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 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
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 60	C 50	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 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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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 55	C 45	Mg 1	N 4	O 5	0
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 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
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 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	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 65	C 55	Mg 1	N 4	O 5	0

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

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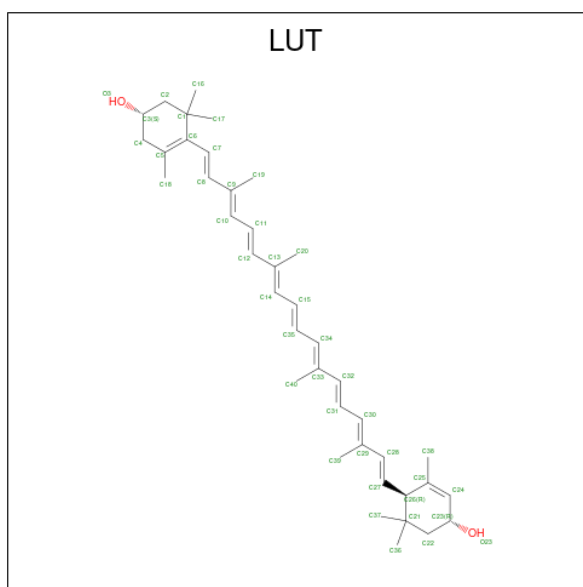
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 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	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	F	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	J	1	Total 49	C 39	Mg 1	N 4	O 5	0

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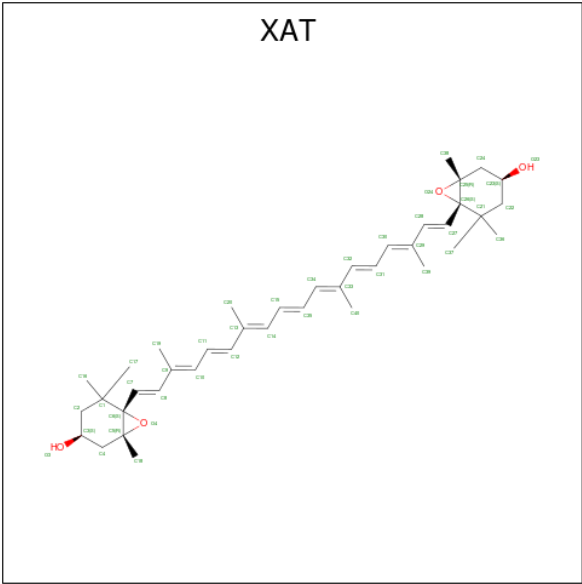
Mol	Chain	Residues	Atoms					AltConf
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			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	L	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: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	1	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	
21	2	1	Total	C	O	0
			42	40	2	
21	2	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	
21	8	1	Total	C	O	0
			42	40	2	
21	9	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: C₄₀H₅₆O₄).



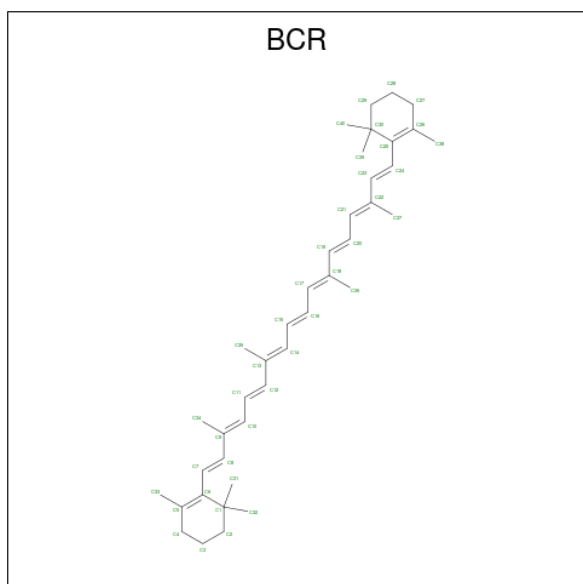
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
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: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



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

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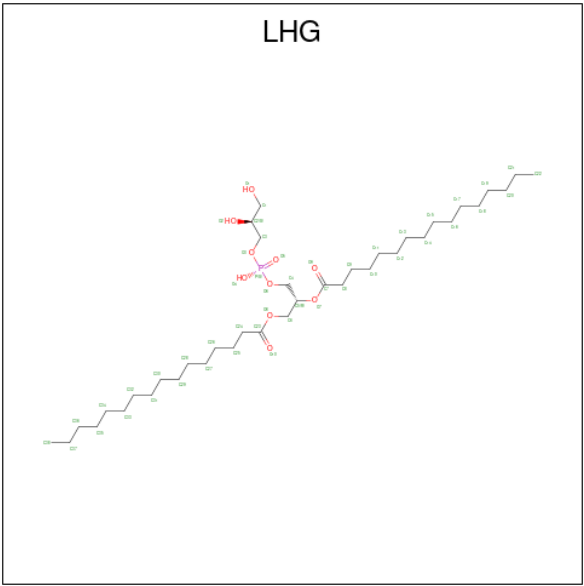
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 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	G	1	Total C 40 40	0
23	H	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	K	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	C	0
			40	40	
23	L	1	Total	C	0
			40	40	
23	L	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



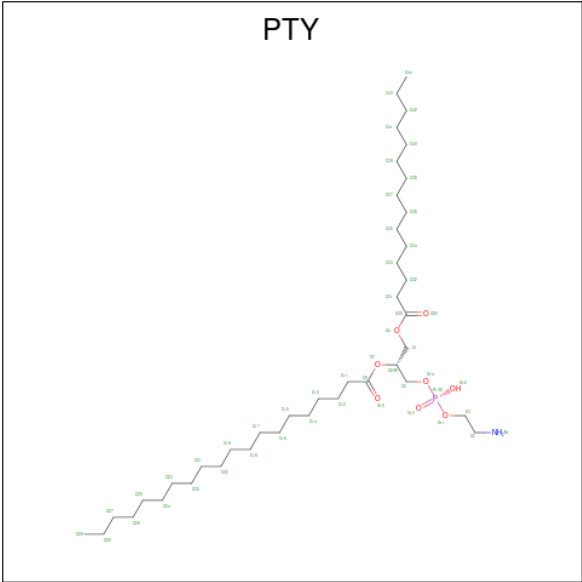
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			25	14	10	1	
24	1	1	Total	C	O	P	0
			44	33	10	1	
24	1	1	Total	C	O	P	0
			31	20	10	1	
24	1	1	Total	C	O	P	0
			46	35	10	1	
24	2	1	Total	C	O	P	0
			44	35	8	1	
24	2	1	Total	C	O	P	0
			36	25	10	1	
24	3	1	Total	C	O	P	0
			17	8	8	1	
24	3	1	Total	C	O	P	0
			39	28	10	1	

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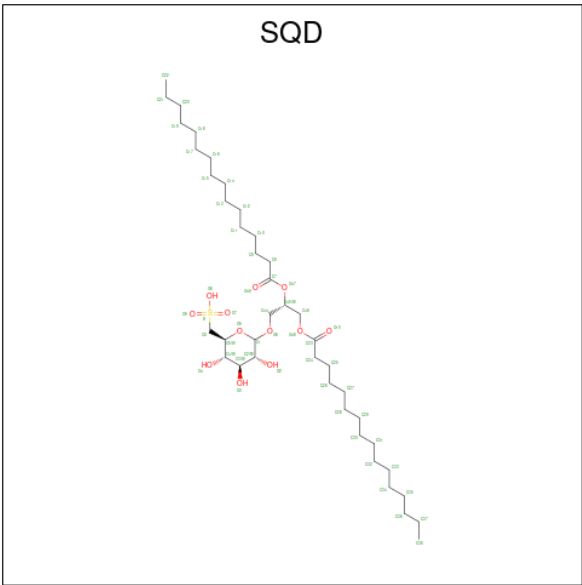
Mol	Chain	Residues	Atoms				AltConf
24	7	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			22	11	10	1	
24	7	1	Total	C	O	P	0
			40	29	10	1	
24	8	1	Total	C	O	P	0
			34	23	10	1	
24	8	1	Total	C	O	P	0
			31	20	10	1	
24	9	1	Total	C	O	P	0
			41	30	10	1	
24	9	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			30	20	9	1	
24	A	1	Total	C	O	P	0
			45	34	10	1	
24	B	1	Total	C	O	P	0
			49	38	10	1	
24	F	1	Total	C	O	P	0
			43	32	10	1	
24	F	1	Total	C	O	P	0
			42	31	10	1	
24	G	1	Total	C	O	P	0
			49	38	10	1	
24	H	1	Total	C	O	P	0
			38	27	10	1	
24	I	1	Total	C	O	P	0
			49	38	10	1	
24	J	1	Total	C	O	P	0
			36	29	6	1	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



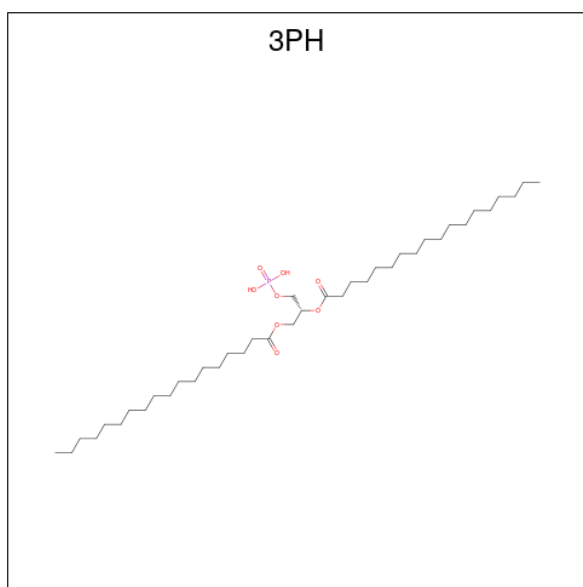
Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	N	O	P	0
			20	10	1	8	1	
25	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	3	1	Total	C	N	O	P	0
			26	16	1	8	1	
25	7	1	Total	C	N	O	P	0
			25	15	1	8	1	
25	8	1	Total	C	N	O	P	0
			24	14	1	8	1	
25	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
25	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
25	F	1	Total	C	N	O	P	0
			22	12	1	8	1	
25	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	L	1	Total	C	N	O	P	0
			20	10	1	8	1	

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



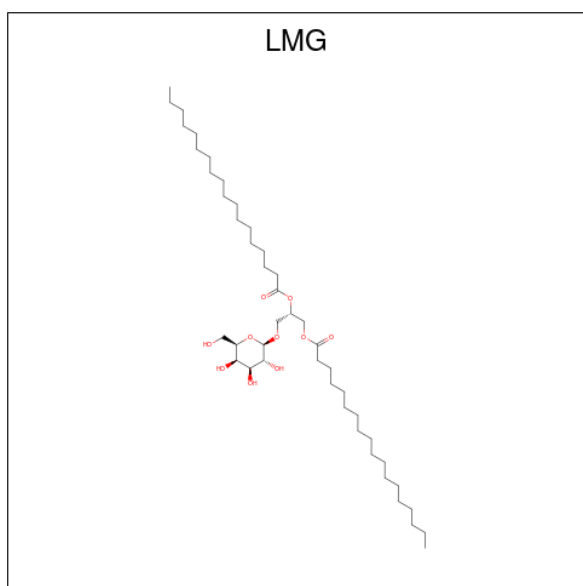
Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	S	0
			41	28	12	1	
26	3	1	Total	C	O	S	0
			35	22	12	1	
26	3	1	Total	C	O	S	0
			32	19	12	1	
26	9	1	Total	C	O	S	0
			37	24	12	1	
26	B	1	Total	C	O	S	0
			31	18	12	1	

- Molecule 27 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



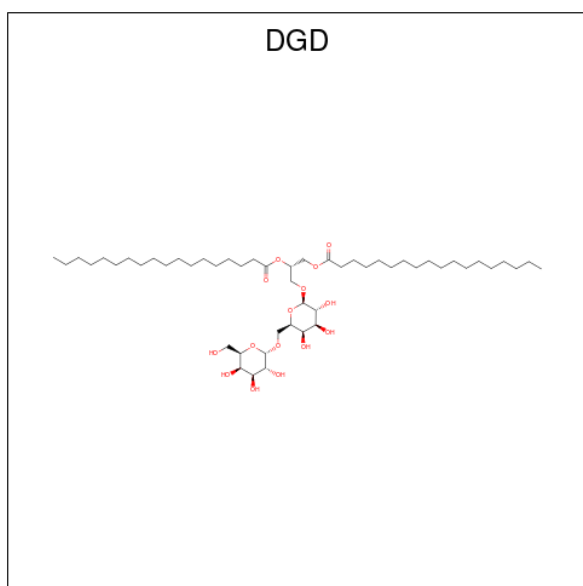
Mol	Chain	Residues	Atoms			AltConf
28	7	1	Total	C	O	0
			40	30	10	
28	7	1	Total	C	O	0
			54	44	10	

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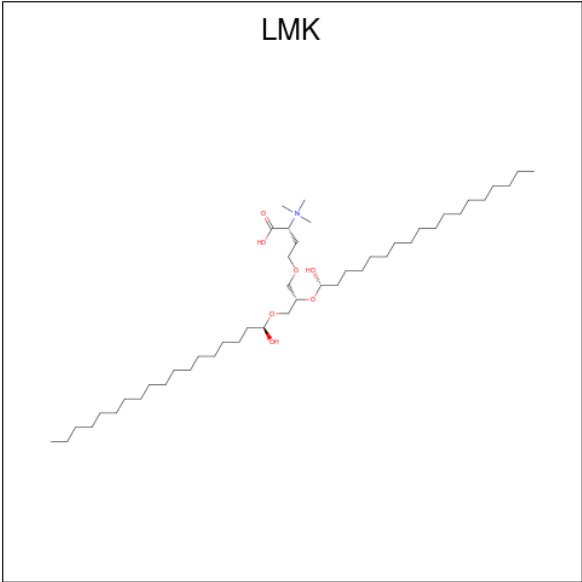
Mol	Chain	Residues	Atoms			AltConf
28	8	1	Total	C	O	0
			50	40	10	
28	A	1	Total	C	O	0
			32	22	10	
28	F	1	Total	C	O	0
			46	36	10	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



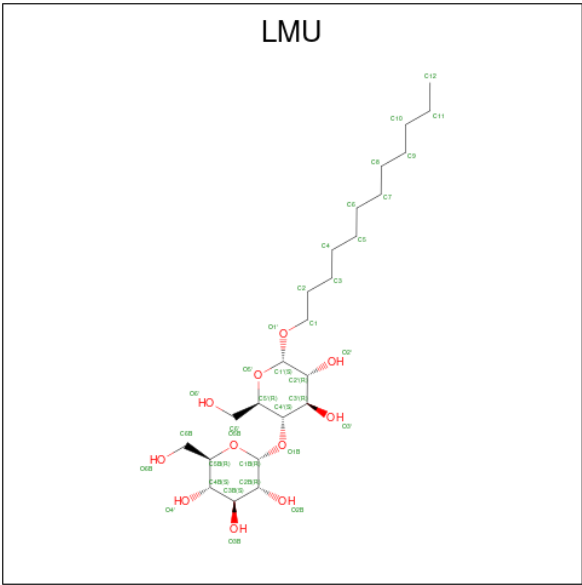
Mol	Chain	Residues	Atoms			AltConf
29	7	1	Total	C	O	0
			47	32	15	
29	A	1	Total	C	O	0
			66	51	15	
29	B	1	Total	C	O	0
			61	46	15	
29	L	1	Total	C	O	0
			58	43	15	

- Molecule 30 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$) (labeled as "Ligand of Interest" by depositor).



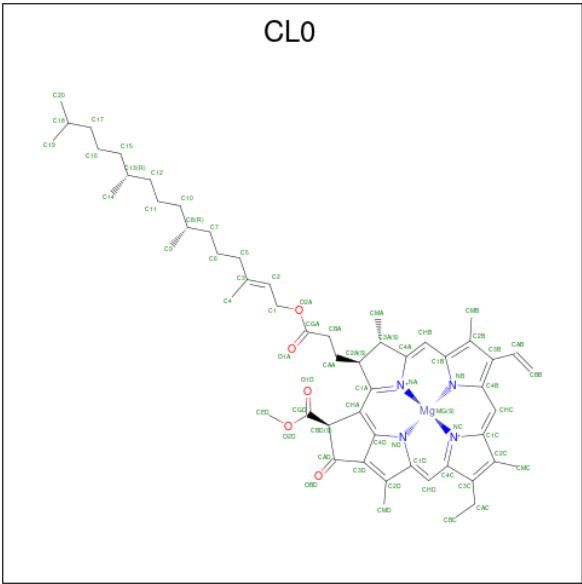
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	8	1	35	27	1	7	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



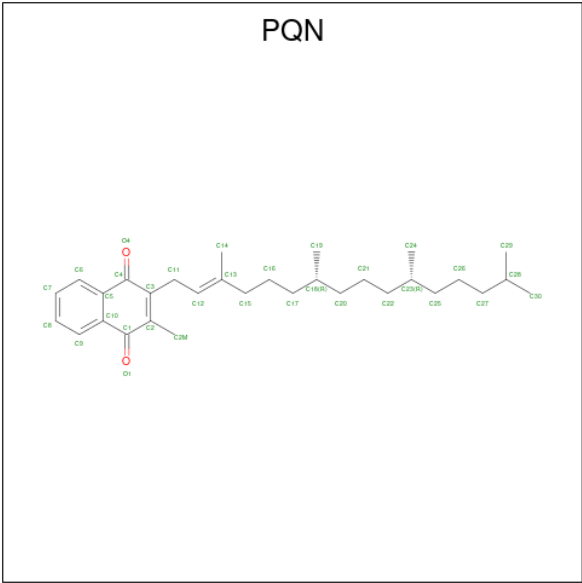
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	9	1	35	24	11	0
31	A	1	35	24	11	0
31	A	1	35	24	11	0

- Molecule 32 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
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



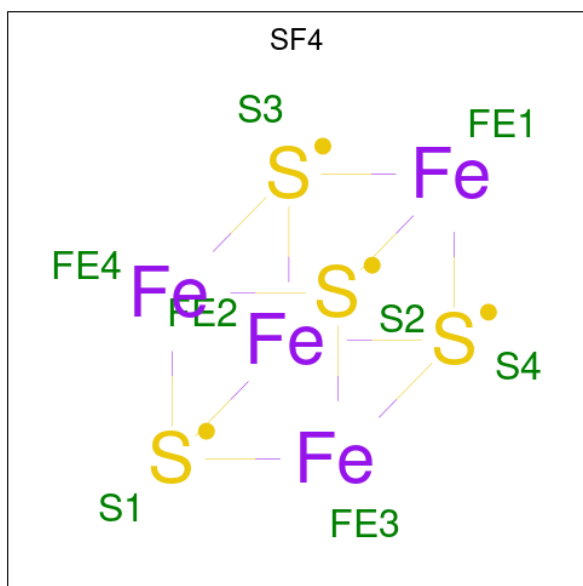
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			33	31	2	

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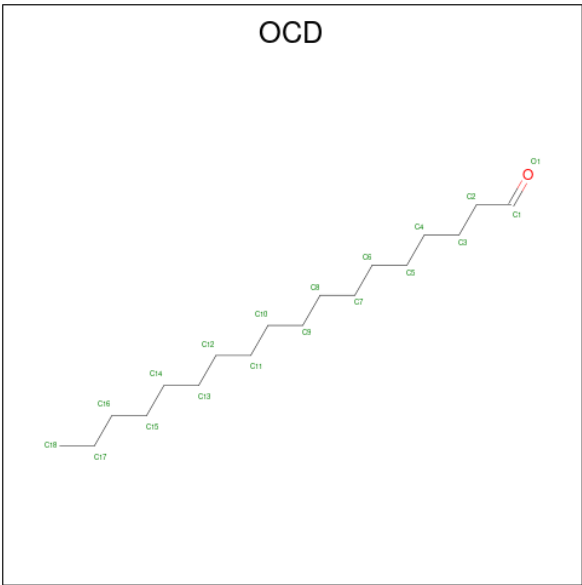
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			33	31	2	

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



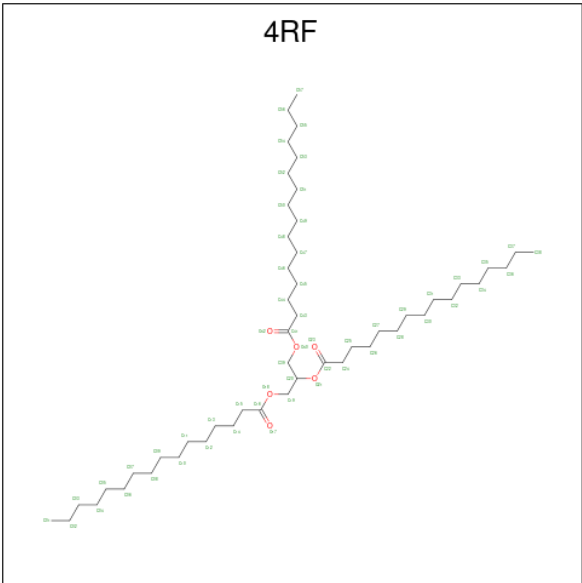
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is octadecanal (CCD ID: OCD) (formula: $\text{C}_{18}\text{H}_{36}\text{O}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	C	0
			11	11	

- Molecule 36 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆) (labeled as "Ligand of Interest" by depositor).

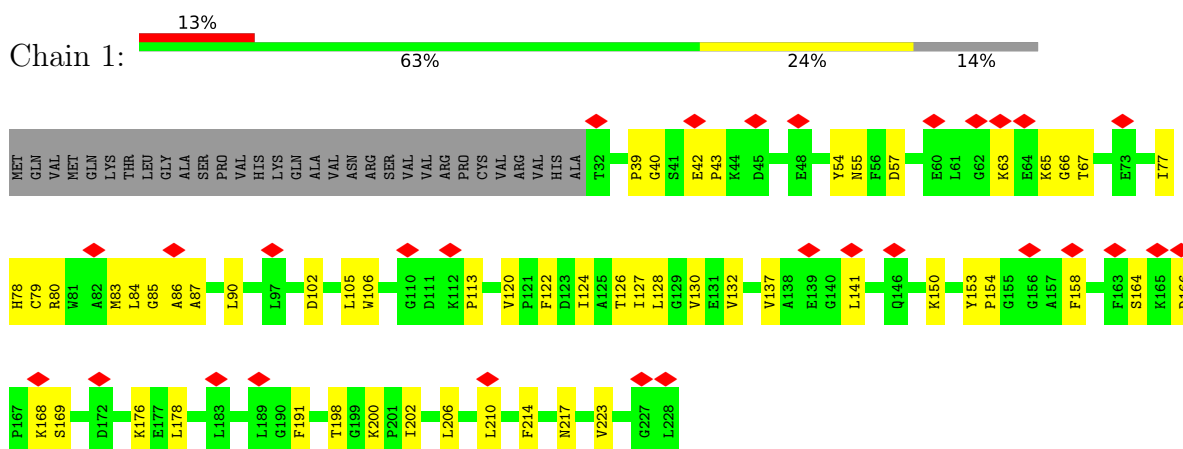


Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			39	33	6	

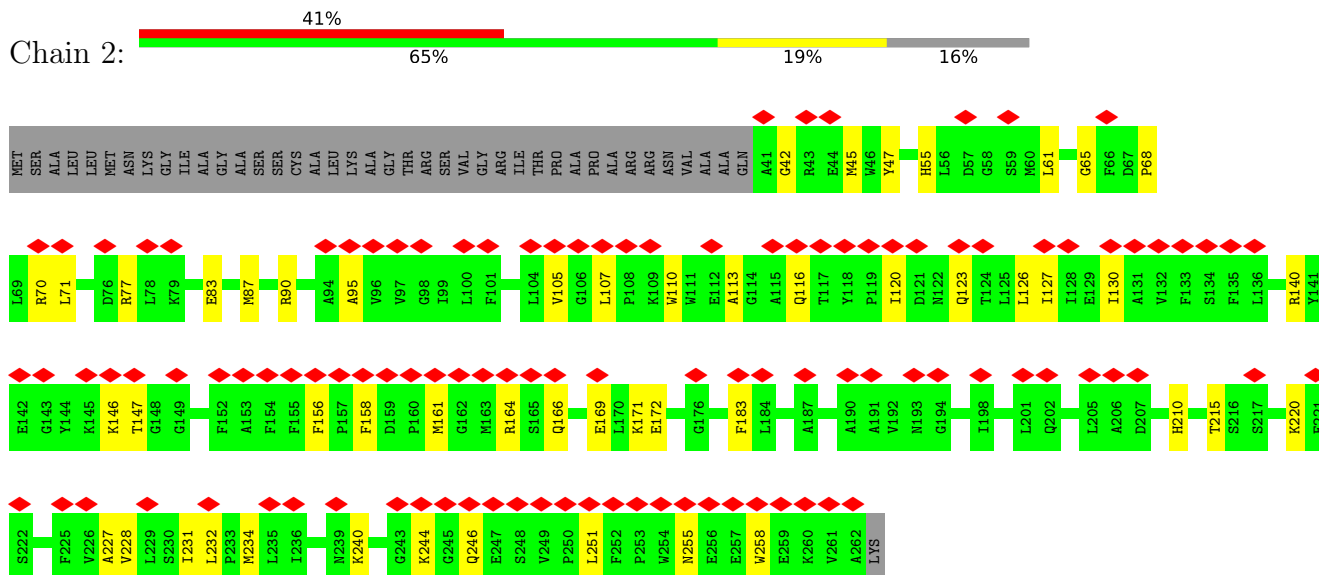
3 Residue-property plots

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

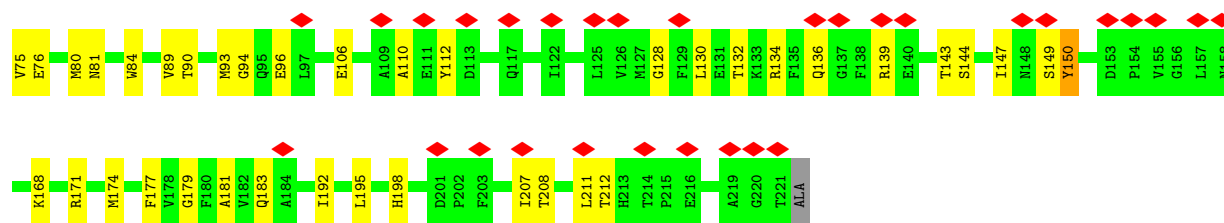


- Molecule 2: LHCA2



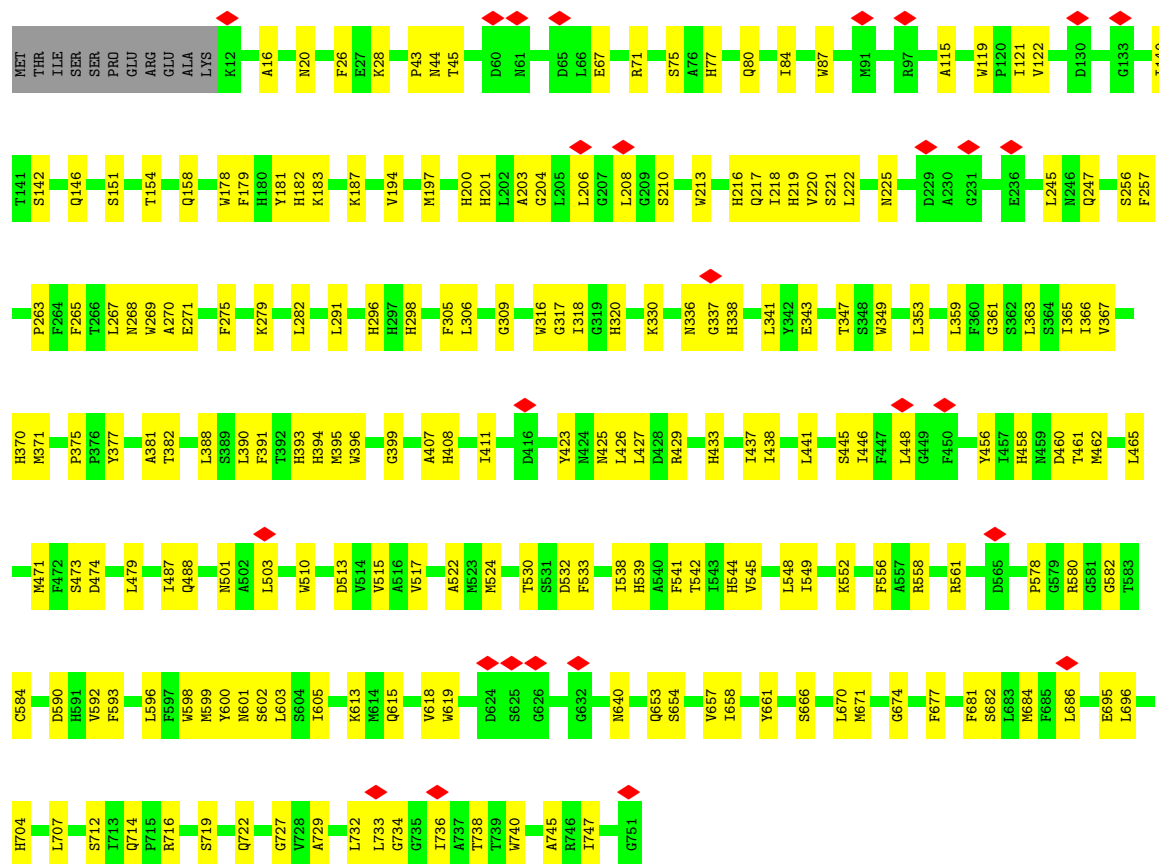
- Molecule 3: LHCA3





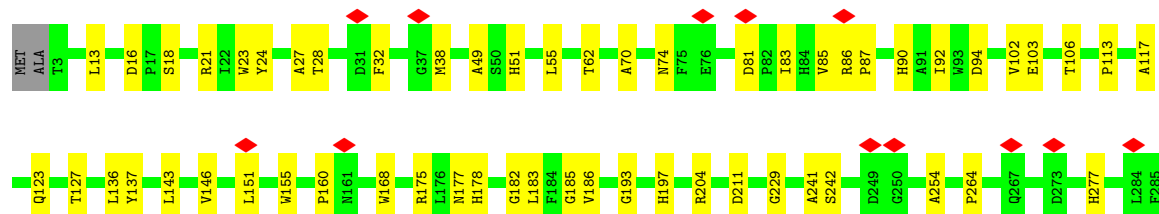
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

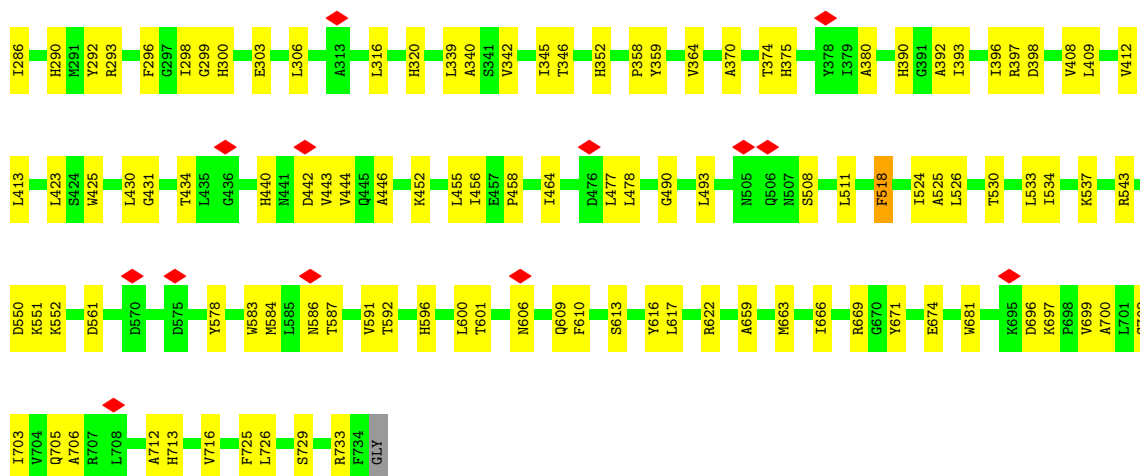
Chain A: 71% 27%



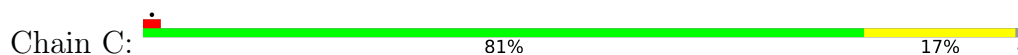
• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 77% 22%

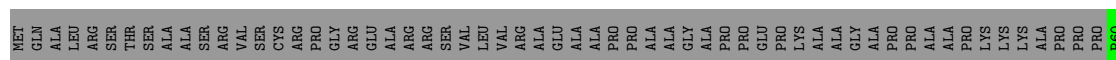




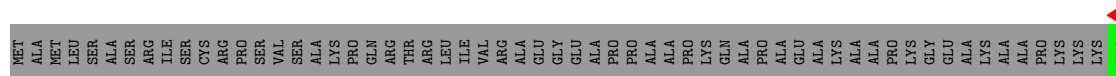
- Molecule 9: Photosystem I iron-sulfur center



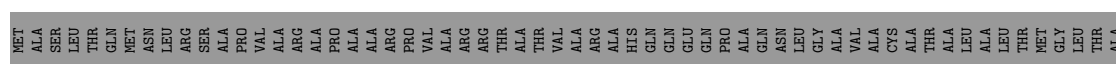
- Molecule 10: PSAD1

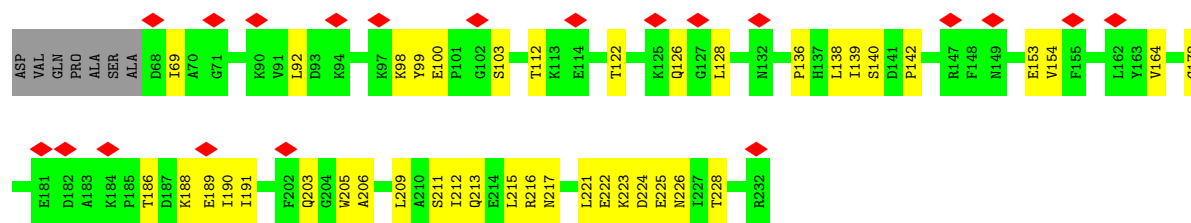


- Molecule 11: PSAE1

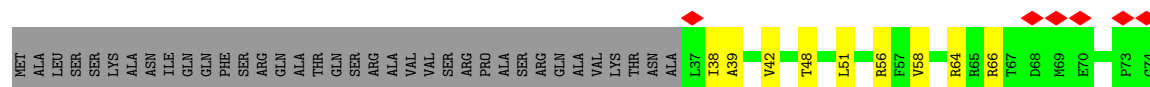


- Molecule 12: PSAF1

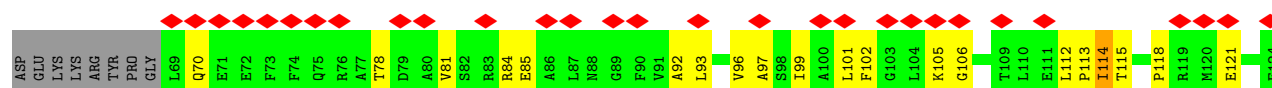
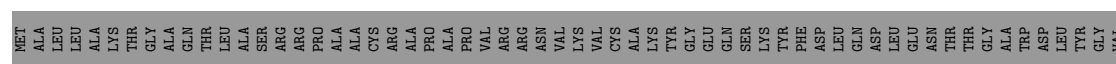
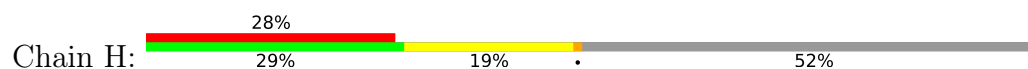




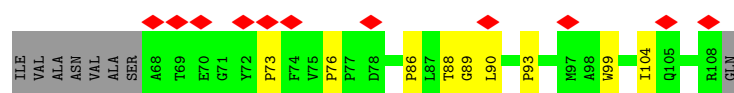
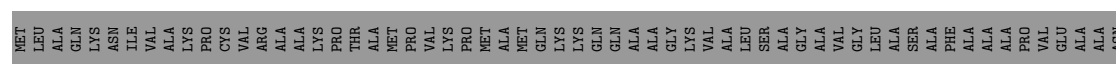
- Molecule 13: PSAG1



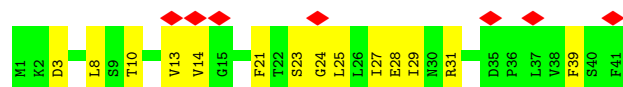
- Molecule 14: PSAH1



- Molecule 15: PSAI1



- Molecule 16: Photosystem I reaction center subunit IX



- Molecule 17: PSAK1

Chain K:

Chain L:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98784	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	0.081	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0165	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: XAT, LMU, LHG, LMG, PQN, PTY, DGD, 3PH, SF4, 4RF, OCD, CL0, LMK, SQD, LUT, CHL, CLA, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.19	0/1537	0.47	0/2084
2	2	0.18	0/1787	0.44	0/2425
3	3	0.19	0/1644	0.42	0/2228
4	7	0.17	0/1659	0.39	0/2254
5	8	0.19	0/1775	0.44	1/2406 (0.0%)
6	9	0.29	0/1499	0.60	0/2043
7	A	0.15	0/6003	0.34	0/8189
8	B	0.16	0/6016	0.35	0/8225
9	C	0.15	0/610	0.36	0/828
10	D	0.15	0/1163	0.35	0/1571
11	E	0.12	0/521	0.28	0/711
12	F	0.19	0/1332	0.47	0/1801
13	G	0.18	0/815	0.47	0/1104
14	H	0.28	0/493	0.75	1/660 (0.2%)
15	I	0.23	0/335	0.62	0/463
16	J	0.23	0/338	0.59	0/461
17	K	0.31	0/592	0.96	4/801 (0.5%)
18	L	0.17	0/1179	0.48	0/1612
All	All	0.18	0/29298	0.44	6/39866 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	F	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	71	ARG	CA-C-N	-11.03	107.45	123.11
17	K	71	ARG	C-N-CA	-11.03	107.45	123.11
17	K	85	LEU	CA-CB-CG	5.87	136.84	116.30
5	8	125	MET	CB-CG-SD	5.73	129.90	112.70
17	K	102	MET	CB-CG-SD	5.51	129.24	112.70
14	H	114	ILE	N-CA-C	-5.40	108.58	113.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F	216	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1498	0	1468	52	0
2	2	1736	0	1704	54	0
3	3	1597	0	1559	63	0
4	7	1609	0	1565	39	0
5	8	1726	0	1678	53	0
6	9	1456	0	1441	51	0
7	A	5807	0	5640	192	0
8	B	5803	0	5556	153	0
9	C	600	0	583	15	0
10	D	1133	0	1141	16	0
11	E	509	0	497	2	0
12	F	1303	0	1331	33	0
13	G	794	0	799	28	0
14	H	488	0	505	30	0
15	I	321	0	316	10	0
16	J	327	0	327	16	0
17	K	584	0	614	41	0
18	L	1149	0	1171	22	0
19	1	98	0	68	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	108	0	88	8	0
19	3	56	0	47	6	0
19	7	211	0	171	16	0
19	8	145	0	97	9	0
19	9	47	0	31	4	0
20	1	659	0	603	29	0
20	2	589	0	467	25	0
20	3	699	0	622	25	0
20	7	647	0	634	21	0
20	8	488	0	434	15	0
20	9	591	0	520	20	0
20	A	2535	0	2641	175	0
20	B	2559	0	2703	148	0
20	F	262	0	225	11	0
20	G	138	0	101	4	0
20	H	45	0	33	0	0
20	J	49	0	38	6	0
20	K	193	0	151	11	0
20	L	340	0	325	13	0
21	1	42	0	56	7	0
21	2	168	0	224	15	0
21	3	42	0	56	2	0
21	7	42	0	56	2	0
21	8	42	0	56	0	0
21	9	42	0	56	4	0
22	1	44	0	56	2	0
22	3	44	0	56	3	0
22	7	44	0	56	6	0
22	8	44	0	56	3	0
22	9	88	0	112	9	0
23	1	40	0	56	2	0
23	3	120	0	168	10	0
23	7	40	0	56	4	0
23	8	40	0	56	4	0
23	A	280	0	389	46	0
23	B	240	0	336	27	0
23	F	80	0	111	9	0
23	G	80	0	112	5	0
23	H	40	0	56	0	0
23	I	40	0	56	3	0
23	J	80	0	112	10	0
23	K	40	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	120	0	168	10	0
24	1	146	0	178	5	0
24	2	80	0	107	4	0
24	3	56	0	62	2	0
24	7	111	0	141	6	0
24	8	65	0	70	3	0
24	9	90	0	129	4	0
24	A	75	0	92	4	0
24	B	49	0	74	0	0
24	F	85	0	113	6	0
24	G	49	0	74	3	0
24	H	38	0	49	2	0
24	I	49	0	74	6	0
24	J	36	0	52	1	0
25	1	55	0	56	2	0
25	3	26	0	25	0	0
25	7	25	0	23	0	0
25	8	45	0	38	0	0
25	B	27	0	27	0	0
25	F	22	0	17	0	0
25	H	78	0	100	6	0
25	L	20	0	13	0	0
26	2	41	0	49	3	0
26	3	67	0	62	5	0
26	9	37	0	38	1	0
26	B	31	0	26	1	0
27	2	33	0	39	4	0
28	7	94	0	134	4	0
28	8	50	0	70	5	0
28	A	32	0	34	2	0
28	F	46	0	62	3	0
29	7	47	0	52	4	0
29	A	66	0	92	4	0
29	B	61	0	83	8	0
29	L	58	0	77	4	0
30	8	35	0	0	0	0
31	9	35	0	46	4	0
31	A	70	0	91	3	0
32	A	65	0	72	8	0
33	A	33	0	46	1	0
33	B	33	0	46	4	0
34	A	8	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	16	0	0	2	0
35	A	11	0	0	0	0
36	A	39	0	53	2	0
All	All	43016	0	43152	1190	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 14.

All (1190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:584:CYS:SG	34:A:846:SF4:FE4	1.05	1.49
2:2:227:ALA:O	2:2:231:ILE:HD12	1.19	1.29
8:B:431:GLY:CA	8:B:526:LEU:HD11	1.74	1.16
1:1:80:ARG:HA	1:1:83:MET:HE3	1.24	1.15
17:K:71:ARG:NH1	17:K:72:LYS:HE2	1.61	1.15
7:A:225:ASN:OD1	7:A:291:LEU:HD21	1.46	1.14
8:B:431:GLY:HA2	8:B:526:LEU:CD1	1.77	1.14
6:9:39:TRP:CE3	6:9:44:ILE:HD13	1.82	1.13
20:2:603:CLA:HED3	14:H:93:LEU:HD11	1.22	1.10
16:J:21:PHE:O	20:J:4002:CLA:HBB2	1.49	1.09
17:K:63:ARG:NH1	17:K:91:PRO:O	1.86	1.08
8:B:431:GLY:HA2	8:B:526:LEU:HD11	1.07	1.06
8:B:303:GLU:HB3	13:G:76:LEU:CD1	1.85	1.06
1:1:80:ARG:HA	1:1:83:MET:CE	1.86	1.05
2:2:227:ALA:O	2:2:231:ILE:CD1	2.04	1.04
20:2:603:CLA:CED	14:H:93:LEU:HD11	1.87	1.03
9:C:17:CYS:HB3	34:C:102:SF4:S2	1.99	1.03
3:3:203:GLU:O	3:3:207:ILE:HG22	1.59	1.02
8:B:182:GLY:HA2	8:B:186:VAL:HG12	1.43	0.98
20:A:805:CLA:NB	20:B:804:CLA:HBB1	1.77	0.97
7:A:204:GLY:O	7:A:208:LEU:HB2	1.65	0.96
8:B:303:GLU:HB3	13:G:76:LEU:HD11	1.43	0.94
3:3:235:LEU:HD22	3:3:249:PHE:N	1.80	0.94
20:A:805:CLA:C1B	20:B:804:CLA:HBB1	1.96	0.93
17:K:70:VAL:O	17:K:82:ARG:NH1	2.02	0.93
7:A:542:THR:HG22	7:A:602:SER:HB2	1.52	0.91
3:3:235:LEU:HD22	3:3:249:PHE:CB	2.02	0.90
3:3:207:ILE:HD13	20:3:407:CLA:HMC3	1.52	0.89
7:A:584:CYS:SG	34:A:846:SF4:S3	2.71	0.89
6:9:39:TRP:HE3	6:9:44:ILE:HD13	1.28	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:39:TRP:HE3	6:9:44:ILE:CD1	1.86	0.87
20:2:603:CLA:HED3	14:H:93:LEU:CD1	2.04	0.87
7:A:584:CYS:SG	34:A:846:SF4:S2	2.73	0.86
6:9:44:ILE:HD12	6:9:44:ILE:O	1.74	0.85
7:A:225:ASN:OD1	7:A:291:LEU:CD2	2.25	0.84
17:K:71:ARG:HH12	17:K:72:LYS:HE2	1.43	0.84
19:7:306:CHL:HBC2	19:7:307:CHL:HHD	1.57	0.83
6:9:143:THR:HG22	6:9:144:SER:N	1.93	0.83
2:2:231:ILE:CD1	21:2:616:LUT:H201	2.08	0.83
1:1:217:ASN:ND2	5:8:122:THR:HG23	1.94	0.83
6:9:39:TRP:CE3	6:9:44:ILE:CD1	2.59	0.83
6:9:143:THR:HG22	6:9:144:SER:H	1.44	0.83
8:B:390:HIS:HE1	20:B:830:CLA:NA	1.76	0.83
8:B:440:HIS:O	8:B:444:VAL:HG23	1.78	0.83
3:3:207:ILE:HD13	20:3:407:CLA:CMC	2.10	0.82
20:7:324:CLA:HBB2	20:8:302:CLA:HHD	1.59	0.82
7:A:584:CYS:HG	34:A:846:SF4:FE4	0.97	0.81
17:K:68:PRO:HB3	17:K:74:ALA:HB2	1.62	0.81
14:H:131:LEU:O	14:H:131:LEU:HD23	1.79	0.81
7:A:542:THR:CG2	7:A:602:SER:HB2	2.11	0.80
20:2:603:CLA:H51	14:H:93:LEU:HD12	1.62	0.80
3:3:235:LEU:HD13	3:3:249:PHE:HB2	1.62	0.80
5:8:108:GLY:O	5:8:112:ILE:HG12	1.82	0.79
7:A:182:HIS:HE1	20:A:814:CLA:NA	1.80	0.78
20:K:203:CLA:H3A	23:K:205:BCR:H363	1.64	0.78
7:A:460:ASP:OD2	20:A:805:CLA:H42	1.84	0.78
20:B:819:CLA:H162	20:B:827:CLA:H3A	1.63	0.78
12:F:139:ILE:N	12:F:153:GLU:OE1	2.11	0.77
20:2:603:CLA:C5	14:H:93:LEU:HD12	2.15	0.76
8:B:303:GLU:CB	13:G:76:LEU:HD11	2.16	0.75
20:A:827:CLA:HBB1	23:A:850:BCR:H16C	1.66	0.75
3:3:235:LEU:HD23	3:3:248:PRO:HB2	1.69	0.75
8:B:431:GLY:CA	8:B:526:LEU:CD1	2.50	0.74
1:1:79:CYS:O	1:1:83:MET:HG3	1.87	0.74
7:A:225:ASN:HB2	7:A:291:LEU:HD22	1.70	0.74
20:1:608:CLA:H3A	24:1:621:LHG:H271	1.70	0.74
2:2:234:MET:HE2	20:9:607:CLA:H3A	1.72	0.72
20:B:808:CLA:H2	15:I:88:THR:HG21	1.72	0.72
6:9:42:ASP:OD1	6:9:43:VAL:N	2.22	0.71
7:A:121:ILE:HD13	23:A:858:BCR:H332	1.72	0.71
8:B:51:HIS:HB3	20:B:814:CLA:HED3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:39:TRP:CZ3	6:9:44:ILE:HD13	2.25	0.71
20:B:834:CLA:H3A	23:J:4001:BCR:H15C	1.71	0.71
8:B:408:VAL:O	8:B:412:VAL:HG23	1.91	0.71
17:K:120:ILE:HD13	20:K:202:CLA:HMB3	1.71	0.71
3:3:235:LEU:HD22	3:3:249:PHE:HB2	1.72	0.71
20:A:823:CLA:HBB1	23:A:847:BCR:H15C	1.71	0.71
20:A:824:CLA:H51	23:A:851:BCR:H17C	1.73	0.70
20:2:608:CLA:HBB2	20:2:610:CLA:H3A	1.72	0.70
3:3:235:LEU:CD2	3:3:249:PHE:N	2.54	0.70
8:B:430:LEU:C	8:B:526:LEU:HD12	2.16	0.70
7:A:121:ILE:HD11	16:J:31:ARG:HB2	1.73	0.70
8:B:339:LEU:HD21	20:B:830:CLA:HAB	1.74	0.70
8:B:303:GLU:HB3	13:G:76:LEU:HD13	1.70	0.70
19:1:601:CHL:HMA2	28:8:301:LMG:H322	1.74	0.69
20:A:812:CLA:HAB	20:B:834:CLA:HMD2	1.74	0.69
7:A:121:ILE:CD1	16:J:31:ARG:HB2	2.22	0.69
23:B:846:BCR:H21C	23:B:846:BCR:H361	1.75	0.69
24:I:201:LHG:H331	23:L:308:BCR:HC32	1.74	0.69
19:8:304:CHL:HBC2	19:8:305:CHL:HHD	1.72	0.69
20:A:827:CLA:H12	23:A:850:BCR:H351	1.75	0.69
9:C:58:CYS:HB3	9:C:63:LEU:HD22	1.75	0.69
20:K:203:CLA:HBB1	23:K:205:BCR:H352	1.73	0.69
17:K:48:ASN:ND2	20:K:203:CLA:OBD	2.27	0.68
1:1:80:ARG:CA	1:1:83:MET:CE	2.69	0.68
2:2:231:ILE:HD13	21:2:616:LUT:H201	1.76	0.68
3:3:235:LEU:CD1	3:3:249:PHE:HB2	2.23	0.68
20:9:601:CLA:HBB2	20:B:813:CLA:H191	1.74	0.68
1:1:217:ASN:HD21	5:8:122:THR:HG23	1.58	0.68
3:3:235:LEU:CD2	3:3:248:PRO:HB2	2.22	0.68
20:A:805:CLA:C4B	20:B:804:CLA:HBB1	2.23	0.68
19:2:601:CHL:HBB2	20:2:602:CLA:HHD	1.76	0.68
2:2:231:ILE:HD11	21:2:616:LUT:H201	1.77	0.67
6:9:143:THR:CG2	6:9:144:SER:H	2.07	0.67
7:A:365:ILE:HD12	7:A:395:MET:HE3	1.75	0.67
7:A:393:HIS:HE1	20:A:831:CLA:ND	1.92	0.67
20:A:835:CLA:HBB2	18:L:109:LEU:HD13	1.75	0.67
2:2:123:GLN:O	2:2:127:ILE:HG12	1.93	0.67
1:1:141:LEU:HD12	20:1:607:CLA:HAB	1.77	0.67
2:2:231:ILE:HD11	21:2:616:LUT:C20	2.25	0.67
20:A:827:CLA:HBB2	24:A:853:LHG:H242	1.76	0.67
29:A:802:DGD:HBH2	23:A:848:BCR:H17C	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:45:MET:HE1	2:2:65:GLY:HA3	1.75	0.67
7:A:225:ASN:CB	7:A:291:LEU:HD22	2.25	0.67
3:3:235:LEU:HD22	3:3:249:PHE:CA	2.25	0.66
1:1:105:LEU:HD21	19:1:606:CHL:HED2	1.75	0.66
7:A:460:ASP:OD2	20:A:805:CLA:C4	2.43	0.66
5:8:169:PRO:HD3	19:8:306:CHL:HMD2	1.77	0.66
3:3:235:LEU:HD13	3:3:249:PHE:CB	2.26	0.66
2:2:90:ARG:NH1	2:2:172:GLU:OE2	2.29	0.65
20:7:303:CLA:HBC1	24:7:320:LHG:H281	1.77	0.65
1:1:42:GLU:H	28:8:301:LMG:HC3	1.61	0.65
20:2:613:CLA:HBA1	25:H:202:PTY:H131	1.79	0.65
8:B:137:TYR:HB3	15:I:73:PRO:HB2	1.78	0.65
5:8:135:GLU:HG2	5:8:138:ARG:HH21	1.60	0.65
20:B:813:CLA:HBB1	20:B:813:CLA:H111	1.78	0.65
2:2:231:ILE:CD1	21:2:616:LUT:C20	2.74	0.64
6:9:62:LEU:HD11	20:B:813:CLA:H122	1.79	0.64
23:A:852:BCR:H291	23:F:5004:BCR:H17C	1.79	0.64
7:A:448:LEU:HB3	7:A:541:PHE:HB2	1.77	0.64
3:3:262:MET:HG3	3:3:266:LYS:HE3	1.77	0.64
5:8:64:GLN:HG2	20:F:5008:CLA:HAA1	1.80	0.64
20:A:804:CLA:HBB1	20:A:844:CLA:C4B	2.27	0.64
4:7:231:LEU:HD13	20:7:313:CLA:H102	1.79	0.64
7:A:456:TYR:CE2	7:A:538:ILE:HD11	2.33	0.64
1:1:80:ARG:CA	1:1:83:MET:HE3	2.16	0.64
29:7:321:DGD:HB32	29:7:321:DGD:HA31	1.80	0.64
20:7:303:CLA:H72	22:7:317:XAT:H10	1.80	0.63
6:9:143:THR:CG2	6:9:144:SER:N	2.61	0.63
20:B:808:CLA:HHB	20:B:809:CLA:HMB3	1.80	0.63
1:1:57:ASP:HB2	20:1:602:CLA:HBA2	1.81	0.63
4:7:120:ILE:HG12	4:7:136:TRP:HB2	1.79	0.63
2:2:55:HIS:HE1	2:2:70:ARG:HG2	1.63	0.63
7:A:601:ASN:HD21	32:A:803:CL0:H68	1.64	0.63
20:L:302:CLA:H121	20:L:305:CLA:HBB1	1.81	0.63
7:A:218:ILE:HA	7:A:222:LEU:HD12	1.81	0.63
3:3:289:ILE:HG23	3:3:290:THR:HG23	1.81	0.62
3:3:176:ASP:HB2	3:3:179:ARG:HG3	1.80	0.62
5:8:57:LEU:HA	12:F:203:GLN:HG2	1.82	0.62
7:A:456:TYR:CD2	7:A:538:ILE:HD11	2.35	0.62
2:2:130:ILE:HG23	20:2:607:CLA:HBB2	1.80	0.62
19:8:304:CHL:HMB2	23:8:316:BCR:H373	1.82	0.62
17:K:63:ARG:NH1	17:K:90:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:824:CLA:H71	23:A:851:BCR:H19C	1.80	0.62
4:7:93:SER:HB2	4:7:99:ARG:HA	1.82	0.62
7:A:661:TYR:OH	8:B:442:ASP:OD1	2.12	0.62
20:B:807:CLA:H91	29:B:850:DGD:HBN1	1.82	0.61
8:B:102:VAL:HG13	8:B:113:PRO:HG3	1.81	0.61
9:C:55:GLU:HB3	9:C:63:LEU:HD13	1.82	0.61
3:3:258:THR:OG1	3:3:261:GLU:HG3	2.00	0.61
19:1:606:CHL:HBB2	20:1:608:CLA:HBC1	1.83	0.61
2:2:71:LEU:O	2:2:77:ARG:NH1	2.34	0.61
7:A:441:LEU:HG	7:A:548:LEU:HB2	1.82	0.61
3:3:286:GLN:HE21	20:3:411:CLA:C4D	1.88	0.61
12:F:203:GLN:HG3	24:F:5002:LHG:H102	1.81	0.60
1:1:90:LEU:HD11	21:1:615:LUT:H10	1.83	0.60
19:9:606:CHL:HED1	31:9:616:LMU:H6D	1.82	0.60
20:A:812:CLA:HBB1	23:J:4003:BCR:HC8	1.83	0.60
19:1:601:CHL:HMD2	23:8:316:BCR:H313	1.82	0.60
17:K:71:ARG:HD2	17:K:93:GLY:HA3	1.83	0.60
7:A:121:ILE:HG23	7:A:122:VAL:N	2.16	0.60
8:B:370:ALA:HB1	8:B:726:LEU:HD11	1.83	0.60
5:8:56:PRO:HB2	24:F:5002:LHG:H112	1.83	0.60
14:H:114:ILE:HG23	14:H:115:THR:HG23	1.84	0.60
20:A:825:CLA:CGD	17:K:74:ALA:HB3	2.32	0.60
5:8:240:SER:OG	20:8:311:CLA:HMD3	2.01	0.60
19:7:302:CHL:H72	24:7:320:LHG:H161	1.82	0.60
19:8:304:CHL:HBA1	23:8:316:BCR:H19C	1.83	0.60
6:9:130:LEU:HD13	22:9:615:XAT:H382	1.83	0.60
7:A:561:ARG:HH12	10:D:81:GLY:H	1.50	0.60
20:3:406:CLA:H42	21:3:415:LUT:H27	1.82	0.60
3:3:235:LEU:CD2	3:3:249:PHE:HB2	2.32	0.59
3:3:235:LEU:CD2	3:3:248:PRO:C	2.75	0.59
2:2:61:LEU:HD21	2:2:169:GLU:HB2	1.85	0.59
1:1:87:ALA:HB2	21:1:615:LUT:H34	1.85	0.59
20:2:603:CLA:H8	26:2:619:SQD:H171	1.85	0.59
10:D:94:THR:HG1	10:D:129:CYS:HG	1.49	0.59
2:2:113:ALA:HA	2:2:116:GLN:HG2	1.83	0.59
8:B:524:ILE:HG12	8:B:591:VAL:HG12	1.84	0.59
1:1:43:PRO:HA	1:1:55:ASN:HD21	1.68	0.59
8:B:178:HIS:CE1	20:B:813:CLA:NA	2.71	0.59
17:K:63:ARG:NH2	17:K:91:PRO:HG2	2.18	0.59
18:L:52:ILE:HG13	18:L:62:GLU:HB2	1.85	0.59
21:2:616:LUT:H24	8:B:155:TRP:CG	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:330:LYS:HG2	7:A:337:GLY:H	1.68	0.59
7:A:396:TRP:CD1	20:A:831:CLA:HAB	2.37	0.58
7:A:542:THR:HG21	7:A:602:SER:HA	1.85	0.58
20:A:836:CLA:HBA1	23:A:851:BCR:H332	1.86	0.58
13:G:64:ARG:NH2	13:G:105:GLY:O	2.37	0.58
1:1:80:ARG:HA	1:1:83:MET:HE2	1.82	0.58
7:A:338:HIS:HA	7:A:341:LEU:HD12	1.84	0.58
22:9:615:XAT:H171	22:9:615:XAT:H193	1.85	0.58
6:9:195:LEU:HB2	21:9:613:LUT:H21	1.84	0.58
20:B:826:CLA:HMA1	23:B:848:BCR:H14C	1.83	0.58
4:7:168:LYS:HA	20:7:324:CLA:HED3	1.86	0.58
20:7:313:CLA:HAB	20:7:313:CLA:H121	1.85	0.58
6:9:90:THR:HG21	21:9:613:LUT:H401	1.85	0.58
20:B:843:CLA:H71	20:B:843:CLA:HBB1	1.85	0.58
17:K:85:LEU:HD23	17:K:86:GLN:H	1.68	0.58
7:A:204:GLY:HA3	20:A:816:CLA:HBB1	1.85	0.58
8:B:530:THR:HG21	8:B:583:TRP:CE2	2.39	0.58
14:H:78:THR:HG21	18:L:88:ASN:HB2	1.86	0.58
20:2:603:CLA:HBC1	19:2:606:CHL:HAB	1.86	0.58
21:2:616:LUT:H361	27:2:620:3PH:H332	1.86	0.58
2:2:140:ARG:HA	2:2:156:PHE:HZ	1.69	0.57
14:H:101:LEU:HD12	29:L:311:DGD:HAG2	1.86	0.57
1:1:84:LEU:HB3	20:1:604:CLA:HAB	1.87	0.57
3:3:235:LEU:HA	3:3:248:PRO:HD2	1.85	0.57
5:8:198:ARG:HA	5:8:201:MET:HE2	1.86	0.57
20:1:610:CLA:NA	24:1:618:LHG:O5	2.37	0.57
20:2:604:CLA:HAB	21:2:617:LUT:H403	1.87	0.57
7:A:353:LEU:HD11	20:A:833:CLA:HBB1	1.87	0.57
9:C:58:CYS:HB3	9:C:63:LEU:CD2	2.34	0.57
2:2:161:MET:N	2:2:161:MET:SD	2.78	0.57
20:B:827:CLA:HBB1	20:B:835:CLA:HMA2	1.85	0.57
7:A:121:ILE:HG23	7:A:122:VAL:H	1.69	0.57
8:B:713:HIS:HE1	20:B:841:CLA:ND	2.02	0.57
23:3:418:BCR:H363	23:A:849:BCR:H313	1.87	0.57
8:B:525:ALA:HB2	20:B:838:CLA:HMA1	1.85	0.57
7:A:84:ILE:HG21	20:A:808:CLA:H61	1.87	0.57
1:1:86:ALA:HB3	21:1:615:LUT:H202	1.87	0.57
4:7:115:LEU:HD13	20:7:305:CLA:HBB2	1.87	0.57
6:9:208:THR:HA	24:9:619:LHG:H261	1.87	0.56
1:1:137:VAL:HG12	13:G:58:VAL:HG21	1.86	0.56
7:A:267:LEU:HD21	17:K:51:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:76:GLU:OE2	6:9:134:ARG:NH2	2.38	0.56
6:9:207:ILE:O	6:9:211:LEU:HB2	2.04	0.56
8:B:90:HIS:CD2	20:B:809:CLA:NA	2.72	0.56
20:B:820:CLA:HBC2	20:B:825:CLA:H172	1.86	0.56
20:B:840:CLA:HAB	33:B:844:PQN:H141	1.86	0.56
10:D:93:VAL:HG22	10:D:122:LYS:HG2	1.88	0.56
12:F:100:GLU:HG2	12:F:103:SER:HB2	1.87	0.56
6:9:106:GLU:HA	19:9:606:CHL:HED3	1.87	0.56
5:8:143:ARG:NH2	28:8:301:LMG:O3	2.38	0.56
5:8:202:VAL:HG21	24:8:319:LHG:H272	1.87	0.56
7:A:151:SER:HB3	7:A:213:TRP:HH2	1.71	0.56
7:A:201:HIS:HE1	20:A:816:CLA:NC	2.02	0.56
7:A:473:SER:HB2	7:A:640:ASN:HD22	1.71	0.56
2:2:110:TRP:CD1	2:2:110:TRP:H	2.23	0.56
6:9:80:MET:HE3	22:9:615:XAT:H372	1.87	0.56
29:A:802:DGD:HBW1	23:A:849:BCR:HC21	1.88	0.56
10:D:96:TRP:HB3	10:D:144:PRO:HB3	1.87	0.56
3:3:195:ASP:OD1	3:3:196:PRO:HD2	2.06	0.56
23:3:418:BCR:H19C	20:A:818:CLA:H101	1.87	0.56
3:3:235:LEU:HD23	3:3:248:PRO:CB	2.35	0.56
4:7:264:ALA:HA	4:7:270:ILE:HG13	1.88	0.56
20:A:808:CLA:H143	23:A:848:BCR:H332	1.88	0.56
8:B:431:GLY:N	8:B:526:LEU:CD1	2.69	0.56
7:A:399:GLY:HA3	7:A:603:LEU:HD11	1.88	0.56
4:7:151:LEU:HB3	5:8:248:GLU:HG2	1.88	0.55
20:A:808:CLA:H72	23:A:849:BCR:H373	1.89	0.55
19:7:306:CHL:HBB2	19:7:307:CHL:HHC	1.88	0.55
19:7:307:CHL:H12	29:7:321:DGD:HE5	1.87	0.55
8:B:303:GLU:CB	13:G:76:LEU:CD1	2.74	0.55
15:I:99:TRP:CE2	24:I:201:LHG:H282	2.40	0.55
2:2:146:LYS:HG3	2:2:147:THR:HG23	1.88	0.55
19:3:401:CHL:H91	20:3:407:CLA:H193	1.88	0.55
4:7:166:GLU:HA	4:7:169:ARG:HG2	1.88	0.55
20:9:602:CLA:H91	23:B:845:BCR:HC42	1.87	0.55
1:1:80:ARG:HG2	1:1:83:MET:CE	2.37	0.55
4:7:205:PRO:HD2	21:7:316:LUT:H22	1.88	0.55
20:1:605:CLA:HBA2	23:1:617:BCR:H21C	1.88	0.55
20:B:817:CLA:H11	20:G:4004:CLA:HED1	1.88	0.55
20:1:604:CLA:HMA2	20:1:605:CLA:HBC3	1.89	0.55
5:8:233:THR:HG23	5:8:235:ALA:H	1.71	0.55
6:9:44:ILE:CD1	6:9:44:ILE:O	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:828:CLA:HBC3	29:B:850:DGD:HBV1	1.88	0.55
14:H:84:ARG:HH12	25:H:201:PTY:H112	1.71	0.55
3:3:196:PRO:HA	3:3:199:LEU:HD12	1.89	0.55
14:H:101:LEU:CD1	29:L:311:DGD:HAG2	2.37	0.55
1:1:158:PHE:HD1	20:1:607:CLA:H2	1.72	0.55
8:B:18:SER:HB2	8:B:699:VAL:CG2	2.37	0.55
18:L:138:LEU:HD13	23:L:308:BCR:H24C	1.89	0.55
20:1:603:CLA:HED1	23:B:847:BCR:H313	1.88	0.55
20:A:811:CLA:H11	23:J:4003:BCR:H383	1.89	0.55
5:8:48:MET:HE1	5:8:70:GLN:HB2	1.88	0.54
7:A:341:LEU:HD11	20:A:827:CLA:HBC3	1.89	0.54
8:B:345:ILE:HG12	20:B:819:CLA:H72	1.89	0.54
6:9:94:GLY:HA3	20:9:604:CLA:HBC3	1.89	0.54
17:K:120:ILE:HD13	20:K:202:CLA:CMB	2.35	0.54
18:L:112:LEU:HD12	18:L:122:VAL:HG21	1.89	0.54
2:2:47:TYR:OH	2:2:240:LYS:NZ	2.41	0.54
8:B:18:SER:HB2	8:B:699:VAL:HG21	1.88	0.54
8:B:32:PHE:HB3	8:B:38:MET:HE3	1.89	0.54
23:A:858:BCR:H11C	20:J:4002:CLA:HMC2	1.89	0.54
8:B:669:ARG:NH1	8:B:700:ALA:O	2.41	0.54
20:3:407:CLA:H203	23:A:849:BCR:H321	1.89	0.54
7:A:296:HIS:HE1	20:A:820:CLA:ND	2.04	0.54
12:F:164:VAL:HG13	20:F:5006:CLA:HAA1	1.89	0.54
17:K:71:ARG:HD2	17:K:93:GLY:CA	2.38	0.54
23:3:418:BCR:H401	23:A:847:BCR:H312	1.89	0.54
20:A:813:CLA:HBB1	20:A:816:CLA:H142	1.88	0.54
20:A:822:CLA:H92	20:A:832:CLA:H91	1.90	0.54
8:B:151:LEU:HD23	23:B:849:BCR:H332	1.90	0.54
8:B:561:ASP:OD1	9:C:52:LYS:NZ	2.40	0.54
8:B:606:ASN:ND2	8:B:609:GLN:OE1	2.41	0.54
20:B:831:CLA:HMC3	20:B:839:CLA:HBB1	1.90	0.54
8:B:320:HIS:CD2	20:B:824:CLA:ND	2.75	0.54
13:G:84:THR:OG1	13:G:87:ASP:OD1	2.25	0.54
17:K:92:ALA:O	17:K:93:GLY:C	2.50	0.54
3:3:147:ALA:HB1	3:3:273:GLY:HA3	1.89	0.54
6:9:81:ASN:HB3	6:9:174:MET:HE2	1.89	0.54
7:A:407:ALA:HB2	7:A:592:VAL:HG11	1.90	0.54
20:A:825:CLA:HED1	17:K:73:VAL:HA	1.90	0.54
2:2:232:LEU:HD21	27:2:620:3PH:H242	1.89	0.54
3:3:132:GLY:O	26:3:421:SQD:O3	2.25	0.54
7:A:44:ASN:OD1	7:A:714:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:71:LEU:HD13	26:2:619:SQD:H162	1.90	0.54
4:7:204:ASP:OD1	21:7:316:LUT:O3	2.25	0.54
7:A:542:THR:HG21	7:A:602:SER:CA	2.38	0.54
13:G:56:ARG:NH1	13:G:102:ASP:OD2	2.40	0.54
3:3:263:LYS:HA	3:3:266:LYS:HD2	1.90	0.53
20:A:805:CLA:C4B	20:B:804:CLA:CBB	2.82	0.53
17:K:63:ARG:NH1	17:K:92:ALA:HB3	2.22	0.53
5:8:144:LYS:HB2	5:8:147:SER:HB3	1.90	0.53
8:B:92:ILE:HB	8:B:113:PRO:HB2	1.88	0.53
13:G:48:THR:HA	13:G:118:GLY:HA3	1.90	0.53
1:1:80:ARG:HG2	1:1:83:MET:HE1	1.91	0.53
26:3:421:SQD:H291	26:3:423:SQD:H81	1.90	0.53
8:B:106:THR:HG21	14:H:118:PRO:HG3	1.89	0.53
8:B:303:GLU:CD	13:G:76:LEU:CD2	2.81	0.53
10:D:148:ARG:HB2	10:D:158:LEU:HD11	1.89	0.53
8:B:340:ALA:HB2	23:B:848:BCR:H372	1.91	0.53
16:J:39:PHE:HA	23:J:4001:BCR:H341	1.90	0.53
18:L:93:GLU:HG3	20:L:304:CLA:HMA3	1.90	0.53
18:L:98:HIS:HE1	20:L:305:CLA:ND	2.06	0.53
2:2:45:MET:CE	2:2:65:GLY:HA3	2.37	0.53
2:2:95:ALA:HB1	21:2:615:LUT:H361	1.90	0.53
7:A:538:ILE:HG21	32:A:803:CL0:H60	1.90	0.53
6:9:40:LEU:HB2	6:9:41:PRO:HD2	1.91	0.53
7:A:45:THR:HB	7:A:716:ARG:HG3	1.91	0.53
8:B:27:ALA:HB1	29:B:850:DGD:HB21	1.89	0.53
8:B:431:GLY:N	8:B:526:LEU:HD12	2.23	0.53
8:B:712:ALA:O	8:B:716:VAL:HG12	2.09	0.53
7:A:515:VAL:HG23	7:A:522:ALA:HB3	1.91	0.53
24:2:621:LHG:HC91	15:I:76:PRO:HB3	1.91	0.53
20:A:817:CLA:HBA1	23:A:848:BCR:HC7	1.90	0.53
20:A:835:CLA:H51	23:B:802:BCR:H372	1.91	0.53
8:B:444:VAL:CG1	8:B:452:LYS:HB2	2.38	0.53
2:2:251:LEU:HD11	24:I:201:LHG:HC91	1.91	0.53
7:A:578:PRO:HA	7:A:582:GLY:HA2	1.91	0.53
32:A:803:CL0:H2	20:B:803:CLA:NC	2.24	0.53
20:B:811:CLA:H112	18:L:125:MET:HB2	1.90	0.53
4:7:110:ALA:O	4:7:114:MET:HG3	2.09	0.53
19:1:601:CHL:H41	20:1:613:CLA:H72	1.90	0.52
3:3:144:VAL:HG21	3:3:243:ALA:HB1	1.91	0.52
8:B:663:MET:HE1	20:B:804:CLA:C4D	2.38	0.52
19:9:606:CHL:HMB2	31:9:616:LMU:H91	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:670:LEU:HD22	8:B:443:VAL:HG12	1.91	0.52
20:A:809:CLA:HED3	20:A:833:CLA:H61	1.91	0.52
20:A:832:CLA:H12	23:A:849:BCR:H24C	1.90	0.52
2:2:68:PRO:HB3	27:2:620:3PH:H241	1.90	0.52
5:8:77:SER:HB2	5:8:197:GLY:HA3	1.92	0.52
18:L:107:ILE:HG12	18:L:120:GLU:HA	1.91	0.52
20:A:817:CLA:H72	20:A:819:CLA:HBB1	1.91	0.52
24:7:325:LHG:H381	28:F:5001:LMG:H292	1.91	0.52
5:8:191:LEU:HD11	5:8:195:LYS:HE3	1.90	0.52
8:B:671:TYR:OH	20:B:804:CLA:OBD	2.27	0.52
13:G:88:ARG:HA	13:G:91:LYS:HD2	1.91	0.52
8:B:123:GLN:O	8:B:127:THR:OG1	2.27	0.52
20:B:808:CLA:HHB	20:B:809:CLA:HHB	1.92	0.52
4:7:144:ILE:HD13	19:7:307:CHL:HMD1	1.91	0.52
4:7:266:ASN:ND2	20:7:313:CLA:OBD	2.43	0.52
20:A:834:CLA:H51	20:L:305:CLA:H43	1.91	0.52
20:2:611:CLA:H101	24:2:618:LHG:H161	1.90	0.52
4:7:221:LYS:HD3	20:7:312:CLA:HBD	1.91	0.52
5:8:242:PRO:HB2	24:J:4004:LHG:H151	1.91	0.52
7:A:456:TYR:CE2	7:A:538:ILE:CD1	2.92	0.52
8:B:716:VAL:HA	29:B:850:DGD:HBG2	1.91	0.52
17:K:70:VAL:O	17:K:82:ARG:CZ	2.56	0.52
18:L:77:ASN:HB3	20:L:304:CLA:HAC1	1.90	0.52
23:3:418:BCR:H21C	20:A:818:CLA:H72	1.92	0.52
7:A:338:HIS:CD2	20:A:827:CLA:ND	2.78	0.52
20:A:815:CLA:HBB1	20:A:815:CLA:H112	1.92	0.52
2:2:158:PHE:N	20:2:608:CLA:OBD	2.43	0.52
20:A:844:CLA:HBC2	8:B:586:ASN:HB2	1.92	0.52
24:3:424:LHG:HC92	20:7:311:CLA:H12	1.92	0.51
1:1:150:LYS:HG3	1:1:154:PRO:HA	1.92	0.51
3:3:310:LEU:HD22	20:3:411:CLA:H2	1.91	0.51
7:A:222:LEU:HD13	7:A:275:PHE:HB2	1.91	0.51
8:B:300:HIS:CD2	20:B:822:CLA:ND	2.77	0.51
7:A:217:GLN:HA	7:A:221:SER:HB2	1.92	0.51
20:B:843:CLA:H151	23:L:303:BCR:H15C	1.93	0.51
12:F:92:LEU:HD21	12:F:112:THR:HG22	1.92	0.51
12:F:122:THR:O	12:F:126:GLN:NE2	2.39	0.51
17:K:63:ARG:HH22	17:K:91:PRO:CD	2.23	0.51
20:1:605:CLA:H3A	23:1:617:BCR:C21	2.41	0.51
7:A:219:HIS:HE1	20:A:818:CLA:ND	2.08	0.51
8:B:87:PRO:HB2	8:B:117:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:838:CLA:HAC2	23:F:5009:BCR:H322	1.91	0.51
12:F:209:LEU:HD12	20:F:5008:CLA:HBB2	1.92	0.51
17:K:67:ALA:N	17:K:78:LYS:HZ1	2.08	0.51
1:1:83:MET:HA	21:1:615:LUT:H201	1.92	0.51
20:1:602:CLA:H13	22:1:616:XAT:H193	1.90	0.51
7:A:532:ASP:OD1	7:A:613:LYS:NZ	2.42	0.51
20:A:804:CLA:HMB1	20:A:804:CLA:H42	1.92	0.51
8:B:143:LEU:HD11	23:B:846:BCR:H292	1.92	0.51
3:3:286:GLN:O	3:3:290:THR:OG1	2.25	0.51
7:A:458:HIS:O	7:A:462:MET:HG2	2.11	0.51
7:A:590:ASP:HA	7:A:593:PHE:HB3	1.92	0.51
20:A:810:CLA:H2A	20:A:812:CLA:HED1	1.92	0.51
20:A:811:CLA:H71	20:A:833:CLA:H162	1.92	0.51
8:B:342:VAL:O	8:B:346:THR:OG1	2.26	0.51
3:3:197:PHE:HZ	28:7:301:LMG:H112	1.75	0.51
3:3:244:TYR:HE2	3:3:266:LYS:HG2	1.75	0.51
7:A:445:SER:HB3	7:A:545:VAL:HG22	1.93	0.51
7:A:671:MET:HE1	23:A:852:BCR:H352	1.93	0.51
8:B:303:GLU:CG	13:G:76:LEU:HD11	2.41	0.51
14:H:105:LYS:HB2	25:H:202:PTY:H322	1.92	0.51
7:A:256:SER:OG	7:A:271:GLU:O	2.26	0.51
19:7:307:CHL:OBD	29:7:321:DGD:O2D	2.28	0.51
20:A:812:CLA:H142	20:A:812:CLA:H91	1.91	0.51
25:1:622:PTY:HC31	24:F:5011:LHG:HC5	1.92	0.51
5:8:62:GLU:OE1	5:8:65:ALA:N	2.44	0.51
8:B:659:ALA:HB1	20:B:804:CLA:HAB	1.92	0.51
6:9:134:ARG:O	6:9:150:TYR:OH	2.29	0.50
7:A:561:ARG:NH1	10:D:81:GLY:O	2.44	0.50
2:2:83:GLU:OE2	2:2:87:MET:HE3	2.11	0.50
7:A:487:ILE:HD11	20:A:838:CLA:H2	1.92	0.50
7:A:501:ASN:HB2	20:A:837:CLA:HED2	1.93	0.50
2:2:183:PHE:CD2	21:2:615:LUT:H32	2.46	0.50
2:2:251:LEU:HB2	2:2:258:TRP:HB3	1.93	0.50
7:A:488:GLN:HG2	7:A:510:TRP:HB3	1.92	0.50
7:A:513:ASP:OD1	7:A:513:ASP:N	2.45	0.50
8:B:352:HIS:ND1	20:B:818:CLA:OBD	2.43	0.50
8:B:430:LEU:HD11	20:B:838:CLA:HMB2	1.94	0.50
20:B:824:CLA:HBB1	20:B:831:CLA:H143	1.94	0.50
16:J:39:PHE:HB2	23:J:4001:BCR:H353	1.92	0.50
3:3:183:ILE:HG22	3:3:186:ALA:H	1.77	0.50
4:7:161:LEU:HB3	23:7:318:BCR:H15C	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:614:XAT:H363	20:B:813:CLA:H121	1.93	0.50
7:A:740:TRP:HB2	20:A:831:CLA:HBB1	1.94	0.50
20:A:841:CLA:H162	20:F:5005:CLA:H11	1.92	0.50
20:B:813:CLA:HBB2	20:B:821:CLA:H8	1.93	0.50
14:H:70:GLN:NE2	20:L:304:CLA:OBD	2.44	0.50
14:H:102:PHE:HA	14:H:106:GLY:HA3	1.94	0.50
7:A:684:MET:HE1	20:A:804:CLA:C4A	2.40	0.50
8:B:413:LEU:HD21	8:B:543:ARG:HD3	1.92	0.50
20:B:812:CLA:HBB2	20:B:814:CLA:HMA3	1.93	0.50
12:F:128:LEU:HG	12:F:136:PRO:HB3	1.94	0.50
17:K:71:ARG:HH12	17:K:72:LYS:CE	2.20	0.50
17:K:71:ARG:HD2	17:K:93:GLY:N	2.27	0.50
2:2:258:TRP:HB2	24:I:201:LHG:H242	1.93	0.50
7:A:20:ASN:OD1	7:A:183:LYS:NZ	2.43	0.50
18:L:155:LYS:HD2	18:L:163:LEU:HD21	1.93	0.50
20:B:834:CLA:H51	23:F:5004:BCR:H382	1.93	0.50
2:2:210:HIS:O	2:2:215:THR:OG1	2.30	0.50
5:8:126:THR:HG21	19:8:304:CHL:HED1	1.94	0.50
7:A:317:GLY:C	17:K:82:ARG:NH2	2.69	0.50
7:A:539:HIS:HE1	7:A:605:ILE:HG22	1.76	0.50
20:B:824:CLA:HAA1	23:B:847:BCR:H16C	1.93	0.50
9:C:30:PRO:HG3	10:D:171:ALA:HA	1.94	0.50
2:2:231:ILE:HD13	21:2:616:LUT:C20	2.40	0.50
3:3:135:ASN:OD1	26:3:421:SQD:O3	2.26	0.50
20:B:808:CLA:H2A	20:B:810:CLA:HED1	1.92	0.50
17:K:89:GLY:HA3	20:K:201:CLA:HBD	1.93	0.49
8:B:458:PRO:HB3	8:B:518:PHE:HB2	1.94	0.49
19:7:306:CHL:CBB	19:7:307:CHL:HHC	2.42	0.49
20:9:603:CLA:H2A	20:9:603:CLA:HED2	1.93	0.49
8:B:143:LEU:HA	8:B:146:VAL:HG12	1.94	0.49
1:1:39:PRO:HB3	5:8:153:THR:HG21	1.93	0.49
4:7:92:LEU:HD12	22:7:317:XAT:H3	1.93	0.49
5:8:232:ASN:HB3	20:8:311:CLA:HED1	1.93	0.49
23:A:850:BCR:H332	23:A:851:BCR:H271	1.95	0.49
8:B:182:GLY:CA	8:B:186:VAL:HG12	2.30	0.49
12:F:98:LYS:HG3	12:F:99:TYR:CE2	2.48	0.49
16:J:25:LEU:O	16:J:29:ILE:HD12	2.11	0.49
17:K:63:ARG:CZ	17:K:90:ASP:OD2	2.61	0.49
5:8:143:ARG:HH22	28:8:301:LMG:HC61	1.77	0.49
20:9:602:CLA:HAB	22:9:614:XAT:H32	1.93	0.49
8:B:716:VAL:HG11	20:B:841:CLA:HMA1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:80:ARG:CA	1:1:83:MET:HE2	2.42	0.49
6:9:177:PHE:CZ	22:9:614:XAT:H10	2.46	0.49
7:A:67:GLU:OE2	7:A:71:ARG:NH2	2.45	0.49
8:B:151:LEU:HG	23:B:849:BCR:H14C	1.95	0.49
20:B:840:CLA:H18	23:I:202:BCR:H353	1.93	0.49
7:A:247:GLN:NE2	7:A:257:PHE:O	2.44	0.49
8:B:229:GLY:HA3	13:G:126:LEU:HB3	1.94	0.49
8:B:440:HIS:HE1	20:B:834:CLA:NA	2.03	0.49
20:B:824:CLA:HBB2	20:B:842:CLA:H71	1.94	0.49
20:1:611:CLA:C2B	21:1:615:LUT:H14	2.42	0.49
3:3:135:ASN:ND2	26:3:421:SQD:O4	2.40	0.49
7:A:200:HIS:HE1	20:A:815:CLA:NA	2.04	0.49
7:A:203:ALA:HB2	7:A:309:GLY:HA3	1.95	0.49
7:A:719:SER:HB3	7:A:722:GLN:HB2	1.95	0.49
8:B:177:ASN:ND2	8:B:292:TYR:O	2.42	0.49
23:L:303:BCR:HC21	20:L:305:CLA:H51	1.94	0.49
5:8:28:SER:OG	5:8:29:MET:N	2.46	0.49
20:8:303:CLA:O1A	19:8:304:CHL:HMD2	2.13	0.49
7:A:598:TRP:CH2	20:A:805:CLA:HAB	2.47	0.49
7:A:615:GLN:OE1	7:A:653:GLN:NE2	2.46	0.49
7:A:740:TRP:NE1	20:A:831:CLA:O1A	2.46	0.49
20:A:804:CLA:HMD3	8:B:534:ILE:HD12	1.94	0.49
20:A:835:CLA:H92	23:B:802:BCR:H362	1.94	0.49
8:B:74:ASN:ND2	8:B:86:ARG:O	2.44	0.49
24:8:321:LHG:H241	24:8:321:LHG:H102	1.95	0.48
7:A:479:LEU:H	7:A:530:THR:HG23	1.77	0.48
23:B:802:BCR:H383	20:B:843:CLA:HHD	1.95	0.48
20:B:832:CLA:H51	12:F:215:LEU:HD22	1.95	0.48
25:H:201:PTY:H361	25:H:201:PTY:H152	1.95	0.48
7:A:375:PRO:HG2	7:A:381:ALA:HB2	1.95	0.48
20:B:819:CLA:H8	20:B:819:CLA:HAB	1.95	0.48
17:K:85:LEU:HD22	17:K:95:THR:HG21	1.94	0.48
3:3:139:LEU:HD13	19:3:401:CHL:HBA2	1.93	0.48
4:7:262:THR:OG1	4:7:263:PHE:N	2.46	0.48
7:A:306:LEU:HG	23:A:847:BCR:H12C	1.95	0.48
9:C:52:LYS:HD3	9:C:67:VAL:HB	1.95	0.48
1:1:164:SER:HB3	20:1:609:CLA:HAA1	1.96	0.48
5:8:83:GLY:O	5:8:87:ILE:HG12	2.13	0.48
7:A:216:HIS:O	7:A:220:VAL:HB	2.14	0.48
23:A:847:BCR:HC8	23:A:848:BCR:H383	1.94	0.48
8:B:702:SER:O	8:B:706:ALA:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:832:CLA:H93	12:F:212:ILE:HD11	1.95	0.48
20:J:4002:CLA:H2	20:J:4002:CLA:H3A	1.96	0.48
28:F:5001:LMG:H132	16:J:8:LEU:HD13	1.95	0.48
3:3:285:ALA:HA	20:A:818:CLA:H62	1.95	0.48
20:A:822:CLA:HAB	20:A:822:CLA:H8	1.94	0.48
8:B:211:ASP:OD1	8:B:211:ASP:N	2.41	0.48
8:B:352:HIS:CD2	20:B:827:CLA:NC	2.81	0.48
8:B:359:TYR:OH	20:B:829:CLA:OBD	2.29	0.48
16:J:23:SER:O	16:J:27:ILE:HG12	2.13	0.48
20:1:612:CLA:HBA1	20:1:612:CLA:H12	1.56	0.48
7:A:658:ILE:HD12	8:B:622:ARG:HG3	1.94	0.48
8:B:303:GLU:CD	13:G:76:LEU:HD22	2.38	0.48
20:B:811:CLA:HAB	15:I:89:GLY:HA3	1.96	0.48
1:1:120:VAL:HG12	1:1:122:PHE:H	1.79	0.48
6:9:139:ARG:HH12	26:9:618:SQD:H61	1.79	0.48
6:9:179:GLY:O	6:9:183:GLN:NE2	2.44	0.48
7:A:269:TRP:O	20:A:820:CLA:H3A	2.14	0.48
7:A:363:LEU:HD11	20:A:822:CLA:H93	1.96	0.48
20:A:821:CLA:H111	20:A:837:CLA:HBA1	1.94	0.48
33:A:845:PQN:H141	20:F:5005:CLA:HBB2	1.95	0.48
10:D:73:PRO:HB3	10:D:114:MET:HA	1.94	0.48
3:3:117:LEU:HD13	20:A:815:CLA:H2	1.96	0.48
3:3:153:GLY:HA2	22:3:416:XAT:H181	1.96	0.48
4:7:209:SER:HB3	20:7:310:CLA:HAA2	1.94	0.48
20:7:324:CLA:HBA1	20:7:324:CLA:H3A	1.57	0.48
6:9:81:ASN:CB	6:9:174:MET:HE2	2.43	0.48
6:9:147:ILE:O	6:9:149:SER:N	2.47	0.48
7:A:558:ARG:NH2	10:D:105:GLU:OE1	2.45	0.48
10:D:94:THR:HG23	10:D:146:PHE:HB3	1.95	0.48
5:8:125:MET:HE3	5:8:125:MET:HA	1.95	0.48
6:9:74:TYR:CG	20:9:602:CLA:H11	2.49	0.48
8:B:697:LYS:NZ	9:C:74:THR:OG1	2.46	0.48
20:B:807:CLA:H71	20:B:807:CLA:H193	1.95	0.48
17:K:58:CYS:HB3	17:K:102:MET:HE2	1.94	0.48
1:1:54:TYR:HE2	19:1:601:CHL:HBC2	1.79	0.47
20:1:610:CLA:HAB	5:8:155:PHE:HE1	1.79	0.47
20:2:603:CLA:HED1	14:H:93:LEU:HD11	1.87	0.47
6:9:53:LEU:HD23	20:9:602:CLA:HED3	1.96	0.47
20:A:830:CLA:H112	20:A:830:CLA:H72	1.58	0.47
8:B:23:TRP:CG	8:B:705:GLN:HE22	2.32	0.47
20:B:809:CLA:H112	20:B:828:CLA:H122	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:619:SQD:H132	25:H:201:PTY:H342	1.96	0.47
3:3:216:GLN:HG3	19:7:302:CHL:HED1	1.96	0.47
4:7:90:LEU:HD22	22:7:317:XAT:H172	1.95	0.47
5:8:57:LEU:HD22	12:F:203:GLN:HA	1.94	0.47
20:9:602:CLA:H62	20:9:602:CLA:H41	1.58	0.47
12:F:211:SER:HB2	23:F:5009:BCR:H391	1.95	0.47
13:G:100:SER:HB2	20:G:4003:CLA:HBA1	1.96	0.47
13:G:117:LEU:HG	23:G:4001:BCR:H371	1.96	0.47
17:K:74:ALA:HA	17:K:78:LYS:HA	1.94	0.47
17:K:116:GLY:O	17:K:120:ILE:HG12	2.13	0.47
19:7:302:CHL:H51	20:7:313:CLA:H71	1.95	0.47
14:H:99:ILE:HG23	15:I:86:PRO:HB2	1.96	0.47
16:J:13:VAL:HG13	16:J:14:VAL:HG13	1.97	0.47
29:L:311:DGD:O5D	29:L:311:DGD:O4D	2.28	0.47
32:A:803:CL0:H66	20:A:805:CLA:C2B	2.43	0.47
20:B:824:CLA:HAB	20:B:831:CLA:HMD1	1.96	0.47
7:A:729:ALA:HA	24:A:854:LHG:H352	1.96	0.47
8:B:21:ARG:NH2	8:B:696:ASP:OD1	2.46	0.47
8:B:24:TYR:O	8:B:28:THR:OG1	2.30	0.47
8:B:49:ALA:HB1	23:B:849:BCR:H312	1.96	0.47
23:B:802:BCR:H21C	20:B:841:CLA:HAC2	1.96	0.47
18:L:63:THR:O	18:L:67:SER:N	2.41	0.47
19:1:606:CHL:HBA1	19:1:606:CHL:H3A	1.65	0.47
19:2:601:CHL:HBB2	20:2:602:CLA:HAC2	1.96	0.47
20:A:813:CLA:H72	20:A:816:CLA:H18	1.96	0.47
8:B:175:ARG:HB2	20:B:814:CLA:HBC2	1.96	0.47
24:1:619:LHG:HC62	24:1:619:LHG:H241	1.55	0.47
2:2:246:GLN:OE1	2:2:246:GLN:N	2.45	0.47
3:3:185:PRO:HG2	20:3:405:CLA:HAB	1.97	0.47
20:3:406:CLA:HHB	23:3:419:BCR:H342	1.97	0.47
20:3:407:CLA:H2A	20:3:407:CLA:HED2	1.96	0.47
4:7:166:GLU:OE2	4:7:169:ARG:NH2	2.41	0.47
6:9:112:TYR:CE2	20:9:605:CLA:HAC1	2.50	0.47
20:A:820:CLA:CHD	20:A:821:CLA:HBB2	2.44	0.47
8:B:601:THR:HG21	8:B:610:PHE:HB2	1.96	0.47
23:B:802:BCR:H271	33:B:844:PQN:H142	1.96	0.47
20:B:803:CLA:H122	20:B:803:CLA:H162	1.54	0.47
20:B:804:CLA:HED2	20:B:804:CLA:HBD	1.74	0.47
17:K:47:THR:OG1	17:K:114:VAL:HG21	2.15	0.47
17:K:73:VAL:HB	17:K:82:ARG:HD3	1.96	0.47
18:L:138:LEU:HD23	18:L:178:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:188:VAL:HG13	3:3:190:LYS:CE	2.45	0.47
7:A:599:MET:HE3	7:A:599:MET:HB3	1.84	0.47
23:A:849:BCR:C25	23:A:849:BCR:H371	2.44	0.47
8:B:62:THR:HG23	8:B:143:LEU:HD13	1.97	0.47
8:B:70:ALA:HB2	8:B:136:LEU:HB2	1.96	0.47
20:B:806:CLA:HBA1	20:B:806:CLA:H3A	1.48	0.47
20:B:809:CLA:H71	20:B:809:CLA:HBB1	1.97	0.47
12:F:69:ILE:HD11	12:F:139:ILE:HG13	1.97	0.47
12:F:188:LYS:HA	12:F:188:LYS:HD3	1.78	0.47
3:3:193:TRP:NE1	20:3:404:CLA:OBD	2.44	0.47
24:7:323:LHG:HC5	24:7:323:LHG:HC82	1.51	0.47
7:A:426:LEU:HB3	20:A:827:CLA:HMC2	1.96	0.47
8:B:83:ILE:O	14:H:132:ARG:NH1	2.48	0.47
8:B:346:THR:HB	8:B:380:ALA:HB2	1.96	0.47
28:7:319:LMG:H292	28:7:319:LMG:HC92	1.49	0.47
20:9:611:CLA:HBB	20:9:612:CLA:HBC3	1.97	0.47
7:A:479:LEU:HD13	7:A:533:PHE:CE2	2.49	0.47
7:A:670:LEU:HD12	20:A:812:CLA:HAC1	1.95	0.47
28:A:801:LMG:H112	28:A:801:LMG:HC8	1.42	0.47
32:A:803:CL0:H51	32:A:803:CL0:H58	1.65	0.47
20:A:812:CLA:H13	23:J:4003:BCR:H391	1.96	0.47
20:A:825:CLA:H2A	17:K:74:ALA:HB3	1.96	0.47
20:B:818:CLA:HBC2	20:B:819:CLA:H203	1.97	0.47
20:B:823:CLA:HAA1	13:G:66:ARG:HH22	1.79	0.47
17:K:71:ARG:NH1	17:K:72:LYS:CE	2.55	0.47
4:7:100:LYS:HA	4:7:196:ASN:HD21	1.80	0.46
6:9:207:ILE:CD1	6:9:211:LEU:HD23	2.45	0.46
20:A:835:CLA:H61	20:B:840:CLA:H52	1.98	0.46
20:B:829:CLA:H3A	20:B:829:CLA:HBA2	1.55	0.46
14:H:97:ALA:O	14:H:101:LEU:HG	2.14	0.46
2:2:83:GLU:O	2:2:87:MET:HG2	2.16	0.46
7:A:365:ILE:HG23	7:A:395:MET:HE1	1.96	0.46
20:A:816:CLA:HAA2	20:A:828:CLA:H51	1.97	0.46
8:B:423:LEU:HD13	8:B:533:LEU:HA	1.96	0.46
20:1:603:CLA:H102	23:B:847:BCR:H311	1.98	0.46
24:1:621:LHG:HC5	24:1:621:LHG:HC82	1.43	0.46
7:A:542:THR:CG2	7:A:602:SER:CB	2.91	0.46
8:B:293:ARG:HA	8:B:299:GLY:HA3	1.98	0.46
20:K:202:CLA:HBA1	20:K:202:CLA:H3A	1.78	0.46
1:1:128:LEU:O	1:1:132:VAL:HG23	2.16	0.46
1:1:223:VAL:HG13	1:1:223:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:77:ARG:NE	14:H:85:GLU:OE2	2.47	0.46
24:2:621:LHG:H251	23:B:849:BCR:H391	1.97	0.46
7:A:393:HIS:HE1	20:A:831:CLA:C1D	2.28	0.46
20:A:836:CLA:ND	23:A:851:BCR:HC31	2.31	0.46
2:2:126:LEU:O	2:2:130:ILE:HG12	2.16	0.46
20:2:603:CLA:HBC3	24:H:203:LHG:H161	1.97	0.46
5:8:240:SER:OG	20:8:311:CLA:CMD	2.62	0.46
7:A:316:TRP:HB3	17:K:97:THR:HG21	1.98	0.46
20:A:817:CLA:H11	23:A:848:BCR:H311	1.98	0.46
20:A:821:CLA:H18	20:A:837:CLA:H12	1.97	0.46
20:A:829:CLA:CAD	20:A:838:CLA:HBB1	2.44	0.46
14:H:81:VAL:HG13	18:L:179:ALA:HB1	1.97	0.46
1:1:198:THR:O	1:1:198:THR:HG23	2.14	0.46
20:A:806:CLA:H142	20:A:806:CLA:H112	1.82	0.46
20:A:827:CLA:HED3	20:A:827:CLA:H2A	1.97	0.46
20:B:807:CLA:H2	20:B:807:CLA:H62	1.67	0.46
20:B:834:CLA:H41	20:B:834:CLA:H62	1.67	0.46
17:K:107:HIS:HB3	23:K:205:BCR:H321	1.97	0.46
29:L:311:DGD:HA22	29:L:311:DGD:HG11	1.44	0.46
2:2:227:ALA:HB1	21:2:616:LUT:H203	1.98	0.46
5:8:79:THR:HG23	22:8:315:XAT:H202	1.98	0.46
24:A:853:LHG:H102	24:A:853:LHG:H252	1.98	0.46
12:F:213:GLN:O	12:F:217:ASN:ND2	2.49	0.46
5:8:201:MET:HE3	20:8:302:CLA:HMC3	1.98	0.46
20:A:841:CLA:H61	23:F:5004:BCR:H14C	1.98	0.46
8:B:425:TRP:CE2	20:B:832:CLA:HAB	2.50	0.46
8:B:703:ILE:H	8:B:703:ILE:HG13	1.62	0.46
20:B:817:CLA:HBA2	20:B:817:CLA:H3A	1.49	0.46
20:1:609:CLA:H141	20:1:609:CLA:H162	1.78	0.46
25:1:622:PTY:HC12	25:1:623:PTY:H112	1.98	0.46
20:3:407:CLA:H192	23:A:849:BCR:H311	1.98	0.46
6:9:198:HIS:CD2	20:9:612:CLA:NC	2.83	0.46
2:2:158:PHE:HB3	20:2:608:CLA:HMD3	1.98	0.46
5:8:52:PHE:HB2	20:8:302:CLA:HMD1	1.98	0.46
6:9:61:PRO:HG3	20:B:813:CLA:H193	1.97	0.46
20:A:809:CLA:H102	20:A:809:CLA:H172	1.98	0.46
20:A:841:CLA:HBB2	12:F:172:GLY:HA3	1.98	0.46
20:B:820:CLA:H193	20:B:825:CLA:H122	1.98	0.46
23:J:4001:BCR:H351	23:J:4001:BCR:H16C	1.98	0.46
5:8:39:THR:O	5:8:44:LYS:NZ	2.49	0.45
5:8:139:TRP:HZ2	20:F:5008:CLA:HHD	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:580:ARG:NH2	10:D:127:GLU:OE2	2.40	0.45
7:A:695:GLU:OE2	8:B:551:LYS:NZ	2.41	0.45
20:A:820:CLA:H11	20:A:820:CLA:H52	1.79	0.45
20:A:841:CLA:H142	20:F:5006:CLA:HAC1	1.98	0.45
20:B:822:CLA:H93	13:G:51:LEU:HD11	1.97	0.45
23:F:5009:BCR:H24C	23:F:5009:BCR:H371	1.80	0.45
28:7:301:LMG:HC8	28:7:301:LMG:H111	1.60	0.45
29:7:321:DGD:HA22	29:7:321:DGD:HG11	1.34	0.45
20:9:603:CLA:H72	20:B:812:CLA:H42	1.99	0.45
7:A:80:GLN:HG2	20:A:808:CLA:H3A	1.98	0.45
7:A:330:LYS:HE3	7:A:336:ASN:HA	1.98	0.45
7:A:461:THR:O	7:A:465:LEU:N	2.49	0.45
7:A:677:PHE:CG	23:A:852:BCR:H363	2.50	0.45
23:A:848:BCR:H403	23:A:849:BCR:HC42	1.98	0.45
20:2:602:CLA:H93	20:2:602:CLA:H61	1.74	0.45
20:2:603:CLA:H52	14:H:93:LEU:HD12	1.96	0.45
3:3:139:LEU:HD22	19:3:401:CHL:H12	1.98	0.45
4:7:188:THR:OG1	4:7:189:ASP:N	2.49	0.45
20:A:804:CLA:H3A	20:A:804:CLA:C2	2.46	0.45
8:B:669:ARG:HB2	33:B:844:PQN:H7	1.98	0.45
20:B:831:CLA:H3A	20:B:832:CLA:OBD	2.16	0.45
12:F:223:LYS:HB3	12:F:225:GLU:CD	2.42	0.45
1:1:65:LYS:HB3	1:1:66:GLY:H	1.66	0.45
6:9:96:GLU:HB3	6:9:192:ILE:HD12	1.97	0.45
24:9:619:LHG:H241	24:9:619:LHG:HC61	1.35	0.45
7:A:43:PRO:O	12:F:186:THR:OG1	2.34	0.45
20:A:815:CLA:HBB1	20:A:815:CLA:H8	1.98	0.45
2:2:171:LYS:NZ	20:2:610:CLA:OBD	2.48	0.45
4:7:136:TRP:HE1	4:7:240:HIS:HB2	1.80	0.45
4:7:166:GLU:HG2	4:7:169:ARG:HE	1.81	0.45
4:7:226:GLY:O	4:7:230:MET:HE3	2.16	0.45
6:9:183:GLN:HE22	20:9:611:CLA:C1D	2.29	0.45
7:A:197:MET:HB2	20:A:816:CLA:HBC2	1.99	0.45
7:A:391:PHE:O	7:A:395:MET:HB2	2.17	0.45
7:A:524:MET:HG2	7:A:618:VAL:HA	1.99	0.45
7:A:549:ILE:HG12	20:B:804:CLA:HMD3	1.98	0.45
8:B:183:LEU:HD13	20:B:814:CLA:HHB	1.99	0.45
8:B:530:THR:HG21	8:B:583:TRP:CZ2	2.52	0.45
20:2:611:CLA:H11	20:2:611:CLA:H51	1.80	0.45
4:7:136:TRP:O	22:7:317:XAT:O23	2.22	0.45
20:9:608:CLA:H11	21:9:613:LUT:H26	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:433:HIS:CE1	20:L:301:CLA:ND	2.85	0.45
7:A:479:LEU:HD21	36:A:859:4RF:H1	1.99	0.45
20:A:827:CLA:H142	20:A:840:CLA:HAA2	1.98	0.45
8:B:204:ARG:HH12	8:B:254:ALA:H	1.64	0.45
20:F:5003:CLA:H142	20:F:5003:CLA:H112	1.85	0.45
20:3:408:CLA:H12	21:3:415:LUT:H373	1.98	0.45
5:8:77:SER:O	5:8:81:MET:HG2	2.16	0.45
24:8:321:LHG:HC5	24:8:321:LHG:HC81	1.56	0.45
7:A:423:TYR:OH	10:D:74:ILE:HG22	2.16	0.45
7:A:582:GLY:HA3	8:B:703:ILE:HD11	1.99	0.45
7:A:605:ILE:HD11	32:A:803:CL0:H38	1.99	0.45
7:A:657:VAL:HG22	7:A:745:ALA:HB3	1.99	0.45
20:A:812:CLA:H92	31:A:856:LMU:H91	1.97	0.45
19:2:601:CHL:H72	19:2:601:CHL:H111	1.76	0.45
5:8:138:ARG:NH1	20:8:307:CLA:O1D	2.48	0.45
5:8:194:ILE:HD12	5:8:194:ILE:HA	1.84	0.45
7:A:26:PHE:HB2	16:J:3:ASP:HB3	1.99	0.45
7:A:115:ALA:HB3	7:A:140:ILE:HG21	1.98	0.45
7:A:146:GLN:HB3	7:A:377:TYR:HB3	1.97	0.45
11:E:81:GLN:HE21	12:F:228:THR:HG1	1.64	0.45
1:1:79:CYS:C	1:1:83:MET:HE2	2.42	0.45
1:1:106:TRP:CE2	1:1:113:PRO:HB3	2.52	0.45
24:1:620:LHG:HC82	20:B:831:CLA:H71	1.99	0.45
7:A:270:ALA:HA	20:A:820:CLA:HAA2	1.99	0.45
20:A:831:CLA:O1D	20:A:832:CLA:HHB	2.17	0.45
20:A:836:CLA:NC	23:A:851:BCR:HC32	2.31	0.45
20:B:835:CLA:HBD	20:B:836:CLA:HMA1	1.98	0.45
20:F:5006:CLA:HBA1	20:F:5006:CLA:H3A	1.55	0.45
5:8:120:PHE:CD1	19:8:305:CHL:HBC2	2.52	0.45
20:8:313:CLA:HBA1	20:8:313:CLA:H3A	1.50	0.45
7:A:87:TRP:HA	20:A:810:CLA:HBB2	1.98	0.45
7:A:425:ASN:HD21	7:A:427:LEU:HB3	1.81	0.45
7:A:704:HIS:HE1	20:A:841:CLA:ND	2.13	0.45
8:B:303:GLU:CD	13:G:76:LEU:HD21	2.42	0.45
8:B:550:ASP:OD2	9:C:66:ARG:NE	2.44	0.45
20:B:814:CLA:H62	20:B:814:CLA:H2	1.61	0.45
10:D:62:LYS:HB2	10:D:62:LYS:HE2	1.81	0.45
1:1:67:THR:HB	20:B:842:CLA:HMC3	1.99	0.44
3:3:244:TYR:CE2	3:3:266:LYS:HG2	2.52	0.44
5:8:220:ASP:OD1	5:8:220:ASP:N	2.49	0.44
7:A:682:SER:OG	7:A:727:GLY:O	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:808:CLA:HBC2	20:A:833:CLA:HMA1	1.99	0.44
20:B:821:CLA:H202	23:B:846:BCR:HC7	2.00	0.44
1:1:166:ASP:HB3	1:1:169:SER:HB3	1.99	0.44
20:3:402:CLA:H143	20:3:402:CLA:H111	1.78	0.44
8:B:298:ILE:HG13	20:B:821:CLA:HED3	1.99	0.44
14:H:101:LEU:O	14:H:106:GLY:N	2.39	0.44
20:1:611:CLA:C4B	21:1:615:LUT:H12	2.47	0.44
24:3:424:LHG:H242	24:3:424:LHG:HC61	1.39	0.44
4:7:162:PHE:O	4:7:166:GLU:HB2	2.18	0.44
7:A:154:THR:N	7:A:158:GLN:OE1	2.51	0.44
7:A:225:ASN:CG	7:A:291:LEU:CD2	2.90	0.44
7:A:279:LYS:HA	7:A:503:LEU:HB2	1.99	0.44
20:A:835:CLA:H61	20:A:835:CLA:H102	1.63	0.44
20:A:837:CLA:H62	20:A:837:CLA:H41	1.78	0.44
8:B:423:LEU:HB3	8:B:533:LEU:HB2	1.99	0.44
8:B:712:ALA:HB1	20:B:830:CLA:H122	2.00	0.44
20:B:814:CLA:H171	23:B:845:BCR:H271	1.99	0.44
20:B:840:CLA:H8	20:B:841:CLA:H121	2.00	0.44
15:I:104:ILE:HD11	23:L:308:BCR:H333	1.98	0.44
26:3:421:SQD:H45	26:3:421:SQD:H81	1.39	0.44
20:8:309:CLA:H91	20:8:310:CLA:HBC3	2.00	0.44
7:A:265:PHE:HA	20:K:203:CLA:HAC2	1.98	0.44
20:A:824:CLA:H161	20:A:824:CLA:H122	1.68	0.44
20:A:834:CLA:HBB2	23:L:303:BCR:H342	1.99	0.44
8:B:490:GLY:HA2	8:B:493:LEU:HD12	1.99	0.44
20:B:824:CLA:HMD1	20:B:825:CLA:HMC1	1.99	0.44
23:G:4005:BCR:H20C	23:G:4005:BCR:H361	1.76	0.44
14:H:112:LEU:HA	14:H:113:PRO:HD3	1.88	0.44
2:2:164:ARG:HG2	20:2:608:CLA:HAA1	2.00	0.44
7:A:596:LEU:HB3	7:A:732:LEU:HD11	1.99	0.44
7:A:707:LEU:HD21	20:A:841:CLA:HMA1	1.99	0.44
8:B:616:TYR:OH	8:B:622:ARG:NH2	2.51	0.44
8:B:725:PHE:O	8:B:729:SER:OG	2.34	0.44
20:B:825:CLA:H92	20:B:825:CLA:H61	1.86	0.44
17:K:77:LEU:HD21	20:K:204:CLA:C3	2.46	0.44
5:8:76:HIS:HD2	22:8:315:XAT:H201	1.83	0.44
20:A:840:CLA:H61	23:A:850:BCR:H373	2.00	0.44
20:B:813:CLA:H62	20:B:813:CLA:H2	1.77	0.44
20:3:405:CLA:H43	20:A:819:CLA:H41	1.99	0.44
23:3:419:BCR:H24C	23:3:419:BCR:H371	1.78	0.44
20:A:807:CLA:H52	20:A:807:CLA:H11	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:808:CLA:H151	23:A:848:BCR:HC41	1.99	0.44
20:A:809:CLA:HED2	20:A:809:CLA:H2A	1.99	0.44
20:A:827:CLA:HMD2	20:A:828:CLA:HAB	2.00	0.44
8:B:168:TRP:HB2	13:G:86:PHE:HB3	1.99	0.44
20:B:818:CLA:H61	20:B:818:CLA:H93	1.85	0.44
20:B:832:CLA:HBA1	12:F:221:LEU:HD21	1.99	0.44
3:3:240:ASP:OD1	3:3:241:ASN:N	2.50	0.44
19:3:401:CHL:HBA2	19:3:401:CHL:H3A	1.63	0.44
5:8:39:THR:HG23	5:8:44:LYS:HZ2	1.82	0.44
6:9:110:ALA:HB3	6:9:112:TYR:HE1	1.82	0.44
7:A:218:ILE:HD13	20:A:818:CLA:HBC2	2.00	0.44
12:F:206:ALA:HB1	12:F:209:LEU:HD23	1.99	0.44
20:3:403:CLA:HAC1	23:3:419:BCR:H23C	2.00	0.44
4:7:164:TRP:CH2	23:7:318:BCR:HC8	2.53	0.44
5:8:131:TYR:HA	5:8:134:VAL:HG22	1.99	0.44
7:A:367:VAL:O	7:A:371:MET:HG3	2.17	0.44
8:B:392:ALA:O	8:B:396:ILE:HG22	2.17	0.44
20:B:827:CLA:H141	20:B:827:CLA:H161	1.72	0.44
12:F:190:ILE:HG13	12:F:191:ILE:HG12	2.00	0.44
20:9:608:CLA:H3A	20:9:608:CLA:HBA2	1.59	0.43
7:A:210:SER:OG	7:A:298:HIS:O	2.33	0.43
20:A:818:CLA:H3A	20:A:818:CLA:HBA2	1.62	0.43
8:B:587:THR:O	8:B:591:VAL:HG13	2.18	0.43
20:B:834:CLA:H151	20:B:834:CLA:H111	1.70	0.43
19:3:401:CHL:H91	20:3:407:CLA:H172	1.99	0.43
19:7:308:CHL:HMA1	23:7:318:BCR:H362	1.99	0.43
5:8:210:GLN:O	5:8:214:THR:OG1	2.31	0.43
7:A:733:LEU:HD22	23:A:852:BCR:H311	2.00	0.43
8:B:444:VAL:HG13	8:B:452:LYS:HB2	2.01	0.43
20:B:814:CLA:H143	20:B:814:CLA:H111	1.84	0.43
16:J:24:GLY:HA3	20:J:4002:CLA:HHC	2.00	0.43
16:J:28:GLU:HG3	20:J:4002:CLA:C1B	2.47	0.43
1:1:168:LYS:HE2	1:1:168:LYS:HB2	1.81	0.43
1:1:200:LYS:HB3	1:1:200:LYS:HE3	1.70	0.43
20:A:821:CLA:H92	20:A:821:CLA:H41	2.00	0.43
20:A:840:CLA:H91	20:A:840:CLA:H112	1.86	0.43
8:B:51:HIS:CE1	20:B:806:CLA:ND	2.85	0.43
8:B:103:GLU:HB3	14:H:121:GLU:HG3	2.01	0.43
8:B:396:ILE:HG13	8:B:552:LYS:HA	2.01	0.43
20:B:806:CLA:H202	20:B:806:CLA:H162	1.85	0.43
20:B:834:CLA:H141	20:B:834:CLA:H161	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:142:PRO:HD3	23:F:5009:BCR:H312	1.99	0.43
1:1:40:GLY:N	5:8:150:GLU:OE1	2.52	0.43
1:1:153:TYR:HB3	20:1:609:CLA:HED2	2.00	0.43
4:7:110:ALA:HA	4:7:230:MET:HE2	2.00	0.43
5:8:135:GLU:O	5:8:139:TRP:HB2	2.19	0.43
7:A:263:PRO:HB3	7:A:268:ASN:HB3	2.00	0.43
7:A:433:HIS:CE1	7:A:437:ILE:HD11	2.53	0.43
20:A:842:CLA:HAC2	23:F:5004:BCR:H342	1.99	0.43
20:B:823:CLA:H62	20:B:823:CLA:H41	1.52	0.43
14:H:125:ASN:OD1	14:H:126:GLY:N	2.51	0.43
18:L:134:LEU:HB3	23:L:308:BCR:H401	2.01	0.43
2:2:166:GLN:HA	2:2:169:GLU:HG3	2.00	0.43
5:8:83:GLY:HA2	22:8:315:XAT:H181	2.01	0.43
20:A:830:CLA:H142	20:A:830:CLA:H111	1.86	0.43
8:B:398:ASP:HA	10:D:190:ILE:HB	2.00	0.43
20:B:809:CLA:HBA2	20:B:809:CLA:H141	2.00	0.43
9:C:27:GLU:N	9:C:41:SER:O	2.48	0.43
2:2:228:VAL:HG11	24:2:621:LHG:H302	2.00	0.43
3:3:137:ARG:NH2	3:3:218:TYR:O	2.52	0.43
7:A:681:PHE:HZ	20:A:842:CLA:HBC2	1.84	0.43
7:A:712:SER:N	12:F:189:GLU:OE2	2.46	0.43
20:A:812:CLA:H61	20:A:812:CLA:H2	1.77	0.43
19:3:401:CHL:H92	20:A:815:CLA:H72	2.01	0.43
7:A:206:LEU:HD11	20:A:832:CLA:H192	2.01	0.43
7:A:282:LEU:HD12	7:A:515:VAL:HG21	2.00	0.43
7:A:426:LEU:HD13	20:A:827:CLA:C1C	2.49	0.43
20:A:827:CLA:H62	20:A:827:CLA:H41	1.70	0.43
20:A:842:CLA:H42	24:A:854:LHG:H172	2.00	0.43
8:B:375:HIS:HB2	20:B:828:CLA:C1B	2.49	0.43
8:B:393:ILE:O	8:B:397:ARG:HB2	2.18	0.43
20:B:822:CLA:H162	20:B:822:CLA:H122	1.73	0.43
23:G:4001:BCR:H371	23:G:4001:BCR:H24C	1.80	0.43
3:3:254:ASN:O	3:3:256:GLY:N	2.52	0.43
20:3:412:CLA:HBA2	20:3:412:CLA:H3A	1.50	0.43
5:8:71:GLN:O	5:8:75:VAL:HG12	2.19	0.43
7:A:121:ILE:CG2	7:A:122:VAL:N	2.82	0.43
20:A:819:CLA:H12	31:A:857:LMU:H81	2.01	0.43
8:B:16:ASP:HB3	8:B:21:ARG:HB2	1.99	0.43
8:B:193:GLY:O	8:B:197:HIS:ND1	2.35	0.43
8:B:508:SER:HA	8:B:511:LEU:HD21	2.00	0.43
12:F:205:TRP:CG	24:F:5002:LHG:H191	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:87:ASP:OD1	13:G:87:ASP:N	2.52	0.43
15:I:90:LEU:HD22	23:L:303:BCR:H291	2.00	0.43
1:1:126:THR:O	1:1:130:VAL:HG12	2.19	0.43
2:2:105:VAL:HG23	2:2:107:LEU:HD23	2.01	0.43
4:7:93:SER:HA	4:7:98:MET:HG2	2.01	0.43
7:A:318:ILE:HD11	20:A:823:CLA:HMA2	2.01	0.43
7:A:366:ILE:HG21	20:A:822:CLA:H201	2.01	0.43
7:A:539:HIS:CD2	20:A:838:CLA:HAB	2.53	0.43
20:A:834:CLA:HED3	8:B:681:TRP:HH2	1.84	0.43
14:H:92:ALA:O	14:H:96:VAL:HG23	2.19	0.43
20:K:203:CLA:HMC2	23:K:205:BCR:H331	2.01	0.43
18:L:202:TYR:HB3	18:L:203:SER:H	1.67	0.43
20:7:310:CLA:H3A	20:7:310:CLA:HBA2	1.53	0.43
19:9:606:CHL:HMB2	31:9:616:LMU:H111	1.99	0.43
7:A:245:LEU:HD21	20:A:819:CLA:HAC1	2.00	0.43
7:A:408:HIS:HA	7:A:411:ILE:HD12	2.01	0.43
20:B:818:CLA:H161	20:G:4004:CLA:HMA2	1.99	0.43
20:B:840:CLA:H62	20:B:843:CLA:H111	2.01	0.43
16:J:8:LEU:HD23	16:J:8:LEU:HA	1.86	0.43
18:L:128:ALA:HB2	18:L:189:VAL:HG11	2.00	0.43
3:3:249:PHE:HZ	23:3:419:BCR:HC8	1.84	0.42
4:7:184:PHE:CE2	19:7:308:CHL:HBB2	2.54	0.42
20:8:303:CLA:NA	23:8:316:BCR:H271	2.34	0.42
20:8:309:CLA:HAC2	20:8:311:CLA:H172	2.01	0.42
6:9:53:LEU:HD11	6:9:75:VAL:HG21	2.01	0.42
7:A:361:GLY:O	7:A:365:ILE:HG12	2.19	0.42
7:A:394:HIS:CD2	20:A:832:CLA:NC	2.87	0.42
7:A:446:ILE:HD11	23:B:802:BCR:H402	2.01	0.42
7:A:686:LEU:HD13	8:B:666:ILE:HD12	2.00	0.42
7:A:747:ILE:HD12	7:A:747:ILE:HA	1.90	0.42
23:A:851:BCR:H20C	23:A:851:BCR:H361	1.92	0.42
8:B:584:MET:HG2	20:B:826:CLA:HBC1	2.01	0.42
23:B:802:BCR:H383	20:B:843:CLA:HMD3	2.01	0.42
20:B:815:CLA:H3A	23:B:846:BCR:H403	2.01	0.42
20:B:830:CLA:H2	29:B:850:DGD:HB52	2.01	0.42
28:F:5001:LMG:H161	16:J:13:VAL:HG23	2.01	0.42
20:8:302:CLA:H3A	20:8:302:CLA:HBA2	1.49	0.42
6:9:112:TYR:HD2	20:9:605:CLA:HMD1	1.84	0.42
20:9:602:CLA:H72	20:B:813:CLA:H52	2.01	0.42
7:A:320:HIS:CD2	20:A:825:CLA:ND	2.87	0.42
8:B:733:ARG:HA	14:H:128:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:823:CLA:H102	23:G:4001:BCR:H381	2.00	0.42
13:G:128:CYS:HB3	24:G:4006:LHG:H251	2.00	0.42
20:L:302:CLA:H41	20:L:302:CLA:H62	1.78	0.42
1:1:80:ARG:N	1:1:83:MET:HE2	2.35	0.42
1:1:102:ASP:HA	1:1:105:LEU:HD23	2.01	0.42
3:3:235:LEU:HD21	3:3:248:PRO:HB2	2.01	0.42
3:3:310:LEU:N	20:3:411:CLA:O1A	2.53	0.42
20:3:412:CLA:H91	20:3:412:CLA:H112	1.78	0.42
7:A:396:TRP:CZ3	7:A:600:TYR:HA	2.54	0.42
7:A:598:TRP:HE1	20:B:804:CLA:C1D	2.32	0.42
20:A:812:CLA:H62	23:A:858:BCR:H363	2.00	0.42
20:A:819:CLA:H2A	20:A:819:CLA:HED2	2.00	0.42
20:A:842:CLA:H41	20:A:842:CLA:H62	1.80	0.42
8:B:430:LEU:O	8:B:434:THR:OG1	2.33	0.42
20:B:819:CLA:H3A	20:B:819:CLA:HBA2	1.38	0.42
20:B:824:CLA:H92	20:B:824:CLA:H61	1.85	0.42
3:3:270:ILE:HD12	3:3:270:ILE:HA	1.93	0.42
20:7:303:CLA:H3A	20:7:303:CLA:HBA2	1.64	0.42
24:9:617:LHG:HC81	24:9:617:LHG:HC5	1.69	0.42
7:A:542:THR:HG21	7:A:602:SER:HB2	1.97	0.42
8:B:185:GLY:HA3	8:B:286:ILE:HG13	2.00	0.42
12:F:225:GLU:CD	12:F:225:GLU:H	2.27	0.42
1:1:124:ILE:HD12	1:1:127:ILE:HD11	2.02	0.42
20:1:607:CLA:H202	20:1:607:CLA:H162	1.92	0.42
20:8:303:CLA:HHB	19:8:304:CHL:HHC	2.00	0.42
7:A:296:HIS:HE1	20:A:820:CLA:C4D	2.32	0.42
7:A:580:ARG:HG2	9:C:78:GLY:HA3	2.01	0.42
7:A:684:MET:HE1	20:A:804:CLA:C1B	2.49	0.42
20:A:812:CLA:H162	20:A:812:CLA:H202	1.84	0.42
20:B:808:CLA:H61	23:I:202:BCR:H282	2.01	0.42
20:B:811:CLA:H61	18:L:125:MET:HG3	2.01	0.42
20:B:828:CLA:H193	29:B:850:DGD:HAW1	2.00	0.42
15:I:93:PRO:HG3	23:I:202:BCR:H19C	2.02	0.42
4:7:168:LYS:HB3	19:7:308:CHL:CMC	2.50	0.42
7:A:305:PHE:HZ	20:A:822:CLA:H112	1.82	0.42
23:A:849:BCR:H371	23:A:849:BCR:C26	2.50	0.42
8:B:81:ASP:HB3	8:B:85:VAL:HG23	2.02	0.42
8:B:94:ASP:HA	20:B:810:CLA:HMA3	2.02	0.42
1:1:85:GLY:HA2	22:1:616:XAT:H381	2.01	0.42
3:3:288:VAL:HB	29:A:802:DGD:HA22	2.01	0.42
4:7:107:LEU:HD13	4:7:107:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:181:ALA:HB1	31:9:616:LMU:H61	2.02	0.42
7:A:359:LEU:HD13	7:A:359:LEU:HA	1.89	0.42
7:A:429:ARG:NH2	18:L:47:GLN:OE1	2.52	0.42
7:A:438:ILE:HG13	7:A:556:PHE:HE2	1.84	0.42
29:A:802:DGD:HA51	20:A:818:CLA:H91	2.02	0.42
8:B:241:ALA:HA	8:B:264:PRO:HG2	2.01	0.42
8:B:306:LEU:HD23	8:B:306:LEU:HA	1.92	0.42
20:G:4004:CLA:HBA2	24:G:4006:LHG:H312	2.01	0.42
23:G:4005:BCR:H24C	23:G:4005:BCR:H371	1.82	0.42
17:K:63:ARG:HH22	17:K:91:PRO:HG2	1.81	0.42
1:1:176:LYS:NZ	20:1:611:CLA:O2D	2.53	0.42
6:9:168:LYS:HA	6:9:171:ARG:HD2	2.02	0.42
6:9:212:THR:HG21	24:9:619:LHG:H242	2.02	0.42
20:9:612:CLA:HBC1	21:9:613:LUT:H162	2.01	0.42
7:A:474:ASP:OD1	7:A:530:THR:OG1	2.34	0.42
20:A:806:CLA:HBB2	20:A:814:CLA:H111	2.02	0.42
23:L:309:BCR:H24C	23:L:309:BCR:H371	1.87	0.42
3:3:182:VAL:HG21	22:3:416:XAT:H172	2.02	0.42
3:3:202:ILE:HG12	20:7:314:CLA:HED1	2.01	0.42
20:7:304:CLA:H51	24:7:325:LHG:H332	2.02	0.42
19:7:308:CHL:H3A	19:7:308:CHL:HBA2	1.74	0.42
20:A:825:CLA:HAA1	17:K:68:PRO:HG3	2.02	0.42
20:A:834:CLA:HAC2	20:L:305:CLA:H193	2.02	0.42
8:B:290:HIS:CD2	20:B:821:CLA:NA	2.88	0.42
20:B:816:CLA:H62	20:B:816:CLA:H2	1.67	0.42
13:G:97:GLU:N	13:G:97:GLU:OE2	2.53	0.42
1:1:63:LYS:HB3	1:1:63:LYS:HE2	1.62	0.42
1:1:206:LEU:O	1:1:210:LEU:HG	2.19	0.42
3:3:188:VAL:HG13	3:3:190:LYS:HE3	2.01	0.42
6:9:84:TRP:HE1	22:9:615:XAT:H371	1.85	0.42
7:A:349:TRP:CD1	20:A:828:CLA:H192	2.55	0.42
20:A:827:CLA:H11	23:A:850:BCR:H362	2.01	0.42
8:B:296:PHE:HA	13:G:96:VAL:HG11	2.01	0.42
20:B:821:CLA:H3A	20:B:821:CLA:HBA2	1.55	0.42
20:B:821:CLA:H143	20:B:821:CLA:H161	1.90	0.42
20:B:826:CLA:HED2	20:B:827:CLA:HBD	2.02	0.42
12:F:215:LEU:HD11	24:F:5011:LHG:HC82	2.01	0.42
16:J:10:THR:O	16:J:13:VAL:HG12	2.20	0.42
20:1:614:CLA:HED3	20:F:5007:CLA:H43	2.02	0.41
7:A:16:ALA:HB1	7:A:187:LYS:HD3	2.02	0.41
7:A:28:LYS:HB2	20:A:814:CLA:HAA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:734:GLY:O	7:A:738:THR:OG1	2.29	0.41
20:A:832:CLA:H122	23:A:849:BCR:H372	2.02	0.41
8:B:464:ILE:HD11	20:B:837:CLA:H2	2.00	0.41
9:C:55:GLU:HB3	9:C:63:LEU:CD1	2.48	0.41
2:2:258:TRP:CE3	24:I:201:LHG:H252	2.55	0.41
20:3:402:CLA:H91	20:3:402:CLA:H112	1.83	0.41
20:8:309:CLA:H2	20:8:310:CLA:HMD2	2.02	0.41
7:A:87:TRP:CZ3	23:A:849:BCR:H391	2.55	0.41
7:A:179:PHE:HA	7:A:183:LYS:HB2	2.03	0.41
7:A:267:LEU:HD11	17:K:111:VAL:HG22	2.01	0.41
7:A:370:HIS:CD2	20:A:830:CLA:NC	2.87	0.41
20:A:829:CLA:H52	20:A:836:CLA:HAB	2.02	0.41
8:B:74:ASN:OD1	8:B:74:ASN:N	2.53	0.41
20:B:827:CLA:H13	23:B:848:BCR:H15C	2.02	0.41
9:C:21:CYS:HB2	34:C:101:SF4:S4	2.60	0.41
12:F:92:LEU:HD12	12:F:92:LEU:HA	1.87	0.41
19:2:606:CHL:HMA2	19:2:606:CHL:HAA1	1.85	0.41
27:2:620:3PH:H321	27:2:620:3PH:H232	2.01	0.41
3:3:169:ILE:HD11	3:3:174:ALA:HB2	2.01	0.41
4:7:221:LYS:HD3	20:7:312:CLA:HAA2	2.02	0.41
5:8:109:LYS:HA	5:8:109:LYS:HD3	1.88	0.41
6:9:67:ASN:HB3	6:9:70:ARG:HB2	2.01	0.41
20:9:607:CLA:H111	20:9:607:CLA:H152	1.77	0.41
20:A:829:CLA:H93	20:A:840:CLA:H51	2.02	0.41
23:A:852:BCR:H20C	23:A:852:BCR:H361	1.89	0.41
8:B:596:HIS:O	8:B:600:LEU:HB2	2.20	0.41
20:B:805:CLA:HHC	20:B:807:CLA:OBD	2.19	0.41
20:1:608:CLA:H42	23:B:847:BCR:HC31	2.01	0.41
6:9:128:GLY:O	6:9:132:THR:OG1	2.34	0.41
6:9:177:PHE:CE2	22:9:614:XAT:H12	2.55	0.41
7:A:388:LEU:HB2	7:A:619:TRP:HH2	1.85	0.41
20:A:813:CLA:H11	20:A:813:CLA:H52	1.79	0.41
20:A:821:CLA:C4D	20:A:830:CLA:HBB1	2.51	0.41
20:A:825:CLA:H121	20:K:202:CLA:HBC1	2.01	0.41
8:B:409:LEU:HD13	20:B:824:CLA:HAC1	2.02	0.41
20:B:838:CLA:HBC2	23:J:4001:BCR:H24C	2.01	0.41
20:B:842:CLA:H2A	20:B:842:CLA:HED3	2.01	0.41
33:B:844:PQN:H262	33:B:844:PQN:H221	1.91	0.41
9:C:38:GLN:HG2	10:D:169:VAL:HG11	2.01	0.41
14:H:131:LEU:O	14:H:131:LEU:CD2	2.60	0.41
23:J:4001:BCR:H24C	23:J:4001:BCR:H371	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:63:ARG:HH22	17:K:91:PRO:CG	2.33	0.41
21:1:615:LUT:H31	21:1:615:LUT:H391	1.88	0.41
2:2:55:HIS:CE1	2:2:70:ARG:HG2	2.51	0.41
3:3:286:GLN:HA	3:3:289:ILE:HG22	2.01	0.41
20:3:414:CLA:HED3	19:7:302:CHL:H43	2.01	0.41
7:A:601:ASN:ND2	32:A:803:CL0:H68	2.31	0.41
7:A:654:SER:HA	7:A:657:VAL:HG23	2.01	0.41
7:A:736:ILE:HG22	23:A:852:BCR:HC32	2.01	0.41
20:A:835:CLA:HAB	20:L:302:CLA:HHB	2.02	0.41
20:A:839:CLA:HBC2	36:A:859:4RF:H23	2.03	0.41
12:F:224:ASP:C	12:F:226:ASN:N	2.78	0.41
1:1:214:PHE:HE2	19:8:304:CHL:HED3	1.85	0.41
2:2:47:TYR:HH	2:2:240:LYS:NZ	2.19	0.41
2:2:244:LYS:HE2	8:B:160:PRO:HG2	2.03	0.41
19:2:601:CHL:HBC3	19:2:601:CHL:HHH	2.03	0.41
4:7:90:LEU:HB2	22:7:317:XAT:H21	2.01	0.41
4:7:159:LEU:HD21	28:7:319:LMG:H431	2.02	0.41
5:8:237:ASN:HD22	5:8:237:ASN:HA	1.70	0.41
20:A:812:CLA:HMA1	16:J:27:ILE:HD12	2.02	0.41
20:A:826:CLA:H11	20:A:826:CLA:H52	1.79	0.41
8:B:242:SER:O	8:B:242:SER:OG	2.31	0.41
8:B:316:LEU:HD22	20:B:831:CLA:HMD3	2.03	0.41
8:B:374:THR:HG23	8:B:592:THR:HG21	2.03	0.41
15:I:99:TRP:CD2	24:I:201:LHG:H302	2.56	0.41
1:1:178:LEU:HD23	1:1:178:LEU:HA	1.94	0.41
20:1:602:CLA:H91	20:1:603:CLA:H151	2.02	0.41
19:2:606:CHL:HAA2	24:H:203:LHG:O9	2.21	0.41
23:3:419:BCR:H20C	23:3:419:BCR:H361	1.84	0.41
7:A:674:GLY:HA2	23:A:852:BCR:H17C	2.03	0.41
8:B:455:LEU:O	12:F:138:LEU:N	2.45	0.41
8:B:609:GLN:O	8:B:613:SER:HB2	2.20	0.41
20:B:819:CLA:H141	20:B:819:CLA:H161	1.84	0.41
12:F:140:SER:HA	12:F:154:VAL:HG21	2.02	0.41
23:K:205:BCR:H20C	23:K:205:BCR:H361	1.82	0.41
20:L:304:CLA:HBA2	20:L:304:CLA:H3A	1.72	0.41
20:1:608:CLA:HBB1	20:B:822:CLA:H151	2.03	0.41
3:3:117:LEU:HD12	22:3:416:XAT:H241	2.02	0.41
3:3:258:THR:OG1	3:3:261:GLU:CG	2.67	0.41
5:8:33:TRP:HZ2	24:F:5002:LHG:HC31	1.84	0.41
6:9:207:ILE:HD12	6:9:211:LEU:HD23	2.02	0.41
7:A:75:SER:OG	7:A:181:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:666:SER:HB2	8:B:446:ALA:HB1	2.02	0.41
20:A:830:CLA:H162	20:A:830:CLA:H121	1.85	0.41
8:B:103:GLU:HG2	14:H:118:PRO:HA	2.02	0.41
8:B:551:LYS:HB2	8:B:551:LYS:HE3	1.92	0.41
20:B:805:CLA:HAA2	26:B:851:SQD:H62	2.03	0.41
13:G:39:ALA:HB3	13:G:42:VAL:HG22	2.03	0.41
2:2:220:LYS:HD3	21:2:616:LUT:H21	2.03	0.41
2:2:255:ASN:O	2:2:258:TRP:NE1	2.54	0.41
3:3:201:PHE:HD2	20:7:314:CLA:HED2	1.86	0.41
20:3:408:CLA:H52	20:3:408:CLA:H11	1.83	0.41
4:7:254:HIS:CD2	20:7:314:CLA:NC	2.89	0.41
19:7:308:CHL:HED3	19:7:308:CHL:HBD	1.85	0.41
6:9:177:PHE:CD2	22:9:614:XAT:H12	2.56	0.41
7:A:178:TRP:CZ2	28:A:801:LMG:H122	2.56	0.41
7:A:390:LEU:HD11	20:A:832:CLA:HED3	2.03	0.41
20:A:809:CLA:H93	20:A:809:CLA:HED1	2.02	0.41
20:A:811:CLA:HAB	20:A:831:CLA:H13	2.03	0.41
20:A:814:CLA:H161	23:A:858:BCR:H371	2.03	0.41
20:A:836:CLA:HBB1	20:A:838:CLA:HED2	2.03	0.41
8:B:83:ILE:HG23	8:B:364:VAL:HG11	2.03	0.41
20:B:820:CLA:H111	20:B:824:CLA:H52	2.03	0.41
23:B:849:BCR:H20C	23:B:849:BCR:H361	1.90	0.41
10:D:133:THR:HG23	10:D:144:PRO:HD2	2.03	0.41
11:E:89:ASP:OD2	11:E:91:SER:OG	2.39	0.41
2:2:183:PHE:CE2	21:2:615:LUT:H32	2.56	0.41
20:3:414:CLA:HAA2	24:7:320:LHG:H371	2.01	0.41
28:8:301:LMG:H112	28:8:301:LMG:HC8	1.64	0.41
20:A:807:CLA:H62	20:A:812:CLA:H192	2.03	0.41
20:A:824:CLA:H162	20:A:824:CLA:H202	1.84	0.41
8:B:13:LEU:HD23	8:B:13:LEU:HA	1.90	0.41
8:B:55:LEU:HG	20:B:814:CLA:HED1	2.03	0.41
20:B:824:CLA:O1A	23:B:847:BCR:H14C	2.20	0.41
23:B:849:BCR:H24C	23:B:849:BCR:H371	1.92	0.41
29:B:850:DGD:HB21	29:B:850:DGD:HG2	1.72	0.41
23:F:5004:BCR:H281	23:J:4001:BCR:C15	2.51	0.41
20:F:5005:CLA:H41	20:F:5005:CLA:H61	1.51	0.41
13:G:129:SER:HA	24:G:4006:LHG:HC61	2.03	0.41
20:L:304:CLA:H92	20:L:304:CLA:H62	1.86	0.41
1:1:77:ILE:HD11	20:1:608:CLA:CAD	2.51	0.40
1:1:191:PHE:CZ	1:1:202:ILE:HG12	2.56	0.40
20:1:612:CLA:H11	20:1:612:CLA:H51	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:171:LYS:NZ	20:2:609:CLA:O2D	2.53	0.40
4:7:187:ILE:HG21	4:7:202:LEU:HD11	2.03	0.40
20:7:313:CLA:H152	20:7:313:CLA:H112	1.72	0.40
6:9:89:VAL:O	6:9:93:MET:HE2	2.20	0.40
7:A:194:VAL:HG11	20:A:828:CLA:HAC2	2.03	0.40
7:A:330:LYS:HE2	7:A:330:LYS:HB3	1.79	0.40
7:A:343:GLU:O	7:A:347:THR:OG1	2.29	0.40
20:A:820:CLA:H41	20:A:820:CLA:H62	1.86	0.40
20:A:828:CLA:H91	20:A:828:CLA:H111	1.89	0.40
8:B:617:LEU:HD21	20:B:803:CLA:H171	2.03	0.40
18:L:155:LYS:H	18:L:155:LYS:HG2	1.67	0.40
18:L:193:TYR:O	18:L:196:THR:OG1	2.31	0.40
19:1:601:CHL:H43	5:8:129:PHE:HB3	2.02	0.40
2:2:42:GLY:O	2:2:45:MET:SD	2.79	0.40
3:3:318:PHE:HE1	7:A:247:GLN:H	1.69	0.40
7:A:119:TRP:CZ3	23:A:858:BCR:HC8	2.56	0.40
7:A:382:THR:HG21	7:A:517:VAL:HB	2.03	0.40
8:B:358:PRO:HG3	20:B:819:CLA:HBA1	2.02	0.40
8:B:456:ILE:HB	8:B:518:PHE:CE1	2.55	0.40
8:B:477:LEU:HG	8:B:478:LEU:H	1.85	0.40
23:3:418:BCR:H373	23:A:849:BCR:HC31	2.03	0.40
19:7:307:CHL:HBB1	22:7:317:XAT:H393	2.04	0.40
7:A:77:HIS:ND1	20:A:816:CLA:OBD	2.45	0.40
7:A:552:LYS:HZ1	8:B:674:GLU:HB2	1.87	0.40
7:A:696:LEU:HD13	8:B:537:LYS:HD2	2.04	0.40
20:A:805:CLA:C1B	20:B:804:CLA:CBB	2.81	0.40
23:A:858:BCR:H11C	20:J:4002:CLA:CMC	2.50	0.40
8:B:277:HIS:HE2	20:B:819:CLA:C2B	2.35	0.40
9:C:58:CYS:CB	9:C:63:LEU:HD22	2.49	0.40
19:2:606:CHL:HBD	19:2:606:CHL:O1A	2.21	0.40
3:3:182:VAL:HG13	3:3:183:ILE:HD12	2.02	0.40
20:3:407:CLA:H8	20:3:407:CLA:H122	1.78	0.40
4:7:150:PRO:HD3	5:8:230:TRP:HB3	2.03	0.40
7:A:119:TRP:HZ2	31:A:856:LMU:H21	1.85	0.40
7:A:142:SER:HA	20:A:831:CLA:HMA2	2.04	0.40
7:A:396:TRP:HZ3	7:A:600:TYR:HA	1.86	0.40
32:A:803:CL0:H70	20:A:805:CLA:C1B	2.51	0.40
20:A:840:CLA:H62	20:A:840:CLA:H41	1.89	0.40
20:A:841:CLA:H93	20:A:841:CLA:H62	1.83	0.40
20:B:820:CLA:H141	20:B:825:CLA:H202	2.04	0.40
20:B:821:CLA:H102	20:B:821:CLA:H13	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:64:ARG:NH2	13:G:110:ASP:OD2	2.35	0.40
25:H:201:PTY:H152	25:H:201:PTY:H182	1.93	0.40
18:L:191:TRP:CE3	18:L:194:ILE:HD11	2.57	0.40
23:L:303:BCR:H20C	23:L:303:BCR:H361	1.92	0.40
20:2:602:CLA:H2	21:2:615:LUT:H182	2.04	0.40
23:7:318:BCR:H24C	23:7:318:BCR:H371	1.92	0.40
7:A:542:THR:HG21	7:A:602:SER:CB	2.52	0.40
20:A:808:CLA:H162	20:A:808:CLA:H141	1.90	0.40
20:A:830:CLA:H143	20:A:836:CLA:H121	2.02	0.40
23:A:851:BCR:H24C	23:A:851:BCR:H371	1.86	0.40
20:B:807:CLA:H43	29:B:850:DGD:HB61	2.02	0.40
20:B:840:CLA:C4D	20:B:843:CLA:HMC2	2.47	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%)	179 (92%)	16 (8%)	0	100	100
2	2	220/263 (84%)	211 (96%)	8 (4%)	1 (0%)	24	54
3	3	206/320 (64%)	201 (98%)	4 (2%)	1 (0%)	24	54
4	7	207/256 (81%)	198 (96%)	9 (4%)	0	100	100
5	8	224/254 (88%)	218 (97%)	6 (3%)	0	100	100
6	9	185/222 (83%)	168 (91%)	15 (8%)	2 (1%)	11	36
7	A	738/751 (98%)	709 (96%)	29 (4%)	0	100	100
8	B	730/735 (99%)	704 (96%)	26 (4%)	0	100	100
9	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
10	D	141/202 (70%)	134 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	62/125 (50%)	60 (97%)	2 (3%)	0	100	100
12	F	163/232 (70%)	152 (93%)	11 (7%)	0	100	100
13	G	103/141 (73%)	96 (93%)	6 (6%)	1 (1%)	12	39
14	H	63/135 (47%)	55 (87%)	7 (11%)	1 (2%)	7	27
15	I	39/109 (36%)	38 (97%)	1 (3%)	0	100	100
16	J	39/41 (95%)	33 (85%)	6 (15%)	0	100	100
17	K	81/123 (66%)	64 (79%)	15 (18%)	2 (2%)	4	17
18	L	154/202 (76%)	145 (94%)	9 (6%)	0	100	100
All	All	3628/4420 (82%)	3438 (95%)	182 (5%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	120	ILE
3	3	255	PHE
6	9	40	LEU
13	G	38	ILE
17	K	92	ALA
17	K	93	GLY
6	9	42	ASP
14	H	130	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	151/178 (85%)	150 (99%)	1 (1%)	76	92
2	2	179/207 (86%)	179 (100%)	0	100	100
3	3	159/236 (67%)	158 (99%)	1 (1%)	78	93
4	7	166/201 (83%)	165 (99%)	1 (1%)	78	93
5	8	173/196 (88%)	171 (99%)	2 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	9	153/183 (84%)	150 (98%)	3 (2%)	48	78
7	A	599/609 (98%)	597 (100%)	2 (0%)	86	96
8	B	593/594 (100%)	591 (100%)	2 (0%)	86	96
9	C	68/69 (99%)	68 (100%)	0	100	100
10	D	123/163 (76%)	122 (99%)	1 (1%)	73	90
11	E	57/101 (56%)	56 (98%)	1 (2%)	51	80
12	F	138/184 (75%)	137 (99%)	1 (1%)	76	92
13	G	81/110 (74%)	81 (100%)	0	100	100
14	H	50/105 (48%)	50 (100%)	0	100	100
15	I	32/77 (42%)	32 (100%)	0	100	100
16	J	36/36 (100%)	36 (100%)	0	100	100
17	K	61/94 (65%)	59 (97%)	2 (3%)	33	67
18	L	120/159 (76%)	120 (100%)	0	100	100
All	All	2939/3502 (84%)	2922 (99%)	17 (1%)	76	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	78	HIS
3	3	214	ARG
4	7	170	LEU
5	8	76	HIS
5	8	201	MET
6	9	38	LEU
6	9	136	GLN
6	9	150	TYR
7	A	471	MET
7	A	544	HIS
8	B	518	PHE
8	B	578	TYR
10	D	173	ARG
11	E	72	LEU
12	F	222	GLU
17	K	73	VAL
17	K	88	THR

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	194	GLN
1	1	221	ASN
3	3	272	ASN
3	3	308	ASN
4	7	196	ASN
4	7	211	ASN
4	7	225	ASN
4	7	240	HIS
5	8	140	GLN
5	8	210	GLN
5	8	232	ASN
5	8	249	GLN
6	9	95	GLN
7	A	283	ASN
7	A	387	GLN
7	A	480	GLN
7	A	539	HIS
8	B	99	GLN
8	B	206	GLN
8	B	267	GLN
8	B	422	HIS
8	B	503	ASN
10	D	177	ASN
12	F	110	GLN
12	F	174	GLN
14	H	75	GLN
18	L	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

291 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$
31	LMU	A	856	-	36,36,36	0.18	0	47,47,47	0.40	0
23	BCR	B	847	-	41,41,41	0.14	0	56,56,56	0.28	0
20	CLA	9	609	24	64,68,73	1.17	7 (10%)	76,107,113	1.18	4 (5%)
25	PTY	H	201	-	45,45,49	0.48	0	48,50,54	0.44	0
20	CLA	8	313	5	55,59,73	1.30	8 (14%)	64,96,113	1.20	4 (6%)
20	CLA	A	838	7	55,59,73	1.34	8 (14%)	64,96,113	1.37	4 (6%)
33	PQN	B	844	-	34,34,34	0.29	0	43,45,45	0.57	1 (2%)
23	BCR	A	848	-	41,41,41	0.43	0	56,56,56	0.99	3 (5%)
20	CLA	7	312	4	56,60,73	1.29	9 (16%)	65,97,113	1.42	5 (7%)
20	CLA	A	816	7	69,73,73	1.14	8 (11%)	82,113,113	1.30	6 (7%)
25	PTY	8	317	-	23,23,49	0.67	0	26,28,54	0.49	0
20	CLA	1	610	24	50,54,73	1.33	7 (14%)	59,90,113	1.20	4 (6%)
20	CLA	A	811	7	69,73,73	1.12	7 (10%)	82,113,113	1.10	5 (6%)
20	CLA	A	810	-	64,68,73	1.23	8 (12%)	76,107,113	1.17	7 (9%)
20	CLA	A	812	7	69,73,73	1.21	8 (11%)	82,113,113	1.33	8 (9%)
20	CLA	B	816	8	59,63,73	1.26	9 (15%)	70,101,113	1.28	4 (5%)
20	CLA	F	5006	-	51,55,73	1.34	8 (15%)	60,91,113	1.27	5 (8%)
21	LUT	9	613	-	42,43,43	0.30	0	51,60,60	0.34	0
23	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.36	0
24	LHG	H	203	-	37,37,48	0.34	0	40,43,54	0.35	0
23	BCR	J	4001	-	41,41,41	0.31	0	56,56,56	0.96	4 (7%)
29	DGD	L	311	-	59,59,67	0.20	0	73,73,81	0.23	0
20	CLA	G	4002	13	51,55,73	1.35	7 (13%)	60,91,113	1.35	5 (8%)
20	CLA	B	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.17	6 (7%)
20	CLA	B	835	-	64,68,73	1.19	8 (12%)	76,107,113	1.24	5 (6%)
20	CLA	B	838	-	64,68,73	1.18	7 (10%)	76,107,113	1.17	5 (6%)
20	CLA	3	409	-	54,58,73	1.31	6 (11%)	64,95,113	1.35	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	837	7	59,63,73	1.27	8 (13%)	70,101,113	1.28	7 (10%)
20	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
24	LHG	7	323	-	21,21,48	0.41	0	24,27,54	0.44	0
20	CLA	7	314	4	54,58,73	1.30	7 (12%)	64,95,113	1.32	6 (9%)
20	CLA	F	5007	12	53,57,73	1.31	7 (13%)	61,93,113	1.32	5 (8%)
20	CLA	A	814	7	69,73,73	1.16	8 (11%)	82,113,113	1.09	5 (6%)
20	CLA	F	5008	12	50,54,73	1.61	8 (16%)	59,90,113	1.43	6 (10%)
25	PTY	L	310	-	19,19,49	0.71	0	22,24,54	0.56	0
20	CLA	2	604	-	54,58,73	1.28	8 (14%)	64,95,113	1.19	6 (9%)
20	CLA	B	832	8	64,68,73	1.22	8 (12%)	76,107,113	1.31	5 (6%)
20	CLA	B	817	8	64,68,73	1.23	9 (14%)	76,107,113	1.30	5 (6%)
20	CLA	L	305	18	69,73,73	1.11	7 (10%)	82,113,113	1.13	8 (9%)
19	CHL	2	601	2	55,69,74	0.80	2 (3%)	52,108,114	2.19	7 (13%)
20	CLA	L	302	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	6 (7%)
20	CLA	A	813	7	59,63,73	1.28	8 (13%)	70,101,113	1.19	4 (5%)
20	CLA	7	309	4	69,73,73	1.14	6 (8%)	82,113,113	1.22	6 (7%)
24	LHG	2	621	-	35,35,48	0.38	0	38,41,54	0.34	0
20	CLA	9	605	6	49,53,73	1.63	11 (22%)	58,89,113	1.38	9 (15%)
20	CLA	B	820	-	69,73,73	1.21	10 (14%)	82,113,113	1.21	6 (7%)
20	CLA	B	809	8	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
20	CLA	1	613	1	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
20	CLA	A	842	7	65,69,73	1.23	8 (12%)	77,108,113	1.23	4 (5%)
20	CLA	B	837	8	55,59,73	1.31	8 (14%)	64,96,113	1.42	6 (9%)
23	BCR	B	802	-	41,41,41	0.23	0	56,56,56	1.02	5 (8%)
20	CLA	3	404	-	50,54,73	1.33	7 (14%)	59,90,113	1.25	4 (6%)
20	CLA	1	614	1	50,54,73	1.35	8 (16%)	59,90,113	1.51	9 (15%)
20	CLA	9	603	6	59,63,73	1.38	9 (15%)	70,101,113	1.31	6 (8%)
24	LHG	1	621	-	45,45,48	0.32	0	48,51,54	0.34	0
20	CLA	L	304	18	69,73,73	1.16	6 (8%)	82,113,113	1.18	5 (6%)
20	CLA	1	603	1	69,73,73	1.16	9 (13%)	82,113,113	1.18	4 (4%)
20	CLA	3	402	3	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
23	BCR	3	417	-	41,41,41	0.19	0	56,56,56	0.37	0
26	SQD	2	619	-	39,41,54	0.20	0	49,52,65	0.22	0
22	XAT	8	315	-	41,47,47	0.16	0	54,74,74	0.68	1 (1%)
24	LHG	3	420	-	16,16,48	0.90	1 (6%)	17,20,54	0.65	0
24	LHG	1	619	-	43,43,48	0.32	0	46,49,54	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	7	325	-	39,39,48	0.34	0	42,45,54	0.38	0
20	CLA	1	612	-	59,63,73	1.39	11 (18%)	70,101,113	1.60	17 (24%)
22	XAT	9	614	-	41,47,47	0.14	0	54,74,74	0.76	2 (3%)
24	LHG	3	424	-	38,38,48	0.34	0	41,44,54	0.34	0
20	CLA	B	840	-	69,73,73	1.20	9 (13%)	82,113,113	1.22	5 (6%)
20	CLA	B	812	-	59,63,73	1.25	7 (11%)	70,101,113	1.24	4 (5%)
20	CLA	2	605	-	49,53,73	1.37	6 (12%)	58,89,113	1.28	4 (6%)
28	LMG	A	801	-	32,32,55	0.21	0	40,40,63	0.27	0
20	CLA	B	819	8	69,73,73	1.14	7 (10%)	82,113,113	1.14	9 (10%)
31	LMU	9	616	-	36,36,36	0.27	0	47,47,47	0.59	0
20	CLA	A	823	7	69,73,73	1.13	8 (11%)	82,113,113	1.21	5 (6%)
20	CLA	B	836	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
20	CLA	B	821	8	69,73,73	1.20	8 (11%)	82,113,113	1.20	6 (7%)
21	LUT	1	615	-	42,43,43	0.22	0	51,60,60	1.47	8 (15%)
20	CLA	2	608	-	49,53,73	1.33	6 (12%)	58,89,113	1.23	5 (8%)
20	CLA	9	610	6	54,58,73	1.33	7 (12%)	64,95,113	1.42	7 (10%)
20	CLA	9	607	6	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
20	CLA	3	406	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	5 (7%)
20	CLA	8	303	-	54,58,73	1.31	9 (16%)	64,95,113	1.39	5 (7%)
20	CLA	B	843	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
20	CLA	K	202	-	59,63,73	1.25	7 (11%)	70,101,113	1.15	4 (5%)
20	CLA	A	839	7	69,73,73	1.13	7 (10%)	82,113,113	1.16	5 (6%)
20	CLA	F	5005	-	59,63,73	1.24	6 (10%)	70,101,113	1.18	5 (7%)
20	CLA	B	827	8	69,73,73	1.20	9 (13%)	82,113,113	1.24	5 (6%)
21	LUT	8	314	-	42,43,43	0.26	0	51,60,60	0.39	0
28	LMG	7	319	-	54,54,55	0.23	0	62,62,63	0.28	0
25	PTY	F	5010	-	21,21,49	0.66	0	24,26,54	0.54	0
33	PQN	A	845	-	34,34,34	0.28	0	43,45,45	0.55	1 (2%)
19	CHL	8	306	-	45,59,74	0.90	2 (4%)	40,96,114	2.06	6 (15%)
22	XAT	9	615	-	41,47,47	0.18	0	54,74,74	1.09	4 (7%)
23	BCR	F	5009	-	41,41,41	0.16	0	56,56,56	0.34	0
20	CLA	8	312	5	50,54,73	1.34	6 (12%)	59,90,113	1.23	4 (6%)
29	DGD	A	802	-	67,67,67	0.17	0	81,81,81	0.16	0
23	BCR	A	851	-	41,41,41	0.19	0	56,56,56	0.46	0
20	CLA	2	609	24	45,49,73	1.39	7 (15%)	54,84,113	1.28	5 (9%)
26	SQD	3	423	-	30,32,54	0.23	0	40,43,65	0.16	0
32	CL0	A	803	7	58,73,73	0.83	2 (3%)	60,113,113	2.17	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	805	-	69,73,73	1.15	8 (11%)	82,113,113	1.10	4 (4%)
20	CLA	A	829	-	60,64,73	1.28	9 (15%)	71,102,113	1.25	5 (7%)
20	CLA	A	831	7	69,73,73	1.12	7 (10%)	82,113,113	1.19	6 (7%)
21	LUT	7	316	-	42,43,43	0.37	1 (2%)	51,60,60	0.55	1 (1%)
20	CLA	B	822	8	69,73,73	1.15	6 (8%)	82,113,113	1.09	6 (7%)
20	CLA	A	832	7	69,73,73	1.19	10 (14%)	82,113,113	1.25	6 (7%)
20	CLA	3	403	-	50,54,73	1.32	7 (14%)	59,90,113	1.36	4 (6%)
30	LMK	8	320	-	34,34,53	0.53	0	34,41,60	0.70	2 (5%)
20	CLA	1	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
20	CLA	7	305	-	54,58,73	1.31	7 (12%)	64,95,113	1.36	6 (9%)
22	XAT	3	416	-	41,47,47	0.19	0	54,74,74	0.91	3 (5%)
25	PTY	3	422	-	25,25,49	0.62	0	28,30,54	0.51	0
20	CLA	1	609	1	69,73,73	1.13	7 (10%)	82,113,113	1.04	4 (4%)
20	CLA	H	204	14	49,53,73	1.35	8 (16%)	58,89,113	1.30	4 (6%)
29	DGD	7	321	-	48,48,67	0.20	0	62,62,81	0.32	0
23	BCR	A	850	-	41,41,41	0.25	0	56,56,56	0.95	3 (5%)
24	LHG	1	620	20	30,30,48	0.36	0	33,36,54	0.33	0
26	SQD	3	421	-	33,35,54	0.26	0	43,46,65	0.32	0
20	CLA	3	413	-	46,50,73	1.41	7 (15%)	53,85,113	1.30	4 (7%)
21	LUT	3	415	-	42,43,43	0.27	0	51,60,60	0.54	1 (1%)
20	CLA	B	828	-	69,73,73	1.14	7 (10%)	82,113,113	1.13	5 (6%)
20	CLA	B	839	-	59,63,73	1.22	7 (11%)	70,101,113	1.30	5 (7%)
20	CLA	K	201	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	4 (6%)
23	BCR	1	617	-	41,41,41	0.14	0	56,56,56	0.33	0
20	CLA	B	824	8	59,63,73	1.23	8 (13%)	70,101,113	1.13	6 (8%)
24	LHG	1	618	20	24,24,48	0.40	0	27,30,54	0.36	0
20	CLA	L	301	7	49,53,73	1.38	8 (16%)	58,89,113	1.30	4 (6%)
23	BCR	G	4001	-	41,41,41	0.18	0	56,56,56	0.39	0
20	CLA	2	622	-	50,54,73	1.31	6 (12%)	59,90,113	1.30	6 (10%)
25	PTY	1	623	-	34,34,49	0.55	0	37,39,54	0.43	0
20	CLA	9	602	6	64,68,73	1.20	8 (12%)	76,107,113	1.14	7 (9%)
24	LHG	2	618	20	43,43,48	0.42	0	46,48,54	0.65	2 (4%)
19	CHL	1	601	-	45,59,74	0.81	1 (2%)	40,96,114	2.39	8 (20%)
20	CLA	B	833	8	69,73,73	1.14	5 (7%)	82,113,113	1.37	9 (10%)
20	CLA	G	4004	-	49,53,73	1.34	8 (16%)	58,89,113	1.36	5 (8%)
20	CLA	A	830	7	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	J	4002	16	53,57,73	1.31	7 (13%)	61,93,113	1.57	7 (11%)
20	CLA	2	610	2	50,54,73	1.33	8 (16%)	59,90,113	1.43	4 (6%)
20	CLA	A	819	-	59,63,73	1.29	8 (13%)	70,101,113	1.34	5 (7%)
20	CLA	A	844	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
20	CLA	B	826	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	6 (7%)
21	LUT	2	616	-	42,43,43	0.23	0	51,60,60	0.72	3 (5%)
19	CHL	3	401	3	50,64,74	0.87	2 (4%)	46,102,114	2.49	8 (17%)
20	CLA	A	821	7	69,73,73	1.20	8 (11%)	82,113,113	1.26	5 (6%)
19	CHL	8	304	-	41,55,74	0.97	2 (4%)	35,91,114	2.79	7 (20%)
20	CLA	7	304	4	59,63,73	1.27	7 (11%)	70,101,113	1.26	5 (7%)
20	CLA	B	829	8	69,73,73	1.17	10 (14%)	82,113,113	1.12	4 (4%)
20	CLA	K	203	17	49,53,73	1.41	9 (18%)	58,89,113	1.47	4 (6%)
23	BCR	F	5004	-	41,41,41	0.15	0	56,56,56	0.33	0
23	BCR	I	202	-	41,41,41	0.16	0	56,56,56	0.32	0
28	LMG	8	301	-	50,50,55	0.22	0	58,58,63	0.28	0
20	CLA	8	310	5	54,58,73	1.35	10 (18%)	64,95,113	1.38	7 (10%)
20	CLA	A	841	7	69,73,73	1.14	8 (11%)	82,113,113	1.16	6 (7%)
23	BCR	K	205	-	41,41,41	0.34	0	56,56,56	0.75	2 (3%)
20	CLA	A	826	7	64,68,73	1.18	7 (10%)	76,107,113	1.10	4 (5%)
23	BCR	J	4003	-	41,41,41	0.15	0	56,56,56	0.26	0
24	LHG	B	852	-	48,48,48	0.31	0	51,54,54	0.32	0
23	BCR	L	303	-	41,41,41	0.15	0	56,56,56	0.27	0
24	LHG	8	321	-	30,30,48	0.38	0	33,36,54	0.39	0
20	CLA	B	834	8	69,73,73	1.16	9 (13%)	82,113,113	1.14	5 (6%)
20	CLA	7	310	4	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
31	LMU	A	857	-	36,36,36	0.19	0	47,47,47	0.21	0
20	CLA	L	307	-	54,58,73	1.27	6 (11%)	64,95,113	1.30	6 (9%)
20	CLA	A	840	7	64,68,73	1.18	7 (10%)	76,107,113	1.12	6 (7%)
20	CLA	A	806	7	69,73,73	1.15	8 (11%)	82,113,113	1.22	5 (6%)
20	CLA	8	302	5	64,68,73	1.21	7 (10%)	76,107,113	1.08	6 (7%)
23	BCR	L	308	-	41,41,41	0.19	0	56,56,56	0.37	0
19	CHL	7	302	-	60,74,74	0.73	3 (5%)	58,114,114	1.96	8 (13%)
20	CLA	7	311	24	64,68,73	1.24	9 (14%)	76,107,113	1.30	6 (7%)
24	LHG	8	319	20	33,33,48	0.34	0	36,39,54	0.34	0
24	LHG	F	5011	-	41,41,48	0.34	0	44,47,54	0.48	0
20	CLA	9	611	-	59,63,73	1.26	8 (13%)	70,101,113	1.30	5 (7%)
20	CLA	3	412	3	69,73,73	1.15	6 (8%)	82,113,113	1.15	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	9	608	6	64,68,73	1.20	7 (10%)	76,107,113	1.19	5 (6%)
20	CLA	B	807	8	69,73,73	1.17	8 (11%)	82,113,113	1.15	6 (7%)
22	XAT	7	317	-	41,47,47	0.18	0	54,74,74	0.81	2 (3%)
24	LHG	F	5002	-	42,42,48	0.31	0	45,48,54	0.32	0
25	PTY	8	318	-	20,20,49	0.66	0	21,24,54	0.54	0
20	CLA	7	313	4	69,73,73	1.22	8 (11%)	82,113,113	1.17	5 (6%)
20	CLA	L	306	-	54,58,73	1.29	7 (12%)	64,95,113	1.33	5 (7%)
24	LHG	J	4004	-	32,35,48	0.23	0	34,37,54	0.33	0
36	4RF	A	859	-	38,38,56	0.43	0	41,41,59	0.38	0
34	SF4	C	101	9	0,12,12	-	-	-	-	-
24	LHG	G	4006	-	48,48,48	0.30	0	51,54,54	0.28	0
20	CLA	B	825	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
21	LUT	2	614	-	42,43,43	0.40	1 (2%)	51,60,60	1.15	2 (3%)
19	CHL	9	606	-	41,55,74	0.93	2 (4%)	35,91,114	2.59	5 (14%)
20	CLA	B	830	8	69,73,73	1.22	8 (11%)	82,113,113	1.18	8 (9%)
25	PTY	7	322	-	24,24,49	0.63	0	27,29,54	0.50	0
20	CLA	2	611	-	64,68,73	1.19	7 (10%)	76,107,113	1.23	4 (5%)
23	BCR	A	847	-	41,41,41	0.17	0	56,56,56	0.65	1 (1%)
23	BCR	3	419	-	41,41,41	0.22	0	56,56,56	0.49	0
19	CHL	7	306	-	40,54,74	0.93	2 (5%)	34,90,114	2.29	6 (17%)
23	BCR	B	846	-	41,41,41	0.38	0	56,56,56	1.31	7 (12%)
27	3PH	2	620	-	32,32,47	0.32	0	35,37,52	0.34	0
20	CLA	A	833	7	69,73,73	1.13	7 (10%)	82,113,113	1.19	5 (6%)
20	CLA	A	835	7	69,73,73	1.15	7 (10%)	82,113,113	1.23	6 (7%)
26	SQD	B	851	-	29,31,54	0.22	0	39,42,65	0.25	0
34	SF4	C	102	9	0,12,12	-	-	-	-	-
20	CLA	9	601	6	50,54,73	1.76	8 (16%)	59,90,113	1.16	4 (6%)
20	CLA	A	824	-	69,73,73	1.15	8 (11%)	82,113,113	1.10	5 (6%)
20	CLA	A	825	7	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)
20	CLA	7	324	5	64,68,73	1.24	7 (10%)	76,107,113	1.30	5 (6%)
20	CLA	7	315	4	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
23	BCR	L	309	-	41,41,41	0.15	0	56,56,56	0.24	0
20	CLA	A	809	7	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.14	6 (7%)
20	CLA	B	815	-	69,73,73	1.14	8 (11%)	82,113,113	1.13	5 (6%)
20	CLA	B	808	8	69,73,73	1.13	7 (10%)	82,113,113	1.18	4 (4%)
26	SQD	9	618	-	35,37,54	0.27	0	45,48,65	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	1	611	1	50,54,73	1.37	9 (18%)	59,90,113	1.40	6 (10%)
20	CLA	3	405	3	54,58,73	1.30	8 (14%)	64,95,113	1.31	5 (7%)
20	CLA	3	411	3	60,64,73	1.26	8 (13%)	70,101,113	1.24	5 (7%)
20	CLA	8	309	24	64,68,73	1.21	8 (12%)	76,107,113	1.23	5 (6%)
34	SF4	A	846	7,8	0,12,12	-	-	-		
19	CHL	8	305	-	41,55,74	0.88	2 (4%)	35,91,114	2.39	8 (22%)
20	CLA	A	820	7	64,68,73	1.18	6 (9%)	76,107,113	1.16	4 (5%)
23	BCR	3	418	-	41,41,41	0.20	0	56,56,56	0.99	2 (3%)
23	BCR	A	849	-	41,41,41	0.29	0	56,56,56	0.95	4 (7%)
20	CLA	2	602	2	60,64,73	1.25	7 (11%)	71,102,113	1.26	4 (5%)
20	CLA	B	813	8	69,73,73	1.17	8 (11%)	82,113,113	1.18	6 (7%)
20	CLA	2	613	-	54,58,73	1.34	8 (14%)	64,95,113	1.32	9 (14%)
23	BCR	B	849	-	41,41,41	0.19	0	56,56,56	0.67	2 (3%)
23	BCR	G	4005	-	41,41,41	0.24	0	56,56,56	0.84	3 (5%)
23	BCR	H	205	-	41,41,41	0.30	0	56,56,56	0.72	2 (3%)
20	CLA	A	808	7	69,73,73	1.12	7 (10%)	82,113,113	1.09	6 (7%)
23	BCR	B	845	-	41,41,41	0.16	0	56,56,56	0.37	0
25	PTY	H	202	-	31,31,49	0.53	0	34,36,54	0.75	1 (2%)
19	CHL	7	308	-	42,56,74	0.86	1 (2%)	36,92,114	2.55	9 (25%)
24	LHG	I	201	-	48,48,48	0.30	0	51,54,54	0.31	0
20	CLA	B	831	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
20	CLA	1	602	1	65,69,73	1.20	8 (12%)	77,108,113	1.17	5 (6%)
20	CLA	3	408	3	64,68,73	1.16	6 (9%)	76,107,113	1.13	5 (6%)
20	CLA	B	818	8	69,73,73	1.15	7 (10%)	82,113,113	1.16	4 (4%)
20	CLA	1	605	-	49,53,73	1.37	6 (12%)	58,89,113	1.36	4 (6%)
20	CLA	3	407	3	69,73,73	1.17	7 (10%)	82,113,113	1.23	5 (6%)
28	LMG	F	5001	-	46,46,55	0.19	0	54,54,63	0.16	0
28	LMG	7	301	-	40,40,55	0.22	0	48,48,63	0.23	0
20	CLA	F	5003	5	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
24	LHG	9	619	-	48,48,48	0.31	0	51,54,54	0.32	0
20	CLA	2	607	2	50,54,73	1.35	7 (14%)	59,90,113	1.21	4 (6%)
20	CLA	A	807	7	69,73,73	1.13	6 (8%)	82,113,113	1.06	5 (6%)
20	CLA	1	608	1	64,68,73	1.19	8 (12%)	76,107,113	1.25	5 (6%)
20	CLA	G	4003	13	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
23	BCR	8	316	-	41,41,41	0.17	0	56,56,56	0.50	0
19	CHL	7	307	-	45,59,74	0.83	3 (6%)	40,96,114	2.54	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	817	-	59,63,73	1.25	6 (10%)	70,101,113	1.33	6 (8%)
20	CLA	A	822	7	69,73,73	1.15	7 (10%)	82,113,113	1.17	7 (8%)
20	CLA	B	810	8	69,73,73	1.16	7 (10%)	82,113,113	1.19	5 (6%)
20	CLA	B	842	24	69,73,73	1.17	7 (10%)	82,113,113	1.24	4 (4%)
21	LUT	2	615	-	42,43,43	0.27	0	51,60,60	0.70	1 (1%)
20	CLA	A	834	7	59,63,73	1.26	8 (13%)	70,101,113	1.25	5 (7%)
24	LHG	A	854	-	44,44,48	0.30	0	47,50,54	0.31	0
35	OCD	A	855	-	10,10,18	0.24	0	9,9,17	0.19	0
20	CLA	A	843	24	54,58,73	1.29	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	9	612	6	49,53,73	1.56	10 (20%)	58,89,113	1.54	8 (13%)
23	BCR	A	852	-	41,41,41	0.15	0	56,56,56	0.34	0
23	BCR	A	858	-	41,41,41	0.24	0	56,56,56	0.42	1 (1%)
20	CLA	A	836	-	64,68,73	1.25	9 (14%)	76,107,113	1.26	5 (6%)
20	CLA	K	204	-	52,56,73	1.34	5 (9%)	61,92,113	1.34	5 (8%)
20	CLA	7	303	4	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
20	CLA	8	311	5	69,73,73	1.51	10 (14%)	82,113,113	1.14	5 (6%)
20	CLA	2	603	2	64,68,73	1.26	8 (12%)	76,107,113	1.37	6 (7%)
20	CLA	3	414	3	50,54,73	1.36	7 (14%)	59,90,113	1.30	4 (6%)
20	CLA	8	308	5	64,68,73	1.16	8 (12%)	76,107,113	1.08	4 (5%)
20	CLA	A	804	-	69,73,73	1.19	10 (14%)	82,113,113	1.16	4 (4%)
20	CLA	A	815	7	66,70,73	1.22	9 (13%)	78,109,113	1.13	5 (6%)
24	LHG	9	617	20	40,40,48	0.33	0	43,46,54	0.36	0
20	CLA	A	827	7	64,68,73	1.20	8 (12%)	76,107,113	1.29	7 (9%)
20	CLA	B	841	8	69,73,73	1.14	7 (10%)	82,113,113	1.08	6 (7%)
20	CLA	B	814	8	69,73,73	1.17	6 (8%)	82,113,113	1.22	4 (4%)
20	CLA	2	612	2	47,52,73	1.39	7 (14%)	55,87,113	1.29	4 (7%)
20	CLA	A	818	7	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
22	XAT	1	616	-	41,47,47	0.15	0	54,74,74	1.04	4 (7%)
24	LHG	7	320	20	48,48,48	0.29	0	51,54,54	0.28	0
20	CLA	3	410	3	56,60,73	1.32	7 (12%)	65,97,113	1.44	7 (10%)
20	CLA	B	823	8	69,73,73	1.13	8 (11%)	82,113,113	1.22	6 (7%)
19	CHL	2	606	-	41,55,74	0.89	2 (4%)	35,91,114	2.34	8 (22%)
20	CLA	1	604	-	54,58,73	1.31	7 (12%)	64,95,113	1.32	6 (9%)
20	CLA	9	604	6	54,58,73	1.31	8 (14%)	64,95,113	1.23	5 (7%)
29	DGD	B	850	-	62,62,67	0.18	0	76,76,81	0.24	0
25	PTY	B	801	-	26,26,49	0.61	0	29,31,54	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	806	8	69,73,73	1.14	7 (10%)	82,113,113	1.33	7 (8%)
21	LUT	2	617	-	42,43,43	0.31	0	51,60,60	0.36	0
23	BCR	7	318	-	41,41,41	0.14	0	56,56,56	0.40	0
20	CLA	8	307	5	50,54,73	1.36	8 (16%)	59,90,113	1.16	4 (6%)
20	CLA	B	811	8	69,73,73	1.13	8 (11%)	82,113,113	1.19	4 (4%)
25	PTY	1	622	-	19,19,49	0.69	0	22,24,54	0.53	0
20	CLA	B	805	8	52,56,73	1.30	8 (15%)	61,92,113	1.30	5 (8%)
24	LHG	A	853	20	29,29,48	0.35	0	33,35,54	0.40	0
19	CHL	1	606	-	41,55,74	0.93	2 (4%)	35,91,114	2.24	9 (25%)

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
31	LMU	A	856	-	-	0/21/61/61	0/2/2/2
23	BCR	B	847	-	-	2/29/63/63	0/2/2/2
20	CLA	9	609	24	1/1/14/20	17/33/109/115	-
25	PTY	H	201	-	-	21/49/49/53	-
20	CLA	8	313	5	1/1/12/20	6/23/99/115	-
20	CLA	A	838	7	1/1/12/20	9/23/99/115	-
33	PQN	B	844	-	-	9/23/43/43	0/2/2/2
23	BCR	A	848	-	-	11/29/63/63	0/2/2/2
20	CLA	7	312	4	1/1/12/20	8/24/100/115	-
20	CLA	A	816	7	-	14/39/115/115	-
25	PTY	8	317	-	-	8/27/27/53	-
20	CLA	1	610	24	1/1/11/20	9/17/93/115	-
20	CLA	A	811	7	1/1/15/20	13/39/115/115	-
20	CLA	A	810	-	1/1/14/20	6/33/109/115	-
20	CLA	A	812	7	1/1/15/20	14/39/115/115	-
20	CLA	B	816	8	1/1/13/20	7/27/103/115	-
20	CLA	F	5006	-	1/1/11/20	9/18/94/115	-
21	LUT	9	613	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	B	848	-	-	2/29/63/63	0/2/2/2
24	LHG	H	203	-	-	8/42/42/53	-
23	BCR	J	4001	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	L	311	-	-	11/47/87/95	0/2/2/2
20	CLA	G	4002	13	1/1/11/20	8/18/94/115	-
20	CLA	B	803	-	1/1/15/20	21/39/115/115	-
20	CLA	B	835	-	1/1/14/20	12/33/109/115	-
20	CLA	B	838	-	1/1/14/20	8/33/109/115	-
20	CLA	3	409	-	1/1/12/20	7/21/97/115	-
20	CLA	A	837	7	1/1/13/20	8/27/103/115	-
20	CLA	A	828	-	1/1/15/20	9/39/115/115	-
24	LHG	7	323	-	-	5/25/25/53	-
20	CLA	7	314	4	1/1/12/20	10/21/97/115	-
20	CLA	F	5007	12	1/1/11/20	7/20/96/115	-
20	CLA	A	814	7	1/1/15/20	18/39/115/115	-
20	CLA	F	5008	12	-	10/17/93/115	-
25	PTY	L	310	-	-	9/22/22/53	-
20	CLA	2	604	-	1/1/12/20	8/21/97/115	-
20	CLA	B	832	8	1/1/14/20	10/33/109/115	-
20	CLA	B	817	8	1/1/14/20	9/33/109/115	-
20	CLA	L	305	18	1/1/15/20	7/39/115/115	-
19	CHL	2	601	2	2/2/19/26	16/33/131/137	-
20	CLA	L	302	-	1/1/15/20	21/39/115/115	-
20	CLA	A	813	7	1/1/13/20	10/27/103/115	-
20	CLA	7	309	4	1/1/15/20	11/39/115/115	-
24	LHG	2	621	-	-	6/40/40/53	-
20	CLA	9	605	6	1/1/11/20	2/15/91/115	-
20	CLA	B	820	-	1/1/15/20	14/39/115/115	-
20	CLA	B	809	8	1/1/15/20	10/39/115/115	-
20	CLA	1	613	1	1/1/13/20	9/27/103/115	-
20	CLA	A	842	7	1/1/14/20	9/35/111/115	-
20	CLA	B	837	8	1/1/12/20	4/23/99/115	-
23	BCR	B	802	-	-	6/29/63/63	0/2/2/2
20	CLA	3	404	-	1/1/11/20	7/17/93/115	-
20	CLA	1	614	1	1/1/11/20	8/17/93/115	-
20	CLA	9	603	6	1/1/13/20	6/27/103/115	-
24	LHG	1	621	-	-	10/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	L	304	18	1/1/15/20	11/39/115/115	-
20	CLA	1	603	1	1/1/15/20	20/39/115/115	-
20	CLA	3	402	3	1/1/15/20	16/39/115/115	-
23	BCR	3	417	-	-	4/29/63/63	0/2/2/2
26	SQD	2	619	-	-	13/36/56/69	0/1/1/1
22	XAT	8	315	-	-	1/31/93/93	0/4/4/4
24	LHG	3	420	-	-	5/19/19/53	-
24	LHG	1	619	-	-	9/48/48/53	-
24	LHG	7	325	-	-	6/44/44/53	-
20	CLA	1	612	-	1/1/13/20	9/27/103/115	-
22	XAT	9	614	-	-	0/31/93/93	0/4/4/4
24	LHG	3	424	-	-	15/43/43/53	-
20	CLA	B	840	-	1/1/15/20	11/39/115/115	-
20	CLA	B	812	-	1/1/13/20	8/27/103/115	-
20	CLA	2	605	-	1/1/11/20	9/15/91/115	-
28	LMG	A	801	-	-	3/26/46/70	0/1/1/1
20	CLA	B	819	8	1/1/15/20	15/39/115/115	-
31	LMU	9	616	-	-	5/21/61/61	0/2/2/2
20	CLA	A	823	7	1/1/15/20	19/39/115/115	-
20	CLA	B	836	-	1/1/12/20	11/21/97/115	-
20	CLA	B	821	8	1/1/15/20	11/39/115/115	-
21	LUT	1	615	-	3/3/12/27	11/29/67/67	0/2/2/2
20	CLA	2	608	-	1/1/11/20	5/15/91/115	-
20	CLA	9	610	6	1/1/12/20	10/21/97/115	-
20	CLA	9	607	6	1/1/15/20	11/39/115/115	-
20	CLA	3	406	-	1/1/13/20	8/27/103/115	-
20	CLA	8	303	-	1/1/12/20	6/21/97/115	-
20	CLA	B	843	-	1/1/15/20	15/39/115/115	-
20	CLA	K	202	-	1/1/13/20	6/27/103/115	-
20	CLA	A	839	7	1/1/15/20	11/39/115/115	-
20	CLA	F	5005	-	1/1/13/20	11/27/103/115	-
20	CLA	B	827	8	1/1/15/20	8/39/115/115	-
21	LUT	8	314	-	3/3/12/27	2/29/67/67	0/2/2/2
28	LMG	7	319	-	-	11/49/69/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PTY	F	5010	-	-	7/25/25/53	-
33	PQN	A	845	-	-	0/23/43/43	0/2/2/2
19	CHL	8	306	-	2/2/17/26	9/21/119/137	-
22	XAT	9	615	-	-	5/31/93/93	0/4/4/4
23	BCR	F	5009	-	-	4/29/63/63	0/2/2/2
20	CLA	8	312	5	1/1/11/20	7/17/93/115	-
29	DGD	A	802	-	-	11/55/95/95	0/2/2/2
23	BCR	A	851	-	-	2/29/63/63	0/2/2/2
20	CLA	2	609	24	1/1/10/20	4/10/86/115	-
26	SQD	3	423	-	-	9/27/47/69	0/1/1/1
32	CL0	A	803	7	-	13/37/135/135	-
20	CLA	A	805	-	1/1/15/20	13/39/115/115	-
20	CLA	A	829	-	1/1/13/20	10/29/105/115	-
20	CLA	A	831	7	1/1/15/20	17/39/115/115	-
21	LUT	7	316	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	B	822	8	1/1/15/20	14/39/115/115	-
20	CLA	A	832	7	1/1/15/20	12/39/115/115	-
20	CLA	3	403	-	1/1/11/20	6/17/93/115	-
30	LMK	8	320	-	-	10/41/41/60	-
20	CLA	1	607	-	1/1/15/20	13/39/115/115	-
20	CLA	7	305	-	1/1/12/20	6/21/97/115	-
22	XAT	3	416	-	-	2/31/93/93	0/4/4/4
25	PTY	3	422	-	-	5/29/29/53	-
20	CLA	1	609	1	1/1/15/20	10/39/115/115	-
20	CLA	H	204	14	1/1/11/20	8/15/91/115	-
29	DGD	7	321	-	-	11/36/76/95	0/2/2/2
23	BCR	A	850	-	-	12/29/63/63	0/2/2/2
24	LHG	1	620	20	-	7/35/35/53	-
26	SQD	3	421	-	-	10/30/50/69	0/1/1/1
20	CLA	3	413	-	1/1/10/20	4/12/88/115	-
21	LUT	3	415	-	3/3/12/27	4/29/67/67	0/2/2/2
20	CLA	B	828	-	1/1/15/20	17/39/115/115	-
20	CLA	B	839	-	1/1/13/20	5/27/103/115	-
20	CLA	K	201	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	1	617	-	-	4/29/63/63	0/2/2/2
20	CLA	B	824	8	1/1/13/20	13/27/103/115	-
24	LHG	1	618	20	-	4/29/29/53	-
20	CLA	L	301	7	1/1/11/20	8/15/91/115	-
23	BCR	G	4001	-	-	5/29/63/63	0/2/2/2
20	CLA	2	622	-	1/1/11/20	5/17/93/115	-
25	PTY	1	623	-	-	8/38/38/53	-
20	CLA	9	602	6	1/1/14/20	18/33/109/115	-
24	LHG	2	618	20	-	5/45/45/53	-
19	CHL	1	601	-	1/1/17/26	4/21/119/137	-
20	CLA	B	833	8	1/1/15/20	13/39/115/115	-
20	CLA	G	4004	-	1/1/11/20	6/15/91/115	-
20	CLA	A	830	7	1/1/15/20	15/39/115/115	-
20	CLA	J	4002	16	1/1/11/20	10/20/96/115	-
20	CLA	2	610	2	1/1/11/20	8/17/93/115	-
20	CLA	A	819	-	1/1/13/20	13/27/103/115	-
20	CLA	A	844	-	1/1/15/20	10/39/115/115	-
20	CLA	B	826	-	1/1/15/20	10/39/115/115	-
21	LUT	2	616	-	3/3/12/27	7/29/67/67	0/2/2/2
19	CHL	3	401	3	2/2/18/26	14/27/125/137	-
20	CLA	A	821	7	1/1/15/20	17/39/115/115	-
19	CHL	8	304	-	1/1/16/26	9/17/115/137	-
20	CLA	7	304	4	1/1/13/20	11/27/103/115	-
20	CLA	B	829	8	1/1/15/20	24/39/115/115	-
20	CLA	K	203	17	1/1/11/20	8/15/91/115	-
23	BCR	F	5004	-	-	0/29/63/63	0/2/2/2
23	BCR	I	202	-	-	4/29/63/63	0/2/2/2
28	LMG	8	301	-	-	8/45/65/70	0/1/1/1
20	CLA	8	310	5	1/1/12/20	10/21/97/115	-
20	CLA	A	841	7	1/1/15/20	17/39/115/115	-
23	BCR	K	205	-	-	9/29/63/63	0/2/2/2
20	CLA	A	826	7	1/1/14/20	15/33/109/115	-
23	BCR	J	4003	-	-	4/29/63/63	0/2/2/2
24	LHG	B	852	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	L	303	-	-	4/29/63/63	0/2/2/2
24	LHG	8	321	-	-	10/35/35/53	-
20	CLA	B	834	8	1/1/15/20	18/39/115/115	-
20	CLA	7	310	4	1/1/15/20	13/39/115/115	-
31	LMU	A	857	-	-	5/21/61/61	0/2/2/2
20	CLA	L	307	-	1/1/12/20	11/21/97/115	-
20	CLA	A	840	7	1/1/14/20	11/33/109/115	-
20	CLA	A	806	7	1/1/15/20	13/39/115/115	-
20	CLA	8	302	5	1/1/14/20	13/33/109/115	-
23	BCR	L	308	-	-	4/29/63/63	0/2/2/2
19	CHL	7	302	-	3/3/20/26	16/39/137/137	-
20	CLA	7	311	24	1/1/14/20	9/33/109/115	-
24	LHG	8	319	20	-	4/38/38/53	-
24	LHG	F	5011	-	-	8/46/46/53	-
20	CLA	9	611	-	1/1/13/20	8/27/103/115	-
20	CLA	3	412	3	1/1/15/20	16/39/115/115	-
20	CLA	9	608	6	1/1/14/20	11/33/109/115	-
20	CLA	B	807	8	1/1/15/20	14/39/115/115	-
22	XAT	7	317	-	-	4/31/93/93	0/4/4/4
24	LHG	F	5002	-	-	12/47/47/53	-
25	PTY	8	318	-	-	11/23/23/53	-
20	CLA	7	313	4	1/1/15/20	11/39/115/115	-
20	CLA	L	306	-	1/1/12/20	7/21/97/115	-
24	LHG	J	4004	-	-	6/35/37/53	-
36	4RF	A	859	-	-	17/41/41/59	-
34	SF4	C	101	9	-	-	0/6/5/5
24	LHG	G	4006	-	-	7/53/53/53	-
20	CLA	B	825	-	1/1/15/20	12/39/115/115	-
21	LUT	2	614	-	3/3/12/27	4/29/67/67	0/2/2/2
19	CHL	9	606	-	1/1/16/26	10/17/115/137	-
20	CLA	B	830	8	1/1/15/20	15/39/115/115	-
25	PTY	7	322	-	-	5/28/28/53	-
20	CLA	2	611	-	1/1/14/20	11/33/109/115	-
23	BCR	A	847	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	3	419	-	-	5/29/63/63	0/2/2/2
19	CHL	7	306	-	1/1/16/26	7/15/113/137	-
23	BCR	B	846	-	-	13/29/63/63	0/2/2/2
27	3PH	2	620	-	-	6/34/34/49	-
20	CLA	A	833	7	1/1/15/20	9/39/115/115	-
20	CLA	A	835	7	1/1/15/20	8/39/115/115	-
26	SQD	B	851	-	-	10/25/45/69	0/1/1/1
34	SF4	C	102	9	-	-	0/6/5/5
20	CLA	9	601	6	1/1/11/20	12/17/93/115	-
20	CLA	A	824	-	1/1/15/20	14/39/115/115	-
20	CLA	A	825	7	1/1/14/20	9/33/109/115	-
20	CLA	7	324	5	1/1/14/20	9/33/109/115	-
20	CLA	7	315	4	1/1/15/20	7/39/115/115	-
23	BCR	L	309	-	-	0/29/63/63	0/2/2/2
20	CLA	A	809	7	1/1/15/20	14/39/115/115	-
20	CLA	B	804	-	1/1/15/20	12/39/115/115	-
20	CLA	B	815	-	1/1/15/20	14/39/115/115	-
20	CLA	B	808	8	1/1/15/20	14/39/115/115	-
26	SQD	9	618	-	-	9/32/52/69	0/1/1/1
20	CLA	1	611	1	1/1/11/20	8/17/93/115	-
20	CLA	3	405	3	1/1/12/20	5/21/97/115	-
20	CLA	3	411	3	1/1/13/20	9/27/103/115	-
20	CLA	8	309	24	1/1/14/20	13/33/109/115	-
34	SF4	A	846	7,8	-	-	0/6/5/5
19	CHL	8	305	-	1/1/16/26	10/17/115/137	-
20	CLA	A	820	7	1/1/14/20	13/33/109/115	-
23	BCR	3	418	-	-	9/29/63/63	0/2/2/2
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
20	CLA	2	602	2	1/1/13/20	10/29/105/115	-
20	CLA	B	813	8	1/1/15/20	13/39/115/115	-
20	CLA	2	613	-	1/1/12/20	9/21/97/115	-
23	BCR	B	849	-	-	7/29/63/63	0/2/2/2
23	BCR	G	4005	-	-	8/29/63/63	0/2/2/2
23	BCR	H	205	-	-	10/29/63/63	0/2/2/2
20	CLA	A	808	7	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
25	PTY	H	202	-	-	16/35/35/53	-
19	CHL	7	308	-	1/1/16/26	6/18/116/137	-
24	LHG	I	201	-	-	17/53/53/53	-
20	CLA	B	831	-	1/1/15/20	15/39/115/115	-
20	CLA	1	602	1	1/1/14/20	12/35/111/115	-
20	CLA	3	408	3	1/1/14/20	14/33/109/115	-
20	CLA	B	818	8	1/1/15/20	18/39/115/115	-
20	CLA	1	605	-	1/1/11/20	6/15/91/115	-
20	CLA	3	407	3	1/1/15/20	15/39/115/115	-
28	LMG	F	5001	-	-	6/41/61/70	0/1/1/1
28	LMG	7	301	-	-	13/35/55/70	0/1/1/1
20	CLA	F	5003	5	1/1/15/20	13/39/115/115	-
24	LHG	9	619	-	-	8/53/53/53	-
20	CLA	2	607	2	1/1/11/20	9/17/93/115	-
20	CLA	A	807	7	1/1/15/20	9/39/115/115	-
20	CLA	1	608	1	1/1/14/20	12/33/109/115	-
20	CLA	G	4003	13	1/1/11/20	8/17/93/115	-
23	BCR	8	316	-	-	4/29/63/63	0/2/2/2
19	CHL	7	307	-	2/2/17/26	10/21/119/137	-
20	CLA	A	817	-	1/1/13/20	9/27/103/115	-
20	CLA	A	822	7	1/1/15/20	13/39/115/115	-
20	CLA	B	810	8	1/1/15/20	12/39/115/115	-
20	CLA	B	842	24	1/1/15/20	11/39/115/115	-
21	LUT	2	615	-	3/3/12/27	6/29/67/67	0/2/2/2
20	CLA	A	834	7	1/1/13/20	7/27/103/115	-
24	LHG	A	854	-	-	11/49/49/53	-
35	OCD	A	855	-	-	0/8/8/16	-
20	CLA	A	843	24	1/1/12/20	10/21/97/115	-
20	CLA	9	612	6	-	8/15/91/115	-
23	BCR	A	852	-	-	4/29/63/63	0/2/2/2
23	BCR	A	858	-	-	6/29/63/63	0/2/2/2
20	CLA	A	836	-	1/1/14/20	14/33/109/115	-
20	CLA	K	204	-	1/1/11/20	10/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	303	4	1/1/14/20	11/33/109/115	-
20	CLA	A	804	-	1/1/15/20	13/39/115/115	-
20	CLA	2	603	2	1/1/14/20	13/33/109/115	-
20	CLA	3	414	3	1/1/11/20	8/17/93/115	-
20	CLA	8	308	5	1/1/14/20	11/33/109/115	-
20	CLA	A	815	7	1/1/14/20	15/36/112/115	-
20	CLA	8	311	5	-	16/39/115/115	-
24	LHG	9	617	20	-	11/45/45/53	-
20	CLA	A	827	7	1/1/14/20	11/33/109/115	-
20	CLA	B	841	8	1/1/15/20	15/39/115/115	-
20	CLA	B	814	8	1/1/15/20	17/39/115/115	-
20	CLA	2	612	2	1/1/10/20	4/14/90/115	-
20	CLA	A	818	7	1/1/15/20	13/39/115/115	-
22	XAT	1	616	-	-	3/31/93/93	0/4/4/4
24	LHG	7	320	20	-	17/53/53/53	-
20	CLA	3	410	3	1/1/12/20	9/24/100/115	-
20	CLA	B	823	8	1/1/15/20	15/39/115/115	-
19	CHL	2	606	-	2/2/16/26	10/17/115/137	-
20	CLA	1	604	-	1/1/12/20	9/21/97/115	-
20	CLA	9	604	6	1/1/12/20	7/21/97/115	-
29	DGD	B	850	-	-	7/50/90/95	0/2/2/2
25	PTY	B	801	-	-	12/30/30/53	-
20	CLA	B	806	8	1/1/15/20	14/39/115/115	-
21	LUT	2	617	-	3/3/12/27	4/29/67/67	0/2/2/2
23	BCR	7	318	-	-	6/29/63/63	0/2/2/2
20	CLA	8	307	5	1/1/11/20	6/17/93/115	-
20	CLA	B	811	8	1/1/15/20	18/39/115/115	-
25	PTY	1	622	-	-	7/22/22/53	-
20	CLA	B	805	8	1/1/11/20	6/19/95/115	-
24	LHG	A	853	20	-	7/33/33/53	-
19	CHL	1	606	-	1/1/16/26	4/17/115/137	-

All (1325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	311	CLA	MG-NC	7.33	2.23	2.06
20	9	601	CLA	MG-NB	6.22	2.18	2.05
20	9	601	CLA	MG-NA	5.53	2.19	2.06
20	9	612	CLA	MG-NA	4.69	2.17	2.06
20	9	603	CLA	MG-NC	4.38	2.16	2.06
20	1	612	CLA	C1D-ND	4.35	1.43	1.37
20	F	5008	CLA	MG-NA	4.27	2.16	2.06
20	F	5008	CLA	MG-ND	-4.06	1.97	2.05
20	9	605	CLA	MG-NA	4.04	2.15	2.06
20	9	603	CLA	C1D-ND	3.89	1.43	1.37
20	9	605	CLA	C1D-ND	3.86	1.42	1.37
20	A	821	CLA	C1D-ND	3.79	1.42	1.37
20	7	324	CLA	C1D-ND	3.78	1.42	1.37
20	8	311	CLA	C1D-ND	3.78	1.42	1.37
20	A	838	CLA	C1D-ND	3.73	1.42	1.37
20	2	622	CLA	C1D-ND	3.70	1.42	1.37
20	G	4002	CLA	C1D-ND	3.70	1.42	1.37
20	2	603	CLA	C1D-ND	3.67	1.42	1.37
20	9	612	CLA	C1D-ND	3.67	1.42	1.37
20	1	611	CLA	C1D-ND	3.67	1.42	1.37
20	2	613	CLA	C4B-NB	3.67	1.42	1.37
20	1	602	CLA	C1D-ND	3.66	1.42	1.37
20	3	407	CLA	C1D-ND	3.65	1.42	1.37
32	A	803	CL0	C3A-C2A	-3.64	1.51	1.54
20	B	820	CLA	C1D-ND	3.63	1.42	1.37
20	7	312	CLA	C1D-ND	3.62	1.42	1.37
20	A	825	CLA	C1D-ND	3.62	1.42	1.37
20	A	836	CLA	C1D-ND	3.62	1.42	1.37
20	3	408	CLA	C1D-ND	3.61	1.42	1.37
20	F	5003	CLA	C1D-ND	3.61	1.42	1.37
20	A	819	CLA	C1D-ND	3.61	1.42	1.37
20	B	817	CLA	C1D-ND	3.61	1.42	1.37
20	J	4002	CLA	C1D-ND	3.61	1.42	1.37
20	9	610	CLA	C1D-ND	3.60	1.42	1.37
20	A	842	CLA	C1D-ND	3.60	1.42	1.37
20	7	304	CLA	C1D-ND	3.58	1.42	1.37
20	3	404	CLA	C1D-ND	3.58	1.42	1.37
20	A	816	CLA	C1D-ND	3.58	1.42	1.37
20	B	843	CLA	C1D-ND	3.58	1.42	1.37
20	1	608	CLA	C1D-ND	3.57	1.42	1.37
20	8	312	CLA	C1D-ND	3.57	1.42	1.37
20	3	410	CLA	C1D-ND	3.57	1.42	1.37
20	B	833	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	409	CLA	C1D-ND	3.56	1.42	1.37
20	7	311	CLA	C1D-ND	3.56	1.42	1.37
20	G	4003	CLA	C1D-ND	3.56	1.42	1.37
20	B	821	CLA	C1D-ND	3.56	1.42	1.37
20	1	603	CLA	C1D-ND	3.55	1.42	1.37
20	3	414	CLA	C1D-ND	3.55	1.42	1.37
20	F	5007	CLA	C1D-ND	3.54	1.42	1.37
20	8	309	CLA	C1D-ND	3.54	1.42	1.37
20	K	204	CLA	C1D-ND	3.54	1.42	1.37
20	3	402	CLA	C1D-ND	3.54	1.42	1.37
20	F	5006	CLA	C1D-ND	3.54	1.42	1.37
20	A	831	CLA	C1D-ND	3.54	1.42	1.37
20	B	818	CLA	C1D-ND	3.54	1.42	1.37
20	K	201	CLA	C1D-ND	3.54	1.42	1.37
20	7	305	CLA	C1D-ND	3.54	1.42	1.37
20	B	836	CLA	C1D-ND	3.54	1.42	1.37
20	9	608	CLA	C1D-ND	3.53	1.42	1.37
20	F	5008	CLA	C1D-ND	3.53	1.42	1.37
20	9	607	CLA	C1D-ND	3.53	1.42	1.37
20	B	837	CLA	C1D-ND	3.53	1.42	1.37
20	B	827	CLA	MG-NA	3.53	2.14	2.06
20	K	203	CLA	C1D-ND	3.52	1.42	1.37
20	3	406	CLA	C1D-ND	3.52	1.42	1.37
20	L	302	CLA	C1D-ND	3.52	1.42	1.37
20	A	815	CLA	C1D-ND	3.52	1.42	1.37
20	8	310	CLA	C1D-ND	3.52	1.42	1.37
20	B	830	CLA	C1D-ND	3.51	1.42	1.37
20	A	837	CLA	C1D-ND	3.51	1.42	1.37
20	H	204	CLA	C1D-ND	3.51	1.42	1.37
19	8	304	CHL	C3A-C2A	-3.51	1.51	1.54
20	3	413	CLA	C1D-ND	3.51	1.42	1.37
20	B	807	CLA	C1D-ND	3.50	1.42	1.37
20	G	4004	CLA	C1D-ND	3.50	1.42	1.37
20	A	841	CLA	C1D-ND	3.50	1.42	1.37
20	1	613	CLA	C1D-ND	3.50	1.42	1.37
20	8	302	CLA	C1D-ND	3.50	1.42	1.37
20	8	303	CLA	C1D-ND	3.50	1.42	1.37
20	B	819	CLA	C1D-ND	3.50	1.42	1.37
20	B	806	CLA	C1D-ND	3.49	1.42	1.37
20	A	844	CLA	C1D-ND	3.49	1.42	1.37
20	2	612	CLA	C1D-ND	3.49	1.42	1.37
20	A	826	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	609	CLA	C1D-ND	3.49	1.42	1.37
20	9	611	CLA	C1D-ND	3.49	1.42	1.37
20	B	840	CLA	C1D-ND	3.49	1.42	1.37
20	B	823	CLA	C1D-ND	3.48	1.42	1.37
20	2	609	CLA	C1D-ND	3.48	1.42	1.37
20	A	827	CLA	C1D-ND	3.48	1.42	1.37
20	A	835	CLA	C1D-ND	3.48	1.42	1.37
20	A	834	CLA	C1D-ND	3.47	1.42	1.37
20	2	605	CLA	C1D-ND	3.47	1.42	1.37
20	A	818	CLA	C1D-ND	3.47	1.42	1.37
20	B	814	CLA	C1D-ND	3.47	1.42	1.37
20	F	5005	CLA	C1D-ND	3.46	1.42	1.37
20	1	610	CLA	C1D-ND	3.46	1.42	1.37
20	A	814	CLA	C1D-ND	3.46	1.42	1.37
20	1	607	CLA	C1D-ND	3.46	1.42	1.37
20	A	843	CLA	C1D-ND	3.46	1.42	1.37
20	2	602	CLA	C1D-ND	3.46	1.42	1.37
20	A	810	CLA	C1D-ND	3.46	1.42	1.37
20	1	605	CLA	C1D-ND	3.45	1.42	1.37
20	2	607	CLA	C1D-ND	3.45	1.42	1.37
20	7	313	CLA	C1D-ND	3.45	1.42	1.37
20	B	810	CLA	C1D-ND	3.45	1.42	1.37
20	B	831	CLA	C1D-ND	3.45	1.42	1.37
20	A	833	CLA	C1D-ND	3.45	1.42	1.37
20	7	315	CLA	C1D-ND	3.44	1.42	1.37
20	3	403	CLA	C1D-ND	3.44	1.42	1.37
20	L	306	CLA	C1D-ND	3.44	1.42	1.37
20	2	610	CLA	C1D-ND	3.44	1.42	1.37
20	B	842	CLA	C1D-ND	3.44	1.42	1.37
20	A	824	CLA	C1D-ND	3.44	1.42	1.37
20	B	827	CLA	C1D-ND	3.44	1.42	1.37
20	L	304	CLA	C1D-ND	3.44	1.42	1.37
20	3	405	CLA	C1D-ND	3.44	1.42	1.37
20	A	805	CLA	C1D-ND	3.43	1.42	1.37
20	7	310	CLA	C1D-ND	3.43	1.42	1.37
20	B	829	CLA	C1D-ND	3.43	1.42	1.37
20	K	202	CLA	C1D-ND	3.43	1.42	1.37
20	B	811	CLA	C1D-ND	3.43	1.42	1.37
20	B	838	CLA	C1D-ND	3.43	1.42	1.37
20	9	602	CLA	C1D-ND	3.42	1.42	1.37
20	A	812	CLA	C1D-ND	3.42	1.42	1.37
20	B	808	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	604	CLA	C1D-ND	3.41	1.42	1.37
20	B	805	CLA	C1D-ND	3.41	1.42	1.37
20	7	303	CLA	C1D-ND	3.41	1.42	1.37
20	A	813	CLA	C1D-ND	3.40	1.42	1.37
20	B	822	CLA	C1D-ND	3.40	1.42	1.37
20	7	314	CLA	C1D-ND	3.40	1.42	1.37
20	B	832	CLA	C1D-ND	3.40	1.42	1.37
20	B	812	CLA	C1D-ND	3.40	1.42	1.37
20	2	604	CLA	C1D-ND	3.40	1.42	1.37
20	A	828	CLA	C1D-ND	3.40	1.42	1.37
20	B	813	CLA	C1D-ND	3.40	1.42	1.37
20	B	816	CLA	C1D-ND	3.40	1.42	1.37
20	9	604	CLA	C1D-ND	3.39	1.42	1.37
20	A	823	CLA	C1D-ND	3.39	1.42	1.37
20	2	608	CLA	C1D-ND	3.38	1.42	1.37
20	9	609	CLA	C1D-ND	3.38	1.42	1.37
20	A	822	CLA	C1D-ND	3.38	1.42	1.37
20	2	611	CLA	C1D-ND	3.38	1.42	1.37
20	A	830	CLA	C1D-ND	3.38	1.42	1.37
20	A	839	CLA	C1D-ND	3.38	1.42	1.37
20	A	832	CLA	C1D-ND	3.37	1.42	1.37
20	A	809	CLA	C1D-ND	3.37	1.42	1.37
20	B	826	CLA	C1D-ND	3.37	1.42	1.37
20	B	828	CLA	C1D-ND	3.37	1.42	1.37
20	A	829	CLA	C1D-ND	3.37	1.42	1.37
20	A	840	CLA	C1D-ND	3.36	1.42	1.37
20	3	411	CLA	C1D-ND	3.36	1.42	1.37
20	8	308	CLA	C1D-ND	3.36	1.42	1.37
20	3	412	CLA	C1D-ND	3.36	1.42	1.37
20	9	601	CLA	C1D-ND	3.35	1.42	1.37
20	L	307	CLA	C1D-ND	3.35	1.42	1.37
20	7	309	CLA	C1D-ND	3.34	1.42	1.37
20	B	824	CLA	C1D-ND	3.34	1.42	1.37
20	8	307	CLA	C1D-ND	3.34	1.42	1.37
20	A	806	CLA	C1D-ND	3.34	1.42	1.37
20	B	809	CLA	C1D-ND	3.34	1.42	1.37
20	1	614	CLA	C1D-ND	3.33	1.42	1.37
20	A	817	CLA	C1D-ND	3.33	1.42	1.37
20	B	835	CLA	C1D-ND	3.33	1.42	1.37
20	8	313	CLA	C1D-ND	3.33	1.42	1.37
20	A	808	CLA	C1D-ND	3.33	1.42	1.37
20	A	820	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	839	CLA	C1D-ND	3.32	1.42	1.37
20	A	842	CLA	C4B-NB	3.31	1.42	1.37
20	8	311	CLA	C4B-NB	3.31	1.42	1.37
19	1	606	CHL	C3A-C2A	-3.30	1.51	1.54
20	B	815	CLA	C1D-ND	3.30	1.42	1.37
20	A	807	CLA	C1D-ND	3.29	1.42	1.37
20	7	313	CLA	MG-ND	-3.28	1.99	2.05
20	9	605	CLA	MG-NB	3.28	2.12	2.05
20	B	803	CLA	C1D-ND	3.28	1.42	1.37
20	B	834	CLA	C1D-ND	3.27	1.42	1.37
20	2	613	CLA	C1D-ND	3.25	1.42	1.37
20	B	825	CLA	C1D-ND	3.25	1.42	1.37
20	1	614	CLA	C4B-NB	3.23	1.42	1.37
20	2	603	CLA	C4B-NB	3.23	1.42	1.37
20	L	301	CLA	C1D-ND	3.23	1.42	1.37
20	8	311	CLA	MG-NB	3.22	2.12	2.05
20	A	811	CLA	C1D-ND	3.20	1.42	1.37
20	9	603	CLA	C4B-NB	3.20	1.42	1.37
20	A	812	CLA	C4B-NB	3.19	1.42	1.37
20	A	804	CLA	C4B-NB	3.17	1.42	1.37
20	2	611	CLA	C4B-NB	3.17	1.42	1.37
20	8	310	CLA	C4B-NB	3.17	1.42	1.37
20	B	841	CLA	C1D-ND	3.16	1.42	1.37
20	3	413	CLA	C4B-NB	3.14	1.42	1.37
20	9	609	CLA	C4B-NB	3.14	1.42	1.37
20	A	813	CLA	C4B-NB	3.13	1.42	1.37
20	3	410	CLA	C4B-NB	3.13	1.42	1.37
20	2	612	CLA	C4B-NB	3.13	1.42	1.37
20	B	840	CLA	C4B-NB	3.12	1.42	1.37
20	3	414	CLA	C4B-NB	3.12	1.42	1.37
20	L	304	CLA	C4B-NB	3.12	1.42	1.37
20	9	612	CLA	C4B-NB	3.12	1.42	1.37
20	B	821	CLA	C4B-NB	3.12	1.42	1.37
20	1	613	CLA	C4B-NB	3.11	1.42	1.37
20	F	5008	CLA	C4B-NB	3.11	1.41	1.37
20	K	201	CLA	C4B-NB	3.11	1.41	1.37
20	2	602	CLA	C4B-NB	3.10	1.41	1.37
20	3	411	CLA	C4B-NB	3.10	1.41	1.37
20	2	609	CLA	C4B-NB	3.10	1.41	1.37
20	8	307	CLA	C4B-NB	3.10	1.41	1.37
20	7	311	CLA	C4B-NB	3.09	1.41	1.37
20	8	309	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	C4B-NB	3.09	1.41	1.37
20	B	830	CLA	C4B-NB	3.09	1.41	1.37
20	B	827	CLA	C4B-NB	3.09	1.41	1.37
20	A	834	CLA	C4B-NB	3.09	1.41	1.37
20	7	303	CLA	C4B-NB	3.08	1.41	1.37
20	B	841	CLA	C4B-NB	3.08	1.41	1.37
20	B	817	CLA	C4B-NB	3.08	1.41	1.37
20	8	313	CLA	C4B-NB	3.07	1.41	1.37
20	A	836	CLA	C4B-NB	3.07	1.41	1.37
20	B	820	CLA	C4B-NB	3.07	1.41	1.37
20	F	5005	CLA	C4B-NB	3.07	1.41	1.37
20	A	833	CLA	C1B-C2B	3.07	1.50	1.43
20	2	607	CLA	C4B-NB	3.07	1.41	1.37
20	2	613	CLA	CHC-C1C	3.07	1.44	1.38
20	7	305	CLA	C4B-NB	3.06	1.41	1.37
20	A	817	CLA	C4B-NB	3.06	1.41	1.37
20	3	405	CLA	C4B-NB	3.06	1.41	1.37
20	L	305	CLA	C1D-ND	3.05	1.41	1.37
20	F	5006	CLA	C4B-NB	3.05	1.41	1.37
20	B	823	CLA	C4B-NB	3.04	1.41	1.37
20	B	804	CLA	MG-NA	-3.04	1.99	2.06
20	B	812	CLA	C4B-NB	3.04	1.41	1.37
20	B	826	CLA	C4B-NB	3.04	1.41	1.37
20	L	306	CLA	C4B-NB	3.04	1.41	1.37
20	1	611	CLA	C4B-NB	3.03	1.41	1.37
20	8	312	CLA	C4B-NB	3.03	1.41	1.37
20	B	836	CLA	C4B-NB	3.03	1.41	1.37
20	7	313	CLA	C4B-NB	3.03	1.41	1.37
20	B	839	CLA	C4B-NB	3.03	1.41	1.37
20	L	301	CLA	C4B-NB	3.03	1.41	1.37
20	1	614	CLA	C3B-C4B	3.02	1.51	1.42
20	3	402	CLA	C4B-NB	3.02	1.41	1.37
20	3	404	CLA	C4B-NB	3.02	1.41	1.37
20	2	605	CLA	C4B-NB	3.02	1.41	1.37
20	A	837	CLA	C4B-NB	3.02	1.41	1.37
20	B	832	CLA	C4B-NB	3.01	1.41	1.37
20	B	842	CLA	C4B-NB	3.01	1.41	1.37
20	B	835	CLA	C4B-NB	3.01	1.41	1.37
20	1	609	CLA	C4B-NB	3.01	1.41	1.37
20	1	603	CLA	C4B-NB	3.01	1.41	1.37
20	B	811	CLA	C4B-NB	3.01	1.41	1.37
20	7	315	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	5007	CLA	C4B-NB	3.01	1.41	1.37
20	A	814	CLA	C4B-NB	3.00	1.41	1.37
20	L	302	CLA	C4B-NB	3.00	1.41	1.37
20	9	605	CLA	MG-ND	-3.00	1.99	2.05
20	A	821	CLA	C4B-NB	3.00	1.41	1.37
20	K	204	CLA	C4B-NB	3.00	1.41	1.37
20	A	840	CLA	C4B-NB	3.00	1.41	1.37
20	3	407	CLA	C4B-NB	3.00	1.41	1.37
20	8	303	CLA	C4B-NB	2.99	1.41	1.37
19	9	606	CHL	C3A-C2A	-2.99	1.52	1.54
20	A	807	CLA	C4B-NB	2.99	1.41	1.37
20	1	610	CLA	C4B-NB	2.99	1.41	1.37
20	9	608	CLA	C4B-NB	2.99	1.41	1.37
20	A	819	CLA	C4B-NB	2.99	1.41	1.37
20	1	604	CLA	C4B-NB	2.98	1.41	1.37
20	3	406	CLA	C4B-NB	2.98	1.41	1.37
20	A	806	CLA	C4B-NB	2.98	1.41	1.37
20	A	822	CLA	C4B-NB	2.98	1.41	1.37
20	B	805	CLA	C4B-NB	2.97	1.41	1.37
20	7	304	CLA	C4B-NB	2.97	1.41	1.37
20	G	4003	CLA	C4B-NB	2.97	1.41	1.37
20	B	809	CLA	C4B-NB	2.97	1.41	1.37
20	B	822	CLA	C4B-NB	2.97	1.41	1.37
20	B	815	CLA	C4B-NB	2.97	1.41	1.37
20	7	310	CLA	C4B-NB	2.97	1.41	1.37
20	A	818	CLA	C4B-NB	2.97	1.41	1.37
20	2	604	CLA	C4B-NB	2.97	1.41	1.37
20	3	412	CLA	C4B-NB	2.97	1.41	1.37
20	B	831	CLA	C4B-NB	2.96	1.41	1.37
20	3	409	CLA	C4B-NB	2.96	1.41	1.37
20	A	820	CLA	C4B-NB	2.96	1.41	1.37
20	G	4002	CLA	C4B-NB	2.96	1.41	1.37
20	B	843	CLA	C4B-NB	2.96	1.41	1.37
20	9	604	CLA	C4B-NB	2.95	1.41	1.37
20	9	611	CLA	C4B-NB	2.95	1.41	1.37
20	7	309	CLA	C4B-NB	2.95	1.41	1.37
20	A	815	CLA	C4B-NB	2.95	1.41	1.37
20	7	304	CLA	MG-NA	2.95	2.13	2.06
20	9	605	CLA	C4B-NB	2.95	1.41	1.37
20	B	807	CLA	C4B-NB	2.95	1.41	1.37
20	7	314	CLA	C4B-NB	2.94	1.41	1.37
20	F	5003	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	605	CLA	C4B-NB	2.93	1.41	1.37
20	A	841	CLA	C4B-NB	2.93	1.41	1.37
19	3	401	CHL	C3A-C2A	-2.93	1.52	1.54
20	B	816	CLA	C4B-NB	2.93	1.41	1.37
20	A	839	CLA	C4B-NB	2.92	1.41	1.37
20	7	324	CLA	C4B-NB	2.92	1.41	1.37
20	A	826	CLA	C4B-NB	2.92	1.41	1.37
20	K	203	CLA	C4B-NB	2.92	1.41	1.37
20	A	825	CLA	C4B-NB	2.92	1.41	1.37
20	B	838	CLA	C4B-NB	2.92	1.41	1.37
19	7	306	CHL	C3A-C2A	-2.92	1.52	1.54
20	2	610	CLA	C4B-NB	2.91	1.41	1.37
20	A	832	CLA	C4B-NB	2.91	1.41	1.37
20	B	818	CLA	C4B-NB	2.91	1.41	1.37
20	A	809	CLA	C4B-NB	2.91	1.41	1.37
19	8	306	CHL	C3A-C2A	-2.91	1.52	1.54
20	K	202	CLA	C4B-NB	2.91	1.41	1.37
20	A	805	CLA	C4B-NB	2.90	1.41	1.37
20	B	808	CLA	C4B-NB	2.90	1.41	1.37
20	3	403	CLA	C4B-NB	2.90	1.41	1.37
20	A	843	CLA	C4B-NB	2.90	1.41	1.37
20	1	608	CLA	C4B-NB	2.90	1.41	1.37
20	A	828	CLA	C4B-NB	2.89	1.41	1.37
20	A	810	CLA	C4B-NB	2.89	1.41	1.37
20	A	830	CLA	C4B-NB	2.89	1.41	1.37
20	B	810	CLA	C4B-NB	2.89	1.41	1.37
20	A	812	CLA	C1B-C2B	2.89	1.49	1.43
20	9	602	CLA	C4B-NB	2.88	1.41	1.37
20	A	804	CLA	C1D-ND	2.88	1.41	1.37
20	A	829	CLA	C4B-NB	2.88	1.41	1.37
20	A	808	CLA	C4B-NB	2.88	1.41	1.37
20	A	824	CLA	C4B-NB	2.88	1.41	1.37
20	B	824	CLA	C4B-NB	2.87	1.41	1.37
20	B	813	CLA	C4B-NB	2.87	1.41	1.37
20	7	312	CLA	C4B-NB	2.87	1.41	1.37
20	B	809	CLA	C1B-C2B	2.87	1.49	1.43
20	9	610	CLA	C4B-NB	2.87	1.41	1.37
20	A	835	CLA	C4B-NB	2.87	1.41	1.37
20	A	838	CLA	C4B-NB	2.87	1.41	1.37
20	A	827	CLA	C4B-NB	2.87	1.41	1.37
20	1	607	CLA	C4B-NB	2.86	1.41	1.37
20	A	831	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	825	CLA	C1B-C2B	2.86	1.49	1.43
20	A	844	CLA	C4B-NB	2.86	1.41	1.37
20	A	843	CLA	C1B-C2B	2.86	1.49	1.43
20	2	608	CLA	C4B-NB	2.86	1.41	1.37
20	A	811	CLA	C4B-NB	2.85	1.41	1.37
20	A	823	CLA	C4B-NB	2.85	1.41	1.37
20	A	827	CLA	C1B-C2B	2.84	1.49	1.43
20	3	411	CLA	MG-ND	-2.84	2.00	2.05
20	A	830	CLA	MG-NA	2.84	2.13	2.06
20	B	833	CLA	C4B-NB	2.84	1.41	1.37
20	H	204	CLA	C1B-C2B	2.84	1.49	1.43
20	B	823	CLA	C1B-C2B	2.84	1.49	1.43
20	B	803	CLA	C4B-NB	2.84	1.41	1.37
20	B	819	CLA	C4B-NB	2.83	1.41	1.37
20	B	814	CLA	C4B-NB	2.83	1.41	1.37
20	B	815	CLA	C1B-C2B	2.83	1.49	1.43
20	B	828	CLA	C4B-NB	2.83	1.41	1.37
20	B	806	CLA	C4B-NB	2.83	1.41	1.37
20	G	4003	CLA	C1B-C2B	2.83	1.49	1.43
20	A	833	CLA	C4B-NB	2.83	1.41	1.37
20	8	302	CLA	C4B-NB	2.83	1.41	1.37
20	B	829	CLA	C4B-NB	2.83	1.41	1.37
20	J	4002	CLA	C1B-C2B	2.83	1.49	1.43
20	G	4004	CLA	C4B-NB	2.82	1.41	1.37
20	K	201	CLA	C1B-C2B	2.82	1.49	1.43
20	A	819	CLA	C1B-C2B	2.82	1.49	1.43
20	9	601	CLA	C4B-NB	2.82	1.41	1.37
20	A	820	CLA	C1B-C2B	2.82	1.49	1.43
20	K	202	CLA	C1B-C2B	2.82	1.49	1.43
20	K	203	CLA	C1B-C2B	2.81	1.49	1.43
20	9	611	CLA	C1B-C2B	2.81	1.49	1.43
20	F	5003	CLA	MG-NA	2.81	2.12	2.06
20	B	825	CLA	C4B-NB	2.81	1.41	1.37
20	2	607	CLA	C1B-C2B	2.80	1.49	1.43
20	H	204	CLA	C4B-NB	2.80	1.41	1.37
20	K	203	CLA	MG-NA	2.80	2.12	2.06
20	B	833	CLA	C1B-C2B	2.79	1.49	1.43
20	L	307	CLA	C4B-NB	2.79	1.41	1.37
20	2	622	CLA	C1B-C2B	2.79	1.49	1.43
20	B	812	CLA	C1B-C2B	2.79	1.49	1.43
20	8	302	CLA	C1B-C2B	2.78	1.49	1.43
20	G	4004	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	806	CLA	C1B-C2B	2.78	1.49	1.43
20	9	612	CLA	C1B-C2B	2.78	1.49	1.43
20	A	838	CLA	MG-NA	2.78	2.12	2.06
20	A	816	CLA	C4B-NB	2.78	1.41	1.37
20	9	607	CLA	C4B-NB	2.78	1.41	1.37
20	A	813	CLA	C1B-C2B	2.78	1.49	1.43
20	L	305	CLA	C4B-NB	2.78	1.41	1.37
20	3	410	CLA	C1B-C2B	2.78	1.49	1.43
20	3	414	CLA	C1B-C2B	2.77	1.49	1.43
20	3	408	CLA	C1B-C2B	2.77	1.49	1.43
20	A	832	CLA	MG-ND	-2.77	2.00	2.05
20	2	609	CLA	C1B-C2B	2.77	1.49	1.43
20	3	408	CLA	C4B-NB	2.77	1.41	1.37
20	A	839	CLA	C1B-C2B	2.76	1.49	1.43
20	1	602	CLA	C4B-NB	2.76	1.41	1.37
20	8	311	CLA	C1B-C2B	2.76	1.49	1.43
20	8	308	CLA	C4B-NB	2.76	1.41	1.37
20	B	832	CLA	MG-ND	-2.76	2.00	2.05
20	L	302	CLA	C1B-C2B	2.76	1.49	1.43
20	2	622	CLA	C4B-NB	2.76	1.41	1.37
20	F	5008	CLA	C1B-C2B	2.75	1.49	1.43
20	7	314	CLA	C1B-C2B	2.75	1.49	1.43
20	7	313	CLA	C1B-C2B	2.75	1.49	1.43
20	A	812	CLA	MG-ND	-2.75	2.00	2.05
20	9	601	CLA	C1B-C2B	2.75	1.49	1.43
20	B	837	CLA	C1B-C2B	2.75	1.49	1.43
20	B	827	CLA	C1B-C2B	2.75	1.49	1.43
20	F	5007	CLA	C1B-C2B	2.75	1.49	1.43
20	B	817	CLA	C1B-C2B	2.75	1.49	1.43
20	L	304	CLA	C1B-C2B	2.75	1.49	1.43
20	3	411	CLA	C1B-C2B	2.75	1.49	1.43
20	A	809	CLA	C1B-C2B	2.75	1.49	1.43
20	7	312	CLA	C1B-C2B	2.74	1.49	1.43
20	2	611	CLA	C1B-C2B	2.74	1.49	1.43
20	3	409	CLA	C1B-C2B	2.74	1.49	1.43
20	A	823	CLA	C1B-C2B	2.74	1.49	1.43
20	1	603	CLA	C1B-C2B	2.74	1.49	1.43
20	B	837	CLA	C4B-NB	2.74	1.41	1.37
20	7	315	CLA	C1B-C2B	2.74	1.49	1.43
20	B	808	CLA	C1B-C2B	2.74	1.49	1.43
20	L	307	CLA	C1B-C2B	2.74	1.49	1.43
20	9	609	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	613	CLA	C1B-C2B	2.73	1.49	1.43
20	A	840	CLA	C1B-C2B	2.73	1.49	1.43
20	7	303	CLA	C1B-C2B	2.73	1.49	1.43
20	B	828	CLA	C1B-C2B	2.73	1.49	1.43
20	B	821	CLA	C1B-C2B	2.73	1.49	1.43
20	8	310	CLA	C1B-C2B	2.73	1.49	1.43
20	2	612	CLA	C1B-C2B	2.73	1.49	1.43
20	9	610	CLA	C1B-C2B	2.73	1.49	1.43
20	2	602	CLA	C1B-C2B	2.73	1.49	1.43
20	3	412	CLA	C1B-C2B	2.73	1.49	1.43
20	1	610	CLA	C1B-C2B	2.73	1.49	1.43
20	8	312	CLA	C1B-C2B	2.73	1.49	1.43
20	A	808	CLA	C1B-C2B	2.73	1.49	1.43
20	K	204	CLA	C1B-C2B	2.73	1.49	1.43
20	B	803	CLA	C1B-C2B	2.72	1.49	1.43
20	B	824	CLA	C1B-C2B	2.72	1.49	1.43
20	2	605	CLA	C1B-C2B	2.72	1.49	1.43
20	A	841	CLA	C1B-C2B	2.72	1.49	1.43
20	9	608	CLA	C1B-C2B	2.72	1.49	1.43
20	B	816	CLA	C1B-C2B	2.72	1.49	1.43
20	J	4002	CLA	C4B-NB	2.72	1.41	1.37
20	7	324	CLA	C1B-C2B	2.72	1.49	1.43
20	A	816	CLA	C1B-C2B	2.72	1.49	1.43
20	A	826	CLA	C1B-C2B	2.72	1.49	1.43
20	A	818	CLA	C1B-C2B	2.72	1.49	1.43
20	7	304	CLA	C1B-C2B	2.71	1.49	1.43
20	7	305	CLA	C1B-C2B	2.71	1.49	1.43
20	J	4002	CLA	C3B-C4B	2.71	1.50	1.42
20	1	612	CLA	C1B-C2B	2.71	1.49	1.43
20	L	306	CLA	C1B-C2B	2.71	1.49	1.43
20	B	811	CLA	C1B-C2B	2.71	1.49	1.43
20	F	5005	CLA	C1B-C2B	2.71	1.49	1.43
20	B	803	CLA	MG-ND	-2.71	2.00	2.05
20	A	805	CLA	C1B-C2B	2.71	1.49	1.43
20	1	602	CLA	C1B-C2B	2.71	1.49	1.43
20	3	406	CLA	C1B-C2B	2.70	1.49	1.43
20	G	4002	CLA	C1B-C2B	2.70	1.49	1.43
20	3	402	CLA	C1B-C2B	2.70	1.49	1.43
20	8	309	CLA	C1B-C2B	2.70	1.49	1.43
20	B	813	CLA	C1B-C2B	2.70	1.49	1.43
20	B	834	CLA	C1B-C2B	2.70	1.49	1.43
20	8	313	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	821	CLA	C1B-C2B	2.70	1.49	1.43
20	A	835	CLA	C1B-C2B	2.70	1.49	1.43
20	B	829	CLA	C1B-C2B	2.70	1.49	1.43
20	9	603	CLA	C1B-C2B	2.70	1.49	1.43
20	F	5006	CLA	C1B-C2B	2.70	1.49	1.43
20	9	605	CLA	C1B-C2B	2.70	1.49	1.43
20	A	831	CLA	C1B-C2B	2.70	1.49	1.43
20	A	806	CLA	C1B-C2B	2.69	1.49	1.43
20	1	608	CLA	C1B-C2B	2.69	1.49	1.43
20	A	836	CLA	C1B-C2B	2.69	1.49	1.43
20	2	613	CLA	C1B-C2B	2.69	1.49	1.43
20	1	612	CLA	C1D-C2D	2.68	1.50	1.45
20	B	810	CLA	C1B-C2B	2.68	1.49	1.43
20	2	603	CLA	C1B-C2B	2.68	1.49	1.43
20	2	610	CLA	C1B-C2B	2.68	1.49	1.43
20	B	822	CLA	C1B-C2B	2.68	1.49	1.43
20	3	405	CLA	C1B-C2B	2.68	1.49	1.43
20	9	604	CLA	C1B-C2B	2.68	1.49	1.43
20	L	305	CLA	C1B-C2B	2.68	1.49	1.43
20	1	609	CLA	C1B-C2B	2.68	1.49	1.43
20	A	824	CLA	C1B-C2B	2.68	1.49	1.43
20	1	612	CLA	C4B-NB	2.68	1.41	1.37
19	7	308	CHL	C3B-C2B	2.68	1.44	1.40
20	1	611	CLA	C1B-C2B	2.68	1.49	1.43
20	7	309	CLA	C1B-C2B	2.68	1.49	1.43
20	3	403	CLA	C1B-C2B	2.68	1.49	1.43
20	B	838	CLA	C1B-C2B	2.67	1.49	1.43
20	7	311	CLA	C1B-C2B	2.67	1.49	1.43
20	3	404	CLA	C1B-C2B	2.67	1.49	1.43
20	L	301	CLA	C1B-C2B	2.67	1.49	1.43
20	3	413	CLA	C1B-C2B	2.67	1.49	1.43
20	8	303	CLA	C1B-C2B	2.67	1.49	1.43
20	A	830	CLA	C1B-C2B	2.67	1.49	1.43
20	2	604	CLA	C1B-C2B	2.66	1.49	1.43
20	A	807	CLA	C1B-C2B	2.65	1.49	1.43
20	2	613	CLA	C3B-C4B	2.65	1.50	1.42
20	B	839	CLA	C1B-C2B	2.65	1.49	1.43
20	B	843	CLA	C1B-C2B	2.65	1.49	1.43
20	A	804	CLA	C1B-C2B	2.65	1.49	1.43
20	A	811	CLA	C1B-C2B	2.65	1.49	1.43
20	A	813	CLA	MG-NC	2.65	2.12	2.06
20	1	605	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	9	607	CLA	C1B-C2B	2.64	1.49	1.43
20	B	835	CLA	C1B-C2B	2.64	1.49	1.43
20	F	5003	CLA	C1B-C2B	2.64	1.49	1.43
20	B	814	CLA	C1B-C2B	2.64	1.49	1.43
20	A	838	CLA	C1B-C2B	2.64	1.49	1.43
20	A	828	CLA	C1B-C2B	2.63	1.49	1.43
20	B	830	CLA	CMB-C2B	-2.63	1.45	1.50
20	B	842	CLA	C1B-C2B	2.63	1.49	1.43
20	2	603	CLA	MG-NC	2.63	2.12	2.06
20	8	308	CLA	C1B-C2B	2.63	1.49	1.43
20	B	840	CLA	C1B-C2B	2.63	1.49	1.43
20	A	815	CLA	C1B-C2B	2.63	1.49	1.43
20	A	810	CLA	C1B-C2B	2.63	1.49	1.43
20	A	842	CLA	C1B-C2B	2.63	1.49	1.43
20	A	829	CLA	C1B-C2B	2.63	1.49	1.43
20	A	834	CLA	C1B-C2B	2.62	1.49	1.43
19	7	307	CHL	CHB-C4A	-2.62	1.35	1.38
20	3	407	CLA	C1B-C2B	2.62	1.49	1.43
20	A	804	CLA	MG-ND	-2.61	2.00	2.05
20	A	817	CLA	C1B-C2B	2.61	1.49	1.43
20	A	822	CLA	C1B-C2B	2.61	1.49	1.43
20	B	831	CLA	C1B-C2B	2.61	1.49	1.43
20	1	607	CLA	C1B-C2B	2.61	1.49	1.43
20	A	832	CLA	C1B-C2B	2.60	1.49	1.43
20	B	826	CLA	C1B-C2B	2.60	1.49	1.43
20	A	814	CLA	C1B-C2B	2.60	1.49	1.43
20	B	807	CLA	C1B-C2B	2.60	1.49	1.43
20	B	830	CLA	C1B-C2B	2.59	1.49	1.43
20	B	818	CLA	C1B-C2B	2.59	1.49	1.43
20	B	805	CLA	C1B-C2B	2.59	1.49	1.43
20	B	825	CLA	MG-ND	-2.58	2.00	2.05
20	2	608	CLA	C1B-C2B	2.58	1.49	1.43
20	B	832	CLA	C1B-C2B	2.58	1.49	1.43
20	1	603	CLA	MG-NA	2.56	2.12	2.06
20	A	804	CLA	CMD-C2D	-2.56	1.45	1.50
20	B	825	CLA	C1B-C2B	2.56	1.49	1.43
20	B	840	CLA	MG-ND	-2.55	2.00	2.05
20	A	804	CLA	CMB-C2B	-2.55	1.45	1.50
20	8	307	CLA	C1B-C2B	2.55	1.49	1.43
20	B	836	CLA	C1B-C2B	2.54	1.49	1.43
20	G	4002	CLA	MG-NA	2.54	2.12	2.06
20	A	829	CLA	MG-ND	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	301	CLA	MG-ND	-2.54	2.00	2.05
20	B	841	CLA	C1B-C2B	2.54	1.49	1.43
19	2	601	CHL	CHB-C4A	-2.53	1.35	1.38
20	B	804	CLA	C4B-NB	2.53	1.41	1.37
20	9	607	CLA	MG-ND	-2.52	2.00	2.05
20	B	807	CLA	MG-ND	-2.51	2.00	2.05
20	A	844	CLA	C1B-C2B	2.51	1.49	1.43
20	8	310	CLA	MG-NA	2.51	2.12	2.06
19	7	302	CHL	CHB-C4A	-2.50	1.35	1.38
20	A	807	CLA	CHC-C1C	2.50	1.43	1.38
20	7	310	CLA	C1B-C2B	2.49	1.49	1.43
20	9	602	CLA	C1B-C2B	2.49	1.49	1.43
19	7	302	CHL	C3A-C2A	-2.49	1.52	1.54
20	1	604	CLA	C1B-C2B	2.49	1.49	1.43
20	B	804	CLA	CHC-C1C	2.48	1.43	1.38
20	8	307	CLA	MG-ND	-2.47	2.00	2.05
20	A	836	CLA	CHC-C1C	2.47	1.43	1.38
20	B	805	CLA	C3B-C4B	2.47	1.49	1.42
20	B	830	CLA	CMD-C2D	-2.47	1.45	1.50
20	9	612	CLA	MG-ND	-2.47	2.00	2.05
19	8	305	CHL	C3A-C2A	-2.45	1.52	1.54
20	B	810	CLA	CMB-C2B	-2.45	1.45	1.50
20	7	310	CLA	C3B-C4B	2.44	1.49	1.42
20	F	5008	CLA	CMB-C2B	-2.44	1.45	1.50
20	2	612	CLA	MG-NA	2.44	2.12	2.06
20	B	820	CLA	MG-ND	-2.43	2.01	2.05
20	B	819	CLA	C1B-C2B	2.43	1.48	1.43
20	B	807	CLA	C3B-C4B	2.43	1.49	1.42
20	B	825	CLA	C3B-C4B	2.43	1.49	1.42
32	A	803	CL0	CHB-C4A	-2.43	1.35	1.38
20	9	602	CLA	CHC-C1C	2.43	1.43	1.38
20	9	602	CLA	C3B-C4B	2.43	1.49	1.42
20	A	837	CLA	C3B-C4B	2.43	1.49	1.42
20	B	820	CLA	C1B-C2B	2.43	1.48	1.43
19	8	304	CHL	CHB-C4A	-2.43	1.35	1.38
20	A	844	CLA	C3B-C4B	2.42	1.49	1.42
20	B	841	CLA	CMB-C2B	-2.42	1.45	1.50
20	9	605	CLA	CMD-C2D	-2.42	1.45	1.50
19	1	601	CHL	CHB-C4A	-2.42	1.35	1.38
19	8	306	CHL	CHB-C4A	-2.42	1.35	1.38
20	L	307	CLA	C3B-C4B	2.41	1.49	1.42
20	B	804	CLA	C1D-ND	2.41	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	831	CLA	C3B-C4B	2.41	1.49	1.42
20	A	829	CLA	CHC-C1C	2.41	1.43	1.38
20	1	614	CLA	CHC-C1C	2.41	1.43	1.38
20	A	810	CLA	MG-NB	-2.41	2.01	2.05
19	3	401	CHL	CHB-C4A	-2.41	1.35	1.38
20	B	835	CLA	C3B-C4B	2.41	1.49	1.42
20	A	837	CLA	C1B-C2B	2.41	1.48	1.43
20	9	605	CLA	CHC-C1C	2.40	1.43	1.38
20	9	608	CLA	CHC-C1C	2.40	1.43	1.38
20	A	817	CLA	CHC-C1C	2.40	1.43	1.38
20	1	613	CLA	MG-NA	2.40	2.12	2.06
19	2	601	CHL	C3A-C2A	-2.40	1.52	1.54
20	2	622	CLA	C3B-C4B	2.40	1.49	1.42
20	7	303	CLA	CHC-C1C	2.40	1.43	1.38
20	F	5003	CLA	C3B-C4B	2.39	1.49	1.42
20	1	604	CLA	C3B-C4B	2.39	1.49	1.42
20	B	840	CLA	MG-NA	2.39	2.12	2.06
20	A	818	CLA	C3B-C4B	2.39	1.49	1.42
20	F	5008	CLA	MG-NC	2.39	2.11	2.06
20	1	612	CLA	C4C-C3C	2.38	1.49	1.45
20	A	812	CLA	CMD-C2D	-2.38	1.45	1.50
20	B	831	CLA	C3B-C4B	2.38	1.49	1.42
20	1	605	CLA	C3B-C4B	2.38	1.49	1.42
20	A	817	CLA	C3B-C4B	2.38	1.49	1.42
20	7	310	CLA	CHC-C1C	2.38	1.43	1.38
20	B	830	CLA	MG-NA	2.38	2.11	2.06
20	3	402	CLA	MG-NA	2.38	2.11	2.06
20	B	818	CLA	CHC-C1C	2.38	1.43	1.38
20	B	822	CLA	C3B-C4B	2.38	1.49	1.42
20	8	308	CLA	C3B-C4B	2.38	1.49	1.42
20	B	825	CLA	CMD-C2D	-2.38	1.45	1.50
20	B	820	CLA	CMB-C2B	-2.38	1.45	1.50
20	A	829	CLA	CMD-C2D	-2.37	1.45	1.50
20	A	808	CLA	CHC-C1C	2.37	1.43	1.38
20	G	4003	CLA	CHC-C1C	2.37	1.43	1.38
20	7	315	CLA	CHC-C1C	2.37	1.43	1.38
20	1	612	CLA	C3B-C4B	2.37	1.49	1.42
20	1	613	CLA	CHC-C1C	2.37	1.43	1.38
20	A	836	CLA	C3B-C4B	2.37	1.49	1.42
20	2	608	CLA	C3B-C4B	2.37	1.49	1.42
19	1	606	CHL	CHB-C4A	-2.37	1.35	1.38
19	2	606	CHL	CHB-C4A	-2.37	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	9	608	CLA	C3B-C4B	2.36	1.49	1.42
20	2	604	CLA	CHC-C1C	2.36	1.43	1.38
20	3	412	CLA	C3B-C4B	2.36	1.49	1.42
20	8	308	CLA	CHC-C1C	2.36	1.43	1.38
20	B	812	CLA	CHC-C1C	2.36	1.43	1.38
20	1	608	CLA	C3B-C4B	2.36	1.49	1.42
20	K	204	CLA	C3B-C4B	2.36	1.49	1.42
20	F	5005	CLA	C3B-C4B	2.36	1.49	1.42
20	B	805	CLA	CHC-C1C	2.36	1.43	1.38
20	B	817	CLA	MG-NC	2.36	2.11	2.06
20	3	409	CLA	C3B-C4B	2.36	1.49	1.42
20	3	414	CLA	C3B-C4B	2.36	1.49	1.42
20	B	838	CLA	C3B-C4B	2.36	1.49	1.42
20	8	313	CLA	MG-ND	-2.36	2.01	2.05
20	1	605	CLA	CHC-C1C	2.36	1.43	1.38
20	9	605	CLA	C3B-C4B	2.35	1.49	1.42
20	A	815	CLA	C3B-C4B	2.35	1.49	1.42
20	A	832	CLA	MG-NA	2.35	2.11	2.06
20	K	202	CLA	C3B-C4B	2.35	1.49	1.42
20	9	605	CLA	C1D-C2D	2.35	1.50	1.45
20	A	836	CLA	MG-NA	2.35	2.11	2.06
20	A	826	CLA	C3B-C4B	2.35	1.49	1.42
19	7	306	CHL	CHB-C4A	-2.35	1.35	1.38
20	8	312	CLA	CHC-C1C	2.35	1.43	1.38
20	A	805	CLA	C3B-C4B	2.35	1.49	1.42
20	K	204	CLA	CHC-C1C	2.34	1.43	1.38
20	A	840	CLA	C3B-C4B	2.34	1.49	1.42
20	1	604	CLA	CHC-C1C	2.34	1.43	1.38
20	8	312	CLA	C3B-C4B	2.34	1.49	1.42
20	B	817	CLA	CHC-C1C	2.34	1.43	1.38
20	7	324	CLA	C3B-C4B	2.34	1.49	1.42
20	7	314	CLA	C3B-C4B	2.34	1.49	1.42
20	B	803	CLA	CMC-C2C	-2.34	1.46	1.50
19	9	606	CHL	CHB-C4A	-2.34	1.35	1.38
20	B	842	CLA	C3B-C4B	2.34	1.49	1.42
20	1	613	CLA	C3B-C4B	2.34	1.49	1.42
20	A	838	CLA	MG-ND	-2.34	2.01	2.05
20	7	312	CLA	C3B-C4B	2.34	1.49	1.42
19	8	305	CHL	CHB-C4A	-2.34	1.35	1.38
20	B	804	CLA	C3B-C4B	2.33	1.49	1.42
20	B	838	CLA	CHC-C1C	2.33	1.43	1.38
20	B	842	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	CHC-C1C	2.33	1.43	1.38
20	K	202	CLA	CHC-C1C	2.33	1.43	1.38
20	8	310	CLA	C3B-C4B	2.33	1.49	1.42
20	K	201	CLA	C3B-C4B	2.33	1.49	1.42
20	9	610	CLA	C3B-C4B	2.33	1.49	1.42
20	A	835	CLA	C3B-C4B	2.33	1.49	1.42
20	A	831	CLA	CHC-C1C	2.33	1.43	1.38
20	7	315	CLA	C3B-C4B	2.33	1.49	1.42
20	2	604	CLA	C3B-C4B	2.33	1.49	1.42
20	2	608	CLA	CHC-C1C	2.33	1.43	1.38
20	A	844	CLA	CHC-C1C	2.33	1.43	1.38
20	B	837	CLA	MG-ND	-2.33	2.01	2.05
20	1	611	CLA	C3B-C4B	2.33	1.49	1.42
20	7	303	CLA	C3B-C4B	2.33	1.49	1.42
20	A	816	CLA	C3B-C4B	2.32	1.49	1.42
20	8	303	CLA	CHC-C1C	2.32	1.43	1.38
20	A	839	CLA	C3B-C4B	2.32	1.49	1.42
20	2	610	CLA	C3B-C4B	2.32	1.49	1.42
20	A	807	CLA	C3B-C4B	2.32	1.49	1.42
20	8	308	CLA	CMC-C2C	-2.32	1.46	1.50
20	B	829	CLA	MG-ND	-2.32	2.01	2.05
20	1	609	CLA	C3B-C4B	2.32	1.49	1.42
20	B	826	CLA	CHC-C1C	2.32	1.43	1.38
20	7	324	CLA	MG-ND	-2.32	2.01	2.05
20	2	609	CLA	C3B-C4B	2.32	1.49	1.42
20	3	407	CLA	C3B-C4B	2.32	1.49	1.42
20	G	4003	CLA	C3B-C4B	2.32	1.49	1.42
20	B	804	CLA	C1B-C2B	2.32	1.48	1.43
20	8	311	CLA	CMD-C2D	-2.32	1.46	1.50
20	8	310	CLA	CHC-C1C	2.32	1.43	1.38
20	B	806	CLA	C3B-C4B	2.32	1.49	1.42
20	B	803	CLA	CMD-C2D	-2.32	1.46	1.50
20	9	607	CLA	C3B-C4B	2.32	1.49	1.42
20	A	828	CLA	C3B-C4B	2.32	1.49	1.42
20	3	414	CLA	CHC-C1C	2.32	1.43	1.38
20	9	603	CLA	C3B-C4B	2.32	1.49	1.42
20	A	824	CLA	C3B-C4B	2.31	1.49	1.42
20	B	832	CLA	C3B-C4B	2.31	1.49	1.42
20	A	814	CLA	C3B-C4B	2.31	1.49	1.42
20	9	604	CLA	C3B-C4B	2.31	1.49	1.42
20	9	601	CLA	C3B-C4B	2.31	1.49	1.42
20	A	837	CLA	MG-ND	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	808	CLA	C3B-C4B	2.31	1.49	1.42
20	F	5006	CLA	C3B-C4B	2.31	1.49	1.42
20	1	602	CLA	C3B-C4B	2.31	1.49	1.42
20	3	404	CLA	C3B-C4B	2.31	1.49	1.42
20	8	307	CLA	C3B-C4B	2.31	1.49	1.42
20	3	413	CLA	C3B-C4B	2.31	1.49	1.42
20	A	829	CLA	C3B-C4B	2.30	1.49	1.42
20	3	412	CLA	CHC-C1C	2.30	1.43	1.38
20	B	817	CLA	C3B-C4B	2.30	1.49	1.42
20	8	302	CLA	C3B-C4B	2.30	1.49	1.42
20	1	612	CLA	CHC-C1C	2.30	1.43	1.38
20	F	5007	CLA	C3B-C4B	2.30	1.49	1.42
20	B	821	CLA	MG-ND	-2.30	2.01	2.05
20	A	809	CLA	C3B-C4B	2.30	1.49	1.42
20	A	814	CLA	CHC-C1C	2.30	1.43	1.38
20	A	821	CLA	C3B-C4B	2.30	1.49	1.42
20	B	814	CLA	C3B-C4B	2.30	1.49	1.42
20	A	805	CLA	CHC-C1C	2.30	1.43	1.38
20	B	813	CLA	C3B-C4B	2.30	1.49	1.42
20	L	301	CLA	CMD-C2D	-2.30	1.46	1.50
20	7	311	CLA	C3B-C4B	2.30	1.49	1.42
20	B	835	CLA	CMD-C2D	-2.29	1.46	1.50
20	3	410	CLA	C3B-C4B	2.29	1.49	1.42
20	3	411	CLA	C3B-C4B	2.29	1.49	1.42
20	B	816	CLA	C3B-C4B	2.29	1.49	1.42
20	3	409	CLA	CHC-C1C	2.29	1.43	1.38
20	7	313	CLA	C3B-C4B	2.29	1.49	1.42
20	B	826	CLA	C3B-C4B	2.29	1.49	1.42
20	B	836	CLA	C3B-C4B	2.29	1.49	1.42
20	2	611	CLA	CHC-C1C	2.29	1.43	1.38
20	A	822	CLA	CMB-C2B	-2.29	1.46	1.50
20	8	303	CLA	C3B-C4B	2.29	1.49	1.42
20	3	402	CLA	C3B-C4B	2.29	1.49	1.42
20	2	612	CLA	CHC-C1C	2.29	1.43	1.38
20	A	820	CLA	C3B-C4B	2.29	1.49	1.42
20	A	841	CLA	C3B-C4B	2.29	1.49	1.42
20	B	827	CLA	C3B-C4B	2.29	1.49	1.42
19	2	606	CHL	C3A-C2A	-2.29	1.52	1.54
20	L	307	CLA	CHC-C1C	2.29	1.43	1.38
20	B	807	CLA	CHC-C1C	2.29	1.43	1.38
20	8	309	CLA	C3B-C4B	2.29	1.49	1.42
20	B	808	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	803	CLA	C3B-C4B	2.28	1.49	1.42
20	1	603	CLA	C3B-C4B	2.28	1.49	1.42
20	F	5007	CLA	CHC-C1C	2.28	1.43	1.38
20	A	811	CLA	C3B-C4B	2.28	1.49	1.42
20	B	812	CLA	C3B-C4B	2.28	1.49	1.42
20	8	313	CLA	C3B-C4B	2.28	1.49	1.42
20	B	829	CLA	C3B-C4B	2.28	1.49	1.42
20	9	612	CLA	C3B-C4B	2.28	1.49	1.42
20	B	824	CLA	CHC-C1C	2.28	1.43	1.38
20	9	609	CLA	CHC-C1C	2.28	1.43	1.38
20	B	834	CLA	C3B-C4B	2.28	1.49	1.42
20	7	305	CLA	C3B-C4B	2.28	1.49	1.42
20	L	305	CLA	C3B-C4B	2.28	1.49	1.42
20	1	607	CLA	C3B-C4B	2.28	1.49	1.42
20	3	408	CLA	C3B-C4B	2.28	1.49	1.42
20	8	311	CLA	CHC-C1C	2.28	1.43	1.38
20	9	610	CLA	MG-NC	2.28	2.11	2.06
20	A	811	CLA	CHC-C1C	2.28	1.43	1.38
20	B	803	CLA	CHC-C1C	2.27	1.43	1.38
20	F	5003	CLA	CHC-C1C	2.27	1.43	1.38
20	2	612	CLA	C3B-C4B	2.27	1.49	1.42
20	A	829	CLA	MG-NB	-2.27	2.01	2.05
20	A	837	CLA	CHC-C1C	2.27	1.43	1.38
20	A	843	CLA	C3B-C4B	2.27	1.49	1.42
20	3	403	CLA	C3B-C4B	2.27	1.49	1.42
24	3	420	LHG	O7-C7	-2.27	1.34	1.42
20	A	804	CLA	CMC-C2C	-2.27	1.46	1.50
20	F	5006	CLA	CHC-C1C	2.27	1.43	1.38
20	A	834	CLA	C3B-C4B	2.27	1.49	1.42
20	A	841	CLA	CHC-C1C	2.27	1.43	1.38
20	A	819	CLA	C3B-C4B	2.27	1.49	1.42
20	3	404	CLA	CHC-C1C	2.27	1.43	1.38
20	A	840	CLA	CHC-C1C	2.27	1.43	1.38
20	2	611	CLA	C3B-C4B	2.27	1.49	1.42
20	1	610	CLA	CHC-C1C	2.27	1.43	1.38
20	A	828	CLA	CMB-C2B	-2.27	1.46	1.50
20	B	821	CLA	CMB-C2B	-2.27	1.46	1.50
20	B	843	CLA	CMB-C2B	-2.27	1.46	1.50
20	7	304	CLA	C3B-C4B	2.27	1.49	1.42
20	7	314	CLA	CHC-C1C	2.26	1.43	1.38
20	A	824	CLA	CHC-C1C	2.26	1.43	1.38
20	B	822	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	819	CLA	C3B-C4B	2.26	1.49	1.42
20	7	311	CLA	MG-ND	-2.26	2.01	2.05
20	3	413	CLA	CMB-C2B	-2.26	1.46	1.50
20	L	304	CLA	CHC-C1C	2.26	1.43	1.38
20	9	609	CLA	C3B-C4B	2.26	1.49	1.42
20	L	306	CLA	C3B-C4B	2.26	1.49	1.42
20	K	203	CLA	C3B-C4B	2.26	1.49	1.42
20	B	834	CLA	MG-ND	-2.26	2.01	2.05
20	A	806	CLA	C3B-C4B	2.26	1.49	1.42
20	B	840	CLA	CMD-C2D	-2.26	1.46	1.50
20	A	808	CLA	CMC-C2C	-2.26	1.46	1.50
20	B	840	CLA	C3B-C4B	2.26	1.49	1.42
20	8	311	CLA	C3B-C4B	2.26	1.49	1.42
20	1	610	CLA	C3B-C4B	2.26	1.49	1.42
20	B	824	CLA	C3B-C4B	2.26	1.49	1.42
20	A	810	CLA	C3B-C4B	2.26	1.49	1.42
20	B	828	CLA	C3B-C4B	2.26	1.49	1.42
20	L	302	CLA	C3B-C4B	2.25	1.49	1.42
20	2	610	CLA	CHC-C1C	2.25	1.43	1.38
20	A	826	CLA	CHC-C1C	2.25	1.43	1.38
20	2	605	CLA	C3B-C4B	2.25	1.49	1.42
20	B	821	CLA	C3B-C4B	2.25	1.49	1.42
20	1	611	CLA	MG-NC	2.25	2.11	2.06
20	B	815	CLA	CHC-C1C	2.25	1.43	1.38
20	B	818	CLA	C3B-C4B	2.25	1.49	1.42
20	L	306	CLA	CHC-C1C	2.25	1.43	1.38
20	3	405	CLA	C3B-C4B	2.25	1.49	1.42
20	7	305	CLA	CHC-C1C	2.25	1.43	1.38
20	1	602	CLA	CHC-C1C	2.25	1.43	1.38
20	3	406	CLA	CMB-C2B	-2.25	1.46	1.50
20	A	823	CLA	C3B-C4B	2.25	1.49	1.42
20	3	410	CLA	CHC-C1C	2.25	1.43	1.38
20	A	806	CLA	CHC-C1C	2.25	1.43	1.38
20	F	5005	CLA	CHC-C1C	2.25	1.43	1.38
20	9	611	CLA	C3B-C4B	2.24	1.49	1.42
20	B	806	CLA	CHC-C1C	2.24	1.43	1.38
20	B	813	CLA	CHC-C1C	2.24	1.43	1.38
20	1	614	CLA	CMB-C2B	-2.24	1.46	1.50
20	A	825	CLA	C3B-C4B	2.24	1.49	1.42
20	K	201	CLA	CHC-C1C	2.24	1.43	1.38
20	L	305	CLA	CHC-C1C	2.24	1.43	1.38
20	A	834	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	831	CLA	CHC-C1C	2.24	1.43	1.38
20	B	834	CLA	CHC-C1C	2.24	1.43	1.38
20	L	304	CLA	C3B-C4B	2.24	1.49	1.42
20	B	815	CLA	CMD-C2D	-2.24	1.46	1.50
20	B	831	CLA	MG-ND	-2.24	2.01	2.05
20	A	837	CLA	CMB-C2B	-2.24	1.46	1.50
20	7	309	CLA	CHC-C1C	2.24	1.43	1.38
20	B	840	CLA	CHC-C1C	2.24	1.43	1.38
20	A	822	CLA	C3B-C4B	2.24	1.49	1.42
20	9	611	CLA	CHC-C1C	2.24	1.43	1.38
20	B	833	CLA	C3B-C4B	2.24	1.49	1.42
20	7	309	CLA	C3B-C4B	2.24	1.49	1.42
20	A	842	CLA	CMB-C2B	-2.23	1.46	1.50
20	A	821	CLA	CHC-C1C	2.23	1.43	1.38
20	3	406	CLA	C3B-C4B	2.23	1.49	1.42
20	H	204	CLA	CHC-C1C	2.23	1.43	1.38
20	G	4004	CLA	C3B-C4B	2.23	1.49	1.42
20	B	828	CLA	CHC-C1C	2.23	1.43	1.38
20	B	837	CLA	C3B-C4B	2.23	1.49	1.42
20	G	4002	CLA	C3B-C4B	2.23	1.49	1.42
20	B	836	CLA	CMB-C2B	-2.23	1.46	1.50
20	2	622	CLA	CHC-C1C	2.23	1.43	1.38
20	9	612	CLA	CHC-C1C	2.23	1.43	1.38
20	B	832	CLA	CHC-C1C	2.23	1.43	1.38
20	A	832	CLA	CMB-C2B	-2.23	1.46	1.50
20	2	609	CLA	CHC-C1C	2.23	1.42	1.38
20	A	832	CLA	C3B-C4B	2.22	1.49	1.42
20	B	823	CLA	C3B-C4B	2.22	1.49	1.42
20	A	830	CLA	C3B-C4B	2.22	1.49	1.42
20	A	819	CLA	CHC-C1C	2.22	1.42	1.38
20	1	611	CLA	CHC-C1C	2.22	1.42	1.38
20	9	601	CLA	CHC-C1C	2.22	1.42	1.38
20	9	607	CLA	CHC-C1C	2.22	1.42	1.38
20	B	814	CLA	CHC-C1C	2.22	1.42	1.38
20	H	204	CLA	CMC-C2C	-2.22	1.46	1.50
20	8	309	CLA	CHC-C1C	2.22	1.42	1.38
20	1	612	CLA	MG-NA	2.22	2.11	2.06
20	A	843	CLA	CHC-C1C	2.22	1.42	1.38
20	B	836	CLA	CHC-C1C	2.22	1.42	1.38
20	A	839	CLA	CHC-C1C	2.22	1.42	1.38
20	1	614	CLA	C1B-C2B	2.22	1.48	1.43
20	9	604	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	301	CLA	C3B-C4B	2.22	1.49	1.42
20	3	413	CLA	CHC-C1C	2.22	1.42	1.38
20	B	815	CLA	C3B-C4B	2.22	1.49	1.42
20	A	818	CLA	CHC-C1C	2.22	1.42	1.38
20	8	307	CLA	CHC-C1C	2.22	1.42	1.38
20	7	312	CLA	MG-NA	2.22	2.11	2.06
20	B	833	CLA	CHC-C1C	2.22	1.42	1.38
20	3	411	CLA	CMB-C2B	-2.21	1.46	1.50
20	1	607	CLA	CHC-C1C	2.21	1.42	1.38
20	K	203	CLA	CHC-C1C	2.21	1.42	1.38
20	B	811	CLA	C3B-C4B	2.21	1.49	1.42
20	B	839	CLA	C3B-C4B	2.21	1.49	1.42
20	B	820	CLA	MG-NB	-2.21	2.01	2.05
20	2	603	CLA	C3B-C4B	2.21	1.49	1.42
20	2	608	CLA	CMD-C2D	-2.21	1.46	1.50
20	B	839	CLA	CHC-C1C	2.21	1.42	1.38
20	B	831	CLA	CMD-C2D	-2.21	1.46	1.50
20	3	406	CLA	CHC-C1C	2.21	1.42	1.38
20	B	826	CLA	CMD-C2D	-2.21	1.46	1.50
20	3	407	CLA	CHC-C1C	2.21	1.42	1.38
20	8	302	CLA	CHC-C1C	2.21	1.42	1.38
20	L	302	CLA	CHC-C1C	2.21	1.42	1.38
20	B	835	CLA	CHC-C1C	2.20	1.42	1.38
20	B	827	CLA	CMB-C2B	-2.20	1.46	1.50
20	B	832	CLA	CMD-C2D	-2.20	1.46	1.50
20	2	605	CLA	CHC-C1C	2.20	1.42	1.38
20	B	842	CLA	CMC-C2C	-2.20	1.46	1.50
20	B	816	CLA	CHC-C1C	2.20	1.42	1.38
20	1	607	CLA	CMB-C2B	-2.20	1.46	1.50
20	A	833	CLA	C3B-C4B	2.20	1.49	1.42
20	A	810	CLA	CHC-C1C	2.20	1.42	1.38
20	A	812	CLA	C3B-C4B	2.20	1.49	1.42
20	H	204	CLA	C3B-C4B	2.20	1.49	1.42
20	F	5005	CLA	CMD-C2D	-2.20	1.46	1.50
20	A	827	CLA	C3B-C4B	2.20	1.49	1.42
20	9	604	CLA	MG-ND	-2.20	2.01	2.05
20	J	4002	CLA	CHC-C1C	2.20	1.42	1.38
20	2	602	CLA	C3B-C4B	2.20	1.49	1.42
20	B	843	CLA	CMD-C2D	-2.20	1.46	1.50
20	1	603	CLA	CHC-C1C	2.19	1.42	1.38
20	A	805	CLA	CMB-C2B	-2.19	1.46	1.50
20	B	819	CLA	CMB-C2B	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	825	CLA	CHC-C1C	2.19	1.42	1.38
20	A	830	CLA	CMC-C2C	-2.19	1.46	1.50
20	A	819	CLA	MG-NA	2.19	2.11	2.06
20	B	830	CLA	MG-ND	-2.19	2.01	2.05
20	B	843	CLA	C3B-C4B	2.19	1.49	1.42
20	A	814	CLA	CMB-C2B	-2.19	1.46	1.50
20	K	203	CLA	CMD-C2D	-2.19	1.46	1.50
20	A	842	CLA	C3B-C4B	2.18	1.49	1.42
20	2	602	CLA	CMB-C2B	-2.18	1.46	1.50
20	B	821	CLA	CMD-C2D	-2.18	1.46	1.50
20	A	842	CLA	CHC-C1C	2.18	1.42	1.38
20	B	836	CLA	MG-ND	-2.18	2.01	2.05
20	B	841	CLA	C3B-C4B	2.17	1.49	1.42
20	B	834	CLA	CMB-C2B	-2.17	1.46	1.50
20	B	820	CLA	C3B-C4B	2.17	1.49	1.42
20	A	822	CLA	CHC-C1C	2.17	1.42	1.38
20	A	828	CLA	CHC-C1C	2.17	1.42	1.38
20	A	812	CLA	CMB-C2B	-2.17	1.46	1.50
20	B	829	CLA	CMD-C2D	-2.17	1.46	1.50
20	2	607	CLA	C3B-C4B	2.17	1.49	1.42
20	8	310	CLA	CMD-C2D	-2.17	1.46	1.50
20	A	836	CLA	MG-NC	2.17	2.11	2.06
20	A	824	CLA	CMB-C2B	-2.17	1.46	1.50
20	B	829	CLA	CMB-C2B	-2.17	1.46	1.50
20	A	806	CLA	CMD-C2D	-2.17	1.46	1.50
20	7	311	CLA	CHC-C1C	2.16	1.42	1.38
20	A	842	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	824	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	834	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	829	CLA	CHC-C1C	2.16	1.42	1.38
20	L	301	CLA	CHC-C1C	2.16	1.42	1.38
20	8	307	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	842	CLA	CMD-C2D	-2.16	1.46	1.50
20	A	833	CLA	CHC-C1C	2.16	1.42	1.38
20	2	605	CLA	CMB-C2B	-2.16	1.46	1.50
20	8	310	CLA	MG-NC	2.16	2.11	2.06
20	A	830	CLA	CHC-C1C	2.16	1.42	1.38
20	9	601	CLA	CMD-C2D	-2.16	1.46	1.50
20	B	827	CLA	CHC-C1C	2.16	1.42	1.38
20	L	304	CLA	CMB-C2B	-2.15	1.46	1.50
20	B	809	CLA	CMD-C2D	-2.15	1.46	1.50
20	3	411	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	804	CLA	C3B-C4B	2.15	1.49	1.42
20	B	822	CLA	CMD-C2D	-2.15	1.46	1.50
20	B	810	CLA	MG-ND	-2.15	2.01	2.05
20	A	815	CLA	CHC-C1C	2.15	1.42	1.38
20	B	809	CLA	C3B-C4B	2.15	1.49	1.42
20	G	4002	CLA	CHC-C1C	2.15	1.42	1.38
20	B	840	CLA	CMB-C2B	-2.15	1.46	1.50
20	8	313	CLA	CHC-C1C	2.15	1.42	1.38
20	9	607	CLA	CMD-C2D	-2.15	1.46	1.50
20	2	603	CLA	CMB-C2B	-2.15	1.46	1.50
20	A	838	CLA	C3B-C4B	2.15	1.49	1.42
20	8	311	CLA	MG-ND	-2.15	2.01	2.05
20	1	609	CLA	CHC-C1C	2.15	1.42	1.38
20	7	304	CLA	CHC-C1C	2.14	1.42	1.38
20	3	403	CLA	CHC-C1C	2.14	1.42	1.38
20	B	818	CLA	CMB-C2B	-2.14	1.46	1.50
20	F	5008	CLA	CMD-C2D	-2.14	1.46	1.50
20	1	603	CLA	CMB-C2B	-2.14	1.46	1.50
20	1	604	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	823	CLA	CHC-C1C	2.14	1.42	1.38
20	B	811	CLA	CHC-C1C	2.14	1.42	1.38
20	K	201	CLA	MG-NA	2.14	2.11	2.06
20	9	610	CLA	CHC-C1C	2.14	1.42	1.38
20	2	604	CLA	CMB-C2B	-2.14	1.46	1.50
20	8	308	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	838	CLA	CMB-C2B	-2.14	1.46	1.50
20	7	312	CLA	CHC-C1C	2.14	1.42	1.38
20	A	819	CLA	CMD-C2D	-2.14	1.46	1.50
20	B	813	CLA	CMB-C2B	-2.14	1.46	1.50
20	7	313	CLA	CHC-C1C	2.14	1.42	1.38
20	A	832	CLA	CMD-C2D	-2.14	1.46	1.50
21	2	614	LUT	C21-C26	2.14	1.62	1.56
20	A	815	CLA	CMB-C2B	-2.14	1.46	1.50
20	A	828	CLA	MG-ND	-2.14	2.01	2.05
20	B	812	CLA	CMD-C2D	-2.13	1.46	1.50
20	B	809	CLA	CMB-C2B	-2.13	1.46	1.50
19	7	307	CHL	C3A-C2A	-2.13	1.52	1.54
20	A	835	CLA	CHC-C1C	2.13	1.42	1.38
20	2	622	CLA	C1D-C2D	2.13	1.49	1.45
20	3	402	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	813	CLA	C3B-C4B	2.13	1.49	1.42
20	1	608	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	4004	CLA	CHC-C1C	2.13	1.42	1.38
20	A	827	CLA	CHC-C1C	2.13	1.42	1.38
20	3	410	CLA	CMB-C2B	-2.13	1.46	1.50
20	A	814	CLA	CMD-C2D	-2.13	1.46	1.50
20	B	806	CLA	CMC-C2C	-2.13	1.46	1.50
20	1	612	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	823	CLA	CHC-C1C	2.13	1.42	1.38
20	3	405	CLA	CHC-C1C	2.13	1.42	1.38
20	9	610	CLA	MG-ND	-2.13	2.01	2.05
20	B	821	CLA	CHC-C1C	2.13	1.42	1.38
20	B	820	CLA	CMD-C2D	-2.13	1.46	1.50
20	K	203	CLA	CMC-C2C	-2.12	1.46	1.50
20	2	607	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	827	CLA	CMC-C2C	-2.12	1.46	1.50
20	A	809	CLA	CHC-C1C	2.12	1.42	1.38
20	1	604	CLA	CMB-C2B	-2.12	1.46	1.50
20	A	840	CLA	CMD-C2D	-2.12	1.46	1.50
20	A	844	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	823	CLA	CMB-C2B	-2.12	1.46	1.50
20	1	614	CLA	CMC-C2C	-2.12	1.46	1.50
20	9	604	CLA	CMB-C2B	-2.12	1.46	1.50
20	L	305	CLA	CMD-C2D	-2.12	1.46	1.50
20	9	608	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	839	CLA	CMD-C2D	-2.12	1.46	1.50
20	A	838	CLA	CHC-C1C	2.12	1.42	1.38
20	A	816	CLA	CHC-C1C	2.12	1.42	1.38
20	A	823	CLA	CMD-C2D	-2.12	1.46	1.50
20	B	806	CLA	CMD-C2D	-2.12	1.46	1.50
20	K	202	CLA	CMD-C2D	-2.11	1.46	1.50
20	7	324	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	820	CLA	CHC-C1C	2.11	1.42	1.38
20	A	836	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	817	CLA	CMC-C2C	-2.11	1.46	1.50
20	B	814	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	815	CLA	CMB-C2B	-2.11	1.46	1.50
20	B	816	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	817	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	804	CLA	MG-NB	-2.11	2.01	2.05
20	7	311	CLA	MG-NA	2.11	2.11	2.06
20	3	410	CLA	CMD-C2D	-2.11	1.46	1.50
20	2	607	CLA	CHC-C1C	2.11	1.42	1.38
20	B	831	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	405	CLA	CMB-C2B	-2.11	1.46	1.50
20	8	303	CLA	CMB-C2B	-2.11	1.46	1.50
20	B	830	CLA	C3B-C4B	2.11	1.48	1.42
20	7	303	CLA	CMB-C2B	-2.11	1.46	1.50
20	8	302	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	843	CLA	CMC-C2C	-2.11	1.46	1.50
20	7	324	CLA	CHC-C1C	2.11	1.42	1.38
20	A	819	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	824	CLA	CMD-C2D	-2.11	1.46	1.50
20	3	406	CLA	CMC-C2C	-2.10	1.46	1.50
20	3	409	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	812	CLA	CHC-C1C	2.10	1.42	1.38
20	3	406	CLA	CMD-C2D	-2.10	1.46	1.50
20	1	608	CLA	CHC-C1C	2.10	1.42	1.38
20	7	312	CLA	CMD-C2D	-2.10	1.46	1.50
20	L	302	CLA	CMB-C2B	-2.10	1.46	1.50
20	7	310	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	816	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	843	CLA	CMD-C2D	-2.10	1.46	1.50
20	3	402	CLA	CHC-C1C	2.10	1.42	1.38
20	A	822	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	818	CLA	CMD-C2D	-2.10	1.46	1.50
20	7	304	CLA	CMB-C2B	-2.10	1.46	1.50
20	B	816	CLA	CMB-C2B	-2.10	1.46	1.50
20	9	604	CLA	CMD-C2D	-2.10	1.46	1.50
20	G	4003	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	820	CLA	CMB-C2B	-2.10	1.46	1.50
20	B	811	CLA	CMB-C2B	-2.10	1.46	1.50
20	2	613	CLA	CMD-C2D	-2.09	1.46	1.50
20	3	411	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	819	CLA	CHC-C1C	2.09	1.42	1.38
20	G	4002	CLA	CMD-C2D	-2.09	1.46	1.50
20	7	313	CLA	CMD-C2D	-2.09	1.46	1.50
20	9	609	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	808	CLA	CHC-C1C	2.09	1.42	1.38
20	2	602	CLA	CMD-C2D	-2.09	1.46	1.50
20	3	406	CLA	MG-ND	-2.09	2.01	2.05
20	2	609	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	817	CLA	CMD-C2D	-2.09	1.46	1.50
20	F	5006	CLA	CMC-C2C	-2.09	1.46	1.50
20	7	311	CLA	CMB-C2B	-2.09	1.46	1.50
20	3	402	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	611	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	826	CLA	CMD-C2D	-2.09	1.46	1.50
20	2	602	CLA	CHC-C1C	2.09	1.42	1.38
20	8	309	CLA	CMD-C2D	-2.09	1.46	1.50
20	L	301	CLA	CMB-C2B	-2.09	1.46	1.50
20	2	607	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	838	CLA	CMD-C2D	-2.09	1.46	1.50
20	K	202	CLA	CMB-C2B	-2.09	1.46	1.50
20	2	613	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	804	CLA	CMB-C2B	-2.08	1.46	1.50
20	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	823	CLA	CMB-C2B	-2.08	1.46	1.50
20	8	313	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	841	CLA	MG-NC	2.08	2.11	2.06
20	8	312	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	832	CLA	CHC-C1C	2.08	1.42	1.38
20	7	305	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	811	CLA	CMD-C2D	-2.08	1.46	1.50
20	9	603	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	807	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	824	CLA	CMC-C2C	-2.08	1.46	1.50
20	A	824	CLA	CMC-C2C	-2.08	1.46	1.50
20	A	835	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
20	B	804	CLA	CMC-C2C	-2.08	1.46	1.50
20	7	309	CLA	CMD-C2D	-2.07	1.46	1.50
20	8	310	CLA	CMC-C2C	-2.07	1.46	1.50
20	B	807	CLA	CMB-C2B	-2.07	1.46	1.50
20	2	610	CLA	CMC-C2C	-2.07	1.46	1.50
20	B	811	CLA	CMC-C2C	-2.07	1.46	1.50
20	B	826	CLA	MG-ND	-2.07	2.01	2.05
20	8	313	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	813	CLA	CMB-C2B	-2.07	1.46	1.50
20	9	611	CLA	CMD-C2D	-2.07	1.46	1.50
20	F	5003	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	407	CLA	CMB-C2B	-2.07	1.46	1.50
20	B	837	CLA	CHC-C1C	2.07	1.42	1.38
20	A	837	CLA	CMD-C2D	-2.07	1.46	1.50
20	L	305	CLA	CMB-C2B	-2.07	1.46	1.50
20	B	809	CLA	CHC-C1C	2.07	1.42	1.38
20	B	810	CLA	C3B-C4B	2.07	1.48	1.42
20	A	842	CLA	MG-NC	2.07	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	609	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	808	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	811	CLA	CMD-C2D	-2.07	1.46	1.50
20	1	602	CLA	CMD-C2D	-2.07	1.46	1.50
20	9	602	CLA	CMD-C2D	-2.07	1.46	1.50
20	G	4004	CLA	CMB-C2B	-2.07	1.46	1.50
20	A	833	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	829	CLA	CMB-C2B	-2.07	1.46	1.50
20	B	810	CLA	CMC-C2C	-2.07	1.46	1.50
20	B	837	CLA	CMB-C2B	-2.07	1.46	1.50
20	F	5006	CLA	CMB-C2B	-2.07	1.46	1.50
20	K	203	CLA	CMB-C2B	-2.07	1.46	1.50
20	7	311	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	805	CLA	CMB-C2B	-2.07	1.46	1.50
20	J	4002	CLA	CMC-C2C	-2.06	1.46	1.50
20	B	828	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	603	CLA	CMD-C2D	-2.06	1.46	1.50
20	9	612	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	833	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	831	CLA	CMD-C2D	-2.06	1.46	1.50
20	7	312	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	827	CLA	CMB-C2B	-2.06	1.46	1.50
20	F	5006	CLA	CMD-C2D	-2.06	1.46	1.50
20	7	315	CLA	CMB-C2B	-2.06	1.46	1.50
20	B	805	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	815	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	818	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	813	CLA	CMD-C2D	-2.06	1.46	1.50
20	L	306	CLA	CMC-C2C	-2.06	1.46	1.50
20	2	603	CLA	CHC-C1C	2.06	1.42	1.38
20	9	602	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	835	CLA	CMB-C2B	-2.06	1.46	1.50
20	H	204	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	816	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	821	CLA	CMB-C2B	-2.06	1.46	1.50
20	9	603	CLA	CHC-C1C	2.06	1.42	1.38
20	3	404	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	807	CLA	CMB-C2B	-2.06	1.46	1.50
20	B	824	CLA	CMB-C2B	-2.06	1.46	1.50
20	B	841	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	813	CLA	MG-NA	2.06	2.11	2.06
20	2	611	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	309	CLA	CMC-C2C	-2.06	1.46	1.50
20	B	834	CLA	CMC-C2C	-2.06	1.46	1.50
20	8	308	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	809	CLA	CMB-C2B	-2.06	1.46	1.50
20	7	303	CLA	CMC-C2C	-2.05	1.46	1.50
20	9	603	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
20	1	609	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	828	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
20	9	605	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	825	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	839	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	829	CLA	MG-NA	2.05	2.11	2.06
20	B	841	CLA	CHC-C1C	2.05	1.42	1.38
20	A	832	CLA	CMC-C2C	-2.05	1.46	1.50
20	B	835	CLA	CMB-C2B	-2.05	1.46	1.50
20	8	303	CLA	MG-NA	2.05	2.11	2.06
21	7	316	LUT	C22-C23	-2.05	1.50	1.52
20	3	405	CLA	CMC-C2C	-2.05	1.46	1.50
20	7	313	CLA	CMB-C2B	-2.05	1.46	1.50
20	7	314	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	814	CLA	CMC-C2C	-2.05	1.46	1.50
20	8	302	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	811	CLA	CMB-C2B	-2.04	1.46	1.50
20	A	813	CLA	CHC-C1C	2.04	1.42	1.38
20	2	604	CLA	CMC-C2C	-2.04	1.46	1.50
20	2	613	CLA	CMB-C2B	-2.04	1.46	1.50
20	B	828	CLA	CMB-C2B	-2.04	1.46	1.50
20	A	834	CLA	CMC-C2C	-2.04	1.46	1.50
20	2	610	CLA	CMB-C2B	-2.04	1.46	1.50
20	A	825	CLA	CMC-C2C	-2.04	1.46	1.50
20	L	302	CLA	CMD-C2D	-2.04	1.46	1.50
20	1	602	CLA	CMB-C2B	-2.04	1.46	1.50
20	1	603	CLA	CMC-C2C	-2.04	1.46	1.50
20	B	820	CLA	CMC-C2C	-2.04	1.46	1.50
20	A	841	CLA	CMB-C2B	-2.04	1.46	1.50
20	1	609	CLA	CMD-C2D	-2.04	1.46	1.50
20	2	603	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	823	CLA	CMC-C2C	-2.04	1.46	1.50
20	3	414	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	806	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	820	CLA	CHC-C1C	2.04	1.42	1.38
20	A	821	CLA	CMC-C2C	-2.04	1.46	1.50
20	B	804	CLA	CMD-C2D	-2.04	1.46	1.50
20	L	306	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	816	CLA	MG-ND	-2.04	2.01	2.05
20	1	613	CLA	CMC-C2C	-2.04	1.46	1.50
20	F	5007	CLA	CMD-C2D	-2.04	1.46	1.50
20	1	614	CLA	C1B-NB	-2.04	1.35	1.37
20	B	827	CLA	CMD-C2D	-2.04	1.46	1.50
20	9	611	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	839	CLA	CMD-C2D	-2.03	1.46	1.50
20	3	403	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	829	CLA	CMC-C2C	-2.03	1.46	1.50
20	8	303	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	830	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	805	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	812	CLA	CMB-C2B	-2.03	1.46	1.50
19	7	307	CHL	CHA-CBD	2.03	1.54	1.51
20	1	613	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	821	CLA	CMD-C2D	-2.03	1.46	1.50
20	1	602	CLA	MG-ND	-2.03	2.01	2.05
20	3	412	CLA	CMD-C2D	-2.03	1.46	1.50
20	9	612	CLA	O2A-CGA	2.03	1.37	1.30
20	B	843	CLA	MG-ND	-2.03	2.01	2.05
20	7	314	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	839	CLA	CMB-C2B	-2.03	1.46	1.50
20	1	612	CLA	MG-NC	2.03	2.11	2.06
20	9	603	CLA	MG-NA	2.03	2.11	2.06
20	8	307	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	835	CLA	CMC-C2C	-2.03	1.46	1.50
20	A	809	CLA	MG-ND	-2.03	2.01	2.05
20	2	611	CLA	CMB-C2B	-2.03	1.46	1.50
20	1	607	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	823	CLA	CMD-C2D	-2.03	1.46	1.50
20	1	611	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	827	CLA	CMD-C2D	-2.03	1.46	1.50
20	1	608	CLA	CMD-C2D	-2.02	1.46	1.50
20	G	4004	CLA	CMC-C2C	-2.02	1.46	1.50
20	7	312	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	816	CLA	CMC-C2C	-2.02	1.46	1.50
20	1	612	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	841	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	816	CLA	CMB-C2B	-2.02	1.46	1.50
20	K	201	CLA	CMB-C2B	-2.02	1.46	1.50
20	1	605	CLA	CMB-C2B	-2.02	1.46	1.50
20	3	414	CLA	CMB-C2B	-2.02	1.46	1.50
20	7	305	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	803	CLA	CMB-C2B	-2.02	1.46	1.50
20	3	405	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	831	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	836	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	806	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	837	CLA	CMD-C2D	-2.02	1.46	1.50
20	J	4002	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	804	CLA	CHC-C1C	2.02	1.42	1.38
20	A	826	CLA	CMB-C2B	-2.02	1.46	1.50
20	9	609	CLA	CMD-C2D	-2.02	1.46	1.50
20	1	611	CLA	CMC-C2C	-2.02	1.46	1.50
20	8	309	CLA	CMB-C2B	-2.02	1.46	1.50
20	A	805	CLA	CMD-C2D	-2.02	1.46	1.50
20	L	307	CLA	CMD-C2D	-2.02	1.46	1.50
20	9	611	CLA	CMC-C2C	-2.02	1.46	1.50
20	A	805	CLA	MG-ND	-2.02	2.01	2.05
20	8	311	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	836	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	832	CLA	CMC-C2C	-2.01	1.46	1.50
20	3	408	CLA	CHC-C1C	2.01	1.42	1.38
20	1	608	CLA	CMB-C2B	-2.01	1.46	1.50
20	8	303	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	843	CLA	CMB-C2B	-2.01	1.46	1.50
20	3	404	CLA	CMB-C2B	-2.01	1.46	1.50
20	2	604	CLA	CMD-C2D	-2.01	1.46	1.50
20	9	602	CLA	MG-ND	-2.01	2.01	2.05
20	A	827	CLA	CMC-C2C	-2.01	1.46	1.50
20	1	610	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	825	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	825	CLA	CMC-C2C	-2.01	1.46	1.50
20	F	5007	CLA	CMB-C2B	-2.01	1.46	1.50
20	2	612	CLA	CMB-C2B	-2.01	1.46	1.50
20	3	408	CLA	CMD-C2D	-2.01	1.46	1.50
20	9	608	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	815	CLA	MG-NA	2.01	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	310	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	819	CLA	CMD-C2D	-2.01	1.46	1.50
20	K	201	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	810	CLA	MG-ND	-2.01	2.01	2.05
20	3	403	CLA	CMD-C2D	-2.01	1.46	1.50
20	9	612	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	840	CLA	CMB-C2B	-2.01	1.46	1.50
20	7	315	CLA	CMD-C2D	-2.01	1.46	1.50
20	3	413	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	815	CLA	MG-ND	-2.01	2.01	2.05
20	2	610	CLA	CMD-C2D	-2.00	1.46	1.50
20	A	834	CLA	CMD-C2D	-2.00	1.46	1.50
20	H	204	CLA	CMD-C2D	-2.00	1.46	1.50
20	A	834	CLA	CMB-C2B	-2.00	1.46	1.50
20	B	808	CLA	CMB-C2B	-2.00	1.46	1.50
20	3	407	CLA	CMD-C2D	-2.00	1.46	1.50
20	1	610	CLA	CMB-C2B	-2.00	1.46	1.50
20	A	810	CLA	CMB-C2B	-2.00	1.46	1.50
20	B	823	CLA	CMC-C2C	-2.00	1.46	1.50
20	G	4004	CLA	CMD-C2D	-2.00	1.46	1.50
20	G	4003	CLA	CMB-C2B	-2.00	1.46	1.50
19	7	302	CHL	CHD-C1D	-2.00	1.36	1.39

All (1101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	803	CL0	C1B-CHB-C4A	14.26	130.49	121.32
19	3	401	CHL	C1B-CHB-C4A	14.07	130.37	121.32
19	8	304	CHL	C1B-CHB-C4A	13.63	130.09	121.32
19	9	606	CHL	C1B-CHB-C4A	13.06	129.72	121.32
19	2	601	CHL	C1B-CHB-C4A	12.30	129.24	121.32
19	1	601	CHL	C1B-CHB-C4A	11.63	128.81	121.32
19	7	308	CHL	C1B-CHB-C4A	11.44	128.68	121.32
19	7	307	CHL	C1B-CHB-C4A	11.22	128.54	121.32
19	7	302	CHL	C1B-CHB-C4A	10.96	128.37	121.32
19	8	305	CHL	C1B-CHB-C4A	10.43	128.03	121.32
19	2	606	CHL	C1B-CHB-C4A	10.36	127.99	121.32
19	7	306	CHL	C1B-CHB-C4A	9.91	127.70	121.32
19	8	306	CHL	C1B-CHB-C4A	9.40	127.37	121.32
19	1	606	CHL	C1B-CHB-C4A	9.21	127.25	121.32
20	A	812	CLA	C4A-NA-C1A	7.56	110.13	106.68
20	2	603	CLA	C4A-NA-C1A	7.46	110.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	4002	CLA	C4A-NA-C1A	7.38	110.05	106.68
20	B	833	CLA	C4A-NA-C1A	7.36	110.03	106.68
19	7	307	CHL	C4D-CHA-CBD	-7.18	101.73	108.97
20	A	828	CLA	C4A-NA-C1A	7.02	109.88	106.68
20	3	410	CLA	C4A-NA-C1A	6.91	109.83	106.68
20	2	610	CLA	C4A-NA-C1A	6.90	109.83	106.68
20	7	312	CLA	C4A-NA-C1A	6.78	109.77	106.68
20	B	817	CLA	C4A-NA-C1A	6.75	109.76	106.68
20	B	832	CLA	C4A-NA-C1A	6.68	109.73	106.68
20	7	324	CLA	C4A-NA-C1A	6.62	109.70	106.68
20	B	806	CLA	C4A-NA-C1A	6.60	109.69	106.68
20	A	819	CLA	C4A-NA-C1A	6.59	109.69	106.68
20	9	610	CLA	C4A-NA-C1A	6.57	109.67	106.68
20	3	406	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	A	816	CLA	C4A-NA-C1A	6.52	109.65	106.68
20	K	203	CLA	C4A-NA-C1A	6.52	109.65	106.68
20	B	837	CLA	C4A-NA-C1A	6.46	109.63	106.68
20	7	305	CLA	C4A-NA-C1A	6.39	109.60	106.68
20	B	842	CLA	C4A-NA-C1A	6.37	109.58	106.68
20	F	5003	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	1	611	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	A	818	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	A	821	CLA	C4A-NA-C1A	6.31	109.56	106.68
20	7	311	CLA	C4A-NA-C1A	6.29	109.55	106.68
20	8	303	CLA	C4A-NA-C1A	6.23	109.52	106.68
20	A	825	CLA	C4A-NA-C1A	6.23	109.52	106.68
20	A	809	CLA	C4A-NA-C1A	6.22	109.52	106.68
20	3	403	CLA	C4A-NA-C1A	6.22	109.52	106.68
20	1	613	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	A	817	CLA	C4A-NA-C1A	6.19	109.50	106.68
20	A	843	CLA	C4A-NA-C1A	6.18	109.50	106.68
20	9	611	CLA	C4A-NA-C1A	6.17	109.49	106.68
20	8	310	CLA	C4A-NA-C1A	6.17	109.49	106.68
20	3	407	CLA	C4A-NA-C1A	6.16	109.49	106.68
20	9	612	CLA	C4A-NA-C1A	6.15	109.48	106.68
20	B	836	CLA	C4A-NA-C1A	6.15	109.48	106.68
20	A	835	CLA	C4A-NA-C1A	6.12	109.47	106.68
20	G	4002	CLA	C4A-NA-C1A	6.11	109.47	106.68
20	A	838	CLA	C4A-NA-C1A	6.10	109.46	106.68
20	B	843	CLA	C4A-NA-C1A	6.10	109.46	106.68
20	3	402	CLA	C4A-NA-C1A	6.09	109.46	106.68
20	B	839	CLA	C4A-NA-C1A	6.09	109.46	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	842	CLA	C4A-NA-C1A	6.04	109.44	106.68
20	B	825	CLA	C4A-NA-C1A	6.04	109.44	106.68
20	3	409	CLA	C4A-NA-C1A	6.02	109.42	106.68
20	A	830	CLA	C4A-NA-C1A	6.00	109.42	106.68
20	L	306	CLA	C4A-NA-C1A	6.00	109.42	106.68
20	B	816	CLA	C4A-NA-C1A	6.00	109.42	106.68
20	B	827	CLA	C4A-NA-C1A	5.99	109.41	106.68
20	A	827	CLA	C4A-NA-C1A	5.96	109.40	106.68
20	9	603	CLA	C4A-NA-C1A	5.89	109.37	106.68
20	1	608	CLA	C4A-NA-C1A	5.89	109.36	106.68
20	2	611	CLA	C4A-NA-C1A	5.88	109.36	106.68
20	G	4003	CLA	C4A-NA-C1A	5.86	109.35	106.68
20	7	304	CLA	C4A-NA-C1A	5.84	109.34	106.68
20	B	808	CLA	C4A-NA-C1A	5.83	109.34	106.68
20	A	836	CLA	C4A-NA-C1A	5.83	109.34	106.68
20	A	806	CLA	C4A-NA-C1A	5.82	109.33	106.68
19	2	601	CHL	C4D-CHA-CBD	-5.82	103.10	108.97
20	1	607	CLA	C4A-NA-C1A	5.81	109.33	106.68
20	B	823	CLA	C4A-NA-C1A	5.81	109.33	106.68
20	B	803	CLA	C4A-NA-C1A	5.80	109.33	106.68
20	B	835	CLA	C4A-NA-C1A	5.79	109.32	106.68
20	8	309	CLA	C4A-NA-C1A	5.76	109.31	106.68
19	1	606	CHL	C4D-CHA-CBD	-5.76	103.16	108.97
20	A	832	CLA	C4A-NA-C1A	5.73	109.30	106.68
20	K	204	CLA	C4A-NA-C1A	5.69	109.27	106.68
20	3	411	CLA	C4A-NA-C1A	5.66	109.26	106.68
20	G	4004	CLA	C4A-NA-C1A	5.64	109.25	106.68
20	A	823	CLA	C4A-NA-C1A	5.62	109.24	106.68
20	B	814	CLA	C4A-NA-C1A	5.62	109.24	106.68
20	A	833	CLA	C4A-NA-C1A	5.61	109.24	106.68
20	K	201	CLA	C4A-NA-C1A	5.60	109.23	106.68
20	B	840	CLA	C4A-NA-C1A	5.58	109.23	106.68
19	2	606	CHL	C4D-CHA-CBD	-5.57	103.35	108.97
20	1	605	CLA	C4A-NA-C1A	5.57	109.22	106.68
20	2	602	CLA	C4A-NA-C1A	5.57	109.22	106.68
20	F	5007	CLA	C4A-NA-C1A	5.56	109.22	106.68
20	3	405	CLA	C4A-NA-C1A	5.56	109.21	106.68
20	A	837	CLA	C4A-NA-C1A	5.51	109.19	106.68
20	7	309	CLA	C4A-NA-C1A	5.50	109.19	106.68
19	8	304	CHL	C4D-CHA-CBD	-5.50	103.42	108.97
19	8	305	CHL	C4D-CHA-CBD	-5.50	103.42	108.97
19	7	308	CHL	C4D-CHA-CBD	-5.50	103.42	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	304	CLA	C4A-NA-C1A	5.45	109.16	106.68
20	B	821	CLA	C4A-NA-C1A	5.42	109.15	106.68
20	3	414	CLA	C4A-NA-C1A	5.41	109.14	106.68
20	7	314	CLA	C4A-NA-C1A	5.40	109.14	106.68
20	B	811	CLA	C4A-NA-C1A	5.39	109.14	106.68
20	7	313	CLA	C4A-NA-C1A	5.37	109.13	106.68
20	B	812	CLA	C4A-NA-C1A	5.32	109.11	106.68
20	1	603	CLA	C4A-NA-C1A	5.32	109.10	106.68
20	A	831	CLA	C4A-NA-C1A	5.29	109.09	106.68
20	B	820	CLA	C4A-NA-C1A	5.27	109.08	106.68
20	A	829	CLA	C4A-NA-C1A	5.25	109.08	106.68
20	A	834	CLA	C4A-NA-C1A	5.23	109.07	106.68
20	L	307	CLA	C4A-NA-C1A	5.23	109.06	106.68
20	B	831	CLA	C4A-NA-C1A	5.17	109.04	106.68
20	2	612	CLA	C4A-NA-C1A	5.16	109.03	106.68
20	A	839	CLA	C4A-NA-C1A	5.15	109.03	106.68
19	7	302	CHL	C4D-CHA-CBD	-5.12	103.80	108.97
20	A	813	CLA	C4A-NA-C1A	5.04	108.98	106.68
21	2	614	LUT	C26-C27-C28	5.01	132.38	124.58
20	3	404	CLA	C4A-NA-C1A	5.01	108.96	106.68
20	9	609	CLA	C4A-NA-C1A	4.99	108.96	106.68
20	F	5006	CLA	C4A-NA-C1A	4.98	108.95	106.68
20	L	301	CLA	C4A-NA-C1A	4.98	108.95	106.68
20	H	204	CLA	C4A-NA-C1A	4.90	108.91	106.68
20	2	622	CLA	C4A-NA-C1A	4.89	108.91	106.68
20	9	608	CLA	C4A-NA-C1A	4.89	108.91	106.68
20	1	602	CLA	C4A-NA-C1A	4.85	108.89	106.68
21	2	614	LUT	C21-C26-C27	4.83	118.37	112.83
20	B	805	CLA	C4A-NA-C1A	4.82	108.88	106.68
20	A	841	CLA	C4A-NA-C1A	4.78	108.86	106.68
20	A	804	CLA	C4A-NA-C1A	4.78	108.86	106.68
20	B	810	CLA	C4A-NA-C1A	4.77	108.86	106.68
20	2	613	CLA	C4A-NA-C1A	4.75	108.85	106.68
20	L	302	CLA	C4A-NA-C1A	4.74	108.84	106.68
20	3	412	CLA	C4A-NA-C1A	4.73	108.84	106.68
20	1	614	CLA	CMB-C2B-C1B	-4.70	118.27	125.42
23	3	418	BCR	C16-C15-C14	4.69	133.11	123.52
20	F	5008	CLA	C4A-NA-C1A	4.65	108.80	106.68
19	7	306	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
22	9	615	XAT	O4-C5-C4	-4.62	109.16	113.49
23	3	418	BCR	C15-C16-C17	4.61	132.95	123.52
20	1	614	CLA	C4A-NA-C1A	4.60	108.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	615	LUT	C35-C15-C14	4.59	132.91	123.52
20	A	820	CLA	C4A-NA-C1A	4.57	108.76	106.68
20	8	311	CLA	C4A-NA-C1A	4.57	108.76	106.68
21	1	615	LUT	C15-C35-C34	-4.55	114.20	123.52
20	1	612	CLA	CAC-C3C-C4C	4.54	130.70	124.79
20	3	413	CLA	C4A-NA-C1A	4.49	108.73	106.68
20	7	303	CLA	C4A-NA-C1A	4.49	108.73	106.68
20	3	408	CLA	C4A-NA-C1A	4.49	108.73	106.68
20	2	605	CLA	C4A-NA-C1A	4.48	108.72	106.68
20	B	815	CLA	C4A-NA-C1A	4.47	108.72	106.68
20	8	312	CLA	C4A-NA-C1A	4.46	108.72	106.68
22	1	616	XAT	C27-C28-C29	4.43	132.40	125.53
20	8	313	CLA	C4A-NA-C1A	4.43	108.70	106.68
20	2	607	CLA	C4A-NA-C1A	4.35	108.66	106.68
20	B	828	CLA	C4A-NA-C1A	4.34	108.66	106.68
19	7	308	CHL	C1A-CHA-C4D	4.33	126.21	118.98
20	B	818	CLA	C4A-NA-C1A	4.32	108.65	106.68
19	7	307	CHL	C1-C2-C3	-4.32	119.77	126.76
19	7	307	CHL	C4D-ND-C1D	4.32	108.50	105.22
19	3	401	CHL	C4D-CHA-CBD	-4.28	104.65	108.97
20	B	838	CLA	C4A-NA-C1A	4.28	108.63	106.68
19	3	401	CHL	C1-C2-C3	-4.26	119.22	126.20
19	1	601	CHL	C1-C2-C3	-4.26	119.87	126.76
20	B	829	CLA	C4A-NA-C1A	4.23	108.61	106.68
19	7	302	CHL	C4D-ND-C1D	4.22	108.42	105.22
20	9	612	CLA	C2A-C1A-CHA	4.21	131.17	123.87
19	1	601	CHL	C4D-ND-C1D	4.20	108.41	105.22
19	8	306	CHL	C1-C2-C3	-4.19	119.98	126.76
23	B	846	BCR	C8-C7-C6	4.17	138.13	127.00
20	A	822	CLA	C4A-NA-C1A	4.16	108.58	106.68
20	1	604	CLA	C4A-NA-C1A	4.15	108.57	106.68
20	F	5005	CLA	C4A-NA-C1A	4.14	108.57	106.68
20	B	813	CLA	C4A-NA-C1A	4.14	108.57	106.68
20	9	607	CLA	C4A-NA-C1A	4.12	108.56	106.68
20	B	807	CLA	C4A-NA-C1A	4.11	108.55	106.68
20	F	5008	CLA	CHB-C4A-NA	4.10	130.32	124.40
20	F	5008	CLA	C2A-C1A-CHA	4.10	130.98	123.87
20	7	315	CLA	C4A-NA-C1A	4.06	108.53	106.68
23	B	846	BCR	C7-C8-C9	4.05	132.23	126.23
19	9	606	CHL	C4D-CHA-CBD	-4.00	104.94	108.97
19	8	305	CHL	C4D-ND-C1D	4.00	108.25	105.22
20	9	604	CLA	C4A-NA-C1A	3.96	108.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	848	BCR	C8-C7-C6	3.95	137.55	127.00
20	L	305	CLA	C4A-NA-C1A	3.95	108.48	106.68
20	1	610	CLA	C4A-NA-C1A	3.94	108.48	106.68
20	A	805	CLA	C4A-NA-C1A	3.92	108.47	106.68
20	B	830	CLA	C4A-NA-C1A	3.92	108.47	106.68
20	2	609	CLA	C4A-NA-C1A	3.90	108.46	106.68
19	2	601	CHL	C1-C2-C3	-3.88	119.85	126.20
19	1	601	CHL	C4D-CHA-CBD	-3.87	105.06	108.97
20	1	612	CLA	C2D-C1D-ND	-3.84	106.33	110.13
20	A	844	CLA	C4A-NA-C1A	3.82	108.42	106.68
19	8	306	CHL	C4D-CHA-CBD	-3.81	105.12	108.97
20	9	612	CLA	CHB-C4A-NA	3.75	129.82	124.40
22	3	416	XAT	O24-C25-C24	-3.74	109.99	113.49
23	A	848	BCR	C7-C8-C9	3.73	131.75	126.23
32	A	803	CL0	C1-C2-C3	-3.72	120.11	126.20
23	A	849	BCR	C24-C23-C22	3.69	131.69	126.23
19	7	302	CHL	C1-C2-C3	-3.67	120.18	126.20
20	A	811	CLA	C4A-NA-C1A	3.64	108.34	106.68
32	A	803	CL0	C4D-CHA-CBD	-3.57	105.37	108.97
20	B	809	CLA	C4A-NA-C1A	3.56	108.30	106.68
21	2	615	LUT	C22-C23-C24	3.56	116.47	111.18
23	A	849	BCR	C23-C24-C25	3.53	136.41	127.00
20	B	834	CLA	C4A-NA-C1A	3.49	108.27	106.68
23	B	846	BCR	C15-C16-C17	3.47	130.62	123.52
20	A	822	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
20	A	824	CLA	C4A-NA-C1A	3.44	108.25	106.68
19	7	308	CHL	C4D-ND-C1D	3.42	107.81	105.22
20	B	804	CLA	C3B-C4B-NB	-3.41	107.49	110.53
20	8	307	CLA	C4A-NA-C1A	3.40	108.23	106.68
20	A	816	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
20	J	4002	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
20	2	608	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
20	1	614	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
20	B	805	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
20	B	809	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
22	1	616	XAT	O24-C25-C24	-3.32	110.38	113.49
19	1	606	CHL	C4D-ND-C1D	3.31	107.73	105.22
20	7	303	CLA	C3B-C4B-NB	-3.31	107.58	110.53
20	A	815	CLA	C4A-NA-C1A	3.29	108.18	106.68
20	B	806	CLA	CHB-C4A-NA	3.29	129.14	124.40
20	2	613	CLA	C3B-C4B-NB	-3.28	107.60	110.53
23	A	850	BCR	C21-C20-C19	3.27	132.68	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	608	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
23	A	850	BCR	C23-C24-C25	3.26	135.70	127.00
20	B	836	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
20	B	817	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
20	1	604	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	9	606	CHL	C3D-C4D-CHA	3.24	113.46	108.54
20	2	608	CLA	CHB-C4A-NA	3.24	129.07	124.40
20	B	834	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
20	1	604	CLA	CHB-C4A-NA	3.22	129.05	124.40
20	7	310	CLA	C3B-C4B-NB	-3.22	107.66	110.53
20	B	825	CLA	CHB-C4A-NA	3.20	129.02	124.40
25	H	202	PTY	C6-O7-C8	3.20	125.45	117.80
20	B	806	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
20	A	807	CLA	C3B-C4B-NB	-3.19	107.69	110.53
22	9	615	XAT	C7-C8-C9	3.18	130.47	125.53
20	A	834	CLA	C3B-C4B-NB	-3.17	107.70	110.53
20	A	832	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
20	8	308	CLA	CHB-C4A-NA	3.16	128.97	124.40
20	A	821	CLA	C3B-C4B-NB	-3.16	107.71	110.53
20	B	831	CLA	C3B-C4B-NB	-3.15	107.71	110.53
33	B	844	PQN	C11-C3-C4	-3.15	115.26	118.58
23	J	4001	BCR	C16-C15-C14	3.15	129.97	123.52
19	2	606	CHL	C3D-C4D-CHA	3.14	113.31	108.54
19	8	304	CHL	C4D-ND-C1D	3.13	107.59	105.22
20	A	817	CLA	C3B-C4B-NB	-3.12	107.74	110.53
20	9	605	CLA	C2D-C1D-ND	-3.12	107.03	110.13
20	A	823	CLA	CHB-C4A-NA	3.12	128.91	124.40
20	2	609	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
20	A	836	CLA	C3B-C4B-NB	-3.12	107.75	110.53
20	B	825	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
23	B	849	BCR	C7-C8-C9	3.11	130.84	126.23
20	B	817	CLA	CHB-C4A-NA	3.11	128.89	124.40
20	1	604	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
20	1	612	CLA	CHD-C1D-C2D	3.11	131.96	125.49
20	L	307	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
20	2	622	CLA	CHB-C4A-NA	3.10	128.87	124.40
20	2	604	CLA	C4A-NA-C1A	3.10	108.09	106.68
20	A	814	CLA	C4A-NA-C1A	3.09	108.09	106.68
20	A	826	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
20	9	610	CLA	CHB-C4A-NA	3.09	128.86	124.40
20	B	807	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	9	614	XAT	C7-C8-C9	3.08	130.31	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
20	B	825	CLA	C3B-C4B-NB	-3.08	107.78	110.53
23	G	4005	BCR	C10-C11-C12	3.07	132.11	123.20
20	A	811	CLA	CHB-C4A-NA	3.07	128.83	124.40
20	K	202	CLA	C3B-C4B-NB	-3.07	107.79	110.53
20	A	815	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
20	K	204	CLA	C3B-C4B-NB	-3.06	107.80	110.53
20	B	838	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	B	802	BCR	C10-C11-C12	3.05	132.05	123.20
20	7	312	CLA	CHB-C4A-NA	3.05	128.80	124.40
20	B	840	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
20	A	810	CLA	CHB-C4A-NA	3.05	128.80	124.40
20	A	834	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
20	B	819	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	B	826	CLA	C4A-NA-C1A	3.04	108.07	106.68
20	A	809	CLA	CHB-C4A-NA	3.04	128.78	124.40
20	B	834	CLA	CHB-C4A-NA	3.03	128.78	124.40
20	9	611	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
20	B	824	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
20	B	818	CLA	C3B-C4B-NB	-3.03	107.82	110.53
20	B	805	CLA	CHB-C4A-NA	3.03	128.77	124.40
20	B	832	CLA	CHB-C4A-NA	3.03	128.77	124.40
20	7	309	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
22	9	615	XAT	C38-C25-C24	-3.03	110.84	114.24
20	7	315	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
20	A	820	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
23	B	802	BCR	C16-C15-C14	3.03	129.71	123.52
20	B	838	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
20	2	611	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
20	A	824	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
20	A	828	CLA	CHB-C4A-NA	3.01	128.74	124.40
20	A	810	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
20	9	608	CLA	C3B-C4B-NB	-3.00	107.85	110.53
20	A	841	CLA	CHB-C4A-NA	3.00	128.73	124.40
19	7	306	CHL	C4D-ND-C1D	3.00	107.50	105.22
20	B	815	CLA	CHB-C4A-NA	3.00	128.73	124.40
20	B	814	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
20	3	409	CLA	C3B-C4B-NB	-3.00	107.86	110.53
20	8	311	CLA	CHB-C4A-NA	2.99	128.72	124.40
20	L	301	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
20	A	831	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
20	1	608	CLA	CHB-C4A-NA	2.99	128.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	302	CLA	CHB-C4A-NA	2.99	128.72	124.40
20	2	612	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	A	829	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	8	307	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	A	840	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	2	605	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	L	302	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	B	849	BCR	C8-C7-C6	2.99	134.98	127.00
20	B	839	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	L	305	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	B	846	BCR	C20-C19-C18	2.99	134.55	126.36
20	3	410	CLA	CHB-C4A-NA	2.99	128.71	124.40
19	7	302	CHL	C3D-C4D-CHA	2.98	113.08	108.54
20	B	821	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
20	B	809	CLA	CHB-C4A-NA	2.98	128.71	124.40
20	9	609	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
20	K	201	CLA	C3B-C4B-NB	-2.98	107.87	110.53
20	B	841	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
33	A	845	PQN	C11-C3-C4	-2.98	115.44	118.58
20	8	302	CLA	CHB-C4A-NA	2.98	128.70	124.40
20	1	614	CLA	CMB-C2B-C3B	2.98	133.56	126.55
20	A	811	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	3	407	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	3	413	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	J	4002	CLA	CHB-C4A-NA	2.97	128.69	124.40
20	A	808	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	B	812	CLA	C3B-C4B-NB	-2.97	107.88	110.53
20	B	835	CLA	CHB-C4A-NA	2.97	128.69	124.40
20	A	827	CLA	CHB-C4A-NA	2.97	128.68	124.40
20	A	815	CLA	C3B-C4B-NB	-2.96	107.88	110.53
20	A	840	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	7	309	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	A	843	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	3	414	CLA	C3B-C4B-NB	-2.95	107.89	110.53
20	9	602	CLA	C3B-C4B-NB	-2.95	107.89	110.53
20	G	4003	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	K	202	CLA	CHB-C4A-NA	2.95	128.66	124.40
20	7	315	CLA	C3B-C4B-NB	-2.95	107.90	110.53
20	B	811	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	B	826	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	B	842	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
20	8	308	CLA	C3B-C4B-NB	-2.94	107.91	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	603	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
20	A	843	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
20	3	411	CLA	CHB-C4A-NA	2.94	128.64	124.40
20	L	307	CLA	C3B-C4B-NB	-2.94	107.91	110.53
20	K	204	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	K	202	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	7	306	CHL	C3D-C4D-CHA	2.93	113.00	108.54
20	9	601	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	G	4004	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
20	3	412	CLA	C3B-C4B-NB	-2.93	107.91	110.53
23	H	205	BCR	C10-C11-C12	2.93	131.69	123.20
20	A	814	CLA	C3B-C4B-NB	-2.93	107.91	110.53
20	9	603	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	B	833	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	2	610	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	A	826	CLA	CHB-C4A-NA	2.93	128.62	124.40
20	F	5006	CLA	C3B-C4B-NB	-2.93	107.92	110.53
20	9	604	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	A	833	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	9	602	CLA	CHB-C4A-NA	2.93	128.62	124.40
20	9	612	CLA	CHA-C1A-NA	-2.92	119.77	126.39
20	B	812	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	B	822	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	B	831	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
20	B	835	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	9	605	CLA	CHD-C1D-C2D	2.91	131.55	125.49
20	B	820	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	A	810	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	3	407	CLA	CHB-C4A-NA	2.91	128.60	124.40
20	A	805	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	1	609	CLA	C3B-C4B-NB	-2.91	107.94	110.53
20	B	837	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	A	806	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
20	B	813	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	A	842	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	3	408	CLA	CHB-C4A-NA	2.90	128.59	124.40
20	2	604	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
19	3	401	CHL	C4D-ND-C1D	2.90	107.42	105.22
20	A	814	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	B	816	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
20	G	4003	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	A	820	CLA	CHB-C4A-NA	2.90	128.58	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	602	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	A	806	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	A	824	CLA	CHB-C4A-NA	2.90	128.58	124.40
20	9	607	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	B	840	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	2	607	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
20	7	314	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	B	824	CLA	CHB-C4A-NA	2.89	128.57	124.40
20	B	818	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	A	841	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
23	B	846	BCR	C21-C20-C19	2.89	131.56	123.20
20	A	819	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	8	310	CLA	CHB-C4A-NA	2.88	128.56	124.40
20	3	407	CLA	C3B-C4B-NB	-2.88	107.95	110.53
20	A	837	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
20	F	5008	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
20	B	813	CLA	C3B-C4B-NB	-2.88	107.96	110.53
20	B	820	CLA	C3B-C4B-NB	-2.88	107.96	110.53
20	B	828	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	2	603	CLA	CHB-C4A-NA	2.88	128.55	124.40
20	3	414	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	L	305	CLA	CHB-C4A-NA	2.88	128.55	124.40
20	7	311	CLA	C3B-C4B-NB	-2.88	107.96	110.53
20	A	823	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	A	836	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
20	2	609	CLA	CHB-C4A-NA	2.87	128.55	124.40
20	1	605	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
20	B	804	CLA	CHB-C4A-NA	2.87	128.55	124.40
20	K	201	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
19	3	401	CHL	C3D-C4D-CHA	2.87	112.91	108.54
20	B	816	CLA	CHB-C4A-NA	2.87	128.54	124.40
20	3	412	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	B	824	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	A	807	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	B	807	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	B	830	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	A	813	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	A	818	CLA	CHB-C4A-NA	2.87	128.54	124.40
20	1	603	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	1	610	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
20	A	825	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
20	B	819	CLA	C4A-NA-C1A	2.86	107.98	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	324	CLA	C3B-C4B-NB	-2.86	107.97	110.53
20	9	612	CLA	C3B-C4B-NB	-2.86	107.97	110.53
20	F	5007	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	J	4002	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	1	610	CLA	C3B-C4B-NB	-2.86	107.98	110.53
20	B	827	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	7	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	8	306	CHL	C3D-C4D-CHA	2.86	112.89	108.54
20	A	830	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	F	5006	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	9	604	CLA	CHB-C4A-NA	2.86	128.53	124.40
20	7	304	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	L	304	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	8	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	9	611	CLA	C3B-C4B-NB	-2.86	107.98	110.53
21	1	615	LUT	C30-C31-C32	2.86	131.48	123.20
22	8	315	XAT	C7-C8-C9	2.86	129.96	125.53
20	B	818	CLA	CHB-C4A-NA	2.86	128.52	124.40
20	9	608	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
20	A	809	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	7	311	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	1	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
20	8	309	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	A	824	CLA	C3B-C4B-NB	-2.85	107.99	110.53
20	B	826	CLA	CHB-C4A-NA	2.85	128.51	124.40
20	9	605	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	7	314	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	A	811	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	1	612	CLA	CHD-C4C-C3C	2.84	128.92	124.77
20	A	807	CLA	CHB-C4A-NA	2.84	128.50	124.40
20	2	602	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	B	806	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
20	F	5008	CLA	CHA-C1A-NA	-2.84	119.96	126.39
20	3	409	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	1	611	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	1	613	CLA	C3B-C4B-NB	-2.84	108.00	110.53
20	F	5005	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	F	5003	CLA	C3B-C4B-NB	-2.84	108.00	110.53
20	8	310	CLA	C3B-C4B-NB	-2.84	108.00	110.53
20	B	810	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	B	822	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
20	8	312	CLA	C3B-C4B-NB	-2.83	108.00	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	607	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	2	604	CLA	C3B-C4B-NB	-2.83	108.00	110.53
20	8	309	CLA	C3B-C4B-NB	-2.83	108.00	110.53
20	B	822	CLA	CHB-C4A-NA	2.83	128.48	124.40
20	1	612	CLA	CMD-C2D-C1D	2.83	129.71	124.73
20	A	827	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	2	604	CLA	CHB-C4A-NA	2.83	128.48	124.40
20	B	827	CLA	C3B-C4B-NB	-2.83	108.01	110.53
20	9	610	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	8	312	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
20	2	611	CLA	CHB-C4A-NA	2.83	128.48	124.40
20	G	4002	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
20	B	842	CLA	C3B-C4B-NB	-2.82	108.01	110.53
20	1	612	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
20	9	607	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
20	A	833	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	B	841	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	B	819	CLA	C1-C2-C3	-2.82	121.58	126.20
20	8	313	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
20	K	203	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
20	A	828	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
20	8	303	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	L	304	CLA	CHB-C4A-NA	2.81	128.46	124.40
20	A	838	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	A	844	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	B	815	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	A	821	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
20	A	822	CLA	O2D-CGD-CBD	2.81	116.14	111.23
20	2	613	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	B	843	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	1	612	CLA	CAC-C3C-C2C	-2.81	122.40	127.56
20	3	413	CLA	C3B-C4B-NB	-2.81	108.02	110.53
20	3	403	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	G	4004	CLA	CHB-C4A-NA	2.81	128.45	124.40
20	9	602	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	8	302	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	B	832	CLA	C3B-C4B-NB	-2.81	108.03	110.53
20	A	840	CLA	C4A-NA-C1A	2.81	107.96	106.68
20	K	203	CLA	CHB-C4A-NA	2.81	128.45	124.40
20	2	612	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	L	306	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	3	404	CLA	O2D-CGD-O1D	-2.80	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	410	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	B	823	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	2	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	L	307	CLA	CHB-C4A-NA	2.80	128.44	124.40
20	7	312	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
20	A	841	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	A	844	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
20	8	302	CLA	C3B-C4B-NB	-2.79	108.03	110.53
20	B	803	CLA	C3B-C4B-NB	-2.79	108.03	110.53
20	B	836	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	F	5005	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	7	324	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	B	805	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	3	408	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
20	1	608	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	3	405	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	K	202	CLA	C4A-NA-C1A	2.79	107.95	106.68
20	B	837	CLA	CHB-C4A-NA	2.79	128.42	124.40
20	2	609	CLA	C3B-C4B-NB	-2.78	108.04	110.53
20	3	405	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	A	812	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	1	613	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	B	832	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	3	403	CLA	CHB-C4A-NA	2.78	128.41	124.40
20	A	839	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	A	819	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	B	821	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	7	313	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	L	301	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	1	611	CLA	C3B-C4B-NB	-2.77	108.06	110.53
20	A	804	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	A	817	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
20	B	812	CLA	CHB-C4A-NA	2.77	128.39	124.40
20	2	611	CLA	C3B-C4B-NB	-2.76	108.06	110.53
20	8	303	CLA	C3B-C4B-NB	-2.76	108.06	110.53
20	A	835	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
20	A	806	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	F	5005	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	8	313	CLA	C3B-C4B-NB	-2.76	108.06	110.53
20	H	204	CLA	CHB-C4A-NA	2.76	128.38	124.40
20	A	831	CLA	C3B-C4B-NB	-2.76	108.07	110.53
20	3	405	CLA	CHB-C4A-NA	2.76	128.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	826	CLA	C3B-C4B-NB	-2.76	108.07	110.53
20	A	829	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
20	9	601	CLA	C3B-C4B-NB	-2.75	108.07	110.53
20	H	204	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
20	7	313	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	8	304	CHL	C3D-C4D-CHA	2.75	112.72	108.54
20	3	410	CLA	C3B-C4B-NB	-2.75	108.08	110.53
20	A	839	CLA	C3B-C4B-NB	-2.75	108.08	110.53
21	2	616	LUT	C22-C23-C24	2.75	115.27	111.18
20	B	807	CLA	CHB-C4A-NA	2.75	128.37	124.40
20	A	804	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
20	1	605	CLA	C3B-C4B-NB	-2.75	108.08	110.53
20	A	837	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	A	812	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	B	838	CLA	CHB-C4A-NA	2.74	128.36	124.40
20	A	818	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	7	313	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	L	304	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	1	611	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	B	804	CLA	CHD-C1D-ND	-2.74	120.95	124.80
20	F	5003	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
20	8	308	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
20	7	314	CLA	CHB-C4A-NA	2.74	128.35	124.40
20	3	411	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
20	F	5007	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	2	605	CLA	CHB-C4A-NA	2.73	128.34	124.40
22	3	416	XAT	C7-C8-C9	2.73	129.77	125.53
21	1	615	LUT	C35-C34-C33	2.73	131.11	127.28
20	B	813	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	B	817	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	9	608	CLA	CHB-C4A-NA	2.73	128.34	124.40
20	9	603	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
20	7	315	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	1	610	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	A	812	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	L	302	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	F	5003	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	B	828	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	A	830	CLA	CHB-C4A-NA	2.72	128.32	124.40
20	A	820	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	A	843	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	8	310	CLA	O2D-CGD-O1D	-2.72	118.56	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	402	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
20	3	411	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	A	831	CLA	CHB-C4A-NA	2.71	128.31	124.40
20	A	808	CLA	CHB-C4A-NA	2.71	128.31	124.40
20	7	312	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	B	828	CLA	CHB-C4A-NA	2.71	128.31	124.40
19	1	601	CHL	C3D-C4D-CHA	2.70	112.65	108.54
20	A	813	CLA	C3B-C4B-NB	-2.70	108.12	110.53
21	1	615	LUT	C10-C11-C12	2.70	131.03	123.20
20	B	826	CLA	C3B-C4B-NB	-2.70	108.12	110.53
20	7	303	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
20	1	607	CLA	CHB-C4A-NA	2.70	128.30	124.40
20	9	610	CLA	C2A-C1A-CHA	2.70	128.55	123.87
20	9	602	CLA	C4A-NA-C1A	2.70	107.91	106.68
20	B	842	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	8	313	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	A	839	CLA	CHB-C4A-NA	2.69	128.29	124.40
20	9	612	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
20	B	805	CLA	O2D-CGD-CBD	2.69	115.94	111.23
20	7	303	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	B	834	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	1	605	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	A	816	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	3	406	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
21	2	616	LUT	C26-C27-C28	2.69	128.76	124.58
20	B	816	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	3	406	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	8	304	CHL	CHA-C1A-C2A	-2.69	127.00	133.31
20	B	804	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
20	B	811	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	9	601	CLA	C4A-NA-C1A	2.68	107.90	106.68
23	H	205	BCR	C11-C12-C13	2.68	133.72	126.36
20	2	603	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	3	404	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	B	803	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	A	823	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	B	829	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
20	A	813	CLA	CHB-C4A-NA	2.68	128.26	124.40
20	A	833	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	B	814	CLA	C3B-C4B-NB	-2.67	108.14	110.53
20	A	830	CLA	C3B-C4B-NB	-2.67	108.14	110.53
20	L	306	CLA	CHB-C4A-NA	2.67	128.26	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	609	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	7	324	CLA	CHB-C4A-NA	2.67	128.25	124.40
23	A	850	BCR	C20-C19-C18	2.67	133.68	126.36
20	B	808	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	9	607	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	8	309	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	B	819	CLA	CHB-C4A-NA	2.67	128.25	124.40
20	B	833	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
20	A	834	CLA	O2D-CGD-CBD	2.66	115.88	111.23
20	3	409	CLA	CHB-C4A-NA	2.66	128.24	124.40
20	2	605	CLA	C3B-C4B-NB	-2.66	108.16	110.53
20	A	814	CLA	CHB-C4A-NA	2.66	128.23	124.40
20	F	5006	CLA	CHB-C4A-NA	2.66	128.23	124.40
20	A	818	CLA	C3B-C4B-NB	-2.65	108.16	110.53
20	B	827	CLA	CHB-C4A-NA	2.65	128.22	124.40
20	3	413	CLA	CHB-C4A-NA	2.65	128.22	124.40
20	3	414	CLA	CHB-C4A-NA	2.64	128.22	124.40
20	1	612	CLA	CHC-C1C-NC	2.64	128.29	124.31
20	A	825	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	1	612	CLA	C4A-NA-C1A	2.64	107.88	106.68
20	7	309	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	2	610	CLA	CHB-C4A-NA	2.64	128.21	124.40
20	A	836	CLA	CHB-C4A-NA	2.64	128.21	124.40
20	9	609	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	7	310	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
20	3	402	CLA	CHB-C4A-NA	2.64	128.20	124.40
20	A	842	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	L	301	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	2	602	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	A	809	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	7	306	CHL	CHA-C1A-C2A	-2.63	127.12	133.31
20	B	835	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
20	2	607	CLA	CHB-C4A-NA	2.63	128.20	124.40
20	3	403	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	A	815	CLA	CHB-C4A-NA	2.63	128.20	124.40
20	A	808	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	1	607	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	B	843	CLA	CHB-C4A-NA	2.63	128.19	124.40
20	9	604	CLA	C3B-C4B-NB	-2.63	108.19	110.53
20	8	312	CLA	CHB-C4A-NA	2.62	128.19	124.40
20	G	4004	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	A	825	CLA	CHB-C4A-NA	2.62	128.18	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	832	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	7	308	CHL	C1C-CHC-C4B	2.62	125.44	116.07
20	8	303	CLA	CHB-C4A-NA	2.62	128.18	124.40
20	1	612	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	B	839	CLA	CHB-C4A-NA	2.62	128.17	124.40
20	A	835	CLA	CHB-C4A-NA	2.61	128.17	124.40
23	B	802	BCR	C15-C14-C13	2.61	130.93	127.28
20	3	412	CLA	CHB-C4A-NA	2.61	128.16	124.40
20	2	608	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	2	622	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
20	7	305	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	3	402	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	3	406	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	B	825	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
20	1	609	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	L	305	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
20	B	829	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	2	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
20	A	840	CLA	C3B-C4B-NB	-2.59	108.22	110.53
20	7	310	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	9	611	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	A	838	CLA	C3B-C4B-NB	-2.59	108.22	110.53
20	B	831	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	1	612	CLA	CHB-C4A-NA	2.58	128.13	124.40
20	A	804	CLA	C3B-C4B-NB	-2.58	108.22	110.53
20	A	817	CLA	CHB-C4A-NA	2.58	128.13	124.40
20	A	841	CLA	C1-C2-C3	-2.58	121.97	126.20
20	A	805	CLA	C3B-C4B-NB	-2.58	108.22	110.53
20	A	838	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	2	622	CLA	C3B-C4B-NB	-2.58	108.23	110.53
20	1	602	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	7	304	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	J	4001	BCR	C15-C14-C13	2.57	130.88	127.28
20	9	603	CLA	C3B-C4B-NB	-2.57	108.24	110.53
20	B	829	CLA	C3B-C4B-NB	-2.57	108.24	110.53
20	K	204	CLA	CHB-C4A-NA	2.57	128.10	124.40
20	1	609	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
20	B	825	CLA	O2D-CGD-CBD	2.56	115.70	111.23
20	G	4003	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	2	601	CHL	C3D-CAD-CBD	-2.56	104.24	107.61
20	B	809	CLA	C3B-C4B-NB	-2.56	108.25	110.53
20	A	829	CLA	CHB-C4A-NA	2.56	128.09	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	814	CLA	CHB-C4A-NA	2.55	128.08	124.40
32	A	803	CL0	C3D-C4D-CHA	2.55	112.42	108.54
20	1	614	CLA	CHB-C4A-NA	2.55	128.08	124.40
20	B	843	CLA	C3B-C4B-NB	-2.55	108.25	110.53
20	1	603	CLA	CHB-C4A-NA	2.55	128.08	124.40
20	A	822	CLA	CHB-C4A-NA	2.55	128.07	124.40
21	1	615	LUT	C26-C27-C28	2.54	128.54	124.58
20	7	305	CLA	CHB-C4A-NA	2.54	128.06	124.40
32	A	803	CL0	C1C-CHC-C4B	2.54	125.14	116.07
22	9	615	XAT	C27-C28-C29	-2.53	121.60	125.53
20	F	5007	CLA	CHB-C4A-NA	2.53	128.06	124.40
20	B	817	CLA	O2D-CGD-CBD	2.53	115.65	111.23
20	A	819	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	A	842	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	B	846	BCR	C16-C17-C18	2.53	130.82	127.28
20	A	834	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	B	810	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	B	802	BCR	C11-C12-C13	2.52	133.28	126.36
20	A	816	CLA	O2D-CGD-CBD	2.52	115.63	111.23
20	A	832	CLA	CHB-C4A-NA	2.52	128.03	124.40
20	B	840	CLA	CHB-C4A-NA	2.52	128.03	124.40
23	A	847	BCR	C15-C16-C17	2.51	128.66	123.52
22	9	614	XAT	O24-C25-C24	-2.51	111.14	113.49
24	2	618	LHG	O3-P-O6	-2.51	100.12	106.67
19	7	307	CHL	C3C-C4C-NC	-2.51	108.52	114.65
20	B	836	CLA	CHB-C4A-NA	2.51	128.02	124.40
20	B	803	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
20	K	203	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	A	810	CLA	C4A-NA-C1A	2.50	107.82	106.68
20	A	835	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	1	612	CLA	C3C-C4C-NC	-2.50	107.23	110.43
20	1	613	CLA	CHB-C4A-NA	2.49	128.00	124.40
20	A	821	CLA	CHB-C4A-NA	2.49	128.00	124.40
20	B	823	CLA	CHB-C4A-NA	2.49	127.99	124.40
20	A	822	CLA	C3B-C4B-NB	-2.49	108.31	110.53
20	7	311	CLA	CHB-C4A-NA	2.49	127.99	124.40
20	8	307	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	7	306	CHL	C3C-C4C-NC	-2.49	108.58	114.65
20	B	821	CLA	CHB-C4A-NA	2.48	127.99	124.40
22	7	317	XAT	C38-C25-C24	-2.48	111.45	114.24
20	1	608	CLA	O2D-CGD-CBD	2.48	115.57	111.23
20	B	815	CLA	C3B-C4B-NB	-2.48	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	828	CLA	C3B-C4B-NB	-2.48	108.32	110.53
19	1	606	CHL	C3C-C4C-NC	-2.48	108.60	114.65
20	B	806	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
20	H	204	CLA	C3B-C4B-NB	-2.47	108.32	110.53
20	L	306	CLA	C3B-C4B-NB	-2.47	108.32	110.53
19	8	304	CHL	C3C-C4C-NC	-2.47	108.61	114.65
20	B	839	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	7	307	CHL	C3D-CAD-CBD	-2.47	104.35	107.61
20	B	820	CLA	CHB-C4A-NA	2.47	127.96	124.40
20	B	813	CLA	C1-C2-C3	-2.47	122.15	126.20
23	A	849	BCR	C21-C20-C19	2.47	130.35	123.20
19	8	306	CHL	C4D-ND-C1D	2.47	107.09	105.22
20	1	614	CLA	CHB-C1B-NB	2.47	127.75	124.05
32	A	803	CL0	C3C-C4C-NC	-2.47	108.62	114.65
19	2	606	CHL	C3C-C4C-NC	-2.46	108.63	114.65
20	B	808	CLA	C3B-C4B-NB	-2.46	108.33	110.53
20	A	807	CLA	C4A-NA-C1A	2.46	107.80	106.68
20	B	837	CLA	C3B-C4B-NB	-2.46	108.33	110.53
20	3	404	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	8	311	CLA	C3B-C4B-NB	-2.46	108.34	110.53
20	2	612	CLA	CHB-C4A-NA	2.46	127.94	124.40
20	A	837	CLA	CHB-C4A-NA	2.46	127.94	124.40
20	L	305	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	8	305	CHL	C3C-C4C-NC	-2.45	108.66	114.65
20	3	408	CLA	C3B-C4B-NB	-2.45	108.34	110.53
20	B	806	CLA	CMB-C2B-C3B	2.44	132.30	126.55
20	A	822	CLA	C1-C2-C3	-2.44	122.19	126.20
20	9	605	CLA	CHD-C1D-ND	-2.44	121.36	124.80
20	2	608	CLA	O2D-CGD-CBD	2.44	115.50	111.23
20	2	602	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	2	601	CHL	C3C-C4C-NC	-2.44	108.69	114.65
20	B	823	CLA	C3B-C4B-NB	-2.44	108.36	110.53
19	7	302	CHL	C3C-C4C-NC	-2.43	108.70	114.65
20	A	827	CLA	C3B-C4B-NB	-2.43	108.36	110.53
20	G	4002	CLA	CHB-C4A-NA	2.43	127.90	124.40
19	7	308	CHL	C3C-C4C-NC	-2.42	108.73	114.65
20	9	602	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
19	9	606	CHL	C3C-C4C-NC	-2.42	108.73	114.65
19	1	601	CHL	C3C-C4C-NC	-2.42	108.73	114.65
19	3	401	CHL	C3C-C4C-NC	-2.41	108.75	114.65
20	A	844	CLA	CMB-C2B-C3B	2.41	132.22	126.55
20	2	613	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	606	CHL	CHA-C1A-C2A	-2.41	127.65	133.31
20	9	605	CLA	C3B-C4B-NB	-2.41	108.38	110.53
20	1	612	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
20	1	603	CLA	C3B-C4B-NB	-2.40	108.39	110.53
23	K	205	BCR	C10-C11-C12	2.40	130.15	123.20
19	2	606	CHL	C4D-ND-C1D	2.40	107.04	105.22
19	8	306	CHL	C3C-C4C-NC	-2.39	108.80	114.65
20	B	831	CLA	C1-C2-C3	-2.39	122.28	126.20
19	7	302	CHL	CHA-C1A-C2A	-2.39	127.69	133.31
20	A	844	CLA	C3B-C4B-NB	-2.39	108.40	110.53
30	8	320	LMK	O2-C4-C3	2.39	117.41	111.88
22	3	416	XAT	C27-C28-C29	2.39	129.24	125.53
20	7	310	CLA	C1-C2-C3	-2.39	122.28	126.20
20	B	811	CLA	C3B-C4B-NB	-2.38	108.40	110.53
20	9	605	CLA	CHB-C4A-NA	2.38	127.84	124.40
19	7	308	CHL	C4C-CHD-C1D	2.38	124.58	116.07
22	1	616	XAT	C7-C8-C9	2.38	129.22	125.53
20	9	601	CLA	CHB-C4A-NA	2.38	127.83	124.40
20	J	4002	CLA	CMB-C2B-C3B	2.38	132.14	126.55
20	G	4004	CLA	CHD-C1D-ND	-2.37	121.47	124.80
20	7	311	CLA	C1-C2-C3	-2.37	122.32	126.20
20	1	604	CLA	C1-C2-C3	-2.37	122.93	126.76
19	8	305	CHL	C3D-C4D-CHA	2.36	112.13	108.54
20	F	5008	CLA	C3B-C4B-NB	-2.36	108.42	110.53
20	1	612	CLA	CHA-C4D-ND	2.36	137.42	132.55
20	K	201	CLA	CHB-C4A-NA	2.36	127.81	124.40
20	B	819	CLA	C3B-C4B-NB	-2.36	108.42	110.53
20	B	806	CLA	C3B-C4B-NB	-2.36	108.43	110.53
32	A	803	CL0	CHA-C1A-C2A	-2.36	127.77	133.31
19	1	606	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
20	B	833	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
20	B	833	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
20	A	810	CLA	C2A-C1A-CHA	2.35	127.94	123.87
20	B	822	CLA	C4A-NA-C1A	2.34	107.75	106.68
20	L	306	CLA	C1-C2-C3	-2.34	122.97	126.76
20	2	604	CLA	C1-C2-C3	-2.34	122.98	126.76
19	2	601	CHL	C3D-C4D-ND	-2.34	109.19	112.94
20	9	610	CLA	C3B-C4B-NB	-2.34	108.44	110.53
20	A	816	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	8	305	CHL	CHA-C1A-C2A	-2.33	127.83	133.31
20	B	831	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
20	A	809	CLA	C1-C2-C3	-2.33	122.38	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	314	CLA	C1-C2-C3	-2.32	123.00	126.76
20	9	603	CLA	C2A-C1A-CHA	2.32	127.89	123.87
20	B	809	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
20	B	836	CLA	C1-C2-C3	-2.31	123.02	126.76
23	K	205	BCR	C11-C12-C13	2.31	132.70	126.36
20	B	822	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
20	B	822	CLA	C1-C2-C3	-2.31	122.42	126.20
20	B	809	CLA	C1-C2-C3	-2.30	122.42	126.20
20	B	824	CLA	C4A-NA-C1A	2.30	107.73	106.68
23	J	4001	BCR	C23-C24-C25	2.30	133.15	127.00
20	A	843	CLA	C1-C2-C3	-2.30	123.04	126.76
20	B	810	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
20	A	831	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
20	8	307	CLA	C3B-C4B-NB	-2.29	108.48	110.53
20	B	833	CLA	C3B-C4B-NB	-2.29	108.49	110.53
20	7	310	CLA	C4A-NA-C1A	2.29	107.72	106.68
21	7	316	LUT	C21-C26-C27	2.28	115.45	112.83
20	A	835	CLA	C1-C2-C3	-2.28	122.46	126.20
20	2	613	CLA	CHD-C4C-NC	2.28	127.76	124.23
23	B	802	BCR	C8-C7-C6	2.28	133.08	127.00
20	9	604	CLA	C1-C2-C3	-2.28	123.08	126.76
20	G	4002	CLA	C3B-C4B-NB	-2.28	108.50	110.53
20	B	841	CLA	C3B-C4B-NB	-2.27	108.50	110.53
20	L	305	CLA	CMB-C2B-C3B	2.27	131.90	126.55
20	L	305	CLA	O2D-CGD-CBD	2.27	115.20	111.23
20	B	830	CLA	C2D-C1D-ND	-2.27	107.88	110.13
20	8	310	CLA	C1-C2-C3	-2.27	123.09	126.76
20	3	408	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
20	A	826	CLA	C4A-NA-C1A	2.27	107.71	106.68
20	9	605	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
21	1	615	LUT	C21-C26-C27	2.26	115.43	112.83
20	A	827	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
20	A	828	CLA	C2A-C1A-CHA	2.26	127.80	123.87
20	7	304	CLA	CHB-C4A-NA	2.26	127.67	124.40
20	B	830	CLA	CHB-C4A-NA	2.26	127.66	124.40
20	9	602	CLA	C1-C2-C3	-2.26	122.50	126.20
20	1	611	CLA	C2A-C1A-CHA	2.26	127.78	123.87
23	A	849	BCR	C20-C19-C18	2.26	132.55	126.36
20	8	302	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
19	8	304	CHL	C1A-CHA-CBD	-2.25	126.59	132.36
19	1	606	CHL	C3D-C4D-CHA	2.25	111.96	108.54
20	F	5007	CLA	O2A-CGA-O1A	-2.25	118.00	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	844	CLA	CHB-C4A-NA	2.25	127.64	124.40
20	A	808	CLA	CHD-C1D-ND	-2.25	121.64	124.80
20	3	405	CLA	C1-C2-C3	-2.25	123.13	126.76
20	B	828	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
23	A	848	BCR	C24-C23-C22	2.24	129.55	126.23
20	3	411	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
20	8	311	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
20	A	808	CLA	C4A-NA-C1A	2.23	107.70	106.68
19	8	305	CHL	C1A-CHA-CBD	-2.23	126.65	132.36
20	B	823	CLA	C1-C2-C3	-2.23	122.54	126.20
20	A	837	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
20	3	410	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
21	1	615	LUT	C32-C33-C34	2.23	122.51	119.01
20	B	830	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
20	L	307	CLA	C1-C2-C3	-2.22	123.17	126.76
20	B	835	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	3	415	LUT	C21-C26-C27	2.22	115.37	112.83
20	B	815	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
20	7	311	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
20	7	324	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
20	1	609	CLA	C4A-NA-C1A	2.21	107.69	106.68
20	9	610	CLA	C1-C2-C3	-2.21	123.19	126.76
20	2	622	CLA	CHD-C1D-ND	-2.21	121.69	124.80
20	B	825	CLA	C2A-C1A-CHA	2.21	127.70	123.87
20	9	605	CLA	CAC-C3C-C4C	2.21	127.66	124.79
24	2	618	LHG	O4-P-O5	2.20	119.41	110.83
20	B	821	CLA	C1-C2-C3	-2.20	122.59	126.20
20	8	302	CLA	C1-C2-C3	-2.20	122.59	126.20
23	J	4001	BCR	C7-C8-C9	2.20	129.49	126.23
30	8	320	LMK	O1-C7-C8	2.20	114.46	109.42
20	1	612	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	B	819	CLA	O2D-CGD-CBD	2.20	115.07	111.23
20	B	821	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
20	B	841	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
20	3	410	CLA	C1-C2-C3	-2.19	122.61	126.20
20	2	613	CLA	C1-C2-C3	-2.18	123.23	126.76
19	1	601	CHL	C1C-CHC-C4B	2.18	123.88	116.07
20	A	805	CLA	CHB-C4A-NA	2.18	127.55	124.40
22	7	317	XAT	C36-C21-C26	2.18	115.94	110.05
20	A	812	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
20	A	832	CLA	C1-C2-C3	-2.18	122.62	126.20
20	B	819	CLA	O2A-CGA-O1A	-2.18	118.18	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	612	CLA	O2A-CGA-O1A	-2.18	117.73	123.33
20	B	810	CLA	C3B-C4B-NB	-2.18	108.59	110.53
20	B	833	CLA	C2A-C1A-CHA	2.17	127.64	123.87
20	8	303	CLA	C1-C2-C3	-2.17	123.25	126.76
20	B	838	CLA	CHD-C1D-ND	-2.17	121.75	124.80
20	9	605	CLA	C3C-C4C-NC	-2.17	107.65	110.43
20	F	5003	CLA	C2A-C1A-CHA	2.17	127.63	123.87
20	B	826	CLA	C1-C2-C3	-2.17	122.64	126.20
20	A	818	CLA	C1-C2-C3	-2.17	122.64	126.20
20	A	835	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	2	601	CHL	C3D-C4D-CHA	2.17	111.83	108.54
20	B	807	CLA	C1-C2-C3	-2.17	122.64	126.20
20	8	310	CLA	C2A-C1A-CHA	2.17	127.63	123.87
23	A	858	BCR	C7-C8-C9	2.16	129.44	126.23
20	B	826	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	3	406	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	A	817	CLA	C1-C2-C3	-2.16	122.67	126.20
20	A	814	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
20	2	613	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
20	L	302	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
20	B	804	CLA	CMB-C2B-C3B	2.15	131.61	126.55
19	9	606	CHL	CHA-C1A-C2A	-2.14	128.27	133.31
20	B	833	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
20	A	818	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
20	9	611	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	G	4005	BCR	C11-C12-C13	2.14	132.23	126.36
20	A	833	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	7	309	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	A	809	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	8	305	CHL	C3D-CAD-CBD	-2.14	104.79	107.61
20	1	612	CLA	CMD-C2D-C3D	-2.13	122.79	127.69
20	B	825	CLA	CHA-C1A-NA	-2.13	121.56	126.39
20	8	309	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
20	A	843	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
20	3	409	CLA	C1-C2-C3	-2.13	123.31	126.76
20	1	604	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
20	2	603	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
20	B	820	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
20	A	807	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
20	B	840	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
20	A	839	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
20	B	839	CLA	O2A-CGA-O1A	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	308	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
20	9	607	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	2	606	CHL	C1A-CHA-CBD	-2.12	126.94	132.36
20	A	822	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
20	A	827	CLA	CHD-C1D-ND	-2.11	121.83	124.80
20	B	833	CLA	CMB-C2B-C3B	2.11	131.52	126.55
20	7	305	CLA	C1-C2-C3	-2.11	123.34	126.76
20	A	812	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
20	A	836	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	2	622	CLA	CHD-C1D-C2D	2.11	129.88	125.49
20	B	830	CLA	CAC-C3C-C4C	2.11	127.53	124.79
20	1	612	CLA	C1D-ND-C4D	2.11	107.79	106.31
20	2	604	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
23	B	846	BCR	C23-C24-C25	2.11	132.62	127.00
20	1	614	CLA	O2D-CGD-CBD	2.11	114.91	111.23
19	7	308	CHL	CHA-C1A-C2A	-2.10	128.36	133.31
20	A	806	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
20	A	817	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
20	1	613	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
20	B	820	CLA	C1-C2-C3	-2.10	122.76	126.20
20	3	410	CLA	C2A-C1A-CHA	2.10	127.51	123.87
19	7	308	CHL	C3D-CAD-CBD	-2.10	104.84	107.61
20	1	611	CLA	CHA-C1A-NA	-2.10	121.64	126.39
20	J	4002	CLA	CBB-CAB-C3B	-2.09	117.07	127.53
20	B	832	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	G	4005	BCR	C15-C16-C17	-2.09	119.24	123.52
20	9	603	CLA	CHA-C1A-NA	-2.09	121.66	126.39
20	A	828	CLA	CHA-C1A-NA	-2.09	121.66	126.39
20	A	827	CLA	C1-C2-C3	-2.09	122.78	126.20
20	A	823	CLA	C1-C2-C3	-2.09	122.78	126.20
20	A	812	CLA	C2A-C1A-CHA	2.09	127.49	123.87
20	B	837	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
20	B	841	CLA	C4A-NA-C1A	2.09	107.63	106.68
20	B	827	CLA	C1-C2-C3	-2.08	122.78	126.20
20	1	613	CLA	C1-C2-C3	-2.08	122.78	126.20
20	A	844	CLA	C1-C2-C3	-2.08	122.78	126.20
19	3	401	CHL	C1A-CHA-CBD	-2.08	127.03	132.36
20	B	823	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	7	312	CLA	C2A-C1A-CHA	2.08	127.48	123.87
20	7	309	CLA	O2D-CGD-CBD	2.08	114.87	111.23
22	1	616	XAT	O24-C26-C27	-2.08	110.92	116.88
20	A	831	CLA	CHD-C1D-ND	-2.08	121.88	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	610	CLA	CHA-C1A-NA	-2.08	121.69	126.39
20	2	613	CLA	CMC-C2C-C1C	2.08	128.28	125.03
20	1	614	CLA	C3B-C4B-NB	-2.08	108.68	110.53
20	7	310	CLA	CAA-CBA-CGA	-2.08	107.31	113.21
20	8	310	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
20	9	612	CLA	O1D-CGD-CBD	2.07	128.61	124.52
20	B	834	CLA	O2D-CGD-CBD	2.07	114.85	111.23
20	A	841	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	A	840	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	B	841	CLA	C1-C2-C3	-2.07	122.81	126.20
20	B	836	CLA	O2D-CGD-CBD	2.07	114.85	111.23
20	A	824	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	A	830	CLA	C1-C2-C3	-2.07	122.81	126.20
20	7	313	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	B	830	CLA	C3B-C4B-NB	-2.07	108.68	110.53
20	9	602	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
20	B	830	CLA	C1-C2-C3	-2.06	122.81	126.20
20	A	840	CLA	C1-C2-C3	-2.06	122.82	126.20
20	B	824	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	1	606	CHL	C3D-CAD-CBD	-2.06	104.89	107.61
20	J	4002	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
20	B	837	CLA	CMB-C2B-C3B	2.06	131.39	126.55
20	G	4002	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
20	3	402	CLA	C1-C2-C3	-2.06	122.83	126.20
19	1	601	CHL	C3D-CAD-CBD	-2.05	104.90	107.61
20	7	314	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	F	5006	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	B	807	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	A	812	CLA	C1-C2-C3	-2.05	122.84	126.20
20	B	803	CLA	C1-C2-C3	-2.05	122.84	126.20
20	L	304	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	A	821	CLA	CAC-C3C-C4C	2.05	127.45	124.79
20	A	832	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
20	3	407	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	L	307	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
21	2	616	LUT	C27-C28-C29	2.04	130.72	126.32
20	9	608	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	A	816	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	L	305	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	2	603	CLA	C2A-C1A-CHA	2.04	127.41	123.87
20	B	803	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	3	401	CHL	C3D-CAD-CBD	-2.04	104.92	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
20	B	824	CLA	C1-C2-C3	-2.03	122.86	126.20
20	1	602	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
20	K	204	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	A	810	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
20	A	829	CLA	C1-C2-C3	-2.03	122.87	126.20
20	7	304	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
20	B	819	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
20	3	412	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	7	302	CHL	C3D-CAD-CBD	-2.02	104.94	107.61
20	2	608	CLA	O2A-CGA-O1A	-2.02	118.12	123.33
19	1	606	CHL	C1A-CHA-CBD	-2.02	127.18	132.36
19	1	606	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
20	7	303	CLA	C1-C2-C3	-2.02	122.88	126.20
20	F	5005	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
20	A	830	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
20	B	804	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
20	A	837	CLA	C1-C2-C3	-2.02	122.89	126.20
20	A	837	CLA	CHB-C1B-NB	2.02	127.07	124.05
20	1	614	CLA	CHD-C1D-ND	-2.02	121.97	124.80
20	7	305	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
20	L	302	CLA	C1-C2-C3	-2.01	122.90	126.20
20	A	819	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
20	A	808	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
20	2	613	CLA	CHD-C1D-ND	-2.01	121.97	124.80
20	A	815	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
19	2	606	CHL	C3D-CAD-CBD	-2.01	104.96	107.61
20	B	819	CLA	CHD-C1D-ND	-2.01	121.98	124.80
20	1	607	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
20	A	810	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
20	B	843	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	2	609	CLA	CAA-C2A-C3A	-2.00	111.64	116.23
20	3	412	CLA	C1-C2-C3	-2.00	122.92	126.20
20	A	811	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	8	302	CLA	C4A-NA-C1A	2.00	107.59	106.68

All (213) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	601	CHL	ND
19	1	606	CHL	NC
19	2	601	CHL	C8

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Mol	Chain	Res	Type	Atom
19	2	601	CHL	NC
19	2	606	CHL	C3A
19	2	606	CHL	NC
19	3	401	CHL	C8
19	3	401	CHL	NC
19	7	302	CHL	C8
19	7	302	CHL	ND
19	7	302	CHL	NA
19	7	306	CHL	NC
19	7	307	CHL	NA
19	7	307	CHL	NC
19	7	308	CHL	NA
19	8	304	CHL	NC
19	8	305	CHL	NC
19	8	306	CHL	ND
19	8	306	CHL	NA
19	9	606	CHL	NC
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	2	602	CLA	ND
20	2	603	CLA	ND
20	2	604	CLA	ND
20	2	605	CLA	ND
20	2	607	CLA	ND
20	2	608	CLA	ND
20	2	609	CLA	ND
20	2	610	CLA	ND
20	2	611	CLA	ND
20	2	612	CLA	ND
20	2	613	CLA	ND
20	2	622	CLA	ND
20	3	402	CLA	ND

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Mol	Chain	Res	Type	Atom
20	3	403	CLA	ND
20	3	404	CLA	ND
20	3	405	CLA	ND
20	3	406	CLA	ND
20	3	407	CLA	ND
20	3	408	CLA	ND
20	3	409	CLA	ND
20	3	410	CLA	ND
20	3	411	CLA	ND
20	3	412	CLA	ND
20	3	413	CLA	ND
20	3	414	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	324	CLA	ND
20	8	302	CLA	ND
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	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	A	804	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	807	CLA	ND
20	A	808	CLA	ND
20	A	809	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	817	CLA	ND
20	A	818	CLA	ND
20	A	819	CLA	ND
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND
20	A	823	CLA	ND
20	A	824	CLA	ND
20	A	825	CLA	ND
20	A	826	CLA	ND
20	A	827	CLA	ND
20	A	828	CLA	ND
20	A	829	CLA	ND
20	A	830	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	836	CLA	ND
20	A	837	CLA	ND
20	A	838	CLA	ND
20	A	839	CLA	ND
20	A	840	CLA	ND
20	A	841	CLA	ND
20	A	842	CLA	ND
20	A	843	CLA	ND
20	A	844	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND

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Mol	Chain	Res	Type	Atom
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
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	837	CLA	ND
20	B	838	CLA	ND
20	B	839	CLA	ND
20	B	840	CLA	ND
20	B	841	CLA	ND
20	B	842	CLA	ND
20	B	843	CLA	ND
20	F	5003	CLA	ND
20	F	5005	CLA	ND
20	F	5006	CLA	ND
20	F	5007	CLA	ND

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Mol	Chain	Res	Type	Atom
20	G	4002	CLA	ND
20	G	4003	CLA	ND
20	G	4004	CLA	ND
20	H	204	CLA	ND
20	J	4002	CLA	ND
20	K	201	CLA	ND
20	K	202	CLA	ND
20	K	203	CLA	ND
20	K	204	CLA	ND
20	L	301	CLA	ND
20	L	302	CLA	ND
20	L	304	CLA	ND
20	L	305	CLA	ND
20	L	306	CLA	ND
20	L	307	CLA	ND
21	1	615	LUT	C23
21	1	615	LUT	C26
21	1	615	LUT	C3
21	2	614	LUT	C23
21	2	614	LUT	C26
21	2	614	LUT	C3
21	2	615	LUT	C23
21	2	615	LUT	C26
21	2	615	LUT	C3
21	2	616	LUT	C23
21	2	616	LUT	C26
21	2	616	LUT	C3
21	2	617	LUT	C23
21	2	617	LUT	C26
21	2	617	LUT	C3
21	3	415	LUT	C23
21	3	415	LUT	C26
21	3	415	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

All (2733) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	601	CHL	C3A-C2A-CAA-CBA
19	1	606	CHL	C1A-C2A-CAA-CBA
19	1	606	CHL	C3A-C2A-CAA-CBA
19	2	606	CHL	C1A-C2A-CAA-CBA
19	2	606	CHL	CHA-CBD-CGD-O1D
19	3	401	CHL	C1A-C2A-CAA-CBA
19	3	401	CHL	C3A-C2A-CAA-CBA
19	3	401	CHL	C1C-C2C-CMC-OMC
19	7	306	CHL	C1C-C2C-CMC-OMC
19	7	306	CHL	C4C-C3C-CAC-CBC
19	7	306	CHL	CBD-CGD-O2D-CED
19	7	307	CHL	C1A-C2A-CAA-CBA
19	7	307	CHL	C3A-C2A-CAA-CBA
19	7	307	CHL	C1C-C2C-CMC-OMC
19	7	307	CHL	C3C-C2C-CMC-OMC
19	7	307	CHL	C1-C2-C3-C4
19	7	307	CHL	C1-C2-C3-C5
19	7	308	CHL	C3A-C2A-CAA-CBA
19	7	308	CHL	C1C-C2C-CMC-OMC
19	7	308	CHL	C3C-C2C-CMC-OMC
19	7	308	CHL	CBD-CGD-O2D-CED
19	7	308	CHL	O1D-CGD-O2D-CED
19	8	304	CHL	C1C-C2C-CMC-OMC
19	8	304	CHL	C3C-C2C-CMC-OMC
19	8	306	CHL	C1A-C2A-CAA-CBA
19	8	306	CHL	C3A-C2A-CAA-CBA
19	8	306	CHL	C1C-C2C-CMC-OMC
19	8	306	CHL	C3C-C2C-CMC-OMC
19	8	306	CHL	C1-C2-C3-C4
19	8	306	CHL	C1-C2-C3-C5
19	9	606	CHL	C1C-C2C-CMC-OMC
19	9	606	CHL	C3C-C2C-CMC-OMC
19	9	606	CHL	C4C-C3C-CAC-CBC
19	9	606	CHL	CHA-CBD-CGD-O1D
19	9	606	CHL	CHA-CBD-CGD-O2D
20	1	603	CLA	C4B-C3B-CAB-CBB
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	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	1	609	CLA	C4B-C3B-CAB-CBB
20	1	610	CLA	C2B-C3B-CAB-CBB
20	1	610	CLA	C4B-C3B-CAB-CBB
20	1	611	CLA	C1A-C2A-CAA-CBA
20	1	611	CLA	C3A-C2A-CAA-CBA
20	1	611	CLA	C2B-C3B-CAB-CBB
20	1	611	CLA	C4B-C3B-CAB-CBB
20	1	612	CLA	CBA-CGA-O2A-C1
20	1	612	CLA	O1A-CGA-O2A-C1
20	1	612	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	C4B-C3B-CAB-CBB
20	1	614	CLA	C1A-C2A-CAA-CBA
20	1	614	CLA	C3A-C2A-CAA-CBA
20	2	602	CLA	C4B-C3B-CAB-CBB
20	2	603	CLA	C4B-C3B-CAB-CBB
20	2	603	CLA	CAD-CBD-CGD-O2D
20	2	604	CLA	CBD-CGD-O2D-CED
20	2	605	CLA	C1A-C2A-CAA-CBA
20	2	605	CLA	C3A-C2A-CAA-CBA
20	2	607	CLA	C1A-C2A-CAA-CBA
20	2	607	CLA	C2B-C3B-CAB-CBB
20	2	607	CLA	C4B-C3B-CAB-CBB
20	2	608	CLA	C1A-C2A-CAA-CBA
20	2	609	CLA	C2B-C3B-CAB-CBB
20	2	609	CLA	C4B-C3B-CAB-CBB
20	2	611	CLA	C1A-C2A-CAA-CBA
20	2	611	CLA	CBD-CGD-O2D-CED
20	2	612	CLA	CAA-CBA-CGA-O1A
20	2	612	CLA	C2B-C3B-CAB-CBB
20	2	612	CLA	C4B-C3B-CAB-CBB
20	2	613	CLA	C4B-C3B-CAB-CBB
20	2	613	CLA	CBD-CGD-O2D-CED
20	2	622	CLA	C2B-C3B-CAB-CBB
20	2	622	CLA	C4B-C3B-CAB-CBB
20	3	402	CLA	CBD-CGD-O2D-CED
20	3	404	CLA	CBA-CGA-O2A-C1
20	3	404	CLA	O1A-CGA-O2A-C1
20	3	405	CLA	C2B-C3B-CAB-CBB
20	3	405	CLA	C4B-C3B-CAB-CBB
20	3	406	CLA	C1A-C2A-CAA-CBA
20	3	407	CLA	C3A-C2A-CAA-CBA
20	3	407	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	3	407	CLA	C4B-C3B-CAB-CBB
20	3	407	CLA	CHA-CBD-CGD-O1D
20	3	407	CLA	CHA-CBD-CGD-O2D
20	3	408	CLA	C2B-C3B-CAB-CBB
20	3	408	CLA	C4B-C3B-CAB-CBB
20	3	409	CLA	C2B-C3B-CAB-CBB
20	3	409	CLA	C4B-C3B-CAB-CBB
20	3	410	CLA	C2B-C3B-CAB-CBB
20	3	410	CLA	C4B-C3B-CAB-CBB
20	3	411	CLA	C2B-C3B-CAB-CBB
20	3	411	CLA	C4B-C3B-CAB-CBB
20	3	412	CLA	C3A-C2A-CAA-CBA
20	3	412	CLA	C2B-C3B-CAB-CBB
20	3	412	CLA	C4B-C3B-CAB-CBB
20	3	412	CLA	CBD-CGD-O2D-CED
20	3	413	CLA	C2B-C3B-CAB-CBB
20	3	413	CLA	C4B-C3B-CAB-CBB
20	3	413	CLA	CBD-CGD-O2D-CED
20	3	414	CLA	C2B-C3B-CAB-CBB
20	3	414	CLA	C4B-C3B-CAB-CBB
20	7	303	CLA	C1A-C2A-CAA-CBA
20	7	303	CLA	C3A-C2A-CAA-CBA
20	7	303	CLA	C2B-C3B-CAB-CBB
20	7	303	CLA	C4B-C3B-CAB-CBB
20	7	303	CLA	CBD-CGD-O2D-CED
20	7	304	CLA	C2B-C3B-CAB-CBB
20	7	304	CLA	C4B-C3B-CAB-CBB
20	7	309	CLA	C1A-C2A-CAA-CBA
20	7	309	CLA	C3A-C2A-CAA-CBA
20	7	310	CLA	C3A-C2A-CAA-CBA
20	7	310	CLA	C4B-C3B-CAB-CBB
20	7	311	CLA	C2B-C3B-CAB-CBB
20	7	311	CLA	C4B-C3B-CAB-CBB
20	7	312	CLA	C4B-C3B-CAB-CBB
20	7	312	CLA	C3-C5-C6-C7
20	7	313	CLA	C2B-C3B-CAB-CBB
20	7	313	CLA	C4B-C3B-CAB-CBB
20	7	314	CLA	C4B-C3B-CAB-CBB
20	7	315	CLA	C2B-C3B-CAB-CBB
20	7	315	CLA	C4B-C3B-CAB-CBB
20	7	324	CLA	C1A-C2A-CAA-CBA
20	7	324	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	8	302	CLA	C1A-C2A-CAA-CBA
20	8	302	CLA	C3A-C2A-CAA-CBA
20	8	307	CLA	C3A-C2A-CAA-CBA
20	8	308	CLA	C1A-C2A-CAA-CBA
20	8	308	CLA	C2B-C3B-CAB-CBB
20	8	308	CLA	C4B-C3B-CAB-CBB
20	8	309	CLA	O1A-CGA-O2A-C1
20	8	309	CLA	C2B-C3B-CAB-CBB
20	8	309	CLA	C4B-C3B-CAB-CBB
20	8	312	CLA	C2B-C3B-CAB-CBB
20	8	312	CLA	C4B-C3B-CAB-CBB
20	8	313	CLA	C1A-C2A-CAA-CBA
20	8	313	CLA	C3A-C2A-CAA-CBA
20	8	313	CLA	C2B-C3B-CAB-CBB
20	8	313	CLA	C4B-C3B-CAB-CBB
20	9	602	CLA	C1A-C2A-CAA-CBA
20	9	602	CLA	C3A-C2A-CAA-CBA
20	9	603	CLA	C4B-C3B-CAB-CBB
20	9	604	CLA	CBD-CGD-O2D-CED
20	9	607	CLA	C4B-C3B-CAB-CBB
20	9	608	CLA	C1A-C2A-CAA-CBA
20	9	608	CLA	C3A-C2A-CAA-CBA
20	9	609	CLA	C2B-C3B-CAB-CBB
20	9	609	CLA	C4B-C3B-CAB-CBB
20	9	610	CLA	CHA-CBD-CGD-O1D
20	9	610	CLA	CHA-CBD-CGD-O2D
20	9	610	CLA	CBD-CGD-O2D-CED
20	9	611	CLA	C4B-C3B-CAB-CBB
20	9	612	CLA	C2B-C3B-CAB-CBB
20	9	612	CLA	C4B-C3B-CAB-CBB
20	A	806	CLA	C4B-C3B-CAB-CBB
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	808	CLA	CAD-CBD-CGD-O1D
20	A	808	CLA	CAD-CBD-CGD-O2D
20	A	809	CLA	C4B-C3B-CAB-CBB
20	A	809	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	C3A-C2A-CAA-CBA
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA
20	A	813	CLA	C2B-C3B-CAB-CBB
20	A	813	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	814	CLA	C1A-C2A-CAA-CBA
20	A	814	CLA	C4B-C3B-CAB-CBB
20	A	815	CLA	C1A-C2A-CAA-CBA
20	A	816	CLA	CBD-CGD-O2D-CED
20	A	817	CLA	CBD-CGD-O2D-CED
20	A	818	CLA	C1A-C2A-CAA-CBA
20	A	818	CLA	C3A-C2A-CAA-CBA
20	A	819	CLA	C1A-C2A-CAA-CBA
20	A	819	CLA	C3A-C2A-CAA-CBA
20	A	820	CLA	CHA-CBD-CGD-O1D
20	A	820	CLA	CHA-CBD-CGD-O2D
20	A	821	CLA	C4B-C3B-CAB-CBB
20	A	822	CLA	CHA-CBD-CGD-O1D
20	A	822	CLA	CHA-CBD-CGD-O2D
20	A	823	CLA	C4B-C3B-CAB-CBB
20	A	823	CLA	CBD-CGD-O2D-CED
20	A	825	CLA	C2B-C3B-CAB-CBB
20	A	825	CLA	C4B-C3B-CAB-CBB
20	A	825	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	C1A-C2A-CAA-CBA
20	A	826	CLA	C4B-C3B-CAB-CBB
20	A	827	CLA	C2B-C3B-CAB-CBB
20	A	827	CLA	C4B-C3B-CAB-CBB
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	CBD-CGD-O2D-CED
20	A	833	CLA	CHA-CBD-CGD-O1D
20	A	833	CLA	CHA-CBD-CGD-O2D
20	A	834	CLA	C2B-C3B-CAB-CBB
20	A	834	CLA	C4B-C3B-CAB-CBB
20	A	837	CLA	C2B-C3B-CAB-CBB
20	A	837	CLA	C4B-C3B-CAB-CBB
20	A	837	CLA	C2-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	A	839	CLA	C2B-C3B-CAB-CBB
20	A	839	CLA	C4B-C3B-CAB-CBB
20	A	840	CLA	C1A-C2A-CAA-CBA
20	A	840	CLA	C4B-C3B-CAB-CBB
20	A	841	CLA	C1A-C2A-CAA-CBA
20	A	841	CLA	C3A-C2A-CAA-CBA
20	A	842	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	843	CLA	CAD-CBD-CGD-O1D
20	A	843	CLA	CAD-CBD-CGD-O2D
20	A	843	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	C1A-C2A-CAA-CBA
20	B	803	CLA	C3A-C2A-CAA-CBA
20	B	803	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	CHA-CBD-CGD-O1D
20	B	805	CLA	CHA-CBD-CGD-O2D
20	B	806	CLA	C1A-C2A-CAA-CBA
20	B	806	CLA	C3A-C2A-CAA-CBA
20	B	806	CLA	CHA-CBD-CGD-O1D
20	B	806	CLA	CHA-CBD-CGD-O2D
20	B	807	CLA	CBD-CGD-O2D-CED
20	B	808	CLA	C2B-C3B-CAB-CBB
20	B	808	CLA	C4B-C3B-CAB-CBB
20	B	808	CLA	CBD-CGD-O2D-CED
20	B	809	CLA	C2B-C3B-CAB-CBB
20	B	809	CLA	C4B-C3B-CAB-CBB
20	B	811	CLA	C11-C10-C8-C7
20	B	812	CLA	C4B-C3B-CAB-CBB
20	B	812	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	O1D-CGD-O2D-CED
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C2B-C3B-CAB-CBB
20	B	813	CLA	C4B-C3B-CAB-CBB
20	B	814	CLA	CBD-CGD-O2D-CED
20	B	814	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	O1A-CGA-O2A-C1
20	B	819	CLA	C1A-C2A-CAA-CBA
20	B	819	CLA	C3A-C2A-CAA-CBA
20	B	820	CLA	C2B-C3B-CAB-CBB
20	B	820	CLA	C4B-C3B-CAB-CBB
20	B	821	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C3A-C2A-CAA-CBA
20	B	821	CLA	C2B-C3B-CAB-CBB
20	B	821	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	822	CLA	C2B-C3B-CAB-CBB
20	B	822	CLA	C4B-C3B-CAB-CBB
20	B	822	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	C2B-C3B-CAB-CBB
20	B	823	CLA	C4B-C3B-CAB-CBB
20	B	824	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	CHA-CBD-CGD-O1D
20	B	826	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C4B-C3B-CAB-CBB
20	B	828	CLA	CBD-CGD-O2D-CED
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C11-C12-C13-C14
20	B	830	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	C4B-C3B-CAB-CBB
20	B	834	CLA	C2B-C3B-CAB-CBB
20	B	834	CLA	C4B-C3B-CAB-CBB
20	B	835	CLA	C1A-C2A-CAA-CBA
20	B	835	CLA	C3A-C2A-CAA-CBA
20	B	836	CLA	CAD-CBD-CGD-O1D
20	B	836	CLA	CAD-CBD-CGD-O2D
20	B	836	CLA	CBD-CGD-O2D-CED
20	B	838	CLA	C2B-C3B-CAB-CBB
20	B	838	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C1A-C2A-CAA-CBA
20	B	841	CLA	C3A-C2A-CAA-CBA
20	B	843	CLA	C2B-C3B-CAB-CBB
20	B	843	CLA	C4B-C3B-CAB-CBB
20	F	5003	CLA	C2B-C3B-CAB-CBB
20	F	5003	CLA	C4B-C3B-CAB-CBB
20	F	5005	CLA	CBD-CGD-O2D-CED
20	F	5006	CLA	C2B-C3B-CAB-CBB
20	F	5006	CLA	C4B-C3B-CAB-CBB
20	F	5007	CLA	C2B-C3B-CAB-CBB
20	F	5007	CLA	C4B-C3B-CAB-CBB
20	F	5008	CLA	C1A-C2A-CAA-CBA
20	F	5008	CLA	CBA-CGA-O2A-C1
20	F	5008	CLA	O1A-CGA-O2A-C1
20	F	5008	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	F	5008	CLA	C4B-C3B-CAB-CBB
20	G	4003	CLA	CBD-CGD-O2D-CED
20	J	4002	CLA	C2B-C3B-CAB-CBB
20	J	4002	CLA	C4B-C3B-CAB-CBB
20	J	4002	CLA	CBD-CGD-O2D-CED
20	K	201	CLA	C4B-C3B-CAB-CBB
20	K	201	CLA	CBD-CGD-O2D-CED
20	K	202	CLA	C2B-C3B-CAB-CBB
20	K	202	CLA	C4B-C3B-CAB-CBB
20	K	203	CLA	C1A-C2A-CAA-CBA
20	K	203	CLA	C3A-C2A-CAA-CBA
20	K	204	CLA	C2B-C3B-CAB-CBB
20	K	204	CLA	C4B-C3B-CAB-CBB
20	L	301	CLA	C1A-C2A-CAA-CBA
20	L	304	CLA	C1A-C2A-CAA-CBA
20	L	304	CLA	C3A-C2A-CAA-CBA
20	L	306	CLA	C1A-C2A-CAA-CBA
20	L	306	CLA	C3A-C2A-CAA-CBA
20	L	307	CLA	C1A-C2A-CAA-CBA
20	L	307	CLA	C3A-C2A-CAA-CBA
20	L	307	CLA	C2B-C3B-CAB-CBB
20	L	307	CLA	C4B-C3B-CAB-CBB
20	L	307	CLA	CAD-CBD-CGD-O1D
20	L	307	CLA	CAD-CBD-CGD-O2D
21	1	615	LUT	C21-C26-C27-C28
21	1	615	LUT	C25-C26-C27-C28
21	2	614	LUT	C21-C26-C27-C28
21	2	614	LUT	C26-C27-C28-C29
21	2	615	LUT	C21-C26-C27-C28
21	2	615	LUT	C25-C26-C27-C28
21	2	616	LUT	C26-C27-C28-C29
21	2	616	LUT	C27-C28-C29-C39
21	3	415	LUT	C21-C26-C27-C28
21	3	415	LUT	C25-C26-C27-C28
21	7	316	LUT	C21-C26-C27-C28
21	7	316	LUT	C25-C26-C27-C28
22	1	616	XAT	O4-C6-C7-C8
22	1	616	XAT	C6-C7-C8-C9
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	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	9	615	XAT	C9-C10-C11-C12
22	9	615	XAT	C26-C27-C28-C29
23	3	418	BCR	C11-C12-C13-C14
23	3	418	BCR	C17-C18-C19-C20
23	7	318	BCR	C13-C14-C15-C16
23	7	318	BCR	C15-C16-C17-C18
23	8	316	BCR	C5-C6-C7-C8
23	A	847	BCR	C11-C12-C13-C14
23	A	847	BCR	C13-C14-C15-C16
23	A	848	BCR	C7-C8-C9-C10
23	A	848	BCR	C13-C14-C15-C16
23	A	849	BCR	C17-C18-C19-C20
23	A	849	BCR	C36-C18-C19-C20
23	A	850	BCR	C15-C16-C17-C18
23	A	850	BCR	C23-C24-C25-C26
23	A	850	BCR	C23-C24-C25-C30
23	A	851	BCR	C15-C16-C17-C18
23	A	858	BCR	C7-C8-C9-C10
23	A	858	BCR	C7-C8-C9-C34
23	A	858	BCR	C11-C12-C13-C14
23	B	802	BCR	C11-C12-C13-C14
23	B	802	BCR	C11-C12-C13-C35
23	B	846	BCR	C21-C22-C23-C24
23	B	849	BCR	C1-C6-C7-C8
23	B	849	BCR	C5-C6-C7-C8
23	B	849	BCR	C6-C7-C8-C9
23	G	4001	BCR	C1-C6-C7-C8
23	G	4001	BCR	C5-C6-C7-C8
23	G	4001	BCR	C19-C20-C21-C22
23	G	4005	BCR	C11-C12-C13-C14
23	G	4005	BCR	C11-C12-C13-C35
23	H	205	BCR	C17-C18-C19-C20
23	H	205	BCR	C36-C18-C19-C20
23	I	202	BCR	C5-C6-C7-C8
23	J	4001	BCR	C5-C6-C7-C8
23	J	4001	BCR	C6-C7-C8-C9
23	J	4001	BCR	C11-C12-C13-C14
23	J	4001	BCR	C11-C12-C13-C35
23	J	4003	BCR	C23-C24-C25-C26
23	K	205	BCR	C1-C6-C7-C8
23	K	205	BCR	C5-C6-C7-C8
23	K	205	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	K	205	BCR	C11-C12-C13-C35
23	L	308	BCR	C21-C22-C23-C24
23	L	308	BCR	C23-C24-C25-C26
23	L	308	BCR	C23-C24-C25-C30
24	1	618	LHG	C3-O3-P-O4
24	1	618	LHG	C3-O3-P-O6
24	1	619	LHG	O10-C23-O8-C6
24	1	619	LHG	C24-C23-O8-C6
24	1	620	LHG	C4-O6-P-O5
24	1	620	LHG	O7-C5-C6-O8
24	1	621	LHG	C3-O3-P-O6
24	1	621	LHG	C4-O6-P-O5
24	1	621	LHG	O6-C4-C5-O7
24	1	621	LHG	O9-C7-O7-C5
24	1	621	LHG	C8-C7-O7-C5
24	2	621	LHG	O7-C5-C6-O8
24	3	420	LHG	C4-C5-O7-C7
24	3	424	LHG	C3-O3-P-O4
24	3	424	LHG	C3-O3-P-O6
24	3	424	LHG	C4-O6-P-O3
24	3	424	LHG	C4-O6-P-O4
24	3	424	LHG	C4-O6-P-O5
24	3	424	LHG	O10-C23-O8-C6
24	3	424	LHG	C24-C23-O8-C6
24	7	320	LHG	C3-O3-P-O4
24	7	320	LHG	C3-O3-P-O5
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	7	320	LHG	C4-O6-P-O5
24	7	323	LHG	C4-O6-P-O3
24	7	323	LHG	C4-O6-P-O4
24	7	323	LHG	O9-C7-O7-C5
24	7	323	LHG	C8-C7-O7-C5
24	7	325	LHG	O10-C23-O8-C6
24	7	325	LHG	C24-C23-O8-C6
24	8	319	LHG	C3-O3-P-O5
24	8	319	LHG	C3-O3-P-O6
24	8	321	LHG	C4-O6-P-O3
24	8	321	LHG	C4-O6-P-O4
24	8	321	LHG	C4-O6-P-O5
24	8	321	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
24	8	321	LHG	C8-C7-O7-C5
24	9	617	LHG	C2-C3-O3-P
24	9	617	LHG	C3-O3-P-O4
24	9	617	LHG	C3-O3-P-O6
24	9	617	LHG	C4-O6-P-O3
24	9	617	LHG	C4-O6-P-O4
24	9	617	LHG	C4-O6-P-O5
24	9	617	LHG	O9-C7-O7-C5
24	9	617	LHG	C8-C7-O7-C5
24	9	619	LHG	C3-O3-P-O4
24	9	619	LHG	C3-O3-P-O6
24	9	619	LHG	C4-O6-P-O3
24	9	619	LHG	C4-O6-P-O4
24	9	619	LHG	O10-C23-O8-C6
24	9	619	LHG	C24-C23-O8-C6
24	A	853	LHG	C3-O3-P-O4
24	A	853	LHG	C3-O3-P-O6
24	A	853	LHG	C4-O6-P-O3
24	A	853	LHG	C4-O6-P-O5
24	A	854	LHG	C3-O3-P-O4
24	A	854	LHG	C3-O3-P-O6
24	A	854	LHG	O7-C5-C6-O8
24	B	852	LHG	C3-O3-P-O4
24	B	852	LHG	C3-O3-P-O6
24	B	852	LHG	C4-O6-P-O3
24	B	852	LHG	C4-O6-P-O4
24	B	852	LHG	C4-O6-P-O5
24	B	852	LHG	O10-C23-O8-C6
24	B	852	LHG	C24-C23-O8-C6
24	F	5002	LHG	C4-O6-P-O3
24	F	5002	LHG	C4-O6-P-O4
24	F	5002	LHG	C4-O6-P-O5
24	F	5011	LHG	C3-O3-P-O5
24	F	5011	LHG	C4-O6-P-O3
24	F	5011	LHG	C4-O6-P-O4
24	F	5011	LHG	C4-O6-P-O5
24	G	4006	LHG	C3-O3-P-O5
24	G	4006	LHG	C4-O6-P-O3
24	G	4006	LHG	C4-O6-P-O5
24	H	203	LHG	O7-C5-C6-O8
24	H	203	LHG	O10-C23-O8-C6
24	H	203	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	I	201	LHG	C3-O3-P-O6
24	I	201	LHG	C4-O6-P-O3
24	I	201	LHG	C4-O6-P-O4
24	I	201	LHG	C4-O6-P-O5
24	J	4004	LHG	O9-C7-O7-C5
24	J	4004	LHG	C8-C7-O7-C5
25	1	622	PTY	C3-O11-P1-O12
25	1	622	PTY	C3-O11-P1-O14
25	1	622	PTY	C5-O14-P1-O11
25	1	622	PTY	C5-O14-P1-O13
25	3	422	PTY	C3-O11-P1-O12
25	3	422	PTY	C5-O14-P1-O11
25	7	322	PTY	O10-C8-O7-C6
25	8	317	PTY	C5-O14-P1-O11
25	8	317	PTY	C5-O14-P1-O13
25	8	318	PTY	N1-C2-C3-O11
25	8	318	PTY	C2-C3-O11-P1
25	8	318	PTY	O30-C30-O4-C1
25	8	318	PTY	C3-O11-P1-O12
25	8	318	PTY	C3-O11-P1-O14
25	8	318	PTY	C5-O14-P1-O13
25	B	801	PTY	C11-C8-O7-C6
25	B	801	PTY	C5-O14-P1-O13
25	F	5010	PTY	C5-O14-P1-O11
25	F	5010	PTY	C5-O14-P1-O12
25	F	5010	PTY	C5-O14-P1-O13
25	H	201	PTY	C3-O11-P1-O12
25	H	201	PTY	C3-O11-P1-O14
25	H	201	PTY	C5-O14-P1-O13
25	H	202	PTY	N1-C2-C3-O11
25	H	202	PTY	C11-C8-O7-C6
25	H	202	PTY	C5-O14-P1-O11
25	H	202	PTY	C5-O14-P1-O13
25	L	310	PTY	O10-C8-O7-C6
25	L	310	PTY	C11-C8-O7-C6
25	L	310	PTY	C5-O14-P1-O11
25	L	310	PTY	C5-O14-P1-O12
26	2	619	SQD	C5-C6-S-O7
26	2	619	SQD	C5-C6-S-O8
26	2	619	SQD	C5-C6-S-O9
26	3	421	SQD	O49-C7-O47-C45
26	3	421	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	3	421	SQD	O5-C5-C6-S
26	9	618	SQD	C2-C1-O6-C44
26	9	618	SQD	O5-C1-O6-C44
26	9	618	SQD	C5-C6-S-O7
26	9	618	SQD	C5-C6-S-O9
26	B	851	SQD	O5-C5-C6-S
27	2	620	3PH	C1-O11-P-O14
27	2	620	3PH	O21-C2-C3-O31
28	7	301	LMG	O9-C10-O7-C8
28	7	301	LMG	C11-C10-O7-C8
28	7	319	LMG	O6-C1-O1-C7
28	7	319	LMG	O9-C10-O7-C8
28	7	319	LMG	C11-C10-O7-C8
28	7	319	LMG	O10-C28-O8-C9
28	7	319	LMG	C29-C28-O8-C9
28	8	301	LMG	O9-C10-O7-C8
28	8	301	LMG	C11-C10-O7-C8
28	8	301	LMG	O10-C28-O8-C9
28	8	301	LMG	C29-C28-O8-C9
28	A	801	LMG	O9-C10-O7-C8
28	A	801	LMG	C11-C10-O7-C8
29	7	321	DGD	C2A-C1A-O1G-C1G
29	7	321	DGD	O1A-C1A-O1G-C1G
29	7	321	DGD	O6D-C1D-O3G-C3G
29	7	321	DGD	O6E-C1E-O5D-C6D
29	B	850	DGD	C2B-C1B-O2G-C2G
29	B	850	DGD	O1B-C1B-O2G-C2G
29	B	850	DGD	O2G-C2G-C3G-O3G
29	L	311	DGD	C2A-C1A-O1G-C1G
29	L	311	DGD	O1A-C1A-O1G-C1G
29	L	311	DGD	O1G-C1G-C2G-O2G
30	8	320	LMK	C2-C3-N4-C5
30	8	320	LMK	C2-C3-N4-C6
30	8	320	LMK	C2-C3-N4-C46
31	9	616	LMU	C2'-C1'-O1'-C1
31	9	616	LMU	O5'-C1'-O1'-C1
20	2	603	CLA	O1D-CGD-O2D-CED
20	2	604	CLA	O1D-CGD-O2D-CED
20	7	305	CLA	O1D-CGD-O2D-CED
20	9	609	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	J	4002	CLA	O1D-CGD-O2D-CED
20	1	605	CLA	O1D-CGD-O2D-CED
20	1	612	CLA	O1D-CGD-O2D-CED
20	2	611	CLA	O1D-CGD-O2D-CED
20	3	402	CLA	O1D-CGD-O2D-CED
20	3	413	CLA	O1D-CGD-O2D-CED
20	8	303	CLA	O1D-CGD-O2D-CED
20	9	612	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	O1D-CGD-O2D-CED
20	B	804	CLA	O1D-CGD-O2D-CED
20	F	5005	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	CBD-CGD-O2D-CED
20	1	610	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	CBD-CGD-O2D-CED
20	2	603	CLA	CBD-CGD-O2D-CED
20	7	305	CLA	CBD-CGD-O2D-CED
20	7	312	CLA	CBD-CGD-O2D-CED
20	7	314	CLA	CBD-CGD-O2D-CED
20	8	303	CLA	CBD-CGD-O2D-CED
20	8	311	CLA	CBD-CGD-O2D-CED
20	9	602	CLA	CBD-CGD-O2D-CED
20	9	603	CLA	CBD-CGD-O2D-CED
20	9	608	CLA	CBD-CGD-O2D-CED
20	9	609	CLA	CBD-CGD-O2D-CED
20	9	612	CLA	CBD-CGD-O2D-CED
20	A	804	CLA	CBD-CGD-O2D-CED
20	A	805	CLA	CBD-CGD-O2D-CED
20	A	819	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CBD-CGD-O2D-CED
20	A	842	CLA	CBD-CGD-O2D-CED
20	B	809	CLA	CBD-CGD-O2D-CED
20	B	815	CLA	CBD-CGD-O2D-CED
20	B	823	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	CBD-CGD-O2D-CED
20	G	4004	CLA	CBD-CGD-O2D-CED
20	K	203	CLA	CBD-CGD-O2D-CED
20	L	307	CLA	CBD-CGD-O2D-CED
20	1	609	CLA	O1A-CGA-O2A-C1
20	7	309	CLA	O1A-CGA-O2A-C1
20	8	303	CLA	O1A-CGA-O2A-C1
20	9	607	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	9	609	CLA	O1A-CGA-O2A-C1
20	A	806	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	O1A-CGA-O2A-C1
20	B	826	CLA	O1A-CGA-O2A-C1
20	L	302	CLA	O1A-CGA-O2A-C1
31	9	616	LMU	O5B-C1B-O1B-C4'
20	2	607	CLA	CBA-CGA-O2A-C1
20	G	4003	CLA	CBA-CGA-O2A-C1
20	1	603	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	O1D-CGD-O2D-CED
20	7	314	CLA	O1D-CGD-O2D-CED
20	9	602	CLA	O1D-CGD-O2D-CED
20	1	609	CLA	CBA-CGA-O2A-C1
20	3	406	CLA	CBA-CGA-O2A-C1
20	7	309	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
20	B	825	CLA	CBA-CGA-O2A-C1
20	B	826	CLA	CBA-CGA-O2A-C1
25	8	317	PTY	C31-C30-O4-C1
20	9	611	CLA	CBD-CGD-O2D-CED
20	2	603	CLA	O1A-CGA-O2A-C1
20	2	604	CLA	O1A-CGA-O2A-C1
20	3	406	CLA	O1A-CGA-O2A-C1
20	3	407	CLA	O1A-CGA-O2A-C1
20	3	410	CLA	O1A-CGA-O2A-C1
20	3	411	CLA	O1A-CGA-O2A-C1
20	7	311	CLA	O1A-CGA-O2A-C1
20	7	324	CLA	O1A-CGA-O2A-C1
20	8	302	CLA	O1A-CGA-O2A-C1
20	8	311	CLA	O1A-CGA-O2A-C1
20	A	804	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	O1A-CGA-O2A-C1
20	A	827	CLA	O1A-CGA-O2A-C1
20	A	831	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	B	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	831	CLA	O1A-CGA-O2A-C1
20	B	833	CLA	O1A-CGA-O2A-C1
20	B	834	CLA	O1A-CGA-O2A-C1
20	F	5006	CLA	O1A-CGA-O2A-C1
20	G	4002	CLA	O1A-CGA-O2A-C1
20	K	202	CLA	O1A-CGA-O2A-C1
20	L	304	CLA	O1A-CGA-O2A-C1
20	L	307	CLA	O1A-CGA-O2A-C1
25	8	317	PTY	O30-C30-O4-C1
25	B	801	PTY	O30-C30-O4-C1
25	F	5010	PTY	O30-C30-O4-C1
20	2	613	CLA	O1D-CGD-O2D-CED
20	3	412	CLA	O1D-CGD-O2D-CED
20	9	604	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	O1D-CGD-O2D-CED
20	A	829	CLA	O1D-CGD-O2D-CED
20	A	831	CLA	O1D-CGD-O2D-CED
20	B	830	CLA	O1D-CGD-O2D-CED
20	B	837	CLA	O1D-CGD-O2D-CED
31	9	616	LMU	C2B-C1B-O1B-C4'
20	A	816	CLA	O1D-CGD-O2D-CED
20	A	823	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	O1D-CGD-O2D-CED
20	A	843	CLA	O1D-CGD-O2D-CED
20	B	807	CLA	O1D-CGD-O2D-CED
20	B	816	CLA	O1D-CGD-O2D-CED
20	B	822	CLA	O1D-CGD-O2D-CED
20	B	836	CLA	O1D-CGD-O2D-CED
20	G	4003	CLA	O1D-CGD-O2D-CED
20	3	407	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	O1A-CGA-O2A-C1
20	3	409	CLA	O1A-CGA-O2A-C1
25	B	801	PTY	O10-C8-O7-C6
25	H	202	PTY	O10-C8-O7-C6
20	B	828	CLA	O1D-CGD-O2D-CED
20	3	403	CLA	CBA-CGA-O2A-C1
20	1	611	CLA	O1A-CGA-O2A-C1
20	3	403	CLA	O1A-CGA-O2A-C1
20	8	307	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	C3-C5-C6-C7
20	3	408	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	7	310	CLA	C3-C5-C6-C7
20	8	311	CLA	C3-C5-C6-C7
20	9	602	CLA	C3-C5-C6-C7
20	9	608	CLA	C3-C5-C6-C7
20	A	810	CLA	C3-C5-C6-C7
20	A	811	CLA	C3-C5-C6-C7
20	A	815	CLA	C3-C5-C6-C7
20	A	827	CLA	C3-C5-C6-C7
20	A	833	CLA	C3-C5-C6-C7
20	A	836	CLA	C3-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7
20	B	810	CLA	C3-C5-C6-C7
20	B	811	CLA	C3-C5-C6-C7
20	B	812	CLA	C3-C5-C6-C7
20	B	824	CLA	C3-C5-C6-C7
20	B	825	CLA	C3-C5-C6-C7
20	B	832	CLA	C3-C5-C6-C7
20	B	843	CLA	C3-C5-C6-C7
32	A	803	CL0	C3-C5-C6-C7
20	9	603	CLA	O1D-CGD-O2D-CED
20	9	610	CLA	O1D-CGD-O2D-CED
20	2	603	CLA	CBA-CGA-O2A-C1
20	3	405	CLA	CBA-CGA-O2A-C1
20	3	410	CLA	CBA-CGA-O2A-C1
20	3	411	CLA	CBA-CGA-O2A-C1
20	7	311	CLA	CBA-CGA-O2A-C1
20	8	302	CLA	CBA-CGA-O2A-C1
20	8	303	CLA	CBA-CGA-O2A-C1
20	8	309	CLA	CBA-CGA-O2A-C1
20	8	311	CLA	CBA-CGA-O2A-C1
20	9	607	CLA	CBA-CGA-O2A-C1
20	9	609	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	809	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	CBA-CGA-O2A-C1
20	A	827	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	B	831	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	G	4002	CLA	CBA-CGA-O2A-C1
20	K	202	CLA	CBA-CGA-O2A-C1
20	L	302	CLA	CBA-CGA-O2A-C1
20	L	304	CLA	CBA-CGA-O2A-C1
25	B	801	PTY	C31-C30-O4-C1
25	F	5010	PTY	C31-C30-O4-C1
19	9	606	CHL	CBD-CGD-O2D-CED
20	1	608	CLA	CBD-CGD-O2D-CED
20	3	408	CLA	CBD-CGD-O2D-CED
20	3	409	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	CBD-CGD-O2D-CED
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	CBD-CGD-O2D-CED
20	A	828	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	CBD-CGD-O2D-CED
20	B	842	CLA	CBD-CGD-O2D-CED
20	F	5008	CLA	CBD-CGD-O2D-CED
20	K	204	CLA	CBD-CGD-O2D-CED
20	L	302	CLA	CBD-CGD-O2D-CED
25	7	322	PTY	C11-C8-O7-C6
19	7	306	CHL	O1D-CGD-O2D-CED
20	B	808	CLA	O1D-CGD-O2D-CED
20	K	201	CLA	O1D-CGD-O2D-CED
20	2	607	CLA	O1A-CGA-O2A-C1
20	7	303	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	O1D-CGD-O2D-CED
20	9	602	CLA	C4-C3-C5-C6
20	A	821	CLA	C4-C3-C5-C6
20	A	823	CLA	C4-C3-C5-C6
20	A	827	CLA	C4-C3-C5-C6
20	B	829	CLA	C4-C3-C5-C6
20	B	834	CLA	C4-C3-C5-C6
20	F	5005	CLA	C4-C3-C5-C6
20	A	821	CLA	C2-C3-C5-C6
20	A	827	CLA	C2-C3-C5-C6
20	B	829	CLA	C2-C3-C5-C6
20	B	834	CLA	C2-C3-C5-C6
19	1	606	CHL	CBA-CGA-O2A-C1
20	1	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	8	307	CLA	CBA-CGA-O2A-C1
20	1	610	CLA	O1D-CGD-O2D-CED
20	A	819	CLA	O1D-CGD-O2D-CED
20	G	4004	CLA	O1D-CGD-O2D-CED
20	A	818	CLA	C2A-CAA-CBA-CGA
20	B	824	CLA	C2A-CAA-CBA-CGA
20	F	5008	CLA	C2A-CAA-CBA-CGA
20	9	611	CLA	C3-C5-C6-C7
20	A	823	CLA	C3-C5-C6-C7
20	B	822	CLA	C3-C5-C6-C7
20	B	834	CLA	C3-C5-C6-C7
20	K	202	CLA	C3-C5-C6-C7
20	L	304	CLA	C3-C5-C6-C7
20	1	604	CLA	CBA-CGA-O2A-C1
20	2	604	CLA	CBA-CGA-O2A-C1
20	3	407	CLA	CBA-CGA-O2A-C1
20	3	408	CLA	CBA-CGA-O2A-C1
20	3	409	CLA	CBA-CGA-O2A-C1
20	7	303	CLA	CBA-CGA-O2A-C1
20	7	324	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	CBA-CGA-O2A-C1
20	A	823	CLA	CBA-CGA-O2A-C1
20	A	831	CLA	CBA-CGA-O2A-C1
20	B	804	CLA	CBA-CGA-O2A-C1
20	B	833	CLA	CBA-CGA-O2A-C1
20	B	834	CLA	CBA-CGA-O2A-C1
20	B	842	CLA	CBA-CGA-O2A-C1
20	F	5005	CLA	CBA-CGA-O2A-C1
20	F	5006	CLA	CBA-CGA-O2A-C1
20	L	307	CLA	CBA-CGA-O2A-C1
19	1	606	CHL	O1A-CGA-O2A-C1
20	F	5007	CLA	CBD-CGD-O2D-CED
23	3	418	BCR	C13-C14-C15-C16
23	A	847	BCR	C15-C16-C17-C18
23	A	848	BCR	C9-C10-C11-C12
23	A	848	BCR	C15-C16-C17-C18
23	A	851	BCR	C13-C14-C15-C16
20	3	405	CLA	O1A-CGA-O2A-C1
20	3	408	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	7	303	CLA	O1A-CGA-O2A-C1
20	7	310	CLA	O1A-CGA-O2A-C1
20	8	310	CLA	O1A-CGA-O2A-C1
20	A	823	CLA	O1A-CGA-O2A-C1
20	B	804	CLA	O1A-CGA-O2A-C1
20	B	842	CLA	O1A-CGA-O2A-C1
20	9	608	CLA	O1D-CGD-O2D-CED
20	G	4003	CLA	O1A-CGA-O2A-C1
20	8	311	CLA	O1D-CGD-O2D-CED
20	2	603	CLA	C3-C5-C6-C7
20	3	402	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	B	833	CLA	C3-C5-C6-C7
20	1	604	CLA	CBD-CGD-O2D-CED
20	1	607	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	CBD-CGD-O2D-CED
20	A	812	CLA	CBD-CGD-O2D-CED
24	7	320	LHG	O2-C2-C3-O3
24	I	201	LHG	O2-C2-C3-O3
20	B	809	CLA	O1D-CGD-O2D-CED
20	L	307	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	CBA-CGA-O2A-C1
20	9	611	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	CBA-CGA-O2A-C1
20	A	821	CLA	CBA-CGA-O2A-C1
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	819	CLA	CBA-CGA-O2A-C1
20	B	835	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	O1A-CGA-O2A-C1
20	F	5005	CLA	O1A-CGA-O2A-C1
19	3	401	CHL	CBD-CGD-O2D-CED
20	2	610	CLA	CBD-CGD-O2D-CED
20	3	414	CLA	CBD-CGD-O2D-CED
20	8	302	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	CBD-CGD-O2D-CED
19	8	305	CHL	CBA-CGA-O2A-C1
20	1	610	CLA	CBA-CGA-O2A-C1
20	3	414	CLA	CBA-CGA-O2A-C1
20	1	608	CLA	C3-C5-C6-C7
20	A	830	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	F	5005	CLA	C3-C5-C6-C7
20	7	304	CLA	CBD-CGD-O2D-CED
20	A	824	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CBD-CGD-O2D-CED
20	B	829	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	O1D-CGD-O2D-CED
20	A	805	CLA	O1D-CGD-O2D-CED
20	B	823	CLA	O1D-CGD-O2D-CED
20	K	203	CLA	O1D-CGD-O2D-CED
20	7	310	CLA	CBA-CGA-O2A-C1
20	8	310	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
20	9	608	CLA	C4-C3-C5-C6
20	9	602	CLA	C2-C3-C5-C6
20	F	5005	CLA	C2-C3-C5-C6
20	1	613	CLA	O1A-CGA-O2A-C1
20	A	811	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	O1A-CGA-O2A-C1
20	A	821	CLA	O1A-CGA-O2A-C1
20	B	814	CLA	O1A-CGA-O2A-C1
20	B	819	CLA	O1A-CGA-O2A-C1
20	B	835	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	CBD-CGD-O2D-CED
20	7	312	CLA	O1D-CGD-O2D-CED
20	9	611	CLA	O1A-CGA-O2A-C1
20	A	812	CLA	O1A-CGA-O2A-C1
20	A	826	CLA	O1A-CGA-O2A-C1
26	2	619	SQD	O5-C1-O6-C44
28	7	301	LMG	O6-C1-O1-C7
20	A	820	CLA	CBA-CGA-O2A-C1
19	8	304	CHL	CBD-CGD-O2D-CED
20	2	605	CLA	CBD-CGD-O2D-CED
20	2	609	CLA	CBD-CGD-O2D-CED
20	8	312	CLA	CBD-CGD-O2D-CED
20	B	811	CLA	CBD-CGD-O2D-CED
20	B	826	CLA	CBD-CGD-O2D-CED
20	B	838	CLA	CBD-CGD-O2D-CED
20	B	840	CLA	CBD-CGD-O2D-CED
20	F	5006	CLA	CBD-CGD-O2D-CED
20	9	611	CLA	O1D-CGD-O2D-CED
20	A	842	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	8	306	CHL	CBD-CGD-O2D-CED
20	1	602	CLA	CBD-CGD-O2D-CED
20	9	601	CLA	CBD-CGD-O2D-CED
20	3	407	CLA	O1D-CGD-O2D-CED
20	A	826	CLA	O1D-CGD-O2D-CED
21	1	615	LUT	C9-C10-C11-C12
20	2	613	CLA	CBA-CGA-O2A-C1
20	7	304	CLA	CBA-CGA-O2A-C1
20	9	602	CLA	CBA-CGA-O2A-C1
20	9	610	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	CBA-CGA-O2A-C1
20	B	811	CLA	CBA-CGA-O2A-C1
20	B	813	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	CBA-CGA-O2A-C1
20	B	836	CLA	CBA-CGA-O2A-C1
20	7	315	CLA	CBD-CGD-O2D-CED
20	A	841	CLA	CBD-CGD-O2D-CED
20	K	204	CLA	O1D-CGD-O2D-CED
19	3	401	CHL	C4-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
19	3	401	CHL	C2-C3-C5-C6
20	A	823	CLA	C2-C3-C5-C6
20	B	823	CLA	C2-C3-C5-C6
20	B	814	CLA	C3-C5-C6-C7
19	7	302	CHL	C11-C10-C8-C9
19	7	302	CHL	C11-C12-C13-C14
20	3	402	CLA	C11-C12-C13-C14
20	A	821	CLA	C6-C7-C8-C9
20	A	841	CLA	C6-C7-C8-C9
20	L	302	CLA	C11-C10-C8-C9
20	L	302	CLA	C14-C13-C15-C16
33	B	844	PQN	C16-C17-C18-C19
33	B	844	PQN	C21-C22-C23-C24
20	3	409	CLA	O1D-CGD-O2D-CED
20	A	814	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	827	CLA	O1D-CGD-O2D-CED
20	B	842	CLA	O1D-CGD-O2D-CED
26	2	619	SQD	C2-C1-O6-C44
29	7	321	DGD	C2D-C1D-O3G-C3G
29	A	802	DGD	O6D-C5D-C6D-O5D
19	9	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	1	608	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	O1D-CGD-O2D-CED
20	2	613	CLA	O1A-CGA-O2A-C1
20	9	610	CLA	O1A-CGA-O2A-C1
21	1	615	LUT	C11-C12-C13-C20
21	2	617	LUT	C7-C8-C9-C19
22	3	416	XAT	C27-C28-C29-C39
22	9	615	XAT	C7-C8-C9-C19
23	A	847	BCR	C11-C12-C13-C35
23	A	848	BCR	C7-C8-C9-C34
23	A	848	BCR	C37-C22-C23-C24
23	A	850	BCR	C36-C18-C19-C20
23	A	858	BCR	C37-C22-C23-C24
23	B	846	BCR	C37-C22-C23-C24
23	J	4001	BCR	C7-C8-C9-C34
23	L	308	BCR	C37-C22-C23-C24
21	1	615	LUT	C11-C12-C13-C14
21	2	616	LUT	C27-C28-C29-C30
21	2	617	LUT	C7-C8-C9-C10
22	3	416	XAT	C27-C28-C29-C30
23	A	848	BCR	C21-C22-C23-C24
23	A	858	BCR	C21-C22-C23-C24
23	J	4001	BCR	C7-C8-C9-C10
19	2	606	CHL	C2A-CAA-CBA-CGA
20	8	313	CLA	C2A-CAA-CBA-CGA
20	A	844	CLA	C2A-CAA-CBA-CGA
20	B	815	CLA	C2A-CAA-CBA-CGA
20	B	832	CLA	C2A-CAA-CBA-CGA
20	3	414	CLA	O1A-CGA-O2A-C1
20	7	304	CLA	O1A-CGA-O2A-C1
20	A	808	CLA	O1A-CGA-O2A-C1
20	B	811	CLA	O1A-CGA-O2A-C1
20	B	813	CLA	O1A-CGA-O2A-C1
29	A	802	DGD	C4D-C5D-C6D-O5D
28	7	301	LMG	O1-C7-C8-O7
20	B	808	CLA	CBA-CGA-O2A-C1
25	H	202	PTY	C31-C30-O4-C1
20	B	826	CLA	C8-C10-C11-C12
20	B	810	CLA	C2-C1-O2A-CGA
20	B	833	CLA	C2-C1-O2A-CGA
20	B	835	CLA	CBD-CGD-O2D-CED
20	9	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	A	811	CLA	C5-C6-C7-C8
20	A	820	CLA	C10-C11-C12-C13
20	A	830	CLA	C8-C10-C11-C12
20	A	835	CLA	C5-C6-C7-C8
20	B	830	CLA	C10-C11-C12-C13
20	B	834	CLA	C10-C11-C12-C13
20	L	304	CLA	C15-C16-C17-C18
20	F	5008	CLA	O1D-CGD-O2D-CED
19	8	305	CHL	O1A-CGA-O2A-C1
20	B	836	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	836	CLA	CBD-CGD-O2D-CED
20	L	301	CLA	CBD-CGD-O2D-CED
19	2	601	CHL	C11-C10-C8-C7
20	3	408	CLA	C6-C7-C8-C10
20	A	823	CLA	C11-C10-C8-C7
20	A	830	CLA	C11-C10-C8-C7
32	A	803	CL0	C11-C12-C13-C15
33	B	844	PQN	C22-C23-C25-C26
20	A	843	CLA	CBA-CGA-O2A-C1
20	B	803	CLA	CBA-CGA-O2A-C1
23	3	418	BCR	C15-C16-C17-C18
23	G	4005	BCR	C9-C10-C11-C12
20	3	408	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	O1D-CGD-O2D-CED
20	L	302	CLA	O1D-CGD-O2D-CED
20	A	832	CLA	C15-C16-C17-C18
20	A	844	CLA	C10-C11-C12-C13
20	B	823	CLA	C8-C10-C11-C12
24	1	619	LHG	C7-C8-C9-C10
36	A	859	4RF	C41-C43-C44-C45
20	9	602	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1
20	1	609	CLA	C5-C6-C7-C8
20	3	407	CLA	C5-C6-C7-C8
20	7	324	CLA	C5-C6-C7-C8
20	B	808	CLA	C15-C16-C17-C18
20	B	815	CLA	C15-C16-C17-C18
20	B	823	CLA	C15-C16-C17-C18
20	B	834	CLA	C8-C10-C11-C12
24	8	321	LHG	C5-C4-O6-P
19	7	306	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	3	405	CLA	C2A-CAA-CBA-CGA
20	3	406	CLA	C2A-CAA-CBA-CGA
20	8	308	CLA	C2A-CAA-CBA-CGA
20	A	832	CLA	C2A-CAA-CBA-CGA
20	A	837	CLA	C2A-CAA-CBA-CGA
20	A	838	CLA	C2A-CAA-CBA-CGA
20	B	819	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
20	B	829	CLA	C2A-CAA-CBA-CGA
20	B	836	CLA	C2A-CAA-CBA-CGA
20	B	843	CLA	C2A-CAA-CBA-CGA
19	2	601	CHL	C5-C6-C7-C8
20	A	826	CLA	C5-C6-C7-C8
20	A	830	CLA	C10-C11-C12-C13
20	B	807	CLA	C8-C10-C11-C12
20	B	811	CLA	C5-C6-C7-C8
24	F	5002	LHG	C23-C24-C25-C26
36	A	859	4RF	C22-C24-C25-C26
19	2	601	CHL	CBD-CGD-O2D-CED
23	B	846	BCR	C6-C7-C8-C9
29	B	850	DGD	O6D-C1D-O3G-C3G
20	7	311	CLA	C5-C6-C7-C8
20	A	812	CLA	C8-C10-C11-C12
20	A	812	CLA	C10-C11-C12-C13
20	A	841	CLA	C13-C15-C16-C17
20	B	822	CLA	C10-C11-C12-C13
20	B	843	CLA	C13-C15-C16-C17
20	L	302	CLA	C5-C6-C7-C8
20	L	302	CLA	C8-C10-C11-C12
20	L	305	CLA	C5-C6-C7-C8
20	G	4002	CLA	C2-C1-O2A-CGA
20	A	820	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	CBA-CGA-O2A-C1
20	A	820	CLA	O1A-CGA-O2A-C1
20	3	402	CLA	C10-C11-C12-C13
20	1	610	CLA	O1A-CGA-O2A-C1
20	8	312	CLA	CBA-CGA-O2A-C1
20	A	831	CLA	C3-C5-C6-C7
20	B	834	CLA	O1D-CGD-O2D-CED
20	F	5007	CLA	O1D-CGD-O2D-CED
20	7	309	CLA	C5-C6-C7-C8
20	A	805	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	A	816	CLA	C15-C16-C17-C18
20	A	831	CLA	C13-C15-C16-C17
20	B	808	CLA	C13-C15-C16-C17
20	B	834	CLA	C5-C6-C7-C8
20	9	608	CLA	C2-C3-C5-C6
20	A	811	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	C13-C15-C16-C17
20	A	808	CLA	C5-C6-C7-C8
20	A	812	CLA	C15-C16-C17-C18
20	A	814	CLA	C15-C16-C17-C18
20	A	828	CLA	C5-C6-C7-C8
20	B	811	CLA	C13-C15-C16-C17
20	B	820	CLA	C8-C10-C11-C12
20	B	825	CLA	C13-C15-C16-C17
20	B	830	CLA	C5-C6-C7-C8
20	F	5003	CLA	C5-C6-C7-C8
20	A	807	CLA	CBA-CGA-O2A-C1
20	A	824	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	CBA-CGA-O2A-C1
20	B	843	CLA	CBA-CGA-O2A-C1
20	F	5003	CLA	CBA-CGA-O2A-C1
19	2	606	CHL	CBD-CGD-O2D-CED
20	3	410	CLA	CBD-CGD-O2D-CED
20	A	813	CLA	CBD-CGD-O2D-CED
20	B	808	CLA	O1A-CGA-O2A-C1
20	1	607	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	C5-C6-C7-C8
20	B	803	CLA	O1A-CGA-O2A-C1
24	7	320	LHG	C1-C2-C3-O3
20	7	315	CLA	C2A-CAA-CBA-CGA
20	A	804	CLA	C2A-CAA-CBA-CGA
20	A	825	CLA	C2A-CAA-CBA-CGA
20	B	840	CLA	C2A-CAA-CBA-CGA
20	J	4002	CLA	C2A-CAA-CBA-CGA
20	K	204	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	O1D-CGD-O2D-CED
20	8	308	CLA	CBA-CGA-O2A-C1
20	A	815	CLA	CBA-CGA-O2A-C1
20	B	838	CLA	CBA-CGA-O2A-C1
19	2	601	CHL	C10-C11-C12-C13
20	1	603	CLA	C10-C11-C12-C13
20	A	816	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	A	827	CLA	C10-C11-C12-C13
20	B	831	CLA	C13-C15-C16-C17
20	B	831	CLA	C15-C16-C17-C18
20	3	414	CLA	O1D-CGD-O2D-CED
19	7	302	CHL	C15-C16-C17-C18
20	A	806	CLA	C15-C16-C17-C18
20	A	820	CLA	C5-C6-C7-C8
20	B	827	CLA	C13-C15-C16-C17
20	B	829	CLA	C15-C16-C17-C18
20	1	604	CLA	O1D-CGD-O2D-CED
20	A	808	CLA	O1D-CGD-O2D-CED
20	2	602	CLA	C5-C6-C7-C8
20	B	807	CLA	C10-C11-C12-C13
20	B	813	CLA	C13-C15-C16-C17
20	B	814	CLA	C5-C6-C7-C8
20	B	816	CLA	C5-C6-C7-C8
20	B	841	CLA	C5-C6-C7-C8
19	3	401	CHL	O1D-CGD-O2D-CED
20	A	842	CLA	C4-C3-C5-C6
20	2	610	CLA	O1D-CGD-O2D-CED
20	A	842	CLA	C10-C11-C12-C13
20	B	824	CLA	C5-C6-C7-C8
20	B	818	CLA	C3-C5-C6-C7
20	A	840	CLA	CBD-CGD-O2D-CED
25	H	201	PTY	C11-C8-O7-C6
20	8	302	CLA	O1D-CGD-O2D-CED
25	H	201	PTY	O10-C8-O7-C6
26	3	421	SQD	C2-C1-O6-C44
28	7	301	LMG	C2-C1-O1-C7
29	7	321	DGD	C2E-C1E-O5D-C6D
20	A	823	CLA	C8-C10-C11-C12
20	A	838	CLA	O1D-CGD-O2D-CED
19	8	304	CHL	CBA-CGA-O2A-C1
20	7	305	CLA	CBA-CGA-O2A-C1
20	7	313	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	C16-C17-C18-C19
20	B	835	CLA	C11-C12-C13-C15
26	B	851	SQD	C24-C23-O48-C46
21	2	615	LUT	C27-C28-C29-C39
23	B	849	BCR	C7-C8-C9-C34
24	1	618	LHG	C2-C3-O3-P
21	2	615	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	B	849	BCR	C7-C8-C9-C10
20	8	308	CLA	O1A-CGA-O2A-C1
20	A	843	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	O1A-CGA-O2A-C1
25	H	202	PTY	O30-C30-O4-C1
20	2	610	CLA	C2A-CAA-CBA-CGA
20	3	403	CLA	C2A-CAA-CBA-CGA
20	3	412	CLA	C2A-CAA-CBA-CGA
20	A	816	CLA	C2A-CAA-CBA-CGA
20	A	841	CLA	C2A-CAA-CBA-CGA
20	F	5006	CLA	C2A-CAA-CBA-CGA
20	3	412	CLA	C8-C10-C11-C12
20	A	805	CLA	C10-C11-C12-C13
20	A	815	CLA	C8-C10-C11-C12
20	8	308	CLA	C11-C12-C13-C14
20	A	817	CLA	C6-C7-C8-C9
20	A	819	CLA	C6-C7-C8-C10
20	B	821	CLA	C16-C17-C18-C19
20	B	841	CLA	C16-C17-C18-C20
20	7	304	CLA	O1D-CGD-O2D-CED
20	B	829	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	O1A-CGA-O2A-C1
20	B	843	CLA	O1A-CGA-O2A-C1
21	1	615	LUT	C12-C13-C14-C15
23	3	418	BCR	C12-C13-C14-C15
23	3	418	BCR	C16-C17-C18-C19
23	A	847	BCR	C11-C10-C9-C8
26	3	421	SQD	O5-C1-O6-C44
20	A	824	CLA	O1D-CGD-O2D-CED
20	B	827	CLA	O1D-CGD-O2D-CED
25	H	201	PTY	C31-C30-O4-C1
24	1	621	LHG	C7-C8-C9-C10
20	3	411	CLA	C3-C5-C6-C7
20	B	824	CLA	O1D-CGD-O2D-CED
20	B	826	CLA	O1D-CGD-O2D-CED
20	3	406	CLA	C2-C1-O2A-CGA
20	8	309	CLA	C2-C1-O2A-CGA
20	A	804	CLA	C2-C1-O2A-CGA
20	B	831	CLA	C2-C1-O2A-CGA
20	9	607	CLA	C16-C17-C18-C20
20	9	608	CLA	C11-C12-C13-C15
20	9	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	A	816	CLA	C16-C17-C18-C19
20	A	817	CLA	C6-C7-C8-C10
20	A	832	CLA	C16-C17-C18-C19
20	B	804	CLA	C16-C17-C18-C20
20	B	821	CLA	C16-C17-C18-C20
20	B	829	CLA	C16-C17-C18-C20
20	B	835	CLA	C11-C12-C13-C14
20	B	841	CLA	C16-C17-C18-C19
20	F	5003	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	C10-C11-C12-C13
20	B	822	CLA	C8-C10-C11-C12
20	B	811	CLA	O1D-CGD-O2D-CED
20	9	601	CLA	CBA-CGA-O2A-C1
20	8	309	CLA	CBD-CGD-O2D-CED
20	8	312	CLA	O1D-CGD-O2D-CED
20	B	804	CLA	C8-C10-C11-C12
24	J	4004	LHG	C11-C10-C9-C8
28	F	5001	LMG	C29-C30-C31-C32
20	2	609	CLA	O1D-CGD-O2D-CED
20	7	312	CLA	CBA-CGA-O2A-C1
19	9	606	CHL	C2C-C3C-CAC-CBC
20	2	611	CLA	C3-C5-C6-C7
19	8	304	CHL	O1D-CGD-O2D-CED
20	2	605	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	C8-C10-C11-C12
20	B	806	CLA	C15-C16-C17-C18
20	1	602	CLA	C4B-C3B-CAB-CBB
20	1	604	CLA	C4B-C3B-CAB-CBB
20	1	608	CLA	C4B-C3B-CAB-CBB
20	2	604	CLA	C4B-C3B-CAB-CBB
20	2	611	CLA	C4B-C3B-CAB-CBB
20	3	402	CLA	C4B-C3B-CAB-CBB
20	3	403	CLA	C4B-C3B-CAB-CBB
20	8	302	CLA	C4B-C3B-CAB-CBB
20	8	307	CLA	C4B-C3B-CAB-CBB
20	8	310	CLA	C4B-C3B-CAB-CBB
20	8	311	CLA	C4B-C3B-CAB-CBB
20	9	608	CLA	C4B-C3B-CAB-CBB
20	A	804	CLA	C4B-C3B-CAB-CBB
20	A	807	CLA	C4B-C3B-CAB-CBB
20	A	812	CLA	C4B-C3B-CAB-CBB
20	A	815	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	819	CLA	C4B-C3B-CAB-CBB
20	A	820	CLA	C4B-C3B-CAB-CBB
20	A	822	CLA	C4B-C3B-CAB-CBB
20	A	835	CLA	C4B-C3B-CAB-CBB
20	A	836	CLA	C4B-C3B-CAB-CBB
20	A	841	CLA	C4B-C3B-CAB-CBB
20	B	803	CLA	C4B-C3B-CAB-CBB
20	B	810	CLA	C4B-C3B-CAB-CBB
20	B	811	CLA	C4B-C3B-CAB-CBB
20	B	818	CLA	C4B-C3B-CAB-CBB
20	B	824	CLA	C4B-C3B-CAB-CBB
20	B	832	CLA	C4B-C3B-CAB-CBB
20	B	835	CLA	C4B-C3B-CAB-CBB
20	B	836	CLA	C4B-C3B-CAB-CBB
20	B	840	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C4B-C3B-CAB-CBB
20	B	842	CLA	C4B-C3B-CAB-CBB
20	G	4003	CLA	C4B-C3B-CAB-CBB
20	G	4004	CLA	C4B-C3B-CAB-CBB
20	K	203	CLA	C4B-C3B-CAB-CBB
20	L	301	CLA	C4B-C3B-CAB-CBB
20	L	302	CLA	C4B-C3B-CAB-CBB
20	L	304	CLA	C4B-C3B-CAB-CBB
19	2	601	CHL	C11-C12-C13-C15
20	9	607	CLA	C16-C17-C18-C19
20	9	608	CLA	C11-C12-C13-C14
20	9	609	CLA	C11-C12-C13-C14
20	A	816	CLA	C16-C17-C18-C20
20	A	818	CLA	C16-C17-C18-C20
20	A	819	CLA	C6-C7-C8-C9
20	A	826	CLA	C11-C12-C13-C15
20	A	832	CLA	C16-C17-C18-C20
20	B	838	CLA	O1A-CGA-O2A-C1
19	7	308	CHL	C2A-CAA-CBA-CGA
20	A	821	CLA	C2A-CAA-CBA-CGA
20	B	822	CLA	C2A-CAA-CBA-CGA
25	H	201	PTY	C31-C32-C33-C34
19	2	601	CHL	C8-C10-C11-C12
25	8	318	PTY	C11-C8-O7-C6
20	A	831	CLA	C11-C10-C8-C7
20	B	813	CLA	C6-C7-C8-C10
25	B	801	PTY	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	H	202	PTY	C11-C12-C13-C14
20	A	807	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	O1A-CGA-O2A-C1
20	B	816	CLA	C3-C5-C6-C7
19	2	606	CHL	C3A-C2A-CAA-CBA
19	9	606	CHL	C3A-C2A-CAA-CBA
20	2	607	CLA	C3A-C2A-CAA-CBA
20	2	608	CLA	C3A-C2A-CAA-CBA
20	2	610	CLA	C3A-C2A-CAA-CBA
20	3	404	CLA	C3A-C2A-CAA-CBA
20	3	406	CLA	C3A-C2A-CAA-CBA
20	8	308	CLA	C3A-C2A-CAA-CBA
20	9	601	CLA	C3A-C2A-CAA-CBA
20	9	610	CLA	C3A-C2A-CAA-CBA
20	9	612	CLA	C3A-C2A-CAA-CBA
20	A	806	CLA	C3A-C2A-CAA-CBA
20	A	808	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	826	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	B	824	CLA	C3A-C2A-CAA-CBA
20	B	837	CLA	C3A-C2A-CAA-CBA
20	F	5003	CLA	C3A-C2A-CAA-CBA
20	F	5005	CLA	C3A-C2A-CAA-CBA
20	F	5008	CLA	C3A-C2A-CAA-CBA
20	G	4003	CLA	C3A-C2A-CAA-CBA
20	H	204	CLA	C3A-C2A-CAA-CBA
20	K	204	CLA	C3A-C2A-CAA-CBA
20	1	614	CLA	CBA-CGA-O2A-C1
20	B	840	CLA	O1D-CGD-O2D-CED
20	8	308	CLA	C11-C12-C13-C15
20	A	826	CLA	C11-C12-C13-C14
20	B	810	CLA	CBD-CGD-O2D-CED
20	G	4002	CLA	CBD-CGD-O2D-CED
24	1	620	LHG	C10-C11-C12-C13
24	B	852	LHG	C26-C27-C28-C29
20	B	828	CLA	CBA-CGA-O2A-C1
20	F	5007	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	A	859	4RF	C43-C41-O40-C39
26	3	423	SQD	C44-C45-C46-O48
26	B	851	SQD	C44-C45-C46-O48
20	7	313	CLA	C3-C5-C6-C7
24	2	621	LHG	C11-C12-C13-C14
24	B	852	LHG	C9-C10-C11-C12
20	A	844	CLA	C13-C15-C16-C17
20	7	305	CLA	O1A-CGA-O2A-C1
20	7	313	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	C2B-C3B-CAB-CBB
20	1	608	CLA	C2B-C3B-CAB-CBB
20	1	613	CLA	C2B-C3B-CAB-CBB
20	2	602	CLA	C2B-C3B-CAB-CBB
20	2	603	CLA	C2B-C3B-CAB-CBB
20	2	613	CLA	C2B-C3B-CAB-CBB
20	7	310	CLA	C2B-C3B-CAB-CBB
20	7	312	CLA	C2B-C3B-CAB-CBB
20	7	314	CLA	C2B-C3B-CAB-CBB
20	9	603	CLA	C2B-C3B-CAB-CBB
20	9	607	CLA	C2B-C3B-CAB-CBB
20	9	611	CLA	C2B-C3B-CAB-CBB
20	A	804	CLA	C2B-C3B-CAB-CBB
20	A	806	CLA	C2B-C3B-CAB-CBB
20	A	809	CLA	C2B-C3B-CAB-CBB
20	A	814	CLA	C2B-C3B-CAB-CBB
20	A	815	CLA	C2B-C3B-CAB-CBB
20	A	821	CLA	C2B-C3B-CAB-CBB
20	A	823	CLA	C2B-C3B-CAB-CBB
20	A	826	CLA	C2B-C3B-CAB-CBB
20	A	835	CLA	C2B-C3B-CAB-CBB
20	A	840	CLA	C2B-C3B-CAB-CBB
20	A	842	CLA	C2B-C3B-CAB-CBB
20	B	811	CLA	C2B-C3B-CAB-CBB
20	B	812	CLA	C2B-C3B-CAB-CBB
20	B	827	CLA	C2B-C3B-CAB-CBB
20	B	831	CLA	C2B-C3B-CAB-CBB
20	B	835	CLA	C2B-C3B-CAB-CBB
20	B	841	CLA	C2B-C3B-CAB-CBB
20	K	201	CLA	C2B-C3B-CAB-CBB
21	2	614	LUT	C1-C6-C7-C8
21	2	614	LUT	C5-C6-C7-C8
21	2	617	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	2	617	LUT	C5-C6-C7-C8
21	9	613	LUT	C1-C6-C7-C8
21	9	613	LUT	C5-C6-C7-C8
23	3	417	BCR	C1-C6-C7-C8
23	3	417	BCR	C5-C6-C7-C8
23	3	417	BCR	C23-C24-C25-C26
23	3	417	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	C23-C24-C25-C26
23	8	316	BCR	C23-C24-C25-C30
23	A	847	BCR	C1-C6-C7-C8
23	A	847	BCR	C5-C6-C7-C8
23	A	848	BCR	C1-C6-C7-C8
23	A	848	BCR	C5-C6-C7-C8
23	B	847	BCR	C23-C24-C25-C30
23	H	205	BCR	C1-C6-C7-C8
23	H	205	BCR	C5-C6-C7-C8
23	I	202	BCR	C1-C6-C7-C8
23	J	4001	BCR	C1-C6-C7-C8
23	J	4003	BCR	C1-C6-C7-C8
23	J	4003	BCR	C23-C24-C25-C30
23	K	205	BCR	C23-C24-C25-C26
23	K	205	BCR	C23-C24-C25-C30
19	7	302	CHL	CBD-CGD-O2D-CED
19	8	305	CHL	CBD-CGD-O2D-CED
19	7	307	CHL	C2C-C3C-CAC-CBC
20	A	815	CLA	C5-C6-C7-C8
20	B	838	CLA	C5-C6-C7-C8
19	3	401	CHL	C2A-CAA-CBA-CGA
20	3	408	CLA	C2A-CAA-CBA-CGA
20	3	411	CLA	C2A-CAA-CBA-CGA
20	7	313	CLA	C2A-CAA-CBA-CGA
20	A	815	CLA	C2A-CAA-CBA-CGA
20	2	603	CLA	C5-C6-C7-C8
20	7	312	CLA	O1A-CGA-O2A-C1
25	H	201	PTY	O30-C30-O4-C1
24	G	4006	LHG	C34-C35-C36-C37
25	8	318	PTY	O10-C8-O7-C6
20	L	302	CLA	C4-C3-C5-C6
20	B	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	F	5006	CLA	O1D-CGD-O2D-CED
26	2	619	SQD	C15-C16-C17-C18
23	A	847	BCR	C10-C11-C12-C13
20	A	842	CLA	C2-C3-C5-C6
25	H	201	PTY	C8-C11-C12-C13
20	B	820	CLA	CBA-CGA-O2A-C1
20	B	840	CLA	CBA-CGA-O2A-C1
20	A	831	CLA	C8-C10-C11-C12
29	A	802	DGD	CAB-CBB-CCB-CDB
20	1	602	CLA	O1D-CGD-O2D-CED
29	A	802	DGD	C2D-C1D-O3G-C3G
20	9	607	CLA	C5-C6-C7-C8
20	B	813	CLA	C15-C16-C17-C18
32	A	803	CL0	C10-C11-C12-C13
20	B	828	CLA	O1A-CGA-O2A-C1
36	A	859	4RF	C04-C05-C06-C07
20	1	607	CLA	C5-C6-C7-C8
20	B	809	CLA	C5-C6-C7-C8
23	A	858	BCR	C11-C12-C13-C35
20	B	813	CLA	C3-C5-C6-C7
19	7	302	CHL	C8-C10-C11-C12
20	A	823	CLA	C2A-CAA-CBA-CGA
32	A	803	CL0	C16-C17-C18-C19
20	9	601	CLA	O1D-CGD-O2D-CED
20	3	412	CLA	C13-C15-C16-C17
26	B	851	SQD	O10-C23-O48-C46
20	F	5007	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C3-C5-C6-C7
31	A	857	LMU	O5'-C5'-C6'-O6'
20	A	833	CLA	C13-C15-C16-C17
24	2	621	LHG	C23-C24-C25-C26
24	3	424	LHG	C24-C25-C26-C27
25	H	202	PTY	C13-C14-C15-C16
28	7	301	LMG	O6-C5-C6-O5
29	A	802	DGD	O6E-C5E-C6E-O5E
31	A	857	LMU	O5B-C5B-C6B-O6B
20	1	603	CLA	C15-C16-C17-C18
20	3	402	CLA	C8-C10-C11-C12
20	B	803	CLA	C10-C11-C12-C13
20	A	813	CLA	C6-C7-C8-C9
20	B	804	CLA	C16-C17-C18-C19
20	B	829	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	7	319	LMG	C36-C37-C38-C39
36	A	859	4RF	O42-C41-O40-C39
20	7	315	CLA	O1D-CGD-O2D-CED
25	H	201	PTY	C14-C15-C16-C17
24	2	618	LHG	C7-C8-C9-C10
26	B	851	SQD	C7-C8-C9-C10
20	1	607	CLA	C13-C15-C16-C17
20	A	841	CLA	C5-C6-C7-C8
20	B	823	CLA	C10-C11-C12-C13
28	A	801	LMG	O6-C5-C6-O5
20	A	808	CLA	C3-C5-C6-C7
20	B	808	CLA	C3-C5-C6-C7
26	2	619	SQD	O47-C45-C46-O48
19	8	306	CHL	O1D-CGD-O2D-CED
20	7	312	CLA	C2-C1-O2A-CGA
24	B	852	LHG	C5-C4-O6-P
20	B	828	CLA	C3-C5-C6-C7
20	2	602	CLA	C2A-CAA-CBA-CGA
20	2	622	CLA	C2A-CAA-CBA-CGA
20	9	602	CLA	C2A-CAA-CBA-CGA
20	9	611	CLA	C2A-CAA-CBA-CGA
20	A	821	CLA	CBD-CGD-O2D-CED
20	8	312	CLA	O1A-CGA-O2A-C1
20	7	310	CLA	C10-C11-C12-C13
20	A	839	CLA	C13-C15-C16-C17
20	L	302	CLA	C13-C15-C16-C17
32	A	803	CL0	C5-C6-C7-C8
24	B	852	LHG	C7-C8-C9-C10
20	7	303	CLA	C11-C12-C13-C15
20	A	841	CLA	O1D-CGD-O2D-CED
20	B	840	CLA	O1A-CGA-O2A-C1
20	A	821	CLA	C3-C5-C6-C7
20	1	604	CLA	C1A-C2A-CAA-CBA
20	1	609	CLA	C1A-C2A-CAA-CBA
20	1	610	CLA	C1A-C2A-CAA-CBA
20	1	612	CLA	C1A-C2A-CAA-CBA
20	1	613	CLA	C1A-C2A-CAA-CBA
20	2	604	CLA	C1A-C2A-CAA-CBA
20	2	610	CLA	C1A-C2A-CAA-CBA
20	3	403	CLA	C1A-C2A-CAA-CBA
20	3	404	CLA	C1A-C2A-CAA-CBA
20	3	407	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	3	412	CLA	C1A-C2A-CAA-CBA
20	7	310	CLA	C1A-C2A-CAA-CBA
20	8	303	CLA	C1A-C2A-CAA-CBA
20	8	307	CLA	C1A-C2A-CAA-CBA
20	8	312	CLA	C1A-C2A-CAA-CBA
20	9	601	CLA	C1A-C2A-CAA-CBA
20	9	604	CLA	C1A-C2A-CAA-CBA
20	9	609	CLA	C1A-C2A-CAA-CBA
20	9	610	CLA	C1A-C2A-CAA-CBA
20	9	612	CLA	C1A-C2A-CAA-CBA
20	A	806	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	811	CLA	C1A-C2A-CAA-CBA
20	A	824	CLA	C1A-C2A-CAA-CBA
20	A	833	CLA	C1A-C2A-CAA-CBA
20	A	836	CLA	C1A-C2A-CAA-CBA
20	A	838	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	832	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	C1A-C2A-CAA-CBA
20	B	837	CLA	C1A-C2A-CAA-CBA
20	F	5003	CLA	C1A-C2A-CAA-CBA
20	F	5005	CLA	C1A-C2A-CAA-CBA
20	G	4003	CLA	C1A-C2A-CAA-CBA
20	H	204	CLA	C1A-C2A-CAA-CBA
20	J	4002	CLA	C1A-C2A-CAA-CBA
20	K	204	CLA	C1A-C2A-CAA-CBA
20	L	302	CLA	C1A-C2A-CAA-CBA
20	L	305	CLA	C1A-C2A-CAA-CBA
20	B	806	CLA	CBA-CGA-O2A-C1
20	B	835	CLA	C5-C6-C7-C8
20	1	608	CLA	C8-C10-C11-C12
20	B	818	CLA	C10-C11-C12-C13
24	1	621	LHG	O6-C4-C5-C6
24	3	424	LHG	O6-C4-C5-C6
25	8	318	PTY	O14-C5-C6-C1
25	B	801	PTY	O14-C5-C6-C1
25	H	202	PTY	O14-C5-C6-C1
20	2	602	CLA	C3-C5-C6-C7
19	7	302	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	7	302	CHL	C11-C12-C13-C15
20	1	603	CLA	C11-C10-C8-C7
20	1	609	CLA	C6-C7-C8-C10
20	7	313	CLA	C6-C7-C8-C10
20	8	302	CLA	C11-C10-C8-C7
20	8	309	CLA	C11-C10-C8-C7
20	9	609	CLA	C6-C7-C8-C10
20	A	806	CLA	C6-C7-C8-C10
20	A	806	CLA	C11-C10-C8-C7
20	A	815	CLA	C12-C13-C15-C16
20	A	818	CLA	C11-C12-C13-C15
20	A	818	CLA	C12-C13-C15-C16
20	A	823	CLA	C11-C12-C13-C15
20	A	828	CLA	C11-C12-C13-C15
20	A	830	CLA	C6-C7-C8-C10
20	A	832	CLA	C12-C13-C15-C16
20	A	839	CLA	C12-C13-C15-C16
20	A	841	CLA	C6-C7-C8-C10
20	B	803	CLA	C6-C7-C8-C10
20	B	803	CLA	C12-C13-C15-C16
20	B	809	CLA	C11-C12-C13-C15
20	B	819	CLA	C11-C10-C8-C7
20	B	830	CLA	C11-C10-C8-C7
20	B	831	CLA	C11-C10-C8-C7
20	B	841	CLA	C12-C13-C15-C16
20	L	302	CLA	C11-C10-C8-C7
20	L	302	CLA	C11-C12-C13-C15
33	B	844	PQN	C17-C18-C20-C21
20	A	813	CLA	C6-C7-C8-C10
29	7	321	DGD	O6E-C5E-C6E-O5E
20	A	819	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	C10-C11-C12-C13
20	A	814	CLA	C13-C15-C16-C17
20	B	833	CLA	C4-C3-C5-C6
20	7	311	CLA	C2-C3-C5-C6
20	B	833	CLA	C2-C3-C5-C6
29	A	802	DGD	C3A-C4A-C5A-C6A
20	B	820	CLA	O1A-CGA-O2A-C1
20	1	613	CLA	C2A-CAA-CBA-CGA
20	2	613	CLA	C2A-CAA-CBA-CGA
20	L	304	CLA	C2A-CAA-CBA-CGA
20	1	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	7	309	CLA	C11-C10-C8-C9
20	7	313	CLA	C6-C7-C8-C9
20	8	302	CLA	C11-C10-C8-C9
20	8	308	CLA	C6-C7-C8-C9
20	9	602	CLA	C11-C10-C8-C9
20	9	609	CLA	C6-C7-C8-C9
20	A	806	CLA	C6-C7-C8-C9
20	A	806	CLA	C11-C10-C8-C9
20	A	821	CLA	C11-C12-C13-C14
20	A	832	CLA	C14-C13-C15-C16
20	B	818	CLA	C11-C10-C8-C9
20	B	819	CLA	C6-C7-C8-C9
20	B	820	CLA	C14-C13-C15-C16
20	B	828	CLA	C11-C10-C8-C9
20	B	830	CLA	C11-C10-C8-C9
20	B	831	CLA	C11-C10-C8-C9
20	B	841	CLA	C14-C13-C15-C16
33	B	844	PQN	C24-C23-C25-C26
20	L	301	CLA	O1D-CGD-O2D-CED
20	A	808	CLA	C8-C10-C11-C12
20	A	829	CLA	C11-C10-C8-C9
24	2	621	LHG	C4-C5-C6-O8
24	3	420	LHG	C4-C5-C6-O8
24	9	619	LHG	C4-C5-C6-O8
24	A	854	LHG	C4-C5-C6-O8
24	H	203	LHG	C4-C5-C6-O8
29	L	311	DGD	O1G-C1G-C2G-C3G
20	B	839	CLA	CBD-CGD-O2D-CED
24	B	852	LHG	C30-C31-C32-C33
20	B	835	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	CBA-CGA-O2A-C1
20	2	602	CLA	CBA-CGA-O2A-C1
20	A	840	CLA	CBA-CGA-O2A-C1
36	A	859	4RF	C13-C14-C15-C16
31	A	857	LMU	C5'-C4'-O1B-C1B
19	1	601	CHL	CHA-CBD-CGD-O1D
19	1	601	CHL	CHA-CBD-CGD-O2D
19	2	606	CHL	CHA-CBD-CGD-O2D
19	8	305	CHL	CHA-CBD-CGD-O1D
19	8	305	CHL	CHA-CBD-CGD-O2D
24	7	320	LHG	C25-C26-C27-C28
24	I	201	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	1	620	LHG	C7-C8-C9-C10
28	7	301	LMG	O8-C28-C29-C30
20	A	810	CLA	C2-C3-C5-C6
20	A	819	CLA	C5-C6-C7-C8
20	A	840	CLA	C10-C11-C12-C13
20	L	304	CLA	C5-C6-C7-C8
23	3	418	BCR	C11-C12-C13-C35
20	A	836	CLA	C11-C12-C13-C15
20	A	819	CLA	O1A-CGA-O2A-C1
20	B	806	CLA	O1A-CGA-O2A-C1
20	B	808	CLA	C8-C10-C11-C12
25	H	202	PTY	C5-C6-O7-C8
36	A	859	4RF	C10-C11-C12-C13
20	8	302	CLA	C5-C6-C7-C8
20	B	832	CLA	C5-C6-C7-C8
19	2	606	CHL	C3C-C2C-CMC-OMC
19	3	401	CHL	C3C-C2C-CMC-OMC
19	7	306	CHL	C3C-C2C-CMC-OMC
19	8	305	CHL	C3C-C2C-CMC-OMC
23	J	4001	BCR	C13-C14-C15-C16
20	7	303	CLA	C11-C12-C13-C14
32	A	803	CL0	C16-C17-C18-C20
31	A	857	LMU	C3'-C4'-O1B-C1B
20	A	836	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	C5-C6-C7-C8
19	3	401	CHL	CBA-CGA-O2A-C1
20	B	832	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	C13-C15-C16-C17
20	A	810	CLA	C4-C3-C5-C6
19	2	601	CHL	O1D-CGD-O2D-CED
20	1	603	CLA	C16-C17-C18-C20
20	A	825	CLA	C11-C12-C13-C14
20	B	840	CLA	C16-C17-C18-C20
24	F	5002	LHG	O7-C5-C6-O8
25	L	310	PTY	O4-C1-C6-O7
26	9	618	SQD	O47-C45-C46-O48
28	7	319	LMG	O7-C8-C9-O8
20	A	810	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	CAA-CBA-CGA-O2A
20	8	311	CLA	C2A-CAA-CBA-CGA
19	8	304	CHL	O1A-CGA-O2A-C1
20	K	204	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	3	422	PTY	C31-C32-C33-C34
25	8	318	PTY	C11-C12-C13-C14
20	A	824	CLA	C8-C10-C11-C12
20	7	314	CLA	CBA-CGA-O2A-C1
19	2	606	CHL	C1C-C2C-CMC-OMC
19	8	305	CHL	C1C-C2C-CMC-OMC
20	3	412	CLA	C5-C6-C7-C8
20	B	820	CLA	C10-C11-C12-C13
20	7	311	CLA	C3-C5-C6-C7
19	2	606	CHL	O1D-CGD-O2D-CED
20	3	410	CLA	O1D-CGD-O2D-CED
23	B	846	BCR	C15-C16-C17-C18
20	3	408	CLA	C11-C12-C13-C14
20	3	411	CLA	C6-C7-C8-C9
24	A	854	LHG	C31-C32-C33-C34
20	B	815	CLA	C4-C3-C5-C6
20	A	829	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	CBA-CGA-O2A-C1
30	8	320	LMK	O9-C10-C11-C12
31	9	616	LMU	C2-C1-O1'-C1'
19	2	601	CHL	C11-C10-C8-C9
20	1	603	CLA	C11-C10-C8-C9
20	1	607	CLA	C11-C12-C13-C14
20	3	408	CLA	C6-C7-C8-C9
20	7	313	CLA	C14-C13-C15-C16
20	8	309	CLA	C11-C10-C8-C9
20	A	815	CLA	C14-C13-C15-C16
20	A	818	CLA	C11-C12-C13-C14
20	A	818	CLA	C14-C13-C15-C16
20	A	822	CLA	C11-C12-C13-C14
20	A	823	CLA	C11-C12-C13-C14
20	A	826	CLA	C11-C10-C8-C9
20	A	828	CLA	C11-C12-C13-C14
20	A	830	CLA	C6-C7-C8-C9
20	A	839	CLA	C14-C13-C15-C16
20	A	844	CLA	C14-C13-C15-C16
20	B	803	CLA	C6-C7-C8-C9
20	B	809	CLA	C11-C12-C13-C14
20	B	814	CLA	C6-C7-C8-C9
20	B	817	CLA	C11-C10-C8-C9
20	B	829	CLA	C6-C7-C8-C9
20	B	842	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	L	302	CLA	C11-C12-C13-C14
33	B	844	PQN	C19-C18-C20-C21
20	A	813	CLA	O1D-CGD-O2D-CED
20	A	811	CLA	C13-C15-C16-C17
20	A	823	CLA	C5-C6-C7-C8
24	7	320	LHG	C2-C3-O3-P
24	G	4006	LHG	C5-C4-O6-P
20	1	605	CLA	C4B-C3B-CAB-CBB
20	1	607	CLA	C4B-C3B-CAB-CBB
20	1	612	CLA	C4B-C3B-CAB-CBB
20	2	608	CLA	C4B-C3B-CAB-CBB
20	2	610	CLA	C4B-C3B-CAB-CBB
20	3	404	CLA	C4B-C3B-CAB-CBB
20	3	406	CLA	C4B-C3B-CAB-CBB
20	7	309	CLA	C4B-C3B-CAB-CBB
20	9	601	CLA	C4B-C3B-CAB-CBB
20	9	604	CLA	C4B-C3B-CAB-CBB
20	A	811	CLA	C4B-C3B-CAB-CBB
20	A	817	CLA	C4B-C3B-CAB-CBB
20	A	824	CLA	C4B-C3B-CAB-CBB
20	A	829	CLA	C4B-C3B-CAB-CBB
20	A	830	CLA	C4B-C3B-CAB-CBB
20	A	832	CLA	C4B-C3B-CAB-CBB
20	A	833	CLA	C4B-C3B-CAB-CBB
20	A	843	CLA	C4B-C3B-CAB-CBB
20	B	807	CLA	C4B-C3B-CAB-CBB
20	B	816	CLA	C4B-C3B-CAB-CBB
20	B	817	CLA	C4B-C3B-CAB-CBB
20	B	825	CLA	C4B-C3B-CAB-CBB
20	F	5005	CLA	C4B-C3B-CAB-CBB
20	1	610	CLA	CAA-CBA-CGA-O2A
20	B	843	CLA	C8-C10-C11-C12
20	2	622	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	C16-C17-C18-C20
20	1	605	CLA	C2A-CAA-CBA-CGA
20	9	609	CLA	C10-C11-C12-C13
20	A	814	CLA	C3-C5-C6-C7
36	A	859	4RF	C12-C13-C14-C15
20	1	608	CLA	C11-C10-C8-C7
20	7	309	CLA	C11-C10-C8-C7
20	8	308	CLA	C6-C7-C8-C10
20	8	311	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	9	602	CLA	C11-C10-C8-C7
20	A	809	CLA	C11-C12-C13-C15
20	A	809	CLA	C12-C13-C15-C16
20	A	812	CLA	C11-C10-C8-C7
20	A	821	CLA	C11-C12-C13-C15
20	A	826	CLA	C11-C10-C8-C7
20	A	841	CLA	C11-C10-C8-C7
20	A	844	CLA	C12-C13-C15-C16
20	B	810	CLA	C11-C12-C13-C15
20	B	814	CLA	C6-C7-C8-C10
20	B	815	CLA	C11-C10-C8-C7
20	B	815	CLA	C11-C12-C13-C15
20	B	817	CLA	C11-C10-C8-C7
20	B	818	CLA	C11-C10-C8-C7
20	B	818	CLA	C11-C12-C13-C15
20	B	818	CLA	C12-C13-C15-C16
20	B	819	CLA	C6-C7-C8-C10
20	B	820	CLA	C12-C13-C15-C16
20	B	828	CLA	C11-C10-C8-C7
20	B	829	CLA	C6-C7-C8-C10
20	B	829	CLA	C11-C12-C13-C15
20	B	841	CLA	C6-C7-C8-C10
20	B	842	CLA	C11-C12-C13-C15
20	3	402	CLA	C5-C6-C7-C8
20	A	822	CLA	C13-C15-C16-C17
20	A	826	CLA	C8-C10-C11-C12
20	B	811	CLA	C10-C11-C12-C13
20	B	825	CLA	C15-C16-C17-C18
20	2	602	CLA	O1A-CGA-O2A-C1
20	2	611	CLA	C3A-C2A-CAA-CBA
20	7	311	CLA	C4-C3-C5-C6
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	832	CLA	C3A-C2A-CAA-CBA
20	F	5006	CLA	C3A-C2A-CAA-CBA
20	J	4002	CLA	C3A-C2A-CAA-CBA
20	L	301	CLA	C3A-C2A-CAA-CBA
20	A	844	CLA	C8-C10-C11-C12
20	A	830	CLA	C2-C3-C5-C6
20	B	819	CLA	C2-C3-C5-C6
20	1	603	CLA	O1A-CGA-O2A-C1
23	B	802	BCR	C13-C14-C15-C16
20	A	836	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	A	840	CLA	O1A-CGA-O2A-C1
22	7	317	XAT	C27-C28-C29-C30
24	2	621	LHG	C7-C8-C9-C10
28	7	301	LMG	C17-C18-C19-C20
20	7	310	CLA	C2A-CAA-CBA-CGA
20	9	601	CLA	C2A-CAA-CBA-CGA
24	I	201	LHG	C4-C5-C6-O8
24	J	4004	LHG	C4-C5-C6-O8
26	2	619	SQD	C44-C45-C46-O48
28	7	301	LMG	O1-C7-C8-C9
28	7	319	LMG	C7-C8-C9-O8
28	F	5001	LMG	C7-C8-C9-O8
29	B	850	DGD	C1G-C2G-C3G-O3G
20	1	603	CLA	C16-C17-C18-C19
20	7	304	CLA	C6-C7-C8-C10
20	A	825	CLA	C11-C12-C13-C15
19	1	601	CHL	C1A-C2A-CAA-CBA
19	2	601	CHL	C1A-C2A-CAA-CBA
19	9	606	CHL	C1A-C2A-CAA-CBA
20	B	823	CLA	C13-C15-C16-C17
20	B	840	CLA	C13-C15-C16-C17
20	3	402	CLA	C4-C3-C5-C6
20	8	309	CLA	C4-C3-C5-C6
20	A	830	CLA	C4-C3-C5-C6
20	B	813	CLA	C4-C3-C5-C6
20	B	819	CLA	C4-C3-C5-C6
20	B	815	CLA	C2-C3-C5-C6
20	A	840	CLA	O1D-CGD-O2D-CED
20	3	411	CLA	C6-C7-C8-C10
20	A	820	CLA	C11-C12-C13-C15
20	B	803	CLA	C16-C17-C18-C19
20	B	822	CLA	C16-C17-C18-C20
20	B	840	CLA	C16-C17-C18-C19
24	8	321	LHG	O6-C4-C5-O7
25	H	202	PTY	O14-C5-C6-O7
20	8	309	CLA	O1D-CGD-O2D-CED
21	1	615	LUT	C1-C6-C7-C8
21	2	615	LUT	C1-C6-C7-C8
21	2	616	LUT	C1-C6-C7-C8
21	8	314	LUT	C1-C6-C7-C8
23	3	418	BCR	C23-C24-C25-C30
23	7	318	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	A	850	BCR	C1-C6-C7-C8
23	B	802	BCR	C23-C24-C25-C30
23	B	845	BCR	C1-C6-C7-C8
23	B	846	BCR	C23-C24-C25-C30
23	G	4001	BCR	C23-C24-C25-C30
23	L	303	BCR	C1-C6-C7-C8
20	A	821	CLA	C5-C6-C7-C8
24	I	201	LHG	C5-C4-O6-P
25	7	322	PTY	C33-C34-C35-C36
19	7	302	CHL	O1D-CGD-O2D-CED
20	1	607	CLA	C10-C11-C12-C13
20	A	818	CLA	C5-C6-C7-C8
20	B	810	CLA	O1D-CGD-O2D-CED
24	A	854	LHG	C26-C27-C28-C29
20	3	408	CLA	C11-C12-C13-C15
20	A	808	CLA	C16-C17-C18-C19
20	B	803	CLA	C16-C17-C18-C20
20	B	817	CLA	CAA-CBA-CGA-O2A
36	A	859	4RF	O40-C41-C43-C44
20	A	844	CLA	C5-C6-C7-C8
24	2	618	LHG	O7-C5-C6-O8
24	7	325	LHG	O7-C5-C6-O8
24	F	5011	LHG	O7-C5-C6-O8
24	I	201	LHG	O7-C5-C6-O8
25	B	801	PTY	O4-C1-C6-O7
29	A	802	DGD	O2G-C2G-C3G-O3G
30	8	320	LMK	O1-C7-C8-O7
24	B	852	LHG	C27-C28-C29-C30
25	H	202	PTY	C12-C13-C14-C15
20	B	832	CLA	O1A-CGA-O2A-C1
20	9	607	CLA	C15-C16-C17-C18
20	A	832	CLA	C5-C6-C7-C8
20	L	302	CLA	C2-C3-C5-C6
32	A	803	CL0	C1-C2-C3-C5
19	2	601	CHL	C11-C12-C13-C14
19	2	601	CHL	CBA-CGA-O2A-C1
20	1	602	CLA	C6-C7-C8-C9
20	1	608	CLA	C11-C10-C8-C9
20	2	602	CLA	C6-C7-C8-C9
20	2	603	CLA	C6-C7-C8-C9
20	A	804	CLA	C6-C7-C8-C9
20	A	805	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	805	CLA	C11-C10-C8-C9
20	A	809	CLA	C14-C13-C15-C16
20	B	803	CLA	C11-C12-C13-C14
20	B	807	CLA	C6-C7-C8-C9
20	B	815	CLA	C11-C10-C8-C9
20	B	818	CLA	C11-C12-C13-C14
20	B	819	CLA	C11-C10-C8-C9
19	3	401	CHL	O1A-CGA-O2A-C1
20	G	4002	CLA	O1D-CGD-O2D-CED
20	7	304	CLA	C6-C7-C8-C9
19	7	302	CHL	C3-C5-C6-C7
20	1	607	CLA	CBA-CGA-O2A-C1
20	J	4002	CLA	O2A-C1-C2-C3
20	A	841	CLA	C15-C16-C17-C18
20	9	601	CLA	O1A-CGA-O2A-C1
23	A	847	BCR	C9-C10-C11-C12
24	9	617	LHG	O8-C23-C24-C25
20	8	309	CLA	C2-C3-C5-C6
20	B	813	CLA	C2-C3-C5-C6
20	B	835	CLA	C8-C10-C11-C12
24	I	201	LHG	C1-C2-C3-O3
24	7	325	LHG	C26-C27-C28-C29
20	A	839	CLA	CBA-CGA-O2A-C1
20	B	841	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	C5-C6-C7-C8
20	F	5003	CLA	C8-C10-C11-C12
25	L	310	PTY	O14-C5-C6-C1
20	A	832	CLA	C8-C10-C11-C12
19	7	302	CHL	C6-C7-C8-C10
20	1	602	CLA	C6-C7-C8-C10
20	1	603	CLA	C6-C7-C8-C10
20	2	603	CLA	C6-C7-C8-C10
20	7	313	CLA	C12-C13-C15-C16
20	8	311	CLA	C11-C12-C13-C15
20	A	804	CLA	C6-C7-C8-C10
20	A	805	CLA	C6-C7-C8-C10
20	A	805	CLA	C11-C10-C8-C7
20	A	822	CLA	C11-C12-C13-C15
20	A	824	CLA	C11-C12-C13-C15
20	A	839	CLA	C6-C7-C8-C10
20	B	803	CLA	C11-C10-C8-C7
20	B	804	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	B	807	CLA	C6-C7-C8-C10
20	B	807	CLA	C12-C13-C15-C16
20	B	808	CLA	C11-C10-C8-C7
20	B	811	CLA	C6-C7-C8-C10
20	B	811	CLA	C11-C12-C13-C15
20	B	820	CLA	C11-C10-C8-C7
20	B	833	CLA	C11-C10-C8-C7
20	B	843	CLA	C6-C7-C8-C10
33	B	844	PQN	C16-C17-C18-C20
33	B	844	PQN	C15-C16-C17-C18
23	A	847	BCR	C7-C8-C9-C10
23	A	850	BCR	C17-C18-C19-C20
20	2	611	CLA	CBA-CGA-O2A-C1
26	3	423	SQD	C5-C6-S-O8
26	9	618	SQD	C5-C6-S-O8
20	B	831	CLA	C8-C10-C11-C12
20	B	840	CLA	C15-C16-C17-C18
20	2	608	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	B	822	CLA	C16-C17-C18-C19
19	8	305	CHL	O1D-CGD-O2D-CED
24	7	320	LHG	O8-C23-C24-C25
20	B	814	CLA	C8-C10-C11-C12
20	B	810	CLA	O2A-C1-C2-C3
20	7	314	CLA	O1A-CGA-O2A-C1
20	A	830	CLA	O1A-CGA-O2A-C1
20	1	607	CLA	O1A-CGA-O2A-C1
20	A	829	CLA	O1A-CGA-O2A-C1
20	F	5003	CLA	C10-C11-C12-C13
25	H	201	PTY	O14-C5-C6-O7
25	L	310	PTY	O14-C5-C6-O7
20	F	5007	CLA	O2A-C1-C2-C3
24	1	620	LHG	C4-C5-C6-O8
24	2	618	LHG	C4-C5-C6-O8
24	7	325	LHG	C4-C5-C6-O8
27	2	620	3PH	C1-C2-C3-O31
20	B	810	CLA	C2A-CAA-CBA-CGA
20	3	402	CLA	C2-C3-C5-C6
24	J	4004	LHG	O7-C5-C6-O8
26	2	619	SQD	O6-C44-C45-O47
29	7	321	DGD	O2G-C2G-C3G-O3G
20	A	824	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	804	CLA	C6-C7-C8-C9
20	B	807	CLA	C14-C13-C15-C16
20	B	808	CLA	C11-C10-C8-C9
20	B	811	CLA	C6-C7-C8-C9
20	B	811	CLA	C11-C12-C13-C14
20	A	820	CLA	C11-C12-C13-C14
28	8	301	LMG	C28-C29-C30-C31
24	B	852	LHG	C12-C13-C14-C15
19	2	601	CHL	O1A-CGA-O2A-C1
20	B	841	CLA	O1A-CGA-O2A-C1
20	B	841	CLA	CAA-CBA-CGA-O2A
20	7	311	CLA	C2-C1-O2A-CGA
20	A	831	CLA	C2-C1-O2A-CGA
20	B	818	CLA	C2-C1-O2A-CGA
20	B	843	CLA	C2-C1-O2A-CGA
23	A	850	BCR	C13-C14-C15-C16
20	A	822	CLA	C16-C17-C18-C20
19	7	302	CHL	C5-C6-C7-C8
20	A	824	CLA	C15-C16-C17-C18
20	B	834	CLA	C13-C15-C16-C17
20	B	839	CLA	O1D-CGD-O2D-CED
20	B	843	CLA	C4-C3-C5-C6
20	L	305	CLA	C4-C3-C5-C6
20	B	808	CLA	C2A-CAA-CBA-CGA
20	1	609	CLA	C10-C11-C12-C13
20	A	839	CLA	O1A-CGA-O2A-C1
20	8	311	CLA	C8-C10-C11-C12
20	B	829	CLA	C3-C5-C6-C7
19	2	606	CHL	C4C-C3C-CAC-CBC
19	8	304	CHL	C4C-C3C-CAC-CBC
26	B	851	SQD	C4-C5-C6-S
25	H	201	PTY	C17-C18-C19-C20
20	1	614	CLA	O1A-CGA-O2A-C1
20	1	602	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	C6-C7-C8-C10
20	A	821	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	C3-C5-C6-C7
20	B	839	CLA	C3-C5-C6-C7
25	1	623	PTY	C11-C12-C13-C14
28	F	5001	LMG	C14-C15-C16-C17
20	3	408	CLA	C1A-C2A-CAA-CBA
20	3	409	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	3	414	CLA	C1A-C2A-CAA-CBA
20	7	314	CLA	C1A-C2A-CAA-CBA
20	7	324	CLA	C4B-C3B-CAB-CBB
20	8	309	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	836	CLA	C1A-C2A-CAA-CBA
20	B	807	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	C4-C3-C5-C6
20	B	818	CLA	C4-C3-C5-C6
23	B	846	BCR	C22-C23-C24-C25
23	A	850	BCR	C21-C22-C23-C24
20	A	812	CLA	C3-C5-C6-C7
19	2	601	CHL	C2A-CAA-CBA-CGA
20	1	602	CLA	C2A-CAA-CBA-CGA
20	2	611	CLA	O1A-CGA-O2A-C1
26	3	423	SQD	C5-C6-S-O9
20	8	309	CLA	C3-C5-C6-C7
20	3	407	CLA	C11-C10-C8-C7
20	3	412	CLA	C11-C12-C13-C15
20	7	310	CLA	C12-C13-C15-C16
20	A	812	CLA	C11-C12-C13-C15
20	A	814	CLA	C12-C13-C15-C16
20	A	815	CLA	C11-C10-C8-C7
20	A	842	CLA	C11-C12-C13-C15
20	A	844	CLA	C11-C10-C8-C7
20	B	806	CLA	C12-C13-C15-C16
20	B	829	CLA	C11-C10-C8-C7
20	B	842	CLA	C11-C10-C8-C7
33	B	844	PQN	C21-C22-C23-C25
25	1	622	PTY	C6-C5-O14-P1
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	833	CLA	CBD-CGD-O2D-CED
24	1	619	LHG	O6-C4-C5-O7
24	3	424	LHG	O6-C4-C5-O7
24	F	5011	LHG	O6-C4-C5-O7
25	8	318	PTY	O14-C5-C6-O7
25	B	801	PTY	O14-C5-C6-O7
20	A	844	CLA	C3-C5-C6-C7
20	8	311	CLA	C6-C7-C8-C9
20	A	815	CLA	C11-C10-C8-C9
20	A	823	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	839	CLA	C6-C7-C8-C9
20	B	803	CLA	C11-C10-C8-C9
20	B	810	CLA	C11-C12-C13-C14
20	B	833	CLA	C11-C10-C8-C9
20	B	841	CLA	C6-C7-C8-C9
20	B	843	CLA	C6-C7-C8-C9
20	1	602	CLA	O1A-CGA-O2A-C1
24	3	420	LHG	O7-C5-C6-O8
24	9	619	LHG	O7-C5-C6-O8
25	1	623	PTY	O4-C1-C6-O7
26	3	423	SQD	O47-C45-C46-O48
26	B	851	SQD	O47-C45-C46-O48
28	F	5001	LMG	O7-C8-C9-O8
25	B	801	PTY	O4-C1-C6-C5
25	L	310	PTY	O4-C1-C6-C5
26	2	619	SQD	O6-C44-C45-C46
26	9	618	SQD	O6-C44-C45-C46
28	7	301	LMG	C7-C8-C9-O8
20	1	603	CLA	C5-C6-C7-C8
20	A	806	CLA	C8-C10-C11-C12
20	A	823	CLA	C10-C11-C12-C13
20	B	823	CLA	C5-C6-C7-C8
20	B	825	CLA	C5-C6-C7-C8
20	B	807	CLA	O1A-CGA-O2A-C1
36	A	859	4RF	C25-C26-C27-C28
20	7	324	CLA	CAD-CBD-CGD-O2D
20	9	602	CLA	CAD-CBD-CGD-O2D
20	9	609	CLA	CAD-CBD-CGD-O2D
20	J	4002	CLA	CBA-CGA-O2A-C1
25	H	201	PTY	C12-C13-C14-C15
29	B	850	DGD	C4B-C5B-C6B-C7B
20	B	806	CLA	C3-C5-C6-C7
20	1	614	CLA	C2A-CAA-CBA-CGA
20	A	820	CLA	C2A-CAA-CBA-CGA
20	L	307	CLA	C2A-CAA-CBA-CGA
30	8	320	LMK	C29-C30-C31-C32
20	J	4002	CLA	O1A-CGA-O2A-C1
19	2	601	CHL	CHA-CBD-CGD-O1D
19	2	601	CHL	CHA-CBD-CGD-O2D
20	1	602	CLA	CHA-CBD-CGD-O1D
20	1	602	CLA	CHA-CBD-CGD-O2D
20	2	603	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	2	607	CLA	CHA-CBD-CGD-O1D
20	2	607	CLA	CHA-CBD-CGD-O2D
20	7	324	CLA	CAD-CBD-CGD-O1D
20	8	310	CLA	CHA-CBD-CGD-O1D
20	8	310	CLA	CHA-CBD-CGD-O2D
20	9	601	CLA	CHA-CBD-CGD-O1D
20	9	601	CLA	CHA-CBD-CGD-O2D
20	9	602	CLA	CAD-CBD-CGD-O1D
20	9	609	CLA	CAD-CBD-CGD-O1D
20	A	807	CLA	CHA-CBD-CGD-O1D
20	A	807	CLA	CHA-CBD-CGD-O2D
20	A	811	CLA	CHA-CBD-CGD-O1D
20	A	811	CLA	CHA-CBD-CGD-O2D
20	A	819	CLA	CHA-CBD-CGD-O1D
20	A	819	CLA	CHA-CBD-CGD-O2D
20	A	838	CLA	CHA-CBD-CGD-O1D
20	A	838	CLA	CHA-CBD-CGD-O2D
20	B	834	CLA	CAD-CBD-CGD-O1D
20	K	204	CLA	CHA-CBD-CGD-O1D
20	K	204	CLA	CHA-CBD-CGD-O2D
20	L	302	CLA	CHA-CBD-CGD-O1D
20	L	302	CLA	CHA-CBD-CGD-O2D
24	1	618	LHG	C4-O6-P-O5
24	1	619	LHG	C3-O3-P-O5
24	1	619	LHG	C4-O6-P-O5
24	1	621	LHG	C3-O3-P-O5
24	3	424	LHG	C3-O3-P-O5
24	8	319	LHG	C3-O3-P-O4
24	8	319	LHG	C4-O6-P-O4
24	8	321	LHG	C3-O3-P-O5
24	A	853	LHG	C4-O6-P-O4
24	G	4006	LHG	C4-O6-P-O4
24	H	203	LHG	C3-O3-P-O5
24	H	203	LHG	C4-O6-P-O5
24	I	201	LHG	C3-O3-P-O5
25	1	622	PTY	C3-O11-P1-O13
25	1	623	PTY	C5-O14-P1-O11
25	1	623	PTY	C5-O14-P1-O12
25	1	623	PTY	C5-O14-P1-O13
25	3	422	PTY	N1-C2-C3-O11
25	3	422	PTY	C5-O14-P1-O13
25	7	322	PTY	C3-O11-P1-O13

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Mol	Chain	Res	Type	Atoms
25	7	322	PTY	C5-O14-P1-O12
25	8	317	PTY	C3-O11-P1-O13
25	8	317	PTY	C5-O14-P1-O12
25	B	801	PTY	C3-O11-P1-O13
25	F	5010	PTY	C3-O11-P1-O13
25	H	201	PTY	C5-O14-P1-O11
25	H	201	PTY	C5-O14-P1-O12
25	H	202	PTY	C5-O14-P1-O12
25	L	310	PTY	C3-O11-P1-O13
20	B	825	CLA	C16-C17-C18-C20
20	1	602	CLA	C2B-C3B-CAB-CBB
20	1	604	CLA	C2B-C3B-CAB-CBB
20	2	604	CLA	C2B-C3B-CAB-CBB
20	2	611	CLA	C2B-C3B-CAB-CBB
20	3	402	CLA	C2B-C3B-CAB-CBB
20	3	403	CLA	C2B-C3B-CAB-CBB
20	3	406	CLA	C2B-C3B-CAB-CBB
20	7	324	CLA	C2B-C3B-CAB-CBB
20	8	302	CLA	C2B-C3B-CAB-CBB
20	8	310	CLA	C2B-C3B-CAB-CBB
20	8	311	CLA	C2B-C3B-CAB-CBB
20	9	601	CLA	C2B-C3B-CAB-CBB
20	9	604	CLA	C2B-C3B-CAB-CBB
20	9	608	CLA	C2B-C3B-CAB-CBB
20	A	807	CLA	C2B-C3B-CAB-CBB
20	A	812	CLA	C2B-C3B-CAB-CBB
20	A	819	CLA	C2B-C3B-CAB-CBB
20	A	820	CLA	C2B-C3B-CAB-CBB
20	A	822	CLA	C2B-C3B-CAB-CBB
20	A	832	CLA	C2B-C3B-CAB-CBB
20	A	833	CLA	C2B-C3B-CAB-CBB
20	A	836	CLA	C2B-C3B-CAB-CBB
20	A	841	CLA	C2B-C3B-CAB-CBB
20	B	803	CLA	C2B-C3B-CAB-CBB
20	B	807	CLA	C2B-C3B-CAB-CBB
20	B	810	CLA	C2B-C3B-CAB-CBB
20	B	818	CLA	C2B-C3B-CAB-CBB
20	B	824	CLA	C2B-C3B-CAB-CBB
20	B	832	CLA	C2B-C3B-CAB-CBB
20	B	836	CLA	C2B-C3B-CAB-CBB
20	B	840	CLA	C2B-C3B-CAB-CBB
20	B	842	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	G	4003	CLA	C2B-C3B-CAB-CBB
20	G	4004	CLA	C2B-C3B-CAB-CBB
20	K	203	CLA	C2B-C3B-CAB-CBB
20	L	301	CLA	C2B-C3B-CAB-CBB
20	L	302	CLA	C2B-C3B-CAB-CBB
20	L	304	CLA	C2B-C3B-CAB-CBB
23	1	617	BCR	C1-C6-C7-C8
23	F	5009	BCR	C23-C24-C25-C30
23	J	4003	BCR	C5-C6-C7-C8
24	1	620	LHG	C2-C3-O3-P
24	1	621	LHG	C5-C4-O6-P
24	2	621	LHG	C5-C4-O6-P
24	7	323	LHG	C2-C3-O3-P
24	7	325	LHG	C2-C3-O3-P
24	8	321	LHG	C2-C3-O3-P
24	F	5011	LHG	C2-C3-O3-P
25	F	5010	PTY	C6-C5-O14-P1
24	7	320	LHG	C28-C29-C30-C31
24	7	320	LHG	C31-C32-C33-C34
19	7	307	CHL	CBD-CGD-O2D-CED
24	7	320	LHG	C10-C11-C12-C13
23	A	849	BCR	C18-C19-C20-C21
23	A	850	BCR	C18-C19-C20-C21
23	B	802	BCR	C10-C11-C12-C13
23	B	846	BCR	C18-C19-C20-C21
23	G	4005	BCR	C10-C11-C12-C13
23	H	205	BCR	C10-C11-C12-C13
23	H	205	BCR	C18-C19-C20-C21
23	K	205	BCR	C10-C11-C12-C13
24	9	617	LHG	C23-C24-C25-C26
20	A	833	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	C16-C17-C18-C19
20	F	5003	CLA	C16-C17-C18-C20
24	1	619	LHG	O6-C4-C5-C6
24	8	321	LHG	O6-C4-C5-C6
19	7	306	CHL	C2C-C3C-CAC-CBC
20	A	809	CLA	C11-C12-C13-C14
20	A	812	CLA	C11-C10-C8-C9
20	A	830	CLA	C11-C10-C8-C9
20	A	842	CLA	C11-C12-C13-C14
20	B	814	CLA	C14-C13-C15-C16
20	B	815	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	818	CLA	C14-C13-C15-C16
20	B	831	CLA	C14-C13-C15-C16
20	A	835	CLA	C6-C7-C8-C10
20	B	803	CLA	C11-C12-C13-C15
20	B	831	CLA	C12-C13-C15-C16
20	2	605	CLA	C2A-CAA-CBA-CGA
20	L	305	CLA	C2-C3-C5-C6
20	A	834	CLA	C6-C7-C8-C9
24	B	852	LHG	O7-C5-C6-O8
26	9	618	SQD	O6-C44-C45-O47
20	L	306	CLA	CBD-CGD-O2D-CED
36	A	859	4RF	C08-C09-C10-C11
20	2	603	CLA	C2A-CAA-CBA-CGA
20	3	414	CLA	C2A-CAA-CBA-CGA
20	H	204	CLA	C2A-CAA-CBA-CGA
20	8	303	CLA	C2-C1-O2A-CGA
20	L	304	CLA	C2-C1-O2A-CGA
20	H	204	CLA	CBD-CGD-O2D-CED
28	7	319	LMG	C10-C11-C12-C13
20	B	825	CLA	C16-C17-C18-C19
20	B	820	CLA	CBD-CGD-O2D-CED
23	B	848	BCR	C21-C22-C23-C24
20	3	412	CLA	CBA-CGA-O2A-C1
20	7	314	CLA	C2A-CAA-CBA-CGA
20	A	809	CLA	C2A-CAA-CBA-CGA
20	2	622	CLA	O1A-CGA-O2A-C1
20	3	412	CLA	C4-C3-C5-C6
32	A	803	CL0	C4-C3-C5-C6
24	2	618	LHG	C24-C25-C26-C27
36	A	859	4RF	C44-C45-C46-C47
26	2	619	SQD	O48-C23-C24-C25
20	7	309	CLA	C14-C13-C15-C16
20	A	812	CLA	C11-C12-C13-C14
20	A	841	CLA	C11-C10-C8-C9
20	A	844	CLA	C11-C10-C8-C9
20	B	842	CLA	C11-C10-C8-C9
20	A	805	CLA	CBA-CGA-O2A-C1
20	2	605	CLA	C4B-C3B-CAB-CBB
20	7	305	CLA	C4B-C3B-CAB-CBB
20	A	838	CLA	C4B-C3B-CAB-CBB
20	G	4002	CLA	C4B-C3B-CAB-CBB
20	3	412	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	7	310	CLA	C16-C17-C18-C20
20	1	603	CLA	C8-C10-C11-C12
20	9	609	CLA	C4-C3-C5-C6
20	B	809	CLA	C4-C3-C5-C6
36	A	859	4RF	C46-C47-C48-C49
20	A	814	CLA	C11-C10-C8-C7
20	A	824	CLA	C12-C13-C15-C16
20	L	302	CLA	C12-C13-C15-C16
20	A	805	CLA	O1A-CGA-O2A-C1
20	F	5003	CLA	C16-C17-C18-C19
20	H	204	CLA	O1D-CGD-O2D-CED
20	L	302	CLA	C10-C11-C12-C13
20	A	805	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	A	840	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C3A-C2A-CAA-CBA
20	B	836	CLA	C3A-C2A-CAA-CBA
32	A	803	CL0	C2-C3-C5-C6
20	L	301	CLA	CAA-CBA-CGA-O2A
21	1	615	LUT	C40-C33-C34-C35
21	2	616	LUT	C40-C33-C34-C35
23	3	419	BCR	C35-C13-C14-C15
23	3	419	BCR	C16-C17-C18-C36
23	A	850	BCR	C35-C13-C14-C15
23	A	852	BCR	C11-C10-C9-C34
23	A	852	BCR	C16-C17-C18-C36
23	B	846	BCR	C11-C10-C9-C34
23	B	846	BCR	C20-C21-C22-C37
23	F	5009	BCR	C16-C17-C18-C36
23	G	4005	BCR	C35-C13-C14-C15
23	G	4005	BCR	C16-C17-C18-C36
23	H	205	BCR	C11-C10-C9-C34
23	H	205	BCR	C20-C21-C22-C37
23	I	202	BCR	C35-C13-C14-C15
23	K	205	BCR	C11-C10-C9-C34
23	L	303	BCR	C11-C10-C9-C34
24	A	854	LHG	C24-C25-C26-C27
20	L	306	CLA	O1D-CGD-O2D-CED
20	A	836	CLA	C2-C1-O2A-CGA
20	A	821	CLA	C10-C11-C12-C13
24	2	618	LHG	C13-C14-C15-C16
20	B	829	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	B	812	CLA	CBA-CGA-O2A-C1
22	1	616	XAT	C7-C8-C9-C10
20	A	814	CLA	C4-C3-C5-C6
20	2	607	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	C8-C10-C11-C12
20	B	833	CLA	C13-C15-C16-C17
20	B	817	CLA	C2A-CAA-CBA-CGA
24	B	852	LHG	C4-C5-C6-O8
30	8	320	LMK	O1-C7-C8-C9
20	B	828	CLA	CAA-CBA-CGA-O1A
20	3	412	CLA	C11-C12-C13-C14
20	9	607	CLA	C6-C7-C8-C9
20	A	814	CLA	C11-C10-C8-C9
20	B	806	CLA	C14-C13-C15-C16
20	B	829	CLA	C11-C10-C8-C9
24	B	852	LHG	C29-C30-C31-C32
20	L	301	CLA	CAA-CBA-CGA-O1A
24	1	620	LHG	O7-C7-C8-C9
25	H	201	PTY	C1-C6-O7-C8
32	A	803	CL0	C1-C2-C3-C4
36	A	859	4RF	C07-C08-C09-C10
20	A	841	CLA	CAA-CBA-CGA-O2A
20	3	412	CLA	C2-C3-C5-C6
20	B	809	CLA	C2-C3-C5-C6
20	1	610	CLA	CAA-CBA-CGA-O1A
20	1	607	CLA	C1A-C2A-CAA-CBA
20	2	612	CLA	C1A-C2A-CAA-CBA
20	8	310	CLA	C1A-C2A-CAA-CBA
20	A	805	CLA	C1A-C2A-CAA-CBA
20	A	837	CLA	C1A-C2A-CAA-CBA
20	A	843	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C1A-C2A-CAA-CBA
20	F	5006	CLA	C1A-C2A-CAA-CBA
21	1	615	LUT	C32-C33-C34-C35
21	2	616	LUT	C32-C33-C34-C35
23	3	419	BCR	C12-C13-C14-C15
23	3	419	BCR	C16-C17-C18-C19
23	A	852	BCR	C11-C10-C9-C8
23	A	852	BCR	C16-C17-C18-C19
23	B	846	BCR	C11-C10-C9-C8
23	B	846	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	F	5009	BCR	C16-C17-C18-C19
23	G	4005	BCR	C16-C17-C18-C19
23	H	205	BCR	C11-C10-C9-C8
23	H	205	BCR	C20-C21-C22-C23
23	I	202	BCR	C12-C13-C14-C15
23	K	205	BCR	C11-C10-C9-C8
23	L	303	BCR	C11-C10-C9-C8
20	K	203	CLA	CAA-CBA-CGA-O1A
20	1	607	CLA	C2B-C3B-CAB-CBB
20	1	612	CLA	C2B-C3B-CAB-CBB
20	7	305	CLA	C2B-C3B-CAB-CBB
20	7	309	CLA	C2B-C3B-CAB-CBB
20	8	307	CLA	C2B-C3B-CAB-CBB
20	A	811	CLA	C2B-C3B-CAB-CBB
20	A	817	CLA	C2B-C3B-CAB-CBB
20	A	829	CLA	C2B-C3B-CAB-CBB
20	A	830	CLA	C2B-C3B-CAB-CBB
20	A	838	CLA	C2B-C3B-CAB-CBB
20	B	817	CLA	C2B-C3B-CAB-CBB
20	B	826	CLA	C2B-C3B-CAB-CBB
20	B	828	CLA	C2B-C3B-CAB-CBB
20	B	829	CLA	C2B-C3B-CAB-CBB
20	G	4002	CLA	C2B-C3B-CAB-CBB
20	H	204	CLA	C2B-C3B-CAB-CBB
20	L	306	CLA	C2B-C3B-CAB-CBB
21	1	615	LUT	C5-C6-C7-C8
21	2	615	LUT	C5-C6-C7-C8
21	2	616	LUT	C5-C6-C7-C8
21	3	415	LUT	C1-C6-C7-C8
21	8	314	LUT	C5-C6-C7-C8
23	1	617	BCR	C5-C6-C7-C8
23	1	617	BCR	C23-C24-C25-C30
23	3	418	BCR	C23-C24-C25-C26
23	7	318	BCR	C5-C6-C7-C8
23	A	847	BCR	C23-C24-C25-C30
23	A	848	BCR	C23-C24-C25-C30
23	A	850	BCR	C5-C6-C7-C8
23	B	802	BCR	C23-C24-C25-C26
23	B	845	BCR	C5-C6-C7-C8
23	B	846	BCR	C23-C24-C25-C26
23	B	847	BCR	C23-C24-C25-C26
23	F	5009	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	G	4001	BCR	C23-C24-C25-C26
23	L	303	BCR	C5-C6-C7-C8
20	2	605	CLA	CAA-CBA-CGA-O2A
20	A	834	CLA	CBA-CGA-O2A-C1
24	1	619	LHG	C5-C4-O6-P
24	F	5002	LHG	C26-C27-C28-C29
20	A	826	CLA	C3-C5-C6-C7
24	B	852	LHG	C31-C32-C33-C34
30	8	320	LMK	N4-C3-C4-O2
19	7	302	CHL	C4-C3-C5-C6
20	2	602	CLA	C4-C3-C5-C6
20	A	831	CLA	C4-C3-C5-C6
20	B	824	CLA	C4-C3-C5-C6
20	7	309	CLA	C12-C13-C15-C16
20	9	607	CLA	C6-C7-C8-C10
20	A	816	CLA	C6-C7-C8-C10
20	B	804	CLA	C12-C13-C15-C16
20	B	814	CLA	C12-C13-C15-C16
32	A	803	CL0	C6-C7-C8-C10
20	1	612	CLA	C2A-CAA-CBA-CGA
29	A	802	DGD	O1G-C1G-C2G-O2G
29	L	311	DGD	C3A-C4A-C5A-C6A
24	3	420	LHG	C6-C5-O7-C7
36	A	859	4RF	C45-C46-C47-C48
28	F	5001	LMG	C11-C12-C13-C14
24	3	420	LHG	C5-C6-O8-C23
20	A	829	CLA	C11-C10-C8-C7
23	B	846	BCR	C11-C12-C13-C35
20	G	4004	CLA	CAA-CBA-CGA-O2A
20	A	836	CLA	C4-C3-C5-C6
20	2	602	CLA	C2-C3-C5-C6
20	9	609	CLA	C2-C3-C5-C6
20	A	804	CLA	C2-C3-C5-C6
19	7	307	CHL	O1D-CGD-O2D-CED
30	8	320	LMK	C8-C7-O1-C1
20	K	201	CLA	CAA-CBA-CGA-O2A
20	K	203	CLA	CAA-CBA-CGA-O2A
20	B	820	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	CBA-CGA-O2A-C1
20	A	822	CLA	C2A-CAA-CBA-CGA
20	2	605	CLA	CAA-CBA-CGA-O1A
20	3	402	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	811	CLA	C11-C10-C8-C9
20	B	833	CLA	C6-C7-C8-C9
20	B	829	CLA	C5-C6-C7-C8
29	A	802	DGD	C2A-C3A-C4A-C5A
21	1	615	LUT	C13-C14-C15-C35
24	1	619	LHG	C10-C11-C12-C13
20	7	304	CLA	C5-C6-C7-C8
20	7	313	CLA	C5-C6-C7-C8
20	A	808	CLA	C4-C3-C5-C6
20	B	821	CLA	C4-C3-C5-C6
20	B	843	CLA	C2-C3-C5-C6
20	A	835	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	O1A-CGA-O2A-C1
24	J	4004	LHG	C14-C15-C16-C17
20	G	4004	CLA	CAA-CBA-CGA-O1A
29	A	802	DGD	O1G-C1G-C2G-C3G
20	9	609	CLA	C5-C6-C7-C8
20	A	834	CLA	O1A-CGA-O2A-C1
20	A	839	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C13-C15-C16-C17
20	7	310	CLA	C16-C17-C18-C19
25	1	623	PTY	C32-C33-C34-C35
24	I	201	LHG	O6-C4-C5-O7
25	1	622	PTY	O14-C5-C6-O7
36	A	859	4RF	O21-C22-C24-C25
20	B	821	CLA	C2-C3-C5-C6
20	B	818	CLA	C15-C16-C17-C18
20	B	826	CLA	C4B-C3B-CAB-CBB
20	B	828	CLA	C4B-C3B-CAB-CBB
20	H	204	CLA	C4B-C3B-CAB-CBB
20	L	306	CLA	C4B-C3B-CAB-CBB
19	8	304	CHL	CHA-CBD-CGD-O1D
19	8	304	CHL	CHA-CBD-CGD-O2D
32	A	803	CL0	CHA-CBD-CGD-O1D
32	A	803	CL0	CHA-CBD-CGD-O2D
20	1	608	CLA	O1A-CGA-O2A-C1
24	A	854	LHG	C28-C29-C30-C31
25	H	201	PTY	O14-C5-C6-C1
26	3	421	SQD	O6-C44-C45-O47
28	7	301	LMG	O7-C8-C9-O8
29	L	311	DGD	O2G-C2G-C3G-O3G
24	7	320	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	B	818	CLA	C2-C3-C5-C6
24	F	5002	LHG	C2-C3-O3-P
20	B	833	CLA	C6-C7-C8-C10
20	9	612	CLA	CAA-CBA-CGA-O1A
20	9	612	CLA	CAA-CBA-CGA-O2A
20	7	310	CLA	C14-C13-C15-C16
20	8	311	CLA	C14-C13-C15-C16
20	A	814	CLA	C14-C13-C15-C16
20	A	832	CLA	C11-C12-C13-C14
20	B	813	CLA	C6-C7-C8-C9
20	B	819	CLA	C11-C12-C13-C14
20	B	831	CLA	C6-C7-C8-C9
26	2	619	SQD	O10-C23-C24-C25
20	A	831	CLA	C5-C6-C7-C8
26	B	851	SQD	C5-C6-S-O8
25	B	801	PTY	C13-C14-C15-C16
20	B	817	CLA	CAA-CBA-CGA-O1A
20	K	201	CLA	CAA-CBA-CGA-O1A
19	7	302	CHL	C2A-CAA-CBA-CGA
20	2	611	CLA	C2A-CAA-CBA-CGA
20	8	302	CLA	C2A-CAA-CBA-CGA
20	L	305	CLA	C2A-CAA-CBA-CGA
20	1	609	CLA	C2-C1-O2A-CGA
20	3	410	CLA	C2-C1-O2A-CGA
20	A	834	CLA	C2-C1-O2A-CGA
20	A	840	CLA	C2-C1-O2A-CGA
20	2	613	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C3A-C2A-CAA-CBA
20	B	830	CLA	C3A-C2A-CAA-CBA
20	9	605	CLA	CAA-CBA-CGA-O2A
20	A	831	CLA	C15-C16-C17-C18
28	F	5001	LMG	C10-C11-C12-C13
20	8	313	CLA	CAA-CBA-CGA-O2A
20	A	815	CLA	CAA-CBA-CGA-O2A
26	B	851	SQD	O47-C7-C8-C9
20	B	833	CLA	C5-C6-C7-C8
20	1	608	CLA	CBA-CGA-O2A-C1
22	7	317	XAT	O24-C26-C27-C28
23	A	850	BCR	C12-C13-C14-C15
23	G	4005	BCR	C12-C13-C14-C15
24	3	424	LHG	C5-C4-O6-P
20	B	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	F	5002	LHG	C4-C5-C6-O8
25	1	623	PTY	O4-C1-C6-C5
29	A	802	DGD	C1G-C2G-C3G-O3G
29	L	311	DGD	C1G-C2G-C3G-O3G
36	A	859	4RF	O42-C41-C43-C44
20	A	840	CLA	C4-C3-C5-C6
20	9	605	CLA	CAA-CBA-CGA-O1A
20	B	826	CLA	C10-C11-C12-C13
20	A	821	CLA	C15-C16-C17-C18
28	8	301	LMG	C17-C18-C19-C20
20	B	806	CLA	CBD-CGD-O2D-CED
20	1	603	CLA	C6-C7-C8-C9
20	3	407	CLA	C11-C10-C8-C9
20	8	311	CLA	C11-C12-C13-C14
20	9	602	CLA	C6-C7-C8-C9
20	A	831	CLA	C6-C7-C8-C9
20	B	806	CLA	C11-C10-C8-C9
20	B	820	CLA	C11-C10-C8-C9
20	7	315	CLA	CAA-CBA-CGA-O2A
20	9	610	CLA	CAA-CBA-CGA-O2A
20	B	843	CLA	CAA-CBA-CGA-O2A
24	A	854	LHG	O8-C23-C24-C25
24	F	5011	LHG	O6-C4-C5-C6
24	I	201	LHG	O6-C4-C5-C6
24	H	203	LHG	C17-C18-C19-C20
19	8	305	CHL	CAA-CBA-CGA-O2A
20	8	310	CLA	CAA-CBA-CGA-O2A
26	2	619	SQD	C18-C19-C20-C21
20	L	305	CLA	CBA-CGA-O2A-C1
20	A	805	CLA	C2A-CAA-CBA-CGA
20	3	402	CLA	C11-C12-C13-C15
20	8	311	CLA	C12-C13-C15-C16
20	A	816	CLA	C11-C10-C8-C7
20	A	831	CLA	C11-C12-C13-C15
20	A	832	CLA	C11-C12-C13-C15
20	A	841	CLA	C12-C13-C15-C16
20	B	831	CLA	C6-C7-C8-C10
20	B	832	CLA	C6-C7-C8-C10
20	B	834	CLA	C11-C12-C13-C15
20	L	305	CLA	O1A-CGA-O2A-C1
19	2	601	CHL	C2C-C3C-CAC-CBC
24	9	617	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	1	605	CLA	C2B-C3B-CAB-CBB
20	2	605	CLA	C2B-C3B-CAB-CBB
20	2	608	CLA	C2B-C3B-CAB-CBB
20	2	610	CLA	C2B-C3B-CAB-CBB
20	3	404	CLA	C2B-C3B-CAB-CBB
20	9	602	CLA	C2B-C3B-CAB-CBB
20	A	824	CLA	C2B-C3B-CAB-CBB
20	A	843	CLA	C2B-C3B-CAB-CBB
20	B	816	CLA	C2B-C3B-CAB-CBB
20	B	825	CLA	C2B-C3B-CAB-CBB
20	B	830	CLA	C2B-C3B-CAB-CBB
20	B	839	CLA	C2B-C3B-CAB-CBB
20	F	5005	CLA	C2B-C3B-CAB-CBB
21	3	415	LUT	C5-C6-C7-C8
23	1	617	BCR	C23-C24-C25-C26
23	3	419	BCR	C23-C24-C25-C26
23	A	848	BCR	C23-C24-C25-C26
23	B	848	BCR	C23-C24-C25-C30
23	B	849	BCR	C23-C24-C25-C26
23	B	849	BCR	C23-C24-C25-C30
23	J	4001	BCR	C23-C24-C25-C26
24	F	5002	LHG	O7-C7-C8-C9
20	3	411	CLA	C2-C1-O2A-CGA
20	8	311	CLA	C2-C1-O2A-CGA
20	9	602	CLA	C2-C1-O2A-CGA
20	A	827	CLA	C2-C1-O2A-CGA
20	B	830	CLA	C2-C1-O2A-CGA
20	K	202	CLA	C2-C1-O2A-CGA
22	7	317	XAT	C26-C27-C28-C29
30	8	320	LMK	C2-C1-O1-C7
20	8	302	CLA	C3-C5-C6-C7
20	A	823	CLA	CAA-CBA-CGA-O2A
20	B	829	CLA	CAA-CBA-CGA-O2A
25	H	202	PTY	C33-C34-C35-C36
20	1	602	CLA	C3-C5-C6-C7
29	B	850	DGD	C5A-C6A-C7A-C8A
20	A	836	CLA	CAA-CBA-CGA-O2A
20	F	5003	CLA	CAA-CBA-CGA-O2A
26	3	421	SQD	O48-C23-C24-C25
19	7	302	CHL	C2-C3-C5-C6
20	A	831	CLA	C2-C3-C5-C6
20	1	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	3	402	CLA	CAA-CBA-CGA-O2A
20	7	314	CLA	CAA-CBA-CGA-O2A
24	I	201	LHG	O7-C7-C8-C9
24	F	5002	LHG	C10-C11-C12-C13
28	7	301	LMG	O10-C28-C29-C30
20	A	807	CLA	C10-C11-C12-C13
20	A	841	CLA	C10-C11-C12-C13
20	A	828	CLA	CAA-CBA-CGA-O2A
20	B	806	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	CAA-CBA-CGA-O2A
26	3	423	SQD	C4-C5-C6-S
24	F	5002	LHG	C11-C12-C13-C14
20	A	818	CLA	C4-C3-C5-C6
25	8	317	PTY	C8-C11-C12-C13
20	9	604	CLA	CAA-CBA-CGA-O2A
27	2	620	3PH	O31-C31-C32-C33
20	B	830	CLA	O1A-CGA-O2A-C1
20	3	407	CLA	C2-C3-C5-C6
25	H	201	PTY	C20-C21-C22-C23
20	1	607	CLA	C8-C10-C11-C12
31	A	857	LMU	C5-C6-C7-C8
25	8	317	PTY	C6-C5-O14-P1
24	7	320	LHG	C7-C8-C9-C10
19	3	401	CHL	CAA-CBA-CGA-O2A
29	L	311	DGD	O1G-C1A-C2A-C3A
26	3	421	SQD	O6-C44-C45-C46
29	7	321	DGD	C1G-C2G-C3G-O3G
20	2	613	CLA	C1A-C2A-CAA-CBA
20	3	410	CLA	C1A-C2A-CAA-CBA
20	7	304	CLA	C1A-C2A-CAA-CBA
20	A	816	CLA	C1A-C2A-CAA-CBA
20	A	828	CLA	C1A-C2A-CAA-CBA
20	A	830	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	820	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C4B-C3B-CAB-CBB
20	B	830	CLA	C4B-C3B-CAB-CBB
20	3	407	CLA	C4-C3-C5-C6
20	A	830	CLA	C5-C6-C7-C8
24	I	201	LHG	O8-C23-C24-C25
27	2	620	3PH	C24-C25-C26-C27
20	A	814	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	C13-C15-C16-C17
20	A	825	CLA	CAA-CBA-CGA-O2A
20	B	830	CLA	CAA-CBA-CGA-O2A
26	3	423	SQD	O48-C23-C24-C25
20	A	816	CLA	C8-C10-C11-C12
20	B	828	CLA	C15-C16-C17-C18
19	3	401	CHL	C6-C7-C8-C9
20	9	602	CLA	C11-C12-C13-C14
20	B	838	CLA	C11-C12-C13-C15
20	B	804	CLA	CAA-CBA-CGA-O2A
24	A	853	LHG	O8-C23-C24-C25
26	3	421	SQD	O47-C7-C8-C9
28	7	319	LMG	O8-C28-C29-C30
29	7	321	DGD	O2G-C1B-C2B-C3B
26	3	423	SQD	C5-C6-S-O7
26	B	851	SQD	C5-C6-S-O7
19	7	307	CHL	C2-C1-O2A-CGA
19	8	306	CHL	C2-C1-O2A-CGA
20	1	613	CLA	C2-C1-O2A-CGA
20	A	816	CLA	C2-C1-O2A-CGA
20	A	824	CLA	C2-C1-O2A-CGA
20	1	614	CLA	CAA-CBA-CGA-O2A
20	2	611	CLA	C11-C10-C8-C7
20	3	402	CLA	C12-C13-C15-C16
20	9	607	CLA	C12-C13-C15-C16
20	A	821	CLA	C6-C7-C8-C10
20	B	819	CLA	C11-C12-C13-C15
20	B	825	CLA	C12-C13-C15-C16
20	B	820	CLA	C13-C15-C16-C17
20	B	825	CLA	O2A-C1-C2-C3
25	H	201	PTY	C5-C6-O7-C8
26	9	618	SQD	C46-C45-O47-C7
20	1	607	CLA	CAA-CBA-CGA-O2A
20	2	610	CLA	CAA-CBA-CGA-O2A
20	9	601	CLA	CAA-CBA-CGA-O2A
20	B	829	CLA	CAA-CBA-CGA-O1A
24	3	424	LHG	C11-C12-C13-C14
24	B	852	LHG	C2-C3-O3-P
25	H	202	PTY	C6-C5-O14-P1
20	1	612	CLA	C3A-C2A-CAA-CBA
20	2	604	CLA	C3A-C2A-CAA-CBA
20	7	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	8	310	CLA	C3A-C2A-CAA-CBA
20	A	810	CLA	C3A-C2A-CAA-CBA
20	A	814	CLA	C3A-C2A-CAA-CBA
20	A	843	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA
20	B	815	CLA	C3A-C2A-CAA-CBA
20	B	822	CLA	C3A-C2A-CAA-CBA
19	8	305	CHL	CAA-CBA-CGA-O1A
24	7	320	LHG	O10-C23-C24-C25
20	B	819	CLA	C13-C15-C16-C17
20	B	839	CLA	CAA-CBA-CGA-O2A
24	3	424	LHG	O8-C23-C24-C25
20	B	824	CLA	C2-C3-C5-C6
20	B	806	CLA	CAA-CBA-CGA-O1A
20	B	841	CLA	CAA-CBA-CGA-O1A
20	F	5003	CLA	CAA-CBA-CGA-O1A
19	7	302	CHL	C6-C7-C8-C9
20	B	803	CLA	C14-C13-C15-C16
20	B	822	CLA	C11-C12-C13-C14
24	F	5002	LHG	O9-C7-C8-C9
25	H	201	PTY	C13-C14-C15-C16
28	8	301	LMG	C11-C12-C13-C14
24	A	854	LHG	C11-C12-C13-C14
29	L	311	DGD	C7A-C8A-C9A-CAA
20	3	402	CLA	CAA-CBA-CGA-O1A
24	I	201	LHG	O9-C7-C8-C9
26	3	423	SQD	O5-C5-C6-S
20	7	314	CLA	CAA-CBA-CGA-O1A
20	7	315	CLA	CAA-CBA-CGA-O1A
20	A	836	CLA	CAA-CBA-CGA-O1A
26	3	423	SQD	O10-C23-C24-C25
20	A	809	CLA	C10-C11-C12-C13
20	H	204	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	C15-C16-C17-C18
19	3	401	CHL	CAA-CBA-CGA-O1A
20	9	610	CLA	CAA-CBA-CGA-O1A
20	B	804	CLA	CAA-CBA-CGA-O1A
20	B	814	CLA	CAA-CBA-CGA-O1A
20	B	843	CLA	CAA-CBA-CGA-O1A
20	1	603	CLA	CAA-CBA-CGA-O1A
20	8	310	CLA	CAA-CBA-CGA-O1A
20	9	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	A	854	LHG	O10-C23-C24-C25
24	I	201	LHG	O10-C23-C24-C25
26	3	421	SQD	O10-C23-C24-C25
28	7	319	LMG	O10-C28-C29-C30
20	F	5008	CLA	CAA-CBA-CGA-O2A
24	G	4006	LHG	O7-C7-C8-C9
25	1	623	PTY	O4-C30-C31-C32
24	A	853	LHG	O10-C23-C24-C25
20	A	839	CLA	C5-C6-C7-C8
20	3	408	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	C2-C3-C5-C6
20	1	614	CLA	CAA-CBA-CGA-O1A
20	A	823	CLA	CAA-CBA-CGA-O1A
20	A	828	CLA	CAA-CBA-CGA-O1A
27	2	620	3PH	O32-C31-C32-C33
20	1	614	CLA	CAD-CBD-CGD-O2D
20	7	303	CLA	CAD-CBD-CGD-O2D
20	9	603	CLA	CAD-CBD-CGD-O2D
20	A	814	CLA	CAD-CBD-CGD-O2D
20	B	808	CLA	CAD-CBD-CGD-O2D
20	B	827	CLA	CAD-CBD-CGD-O2D
20	B	831	CLA	CAD-CBD-CGD-O2D
24	H	203	LHG	O8-C23-C24-C25
29	L	311	DGD	O2G-C1B-C2B-C3B
29	L	311	DGD	O1A-C1A-C2A-C3A
20	B	821	CLA	C13-C15-C16-C17
20	A	828	CLA	C8-C10-C11-C12
20	B	834	CLA	C2-C1-O2A-CGA
20	B	830	CLA	CAA-CBA-CGA-O1A
20	3	410	CLA	CAA-CBA-CGA-O2A
20	B	842	CLA	CAA-CBA-CGA-O2A
19	7	302	CHL	C1-C2-C3-C4
20	A	825	CLA	CAA-CBA-CGA-O1A
24	3	424	LHG	O10-C23-C24-C25
20	B	812	CLA	C4-C3-C5-C6
20	B	807	CLA	CAA-CBA-CGA-O2A
25	H	201	PTY	C12-C11-C8-O7
29	7	321	DGD	O1B-C1B-C2B-C3B
20	3	404	CLA	CAA-CBA-CGA-O2A
20	G	4002	CLA	CAA-CBA-CGA-O2A
20	L	306	CLA	CAA-CBA-CGA-O2A
24	1	621	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
28	8	301	LMG	O8-C28-C29-C30
28	7	301	LMG	C18-C19-C20-C21
20	1	605	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

258 monomers are involved in 706 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	856	LMU	2	0
23	B	847	BCR	5	0
25	H	201	PTY	4	0
20	8	313	CLA	1	0
20	A	838	CLA	4	0
33	B	844	PQN	4	0
23	A	848	BCR	7	0
20	7	312	CLA	2	0
20	A	816	CLA	7	0
20	1	610	CLA	2	0
20	A	811	CLA	3	0
20	A	810	CLA	2	0
20	A	812	CLA	12	0
20	B	816	CLA	1	0
20	F	5006	CLA	3	0
21	9	613	LUT	4	0
23	B	848	BCR	3	0
24	H	203	LHG	2	0
23	J	4001	BCR	7	0
29	L	311	DGD	4	0
20	B	803	CLA	3	0
20	B	835	CLA	2	0
20	B	838	CLA	4	0
20	A	837	CLA	4	0
20	A	828	CLA	5	0
24	7	323	LHG	1	0
20	7	314	CLA	3	0
20	F	5007	CLA	1	0
20	A	814	CLA	4	0
20	F	5008	CLA	3	0
20	2	604	CLA	1	0
20	B	832	CLA	5	0
20	B	817	CLA	2	0
20	L	305	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	601	CHL	4	0
20	L	302	CLA	3	0
20	A	813	CLA	3	0
24	2	621	LHG	3	0
20	9	605	CLA	2	0
20	B	820	CLA	4	0
20	B	809	CLA	6	0
20	1	613	CLA	1	0
20	A	842	CLA	4	0
20	B	837	CLA	1	0
23	B	802	BCR	7	0
20	3	404	CLA	1	0
20	1	614	CLA	1	0
20	9	603	CLA	2	0
24	1	621	LHG	2	0
20	L	304	CLA	5	0
20	1	603	CLA	3	0
20	3	402	CLA	2	0
26	2	619	SQD	3	0
22	8	315	XAT	3	0
24	1	619	LHG	1	0
24	7	325	LHG	2	0
20	1	612	CLA	2	0
22	9	614	XAT	5	0
24	3	424	LHG	2	0
20	B	840	CLA	6	0
20	B	812	CLA	2	0
28	A	801	LMG	2	0
20	B	819	CLA	8	0
31	9	616	LMU	4	0
20	A	823	CLA	2	0
20	B	836	CLA	1	0
20	B	821	CLA	7	0
21	1	615	LUT	7	0
20	2	608	CLA	4	0
20	9	607	CLA	2	0
20	3	406	CLA	2	0
20	8	303	CLA	3	0
20	B	843	CLA	6	0
20	K	202	CLA	4	0
20	A	839	CLA	1	0
20	F	5005	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	827	CLA	6	0
28	7	319	LMG	2	0
33	A	845	PQN	1	0
19	8	306	CHL	1	0
22	9	615	XAT	4	0
23	F	5009	BCR	4	0
29	A	802	DGD	4	0
23	A	851	BCR	8	0
20	2	609	CLA	1	0
26	3	423	SQD	1	0
32	A	803	CL0	8	0
20	A	805	CLA	10	0
20	A	829	CLA	3	0
20	A	831	CLA	8	0
21	7	316	LUT	2	0
20	B	822	CLA	4	0
20	A	832	CLA	7	0
20	3	403	CLA	1	0
20	1	607	CLA	3	0
20	7	305	CLA	1	0
22	3	416	XAT	3	0
20	1	609	CLA	3	0
29	7	321	DGD	4	0
23	A	850	BCR	5	0
24	1	620	LHG	1	0
26	3	421	SQD	5	0
21	3	415	LUT	2	0
20	B	828	CLA	4	0
20	B	839	CLA	1	0
20	K	201	CLA	1	0
23	1	617	BCR	2	0
20	B	824	CLA	10	0
24	1	618	LHG	1	0
20	L	301	CLA	1	0
23	G	4001	BCR	3	0
25	1	623	PTY	1	0
20	9	602	CLA	6	0
24	2	618	LHG	1	0
19	1	601	CHL	5	0
20	G	4004	CLA	3	0
20	A	830	CLA	6	0
20	J	4002	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	610	CLA	2	0
20	A	819	CLA	5	0
20	A	844	CLA	2	0
20	B	826	CLA	3	0
21	2	616	LUT	10	0
19	3	401	CHL	6	0
20	A	821	CLA	5	0
19	8	304	CHL	7	0
20	7	304	CLA	1	0
20	B	829	CLA	2	0
20	K	203	CLA	5	0
23	F	5004	BCR	5	0
23	I	202	BCR	3	0
28	8	301	LMG	5	0
20	8	310	CLA	2	0
20	A	841	CLA	7	0
23	K	205	BCR	5	0
20	A	826	CLA	1	0
23	J	4003	BCR	3	0
23	L	303	BCR	5	0
24	8	321	LHG	2	0
20	B	834	CLA	7	0
20	7	310	CLA	2	0
31	A	857	LMU	1	0
20	A	840	CLA	5	0
20	A	806	CLA	2	0
20	8	302	CLA	4	0
23	L	308	BCR	4	0
19	7	302	CHL	4	0
20	7	311	CLA	1	0
24	8	319	LHG	1	0
24	F	5011	LHG	2	0
20	9	611	CLA	2	0
20	3	412	CLA	2	0
20	9	608	CLA	2	0
20	B	807	CLA	5	0
22	7	317	XAT	6	0
24	F	5002	LHG	4	0
20	7	313	CLA	5	0
24	J	4004	LHG	1	0
36	A	859	4RF	2	0
34	C	101	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	4006	LHG	3	0
20	B	825	CLA	5	0
19	9	606	CHL	4	0
20	B	830	CLA	4	0
20	2	611	CLA	2	0
23	A	847	BCR	4	0
23	3	419	BCR	5	0
19	7	306	CHL	3	0
23	B	846	BCR	4	0
27	2	620	3PH	4	0
20	A	833	CLA	4	0
20	A	835	CLA	6	0
26	B	851	SQD	1	0
34	C	102	SF4	1	0
20	9	601	CLA	1	0
20	A	824	CLA	4	0
20	A	825	CLA	6	0
20	7	324	CLA	3	0
23	L	309	BCR	1	0
20	A	809	CLA	4	0
20	B	804	CLA	11	0
20	B	815	CLA	1	0
20	B	808	CLA	5	0
26	9	618	SQD	1	0
20	1	611	CLA	3	0
20	3	405	CLA	2	0
20	3	411	CLA	3	0
20	8	309	CLA	3	0
34	A	846	SF4	4	0
19	8	305	CHL	2	0
20	A	820	CLA	7	0
23	3	418	BCR	5	0
23	A	849	BCR	12	0
20	2	602	CLA	4	0
20	B	813	CLA	9	0
20	2	613	CLA	1	0
23	B	849	BCR	6	0
23	G	4005	BCR	2	0
20	A	808	CLA	7	0
23	B	845	BCR	2	0
25	H	202	PTY	2	0
19	7	308	CHL	5	0

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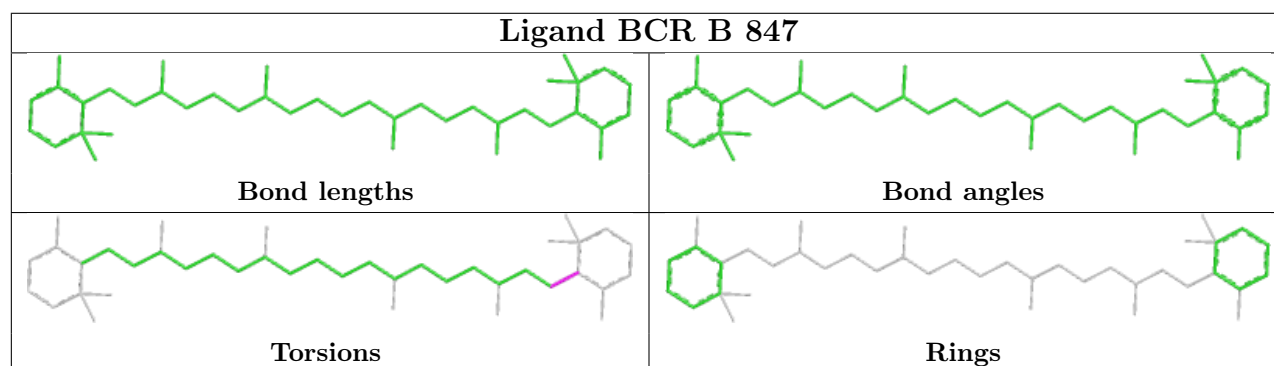
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	B	831	CLA	6	0
20	1	602	CLA	3	0
20	3	408	CLA	2	0
20	B	818	CLA	4	0
20	1	605	CLA	3	0
20	3	407	CLA	8	0
28	F	5001	LMG	3	0
28	7	301	LMG	2	0
20	F	5003	CLA	1	0
24	9	619	LHG	3	0
20	2	607	CLA	1	0
20	A	807	CLA	2	0
20	1	608	CLA	5	0
20	G	4003	CLA	1	0
23	8	316	BCR	4	0
19	7	307	CHL	7	0
20	A	817	CLA	3	0
20	A	822	CLA	5	0
20	B	810	CLA	2	0
20	B	842	CLA	3	0
21	2	615	LUT	4	0
20	A	834	CLA	4	0
24	A	854	LHG	2	0
20	9	612	CLA	3	0
23	A	852	BCR	7	0
23	A	858	BCR	6	0
20	A	836	CLA	6	0
20	K	204	CLA	1	0
20	7	303	CLA	3	0
20	8	311	CLA	4	0
20	2	603	CLA	10	0
20	3	414	CLA	2	0
20	A	804	CLA	6	0
20	A	815	CLA	5	0
24	9	617	LHG	1	0
20	A	827	CLA	12	0
20	B	841	CLA	4	0
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20	A	818	CLA	7	0
22	1	616	XAT	2	0
24	7	320	LHG	3	0

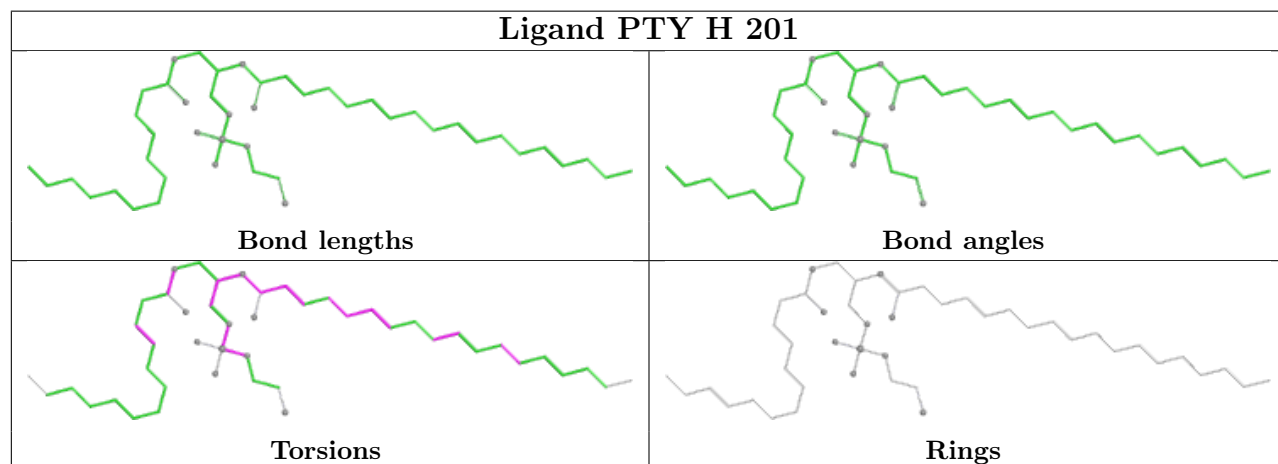
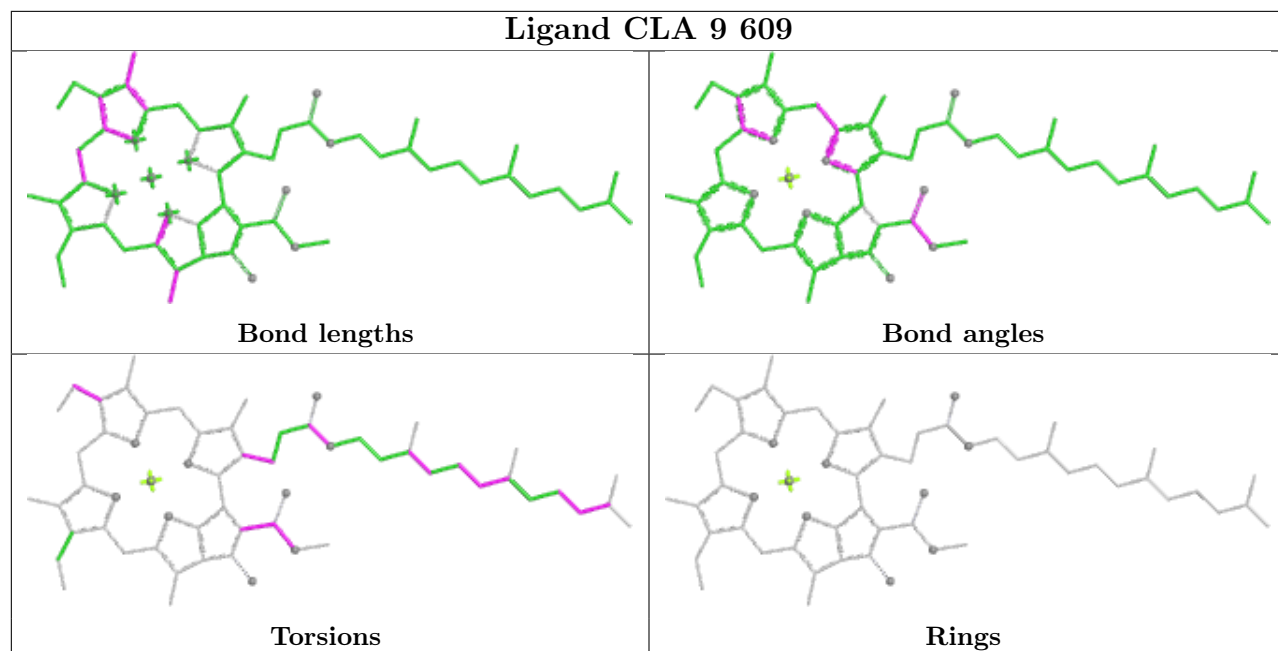
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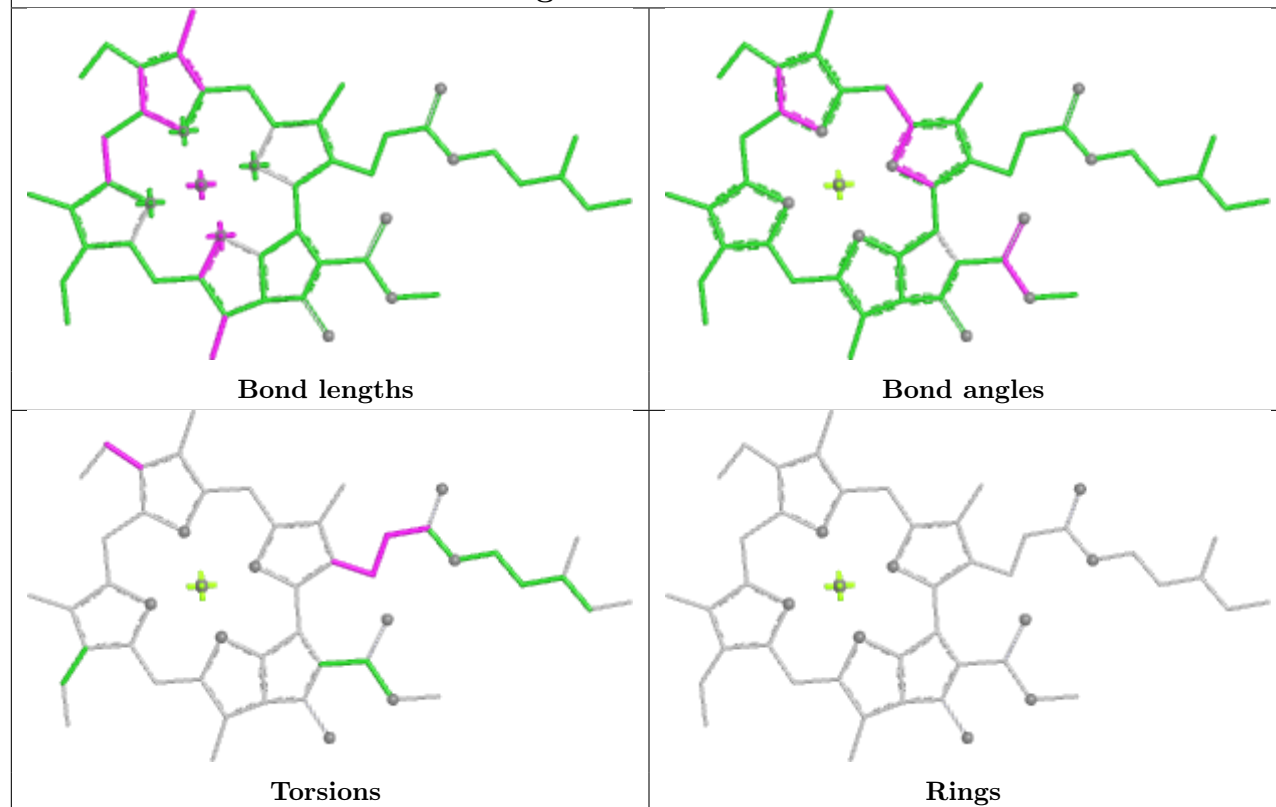
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	823	CLA	3	0
19	2	606	CHL	4	0
20	1	604	CLA	2	0
20	9	604	CLA	1	0
29	B	850	DGD	8	0
20	B	806	CLA	3	0
21	2	617	LUT	1	0
23	7	318	BCR	4	0
20	8	307	CLA	1	0
20	B	811	CLA	3	0
25	1	622	PTY	2	0
20	B	805	CLA	2	0
24	A	853	LHG	2	0
19	1	606	CHL	3	0

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.

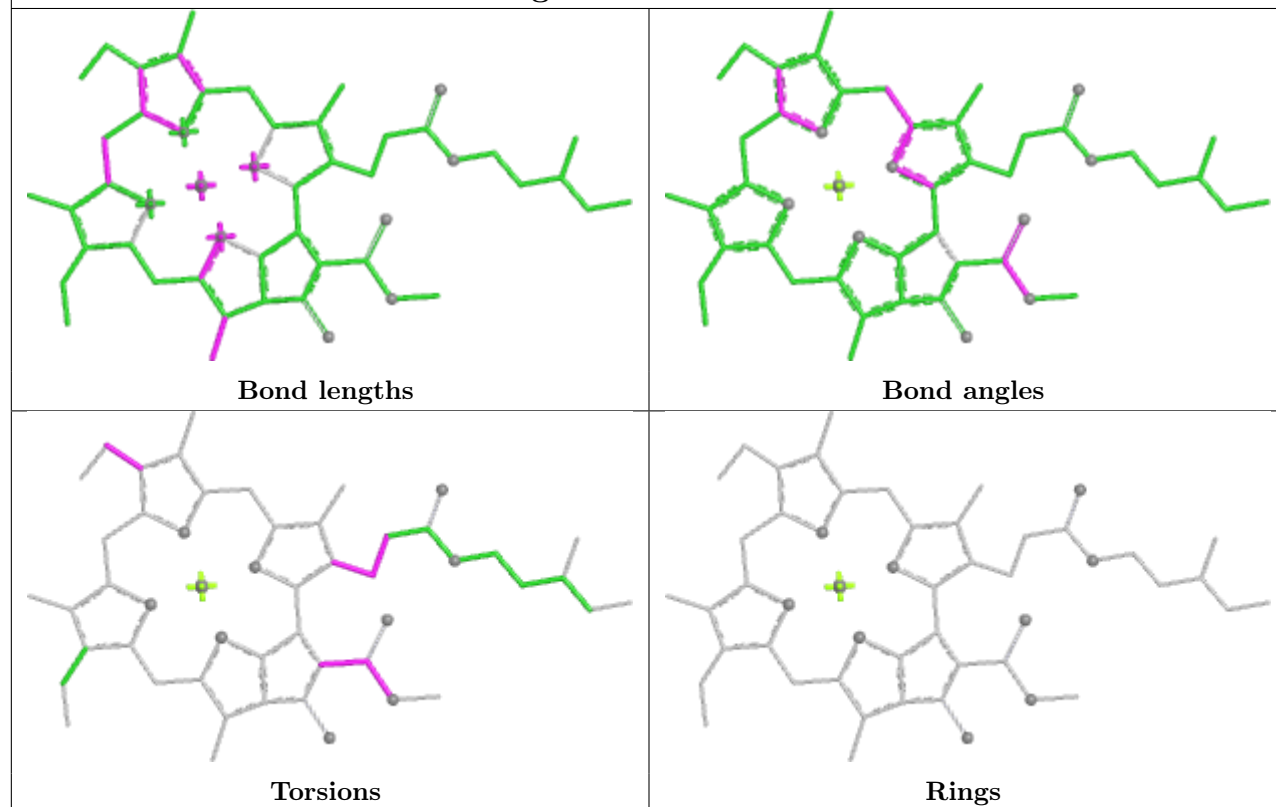


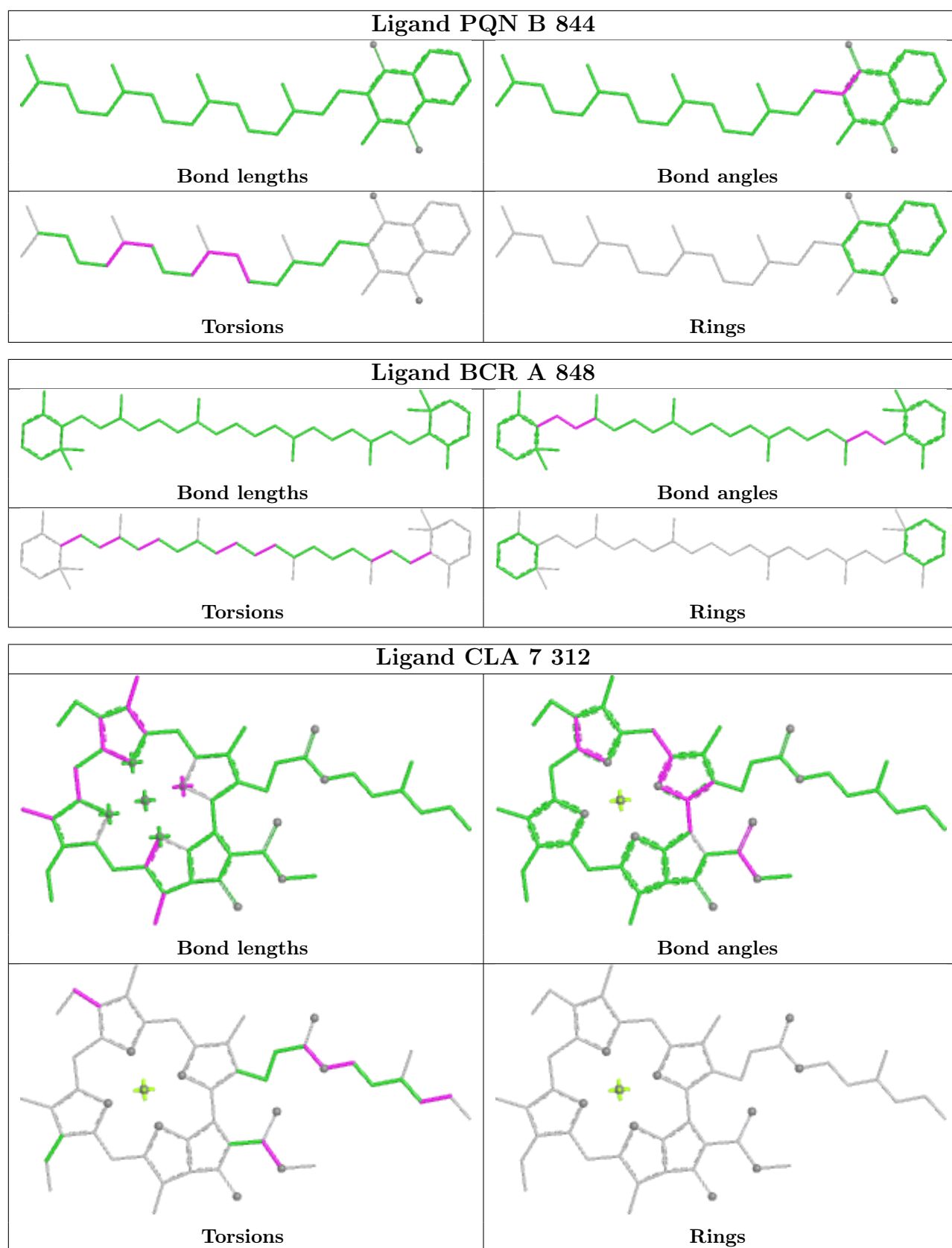


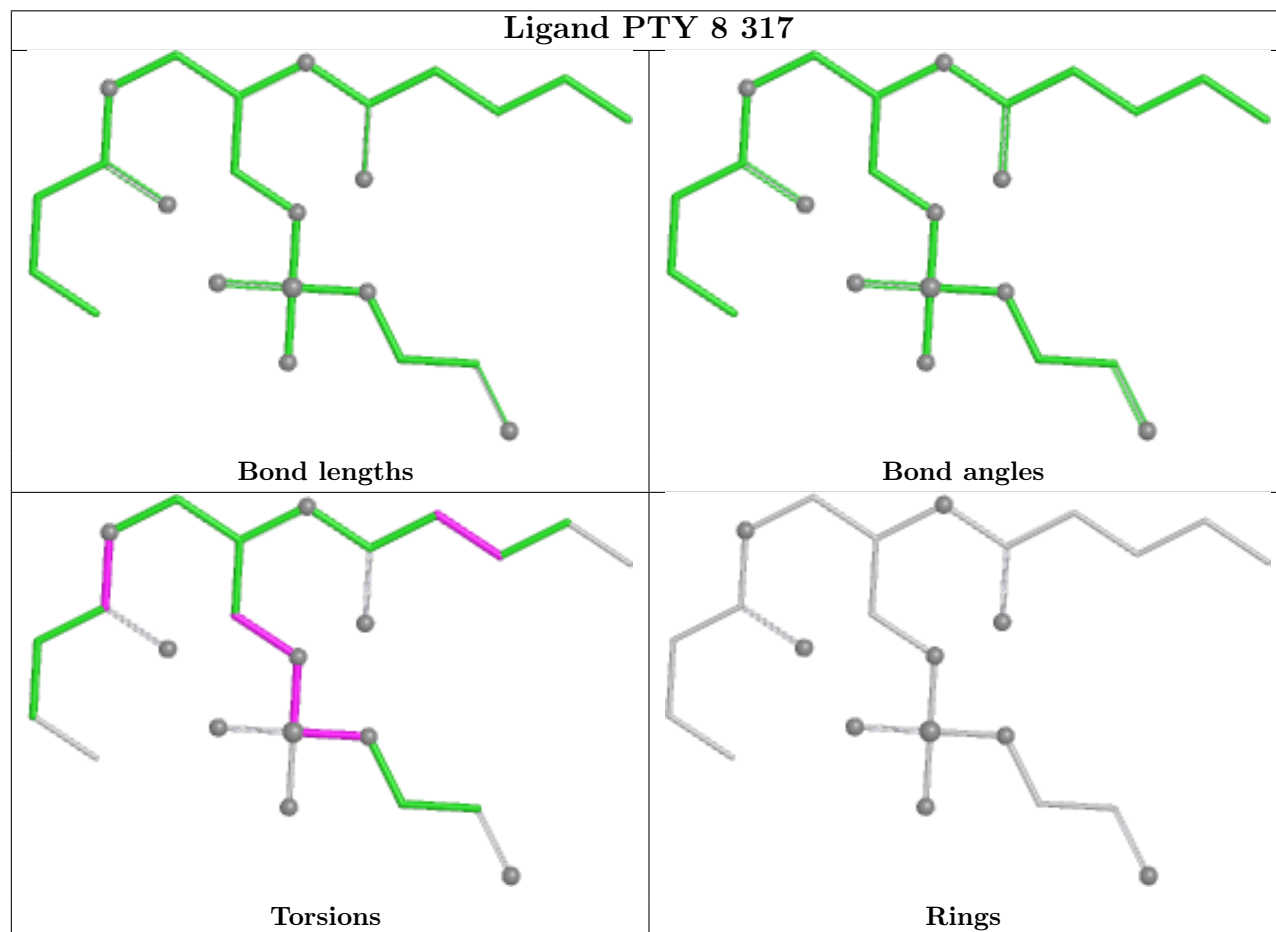
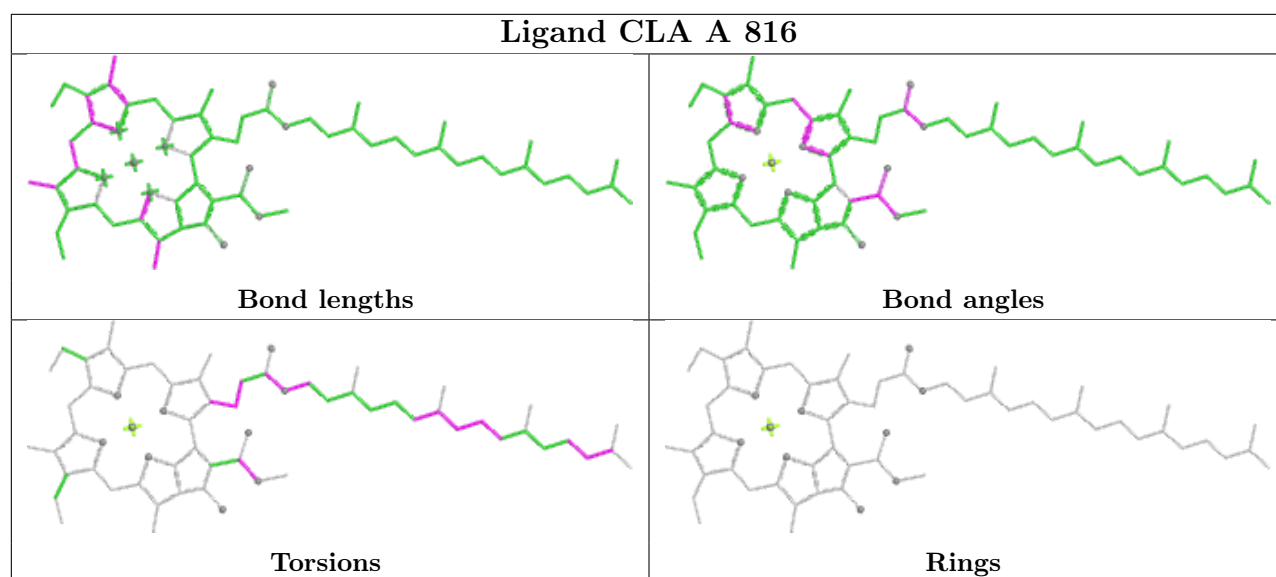
Ligand CLA 8 313



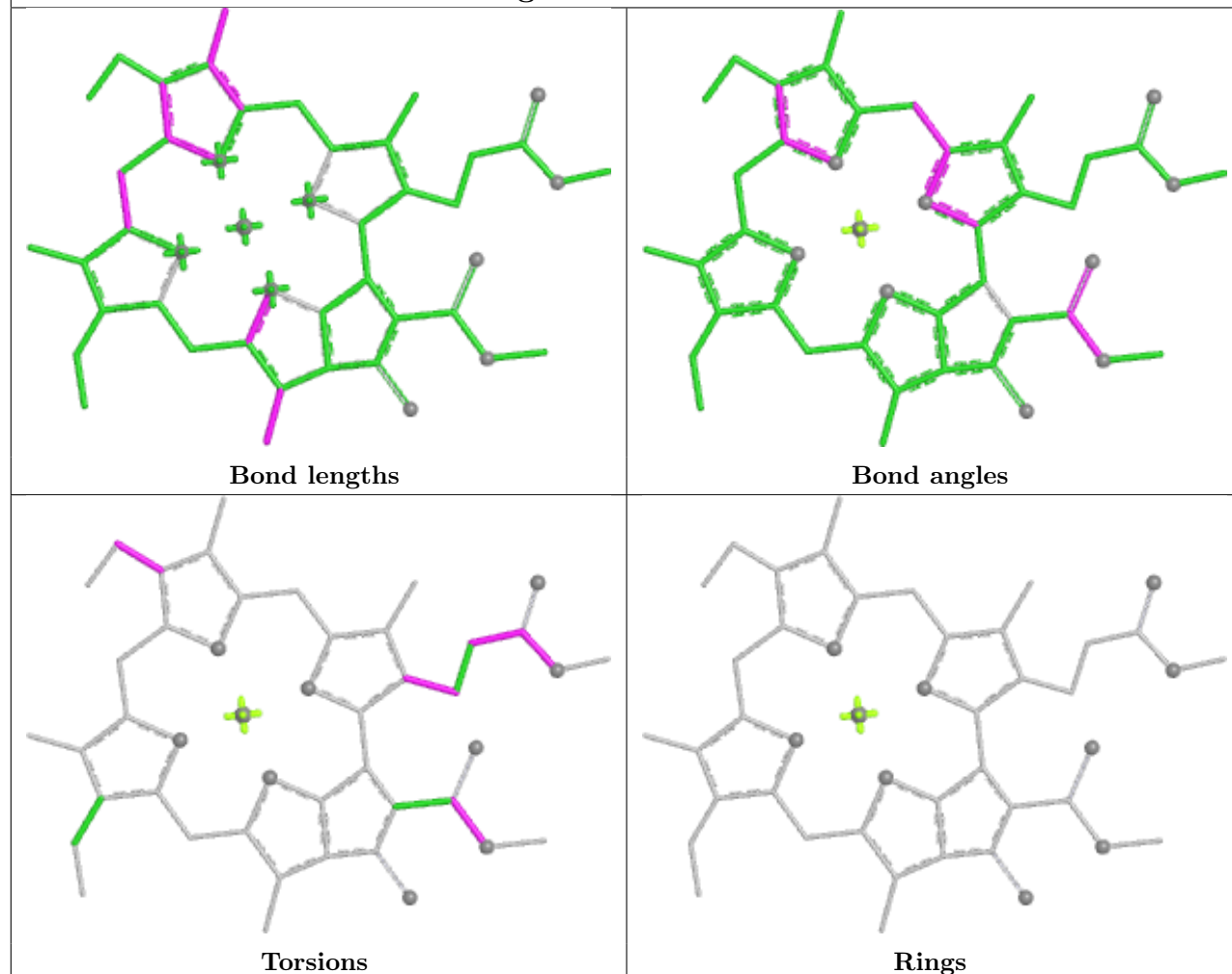
Ligand CLA A 838



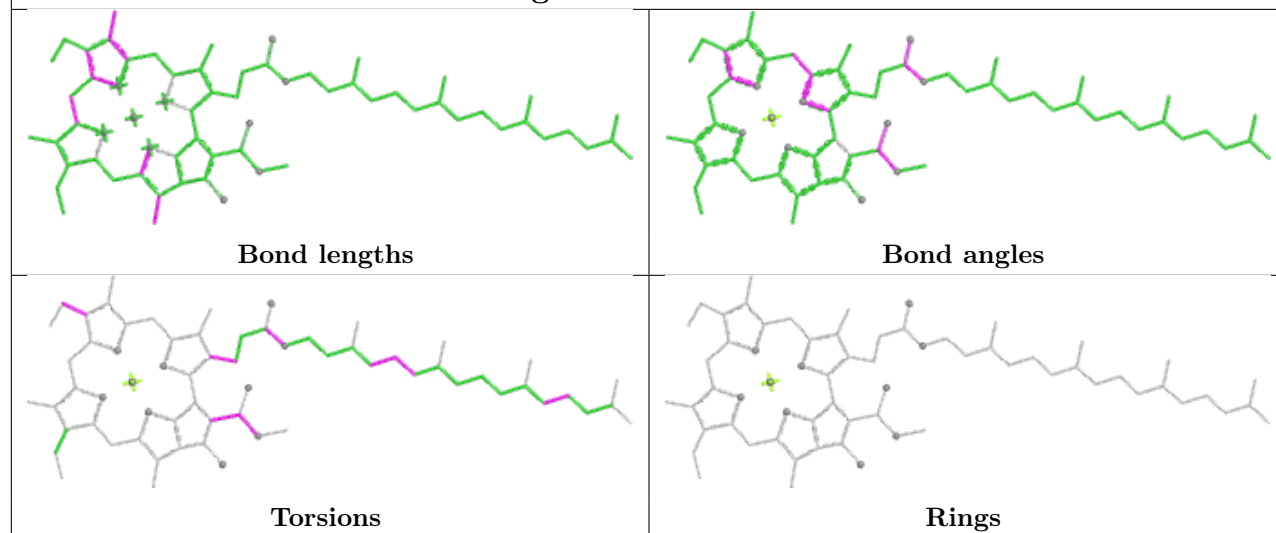


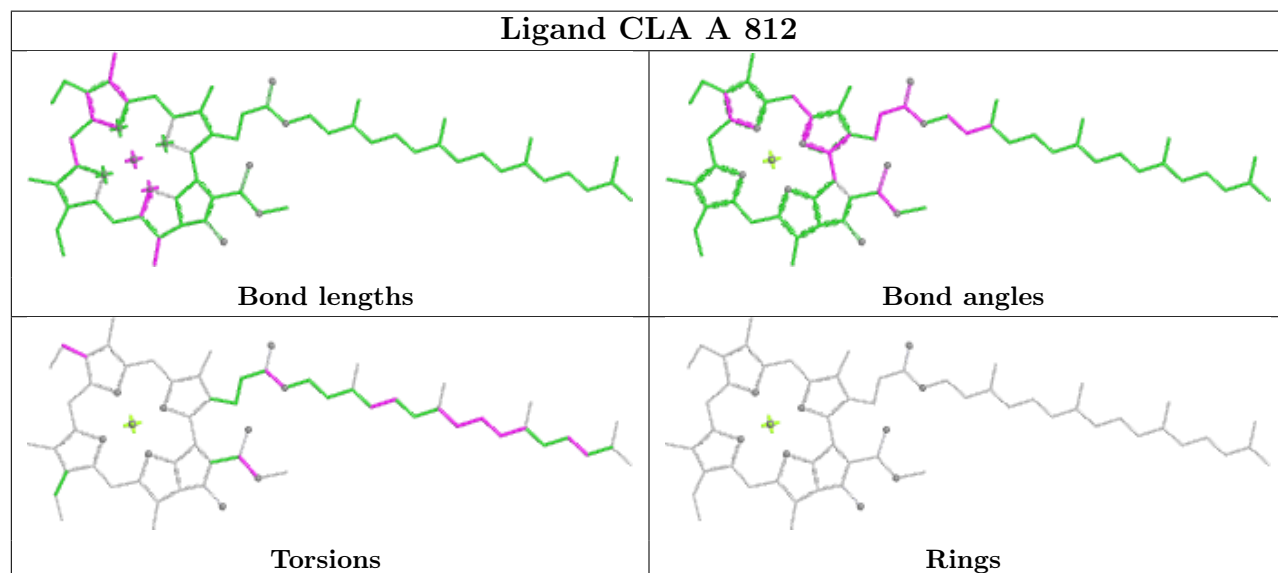
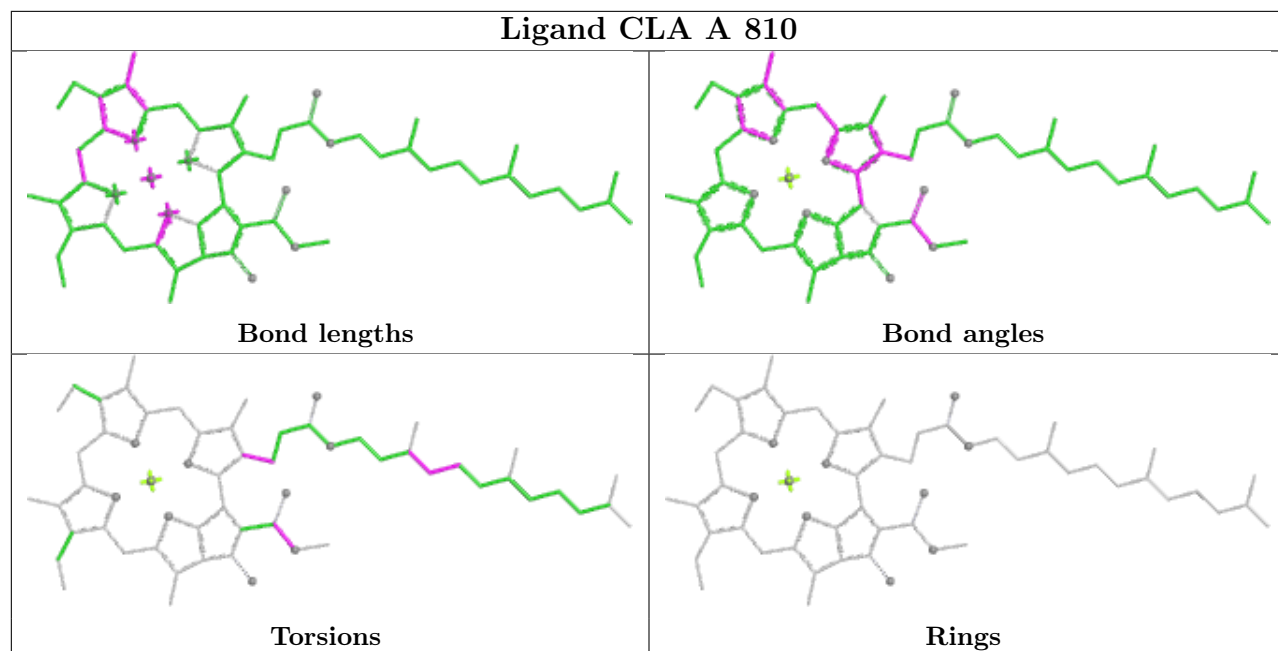


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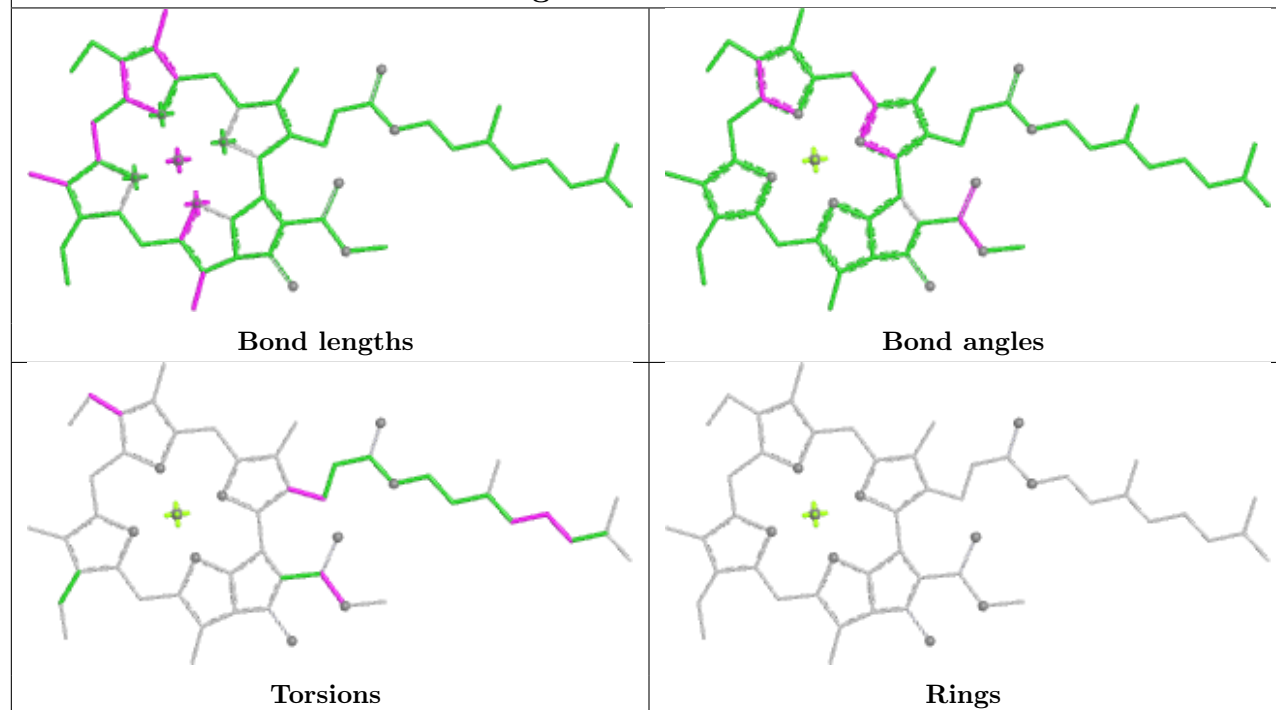


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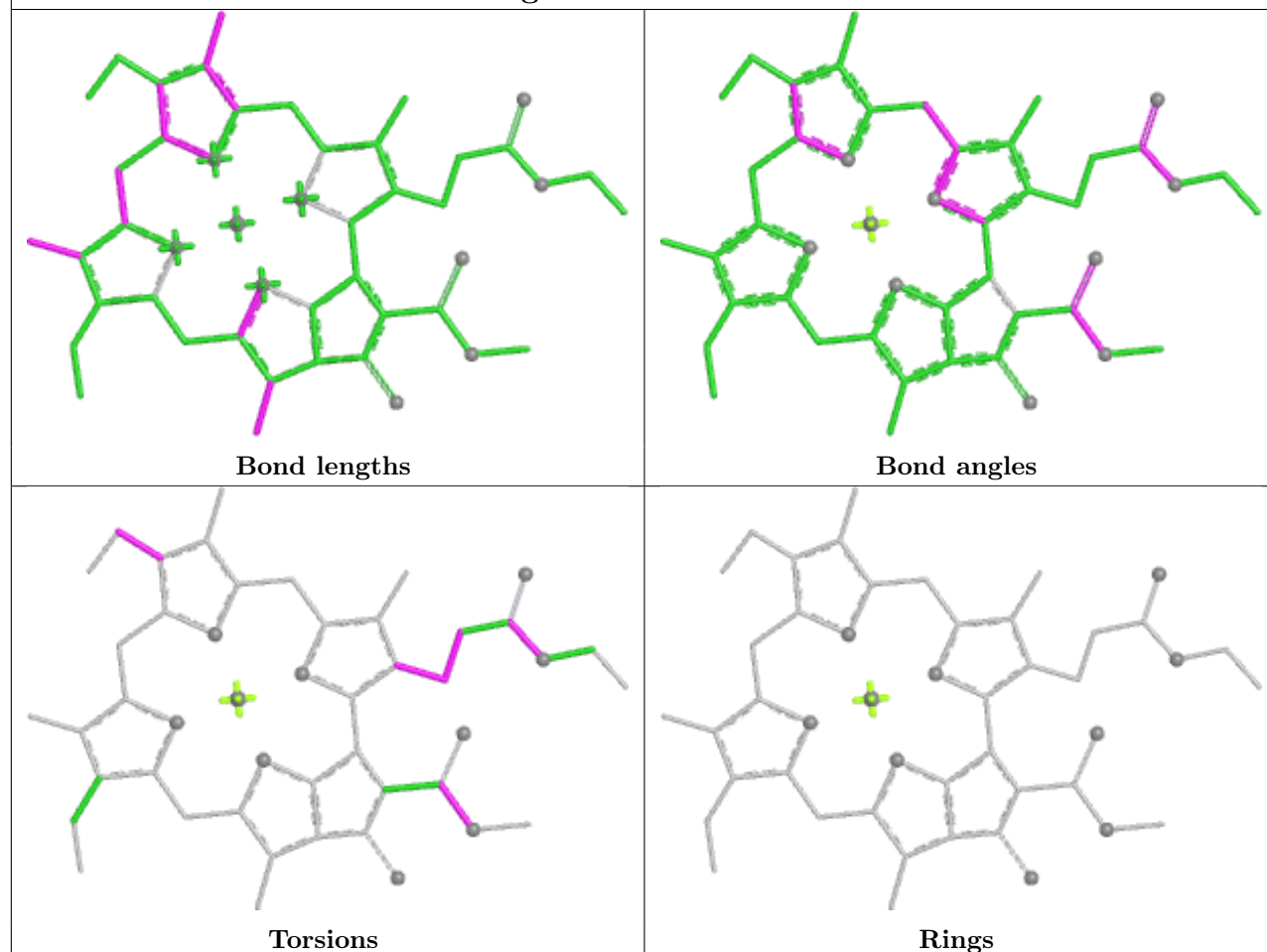


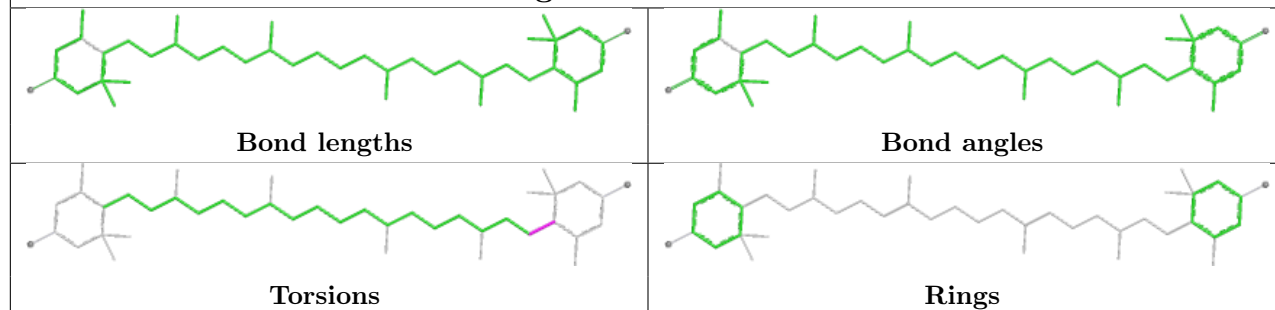
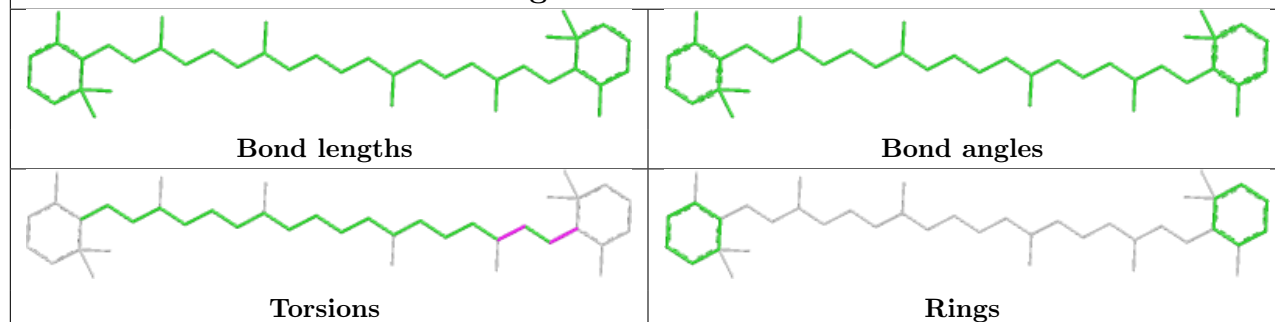
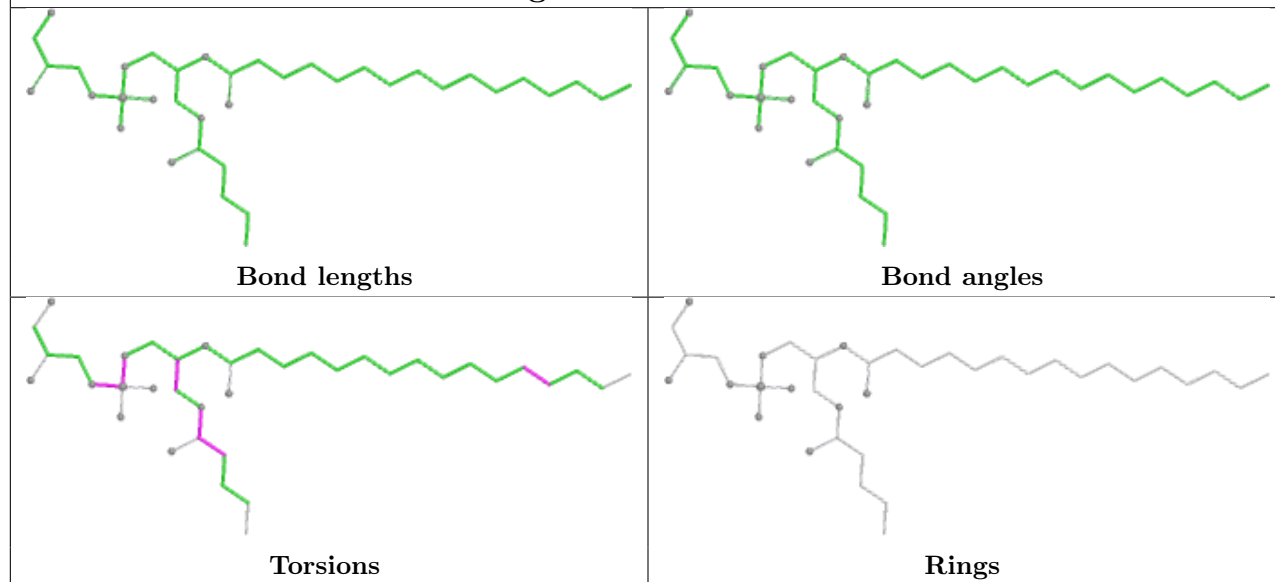
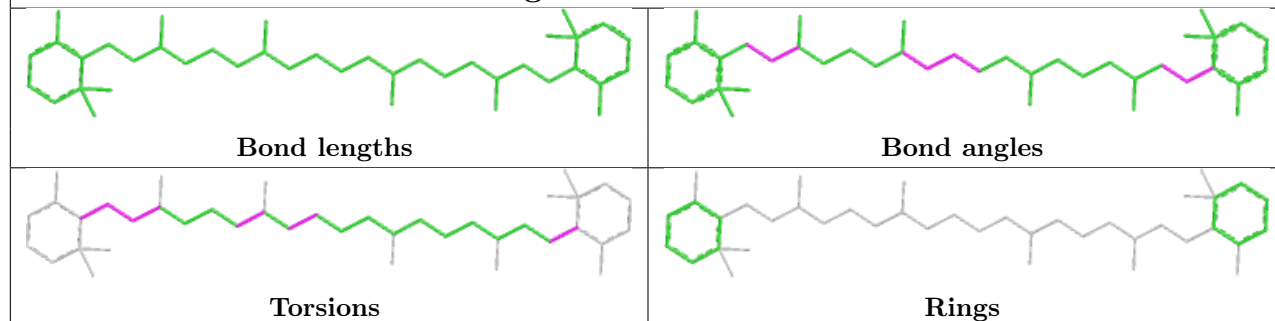


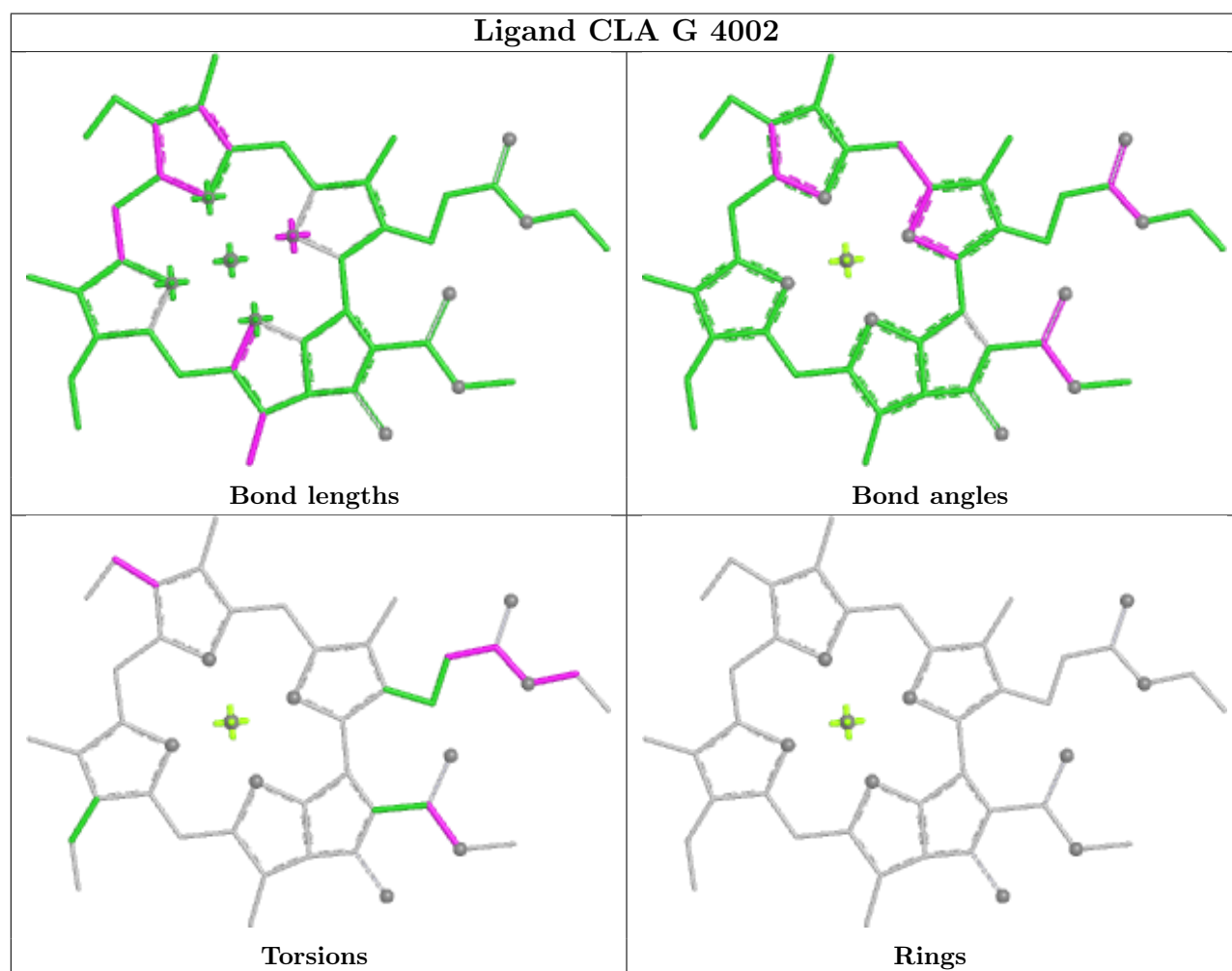
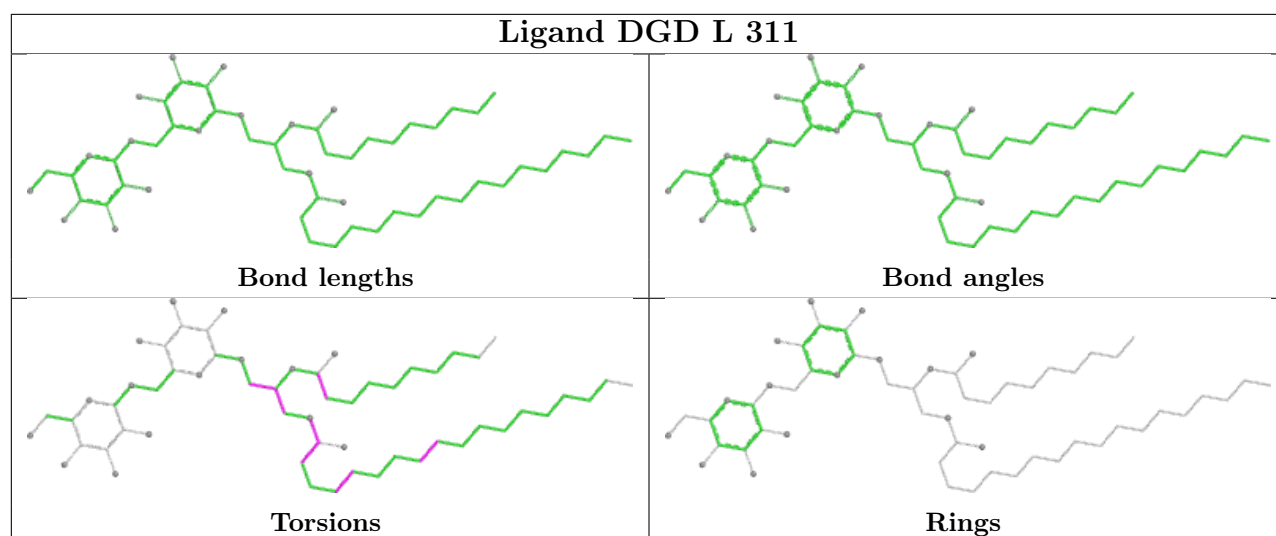
Ligand CLA B 816

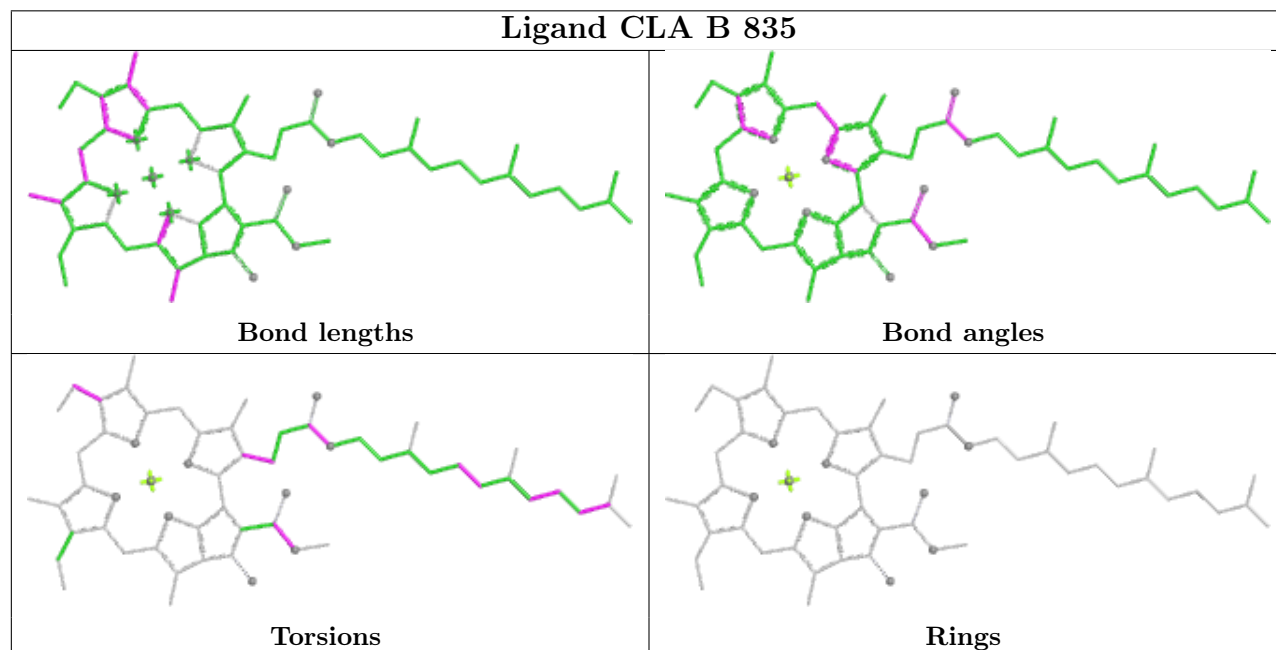
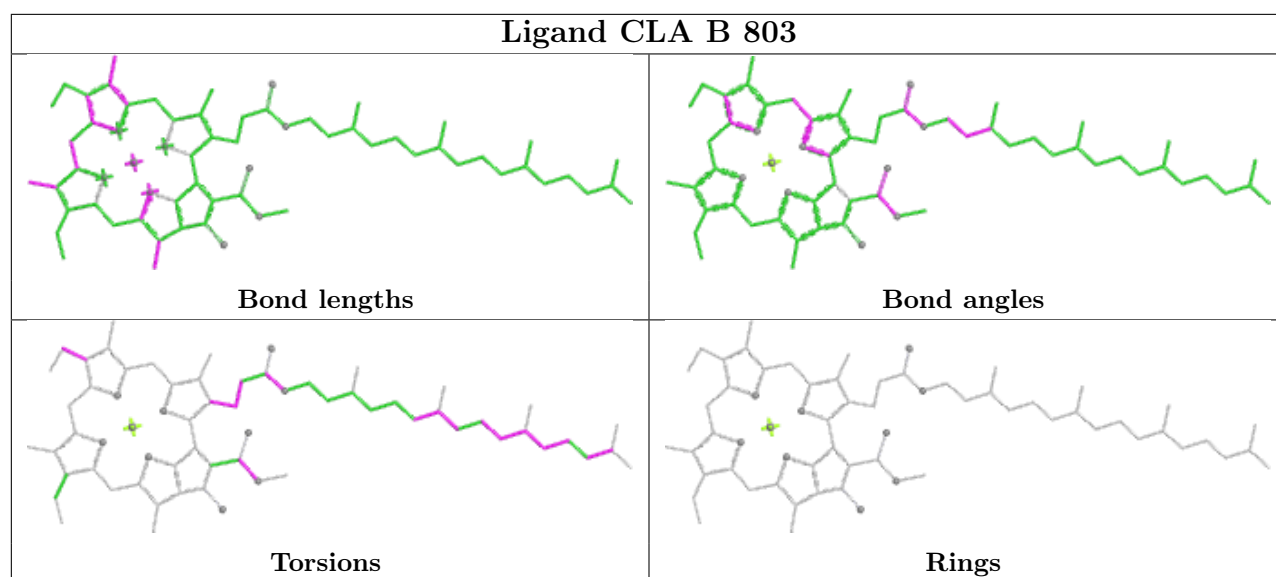


Ligand CLA F 5006

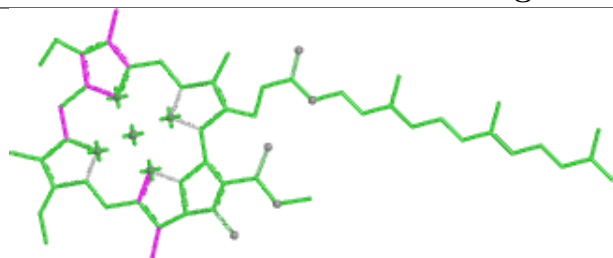


Ligand LUT 9 613**Ligand BCR B 848****Ligand LHG H 203****Ligand BCR J 4001**

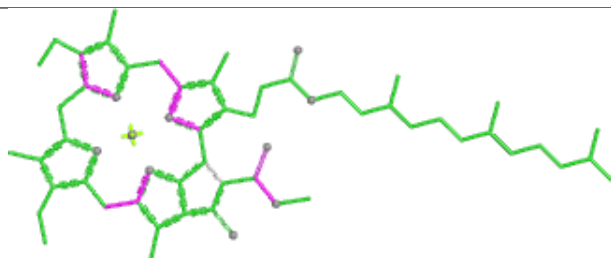




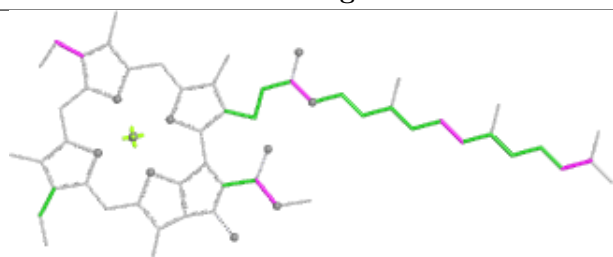
Ligand CLA B 838



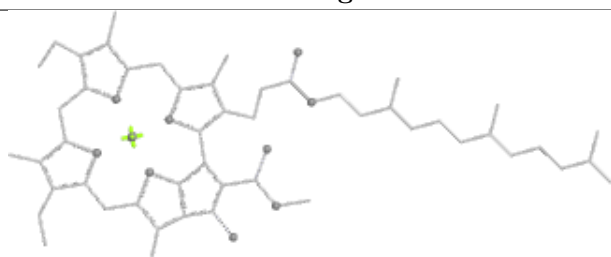
Bond lengths



Bond angles

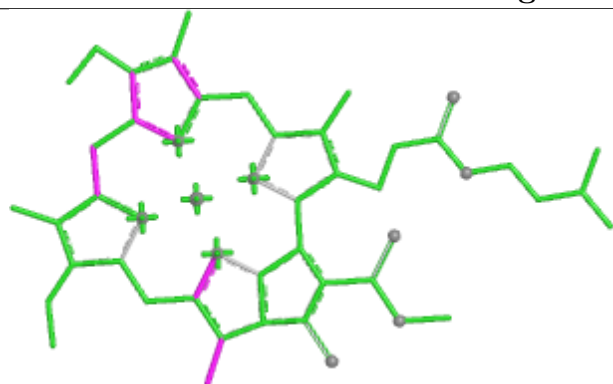


Torsions

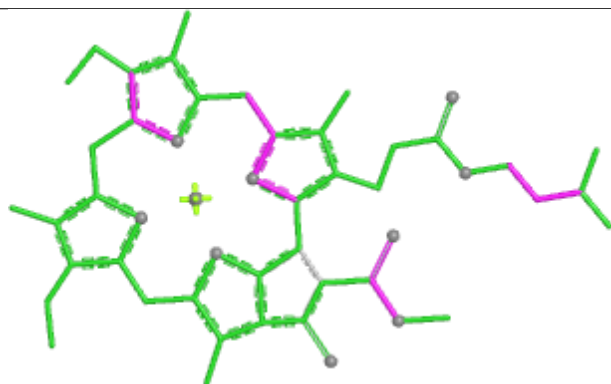


Rings

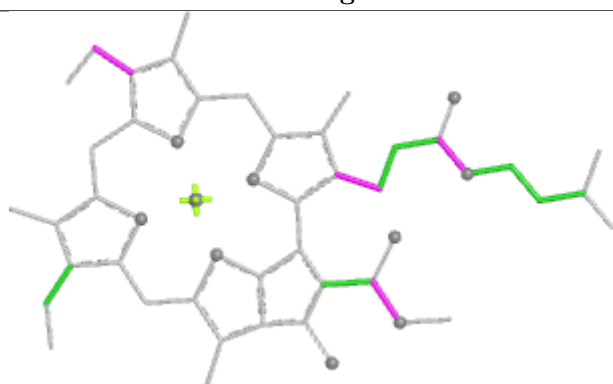
Ligand CLA 3 409



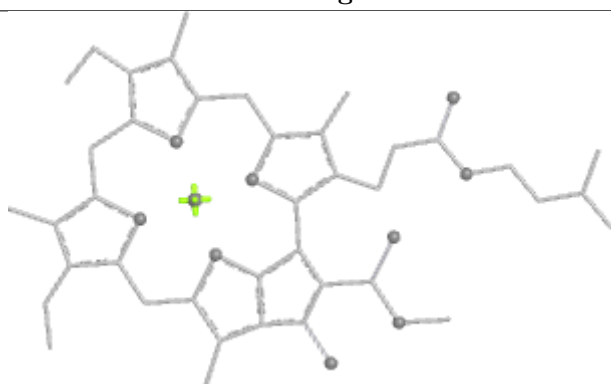
Bond lengths



Bond angles

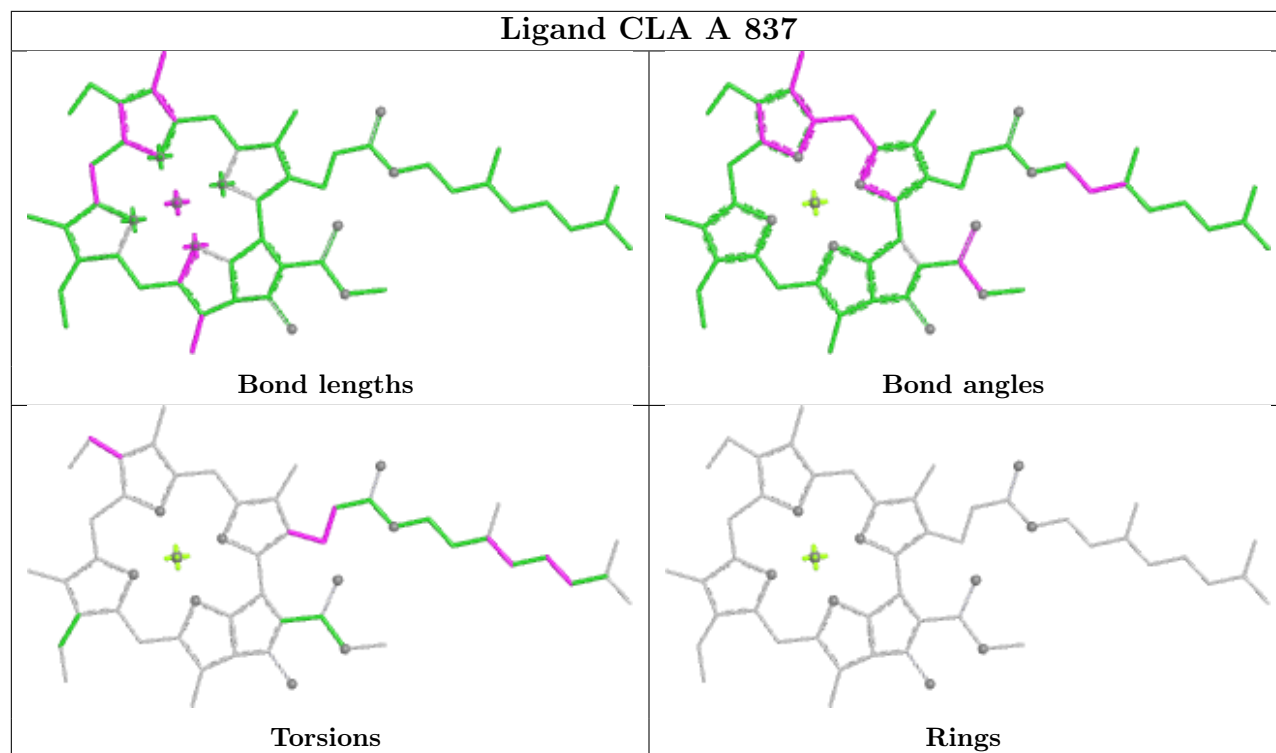


Torsions

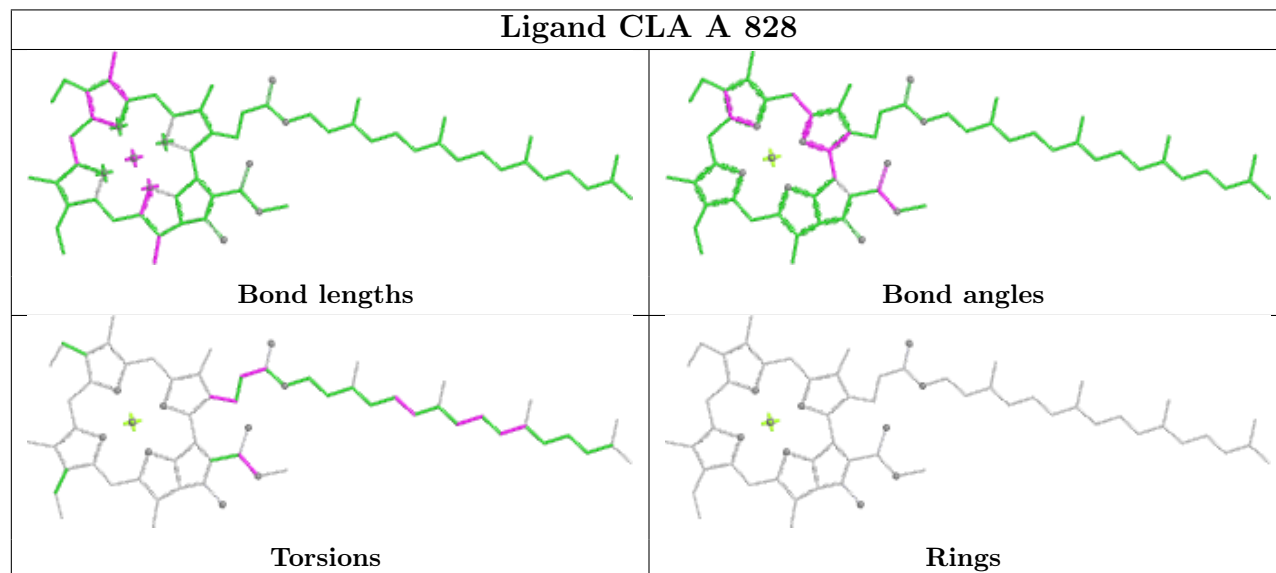


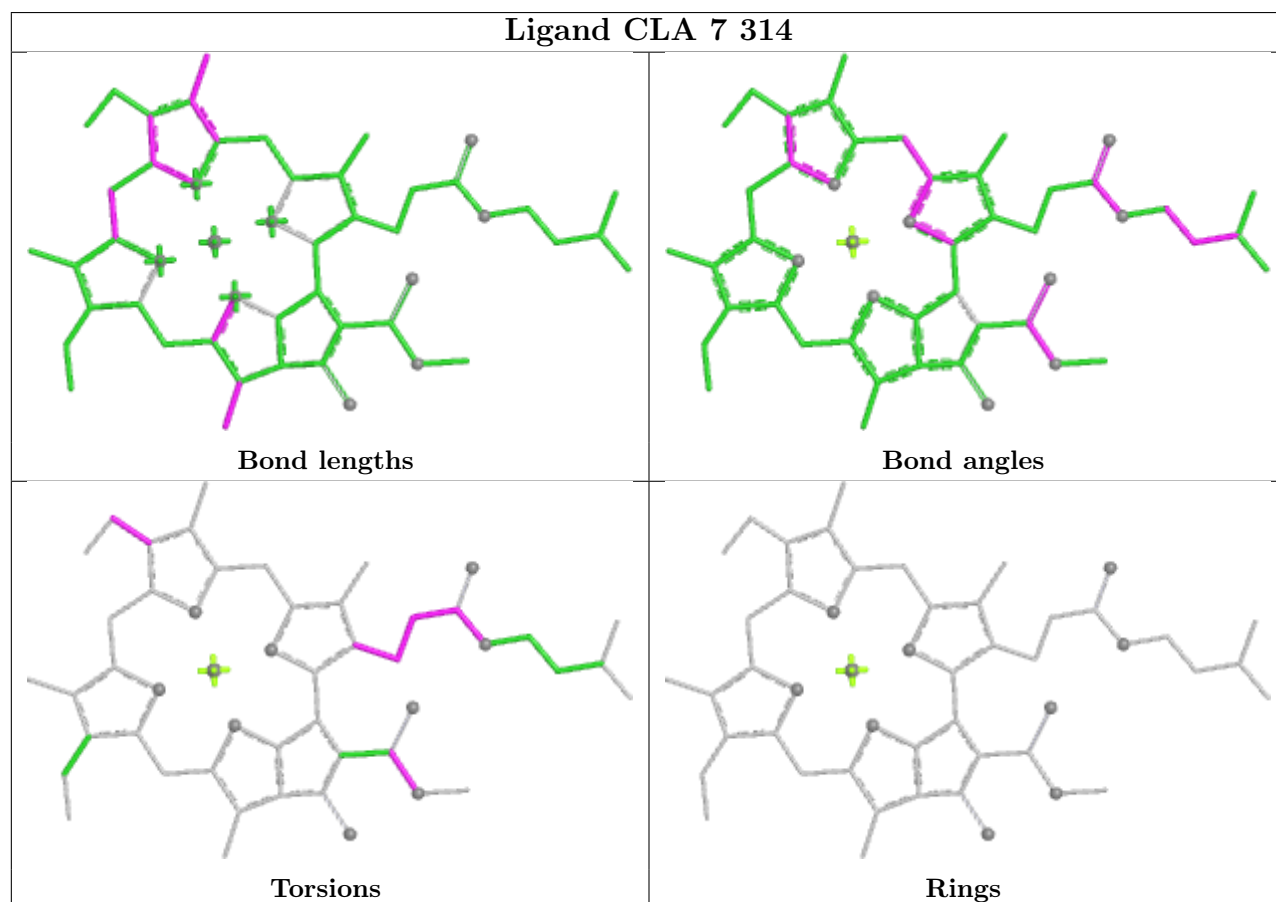
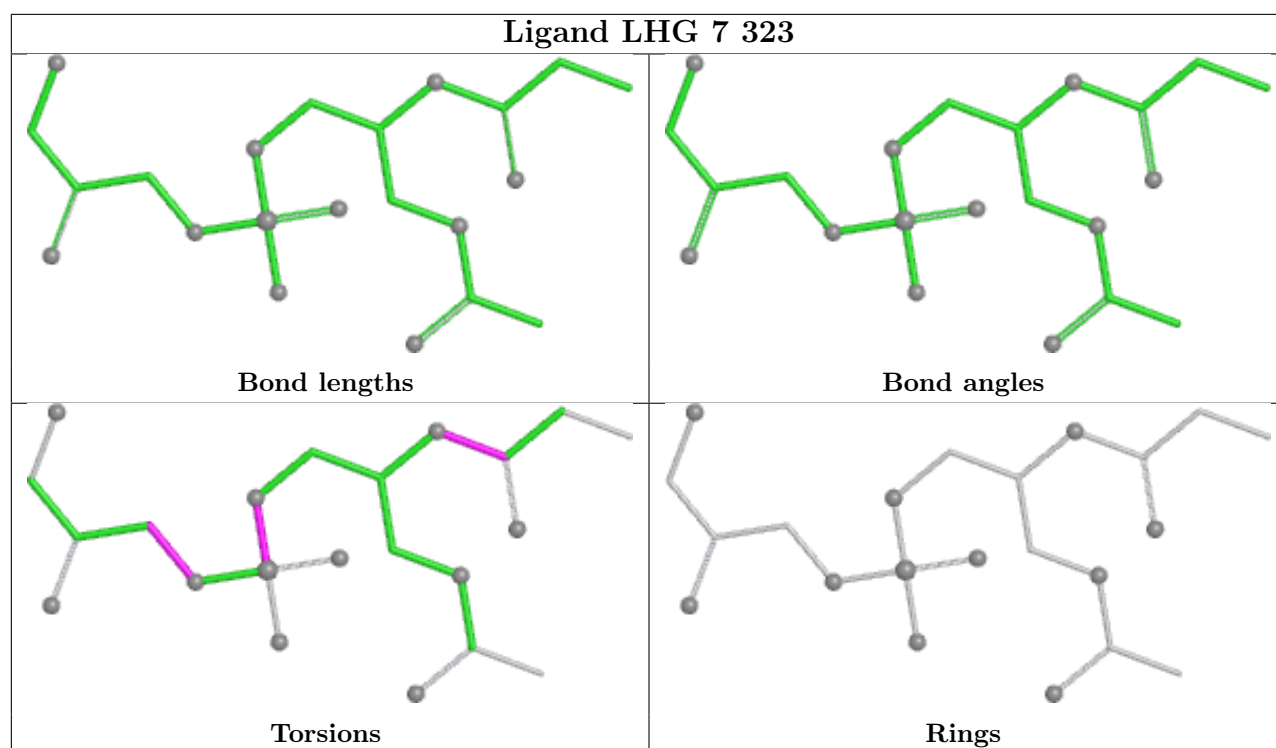
Rings

Ligand CLA A 837

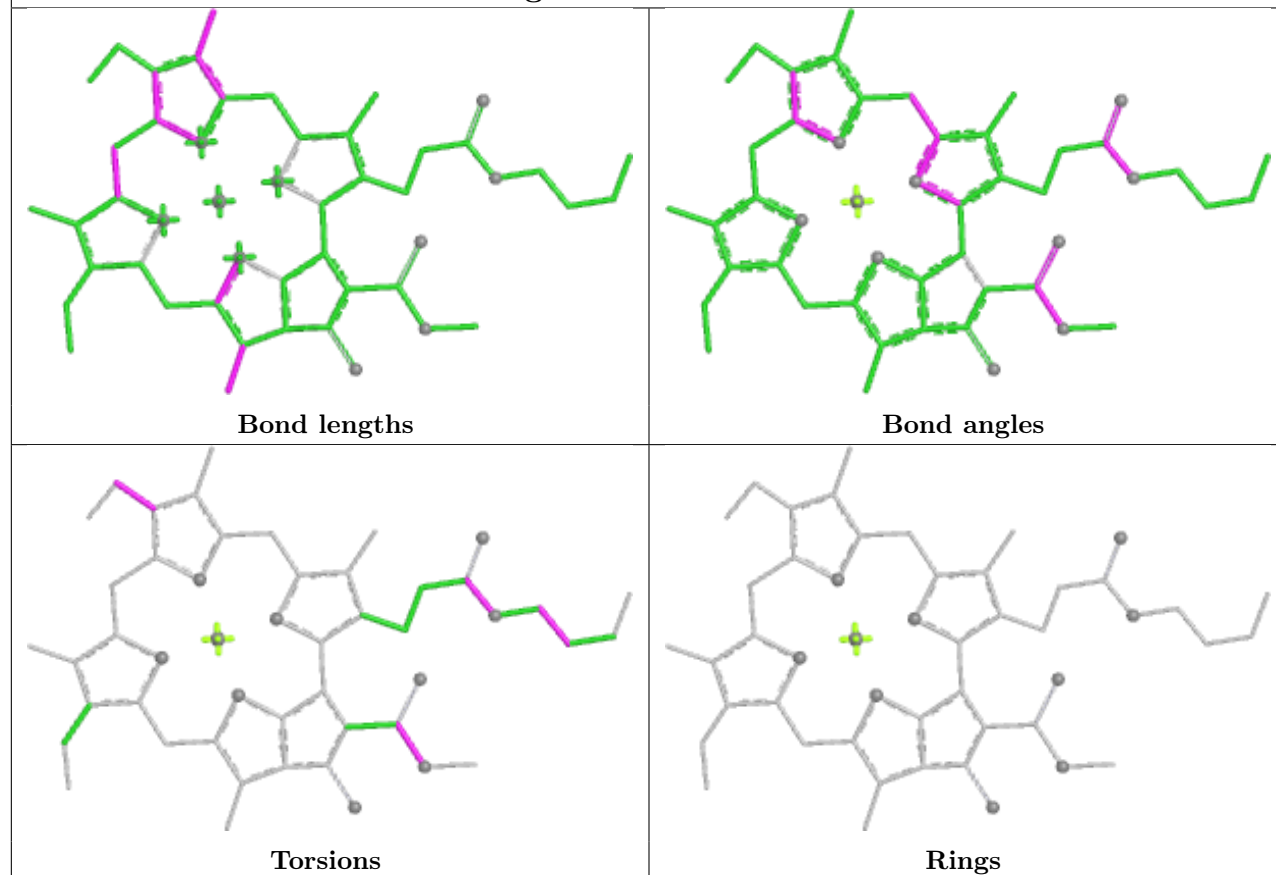


Ligand CLA A 828

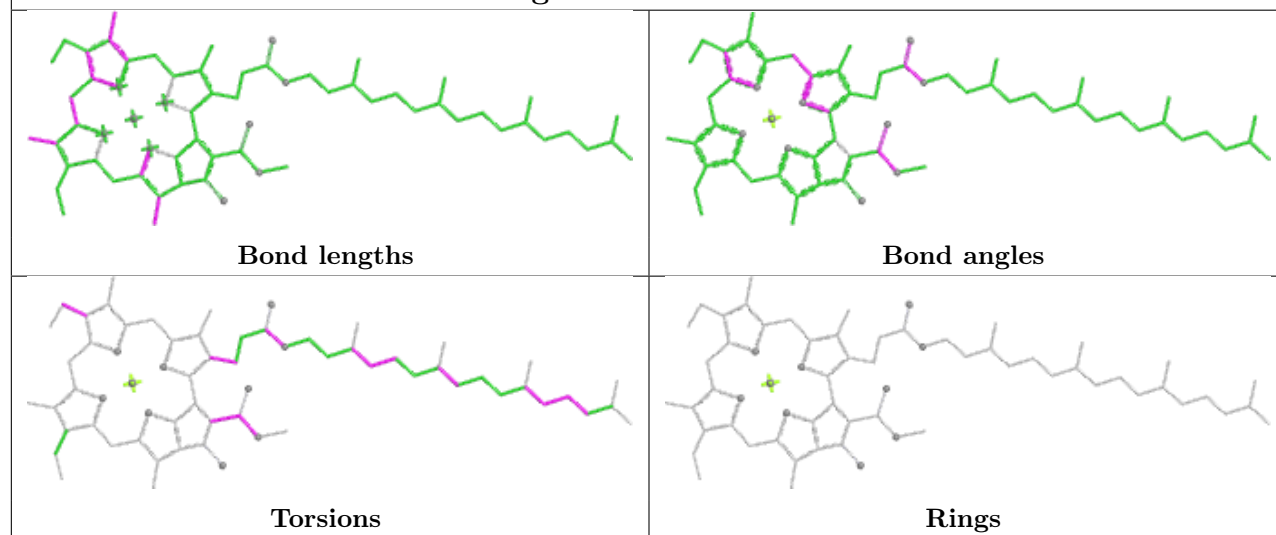


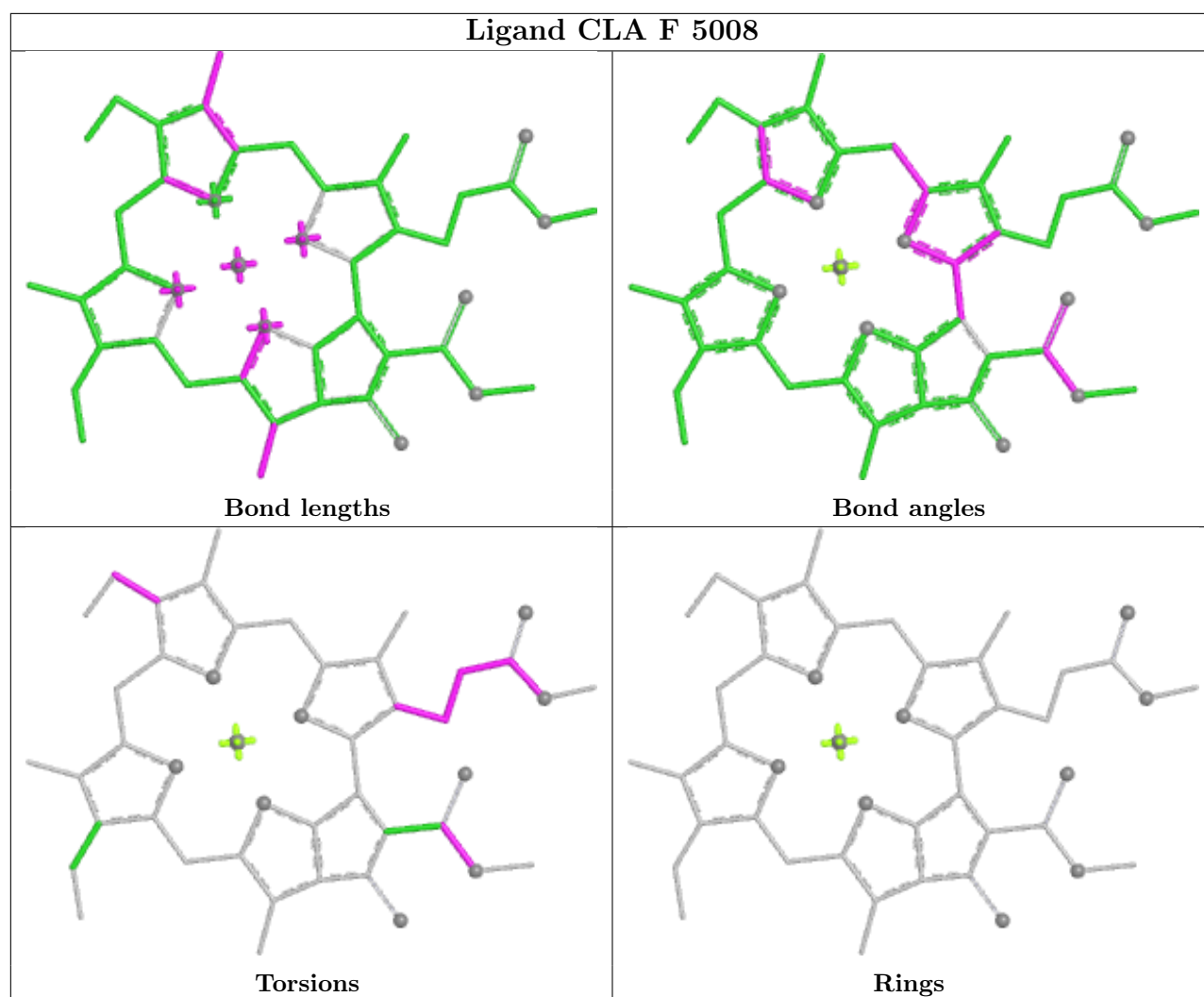


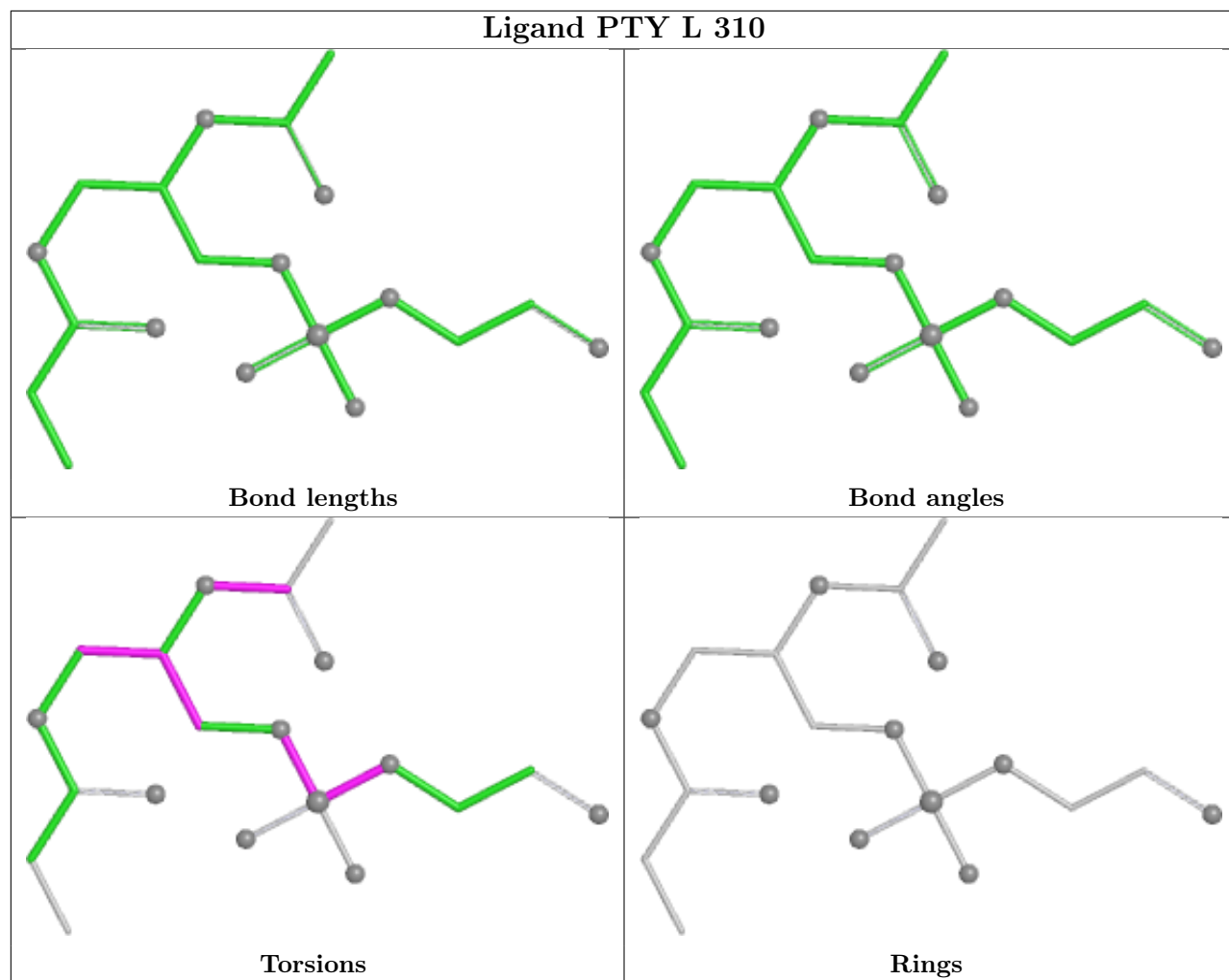
Ligand CLA F 5007



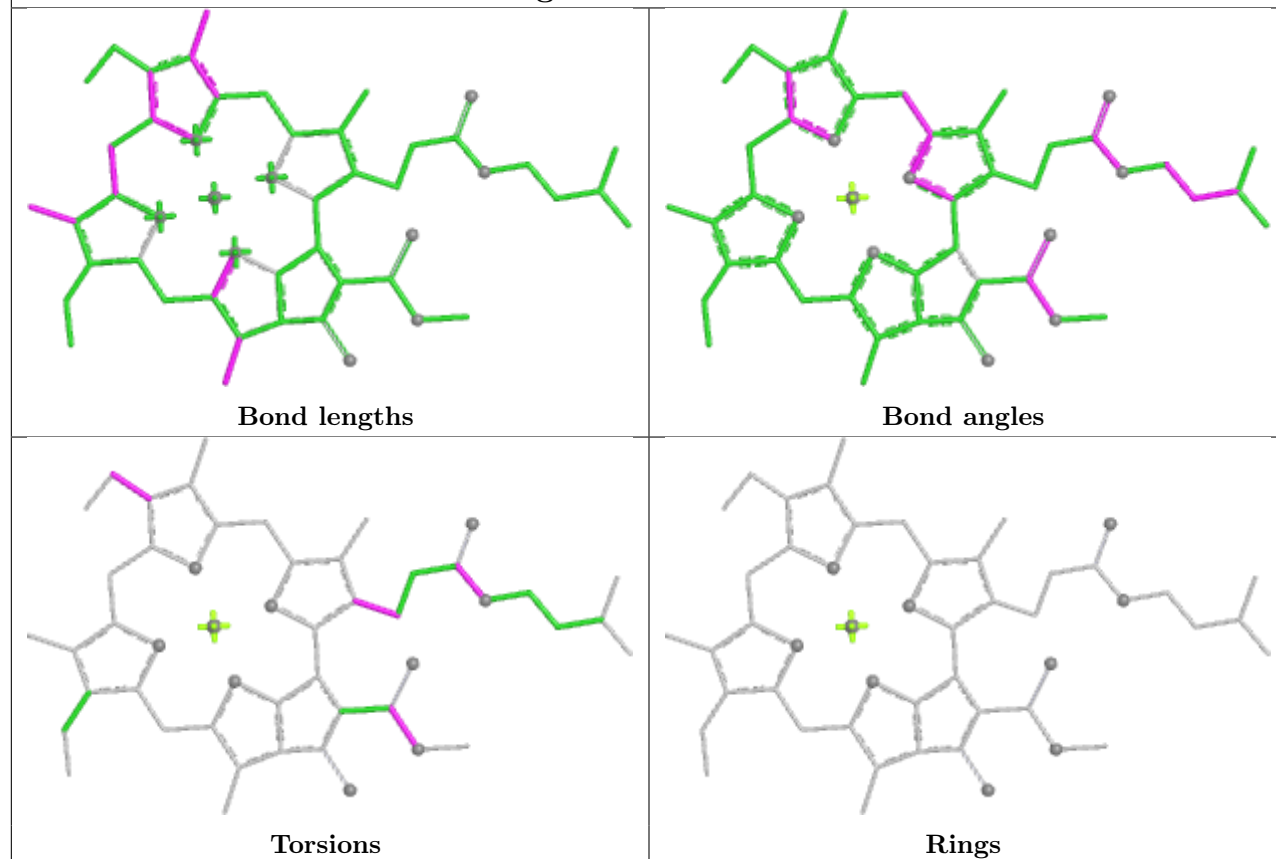
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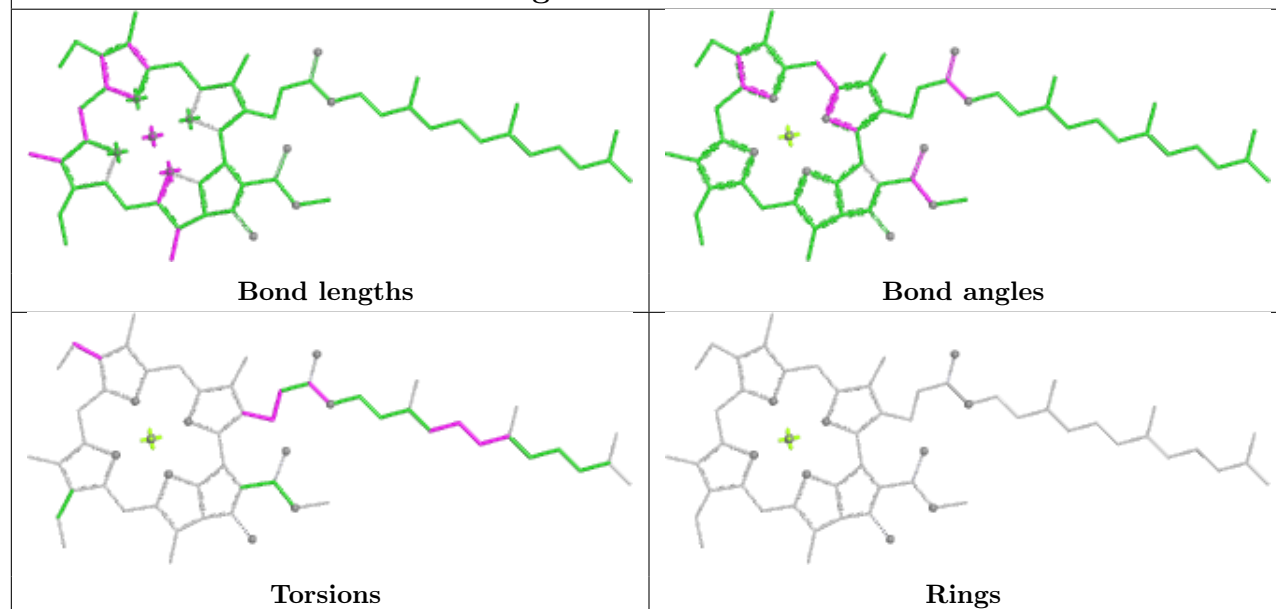




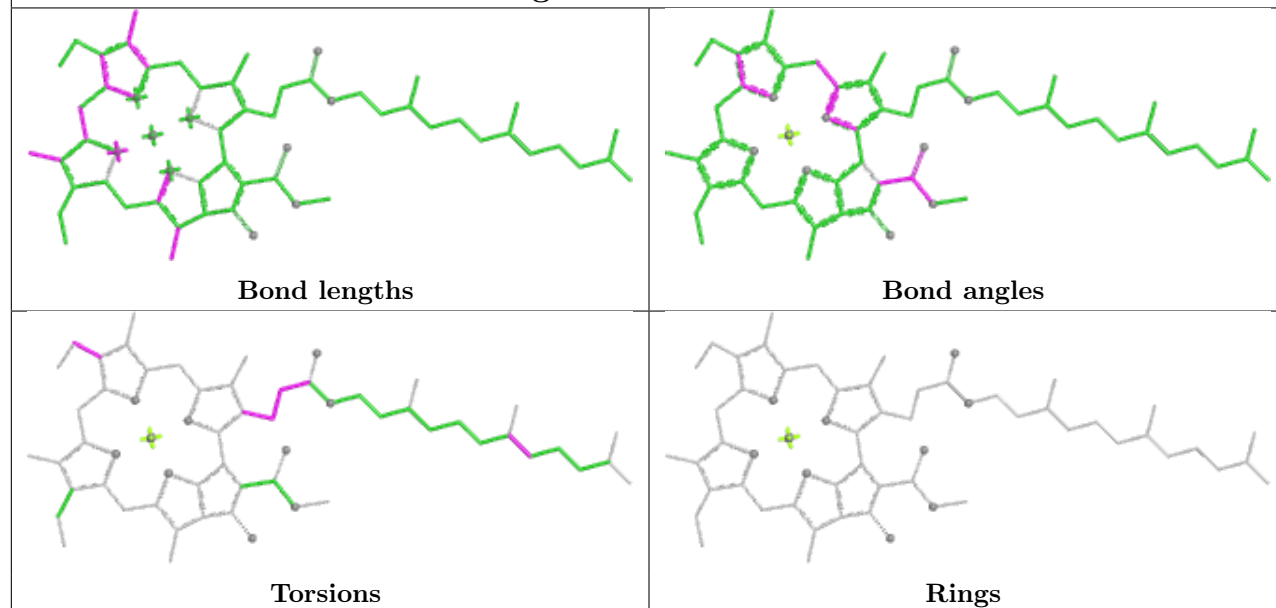
Ligand CLA 2 604



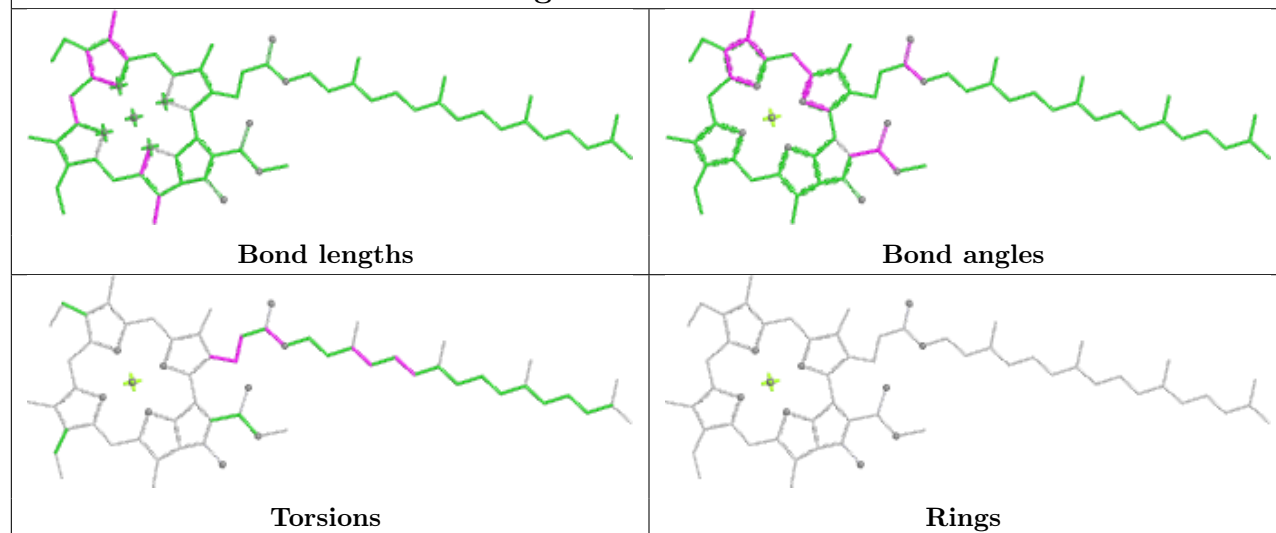
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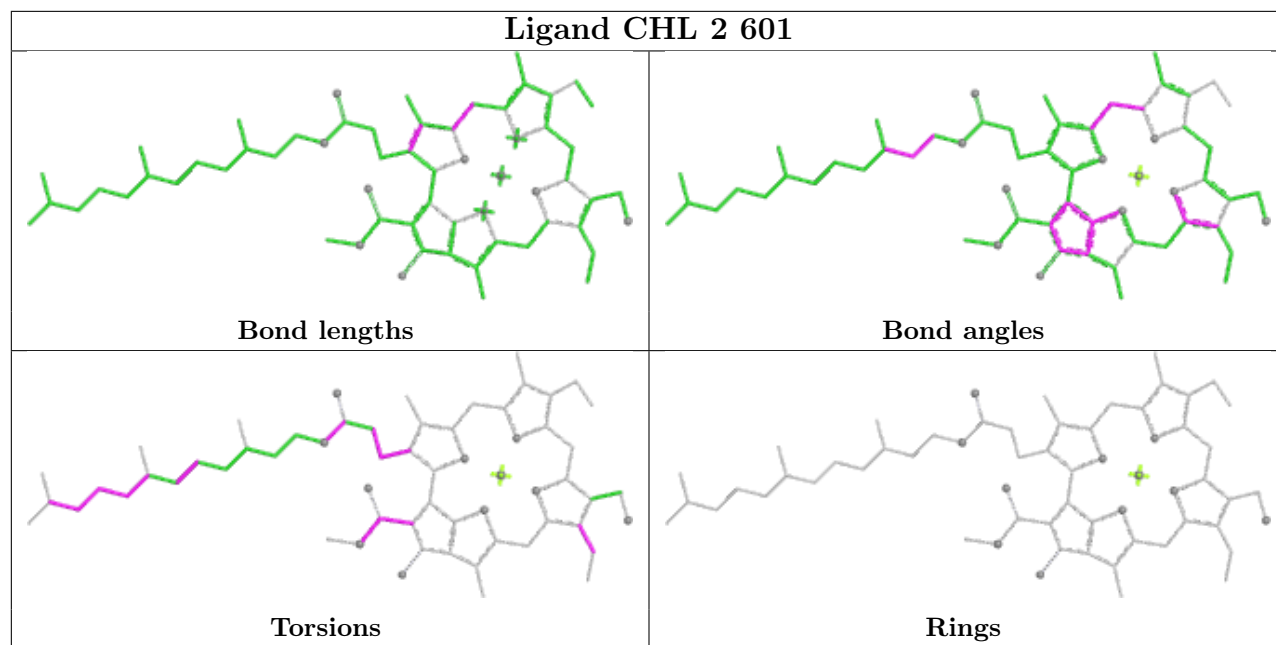
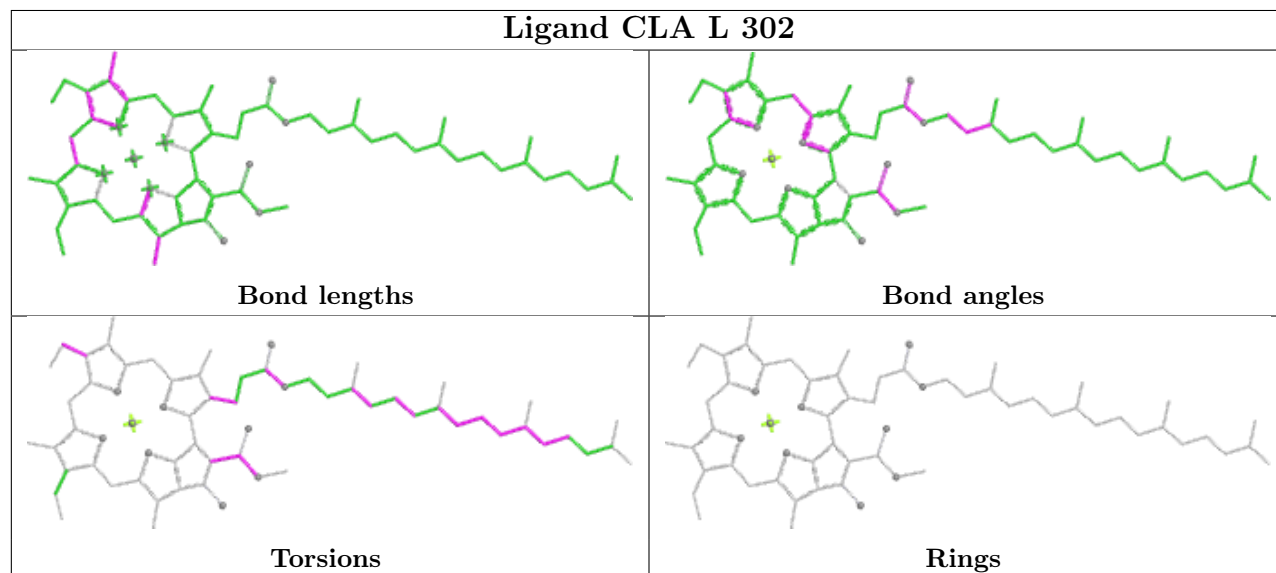


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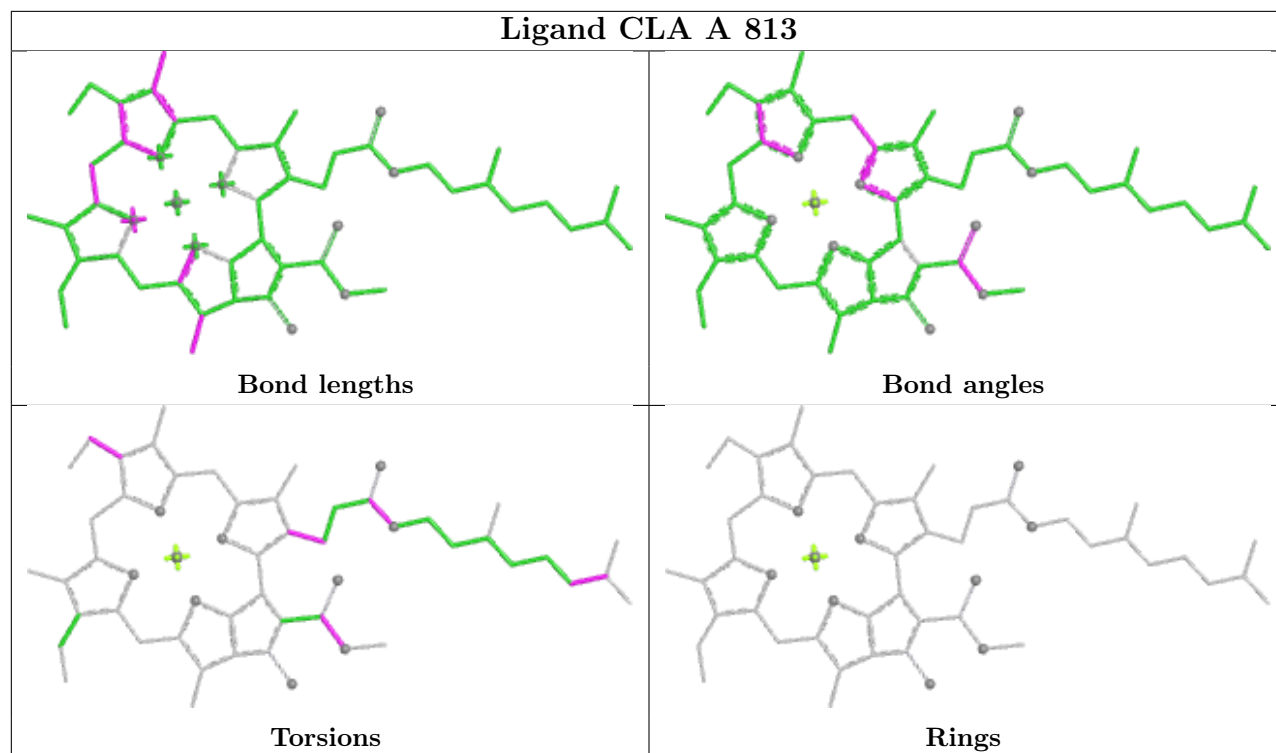


Ligand CLA L 305

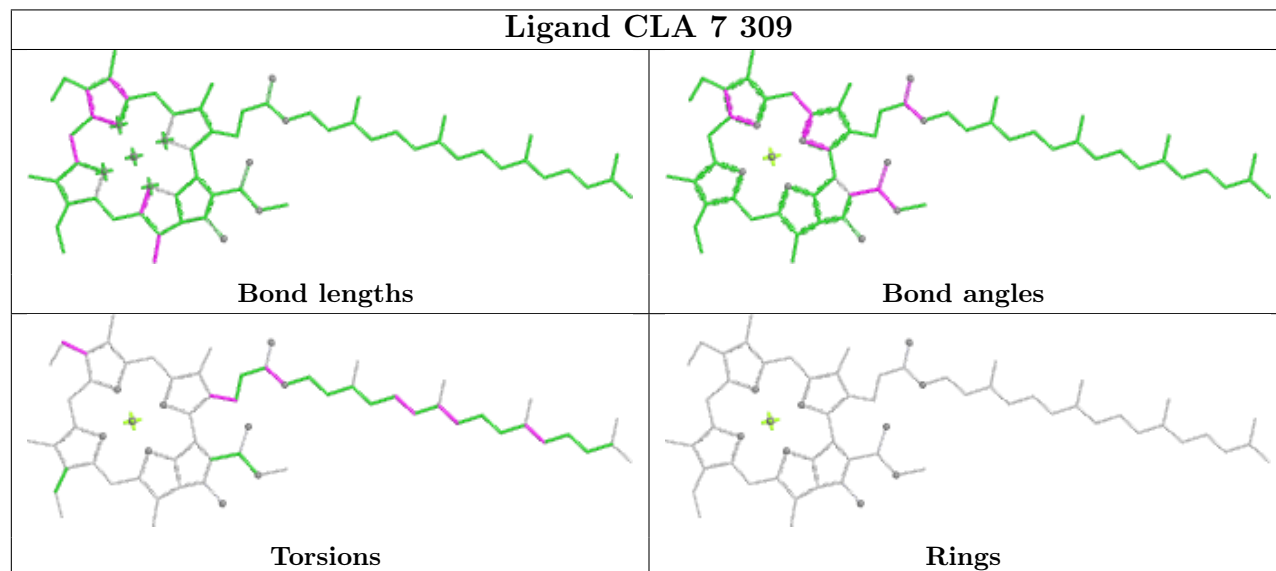


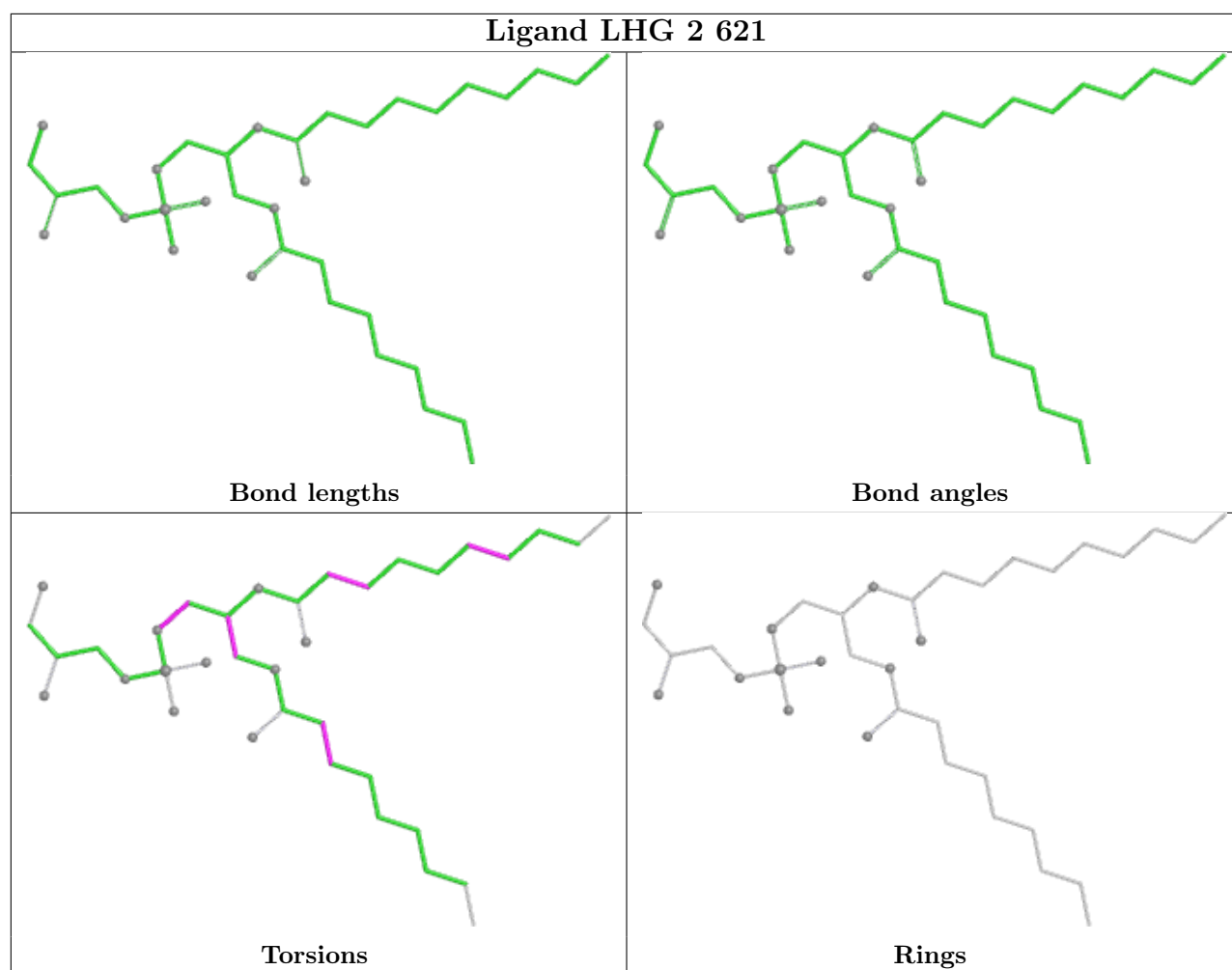
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Ligand CLA A 813

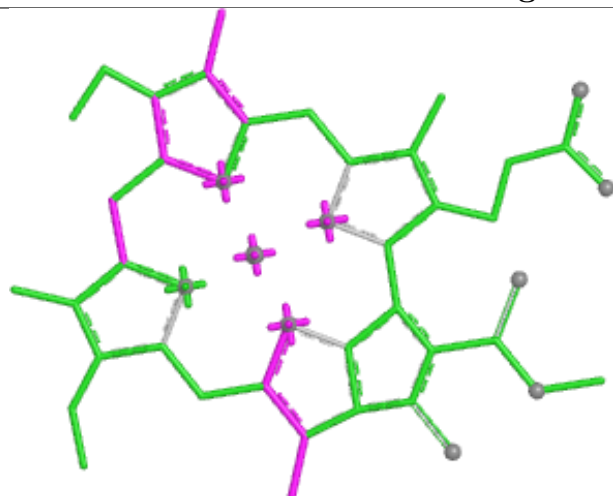


Ligand CLA 7 309

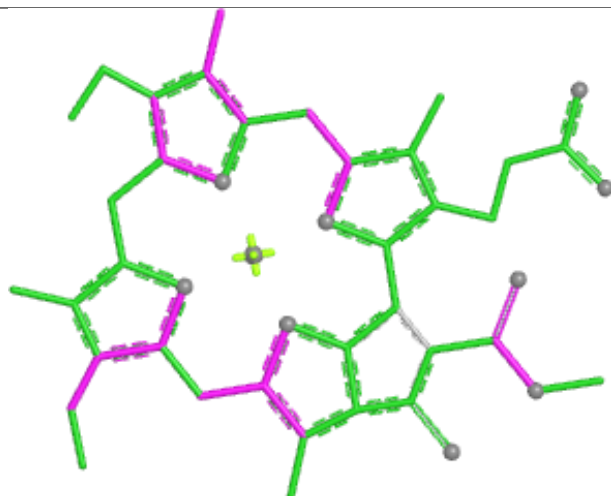




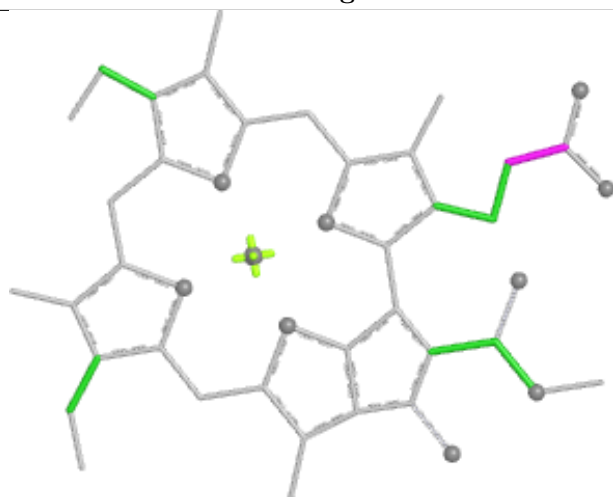
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Bond lengths



Bond angles

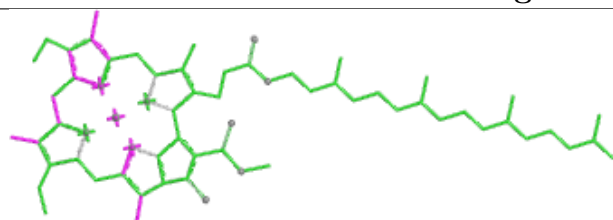


Torsions

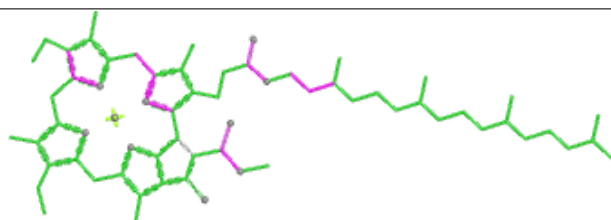


Rings

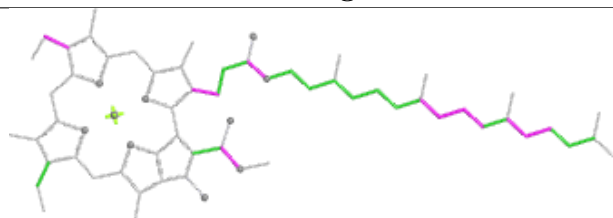
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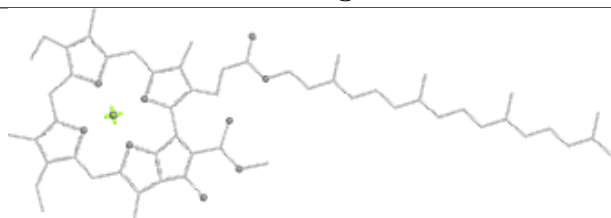
Bond lengths



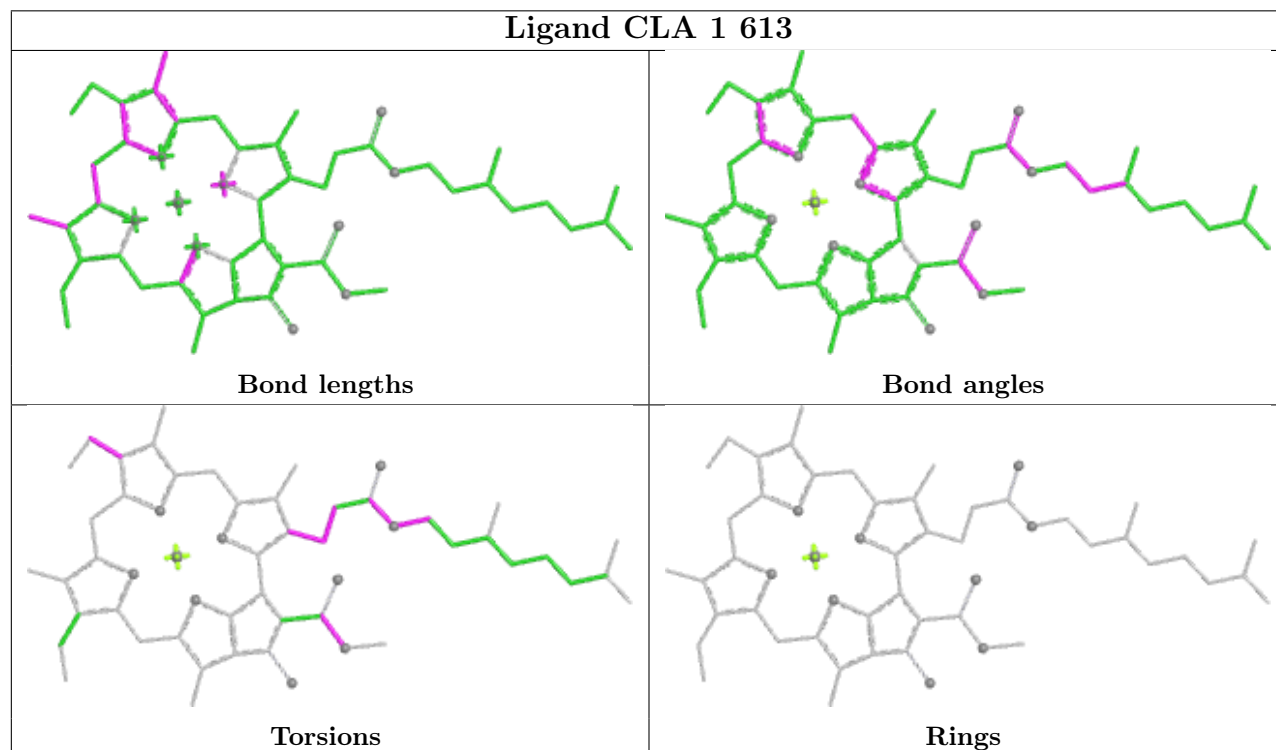
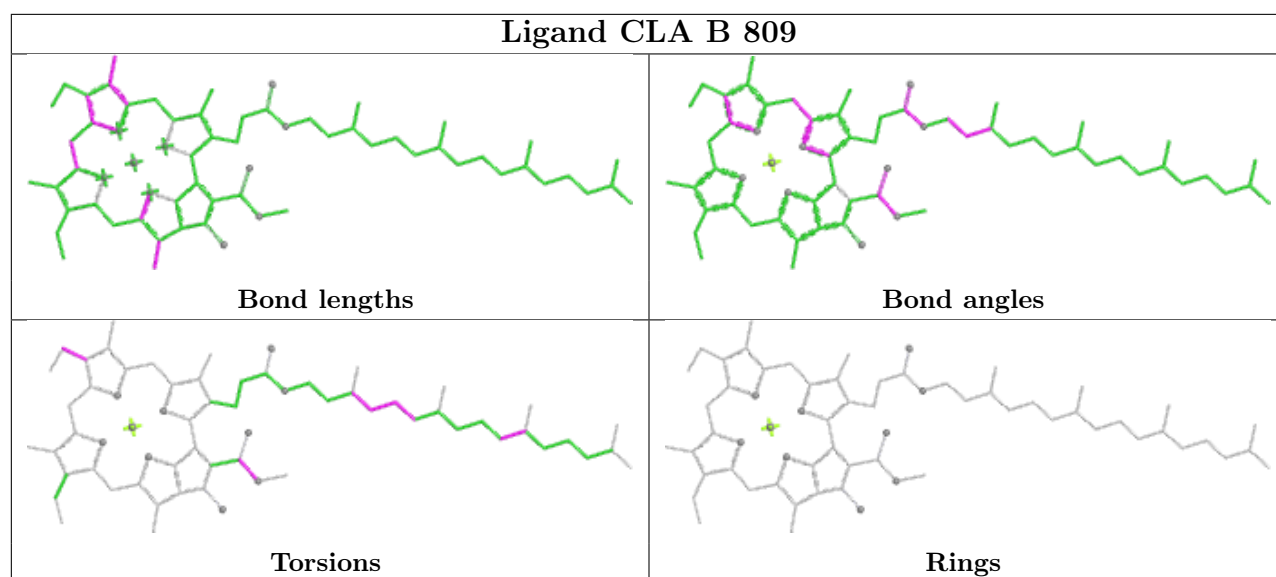
Bond angles



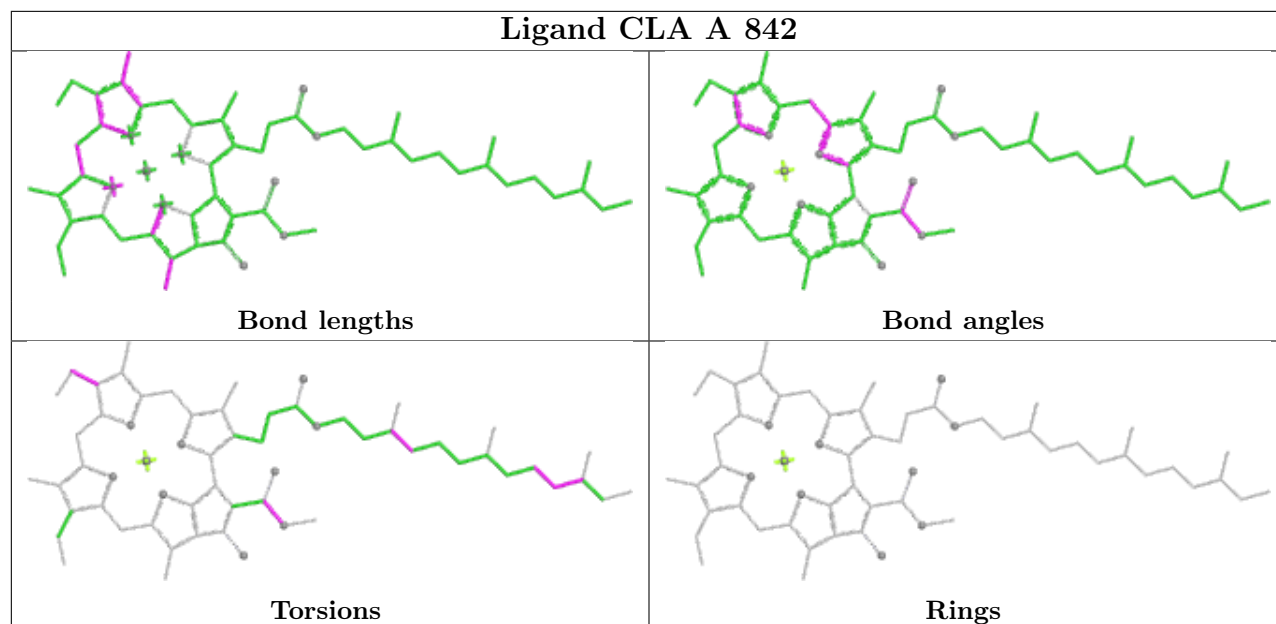
Torsions



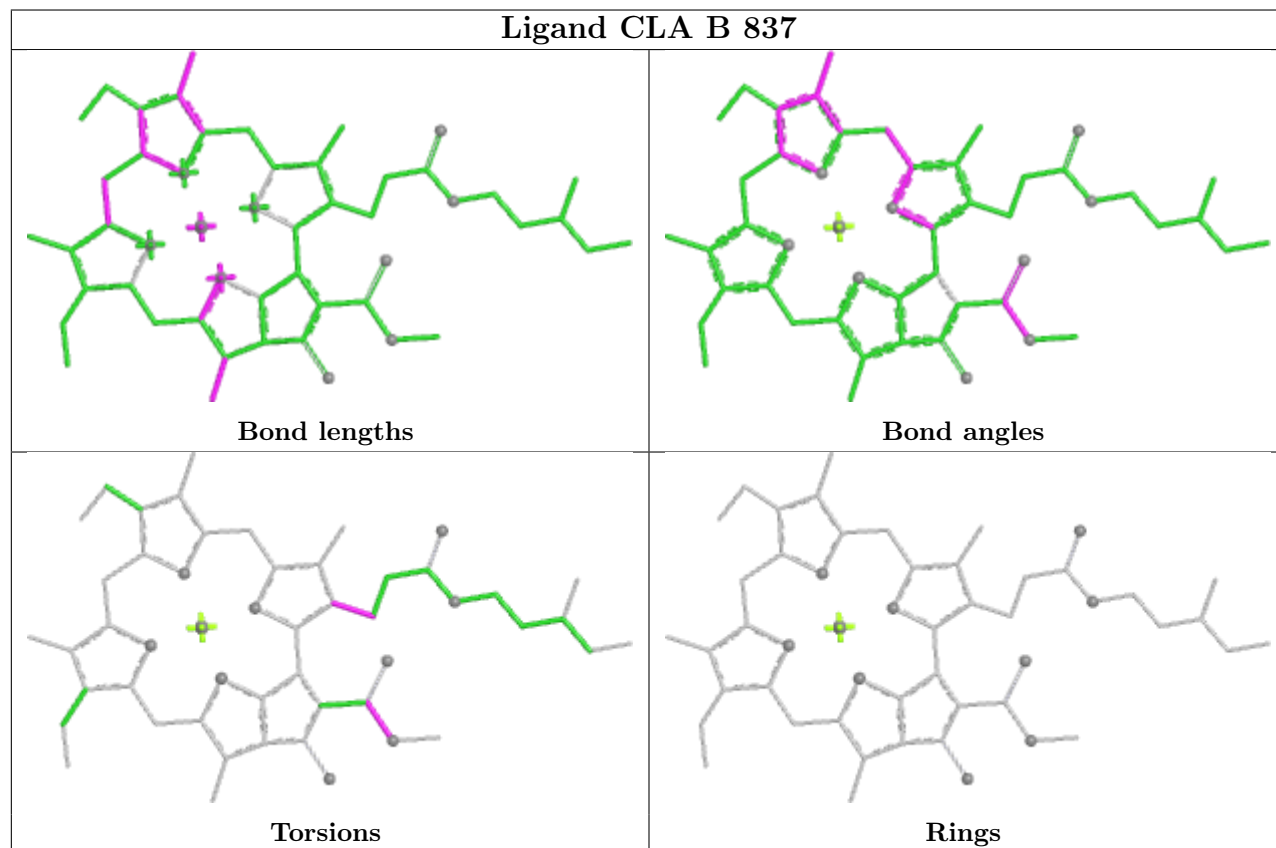
Rings

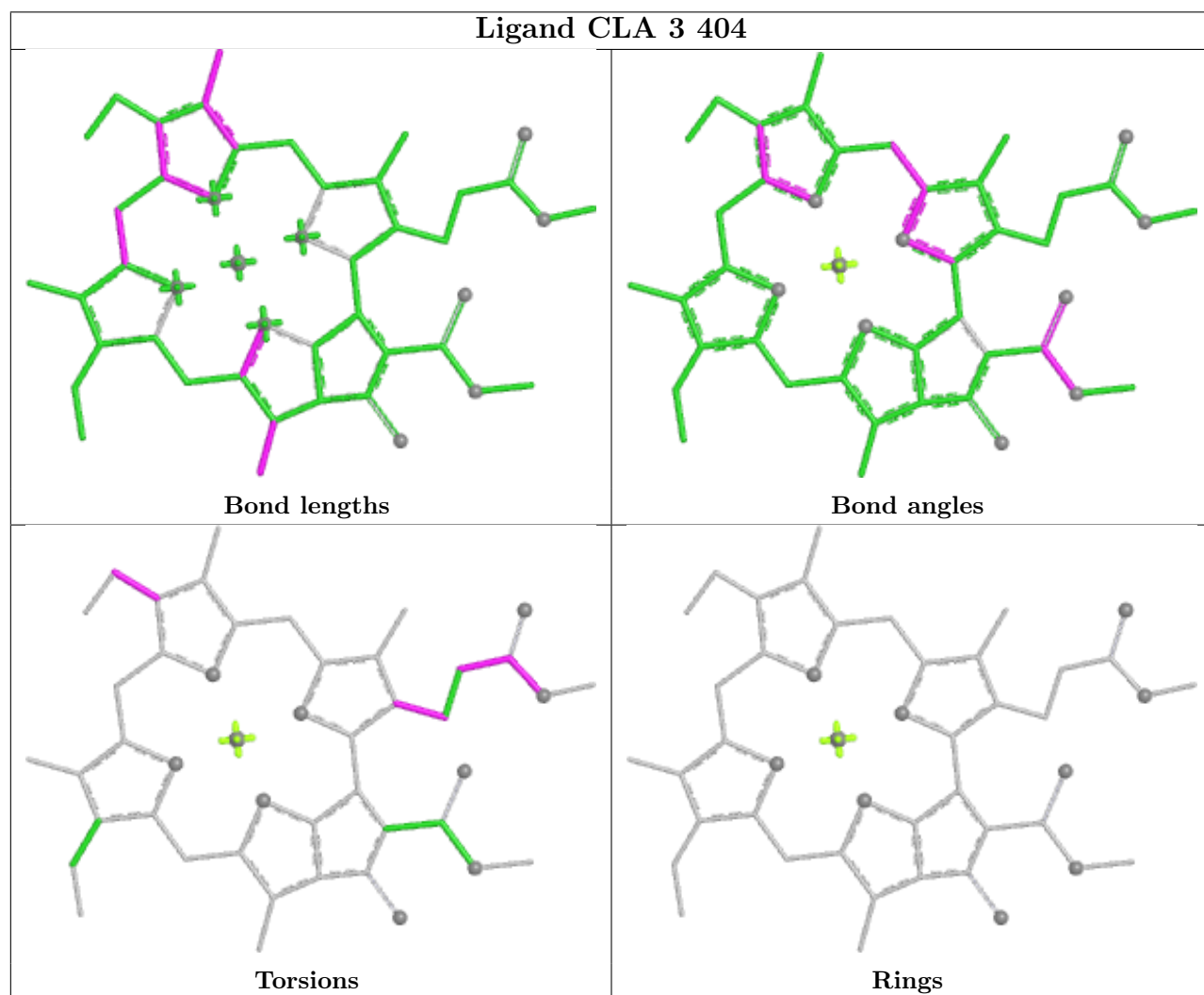
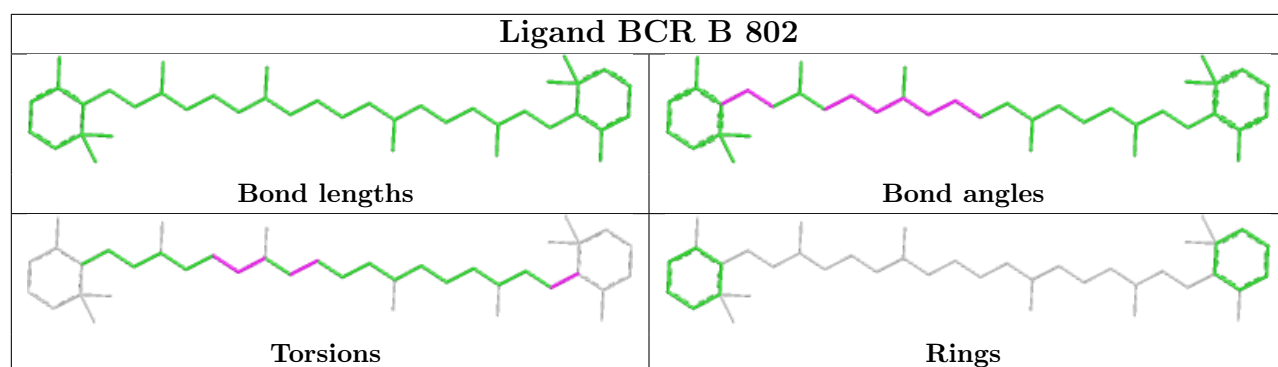


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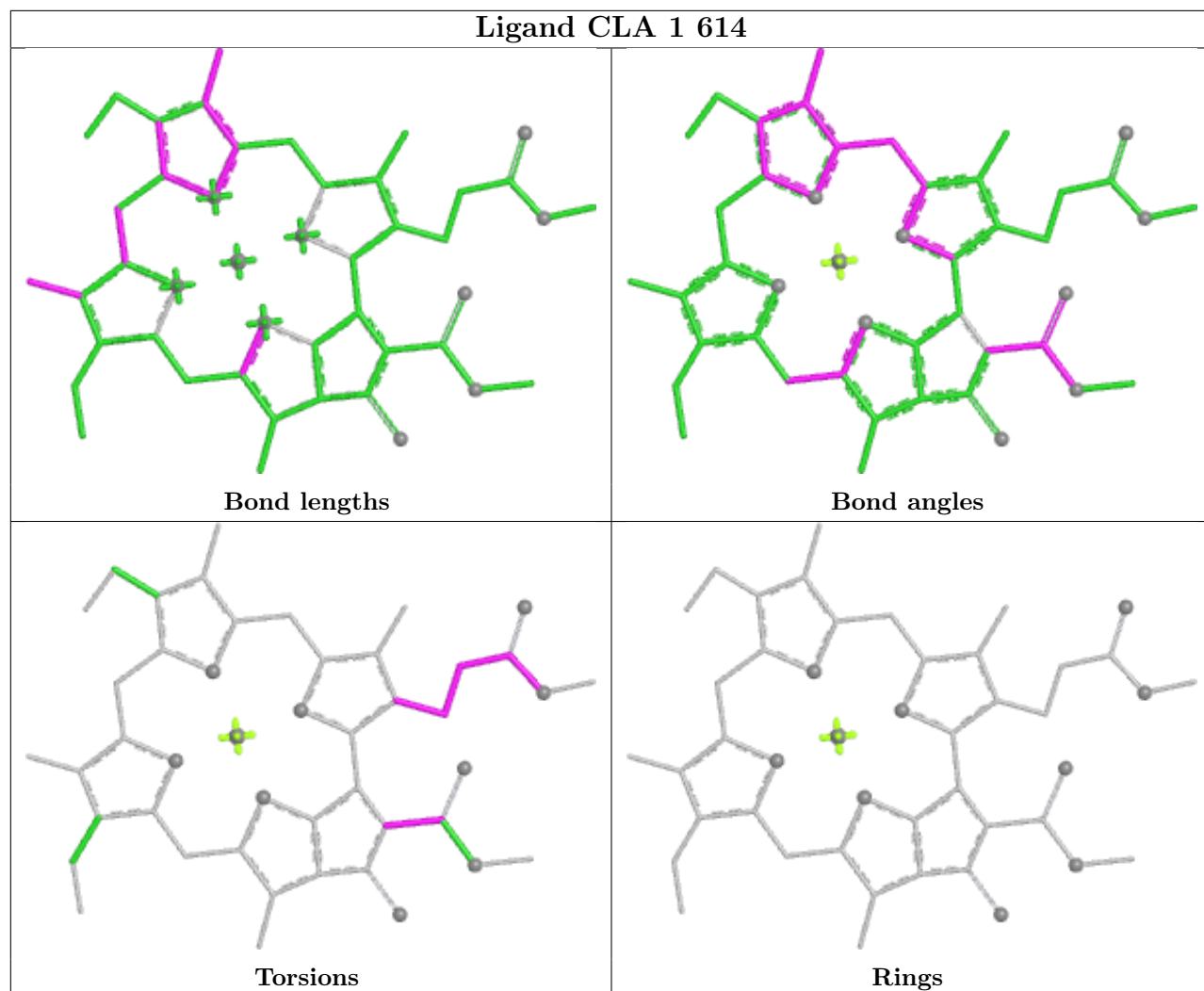


Ligand CLA B 837

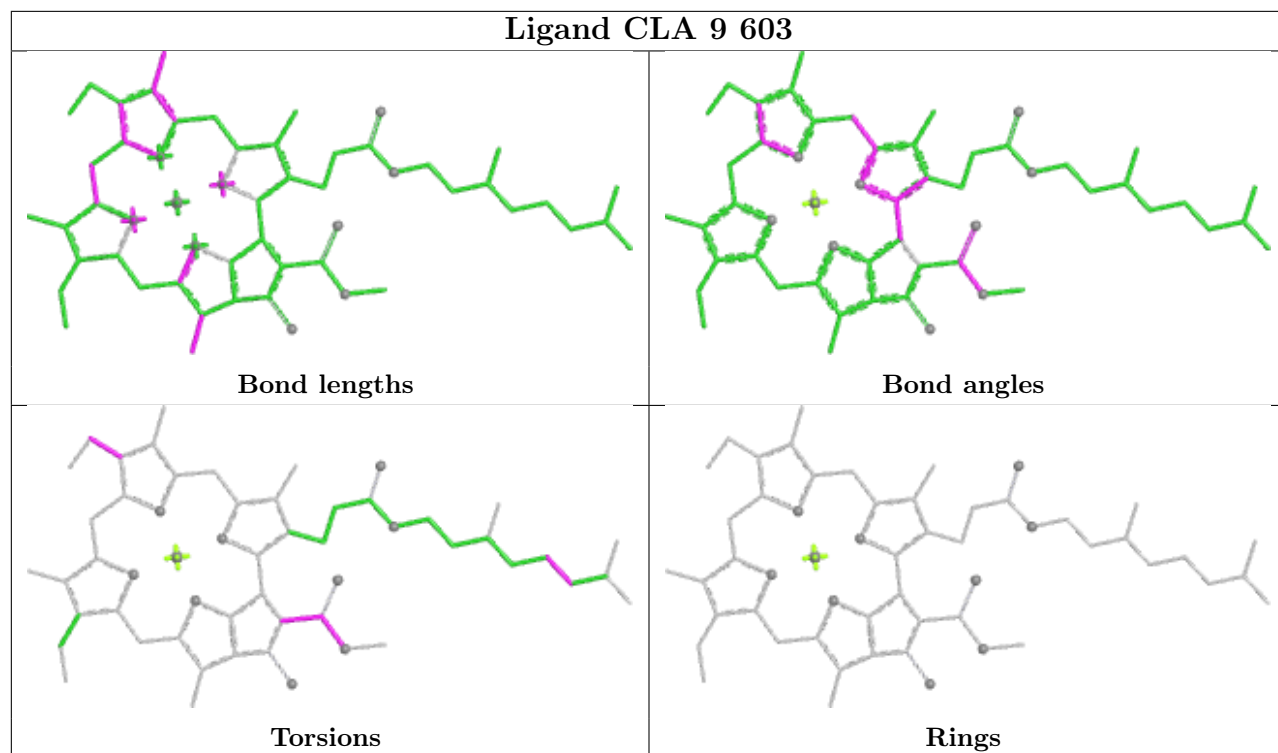




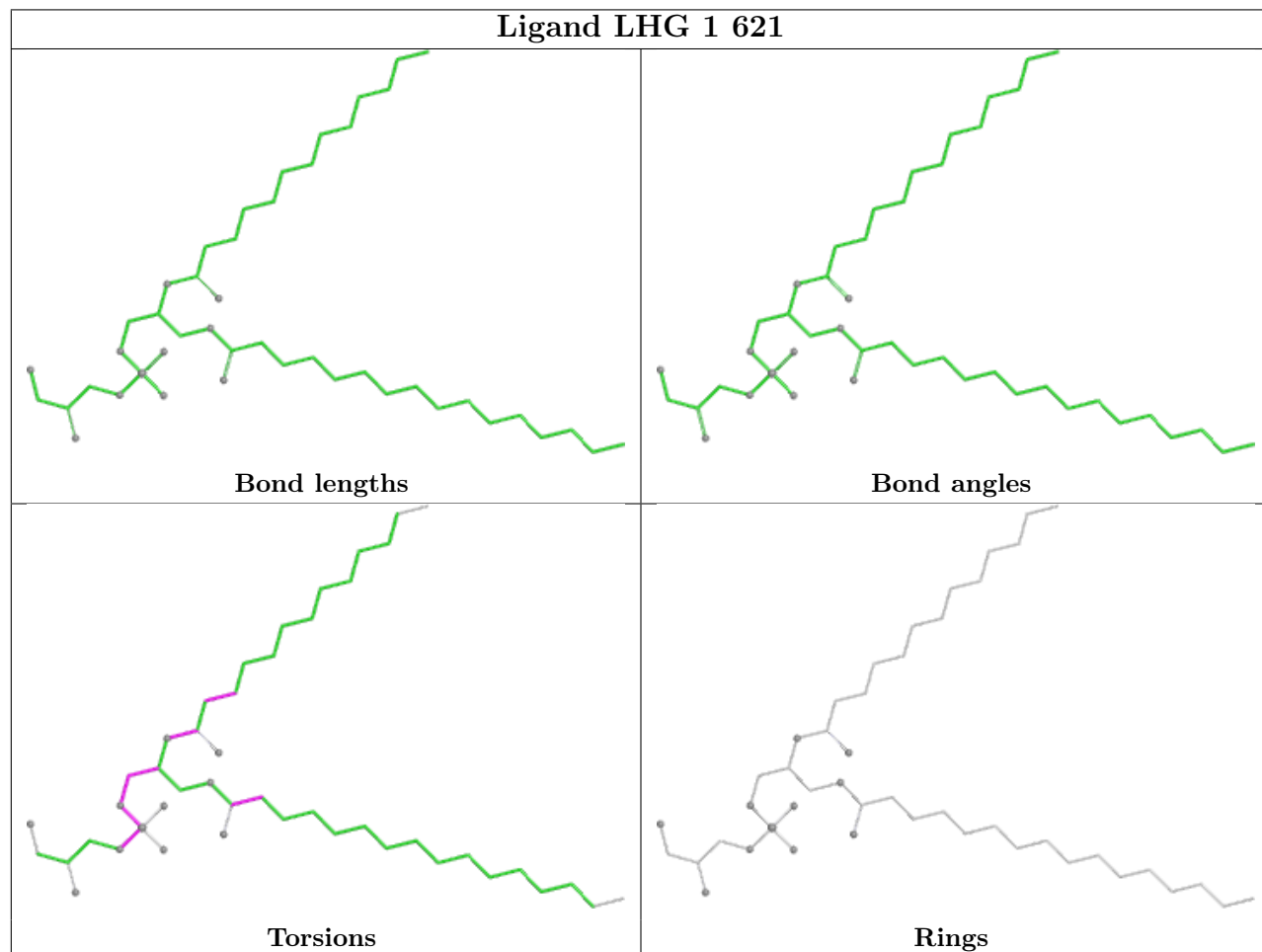
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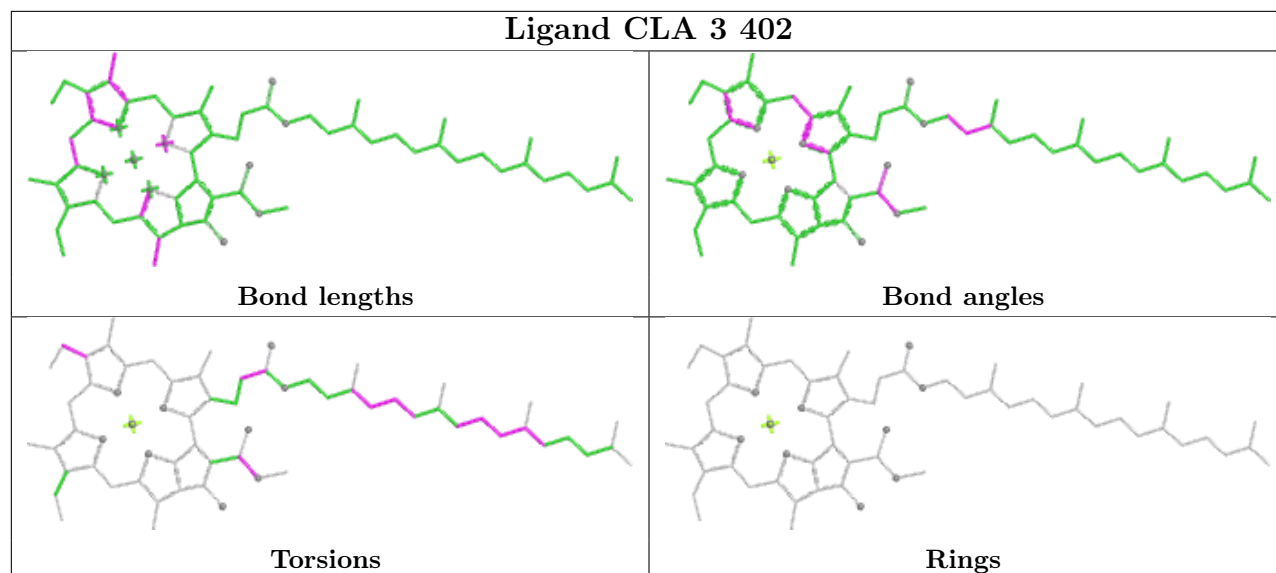
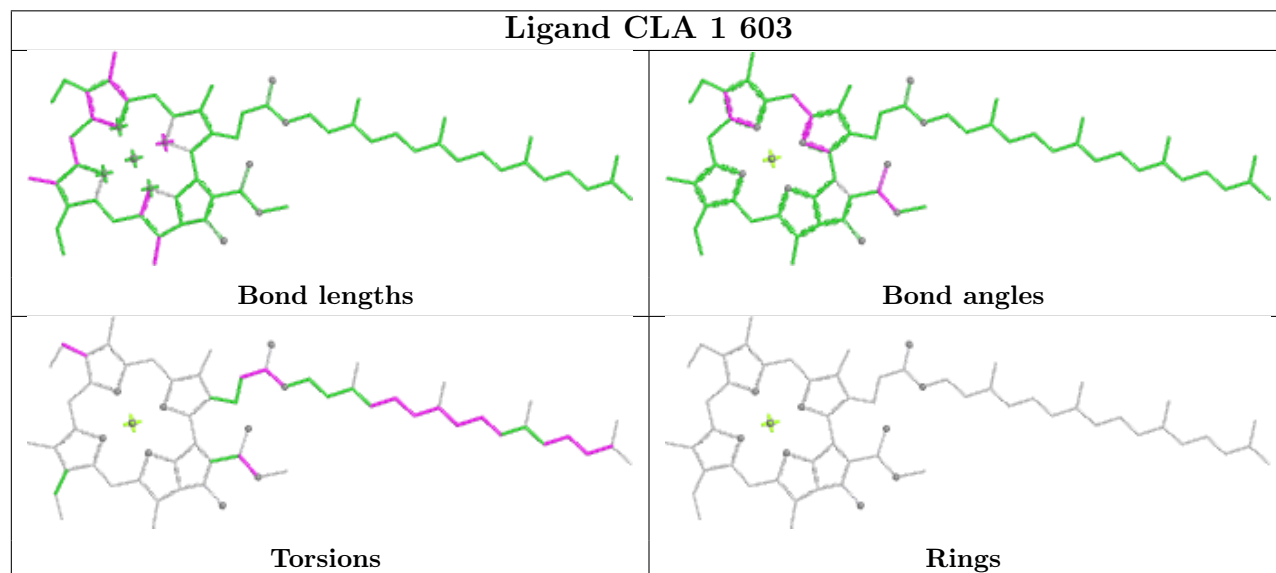
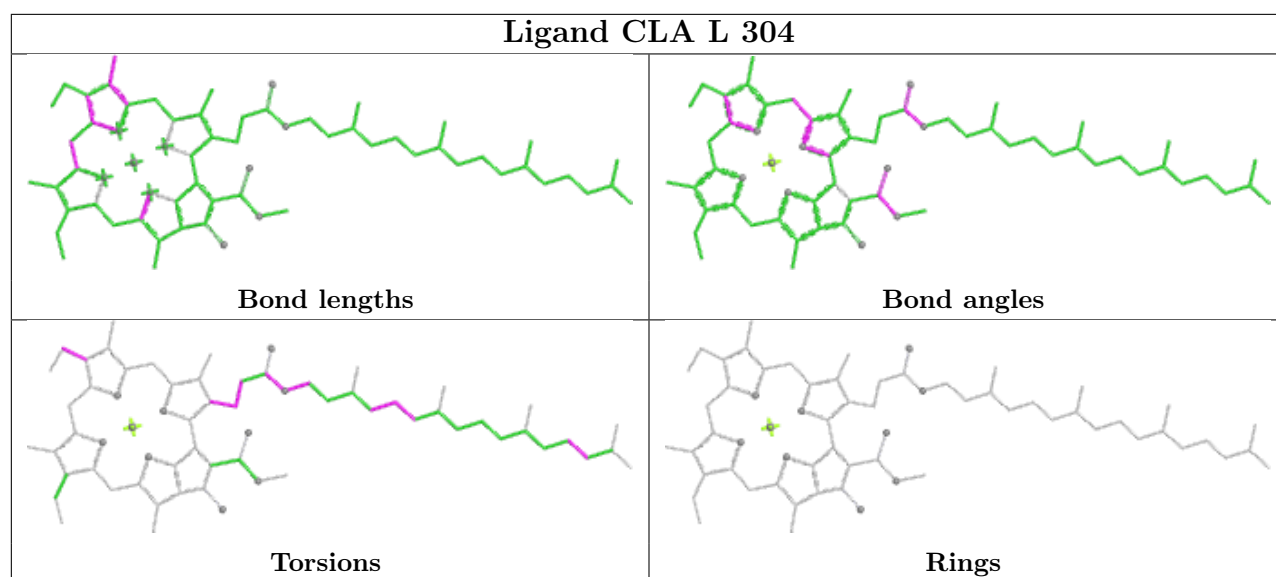


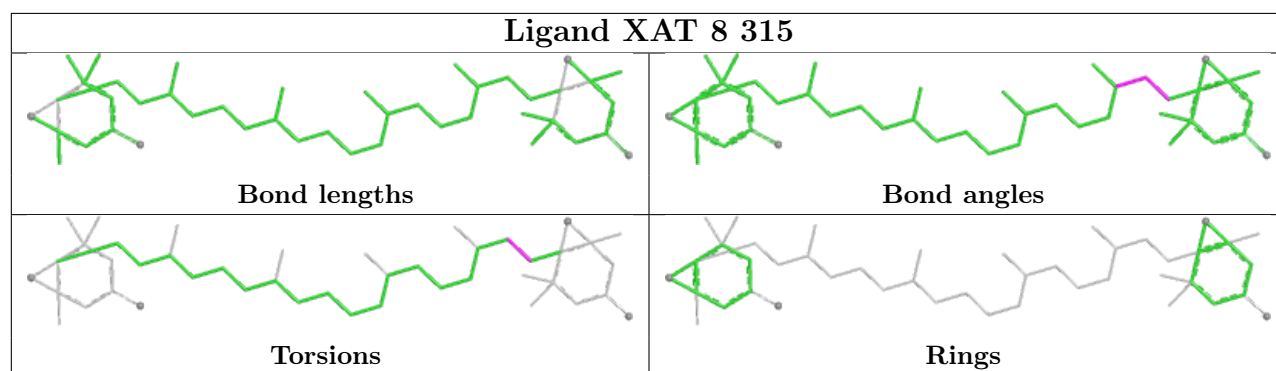
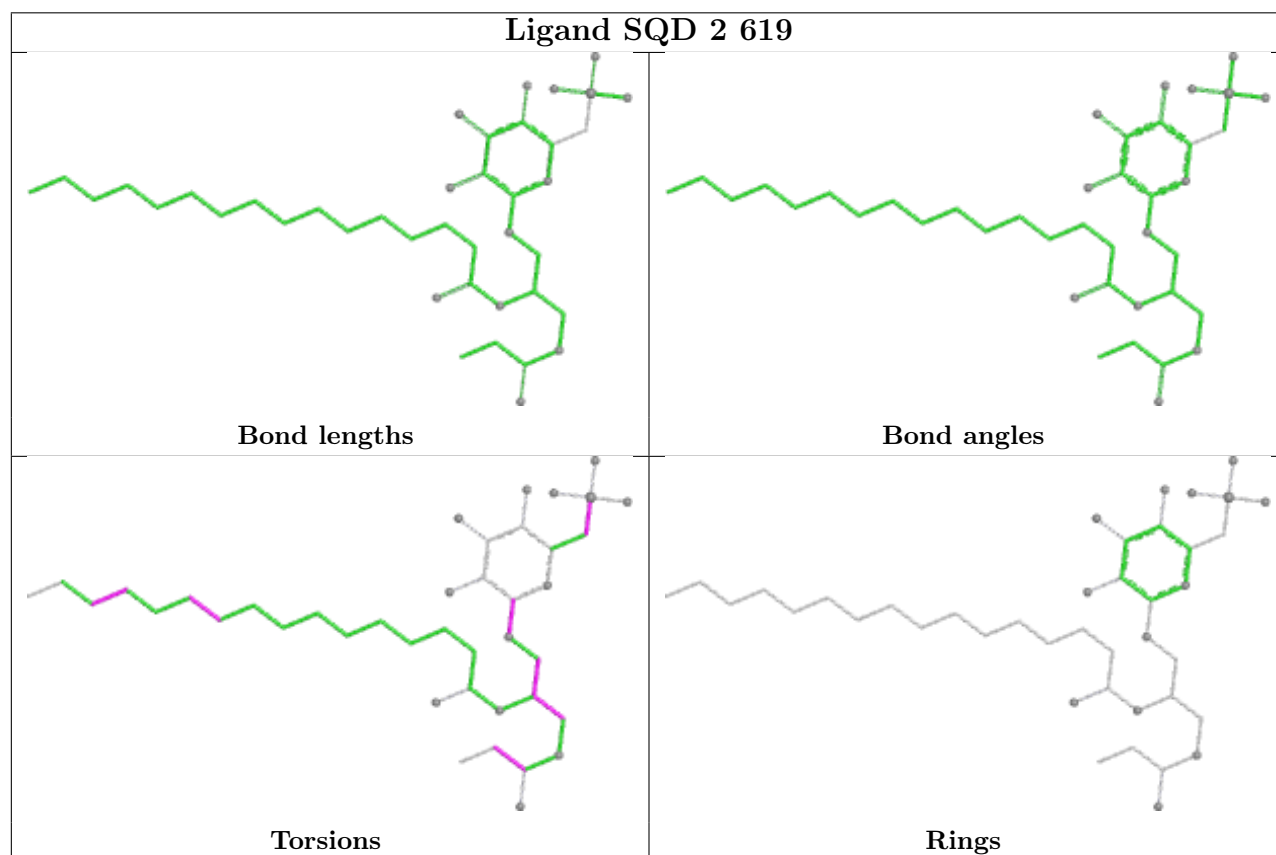
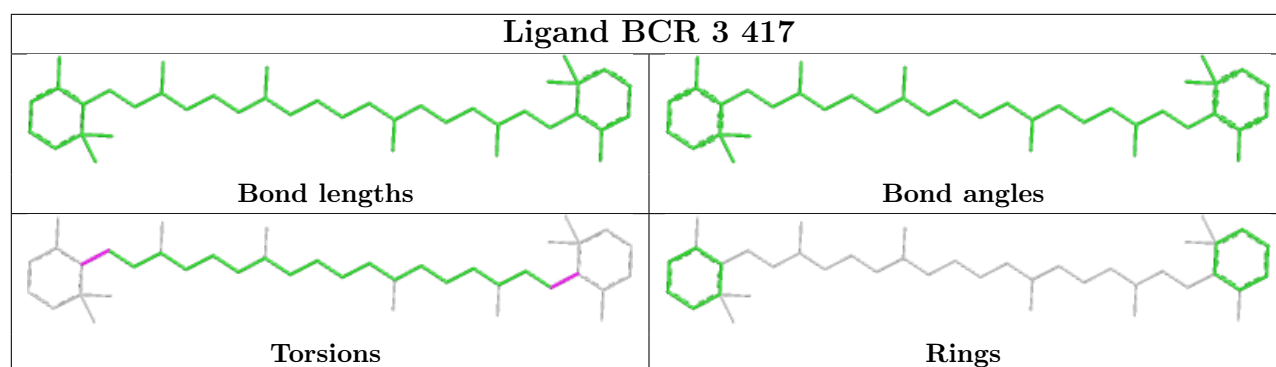
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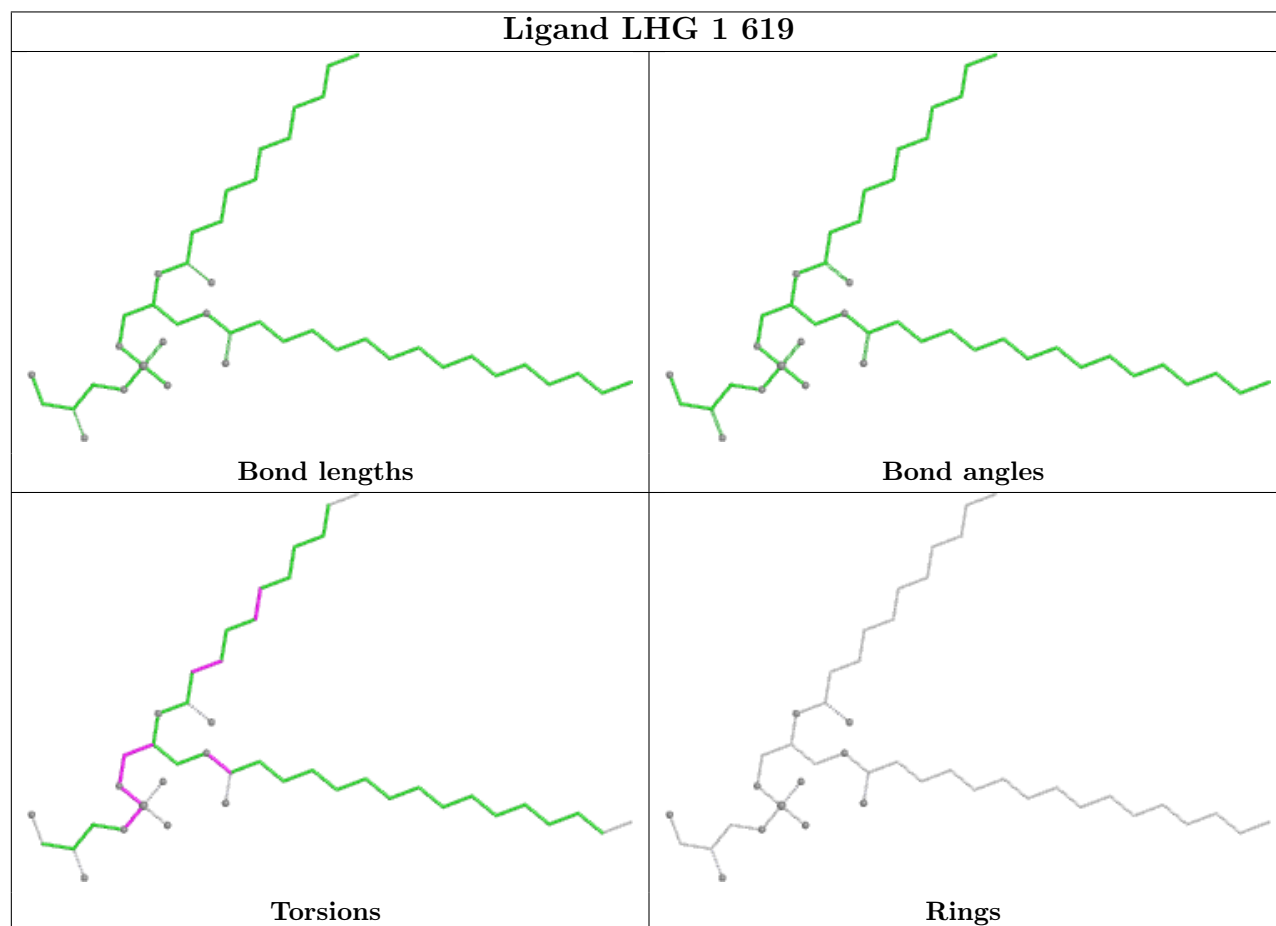
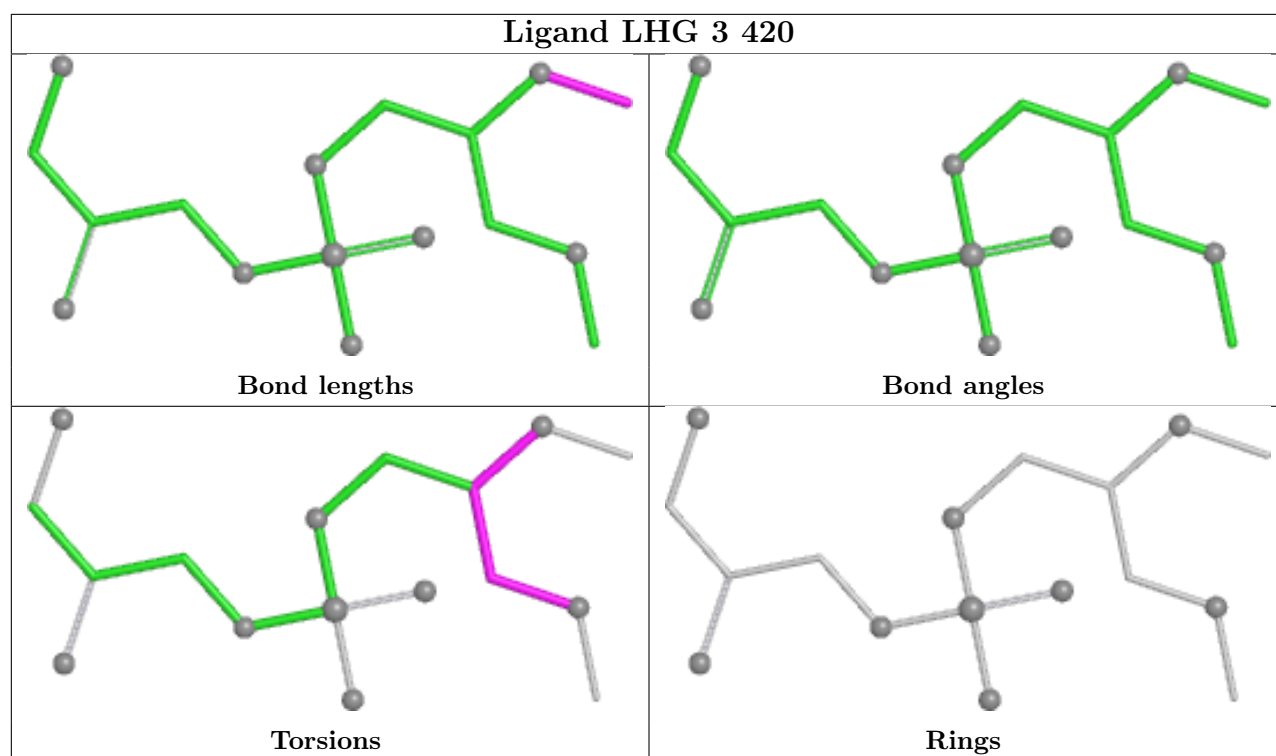


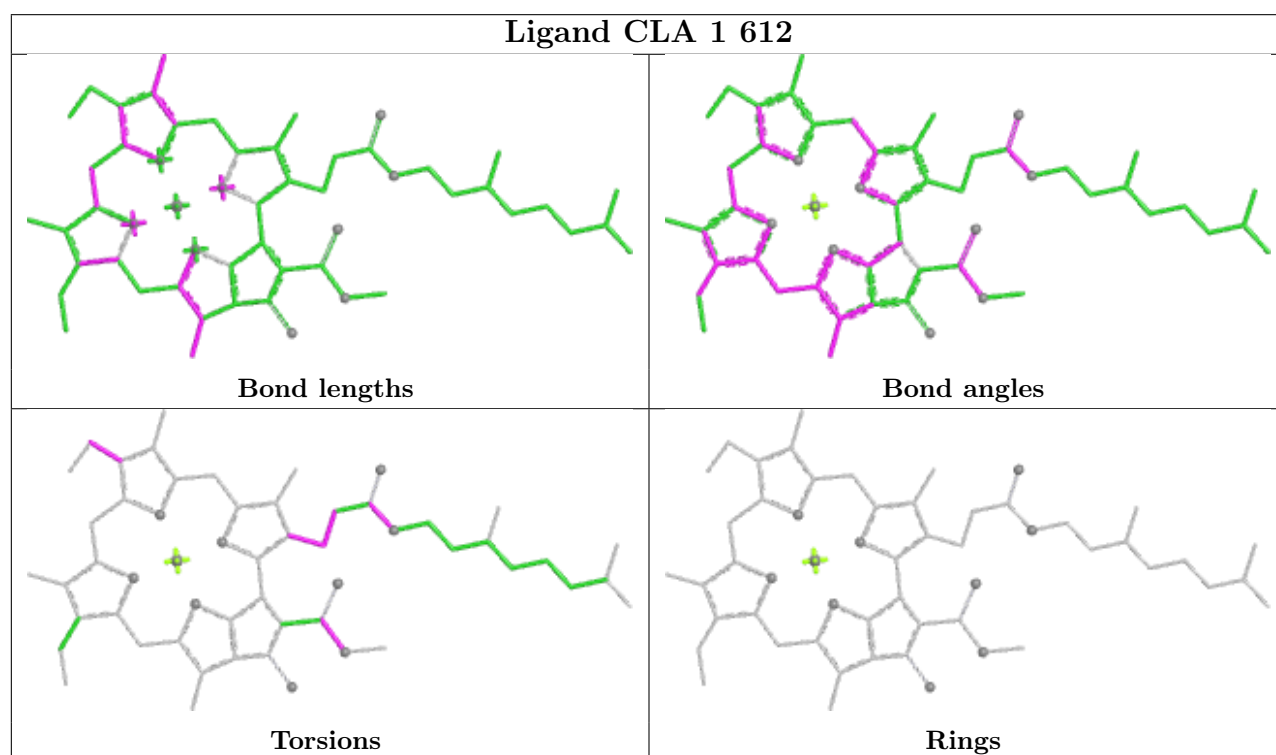
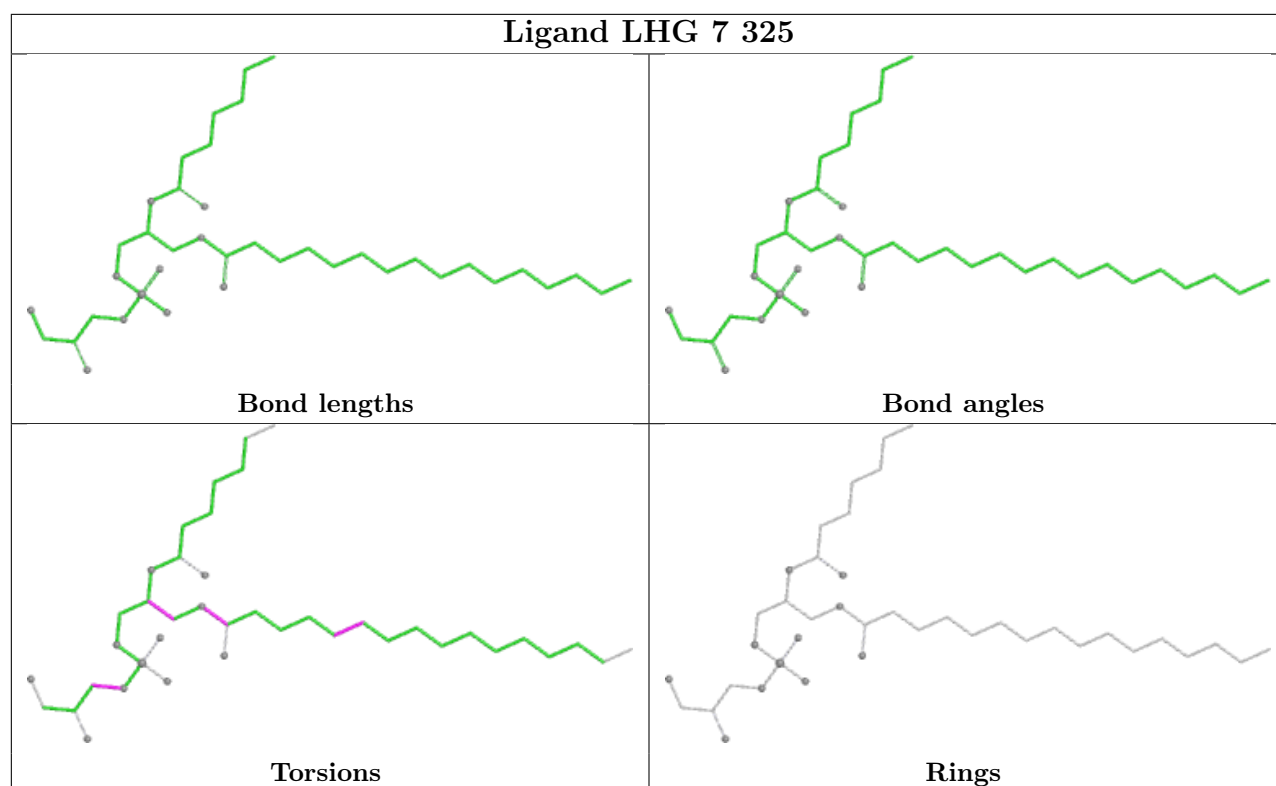
Ligand LHG 1 621

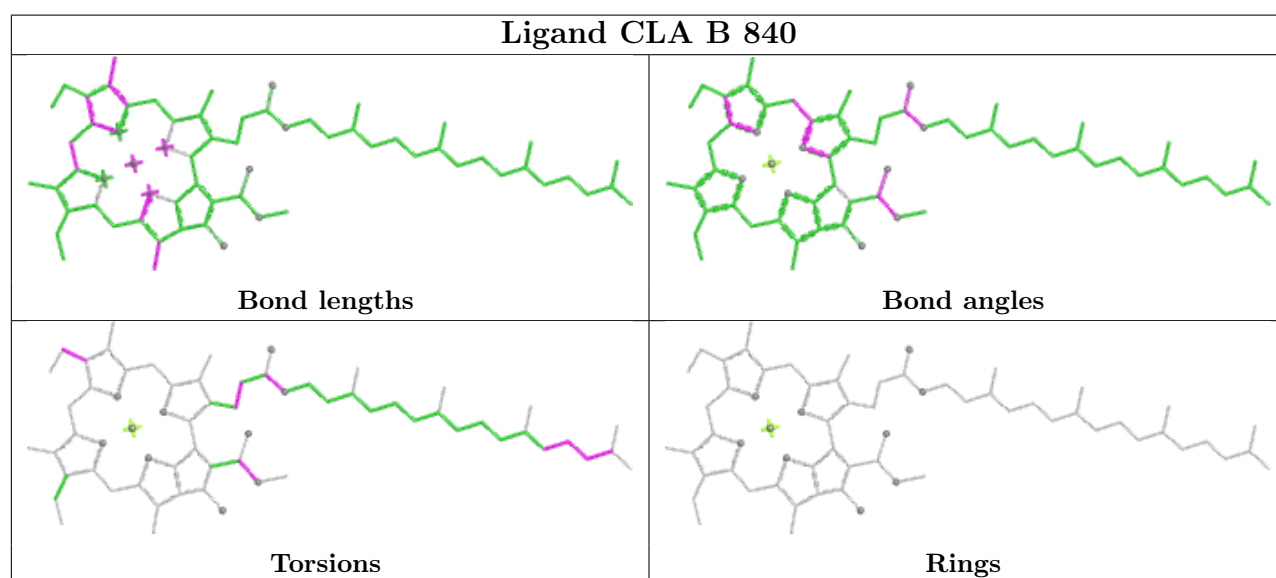
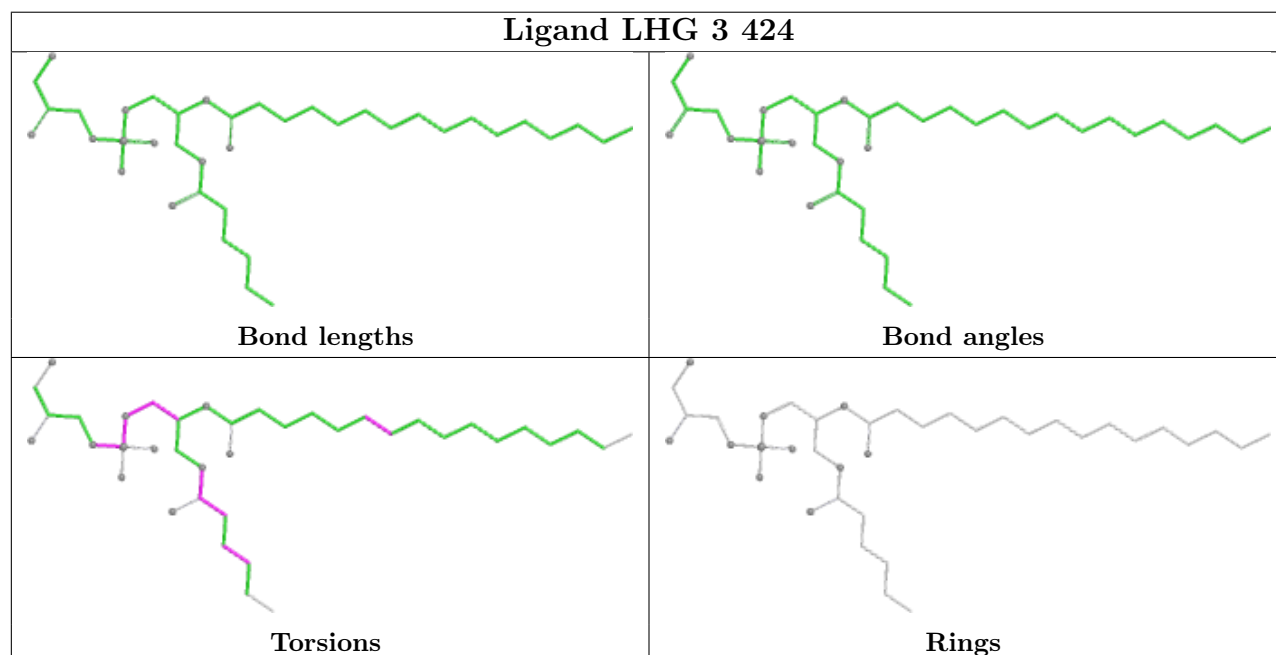
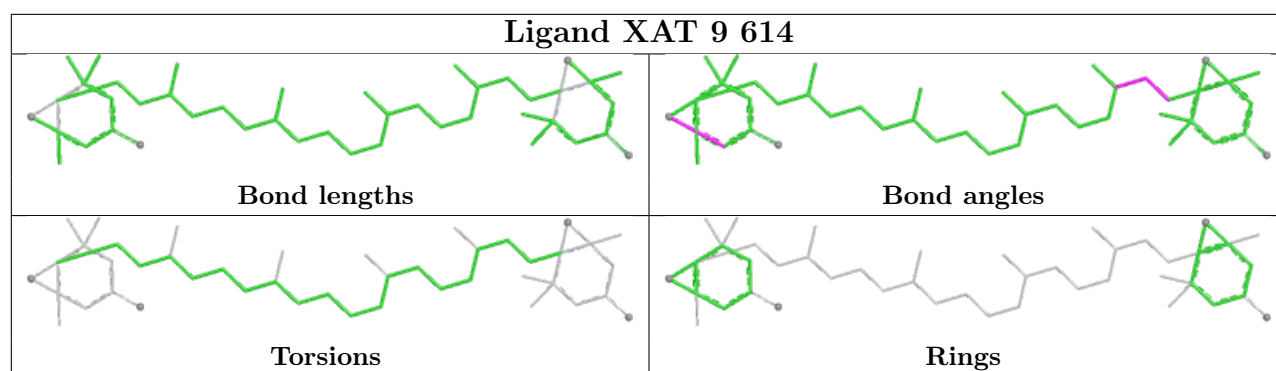


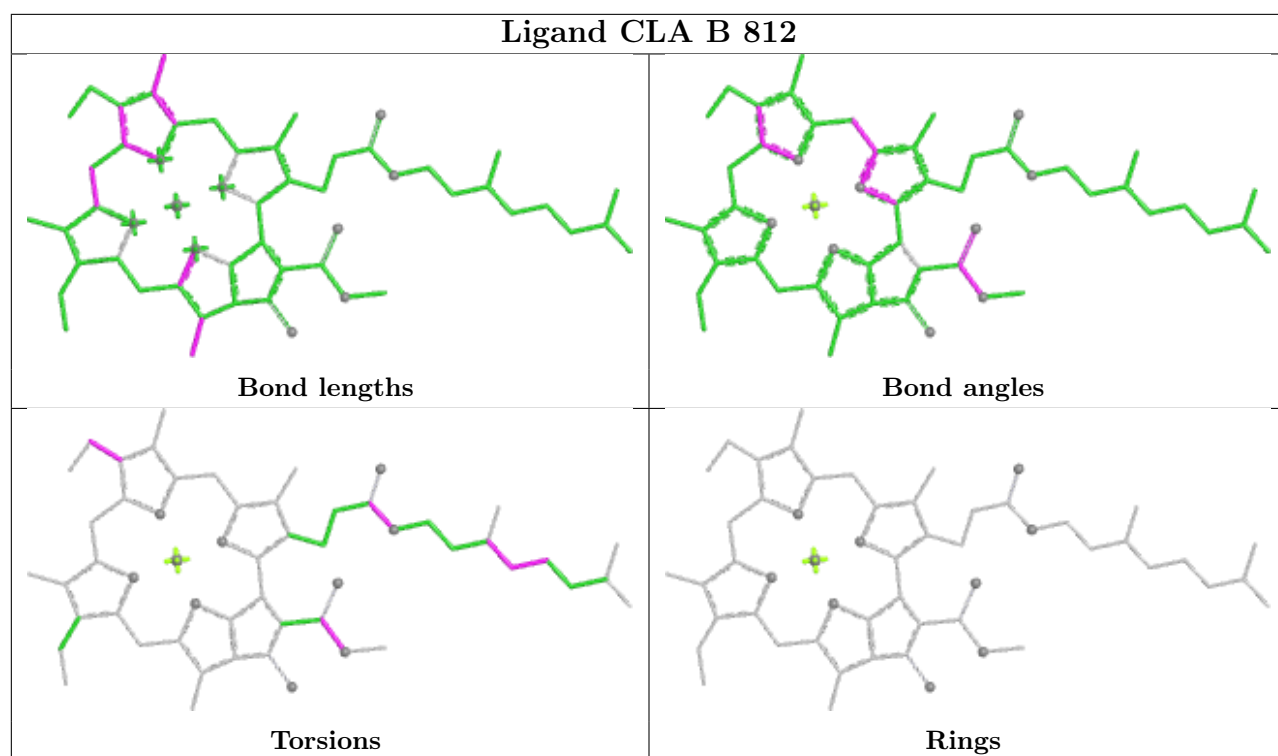




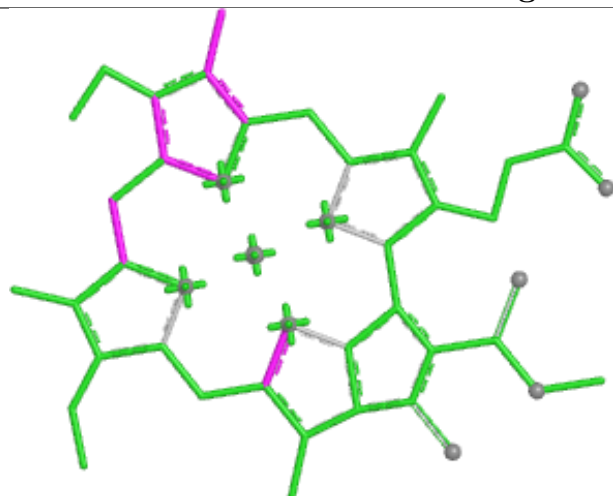




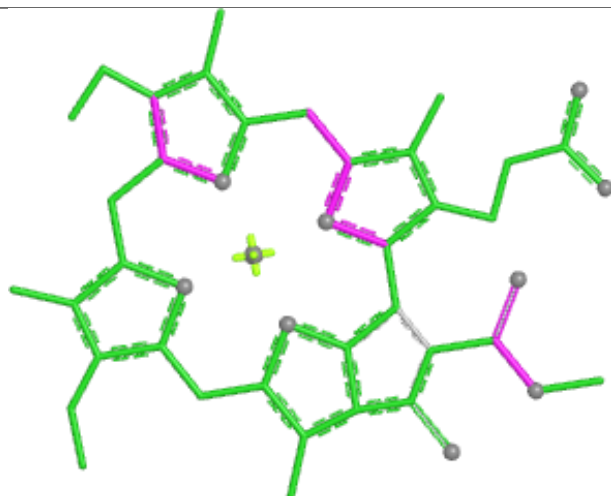




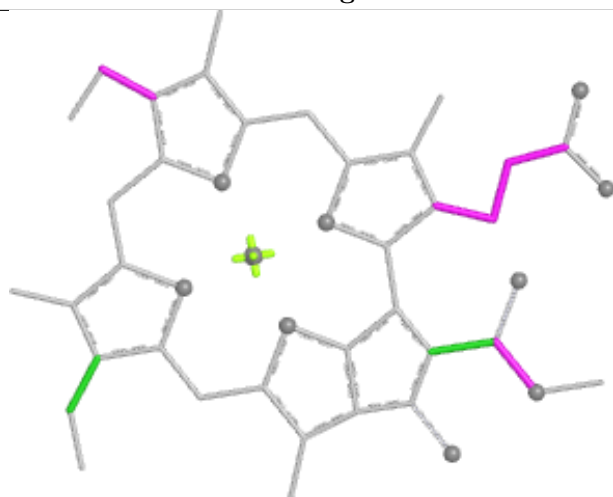
Ligand CLA 2 605



Bond lengths



Bond angles

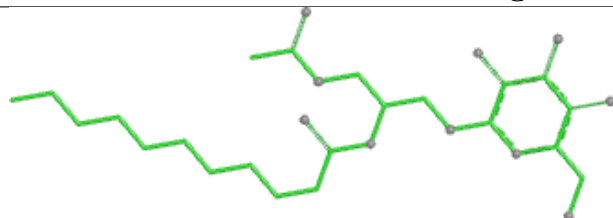


Torsions

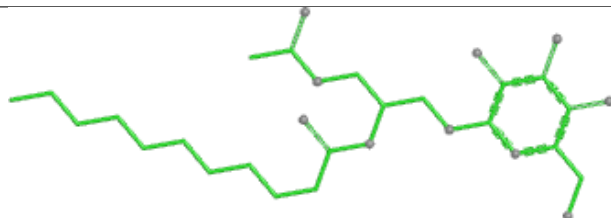


Rings

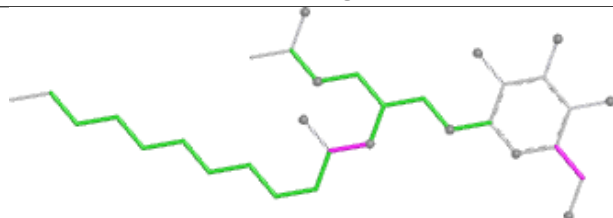
Ligand LMG A 801



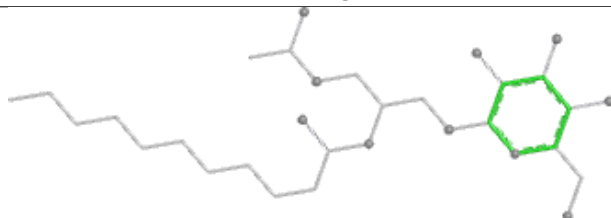
Bond lengths



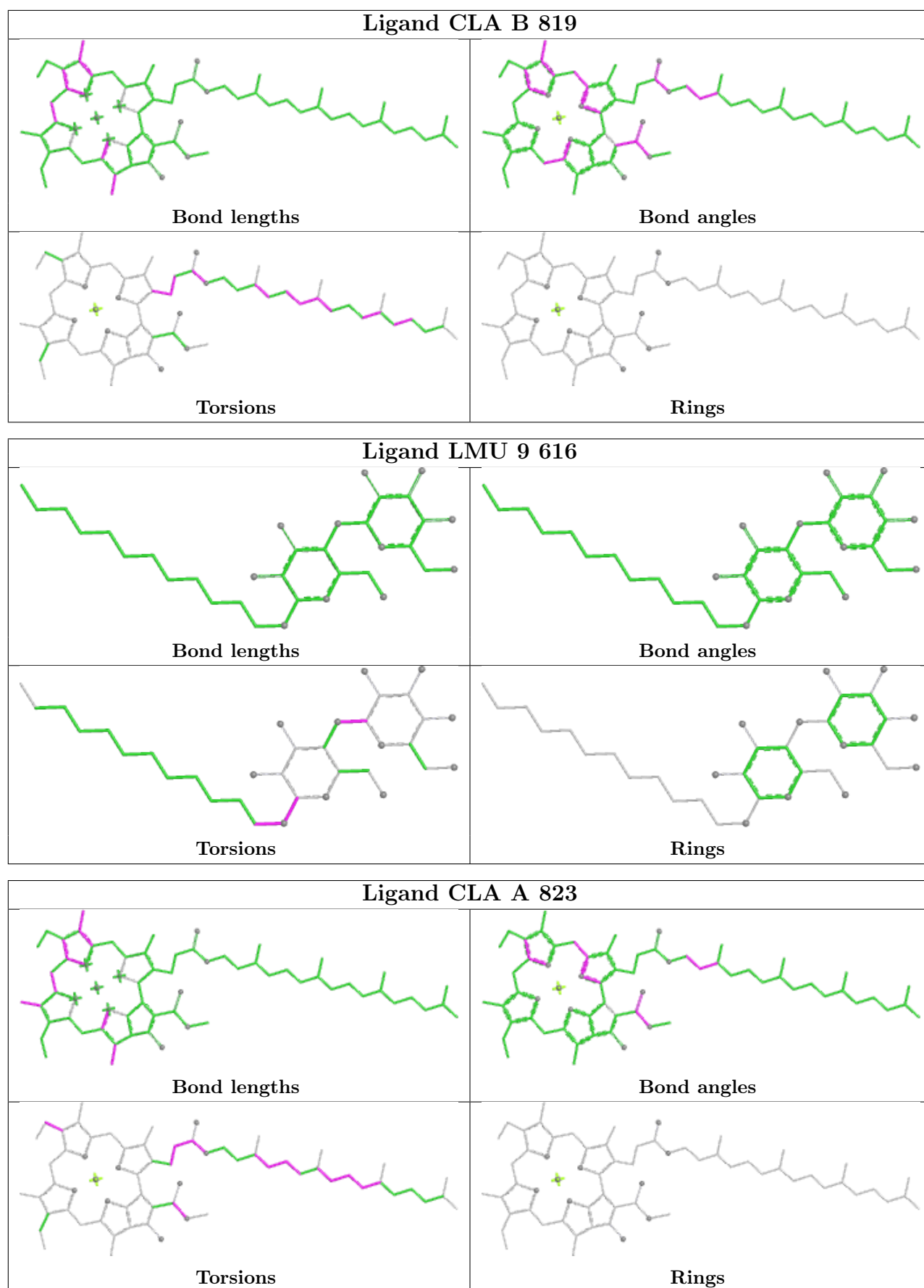
Bond angles



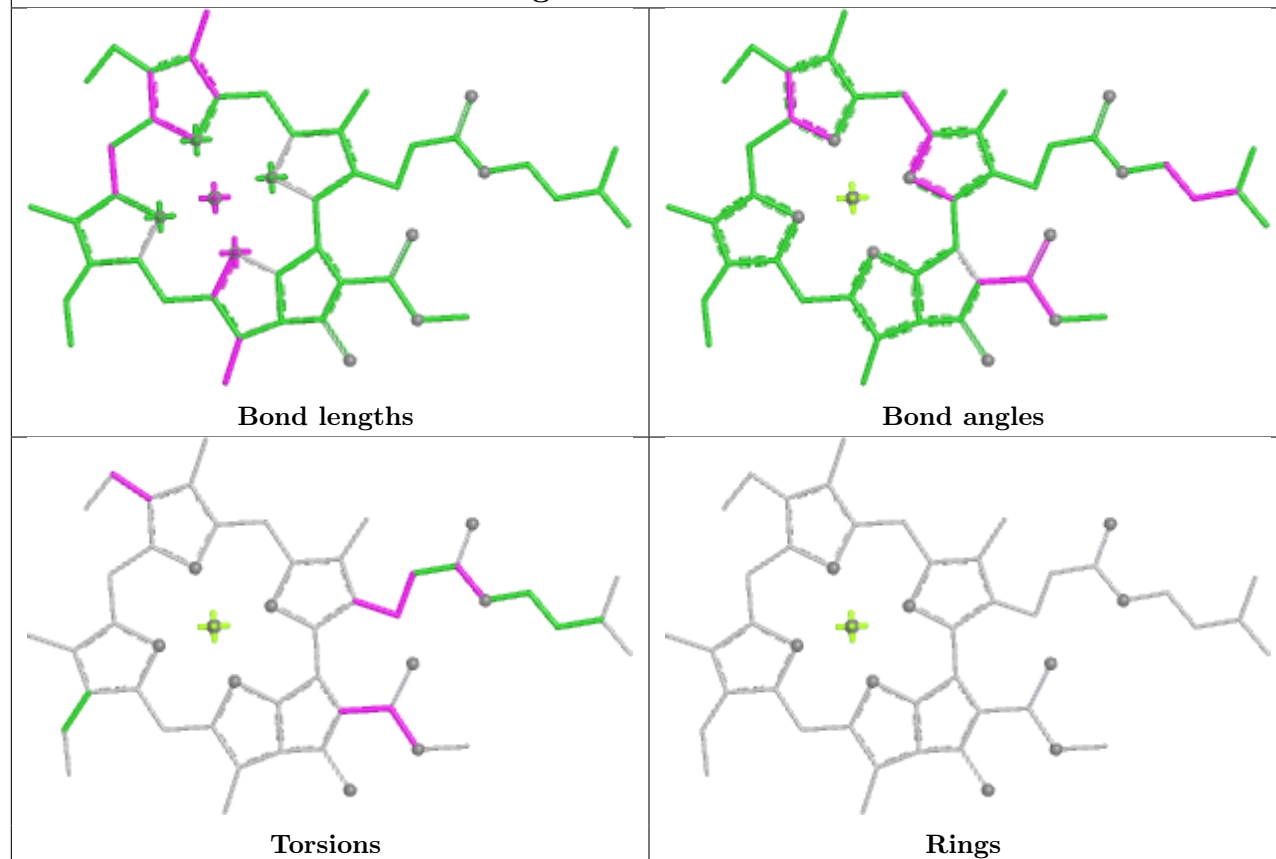
Torsions



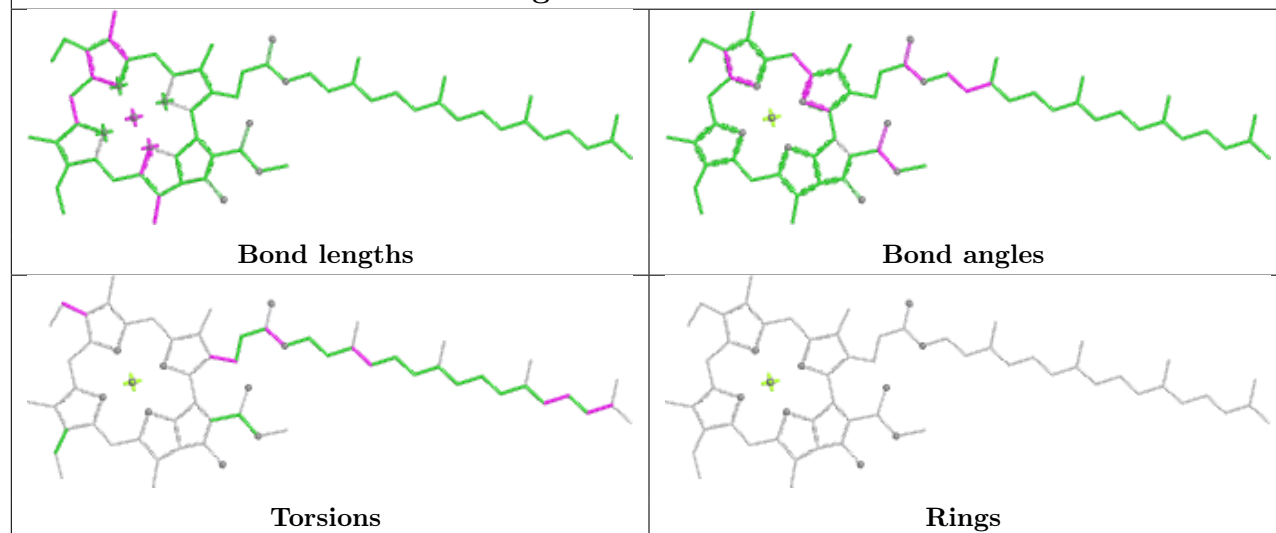
Rings



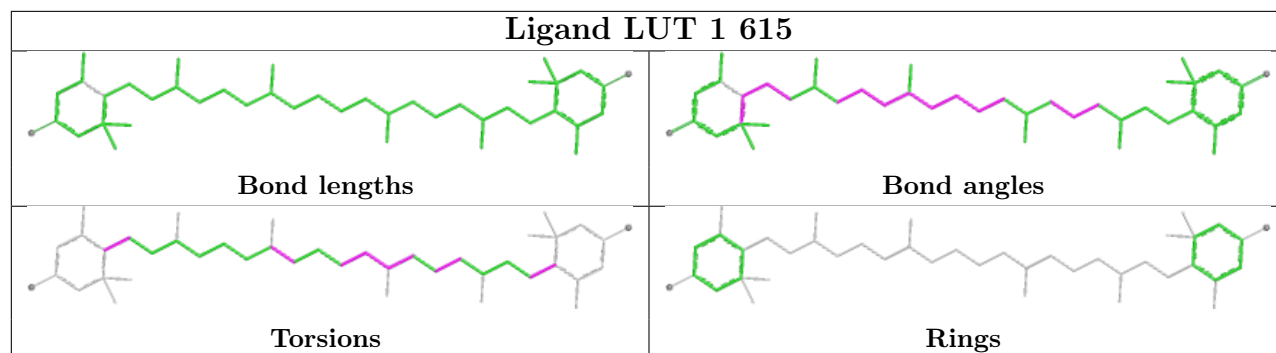
Ligand CLA B 836



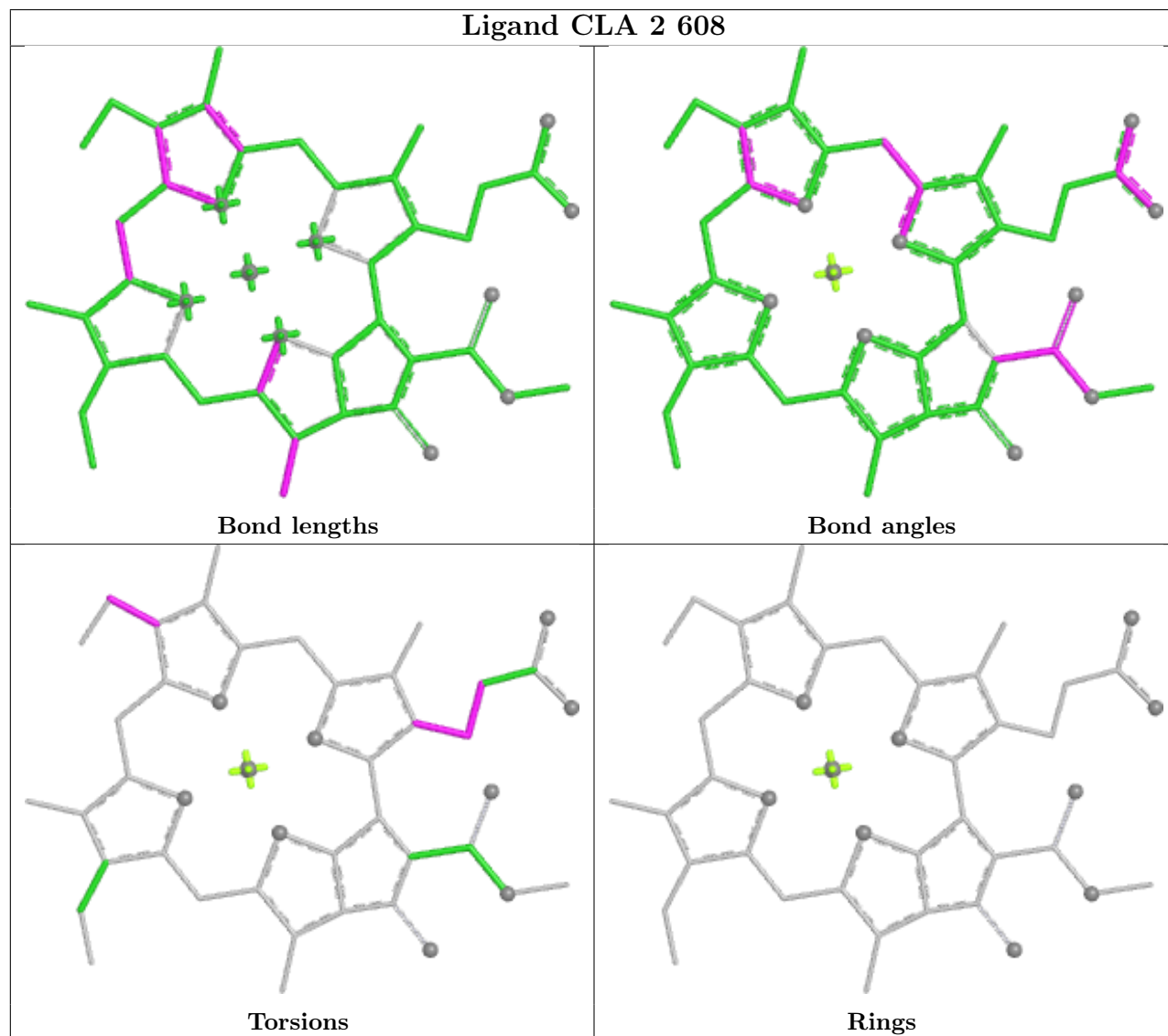
Ligand CLA B 821



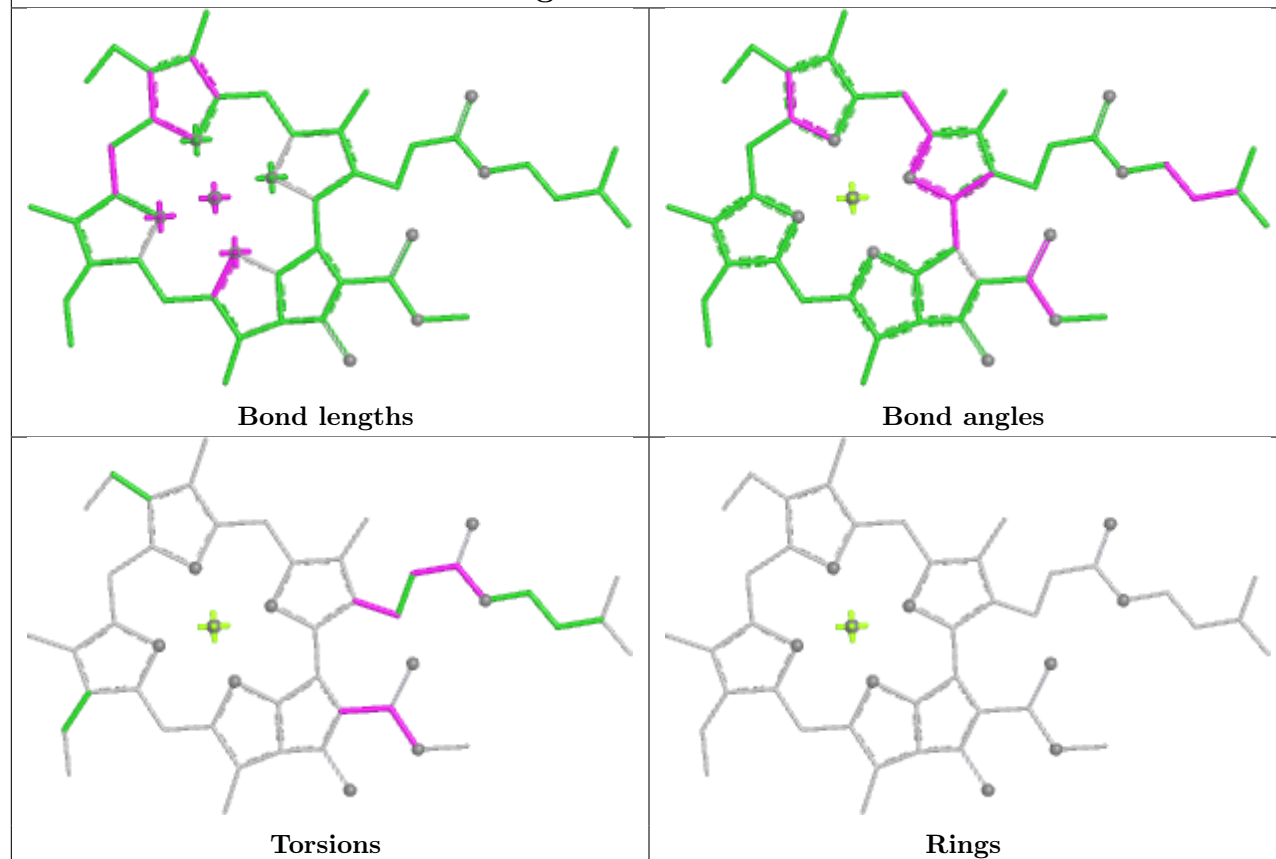
Ligand LUT 1 615



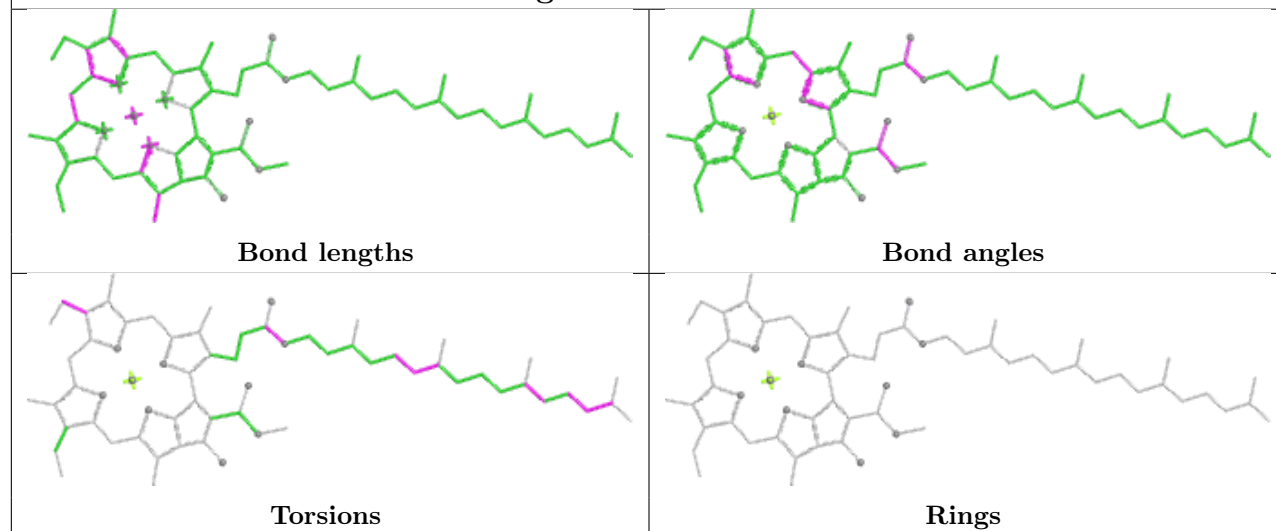
Ligand CLA 2 608



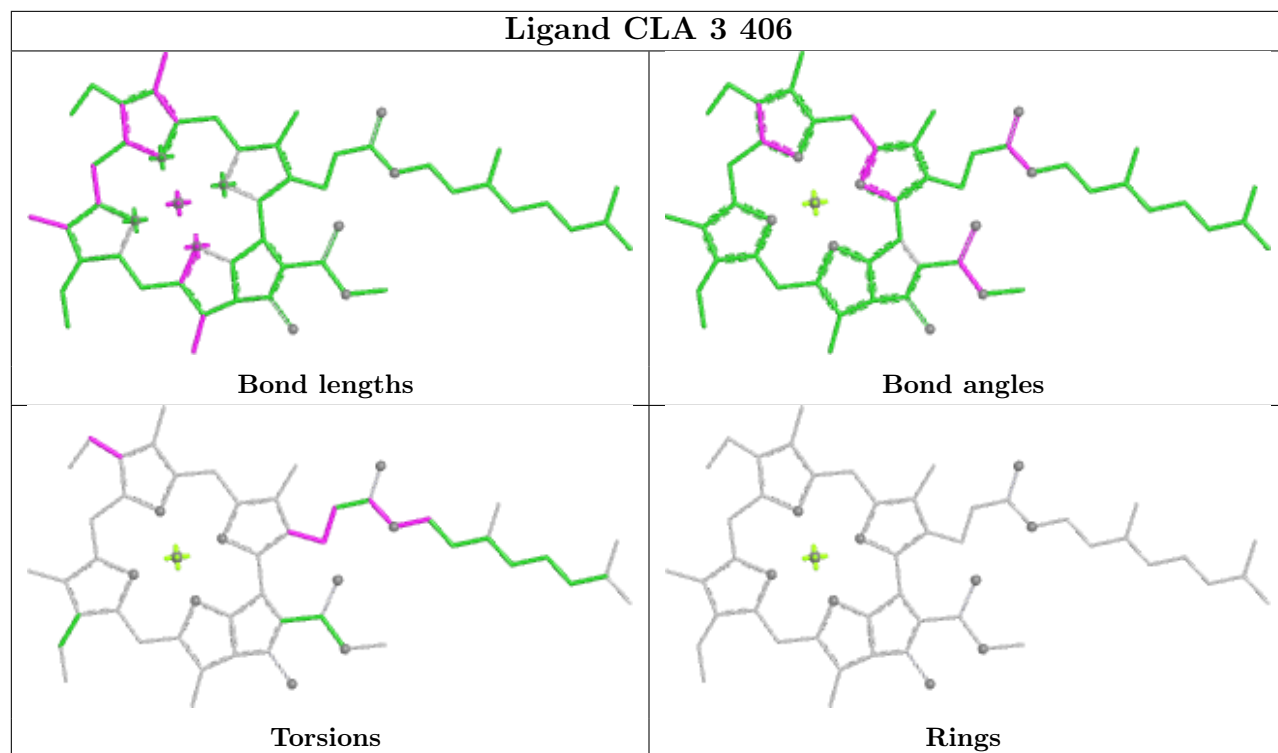
Ligand CLA 9 610



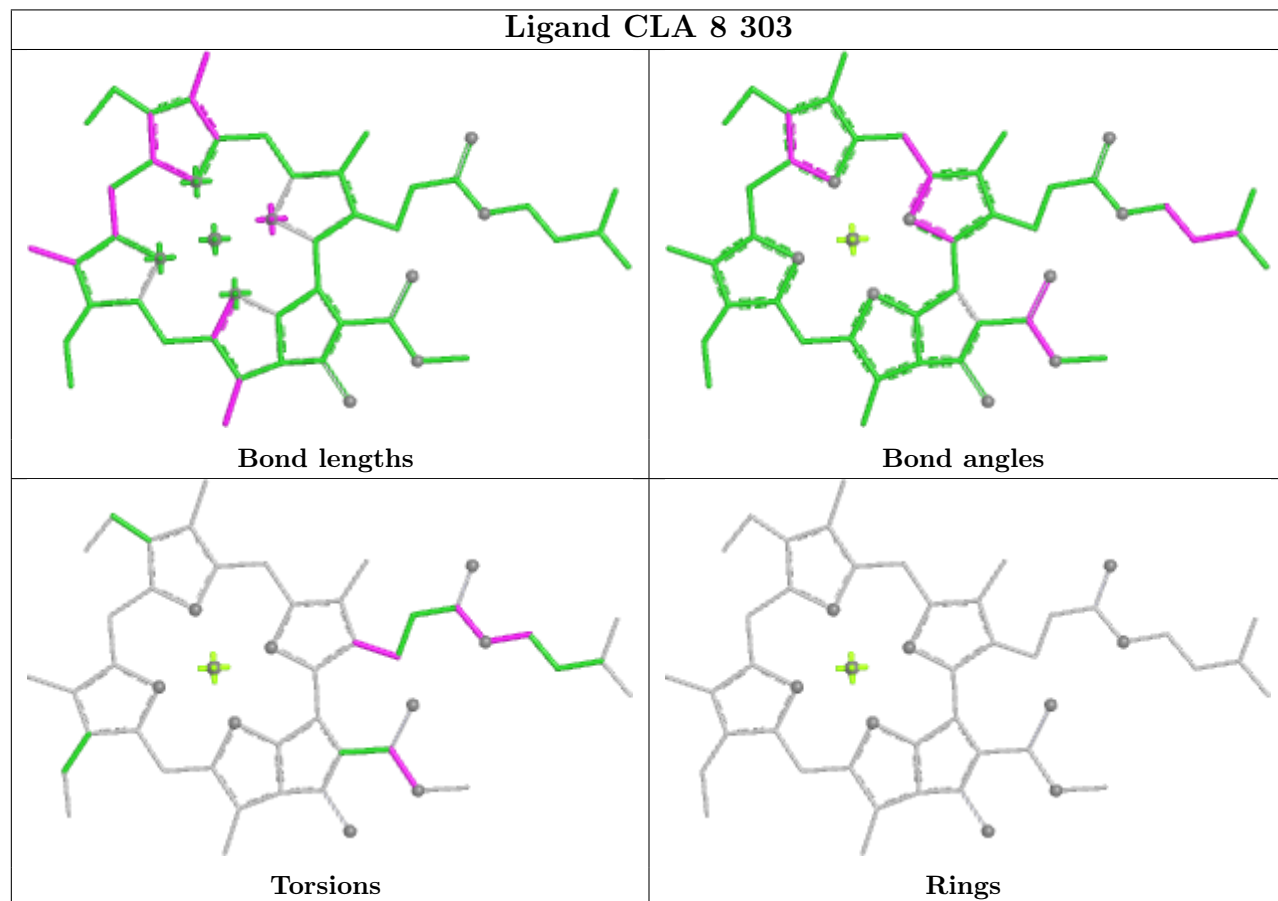
Ligand CLA 9 607

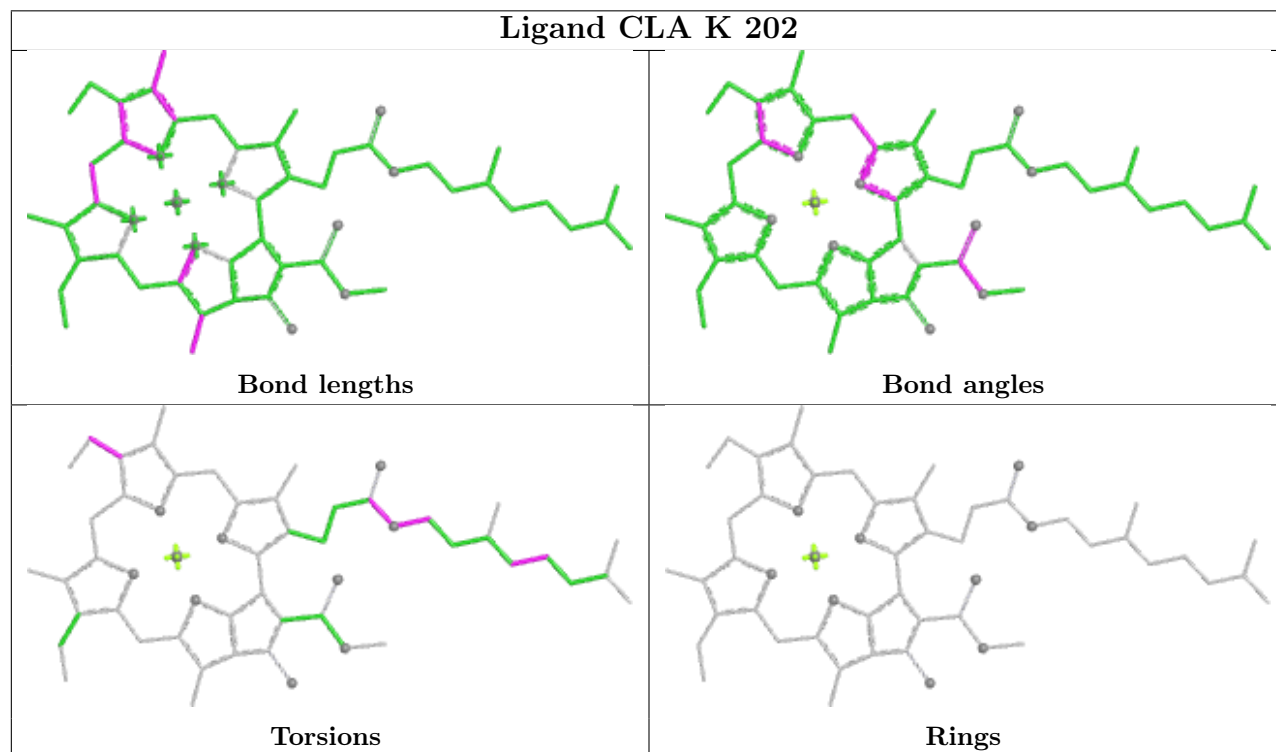
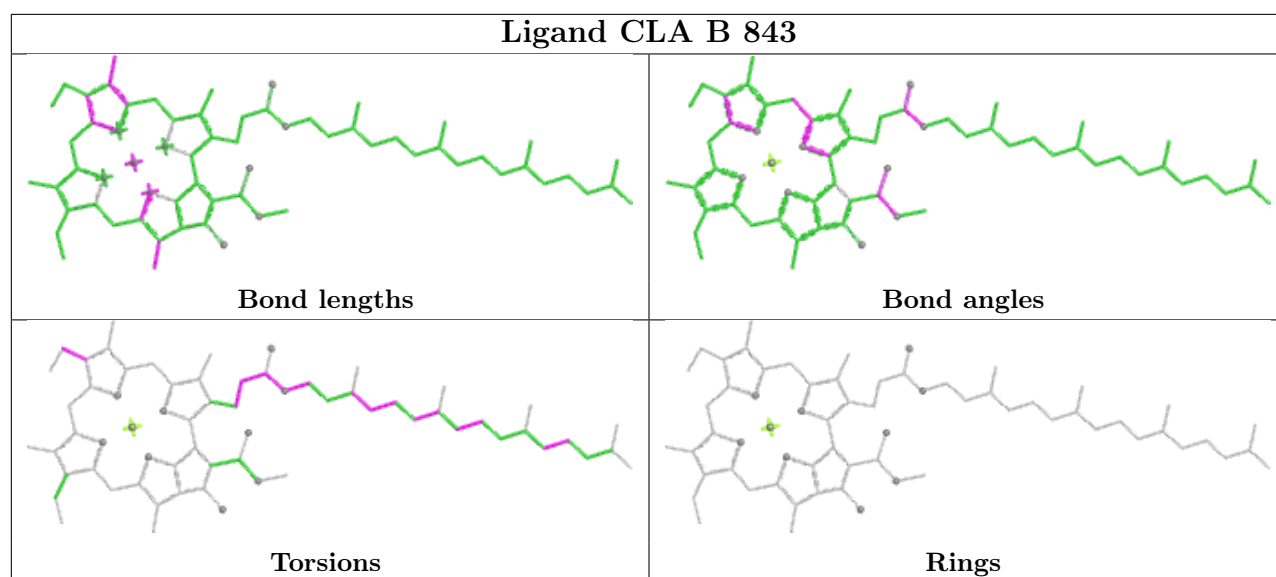


Ligand CLA 3 406

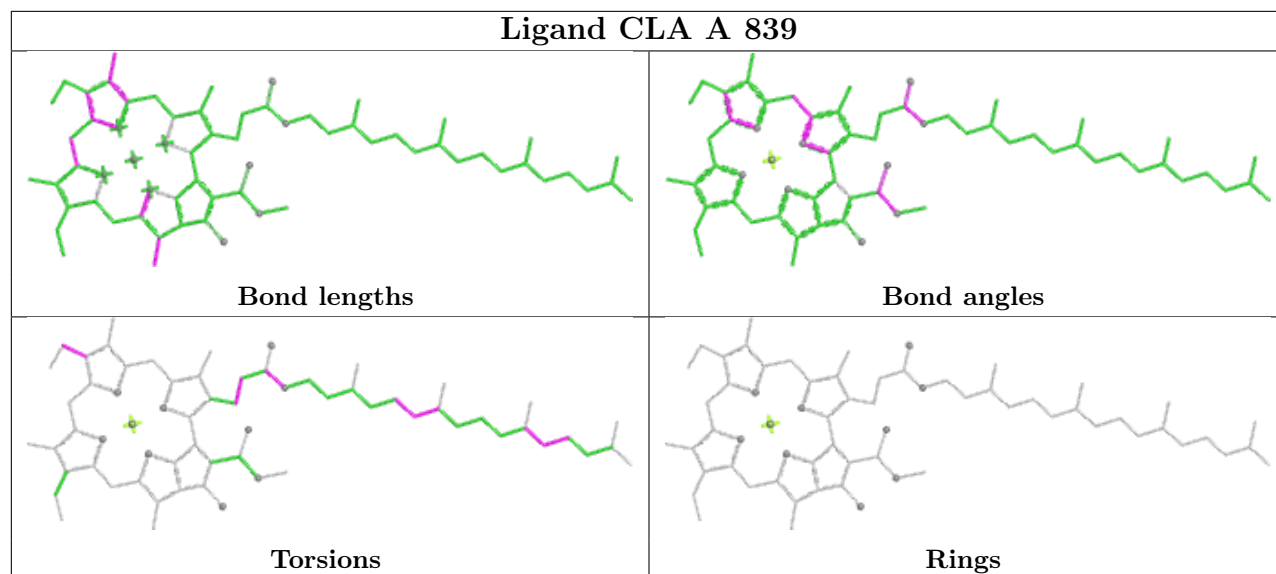


Ligand CLA 8 303

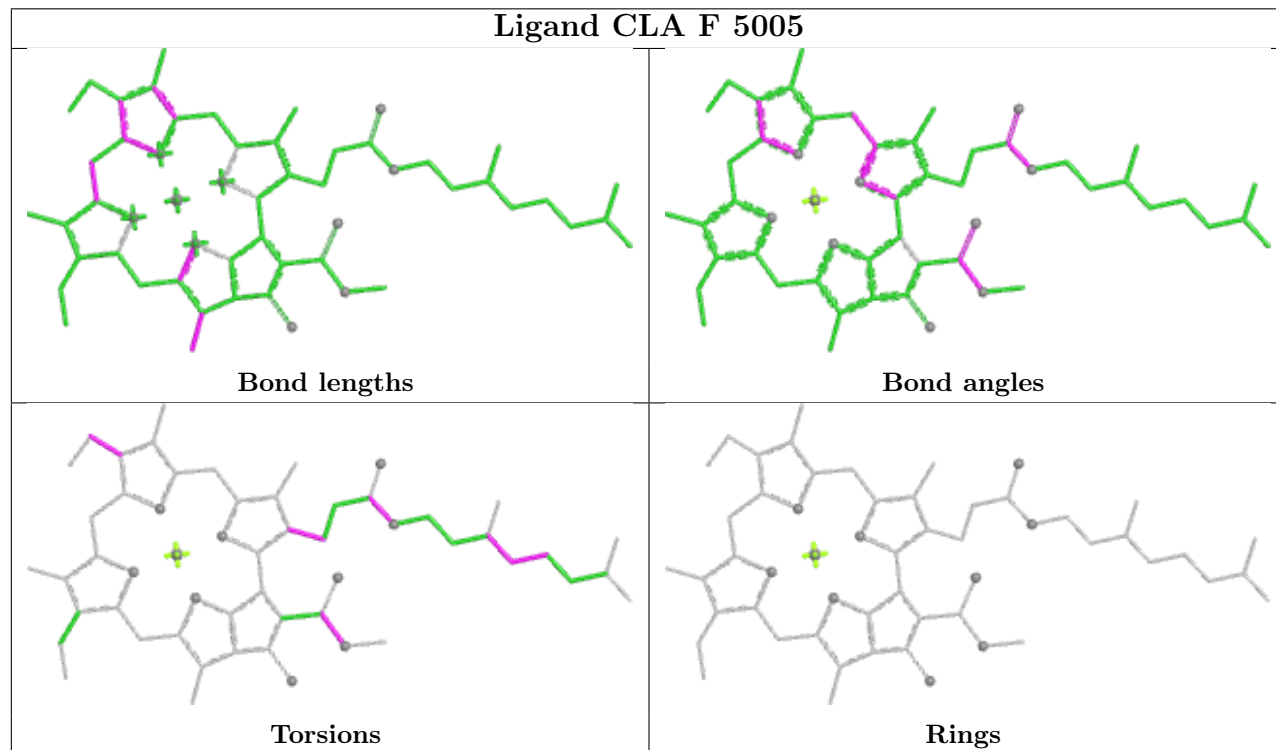


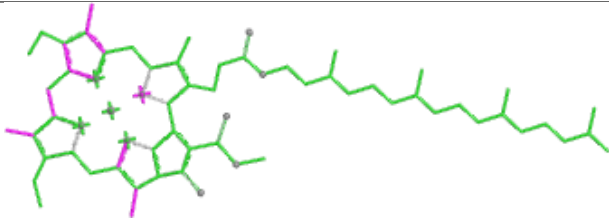
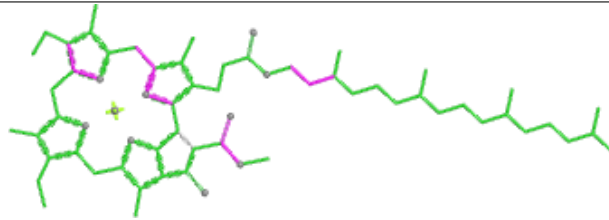
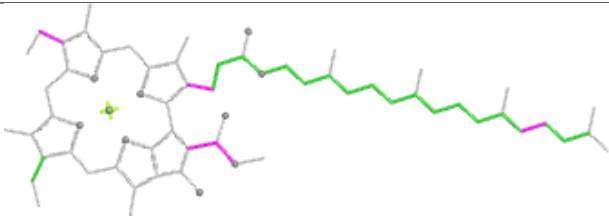
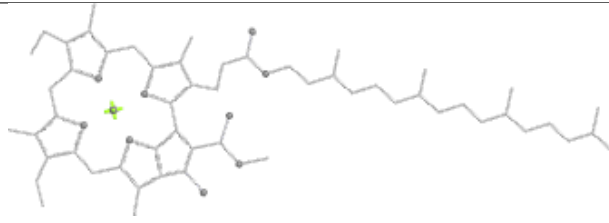


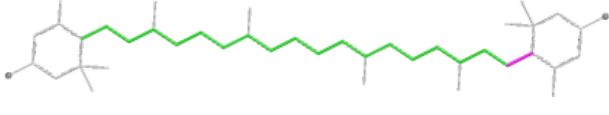
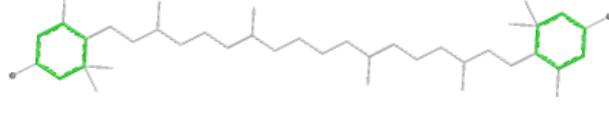
Ligand CLA A 839

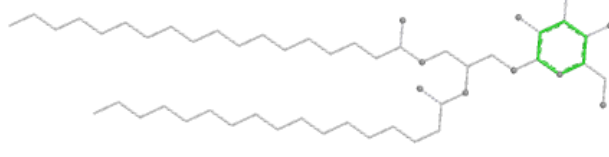


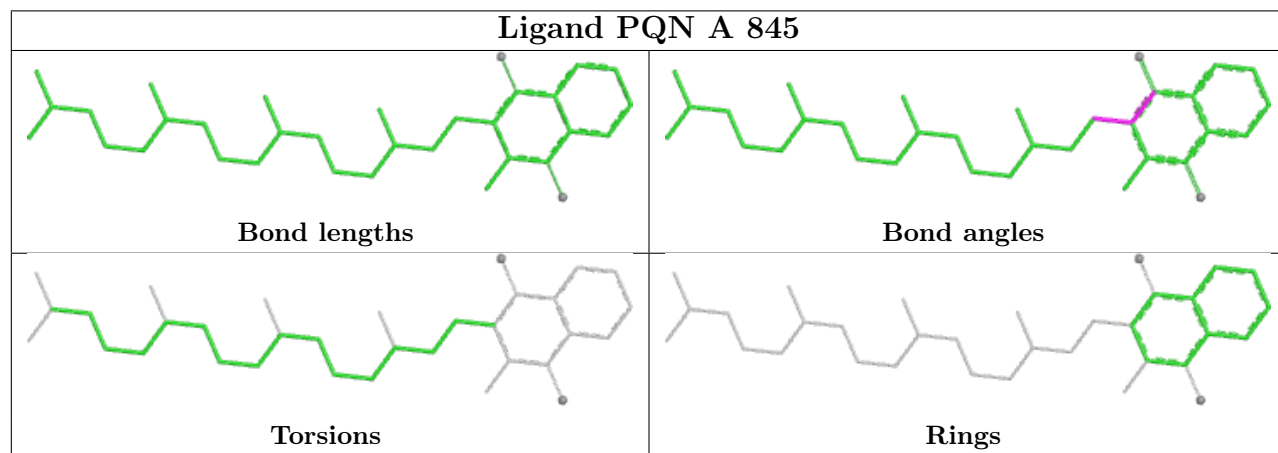
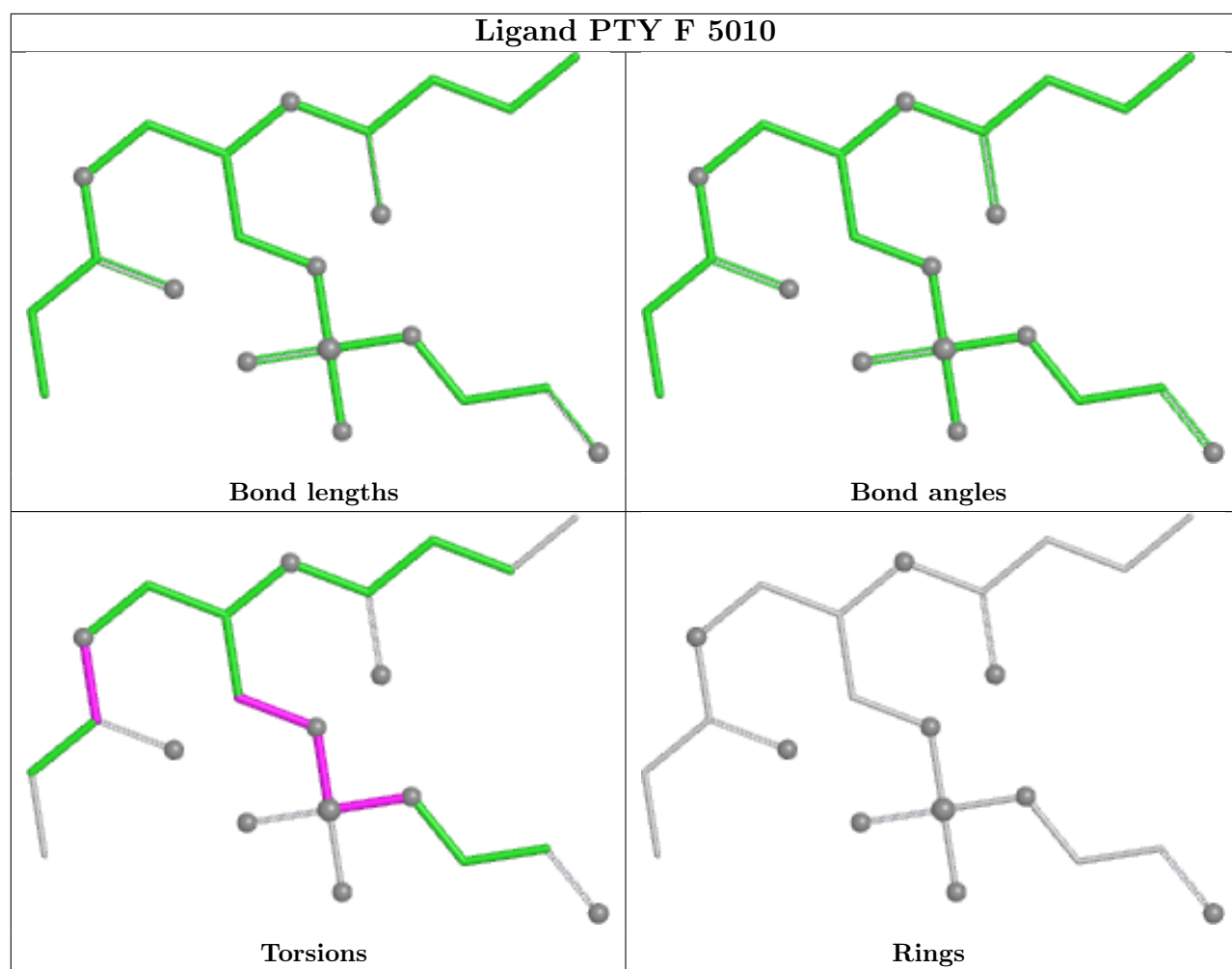
Ligand CLA F 5005

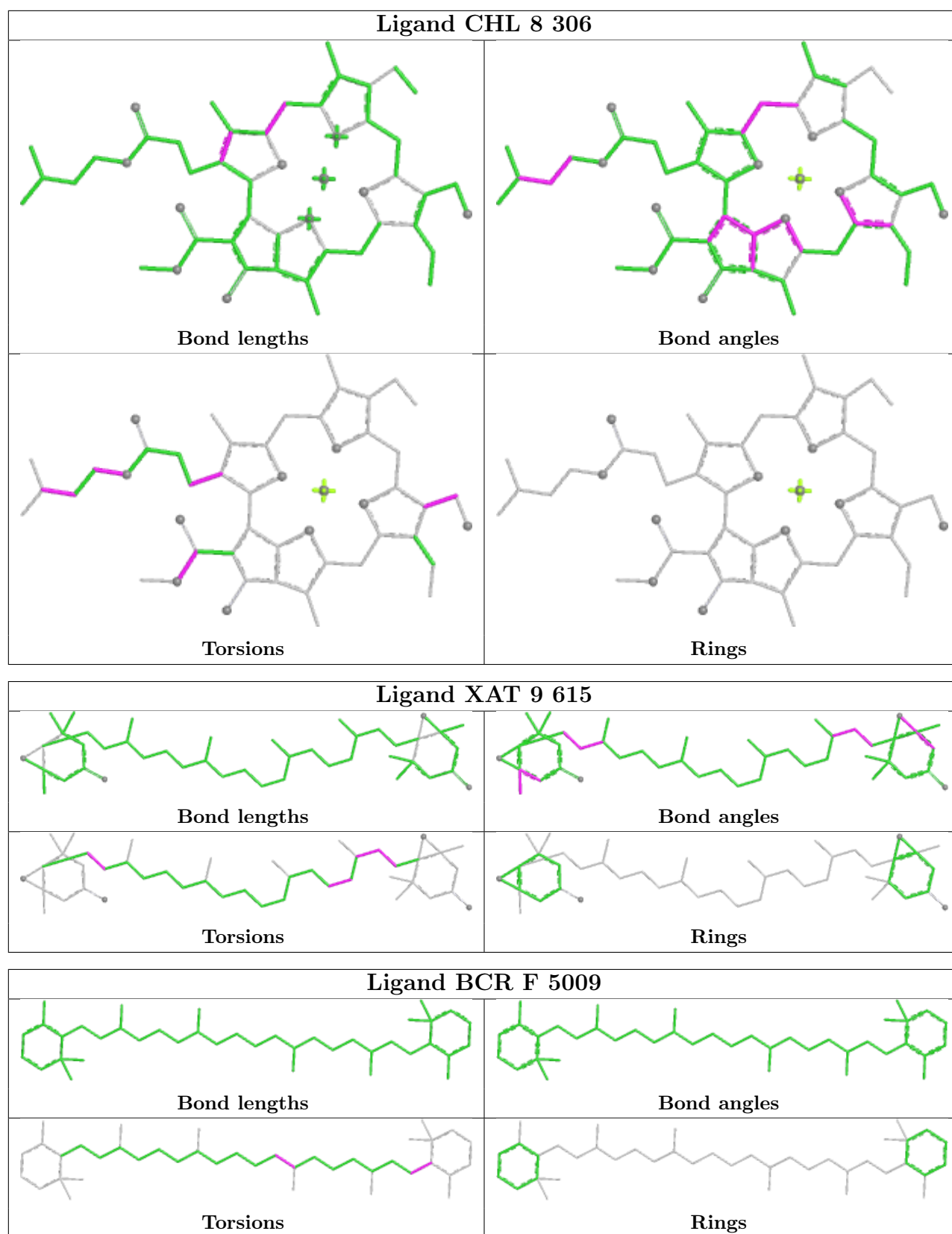


Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

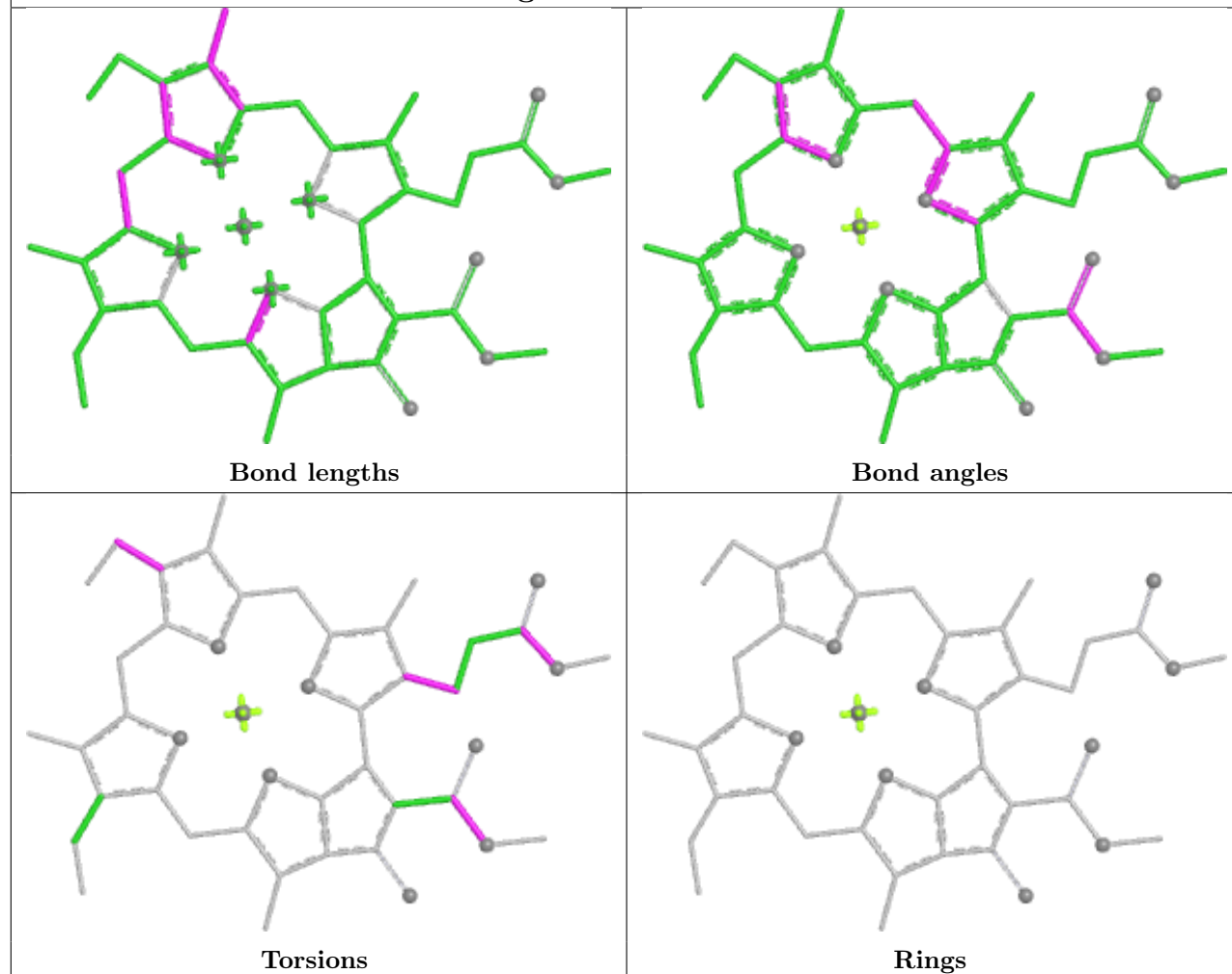
Ligand LUT 8 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 7 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

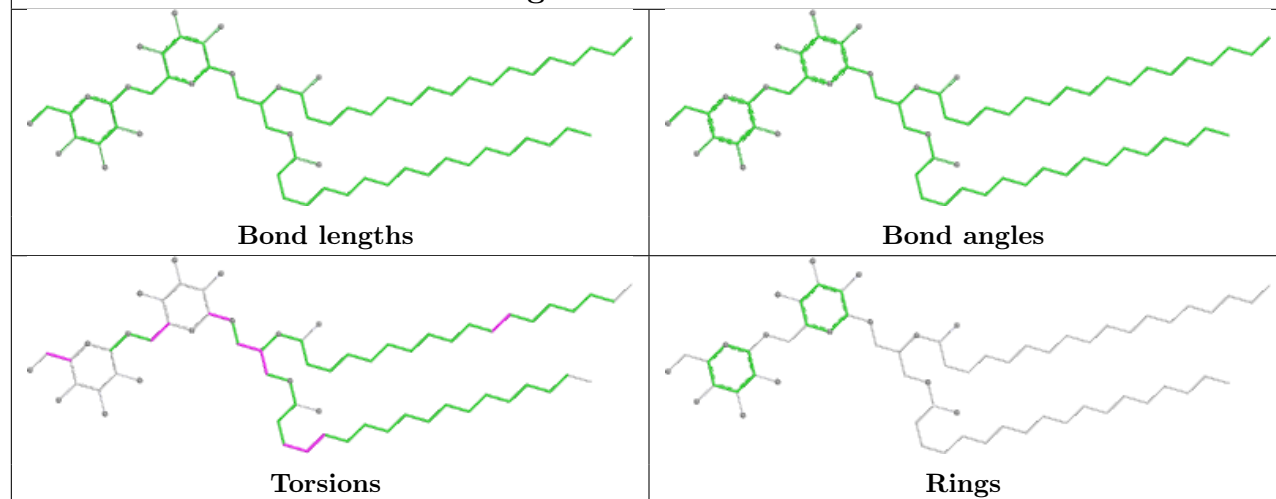


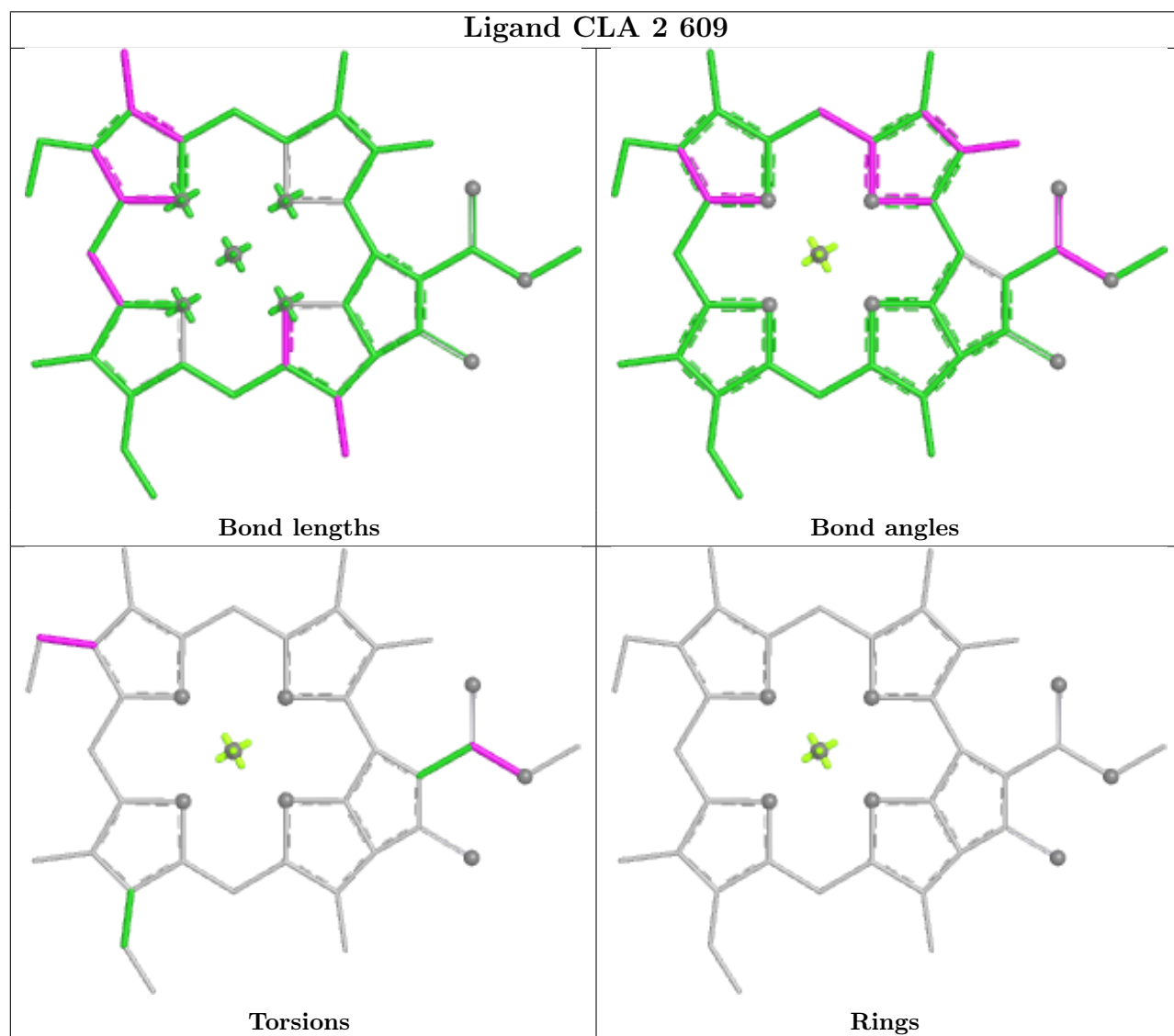
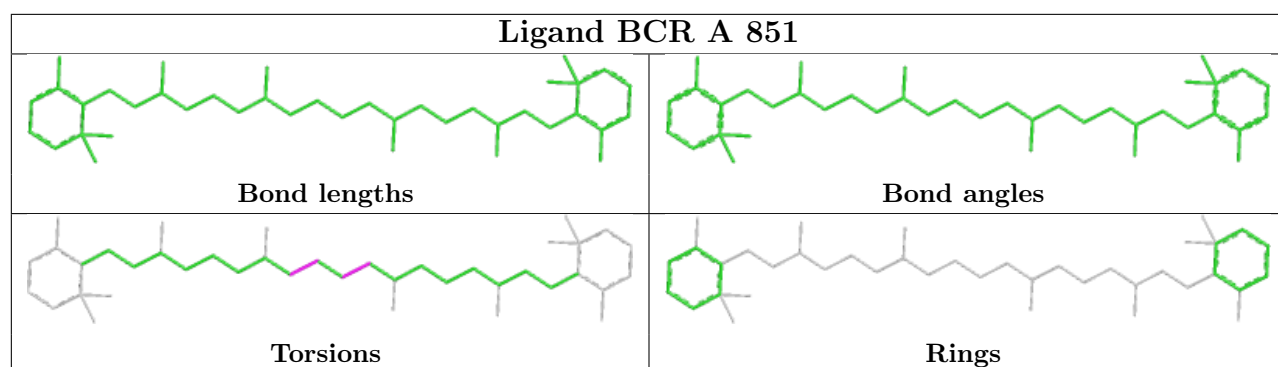


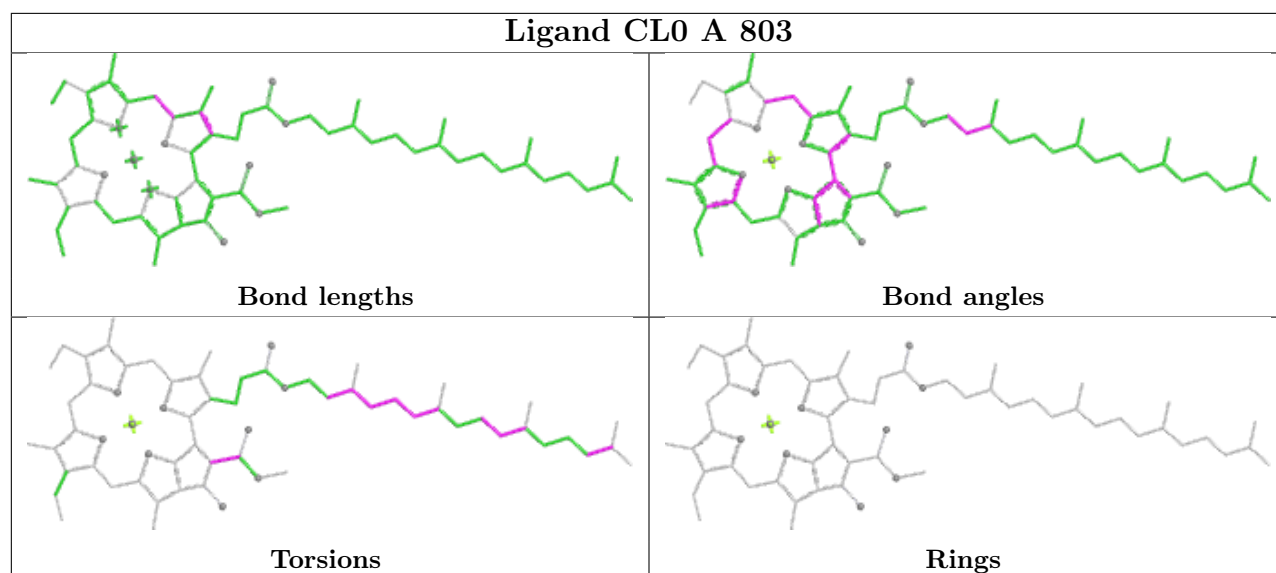
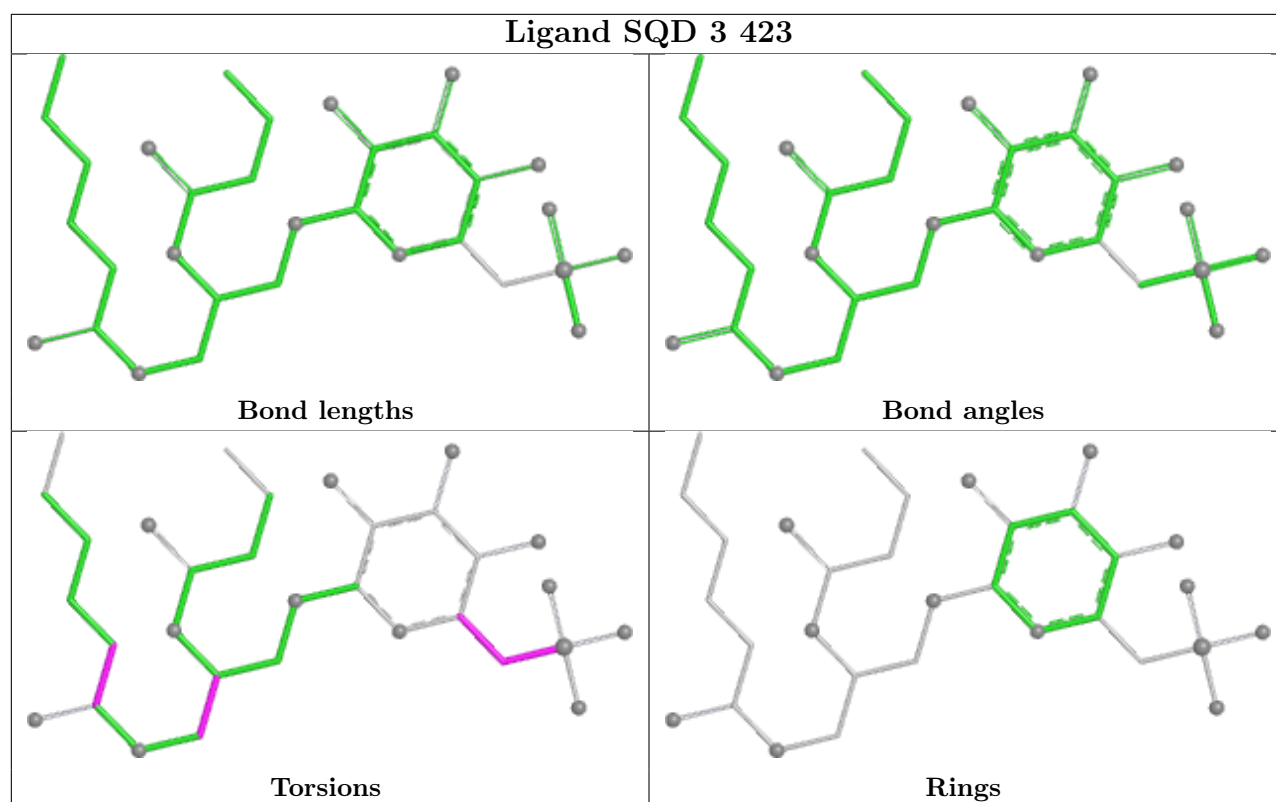
Ligand CLA 8 312

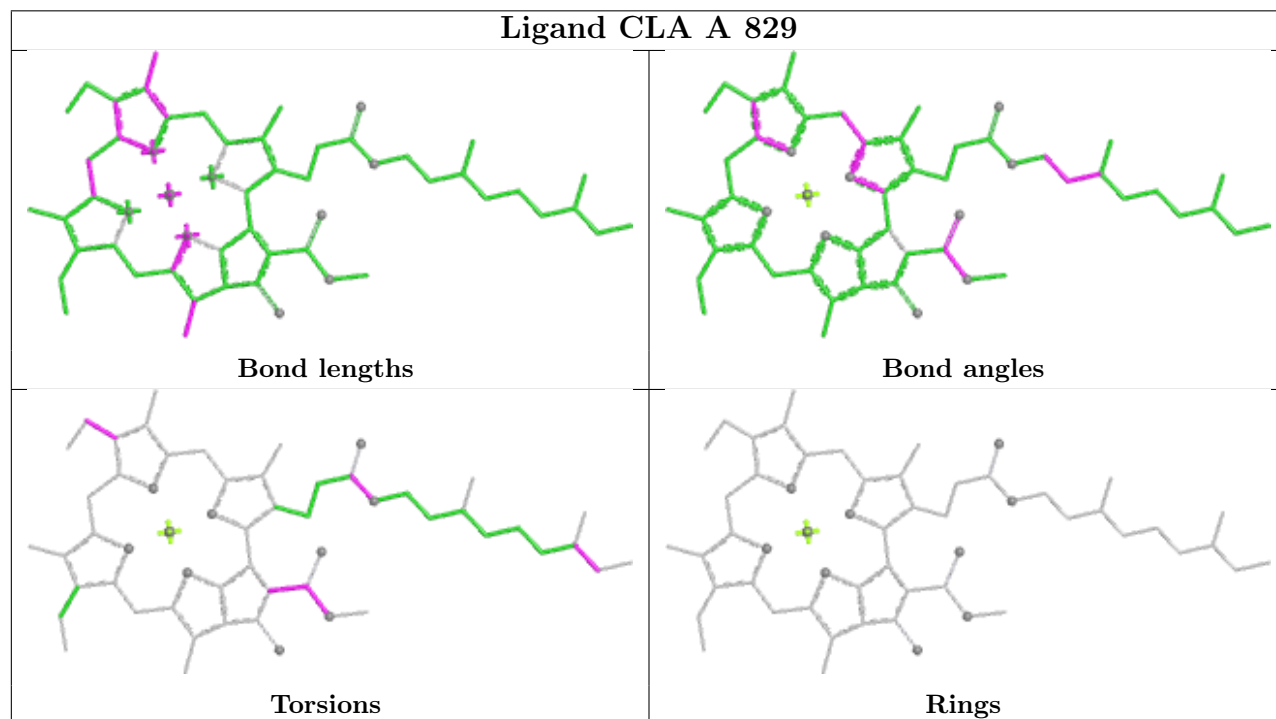
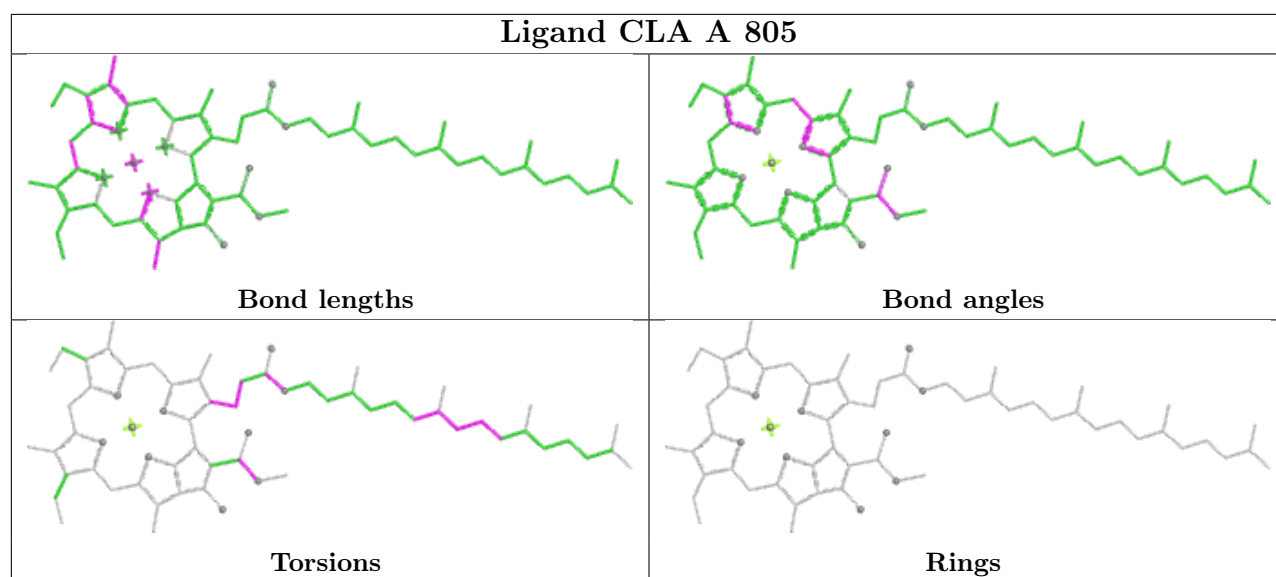


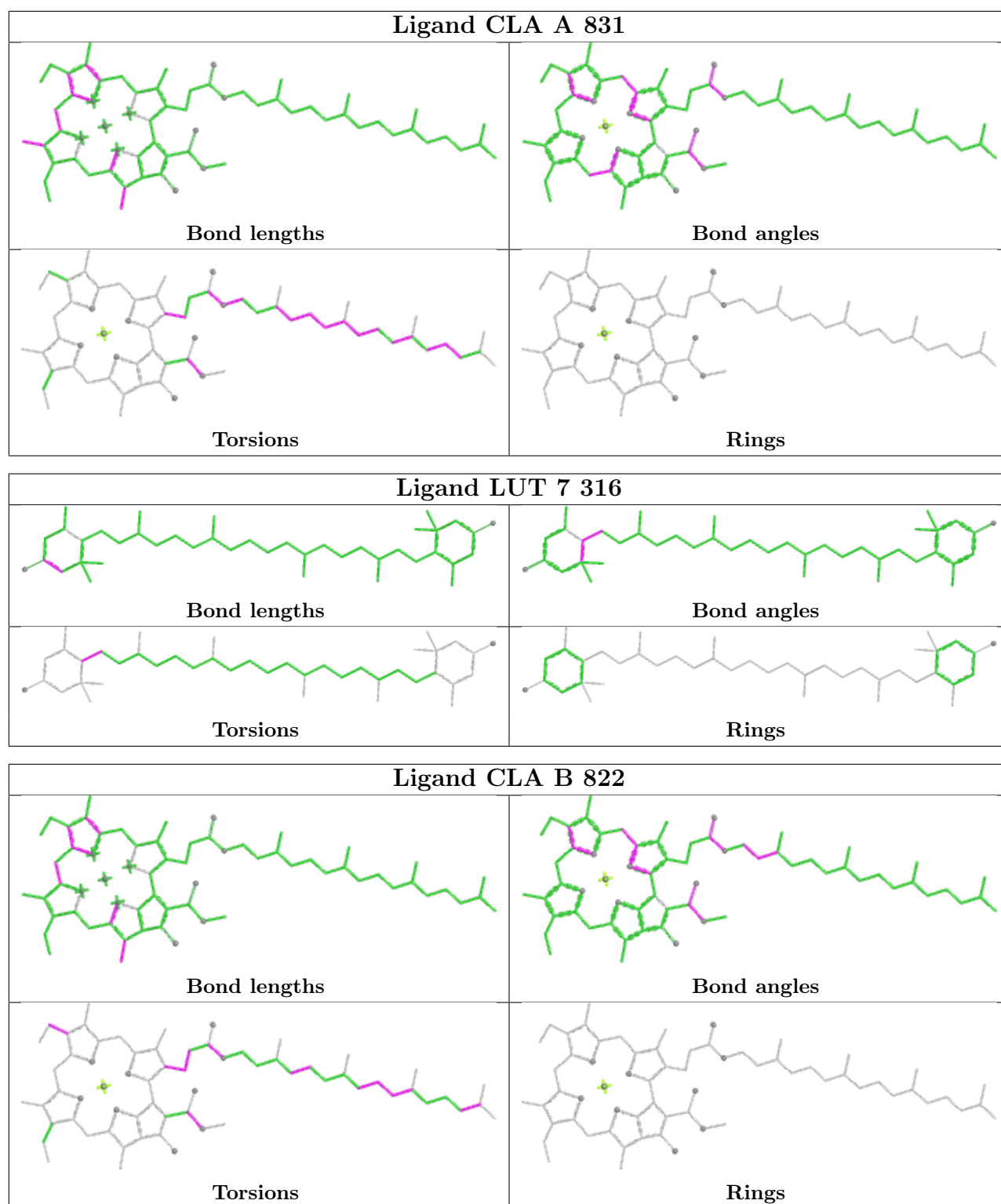
Ligand DGD A 802



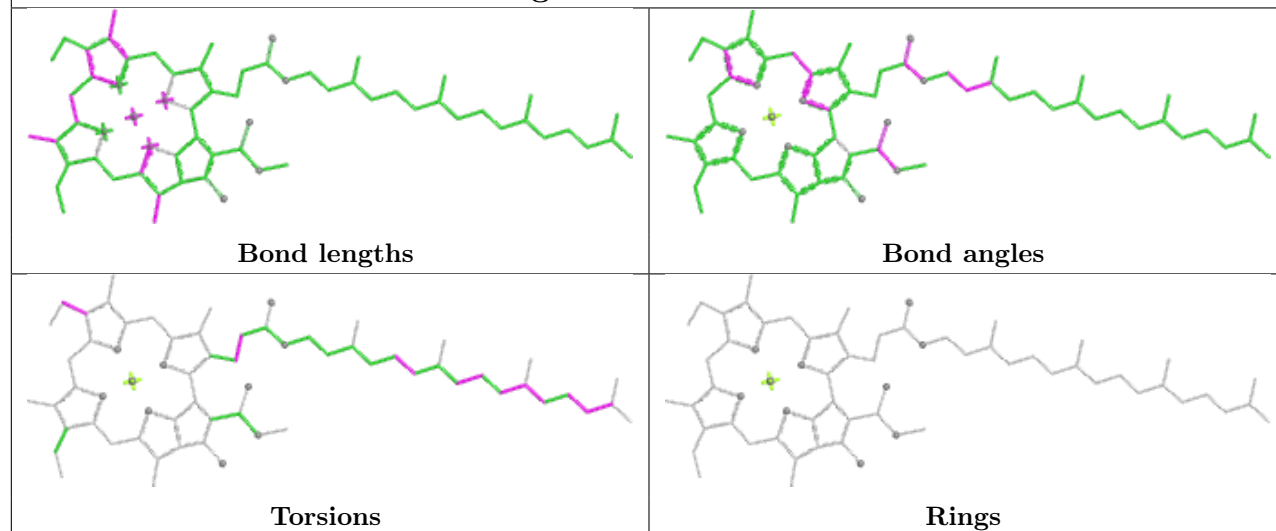




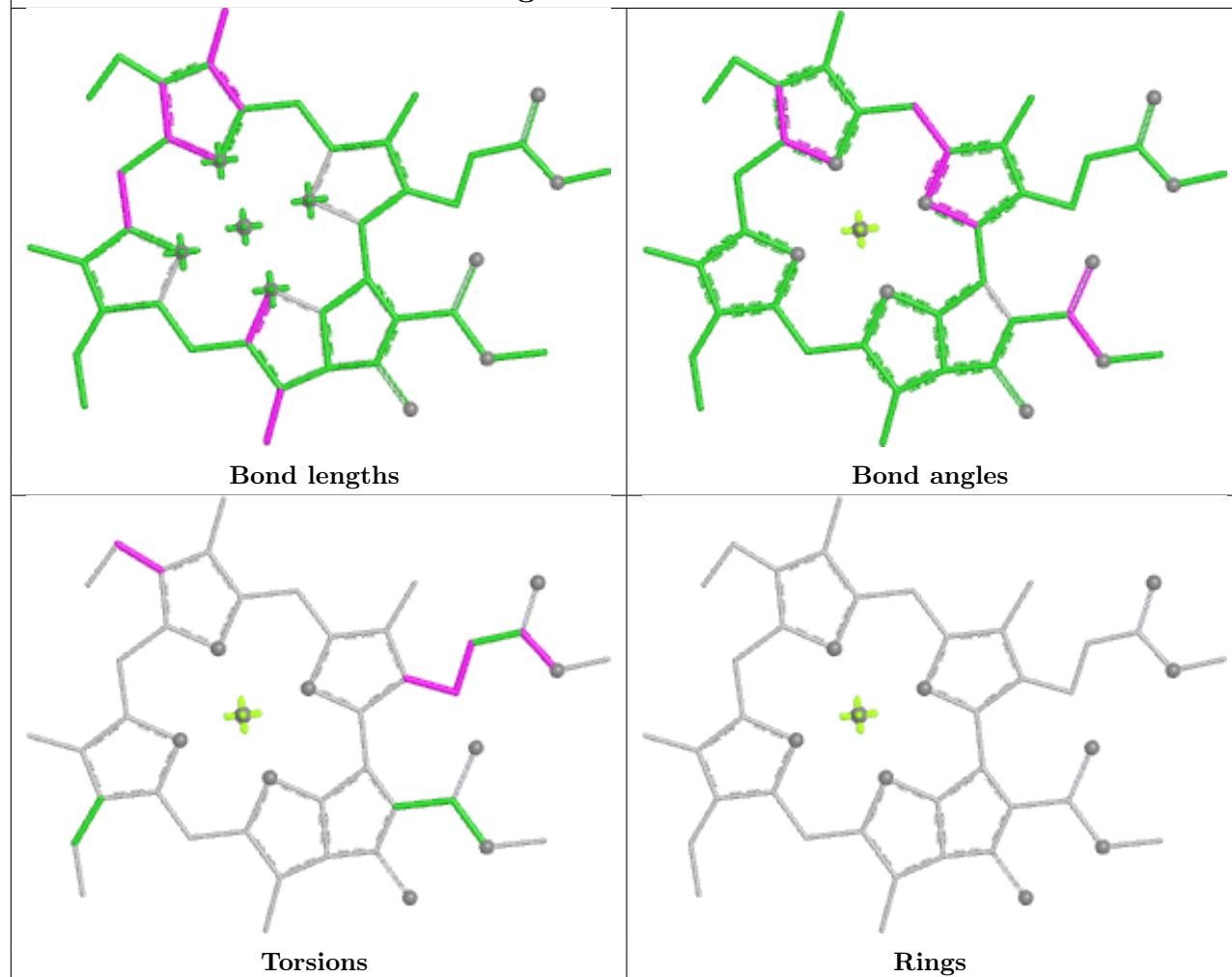


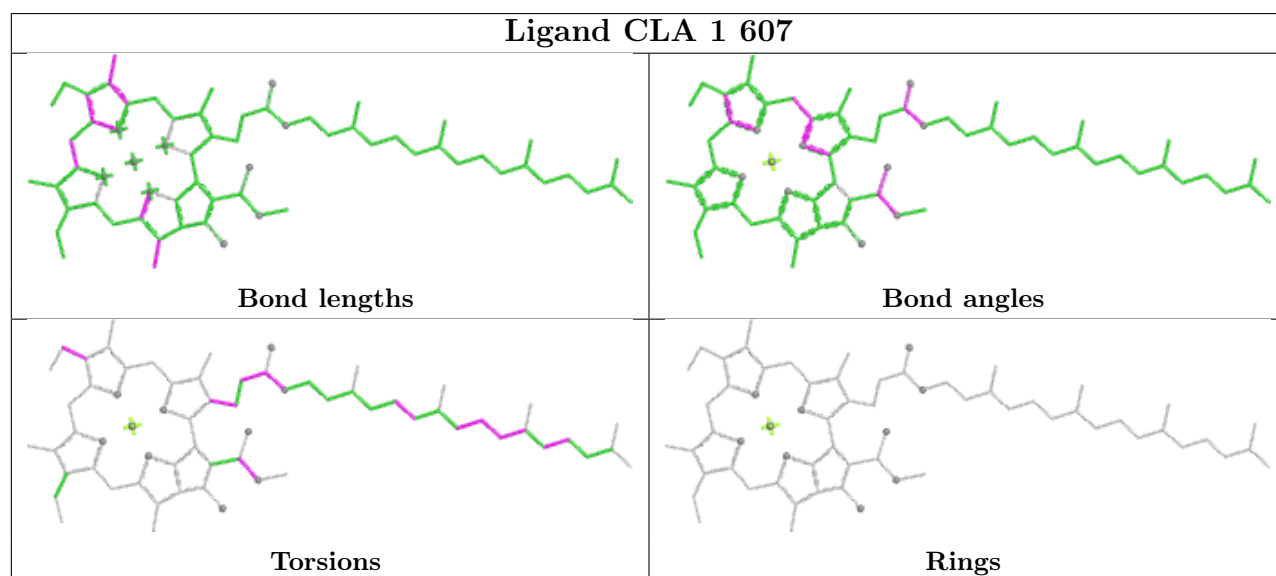
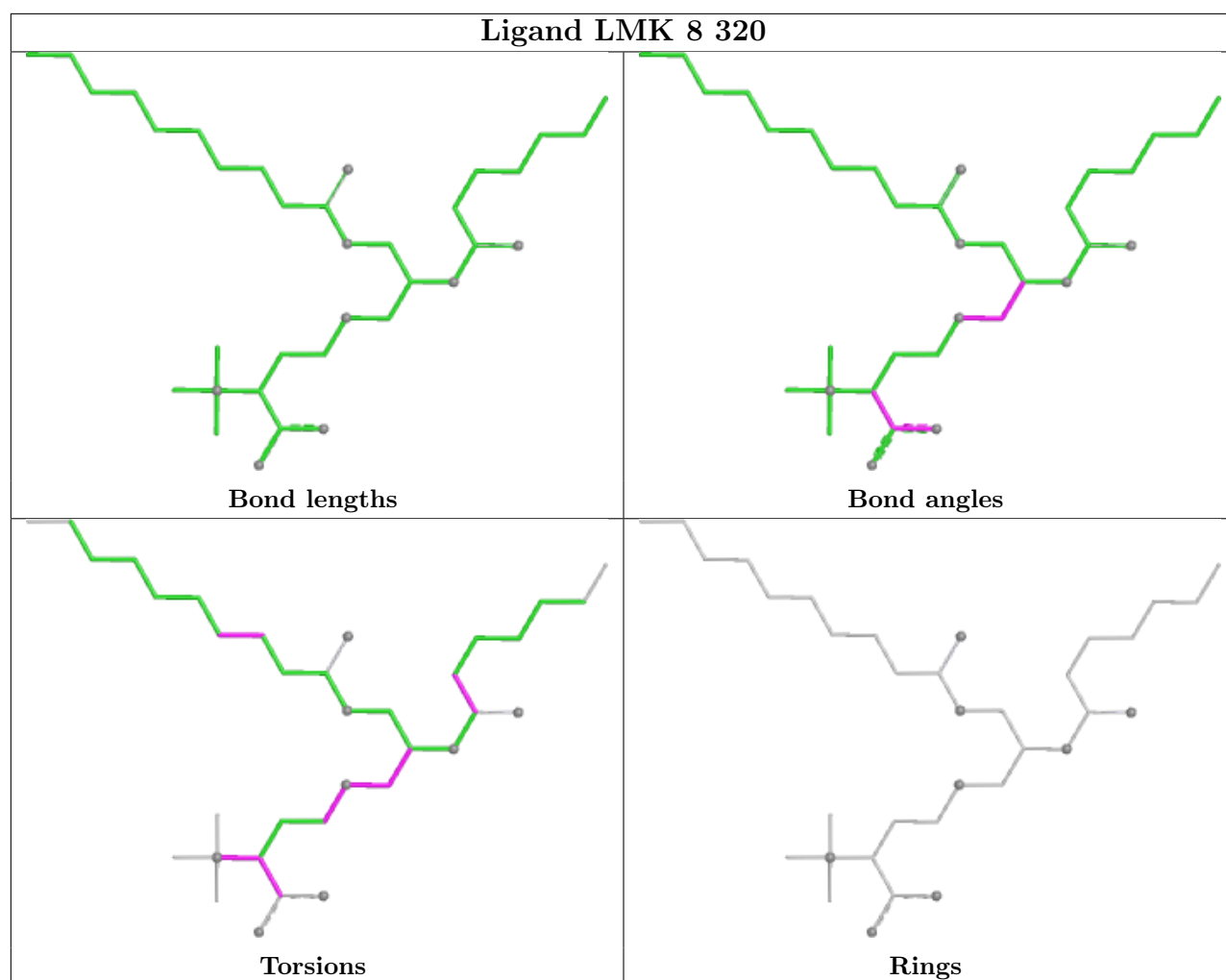


Ligand CLA A 832

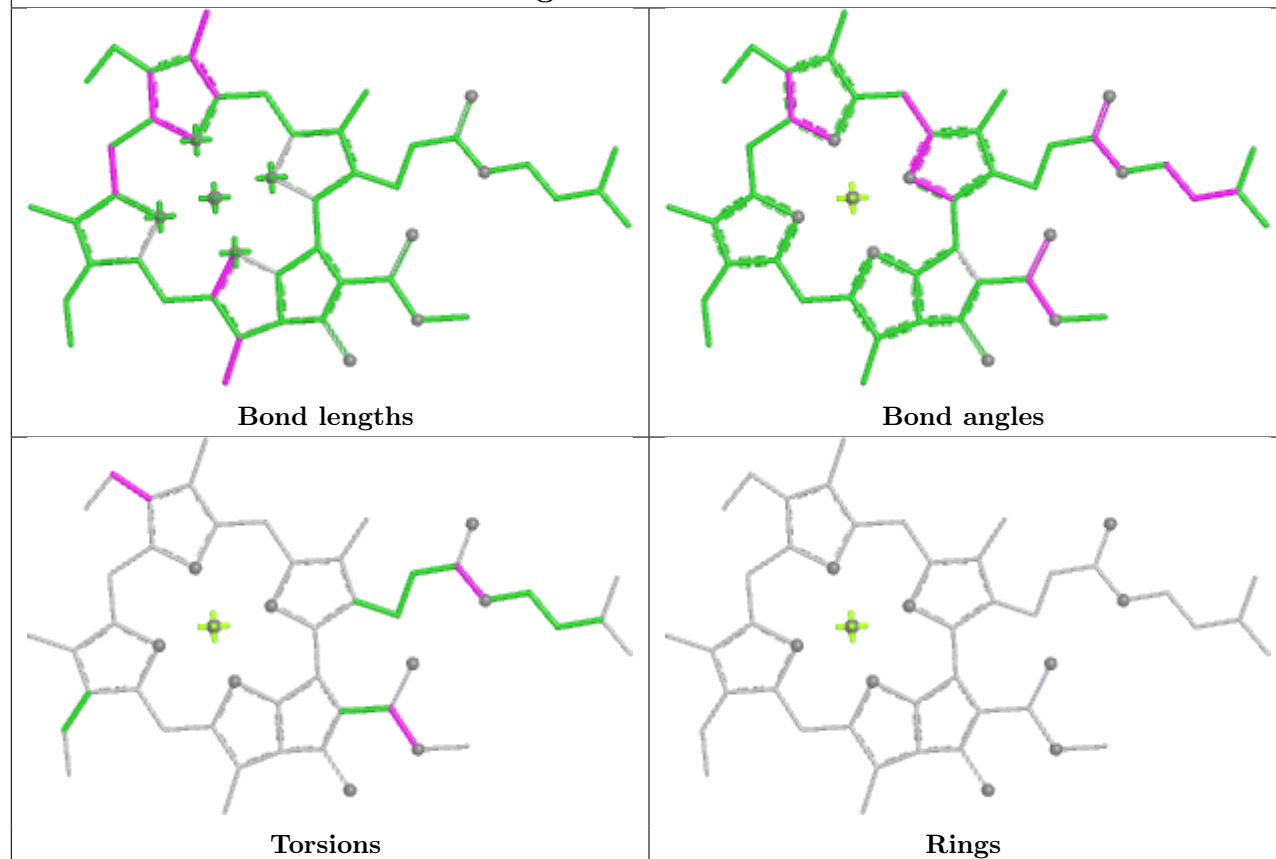


Ligand CLA 3 403

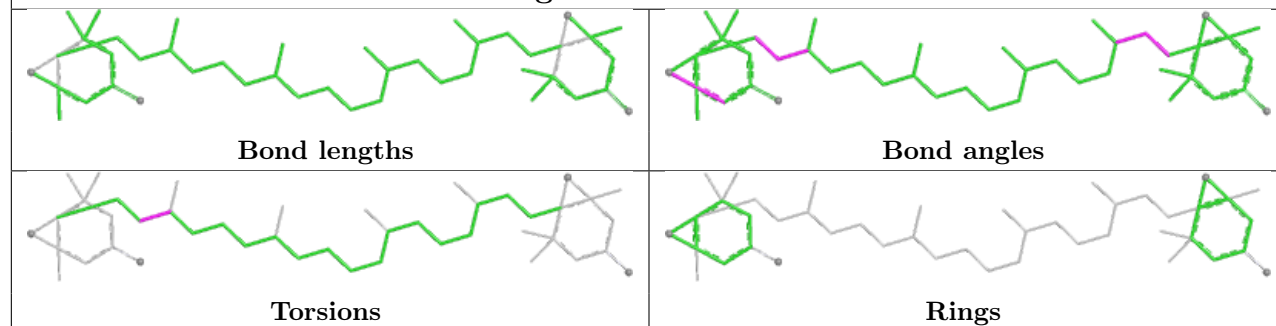




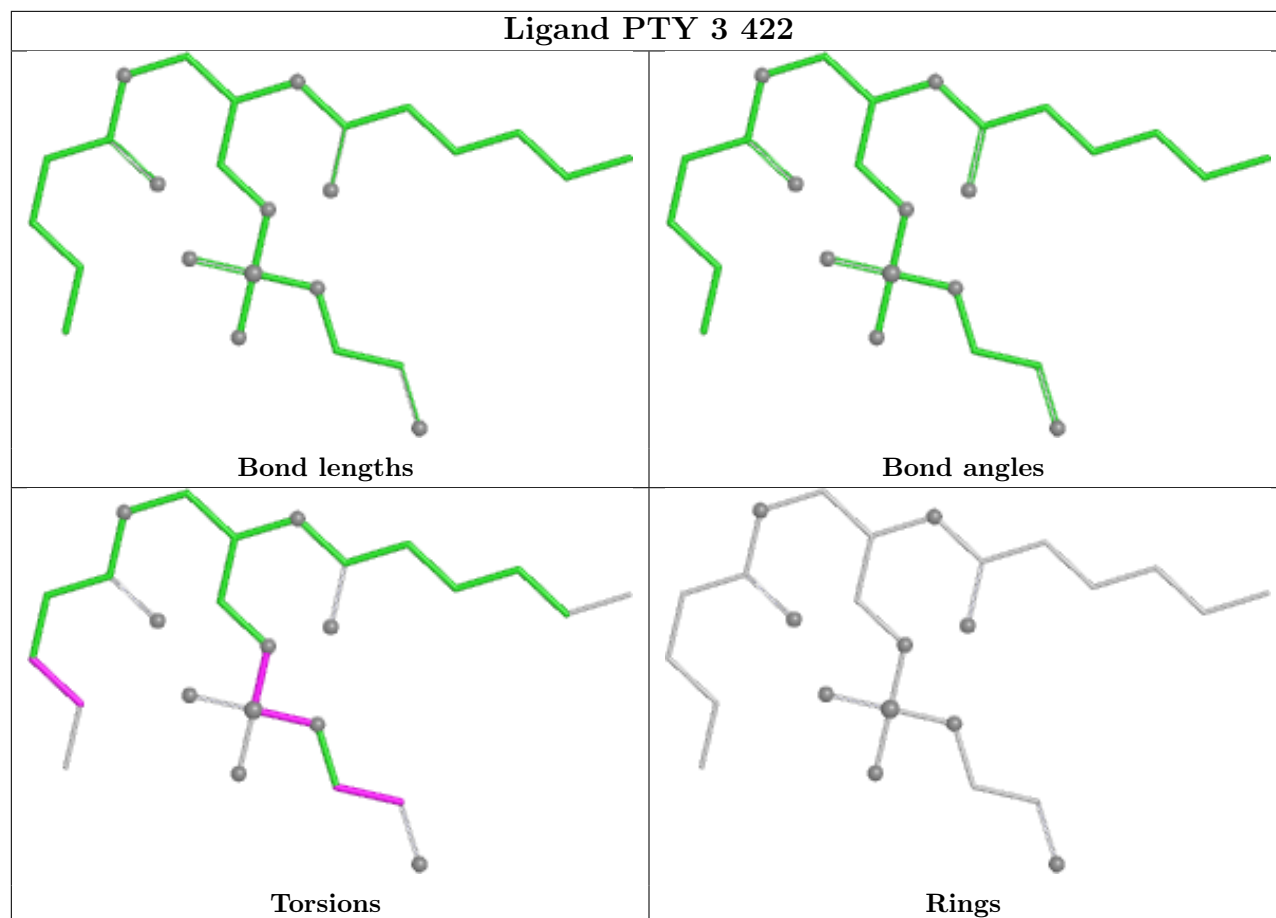
Ligand CLA 7 305



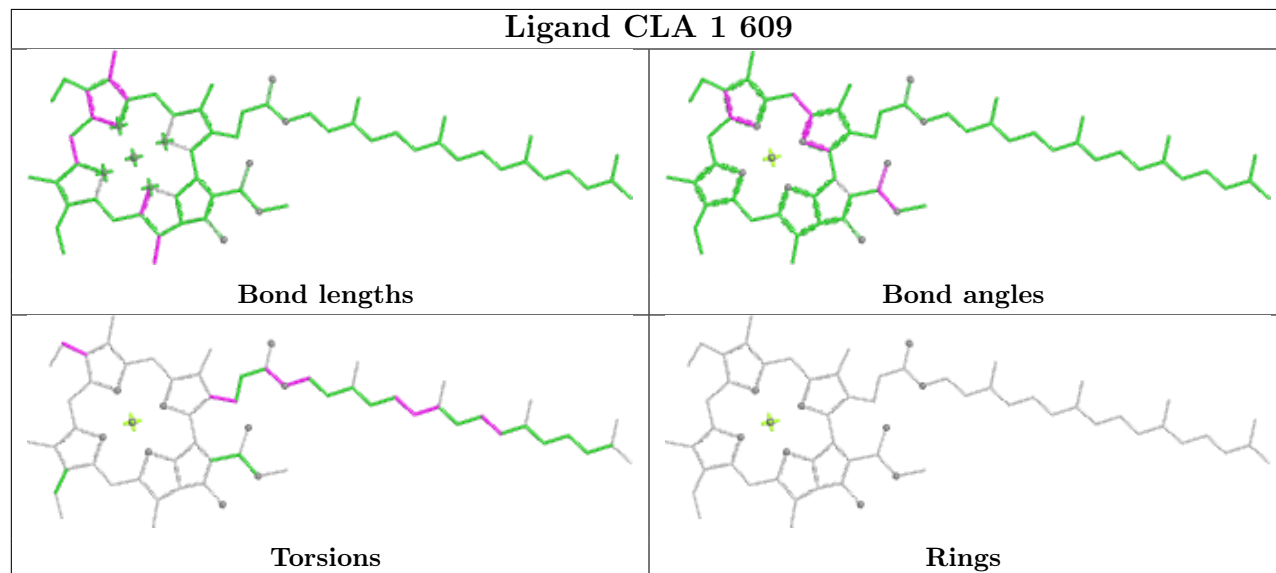
Ligand XAT 3 416



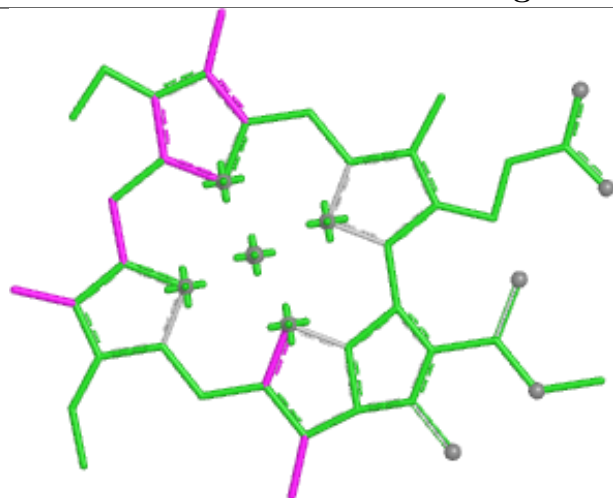
Ligand PTY 3 422



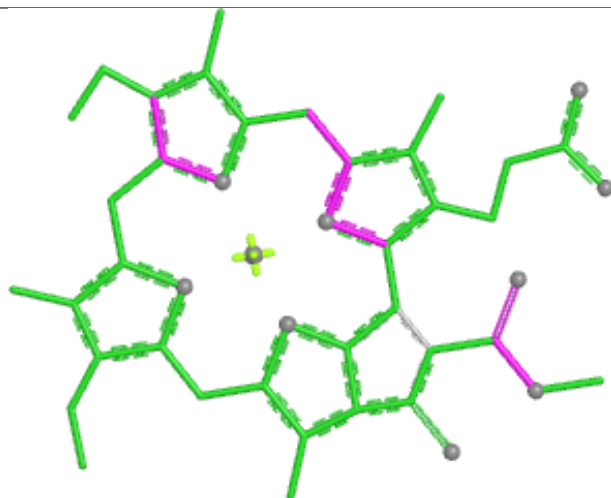
Ligand CLA 1 609



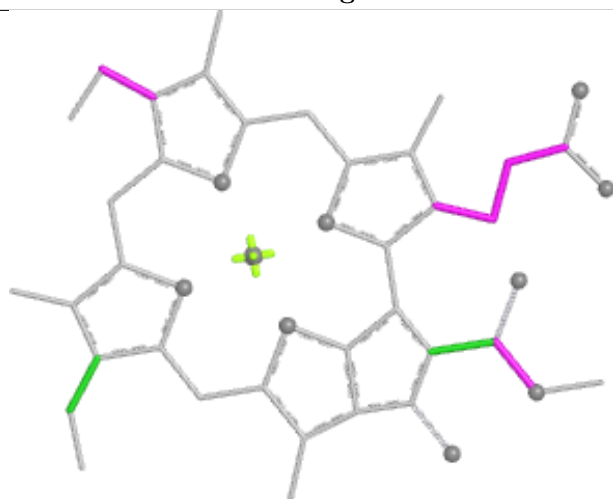
Ligand CLA H 204



Bond lengths



Bond angles

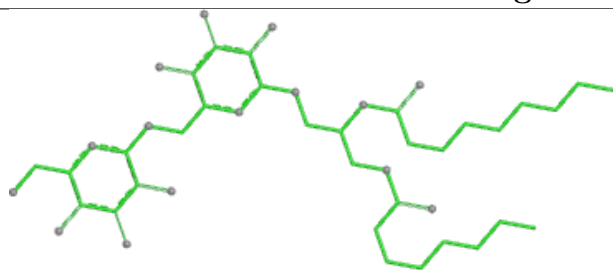


Torsions

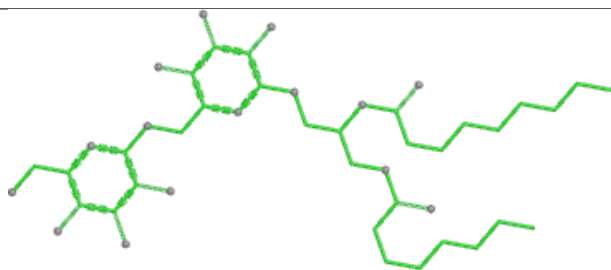


Rings

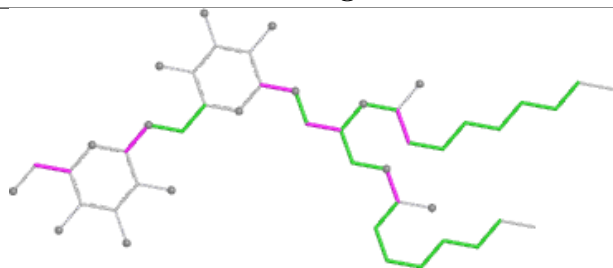
Ligand DGD 7 321



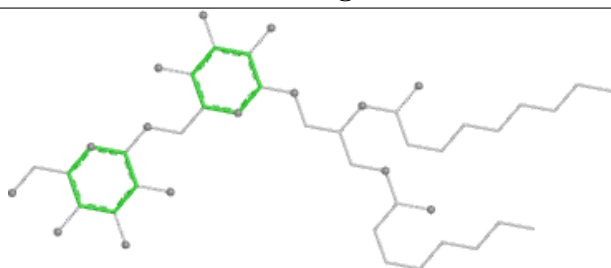
Bond lengths



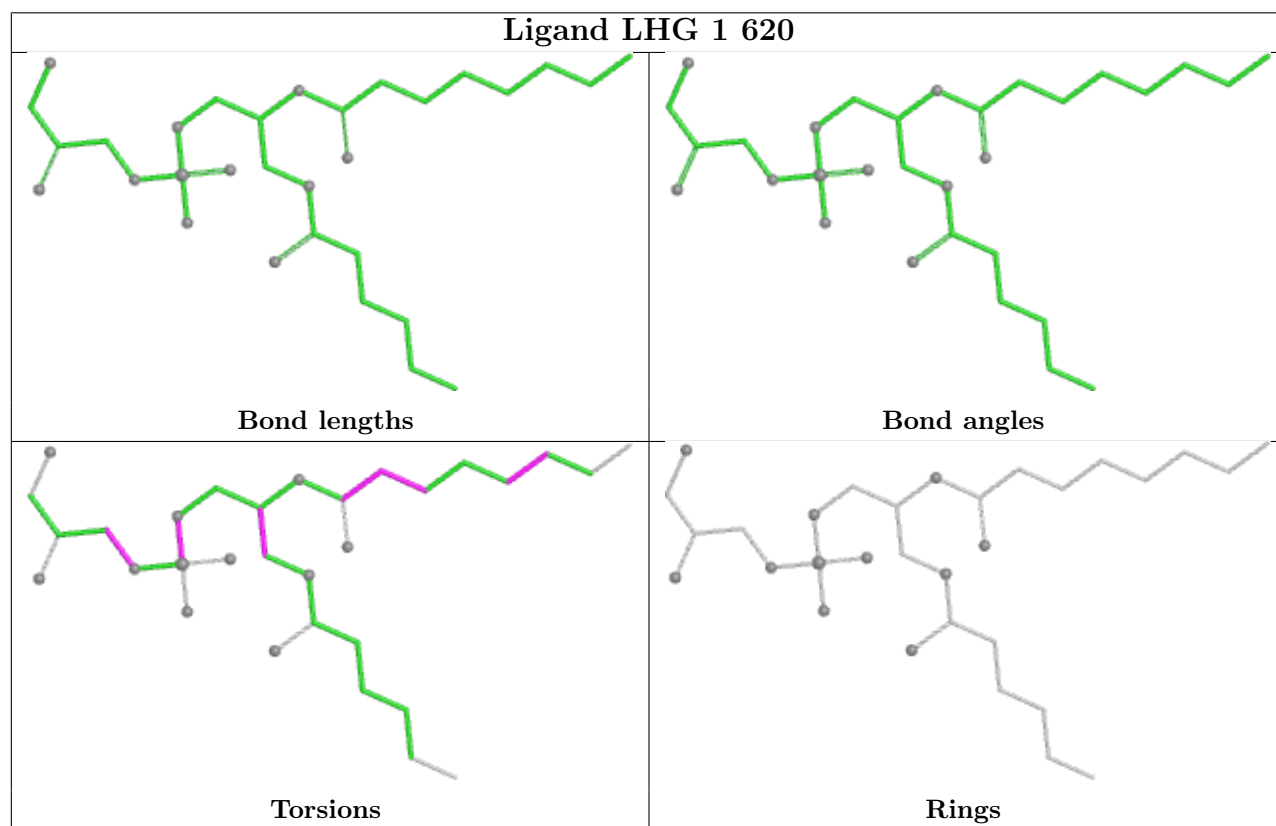
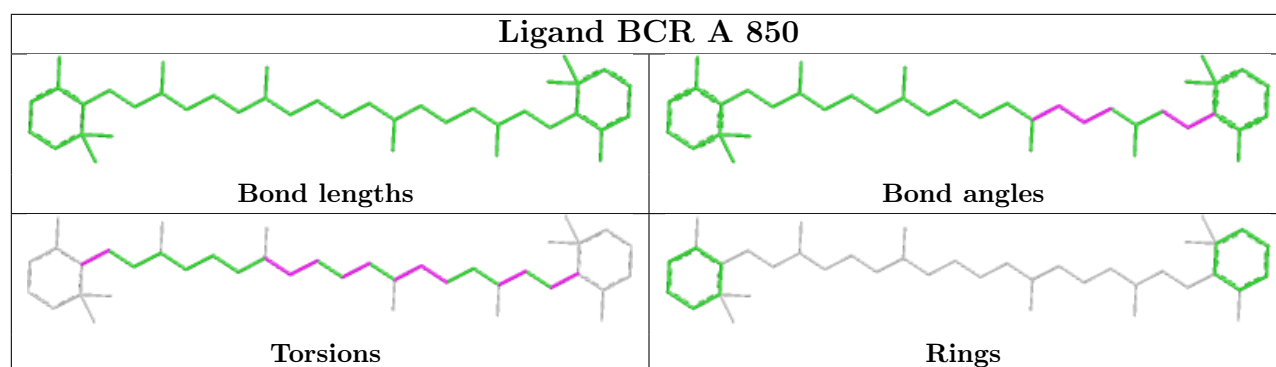
Bond angles

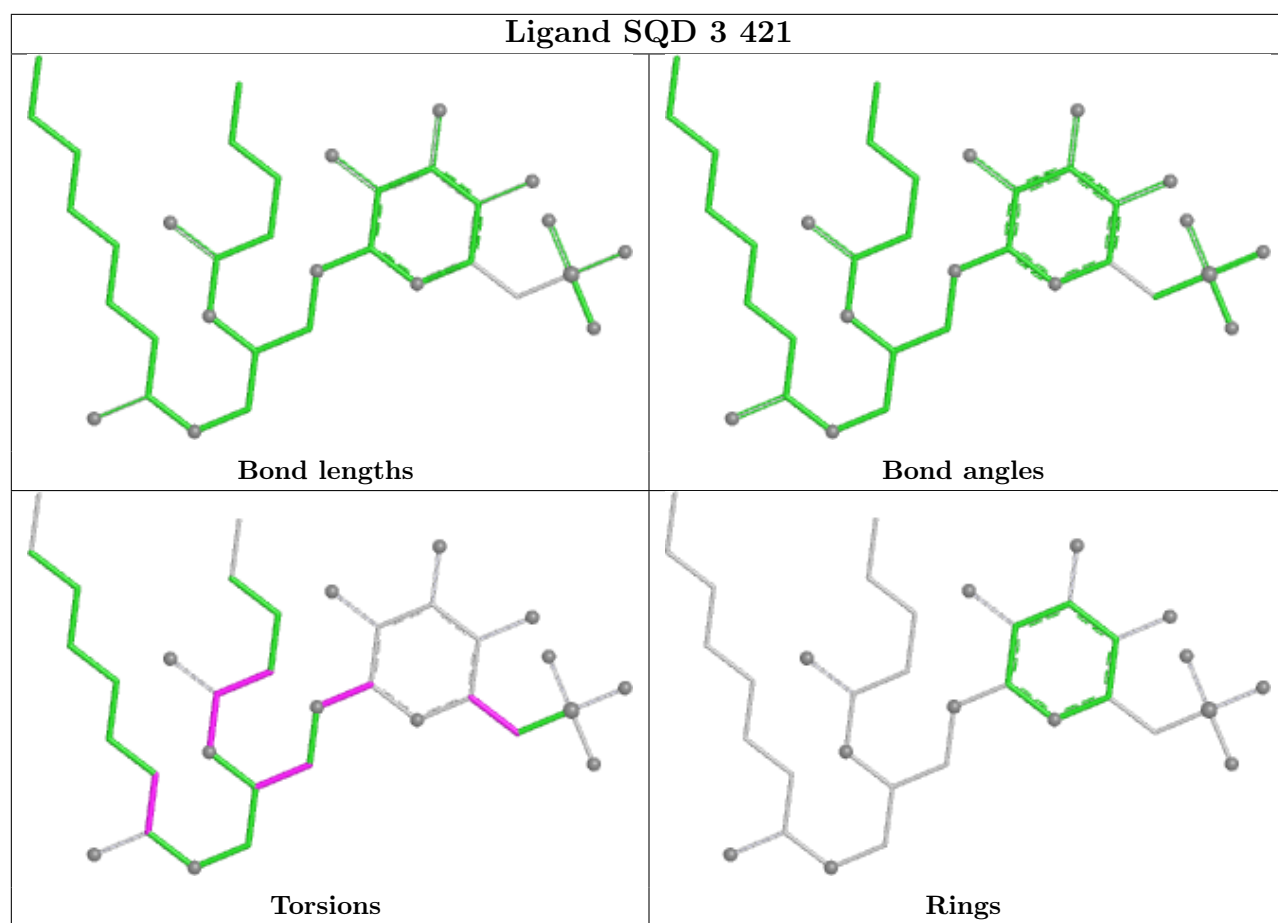


Torsions

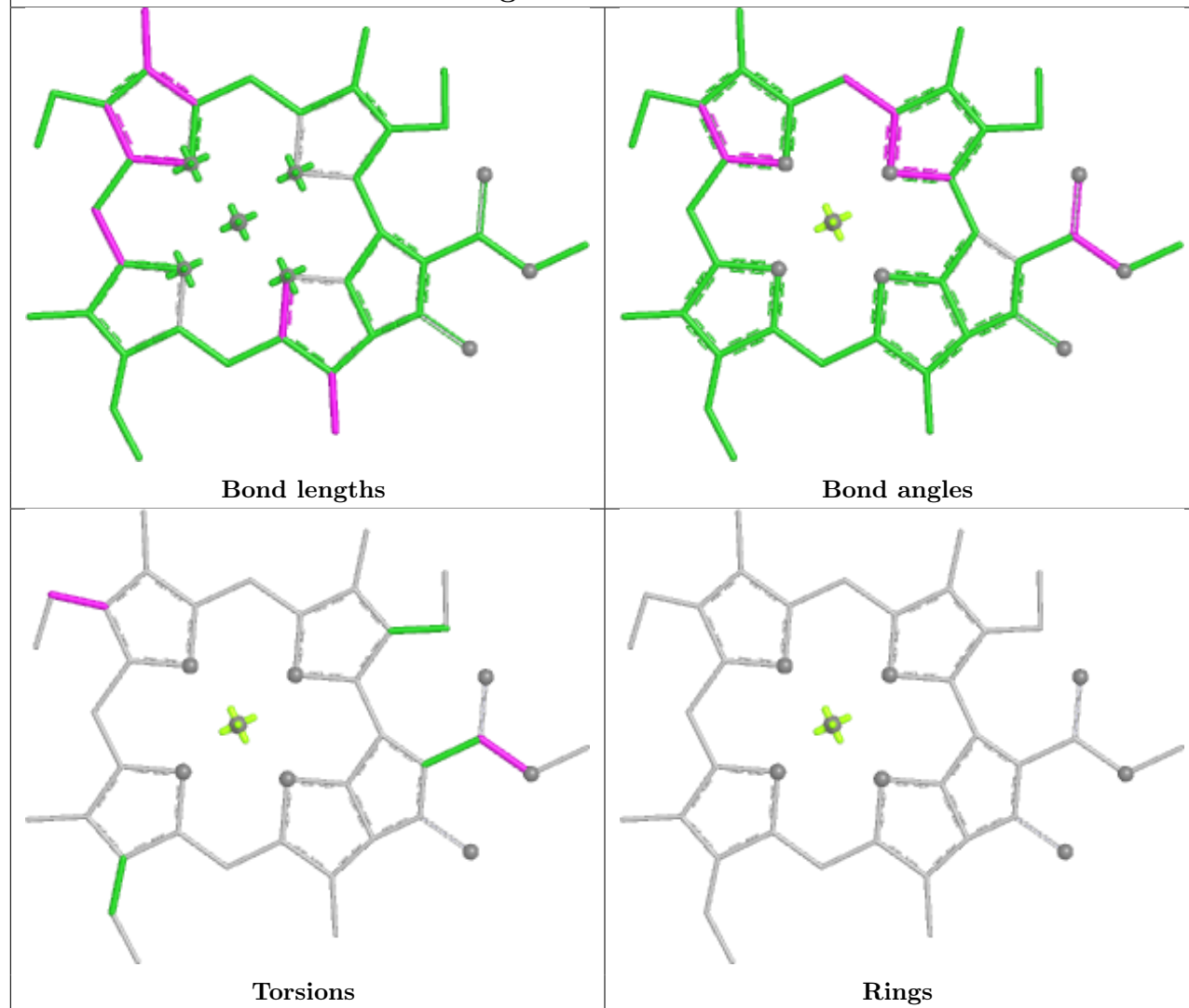


Rings

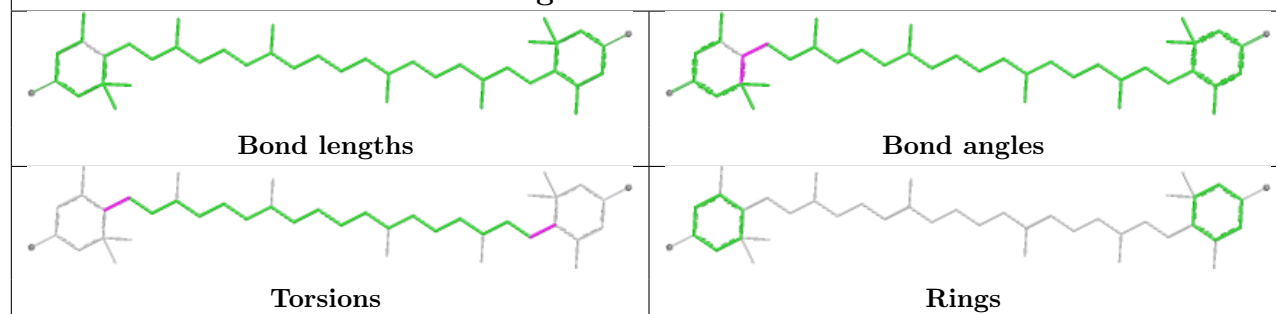




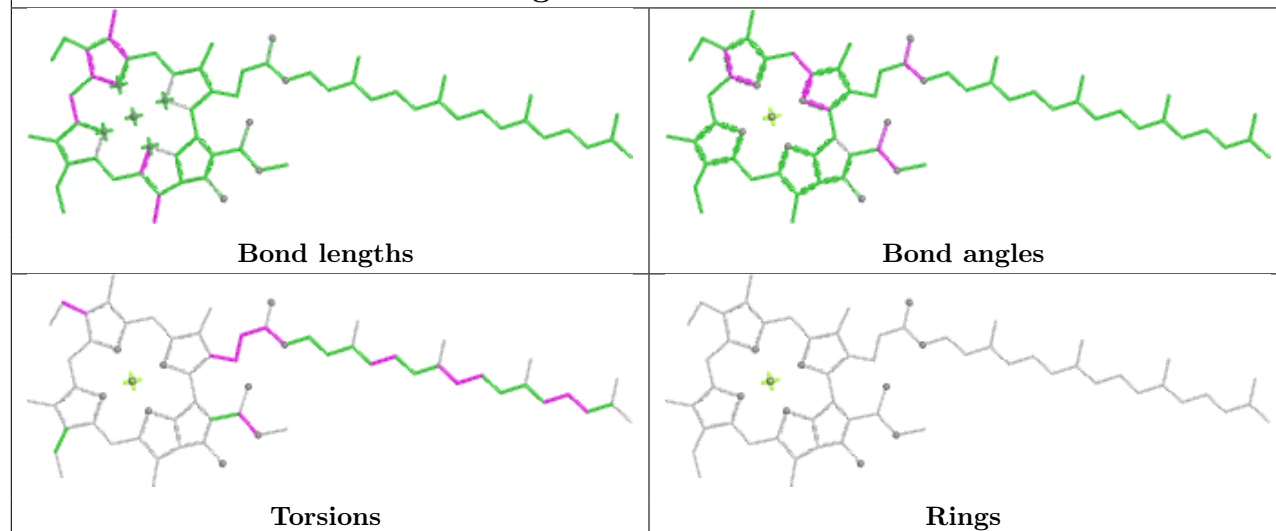
Ligand CLA 3 413



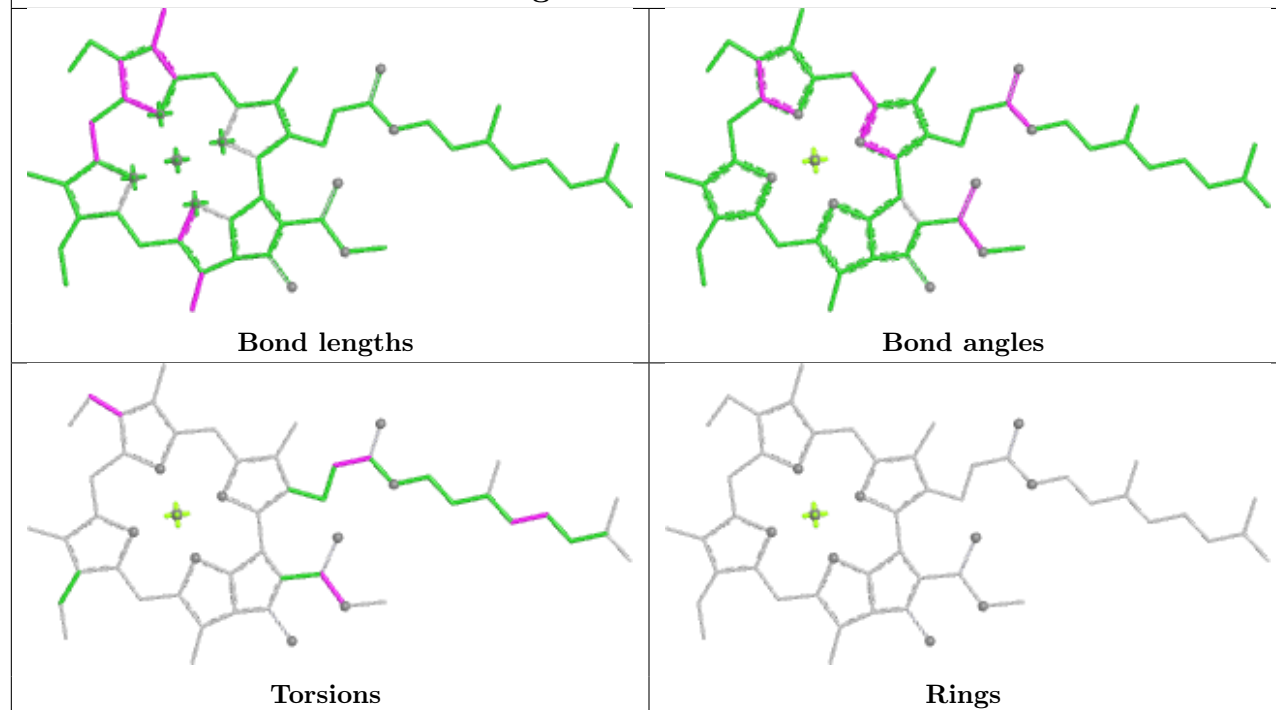
Ligand LUT 3 415

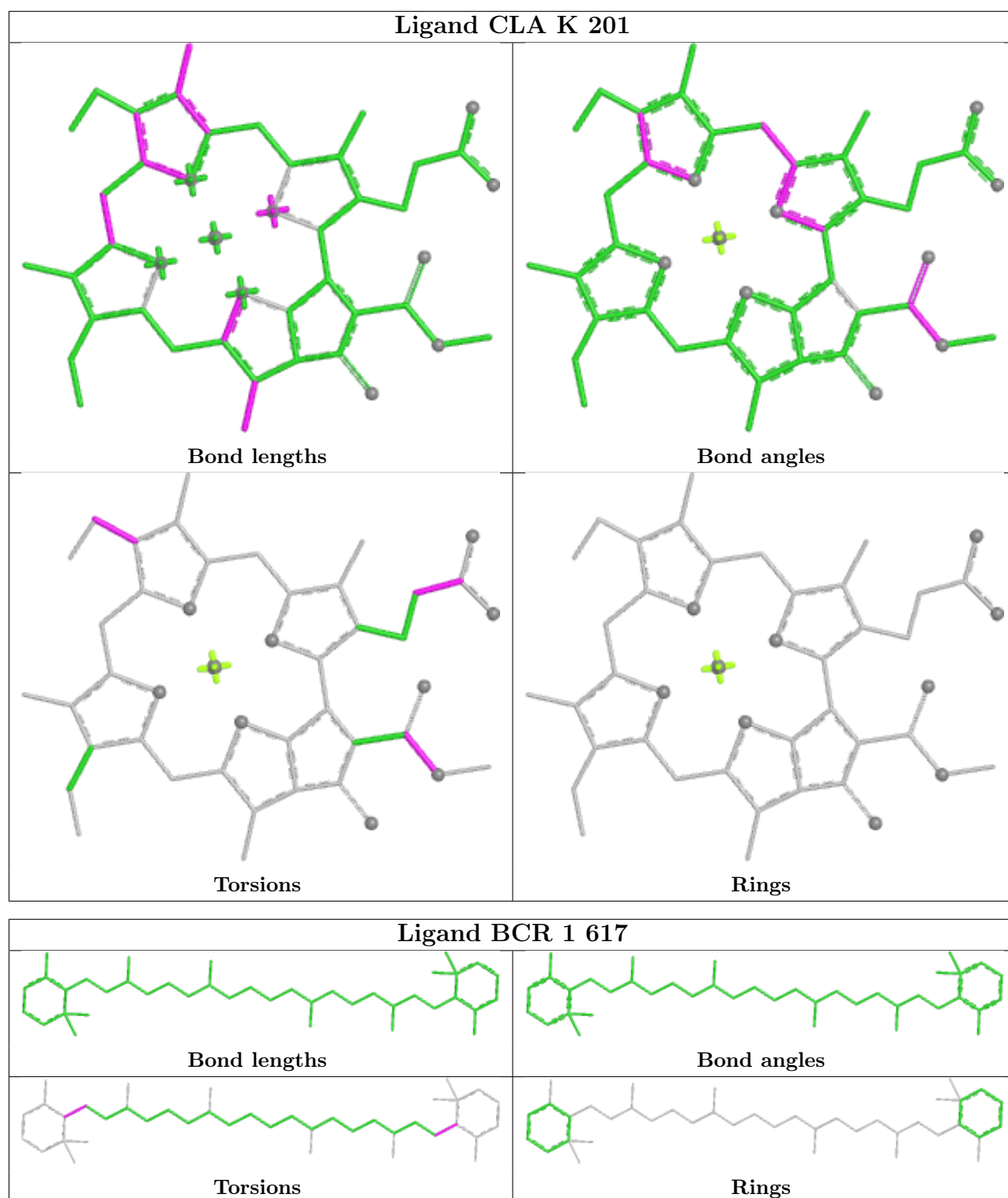


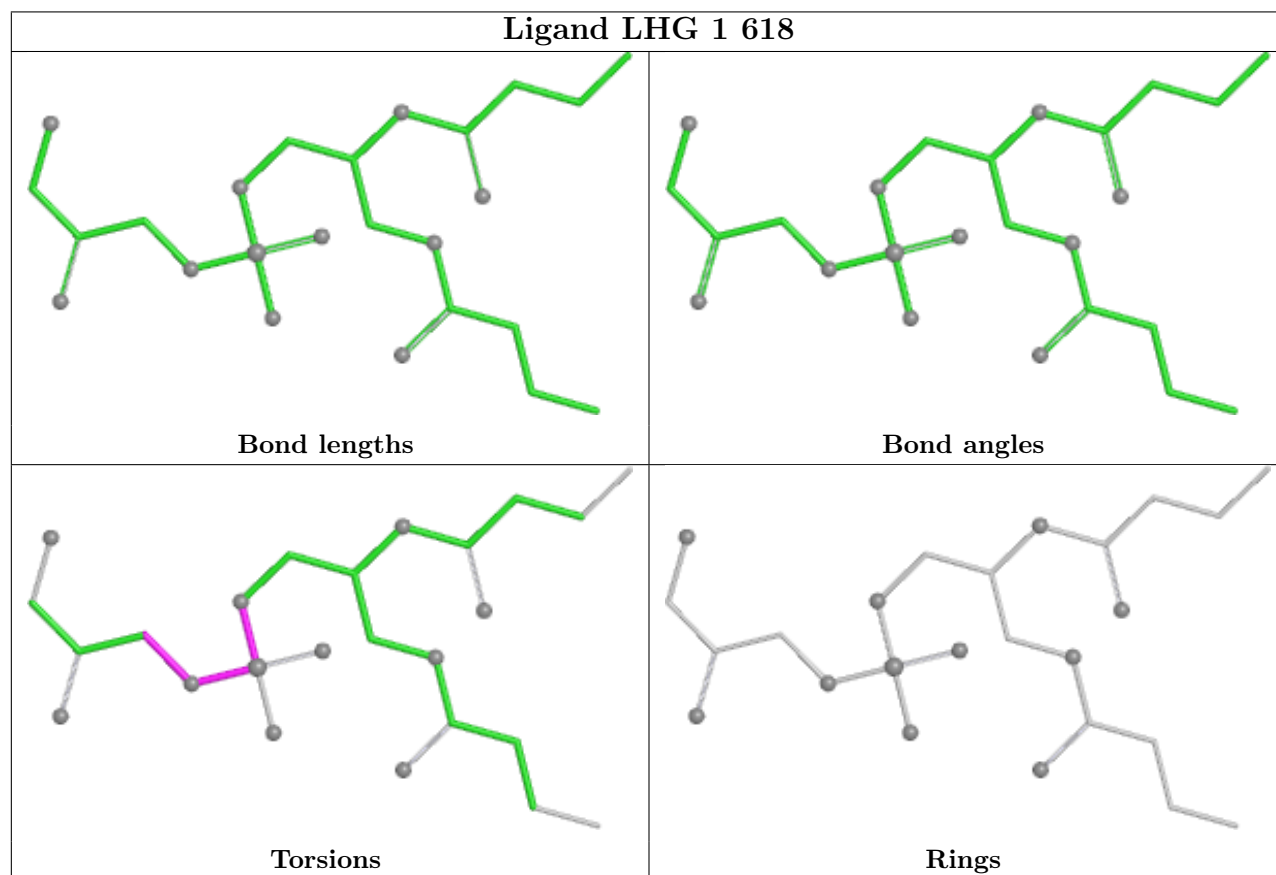
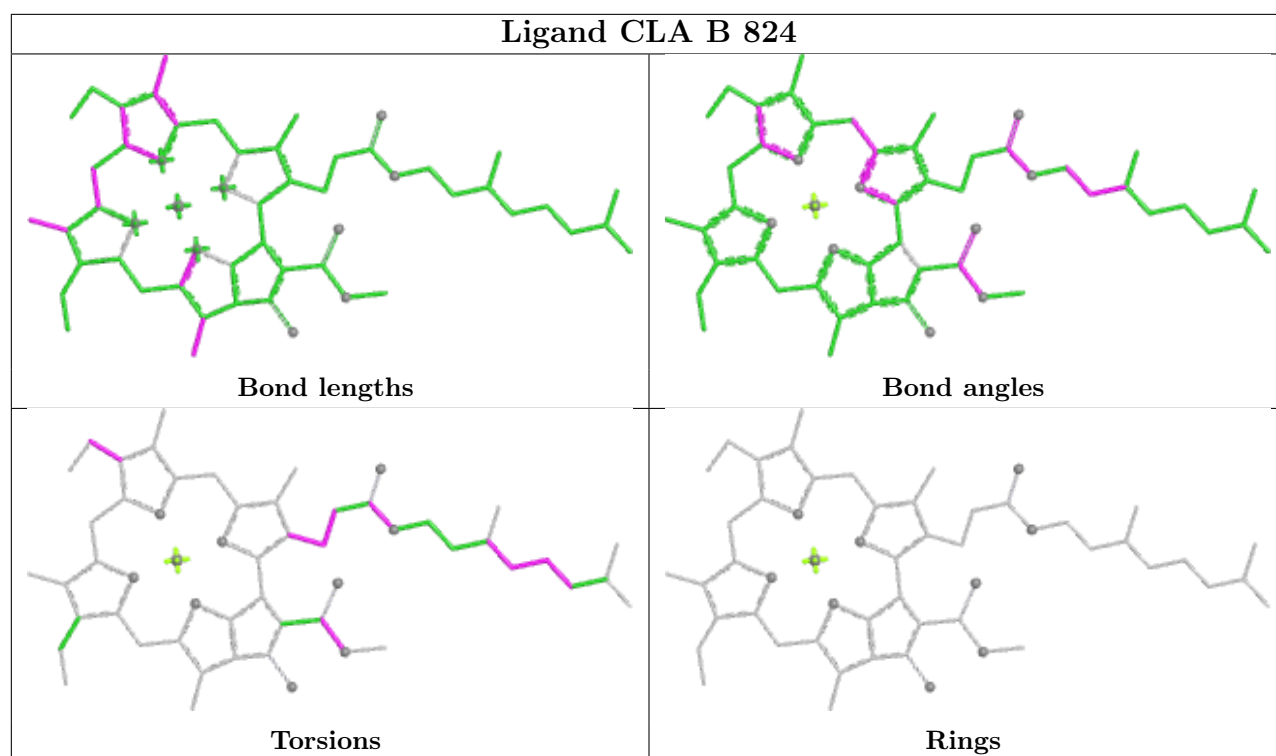
Ligand CLA B 828



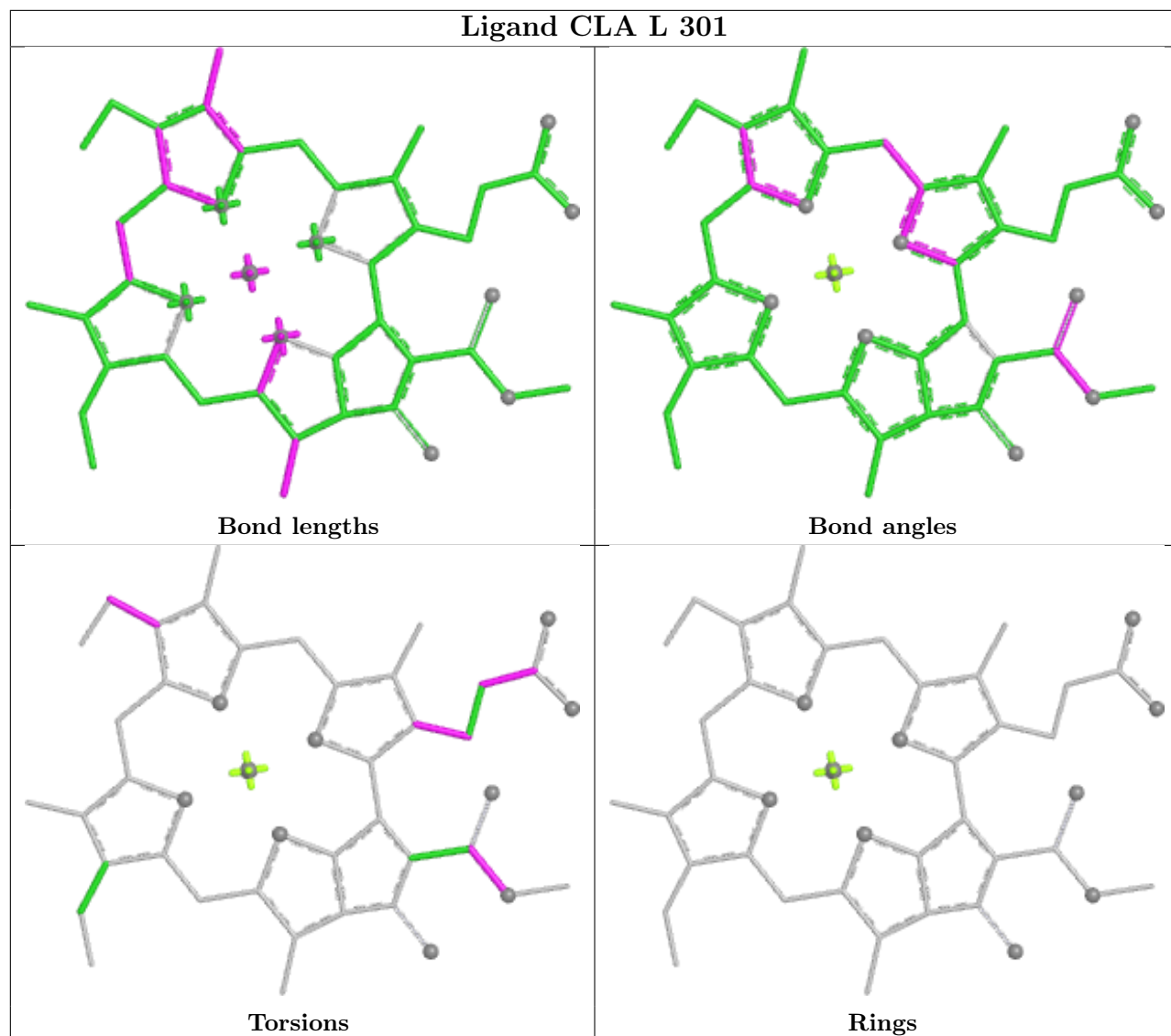
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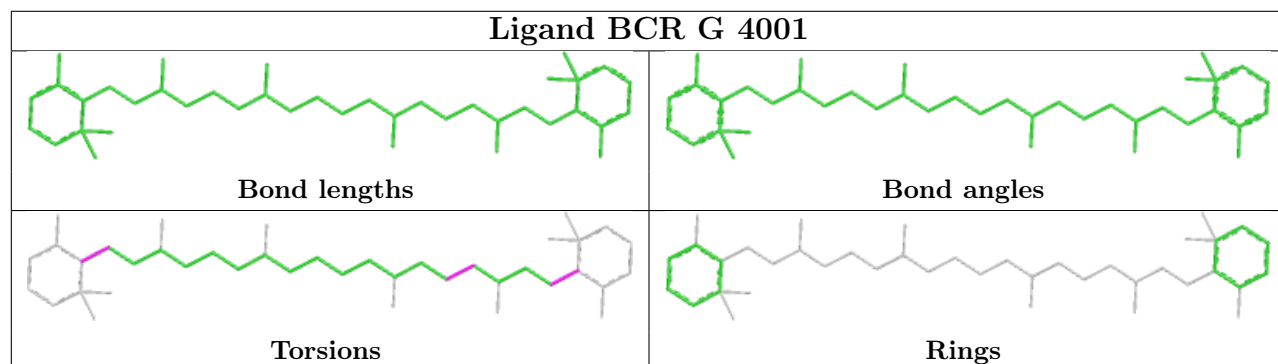




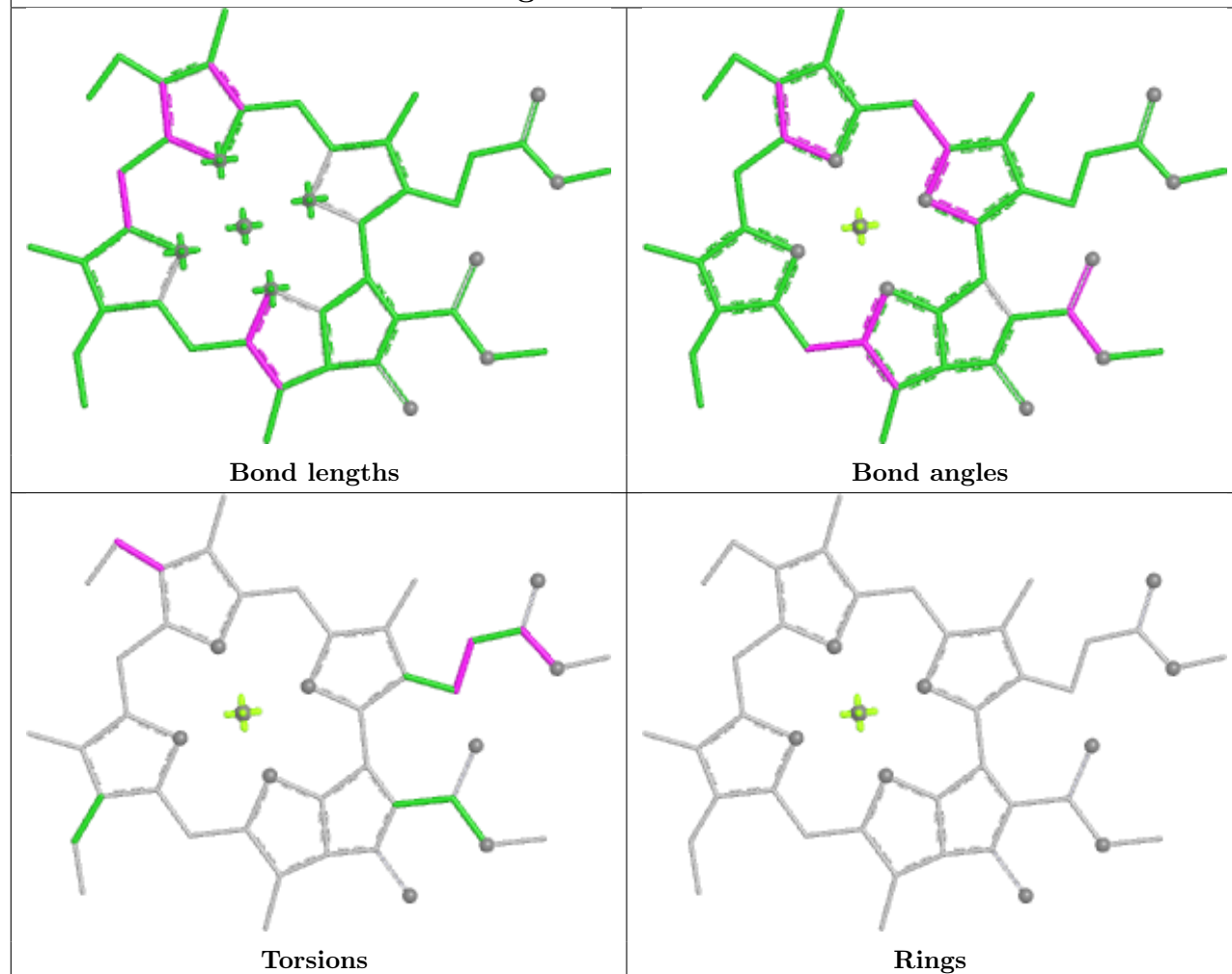
Ligand CLA L 301



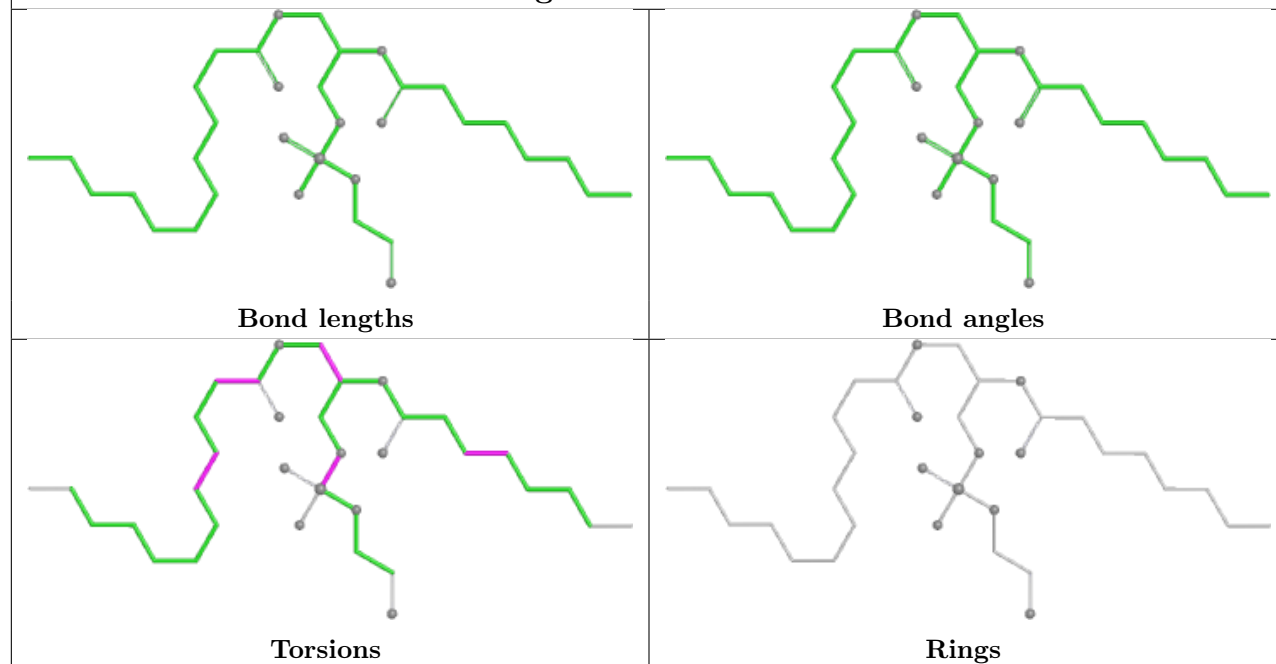
Ligand BCR G 4001

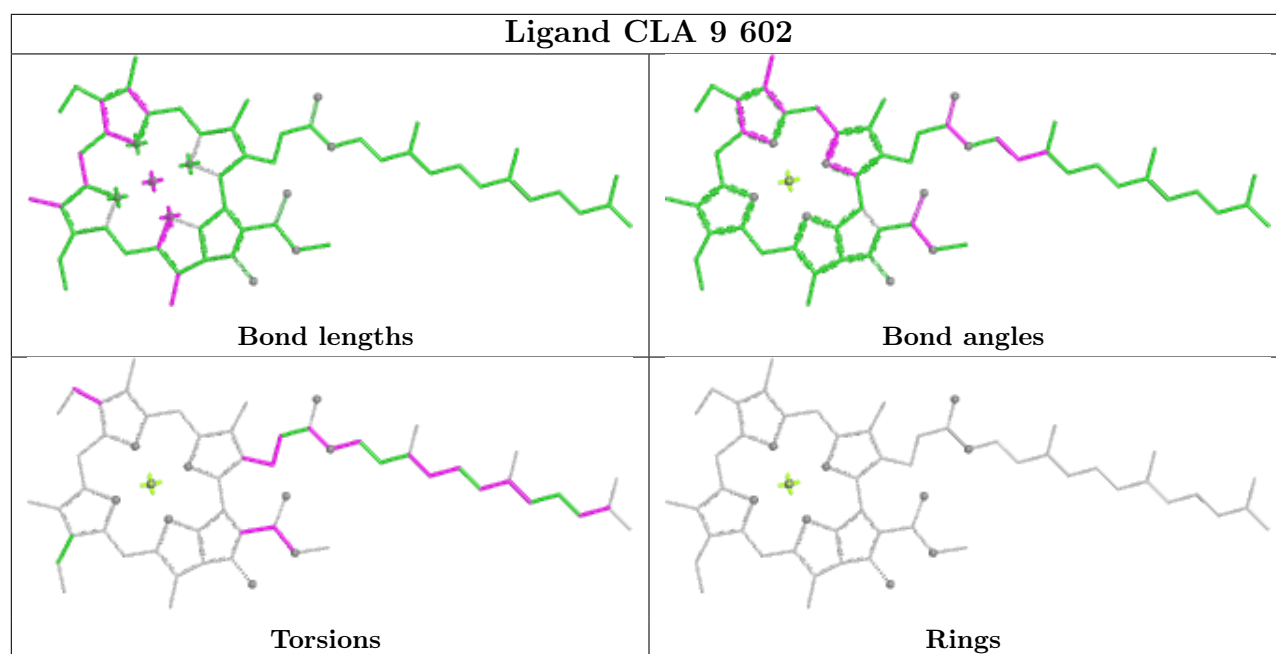


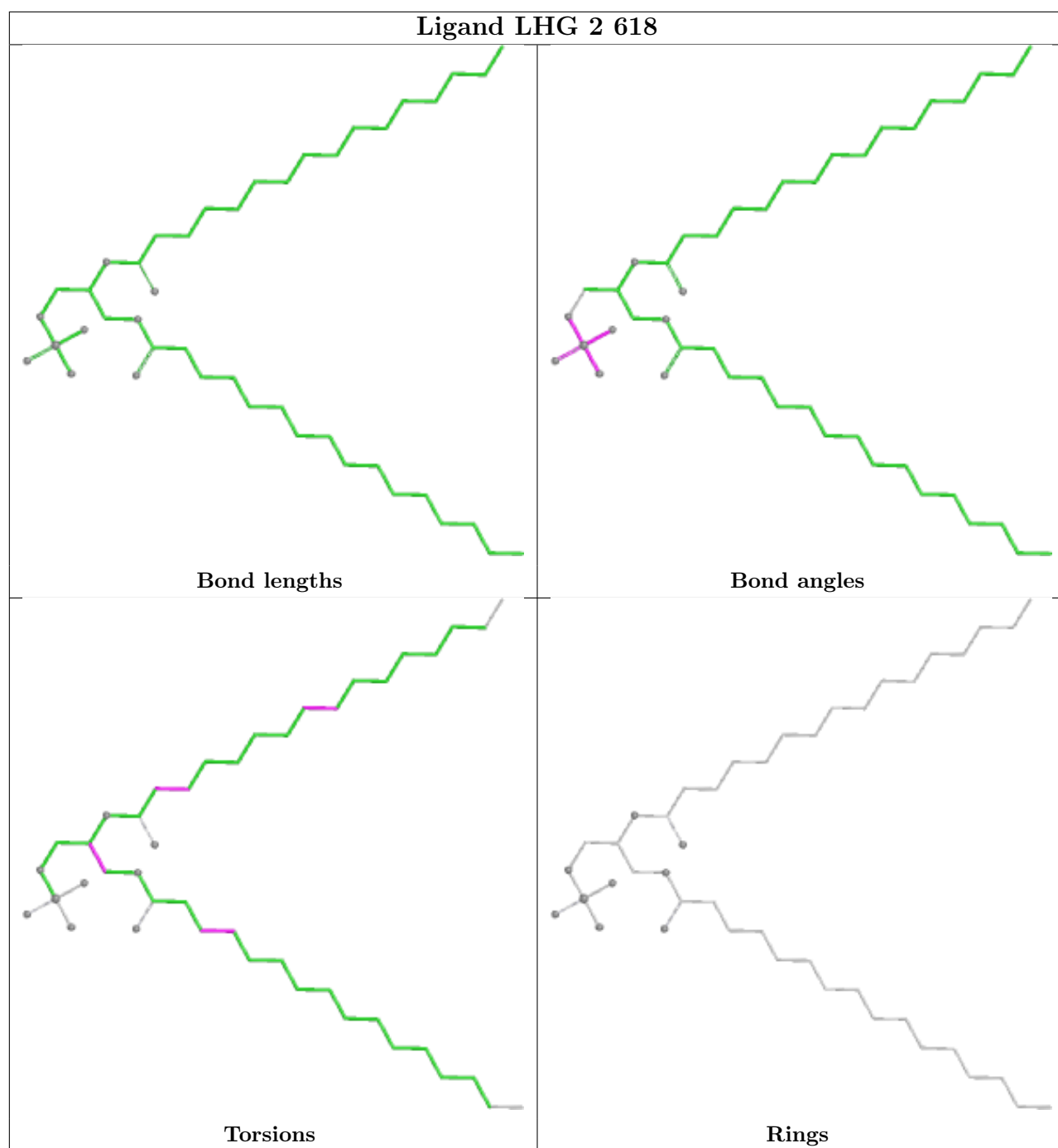
Ligand CLA 2 622



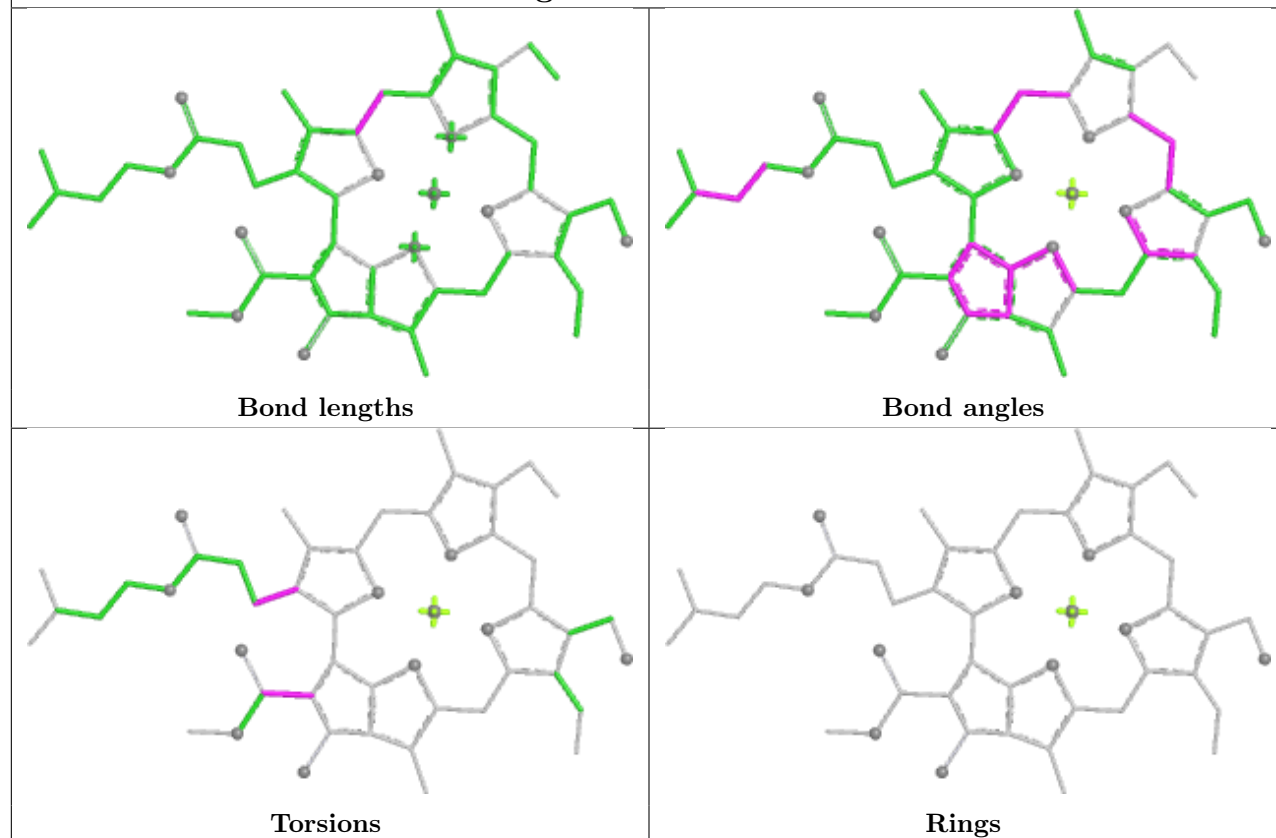
Ligand PTY 1 623



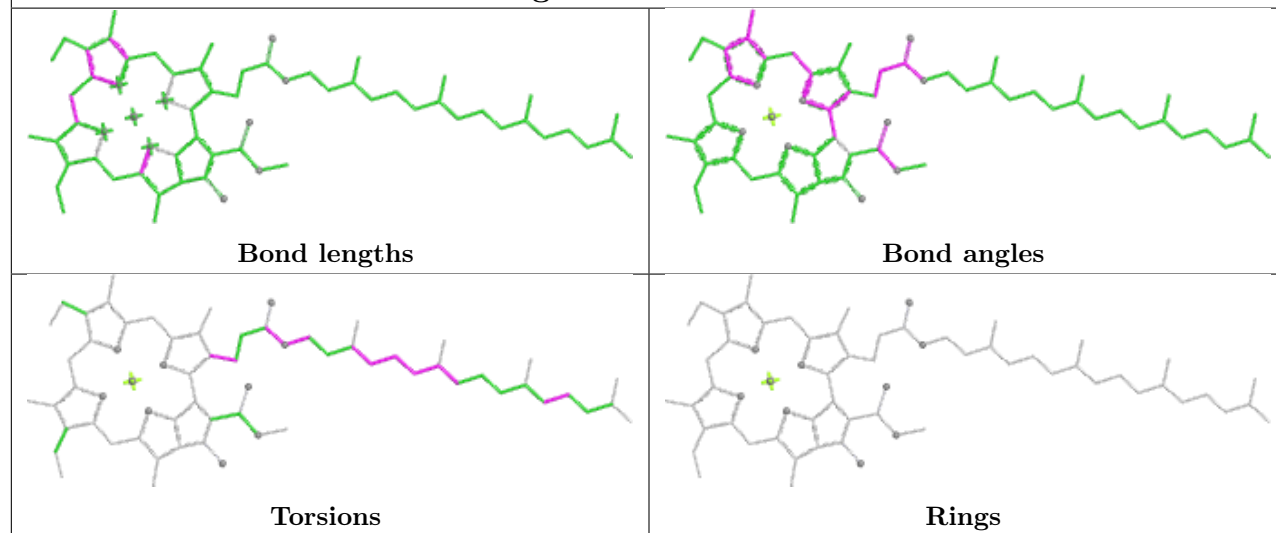




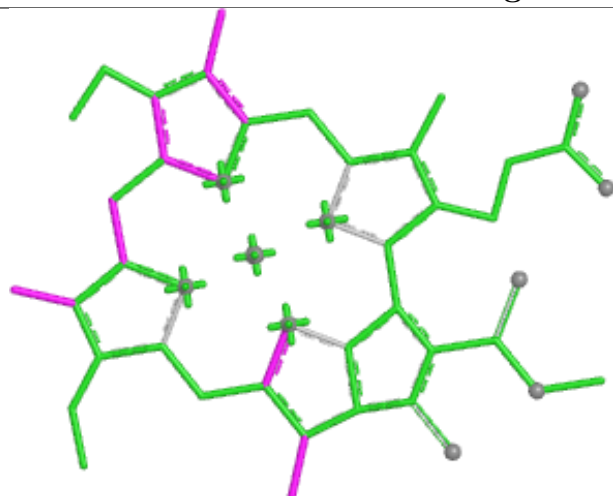
Ligand CHL 1 601



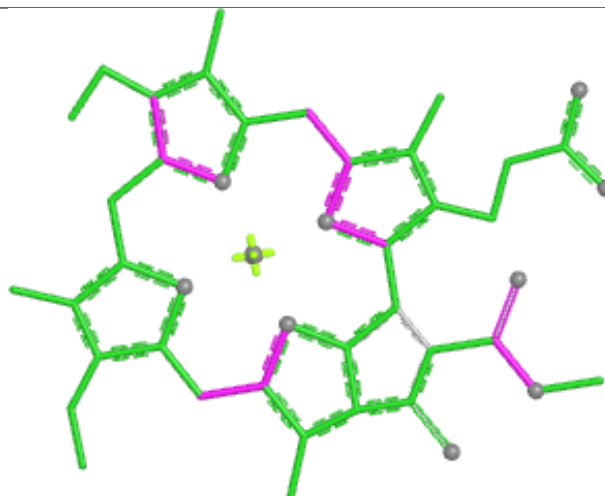
Ligand CLA B 833



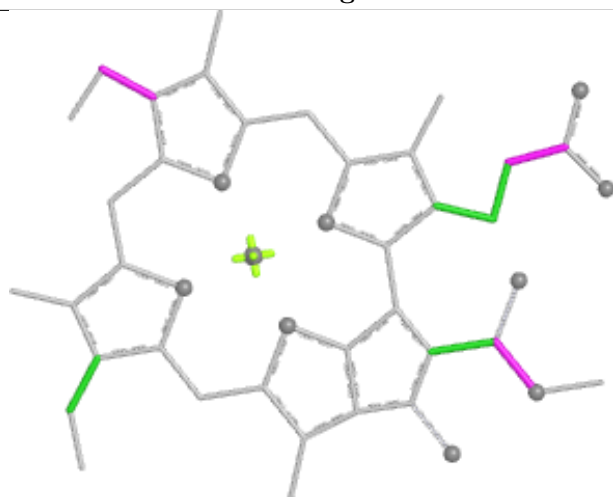
Ligand CLA G 4004



Bond lengths



Bond angles

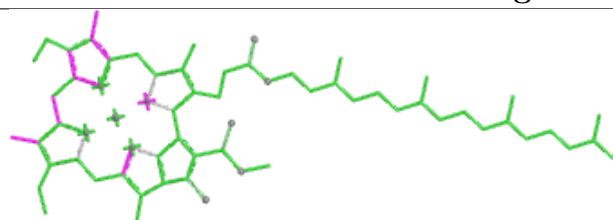


Torsions

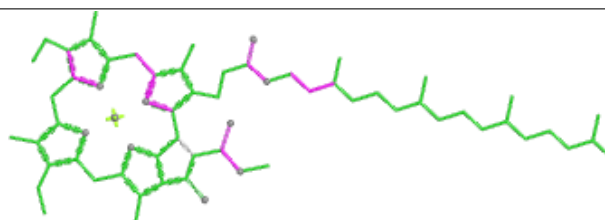


Rings

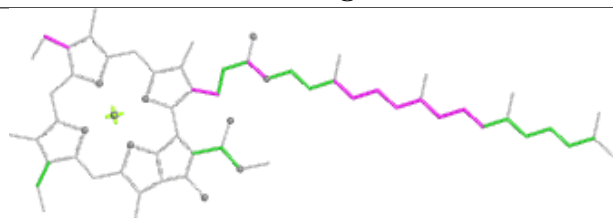
Ligand CLA A 830



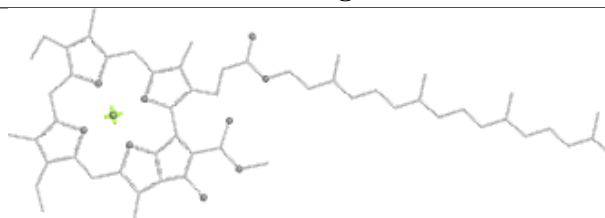
Bond lengths



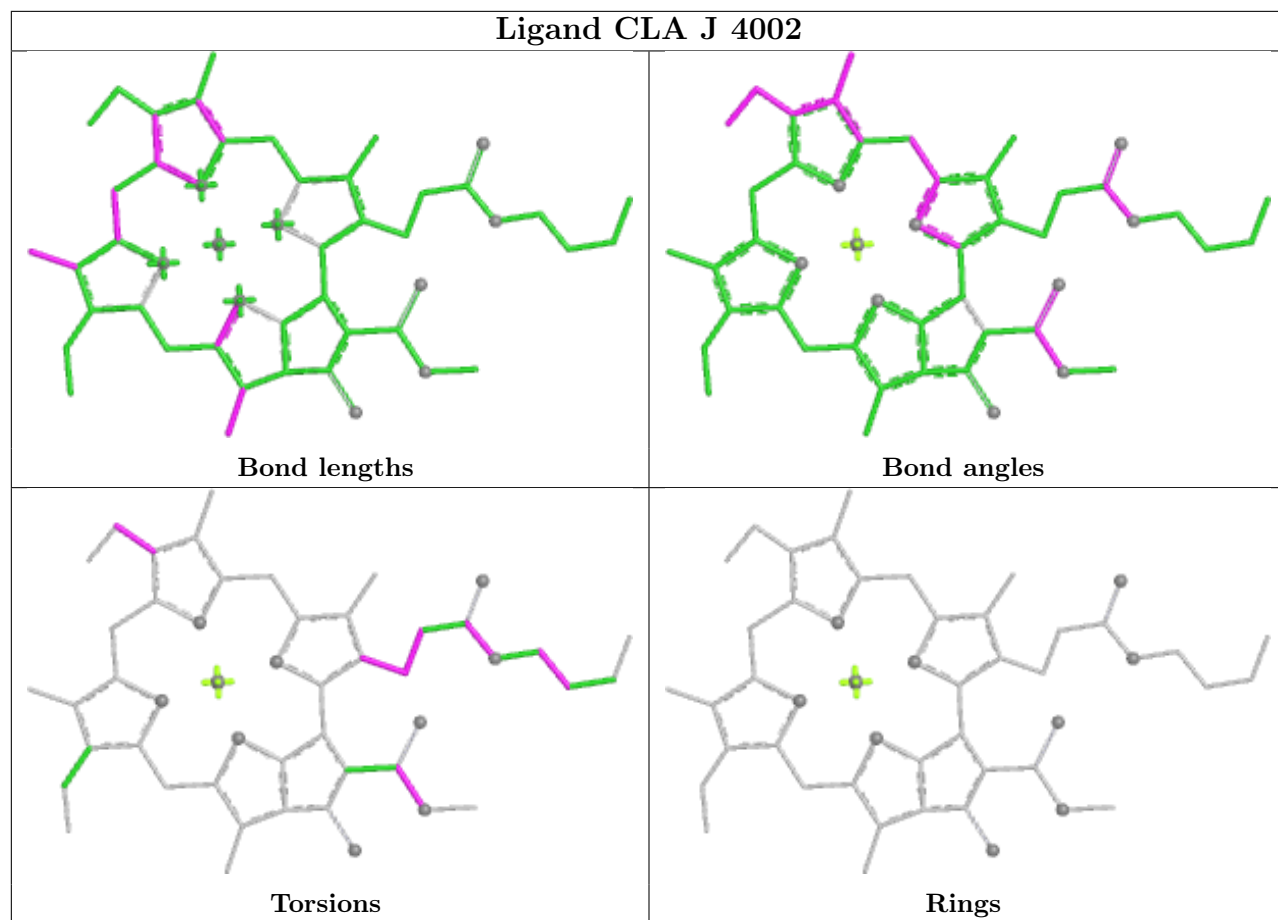
Bond angles



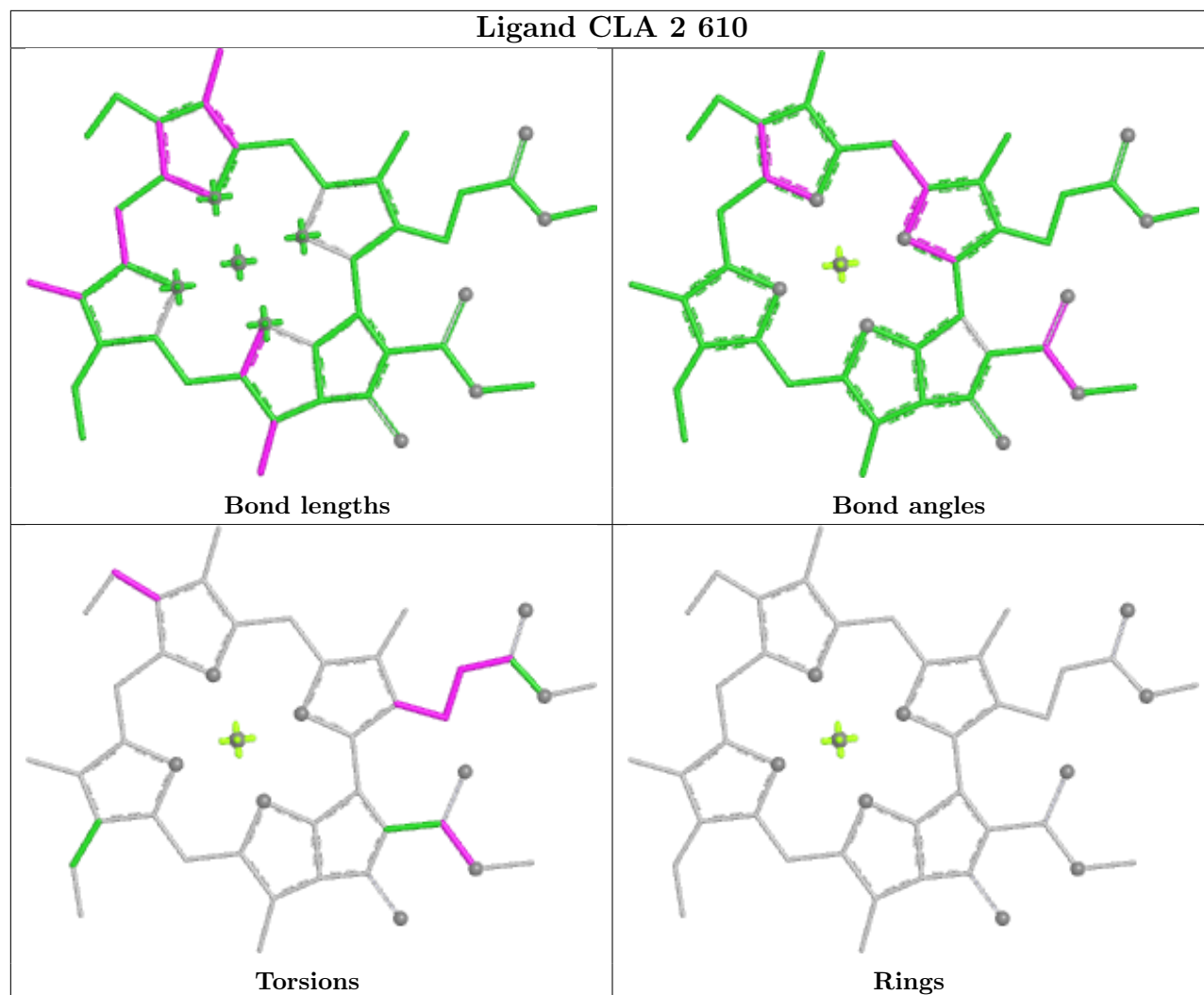
Torsions



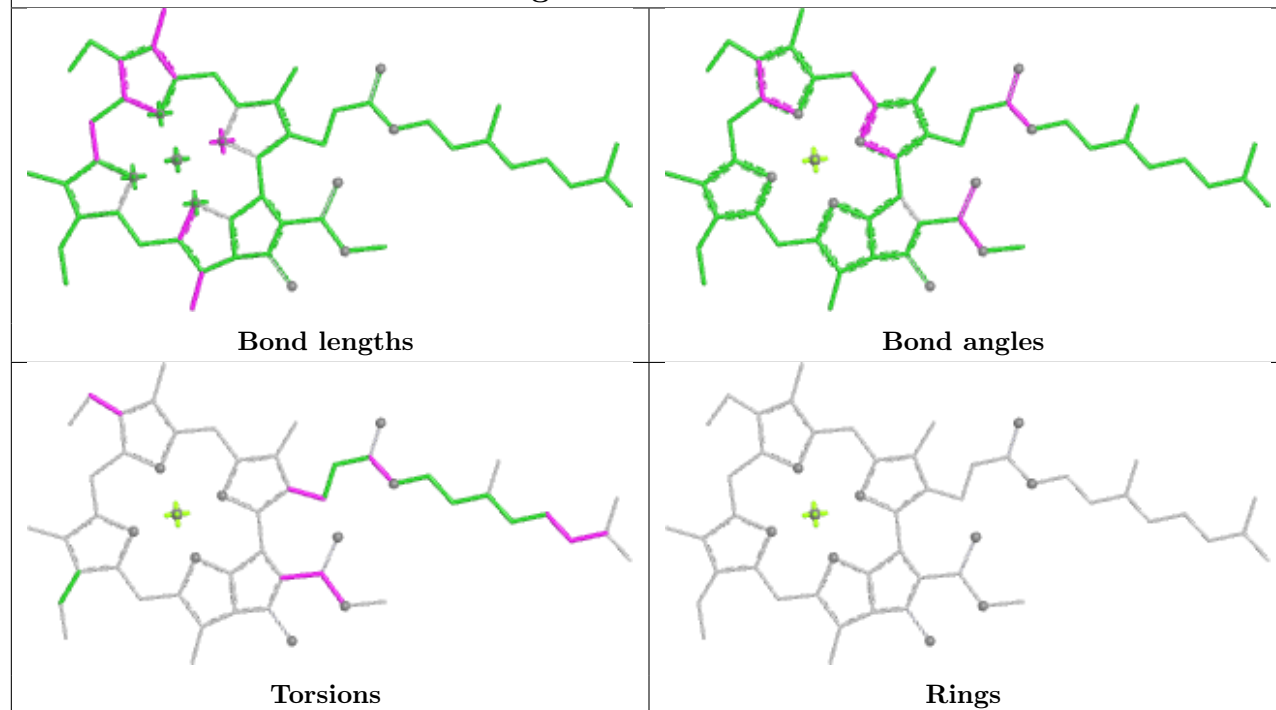
Rings



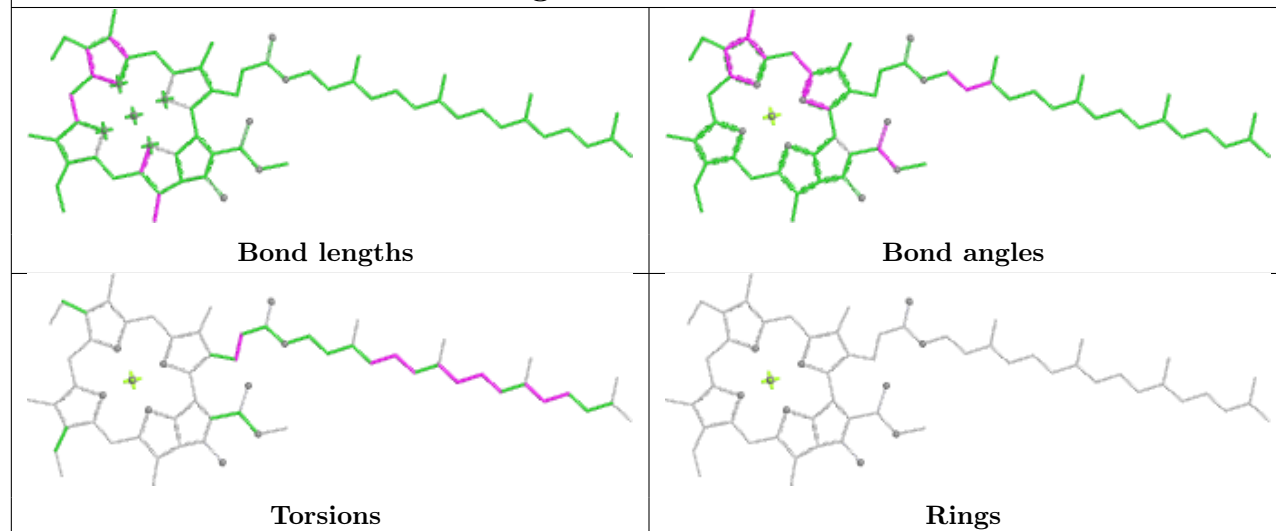
Ligand CLA 2 610

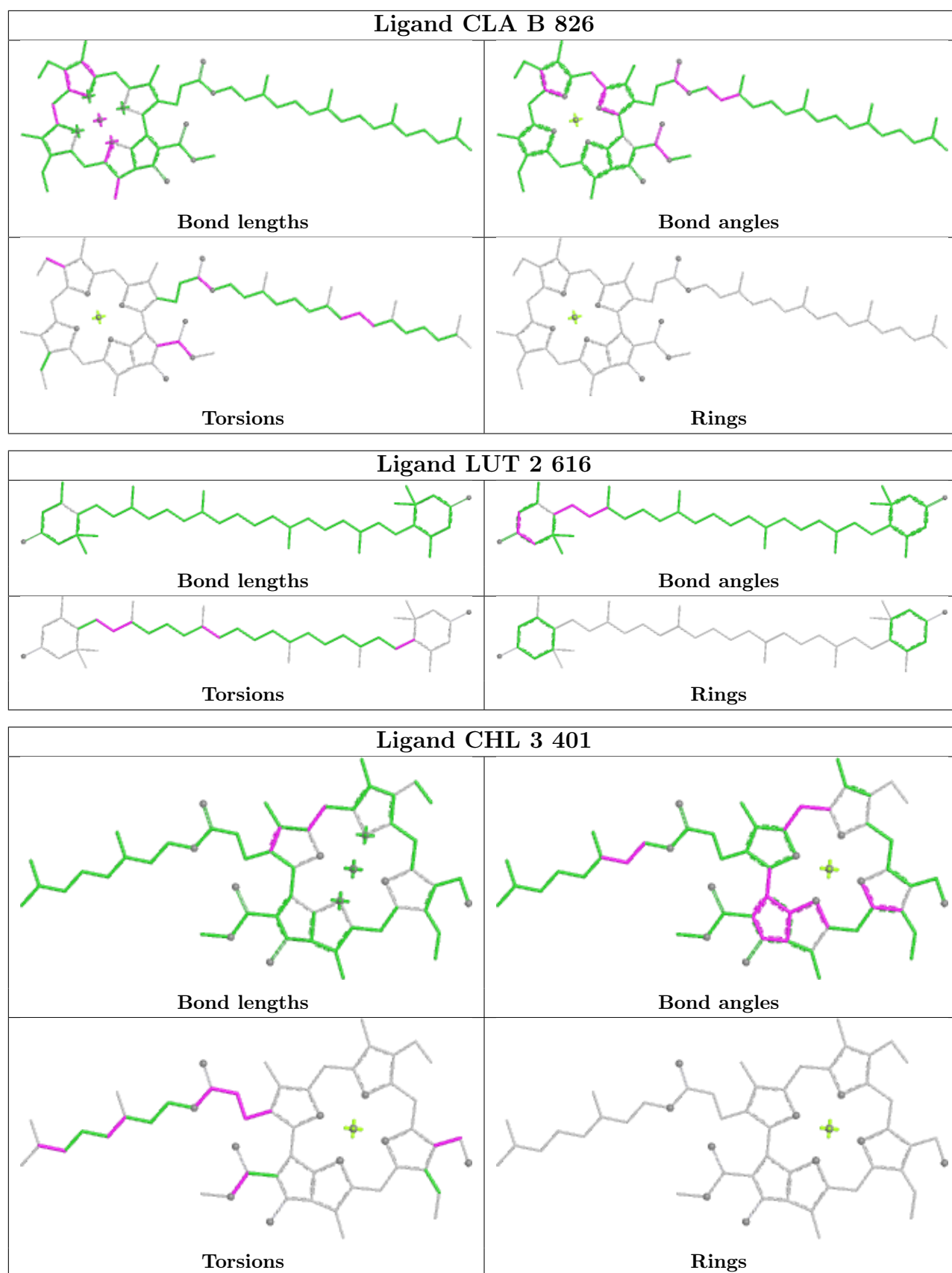


Ligand CLA A 819

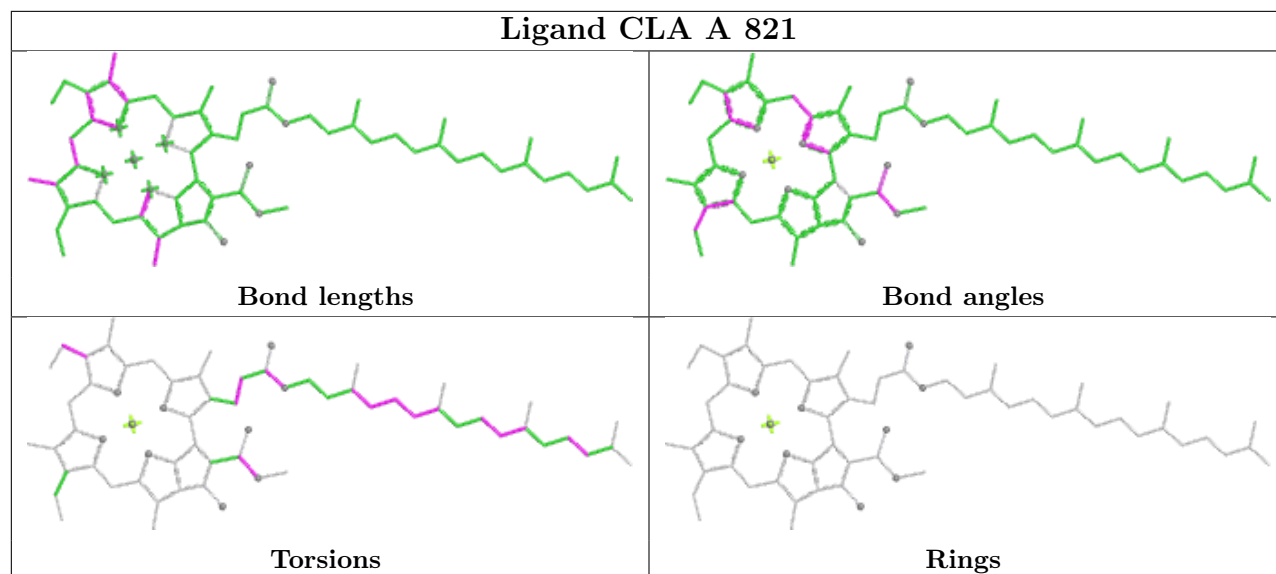


Ligand CLA A 844

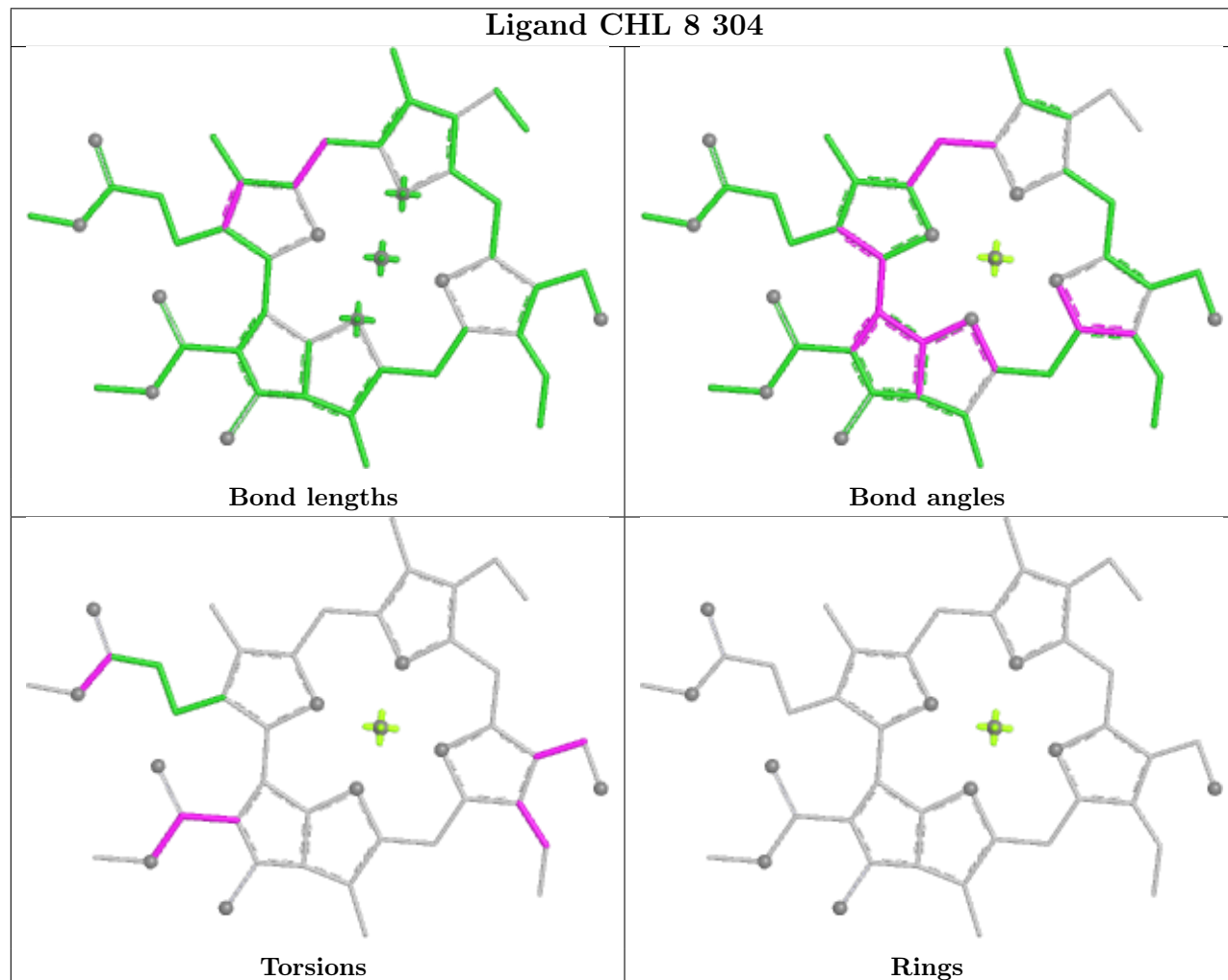




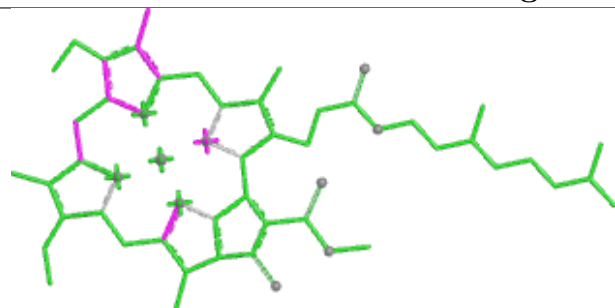
Ligand CLA A 821



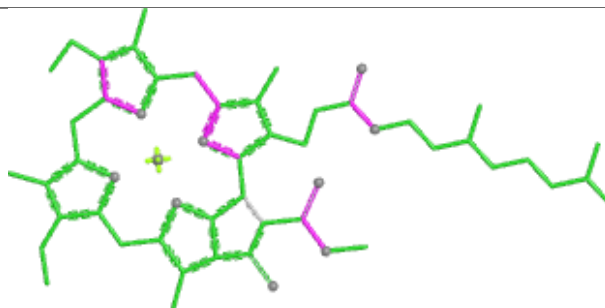
Ligand CHL 8 304



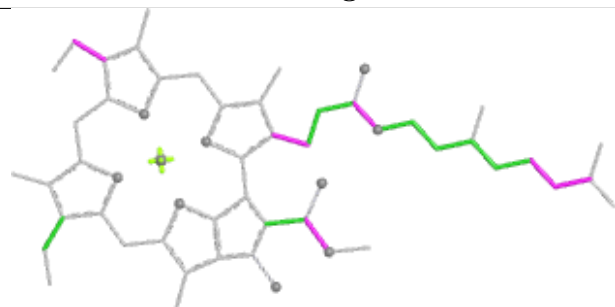
Ligand CLA 7 304



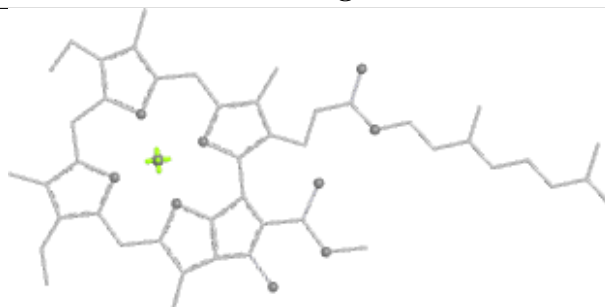
Bond lengths



Bond angles

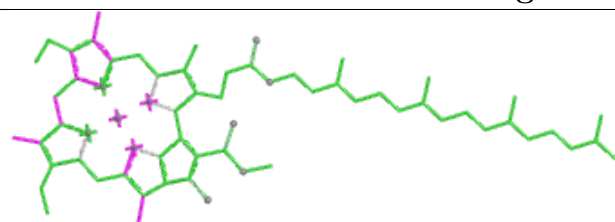


Torsions

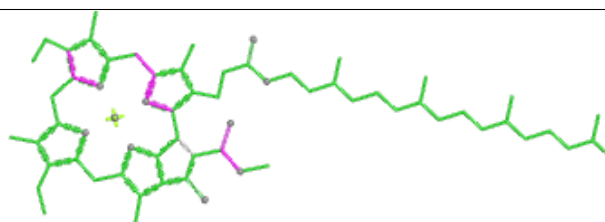


Rings

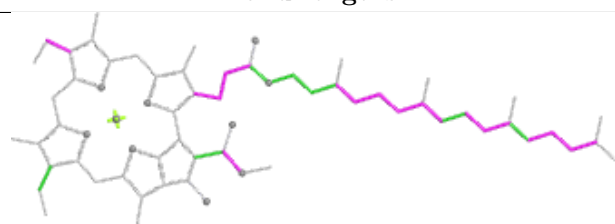
Ligand CLA B 829



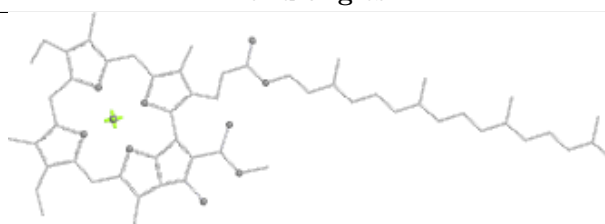
Bond lengths



Bond angles

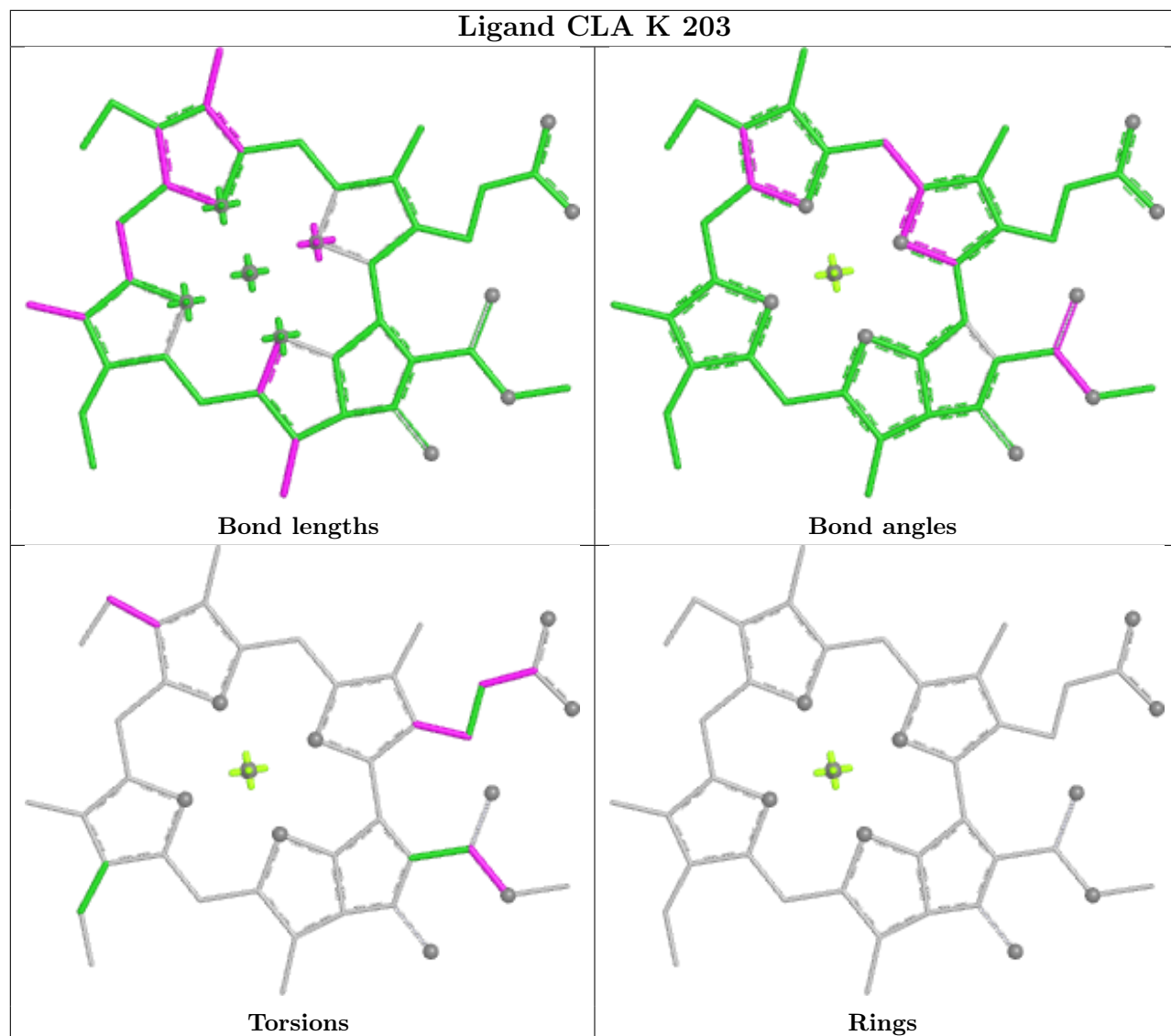


Torsions

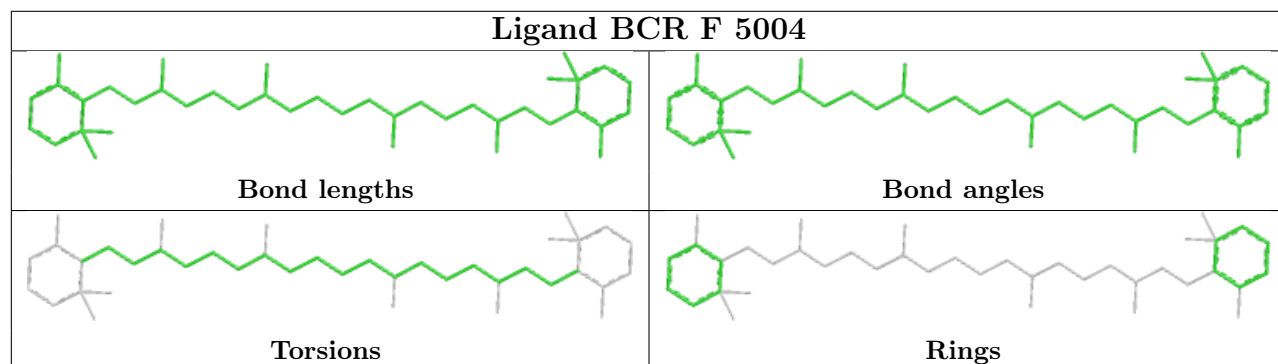


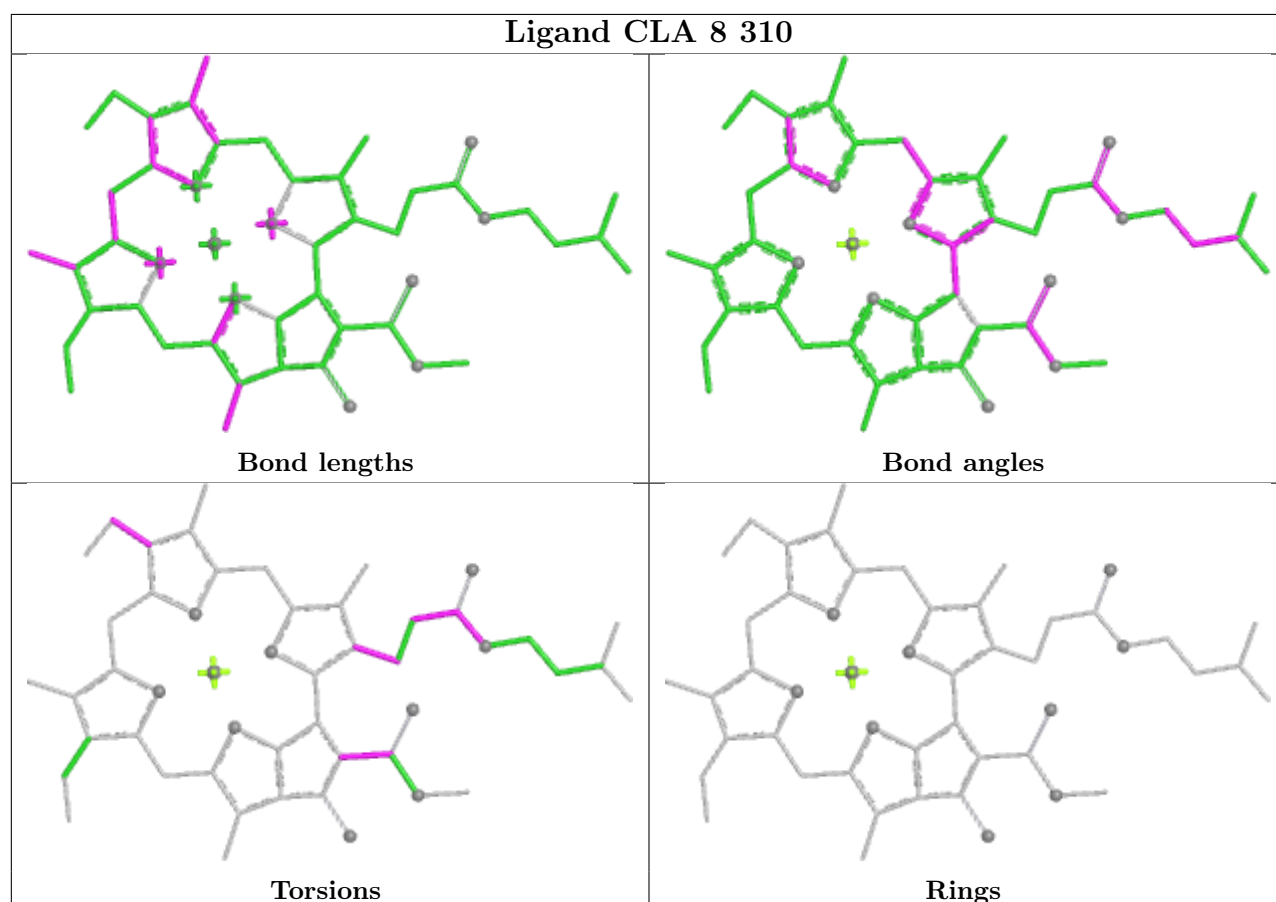
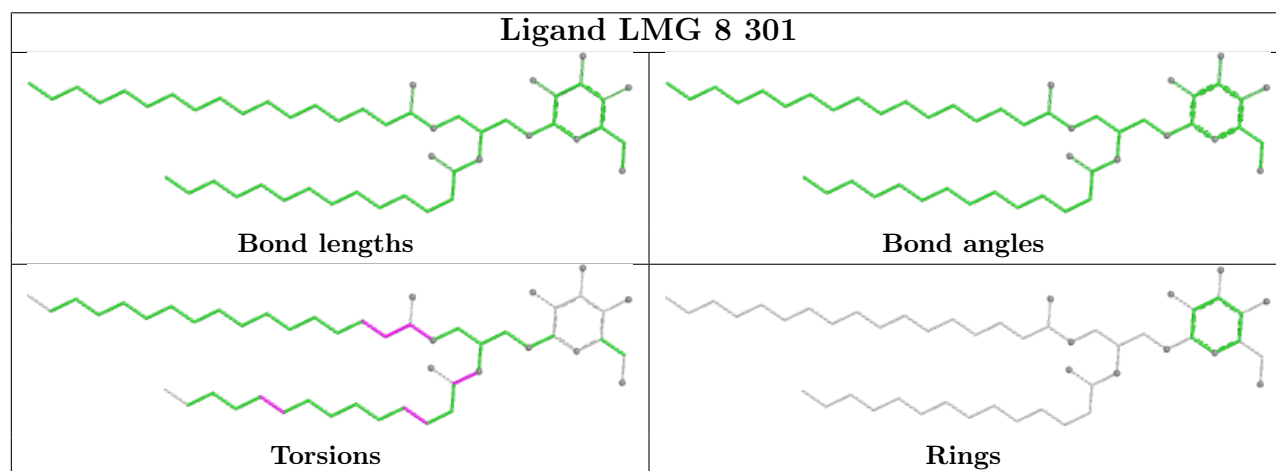
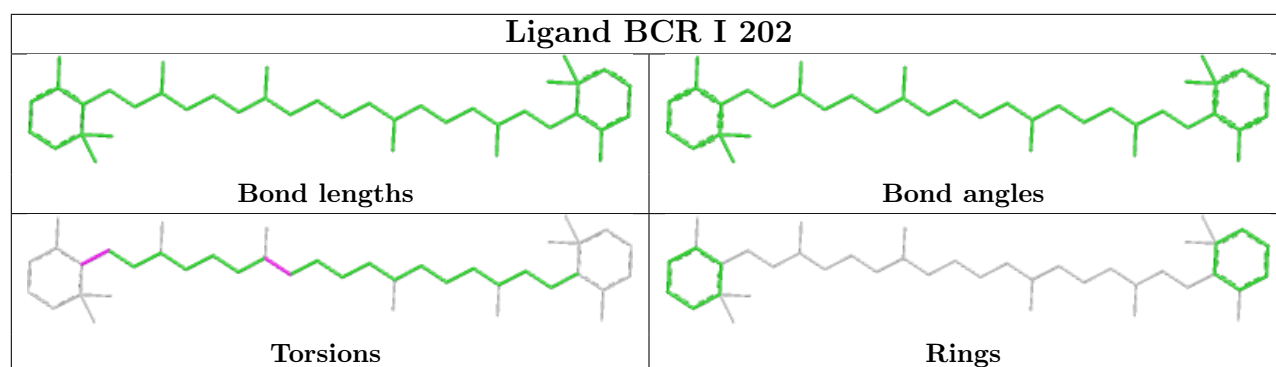
Rings

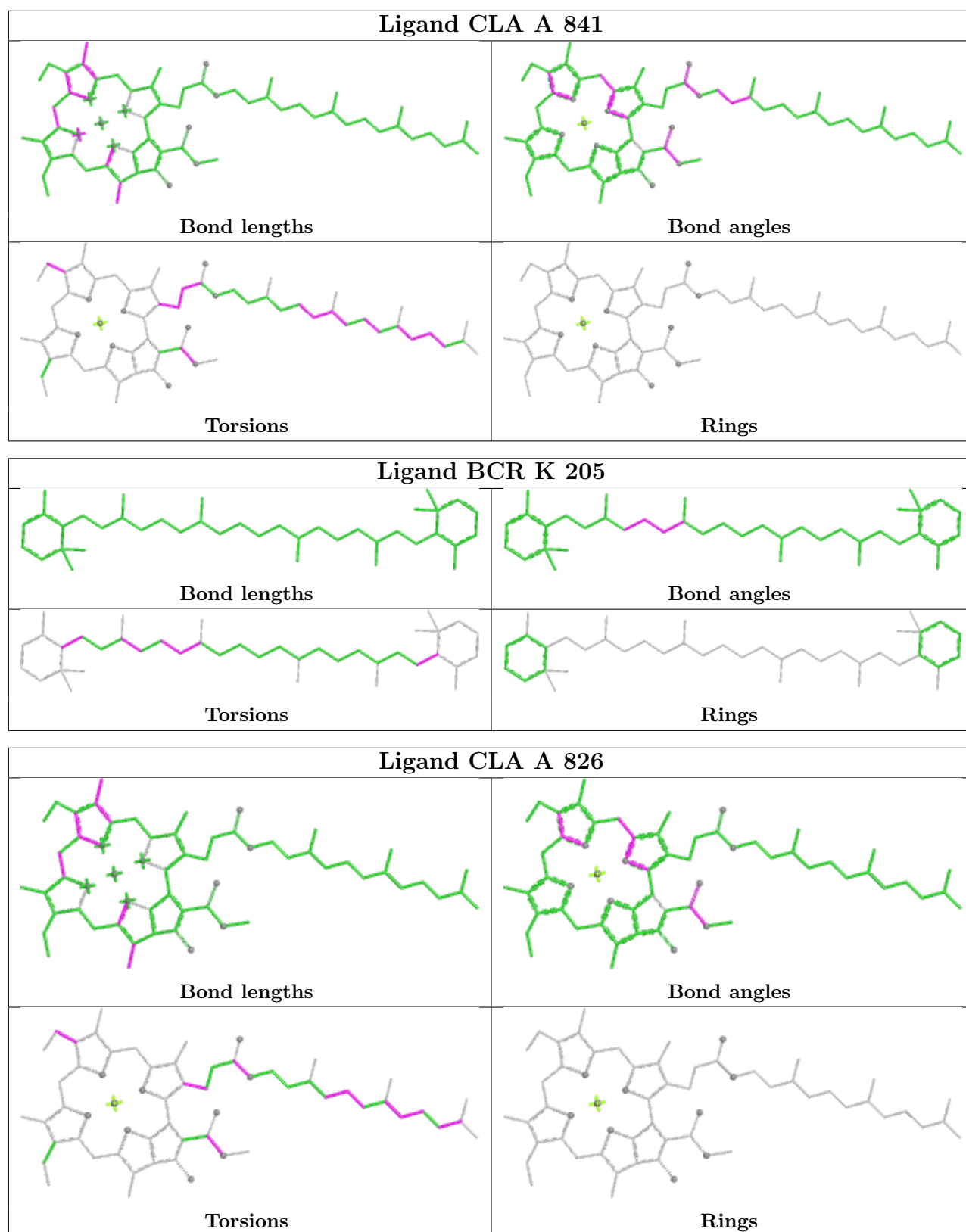
Ligand CLA K 203

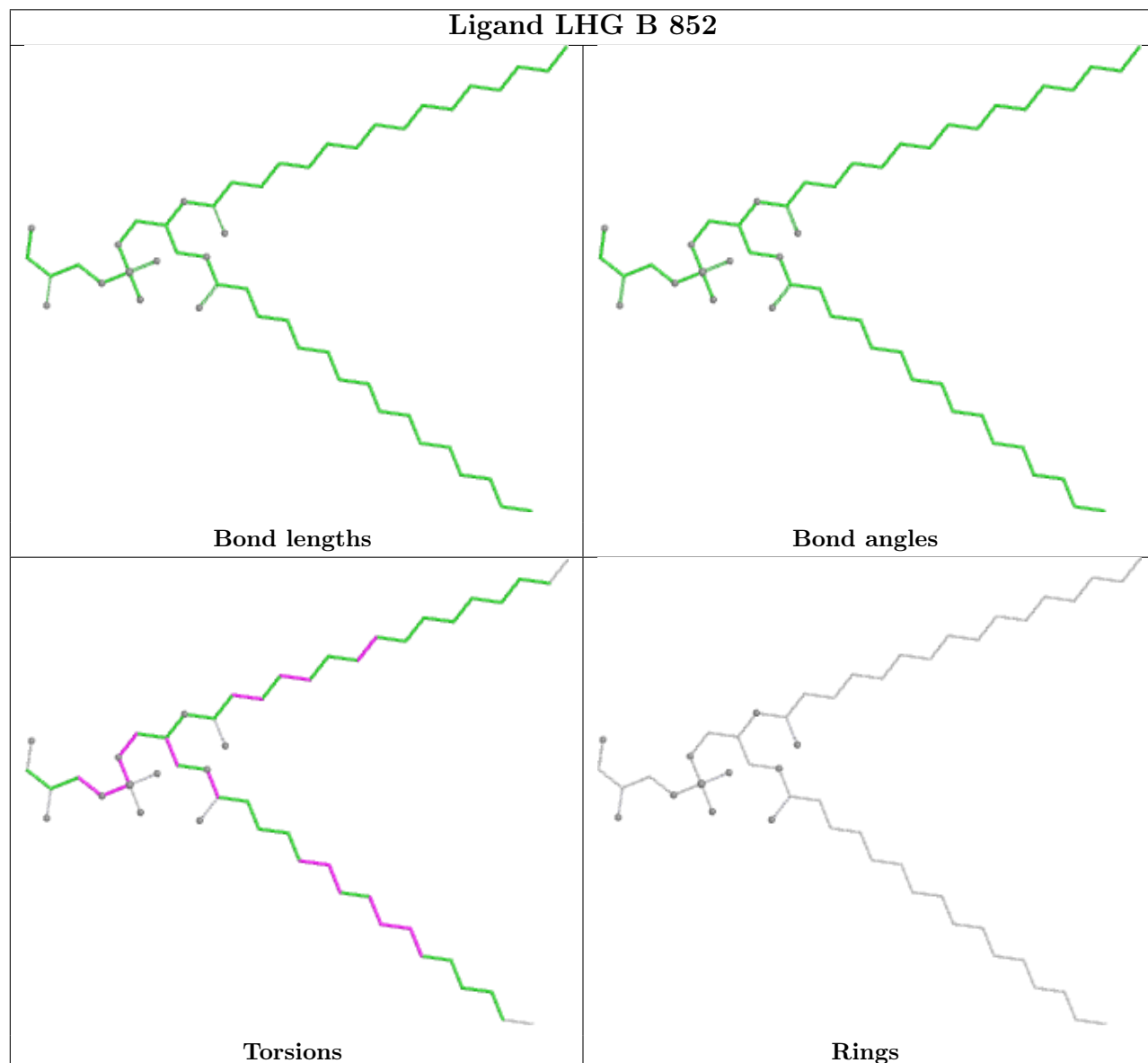
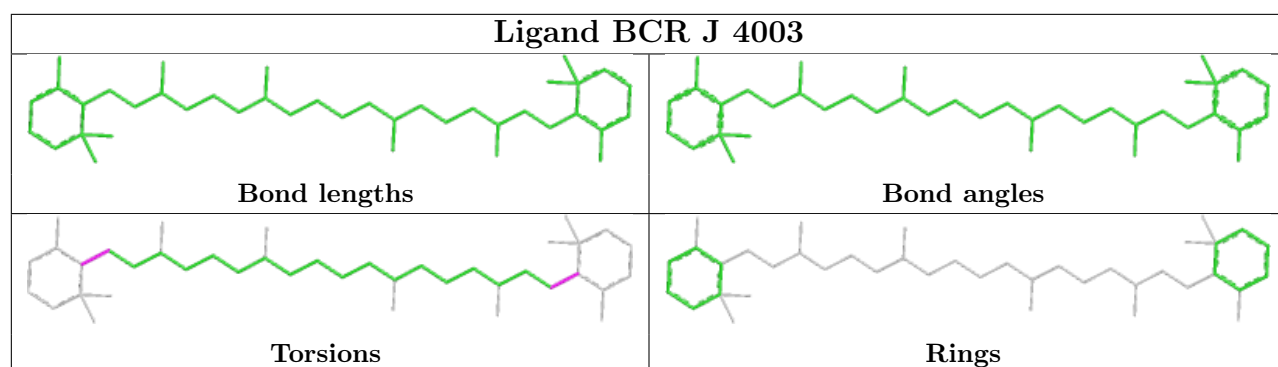


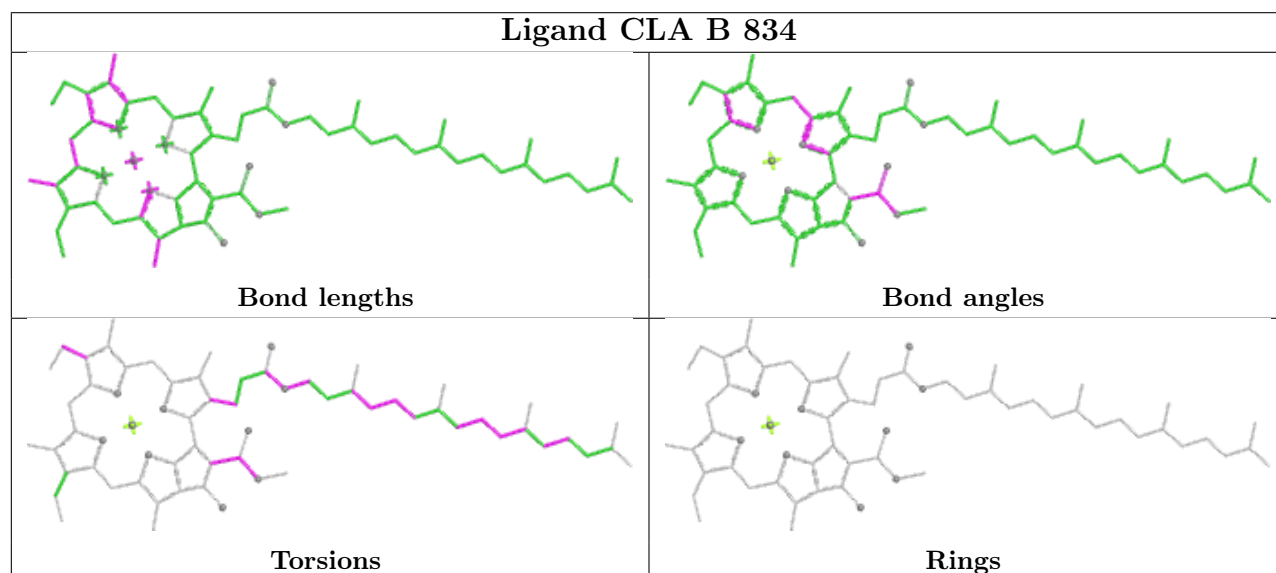
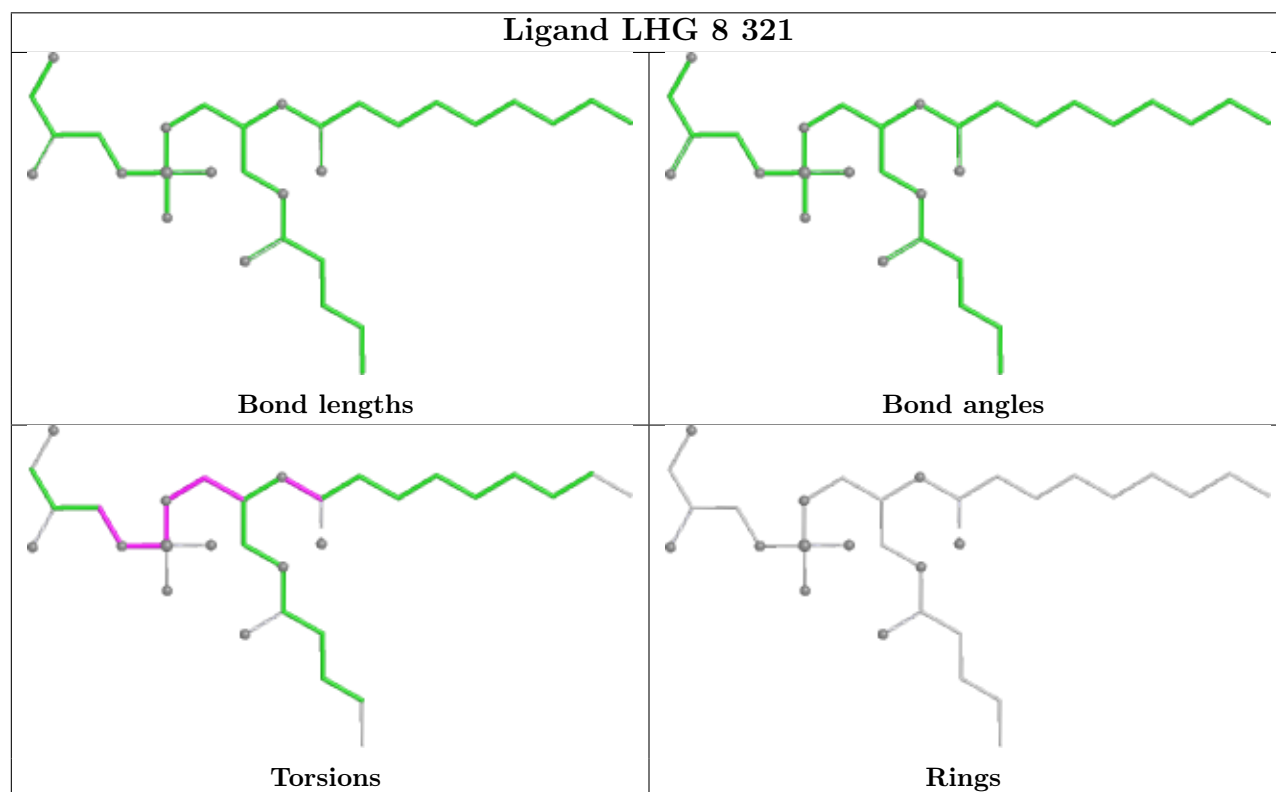
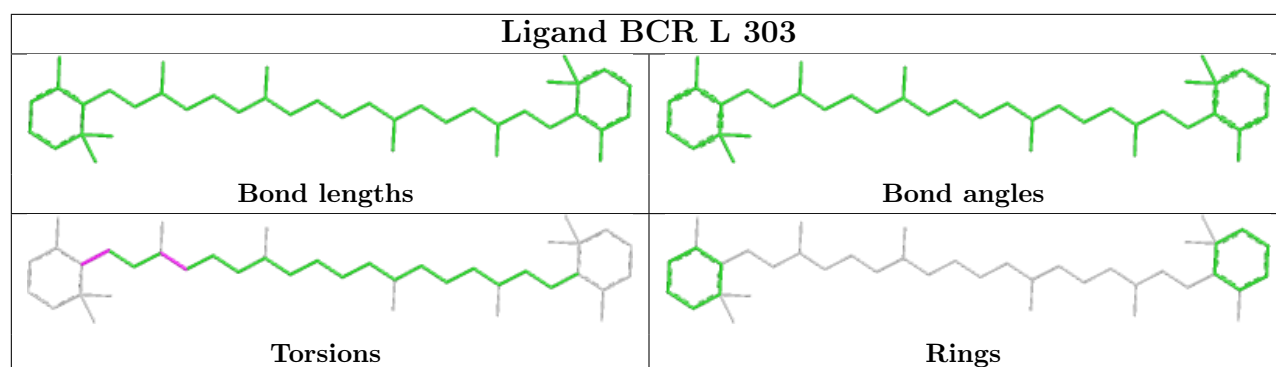
Ligand BCR F 5004

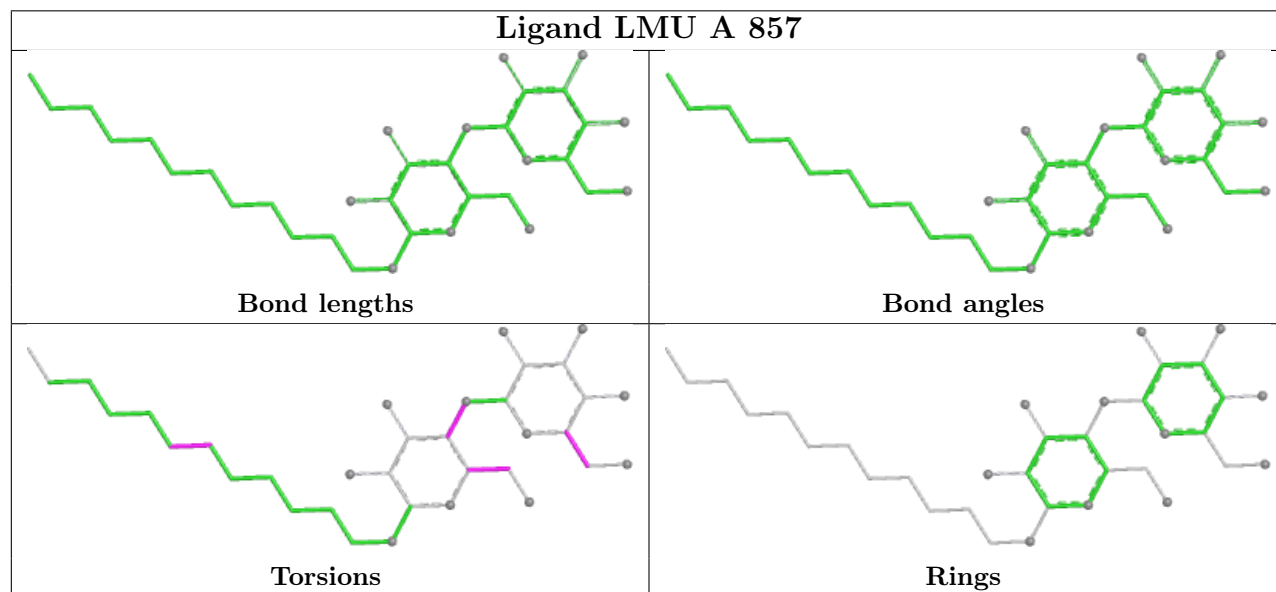
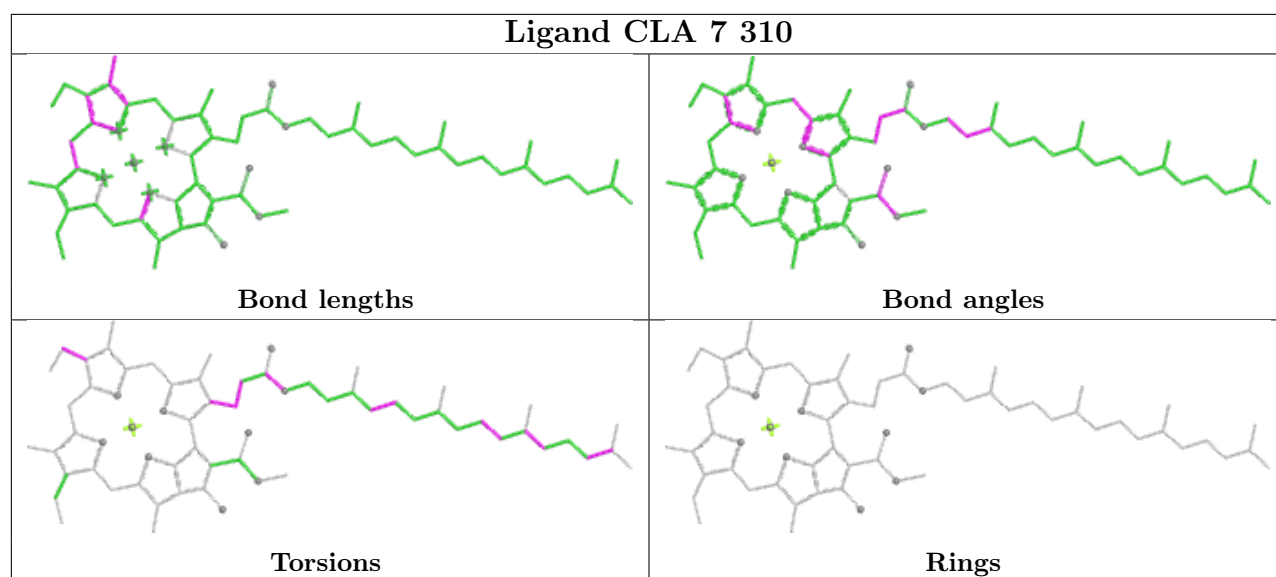




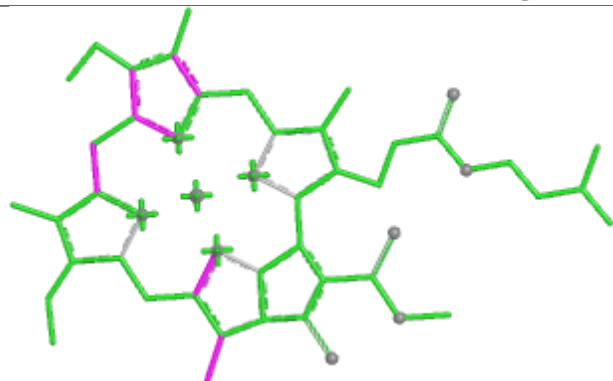




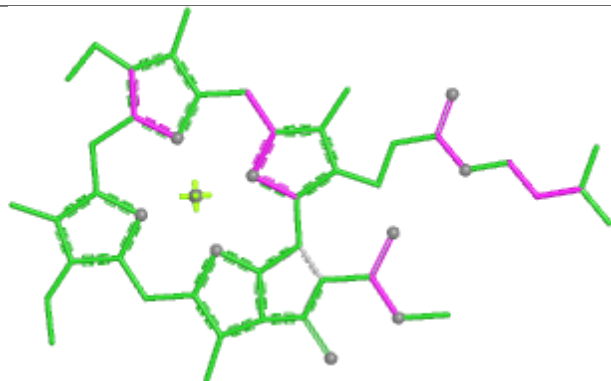




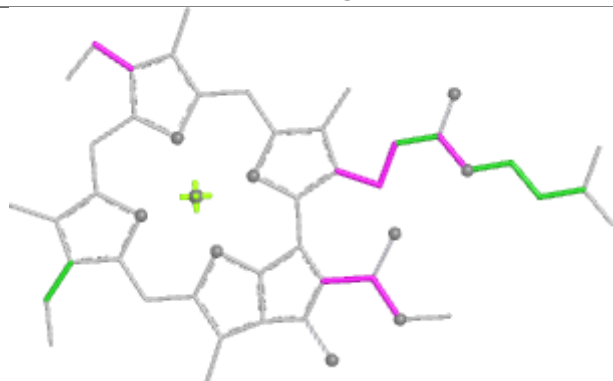
Ligand CLA L 307



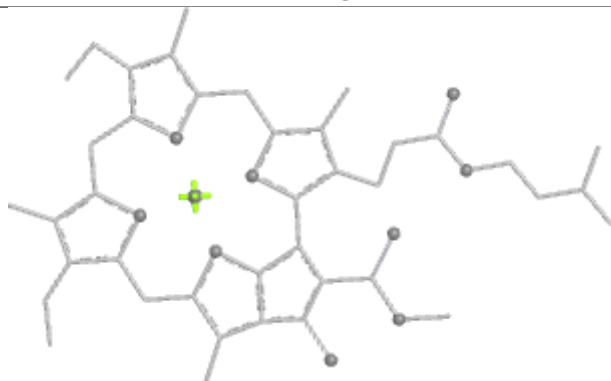
Bond lengths



Bond angles

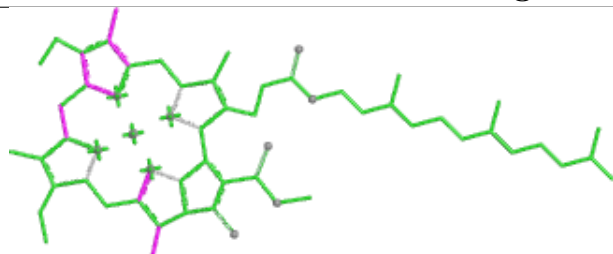


Torsions

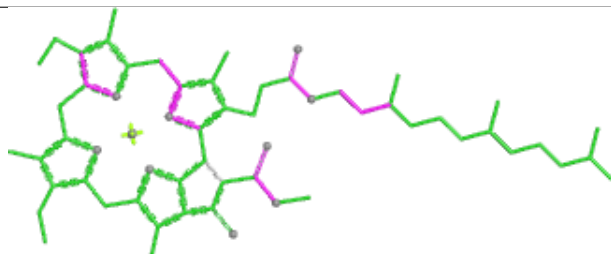


Rings

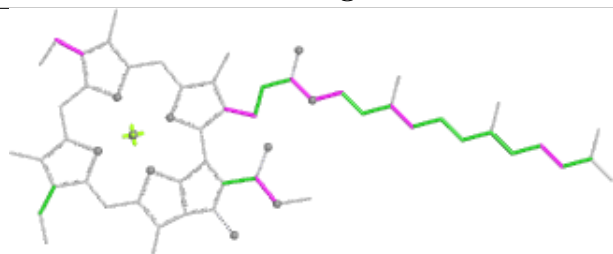
Ligand CLA A 840



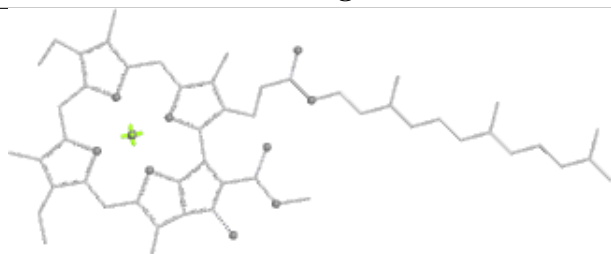
Bond lengths



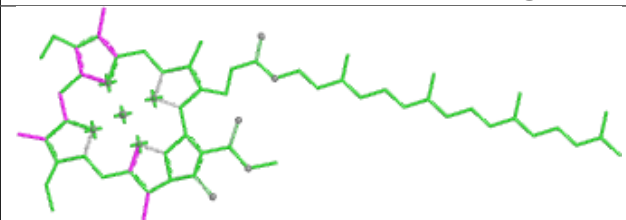
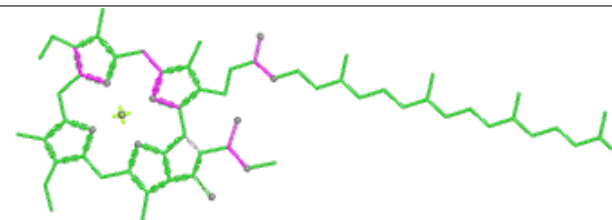
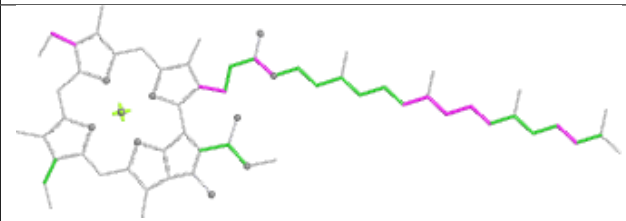
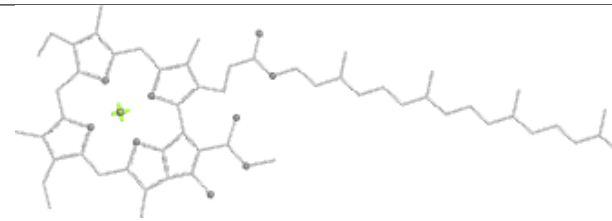
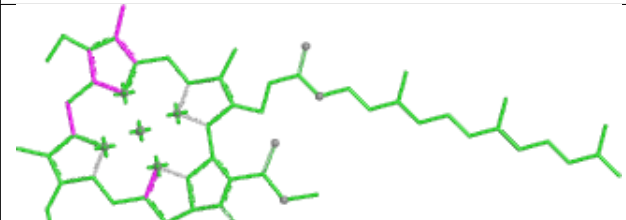
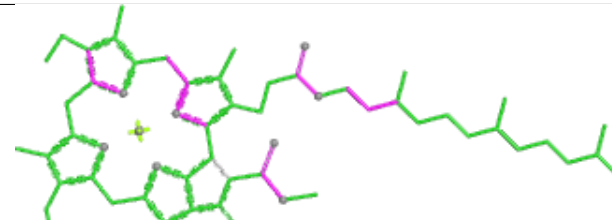
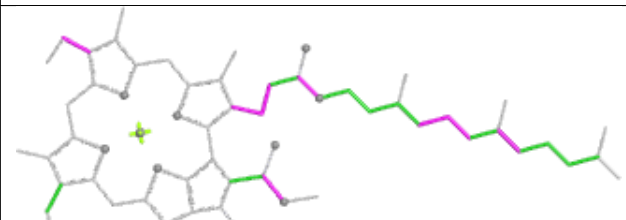
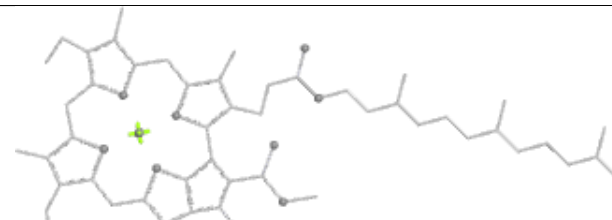
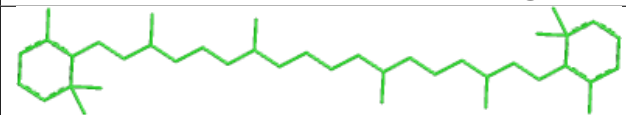
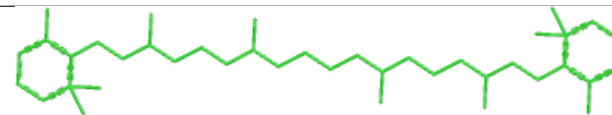
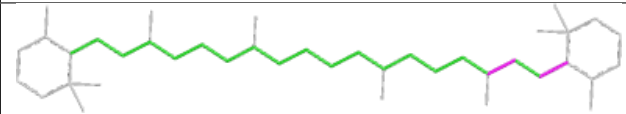
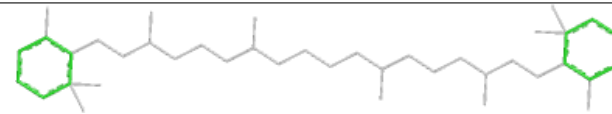
Bond angles

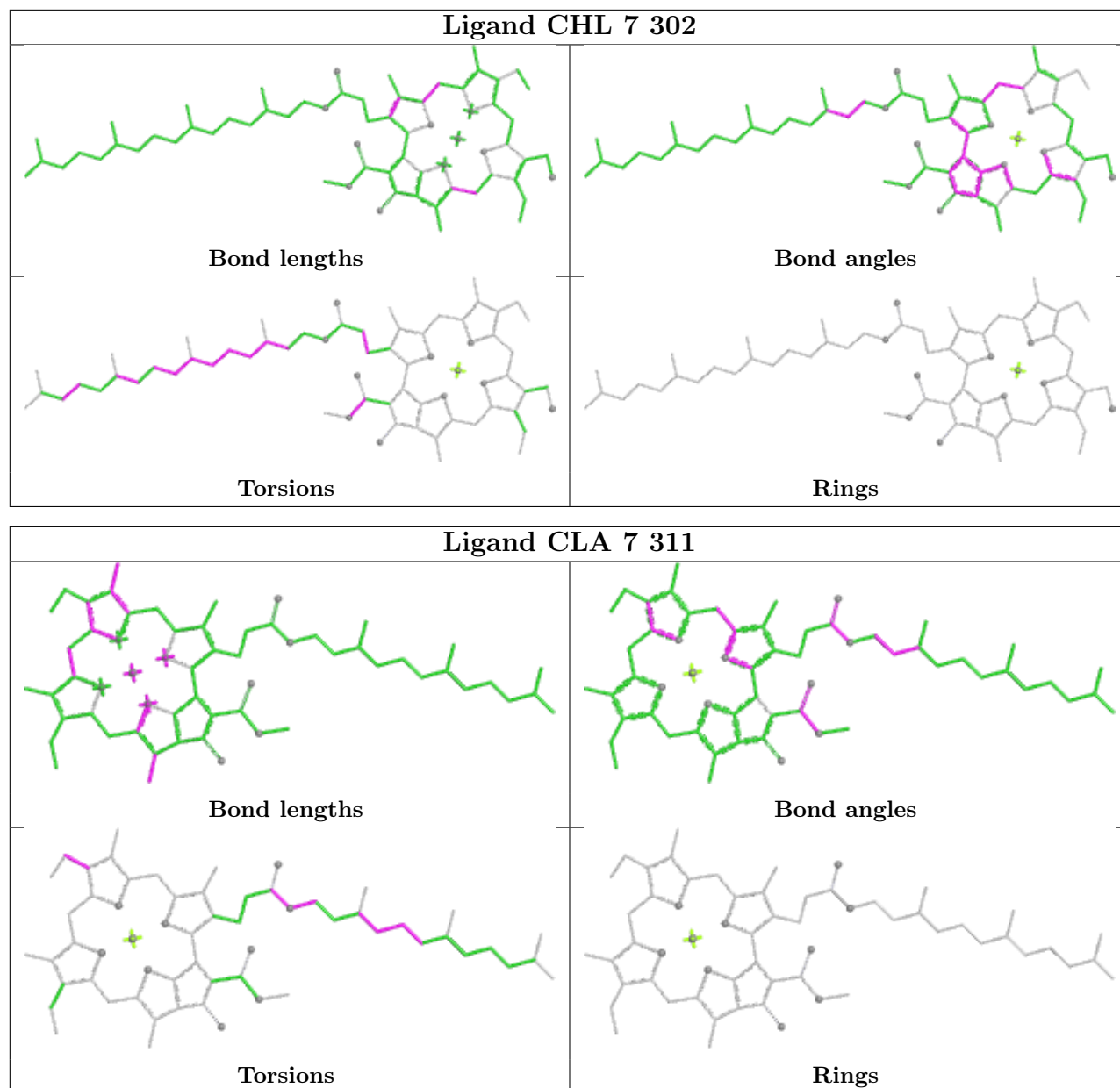


Torsions

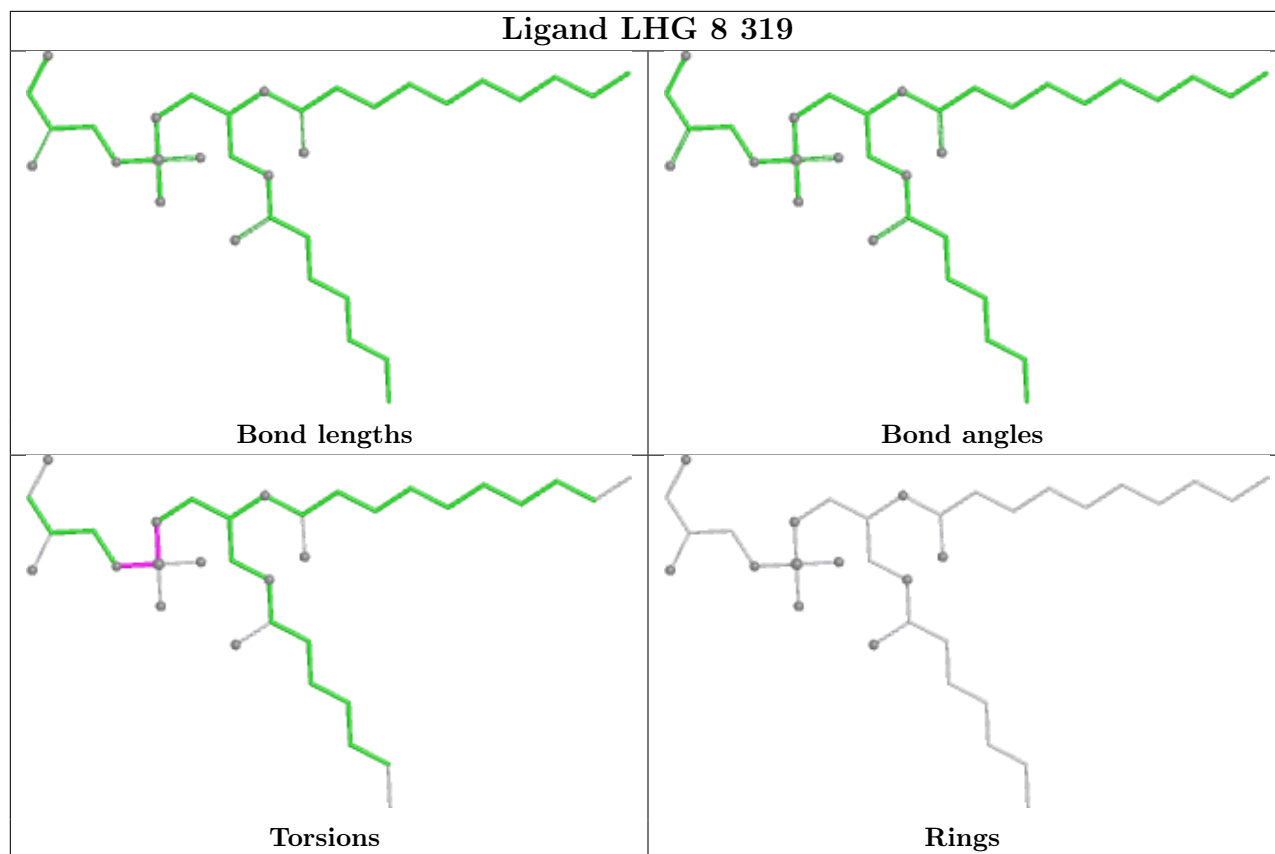


Rings

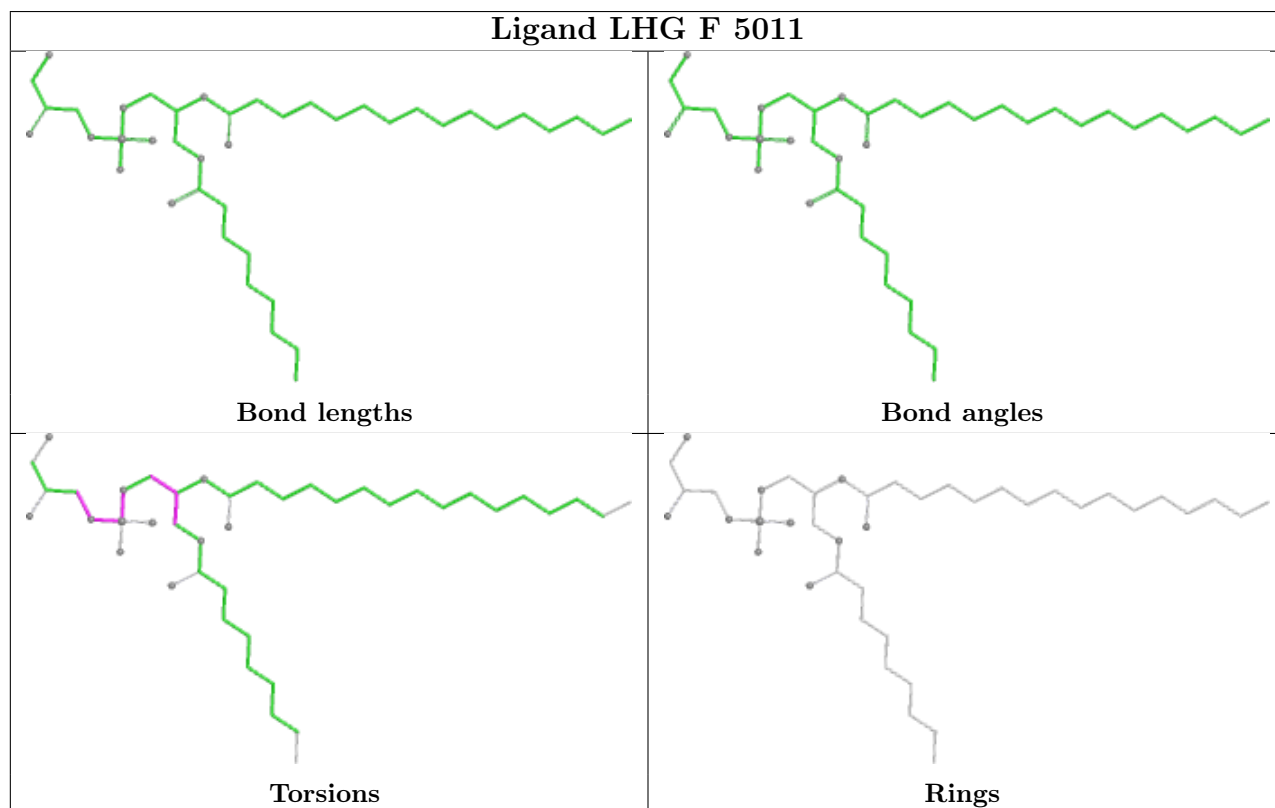
Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA 8 302	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR L 308	
	
Bond lengths	Bond angles
	
Torsions	Rings



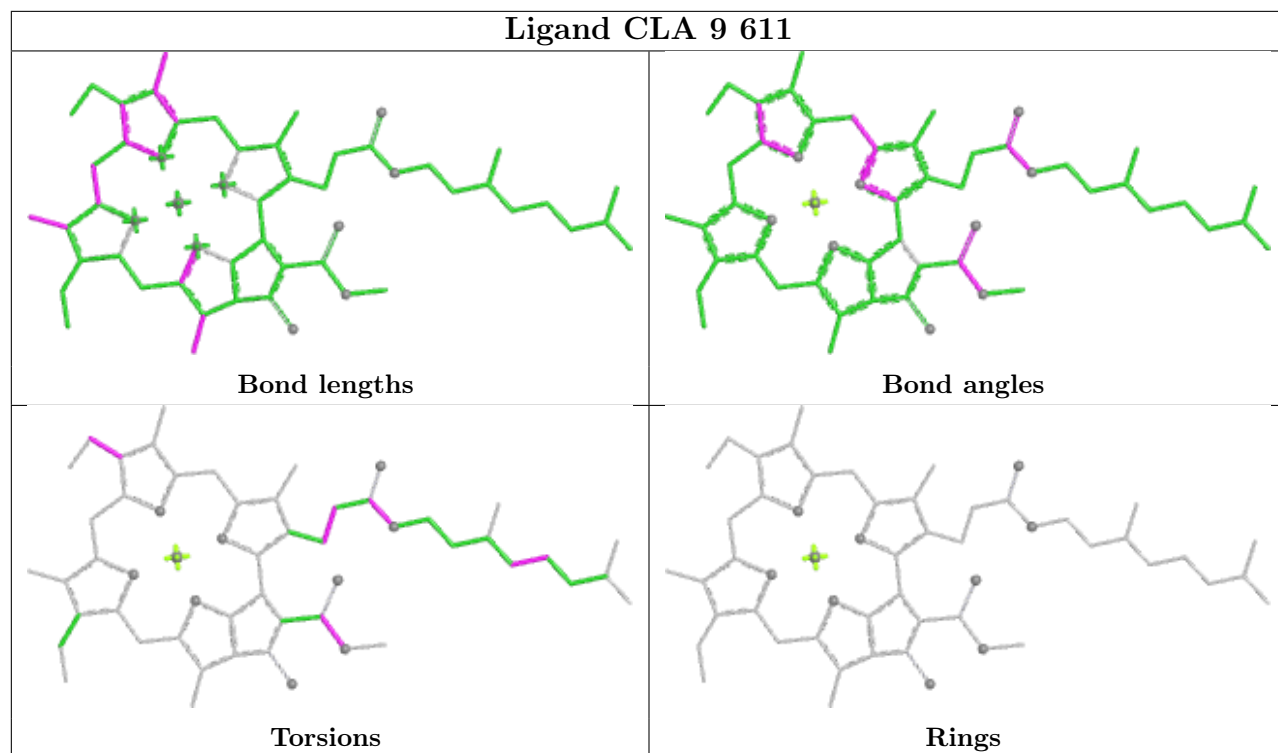
Ligand LHG 8 319



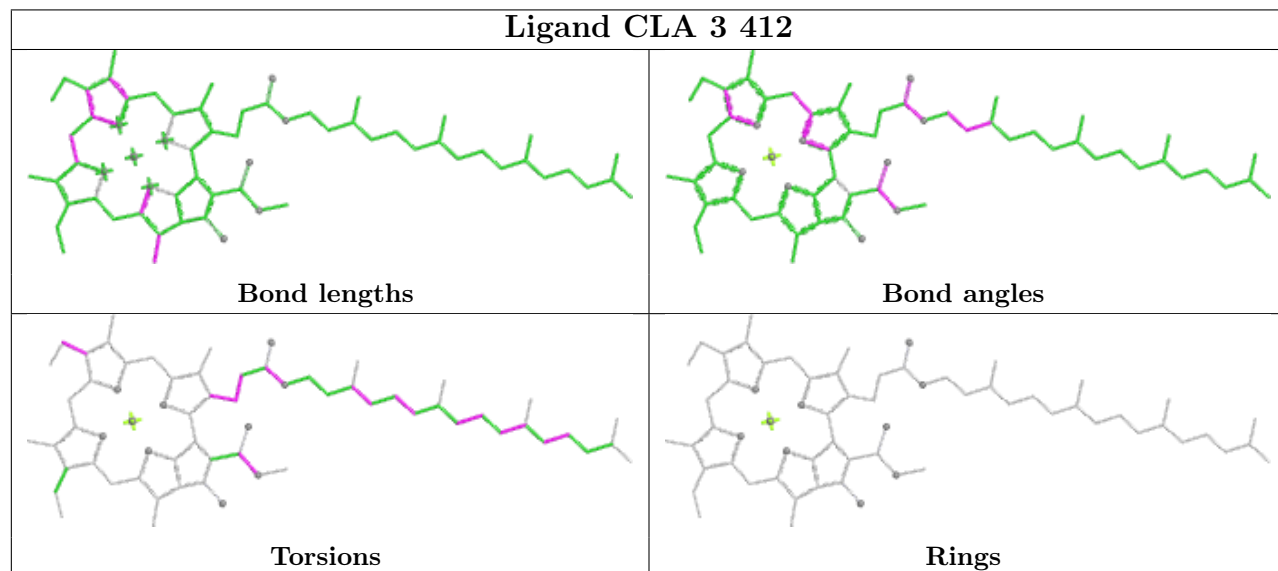
Ligand LHG F 5011



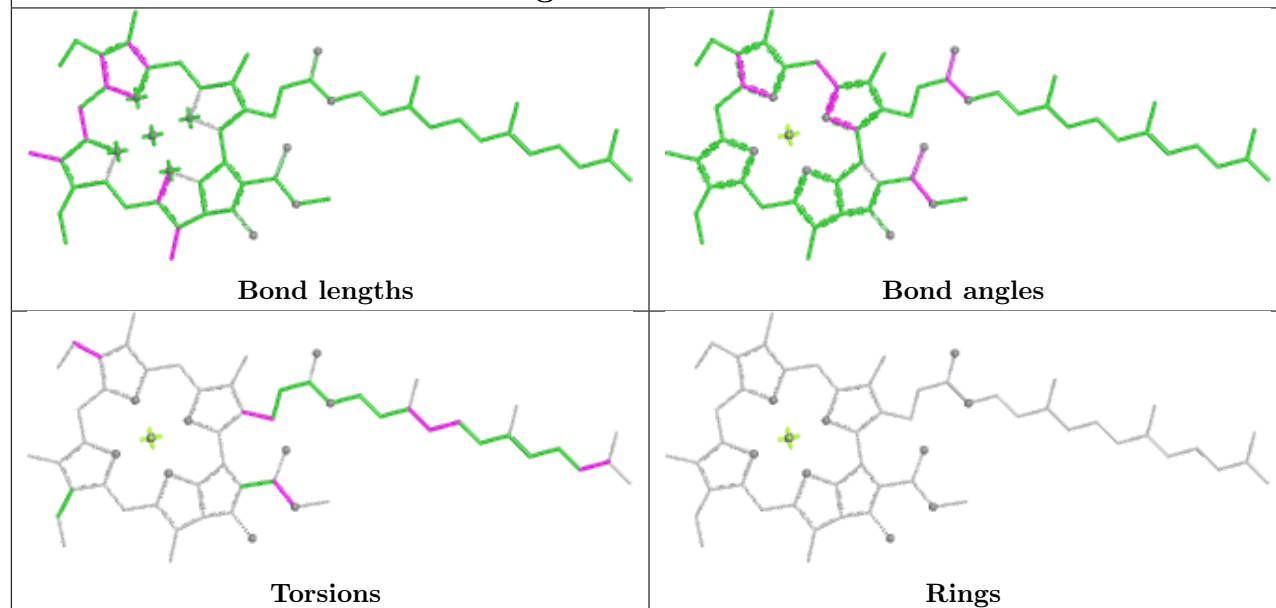
Ligand CLA 9 611



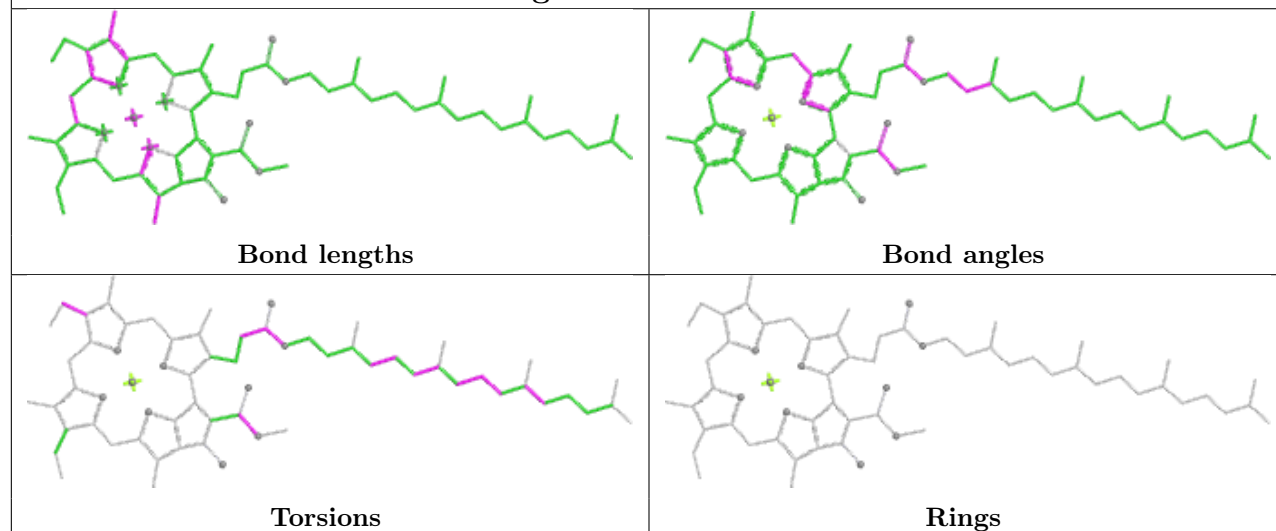
Ligand CLA 3 412



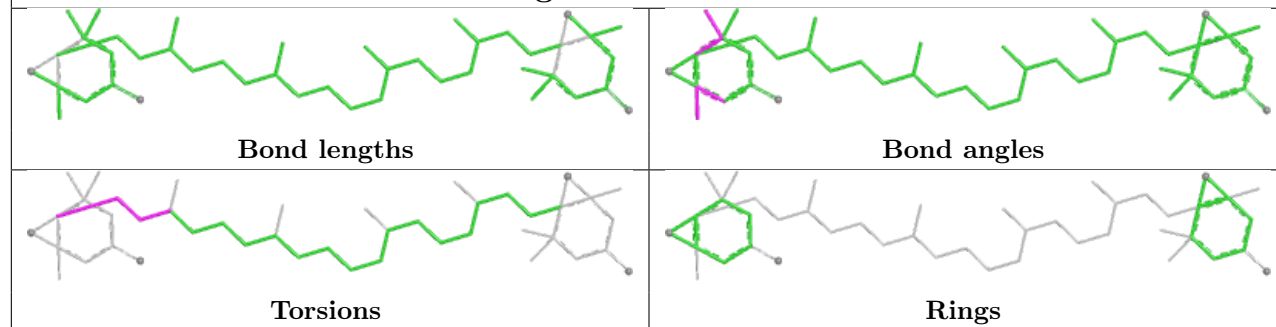
Ligand CLA 9 608

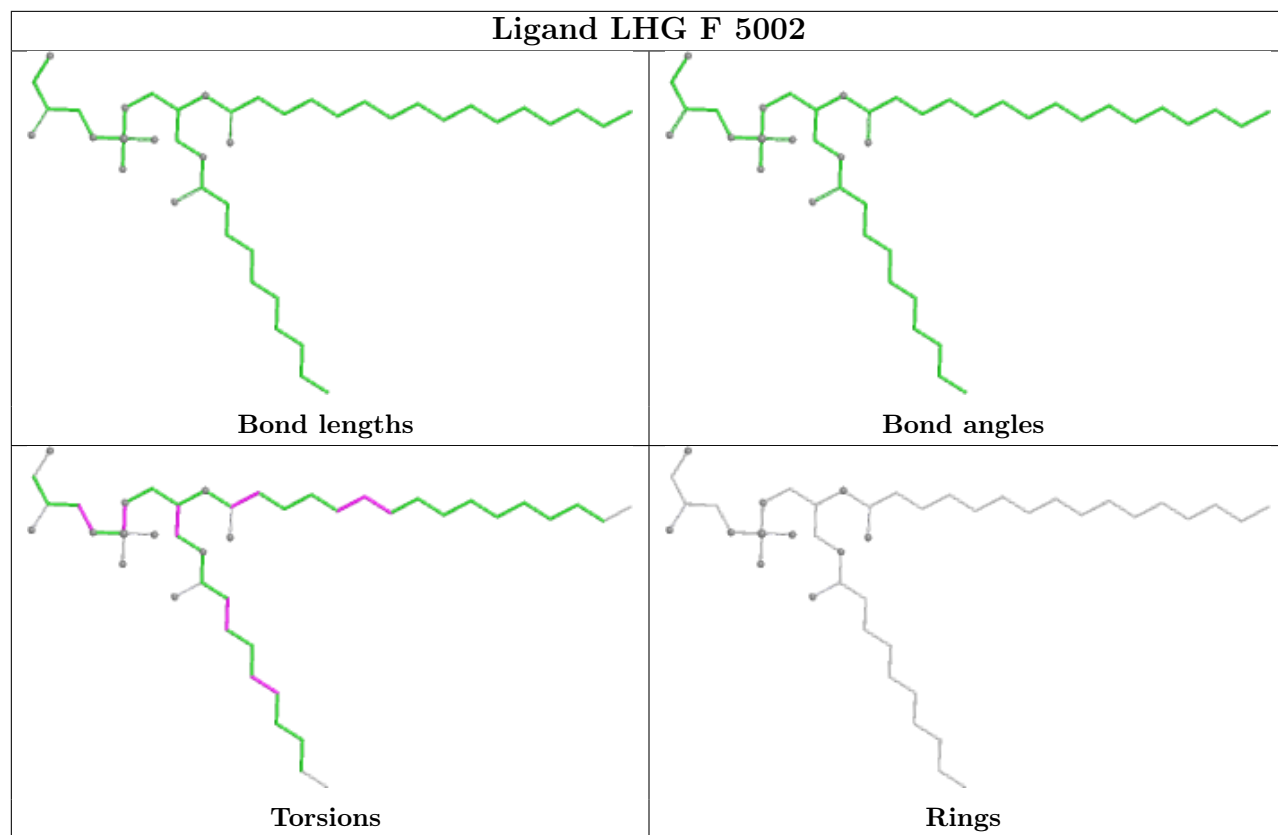


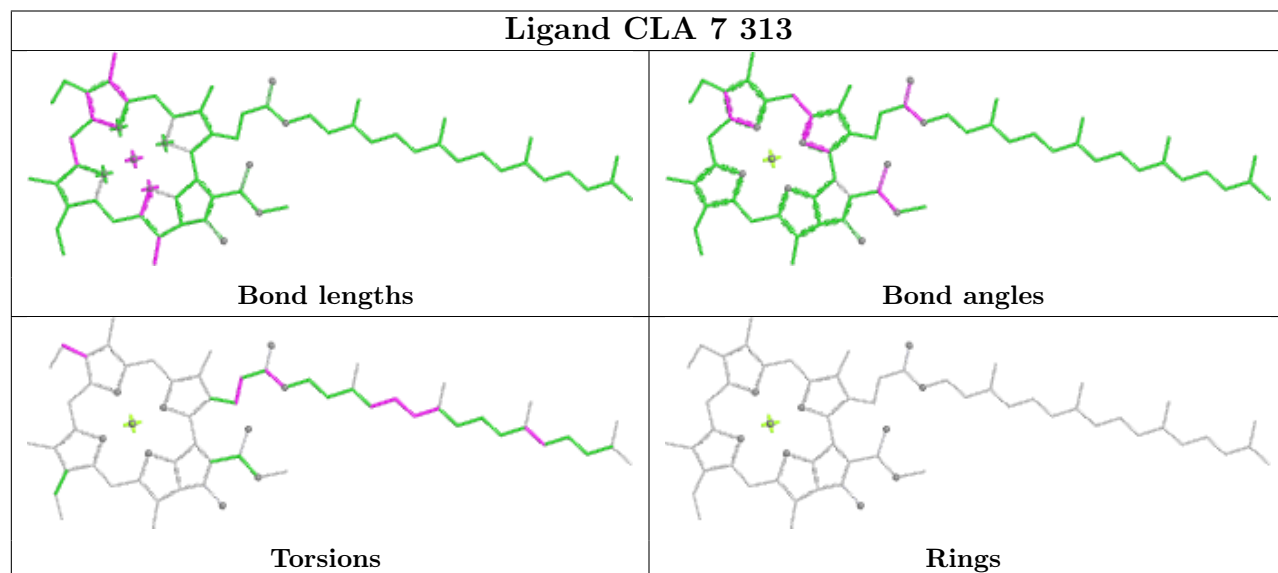
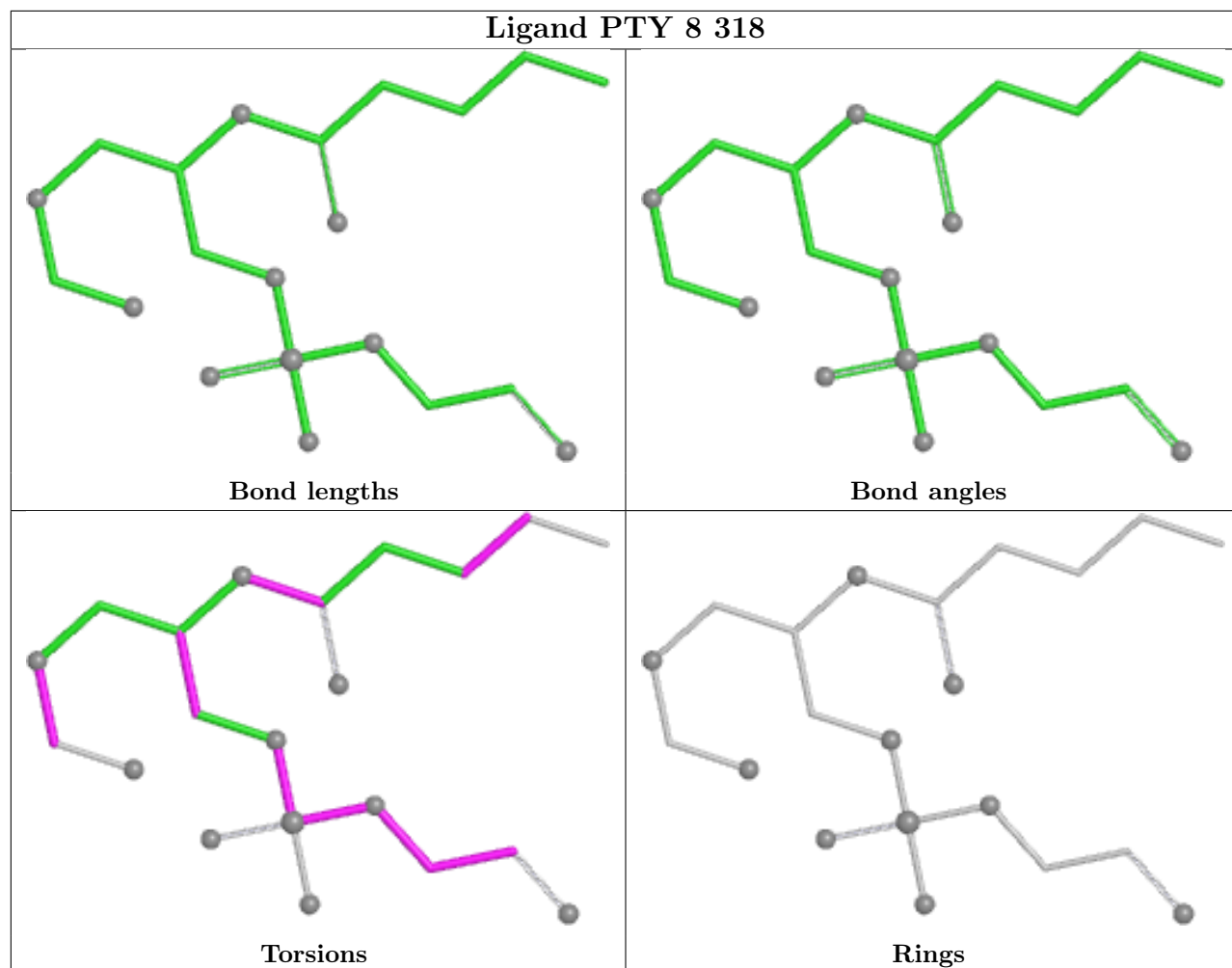
Ligand CLA B 807



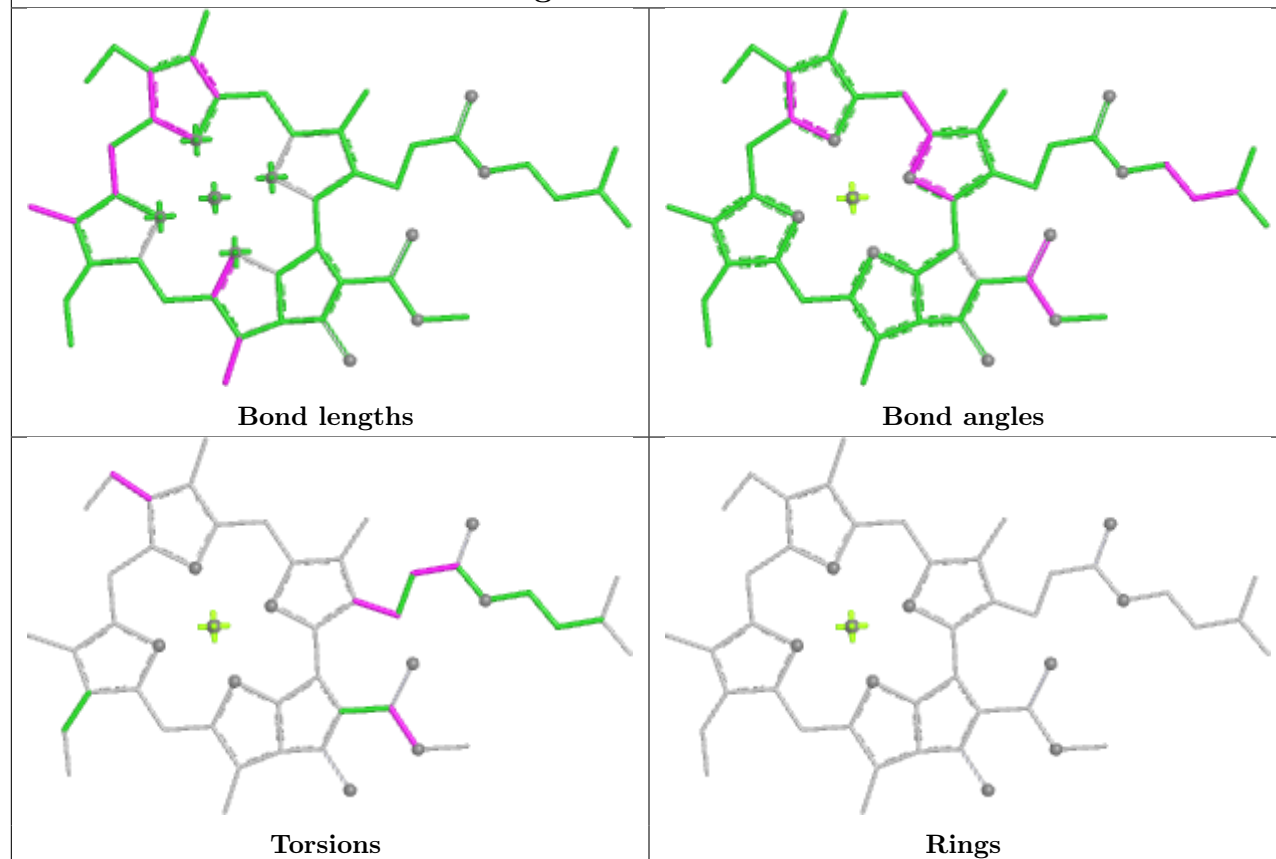
Ligand XAT 7 317



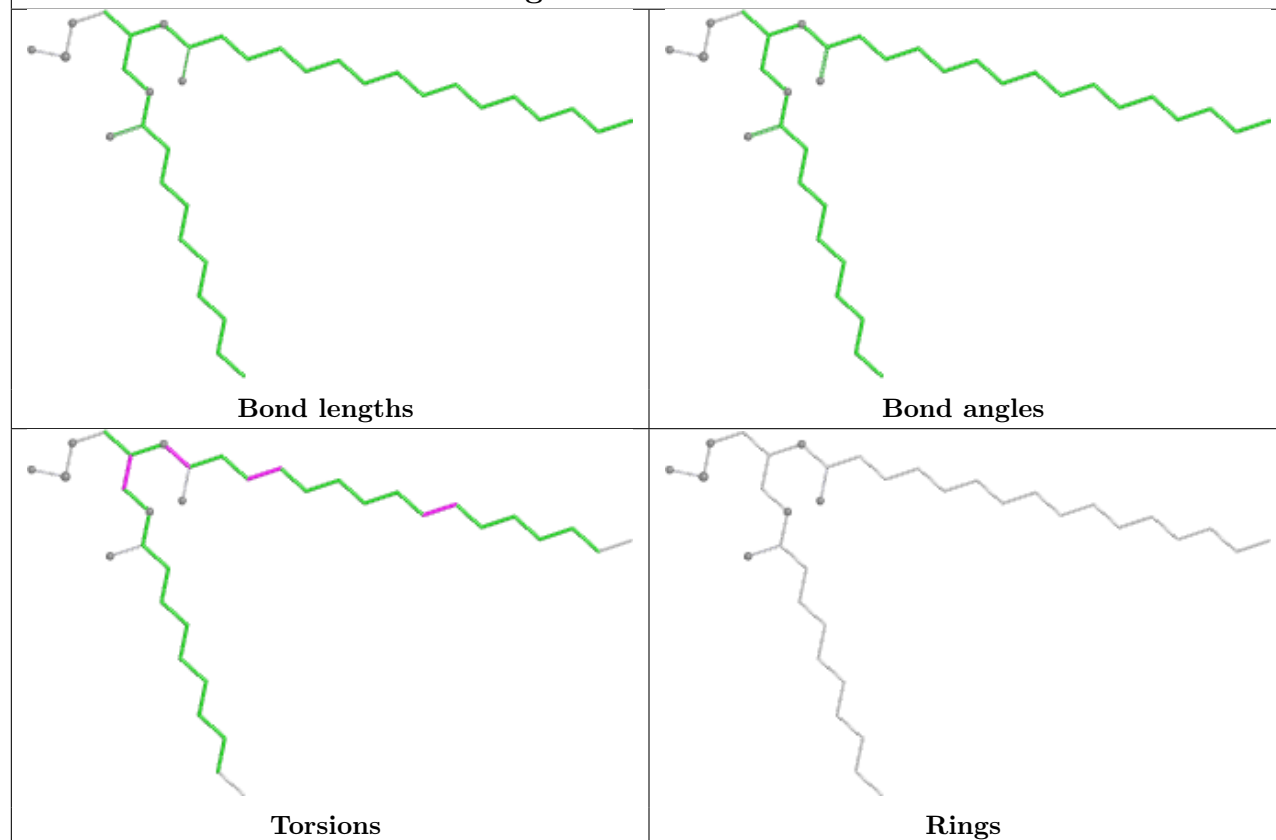


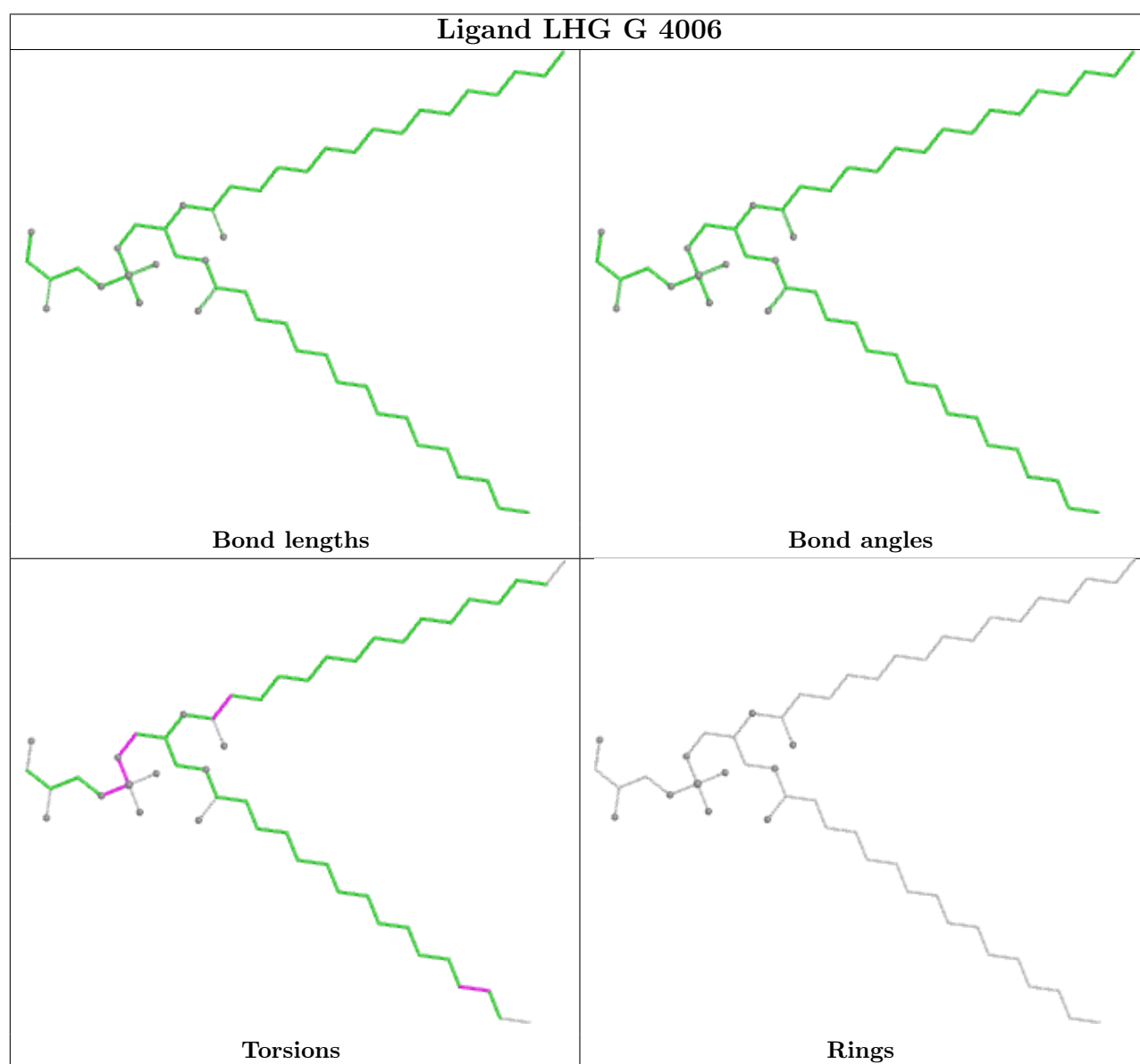
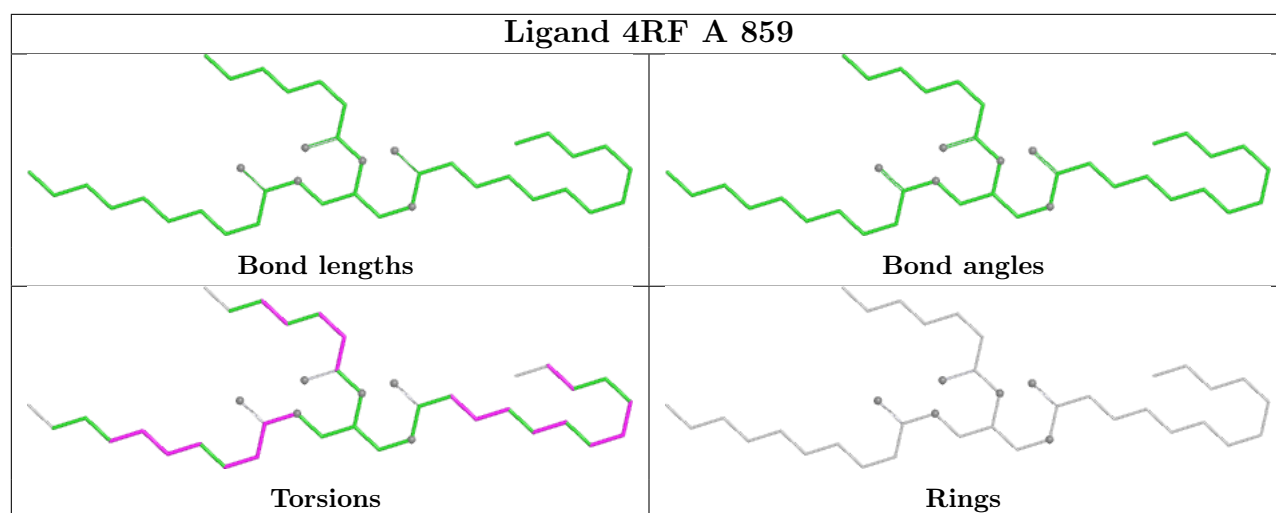


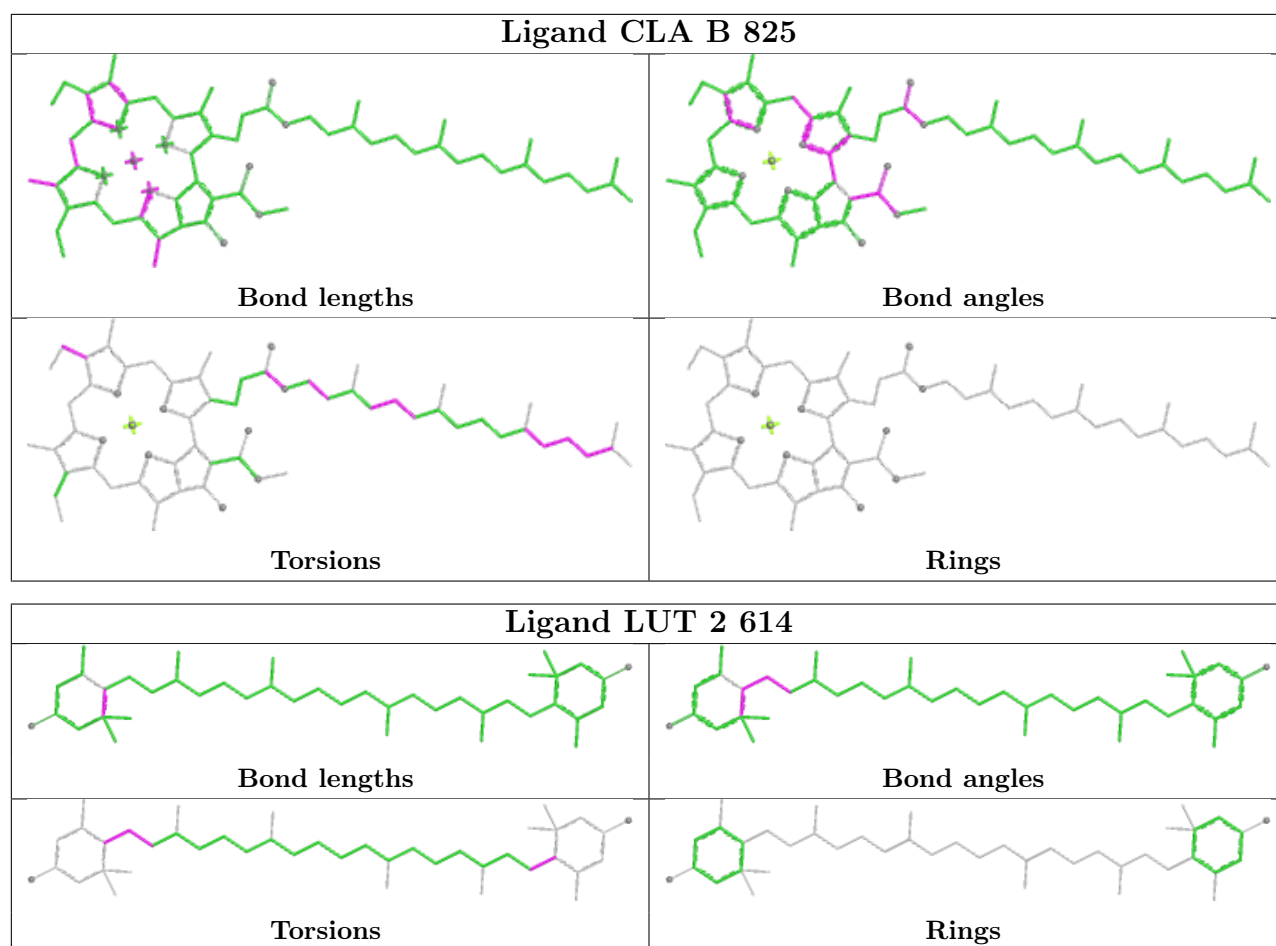
Ligand CLA L 306



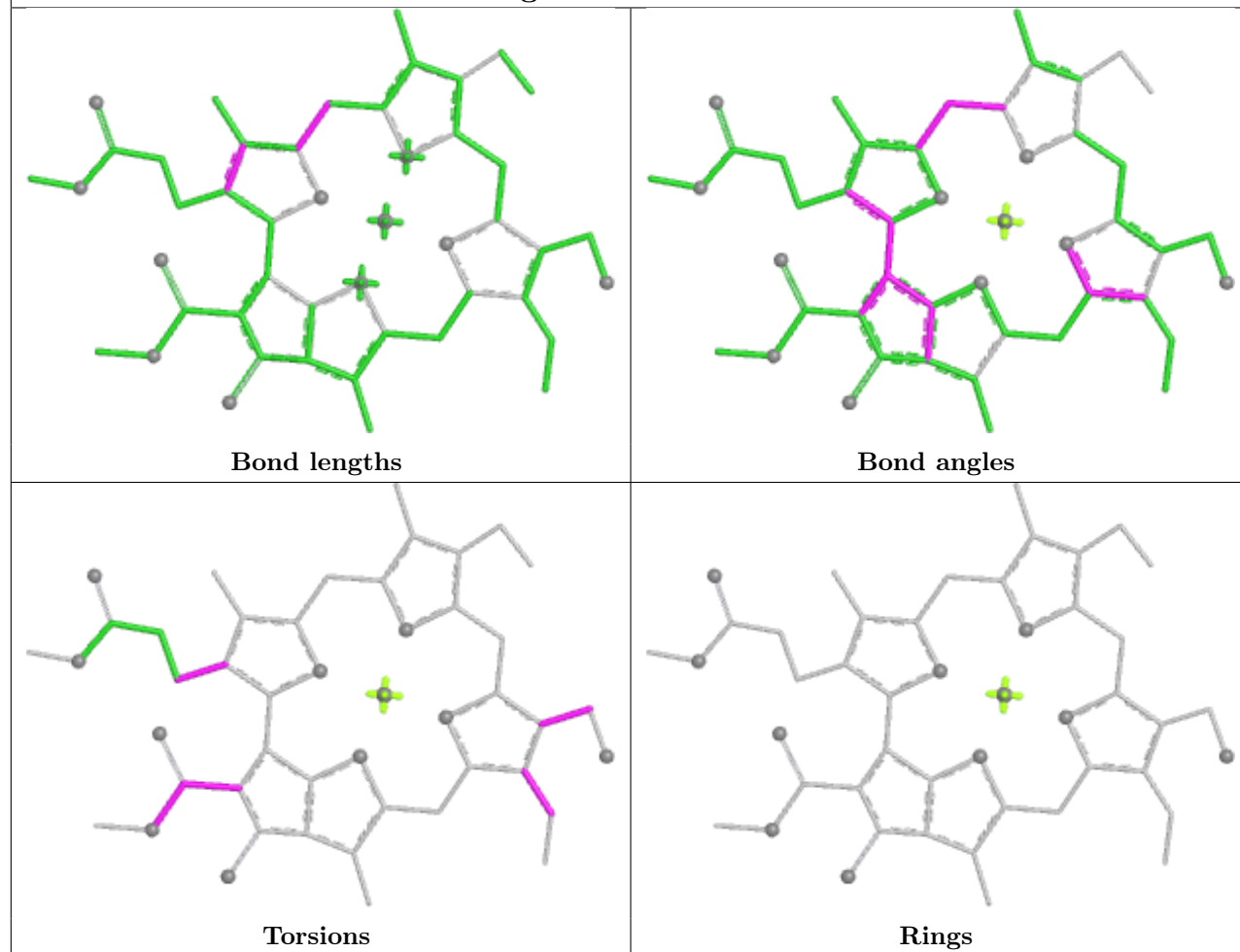
Ligand LHG J 4004



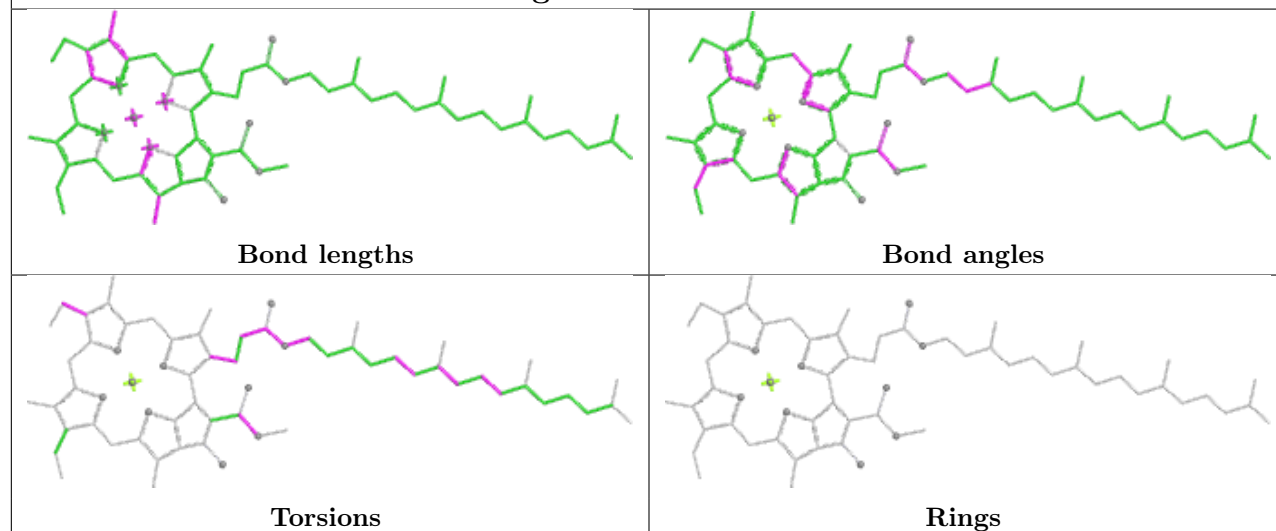


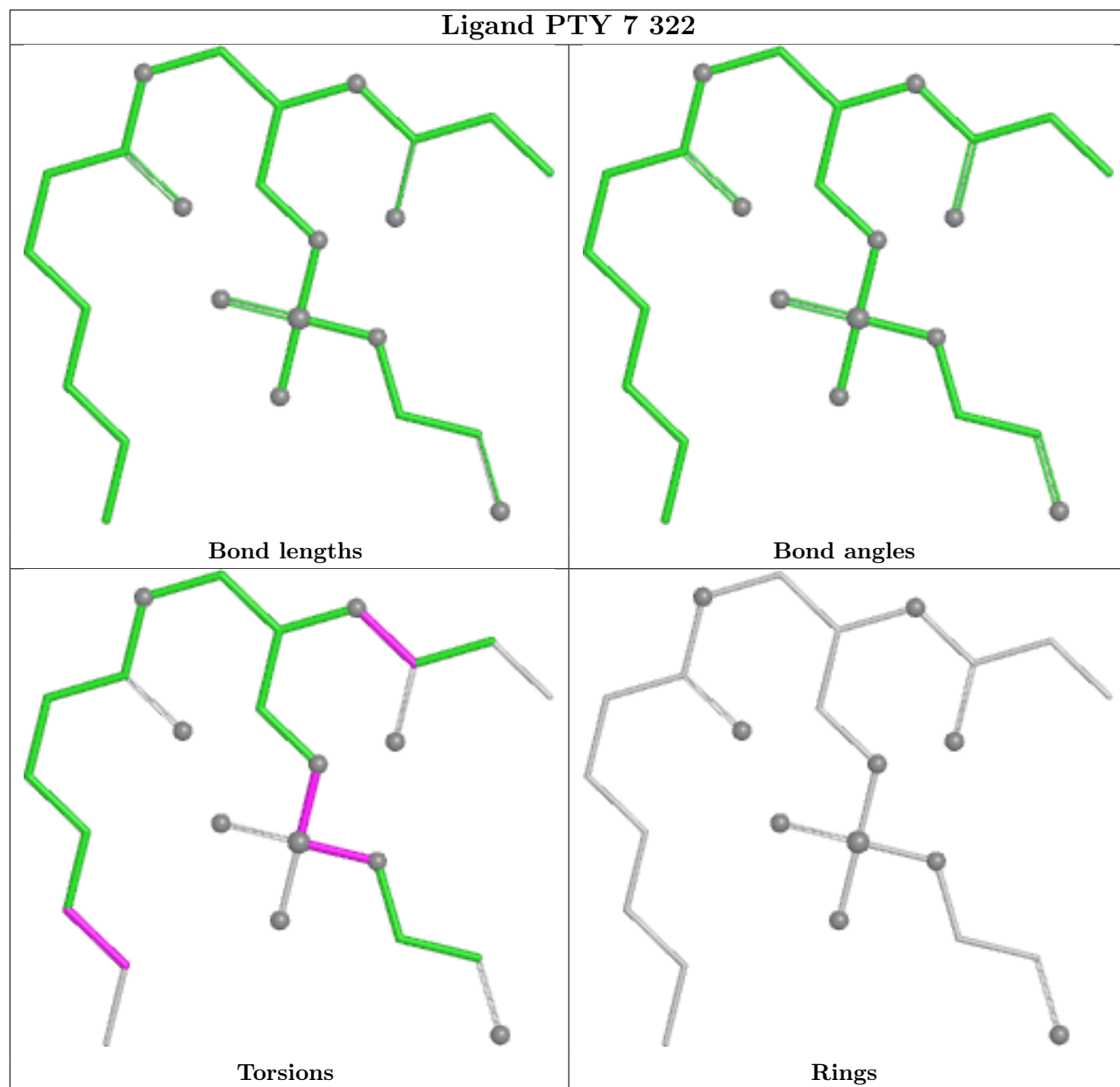


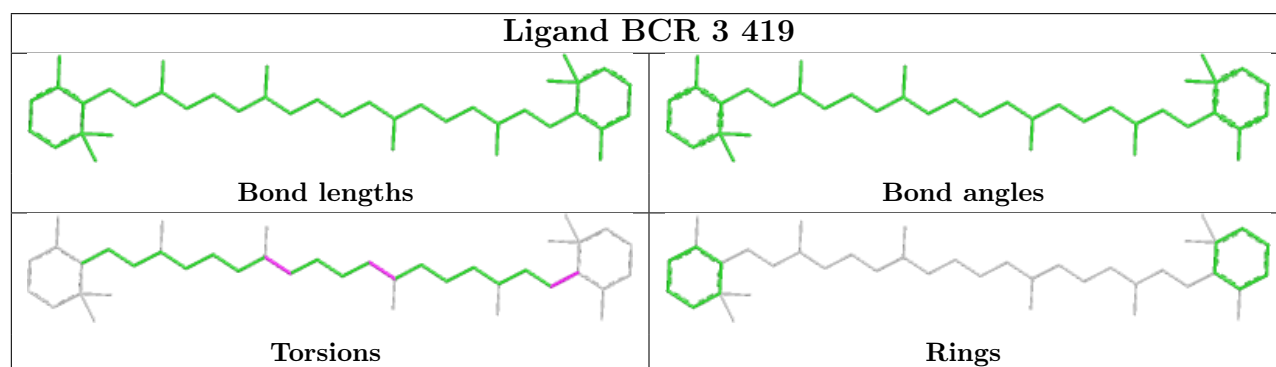
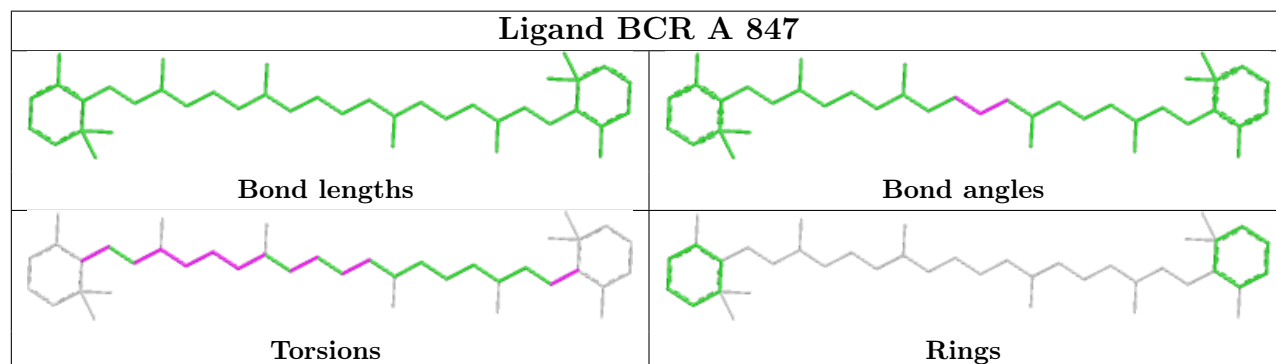
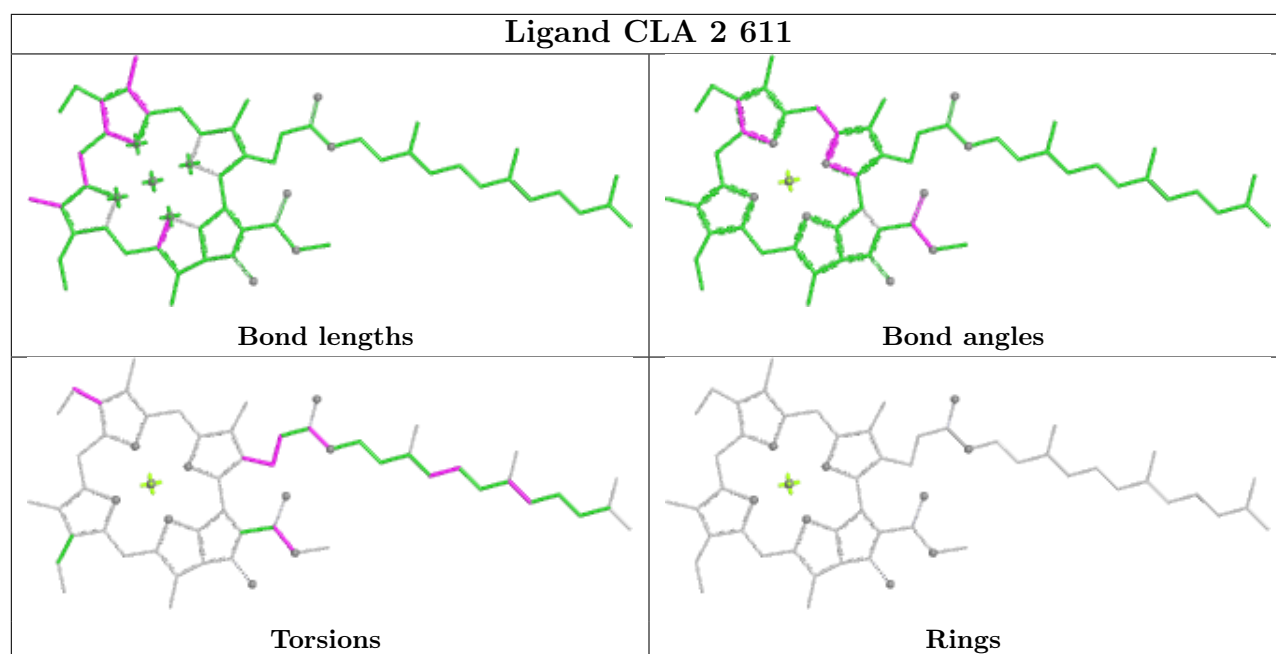
Ligand CHL 9 606



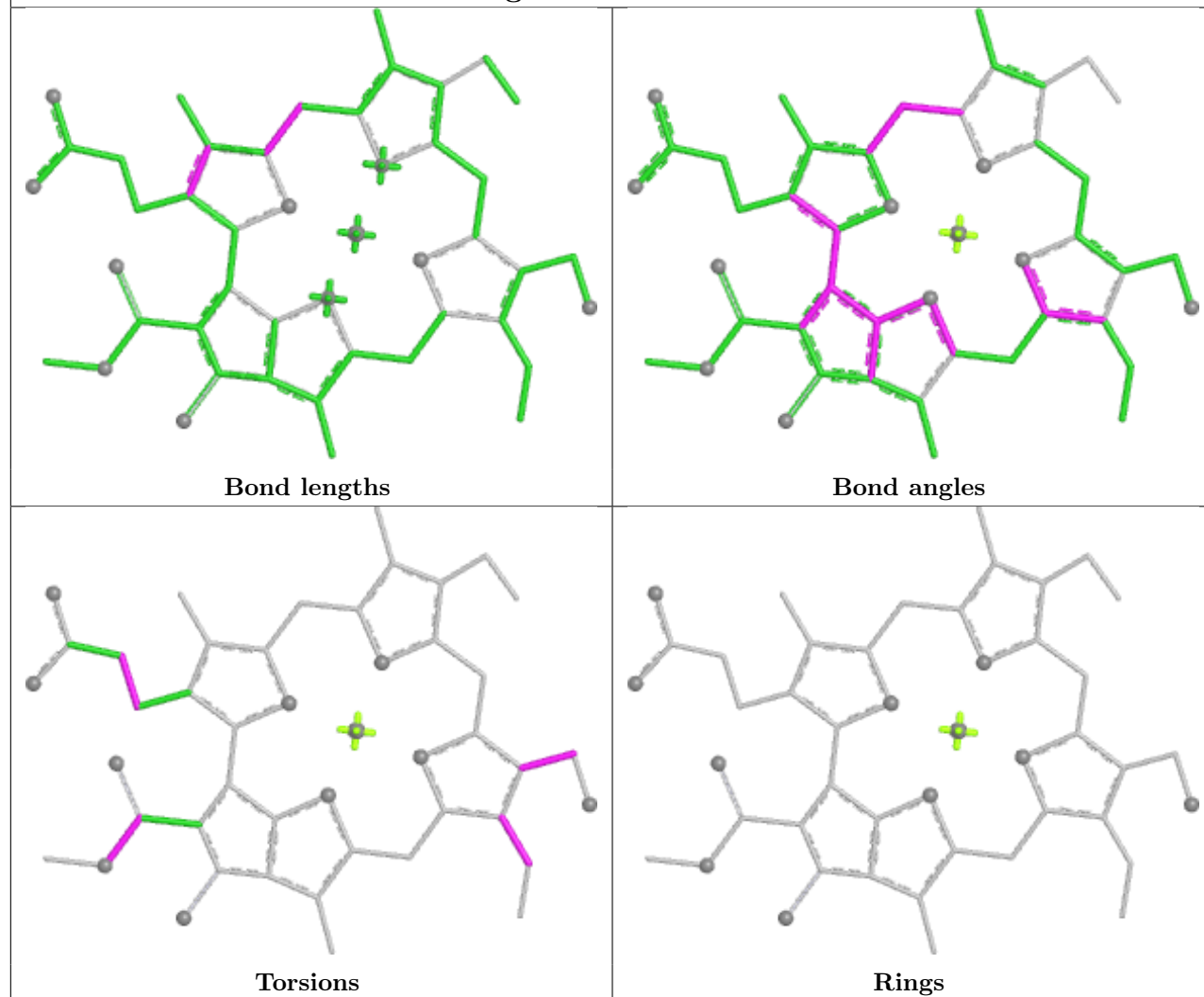
Ligand CLA B 830



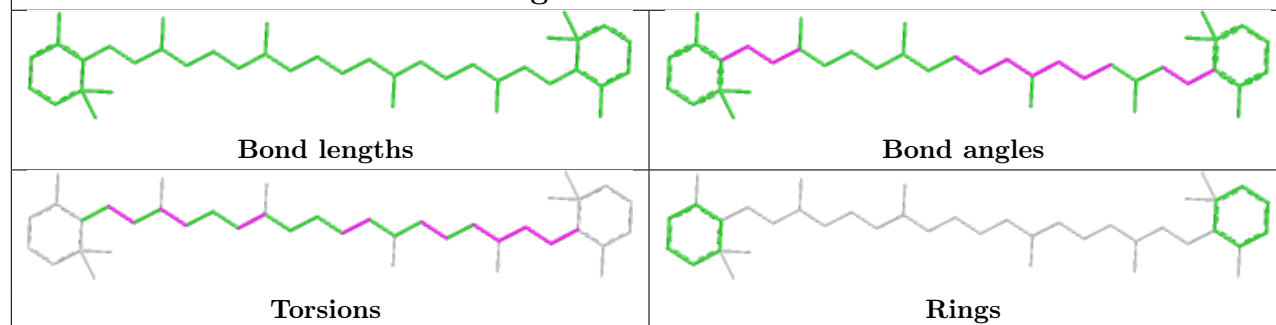


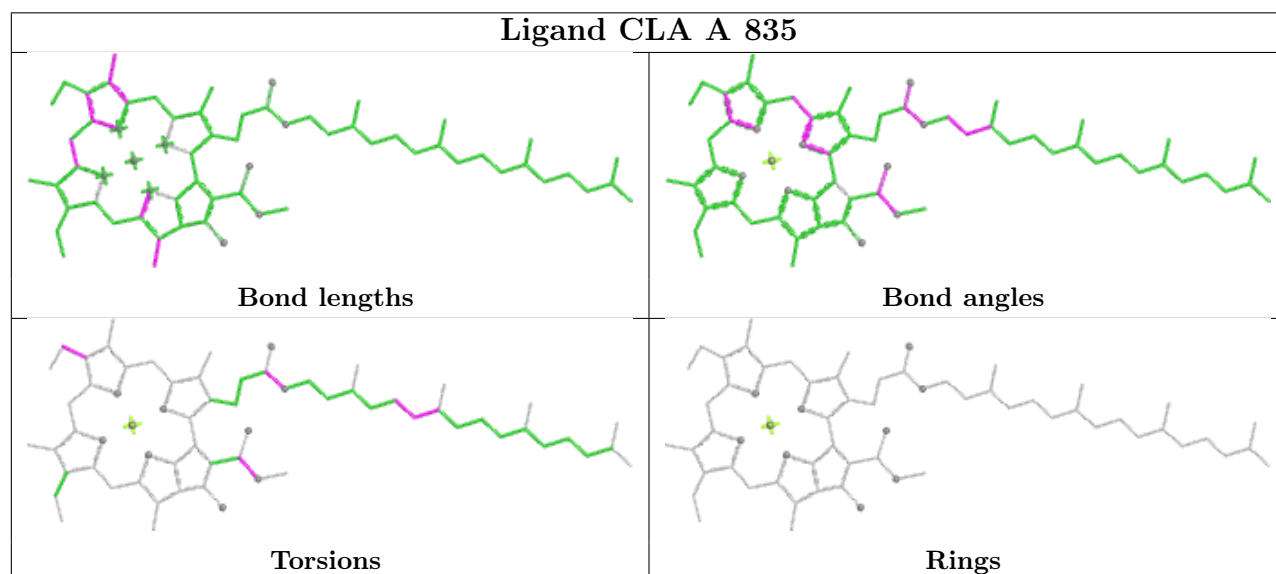
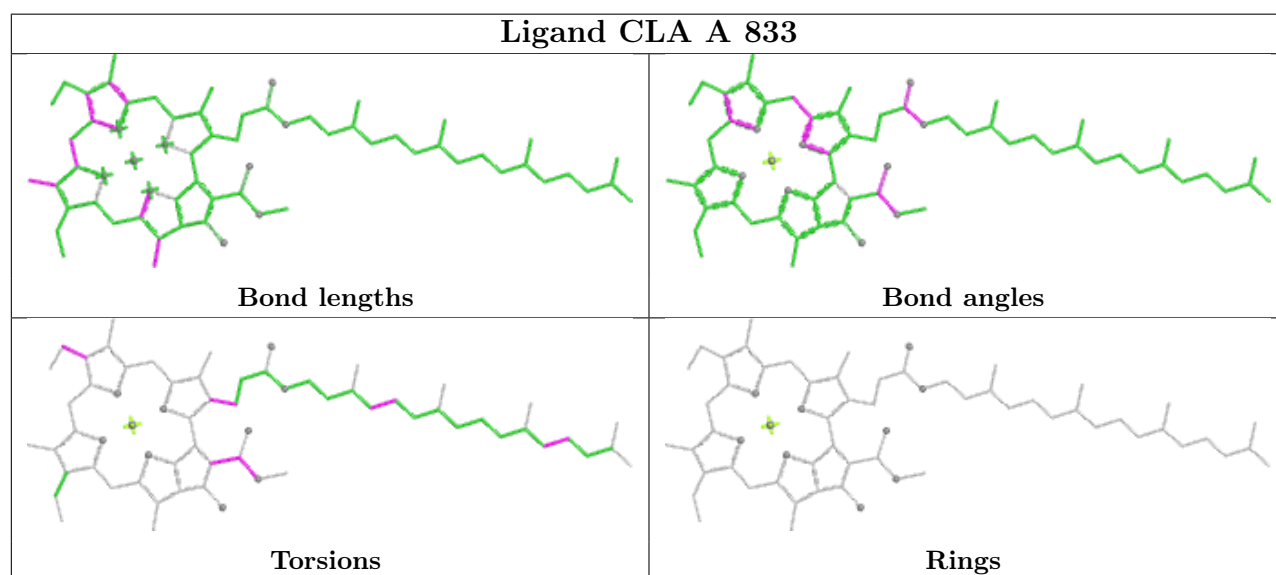
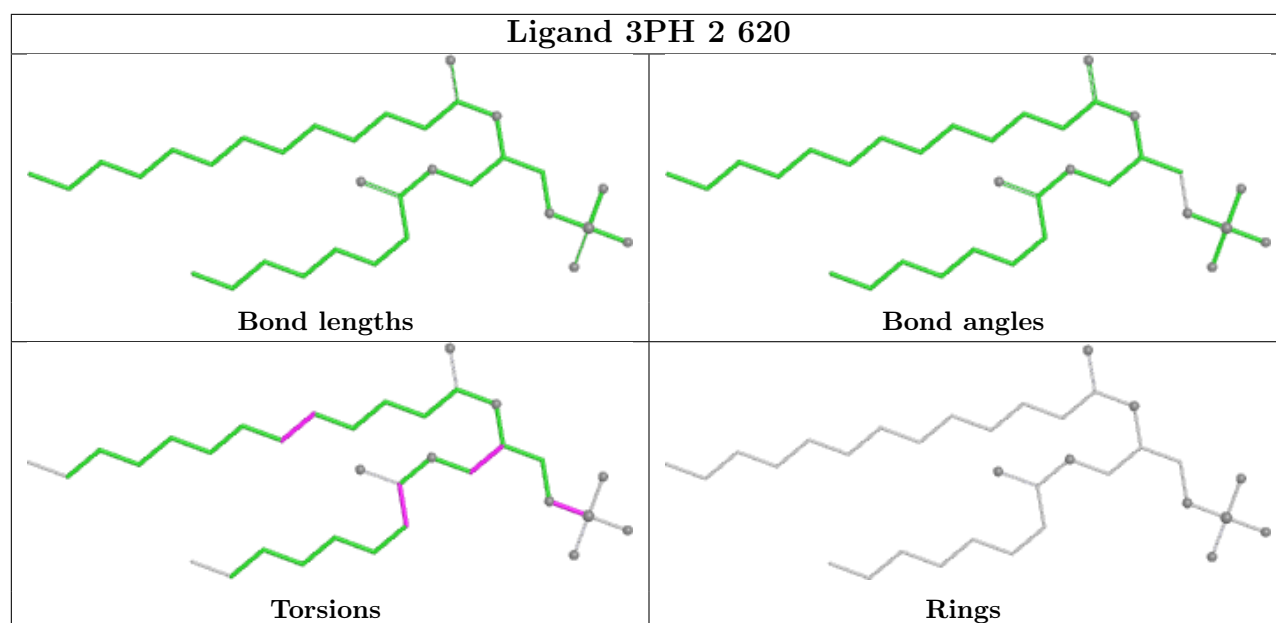


Ligand CHL 7 306

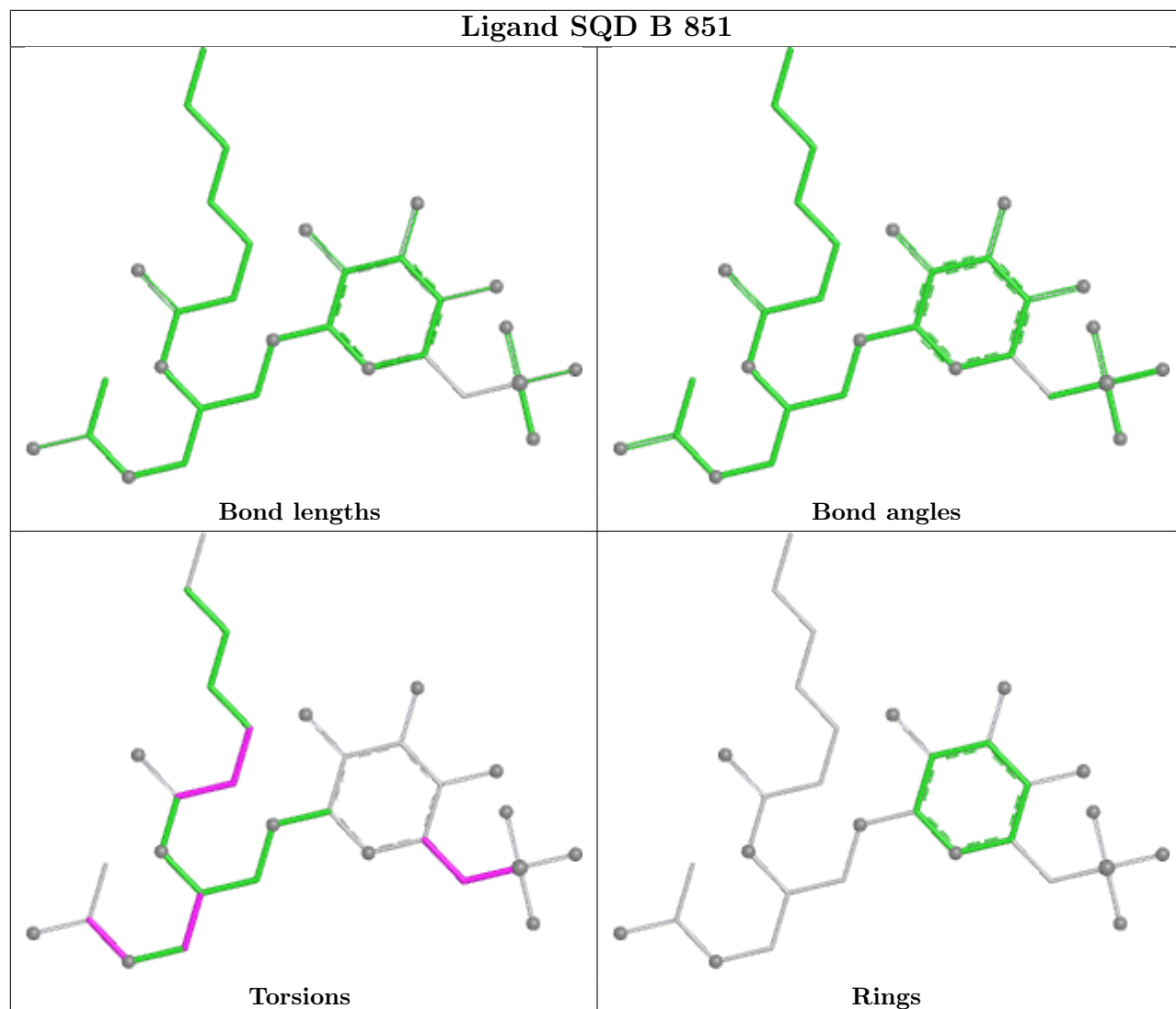


Ligand BCR B 846

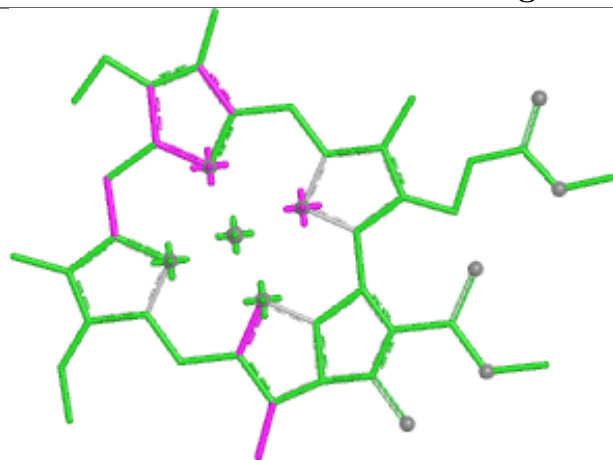




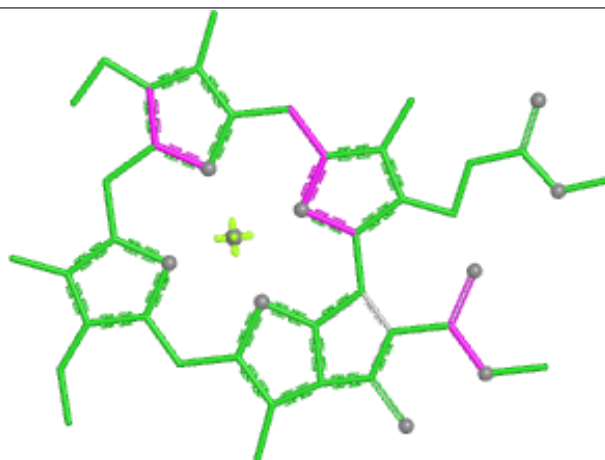
Ligand SQD B 851



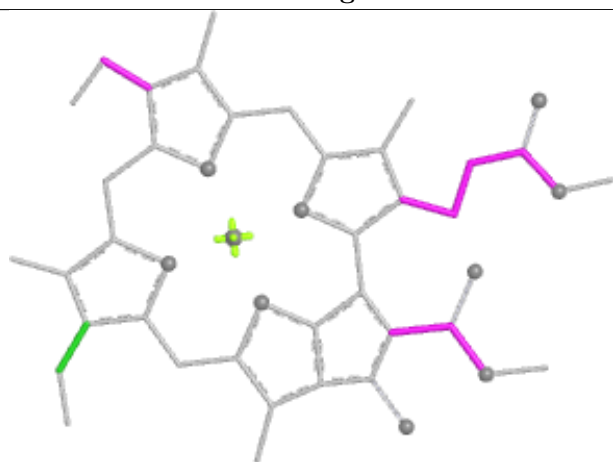
Ligand CLA 9 601



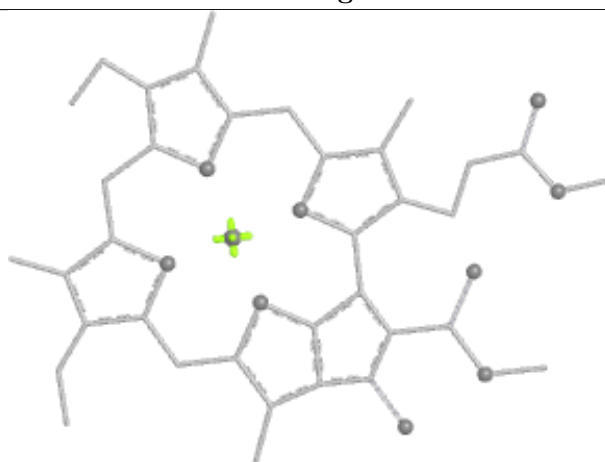
Bond lengths



Bond angles

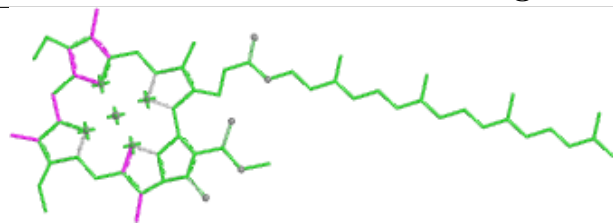


Torsions

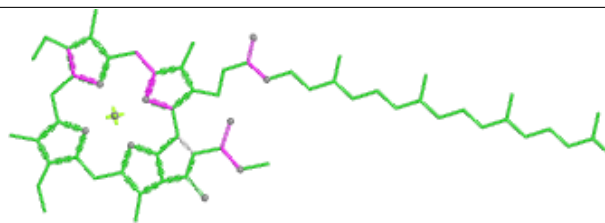


Rings

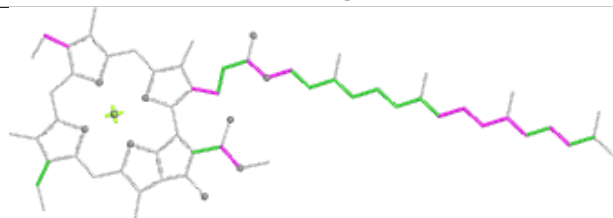
Ligand CLA A 824



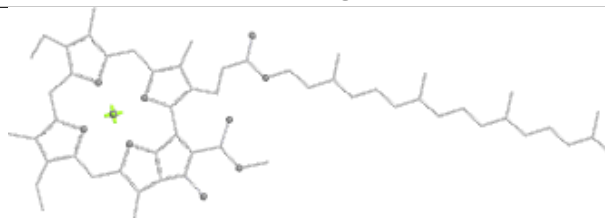
Bond lengths



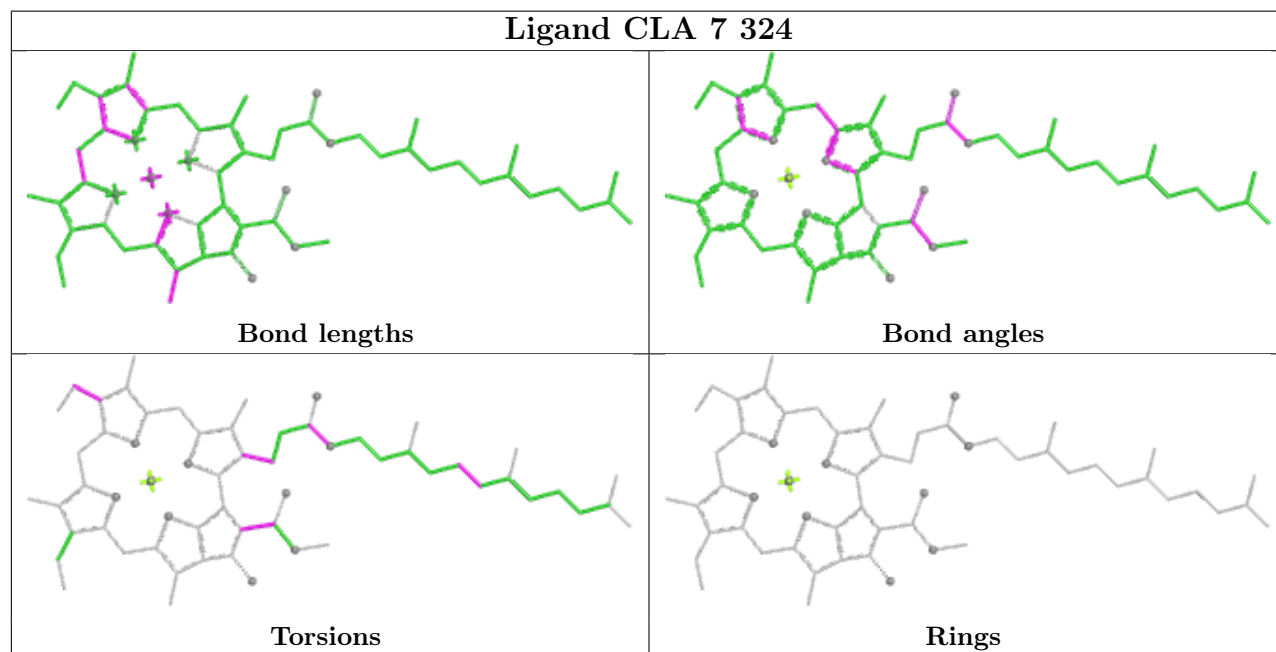
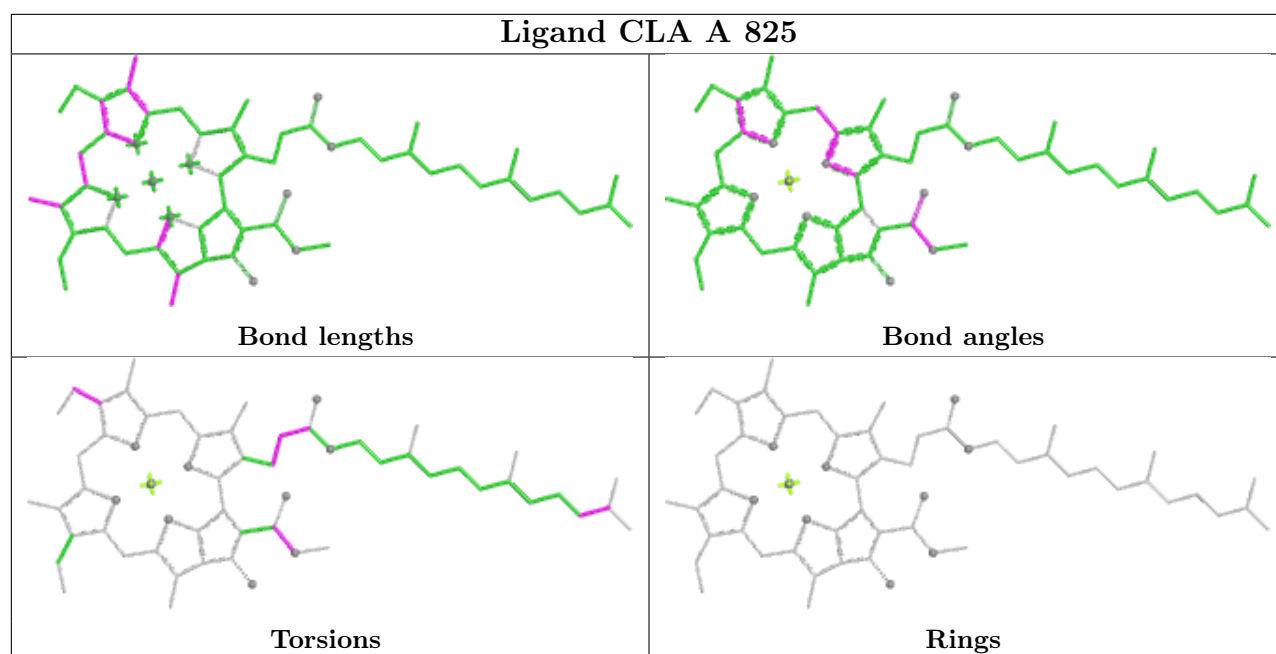
Bond angles

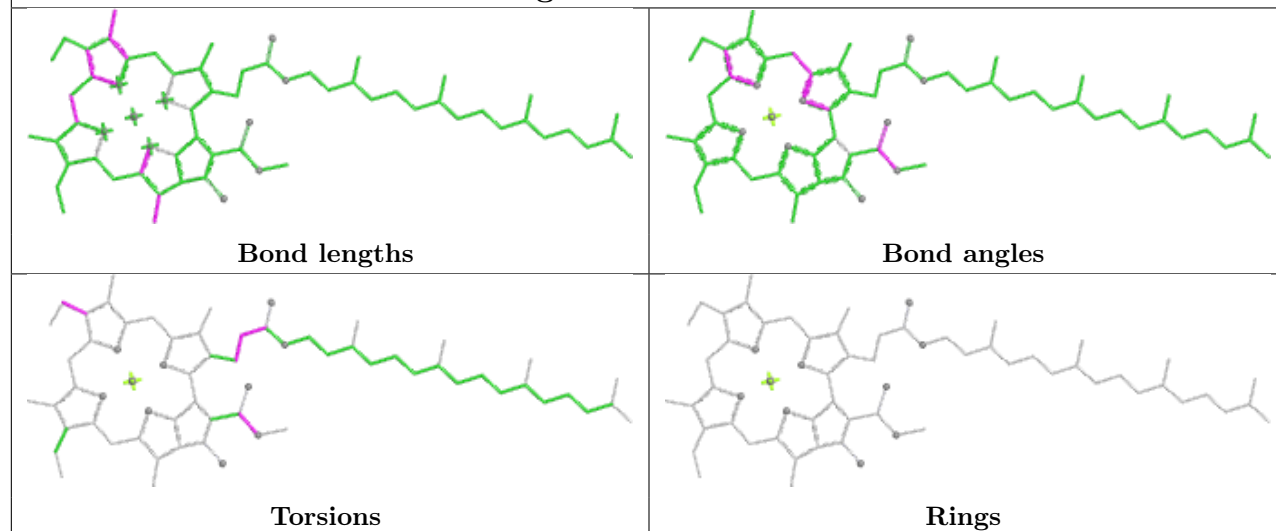
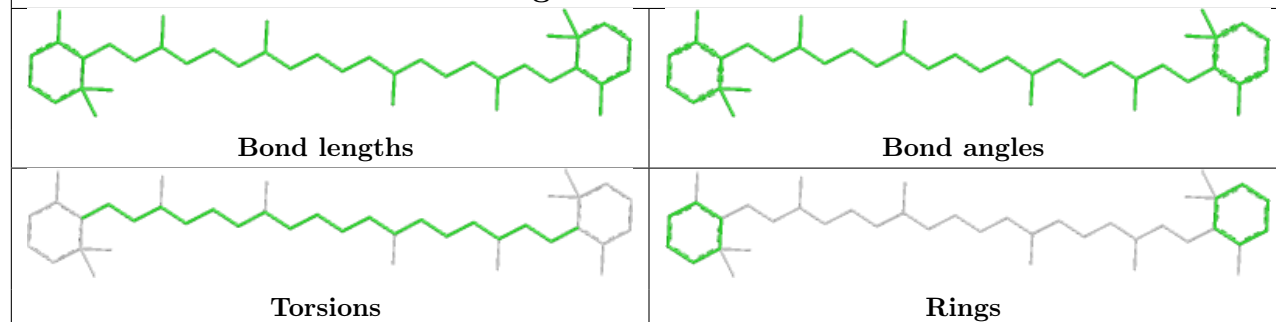
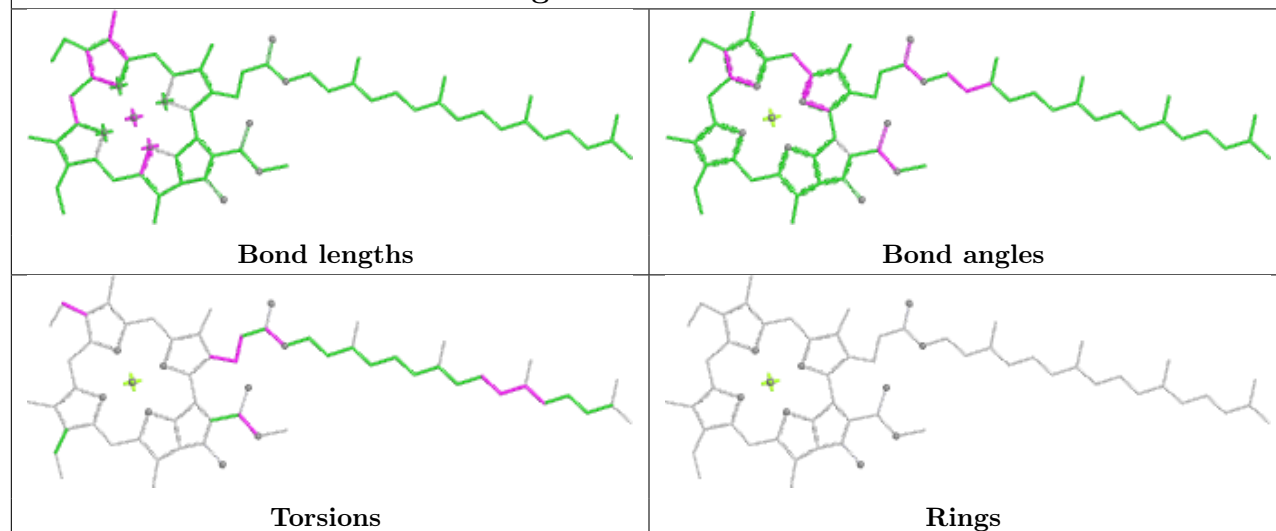


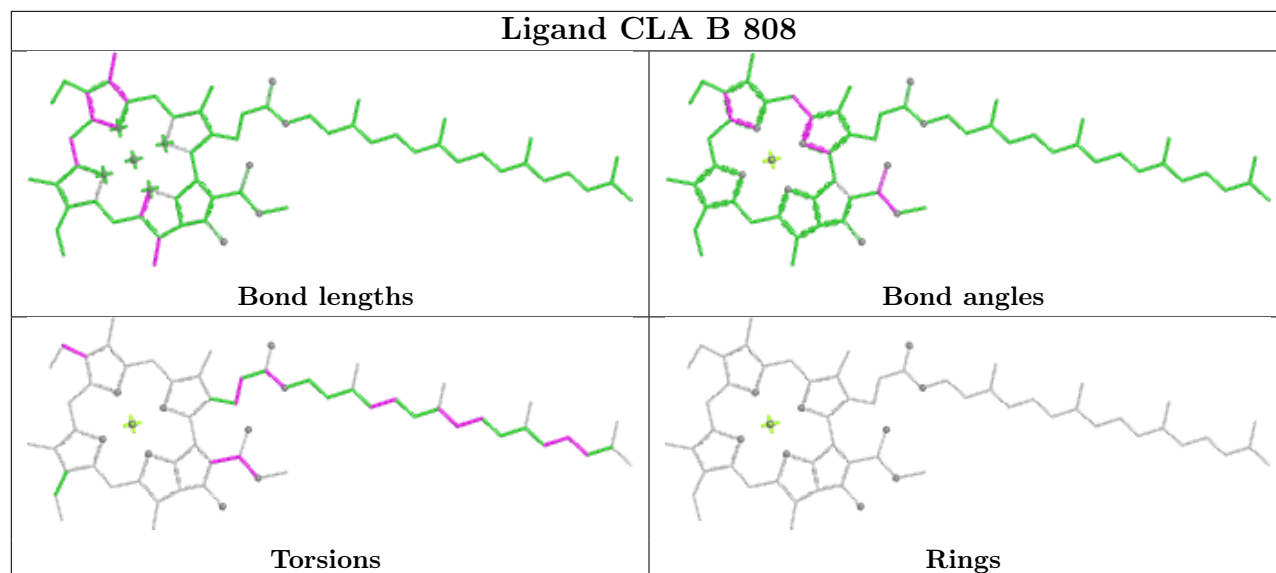
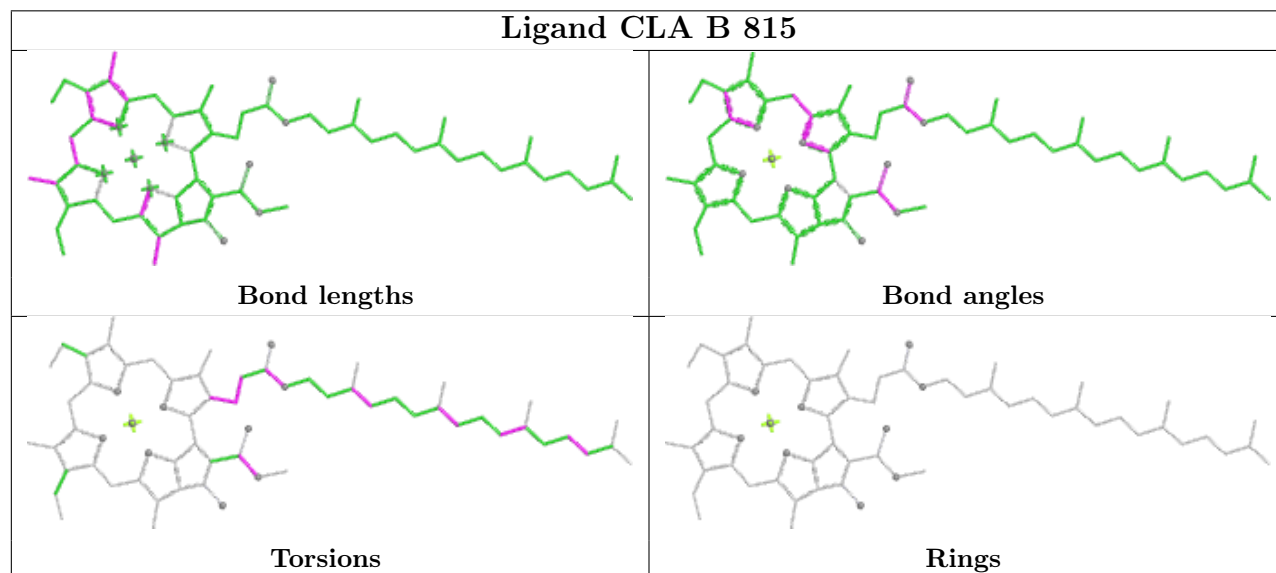
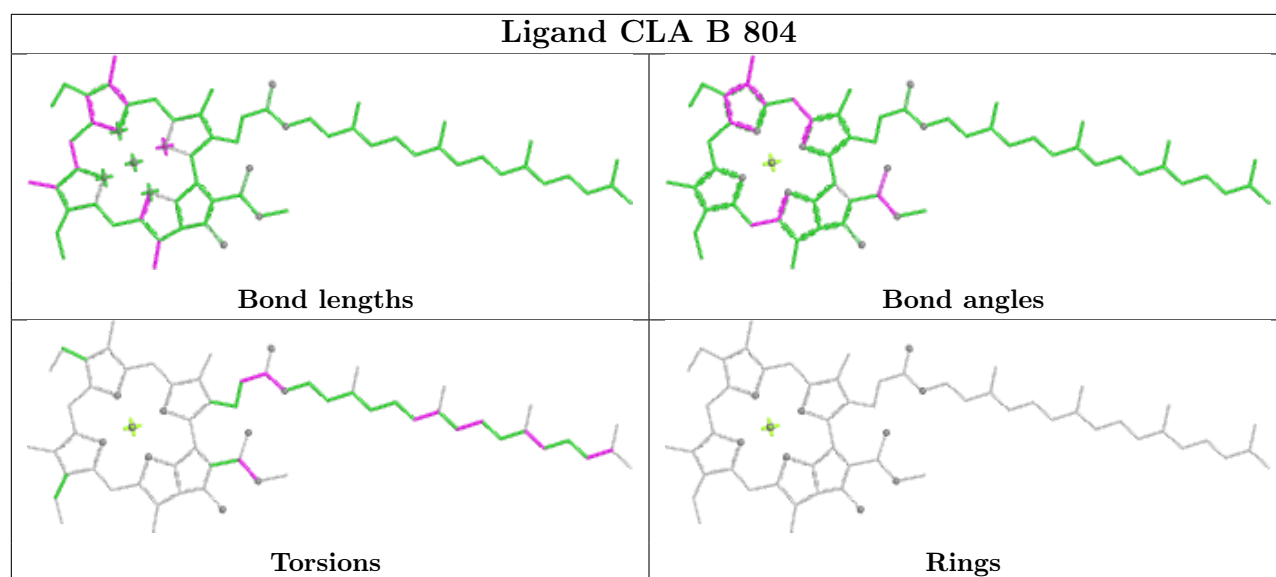
Torsions

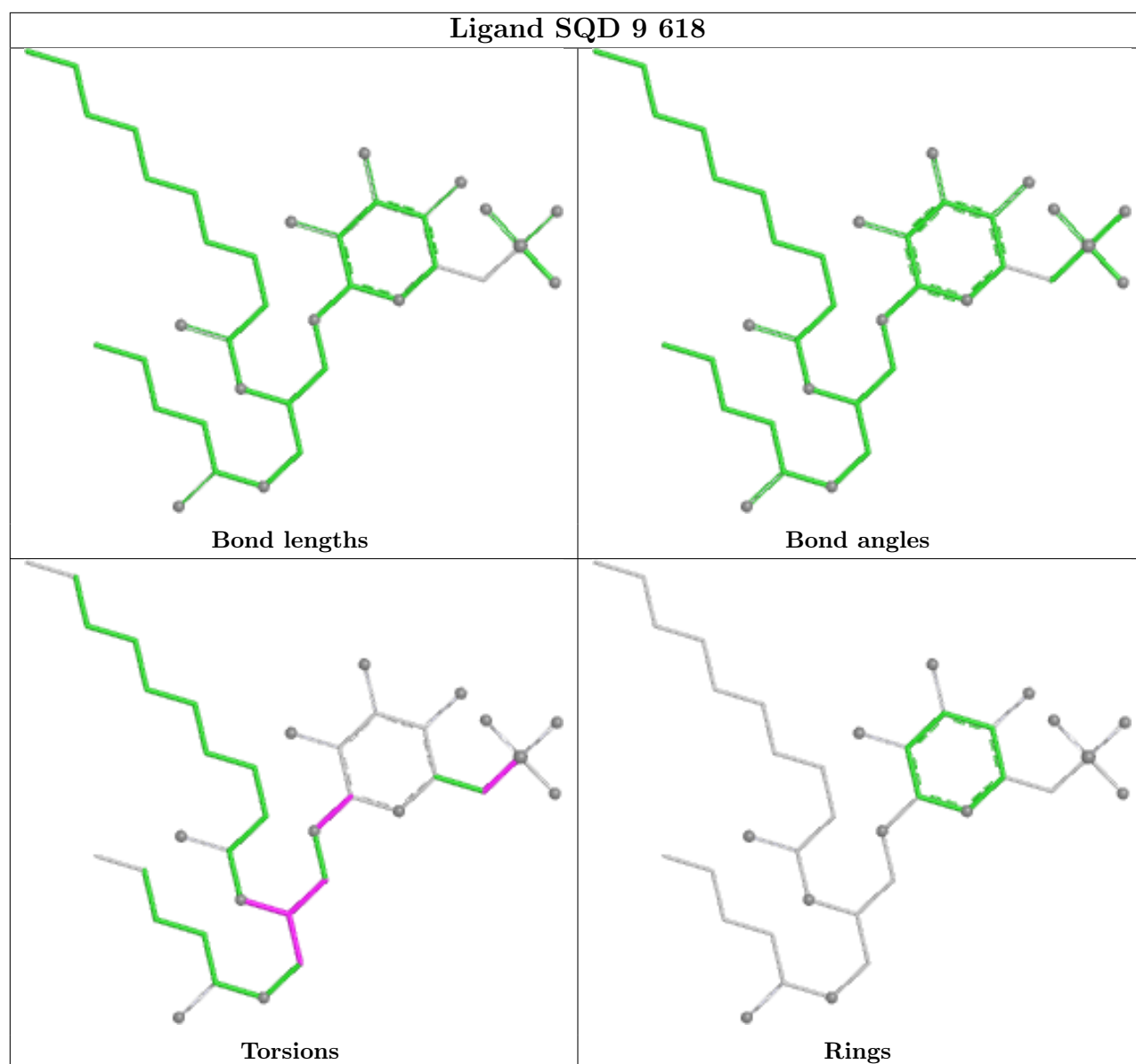


Rings

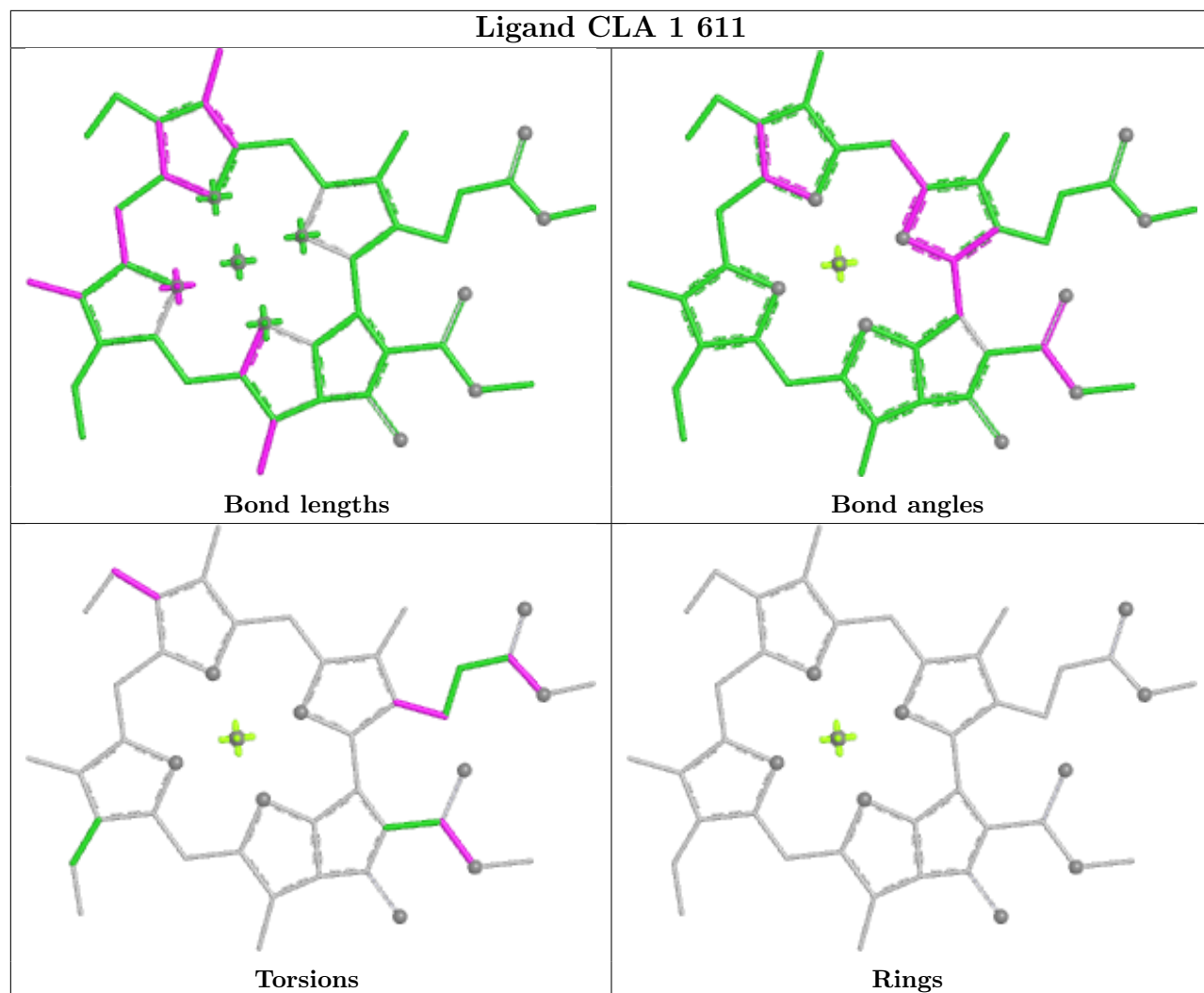


Ligand CLA 7 315**Ligand BCR L 309****Ligand CLA A 809**

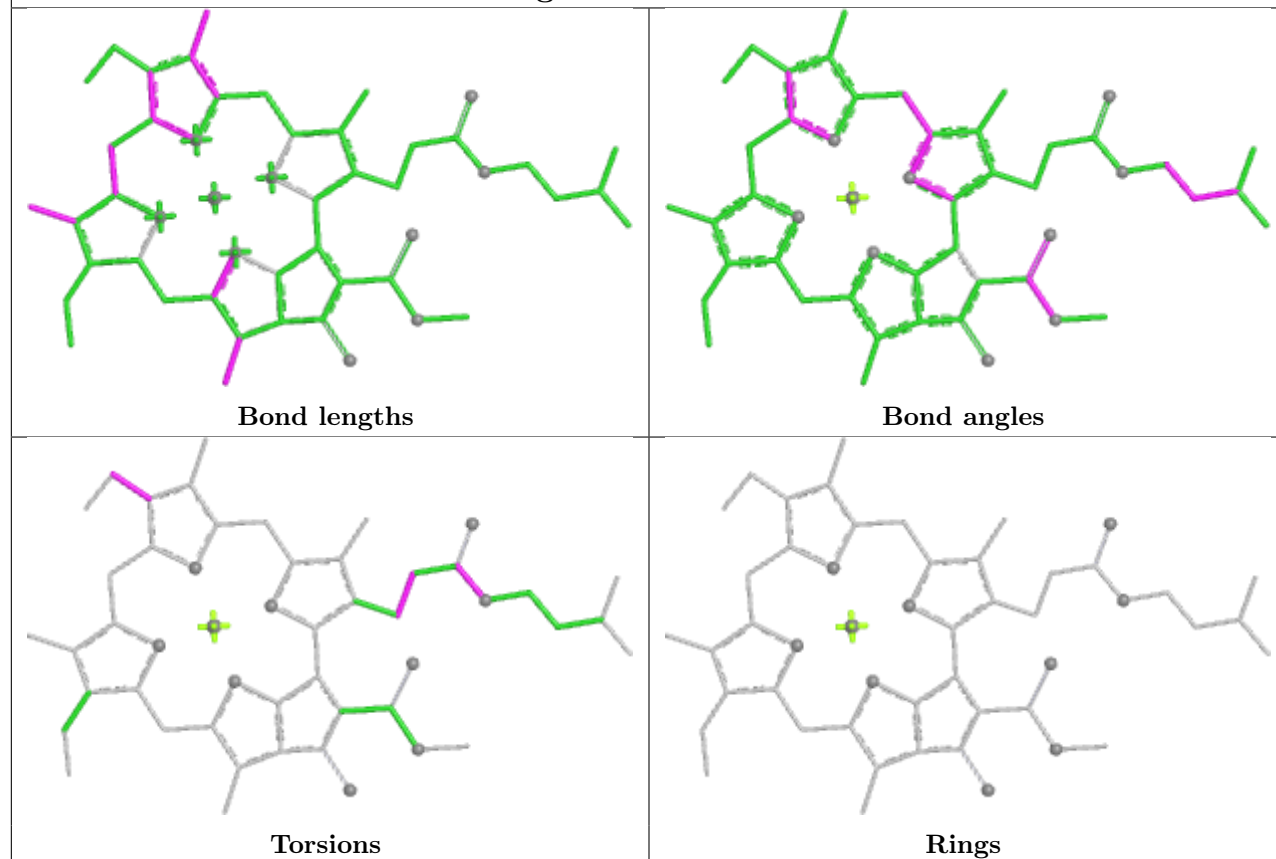




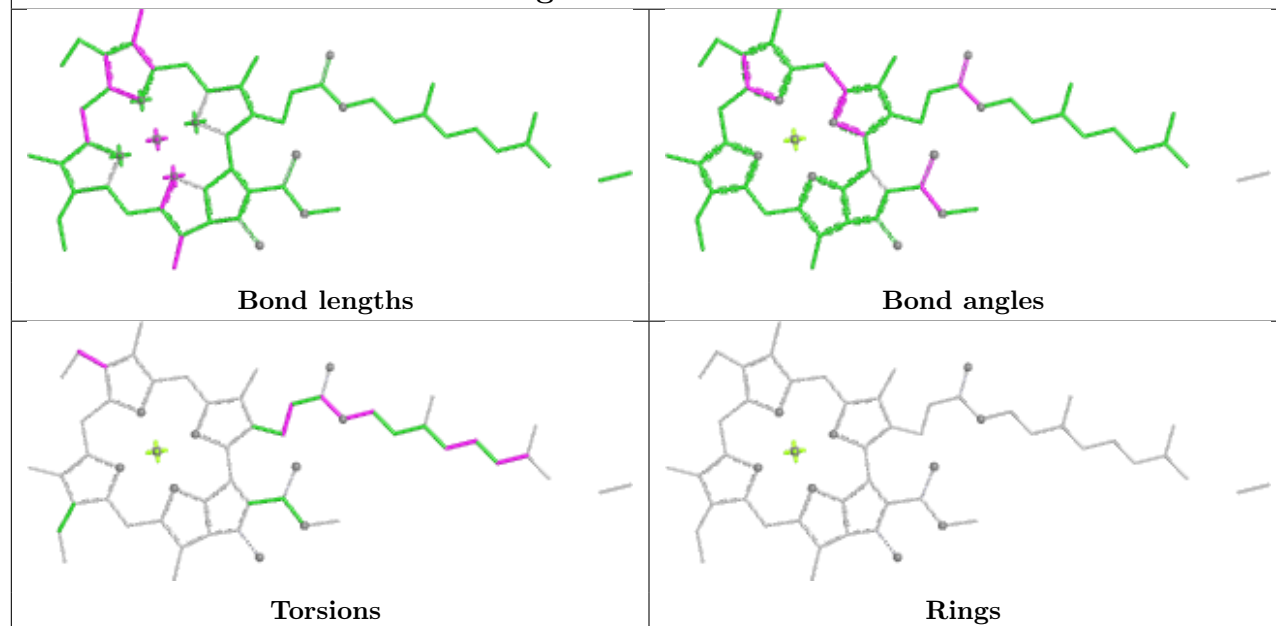
Ligand CLA 1 611



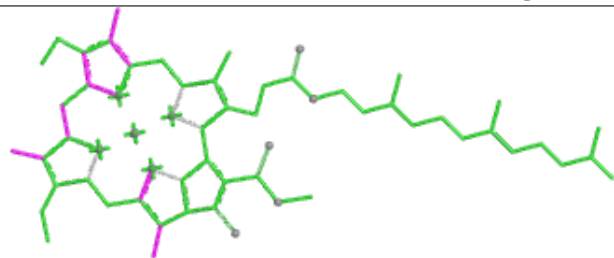
Ligand CLA 3 405



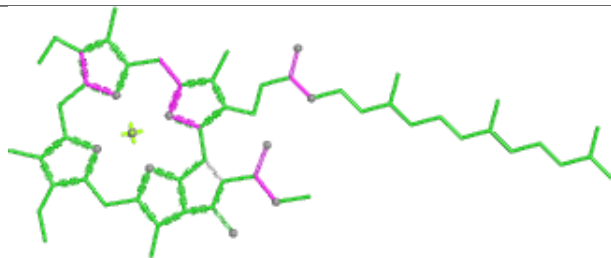
Ligand CLA 3 411



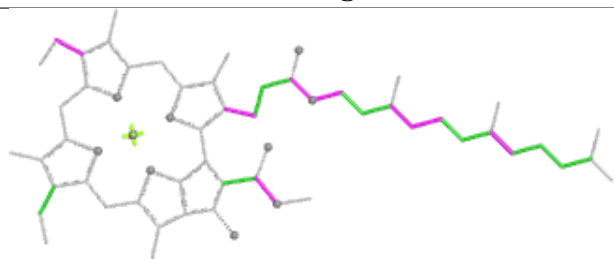
Ligand CLA 8 309



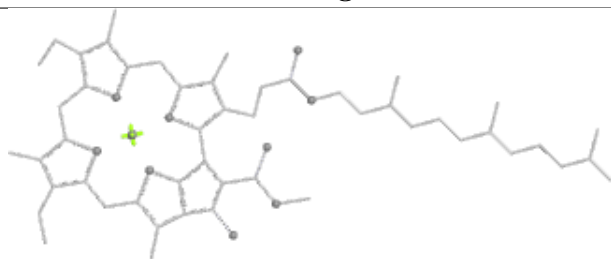
Bond lengths



Bond angles

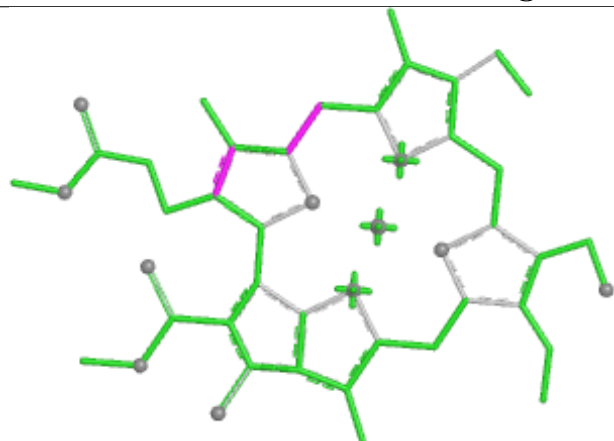


Torsions

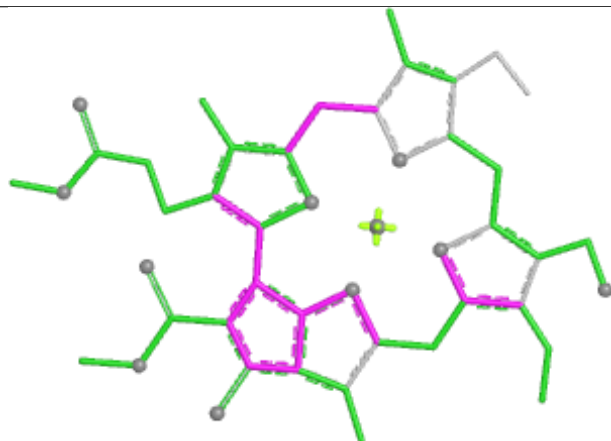


Rings

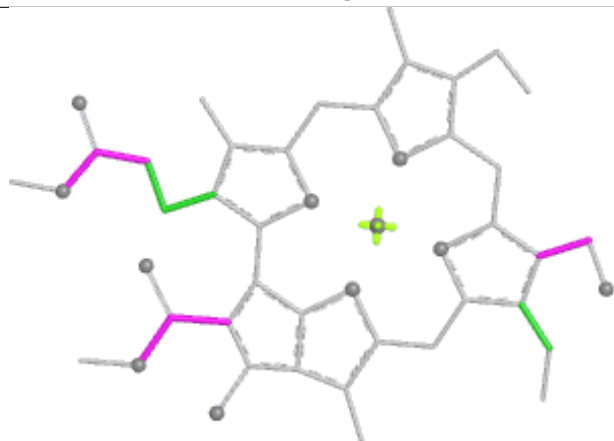
Ligand CHL 8 305



Bond lengths



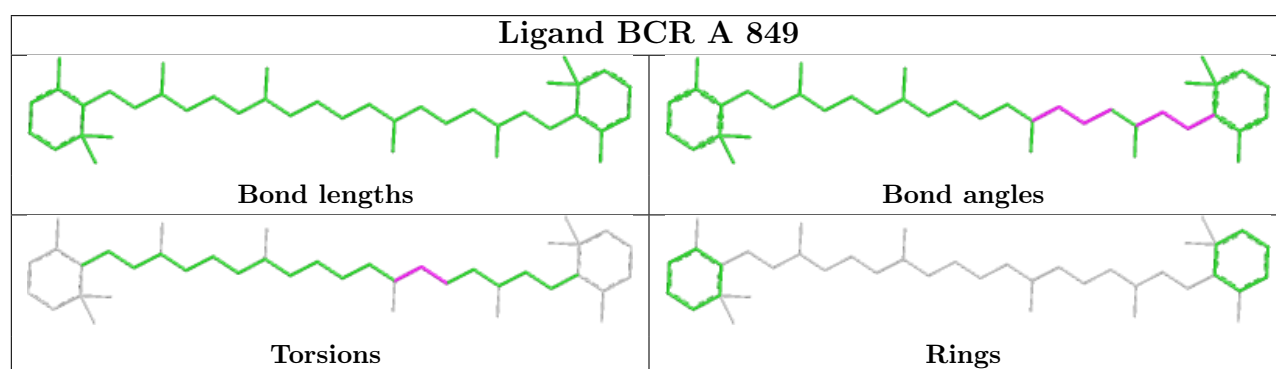
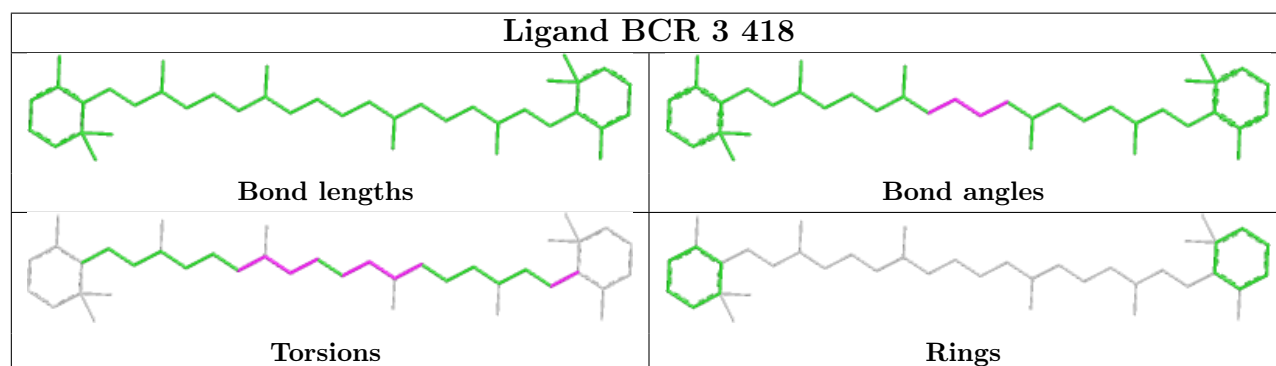
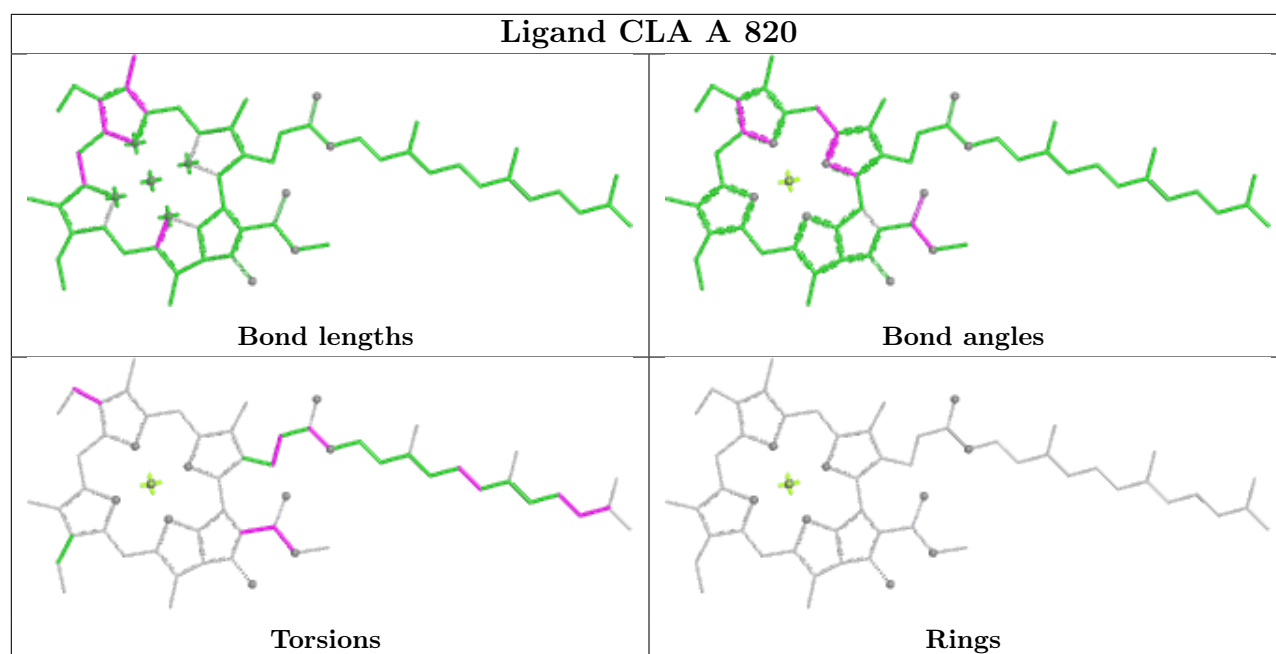
Bond angles

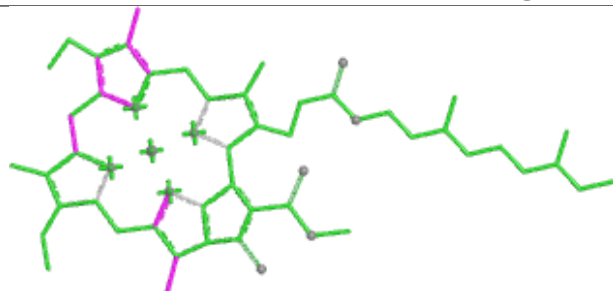


Torsions

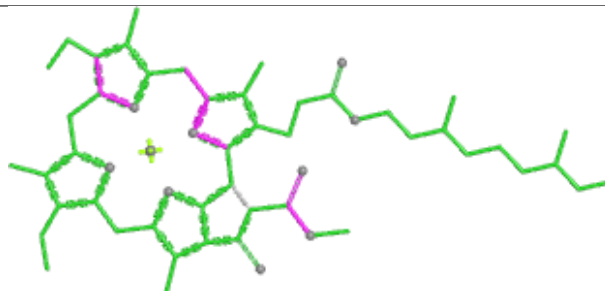


Rings

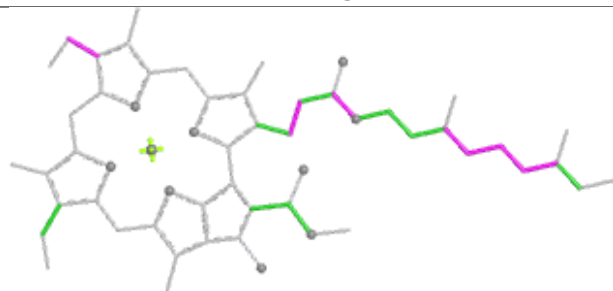


Ligand CLA 2 602

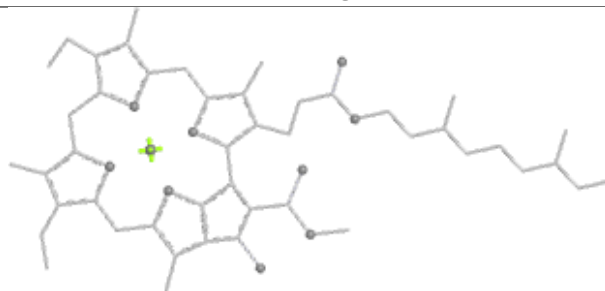
Bond lengths



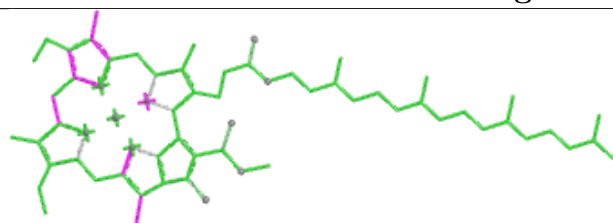
Bond angles



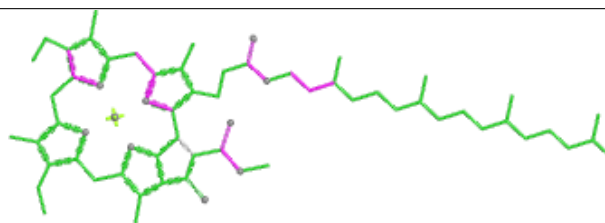
Torsions



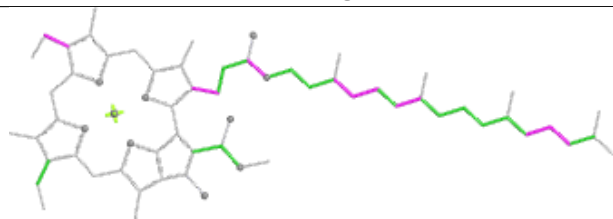
Rings

Ligand CLA B 813

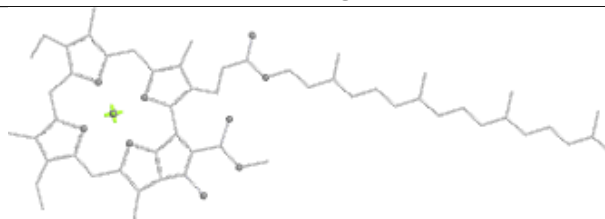
Bond lengths



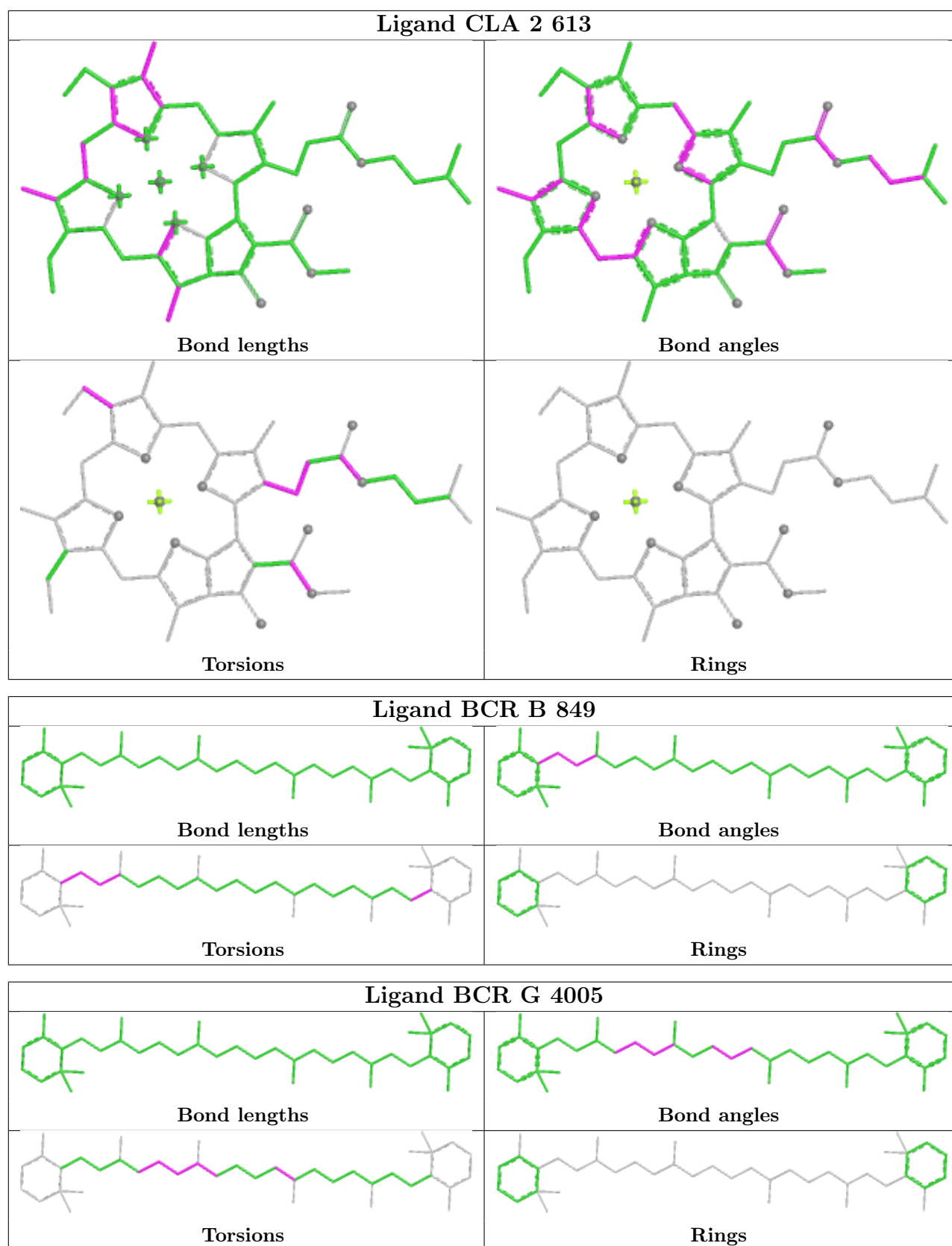
Bond angles

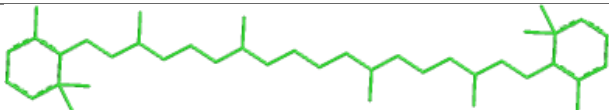
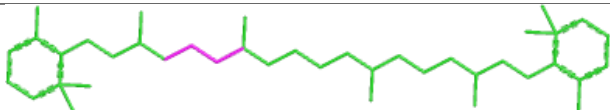
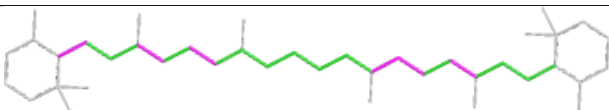
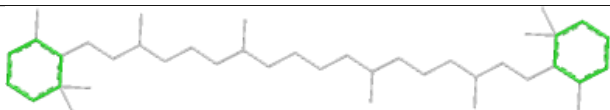


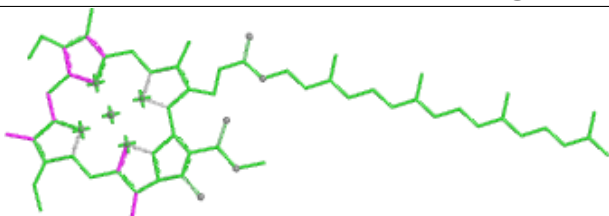
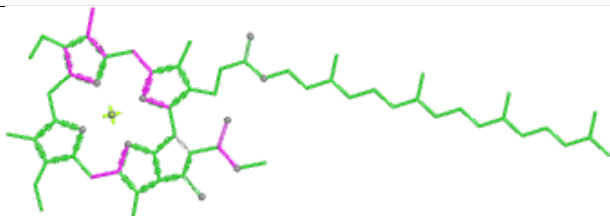
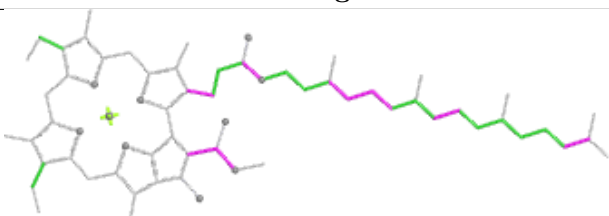
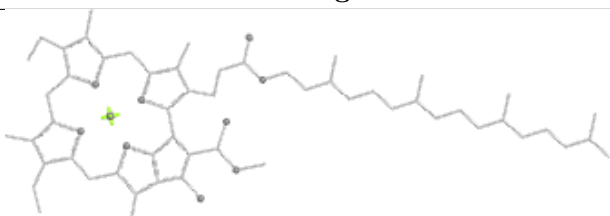
Torsions

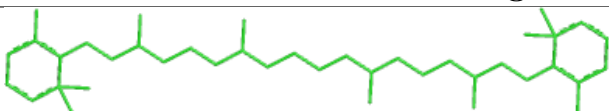
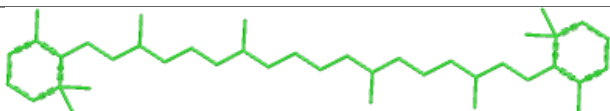
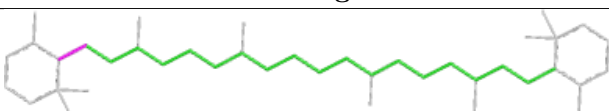
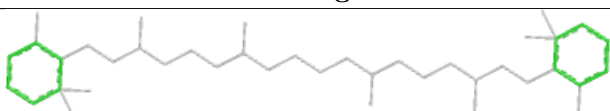


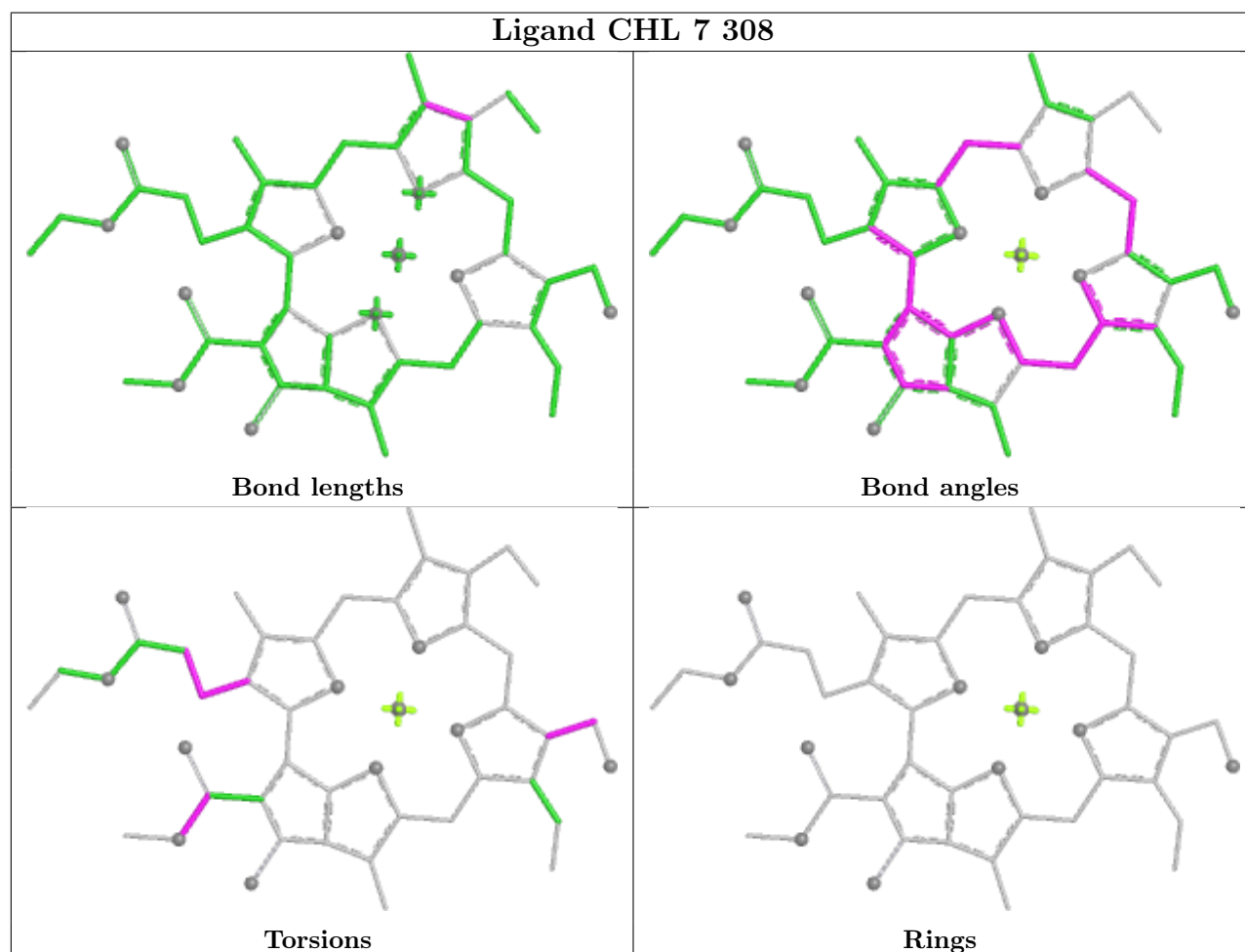
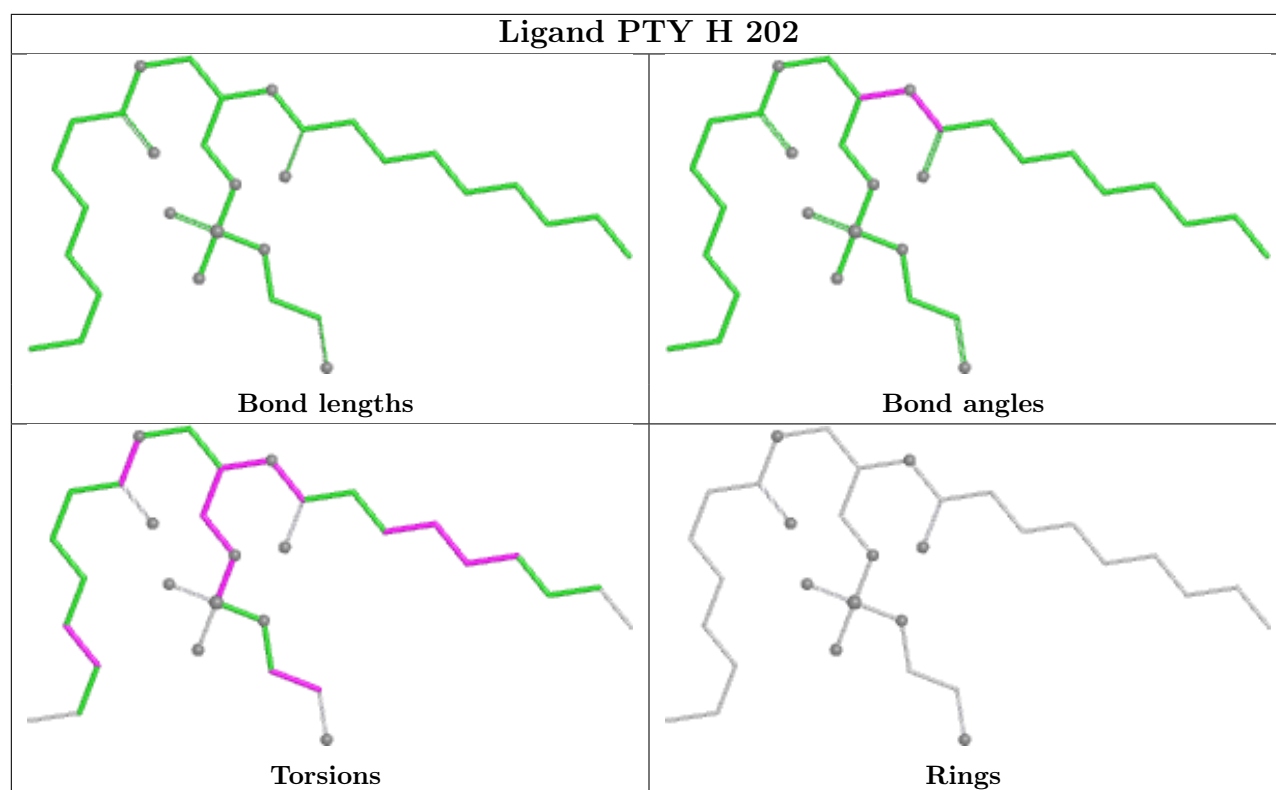
Rings

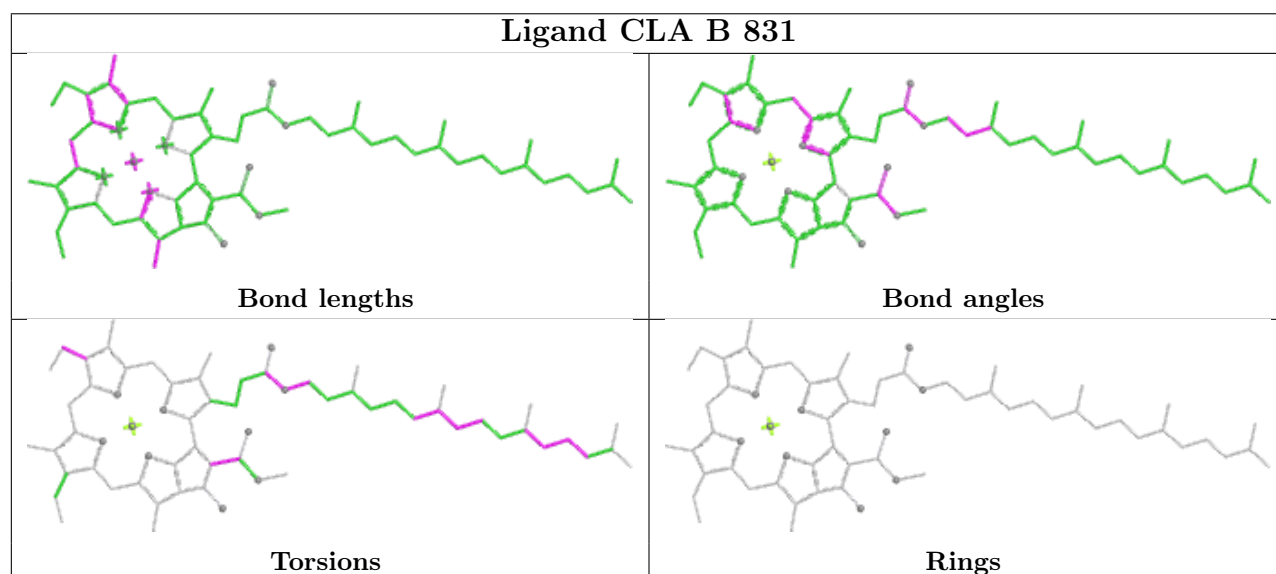
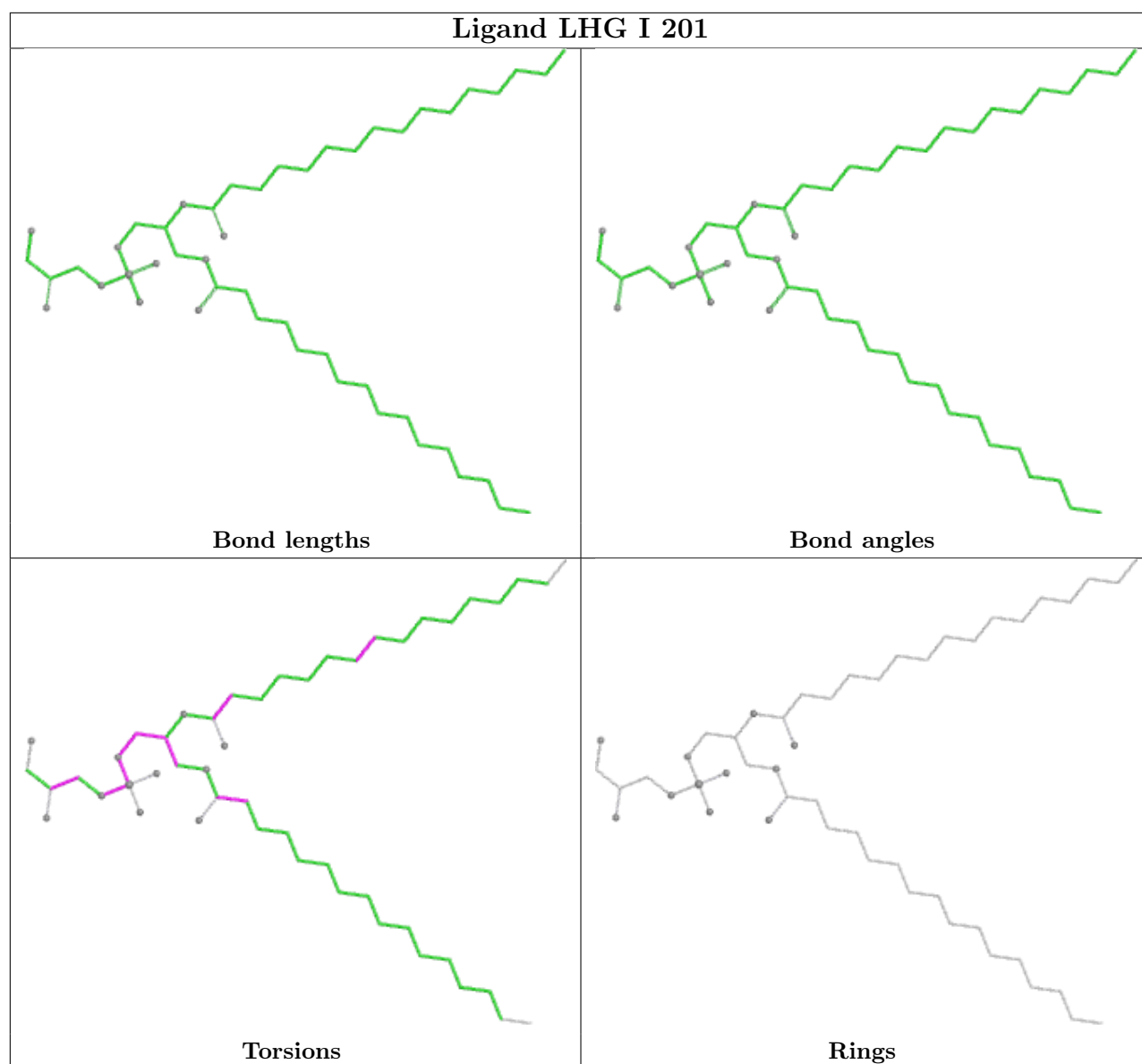


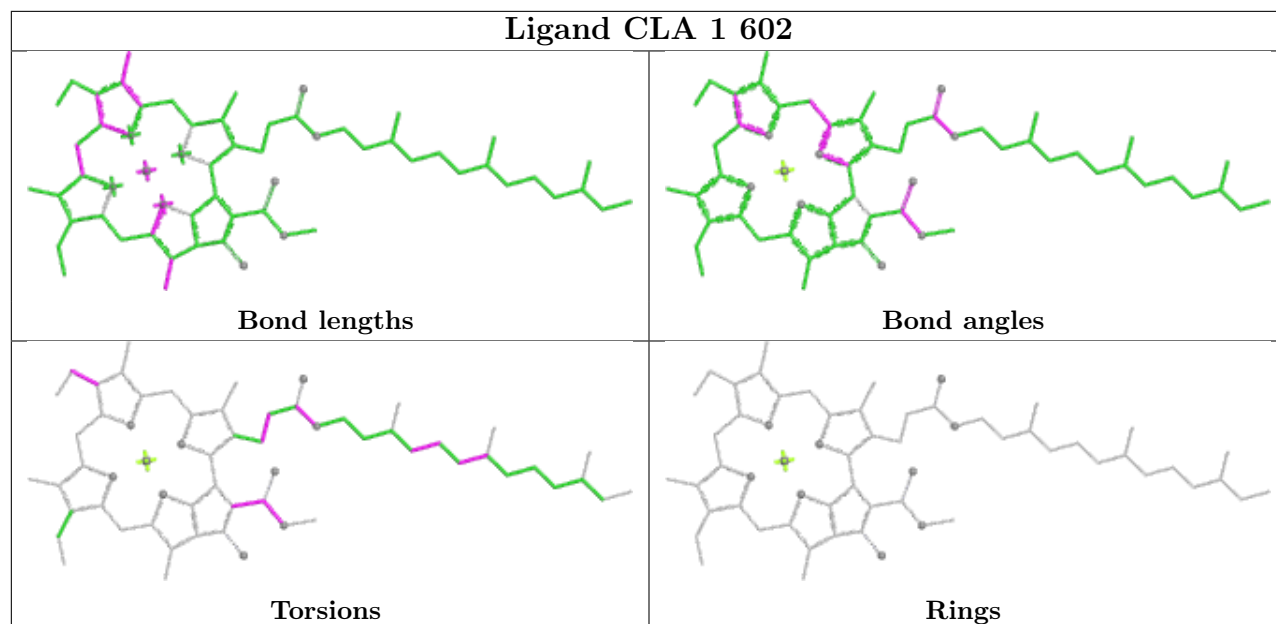
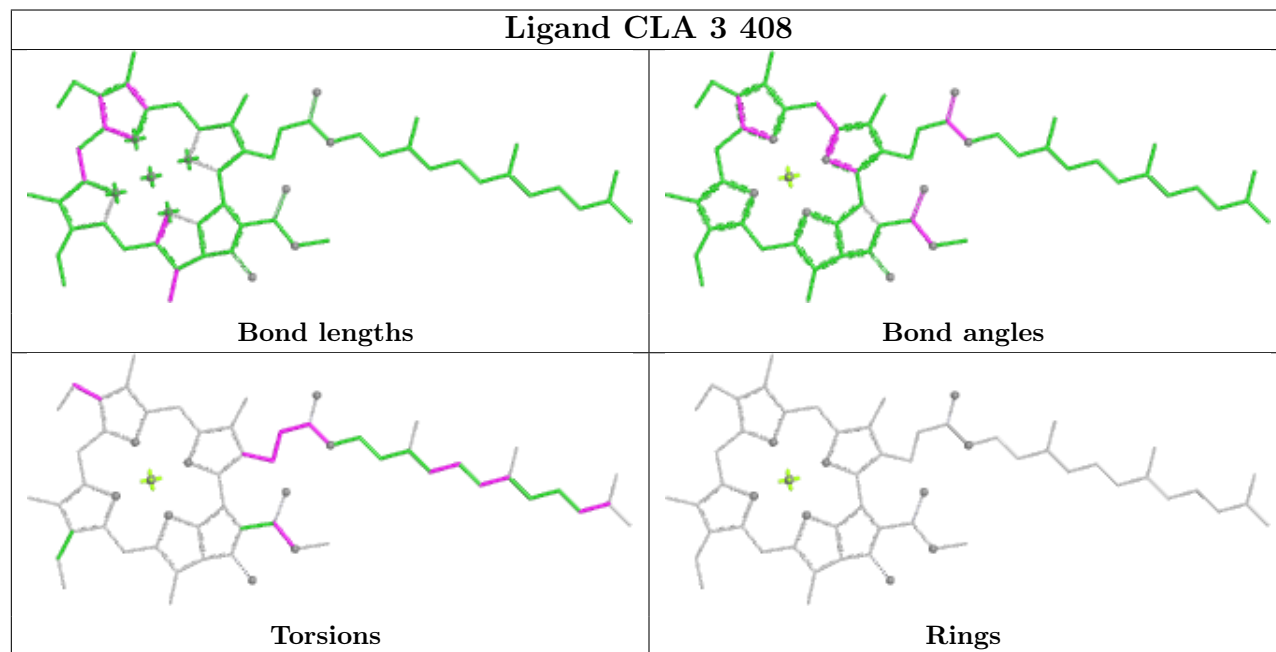
Ligand BCR H 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

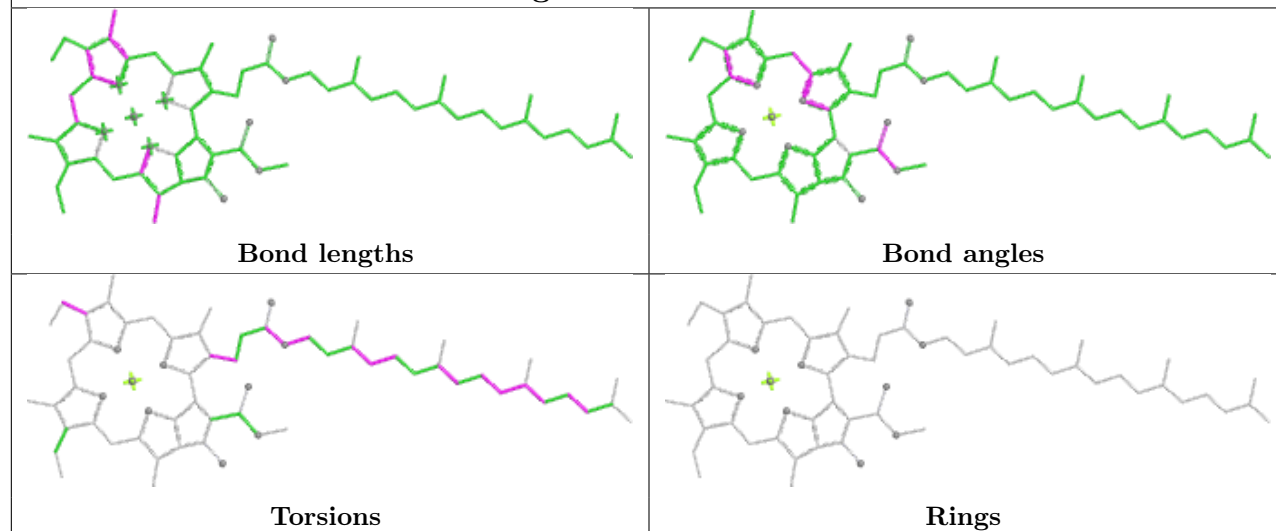
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings



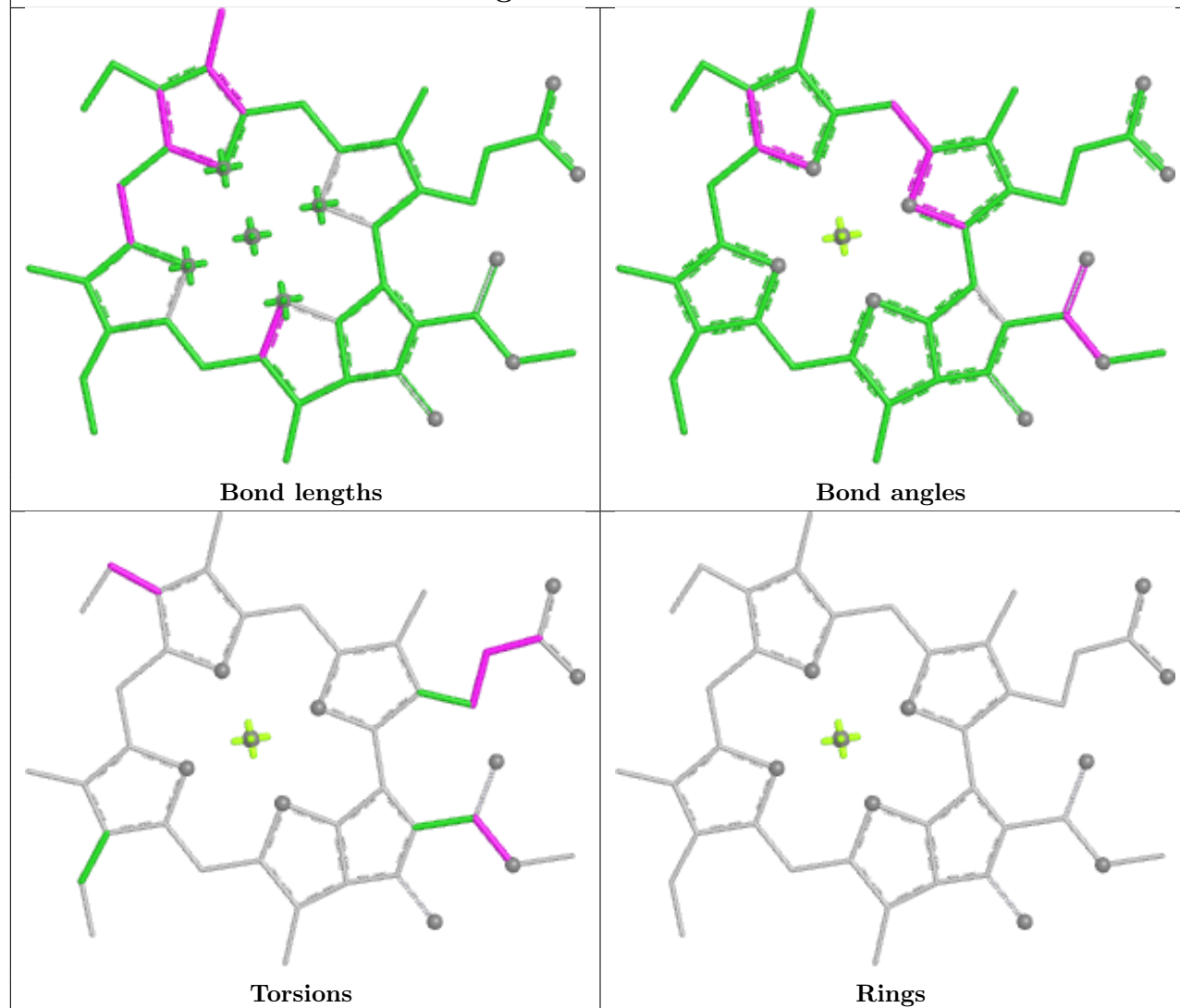


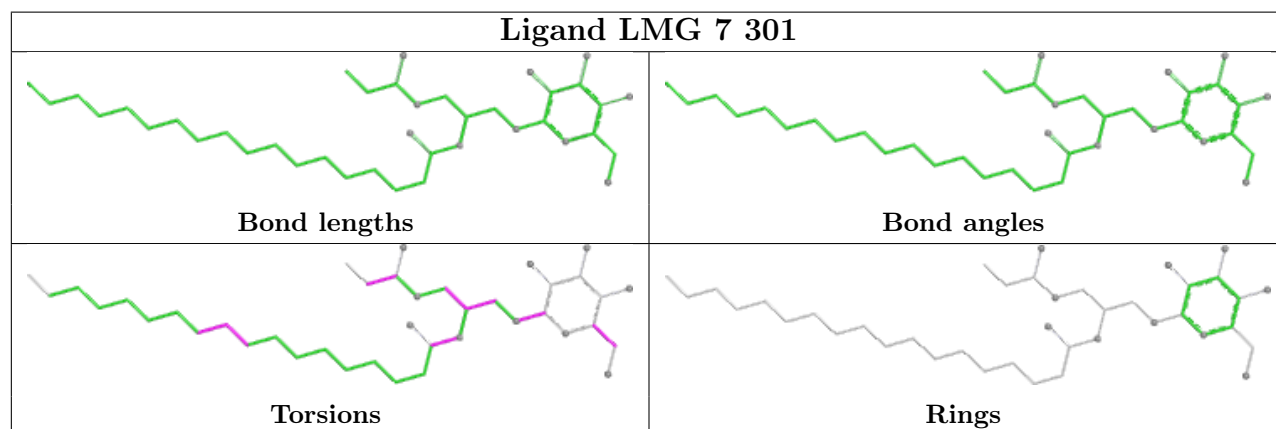
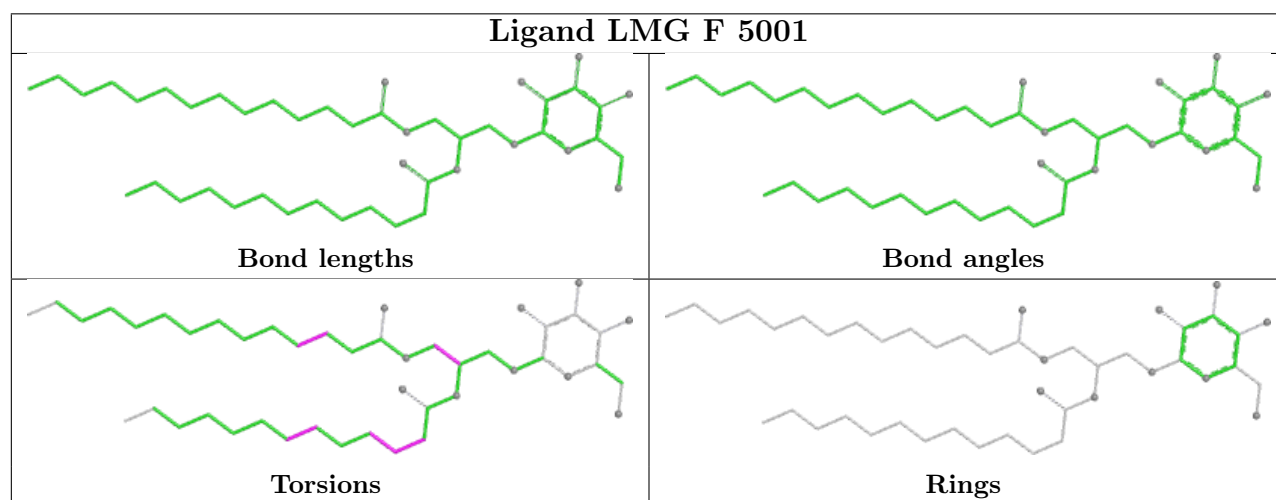
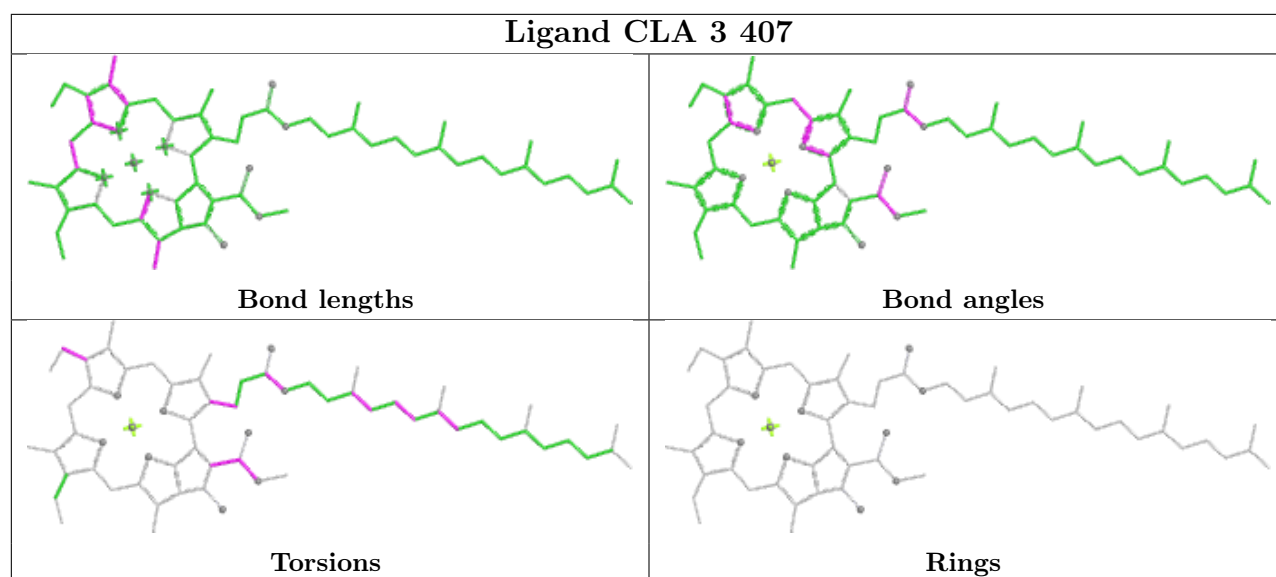
Ligand CLA 1 602**Ligand CLA 3 408**

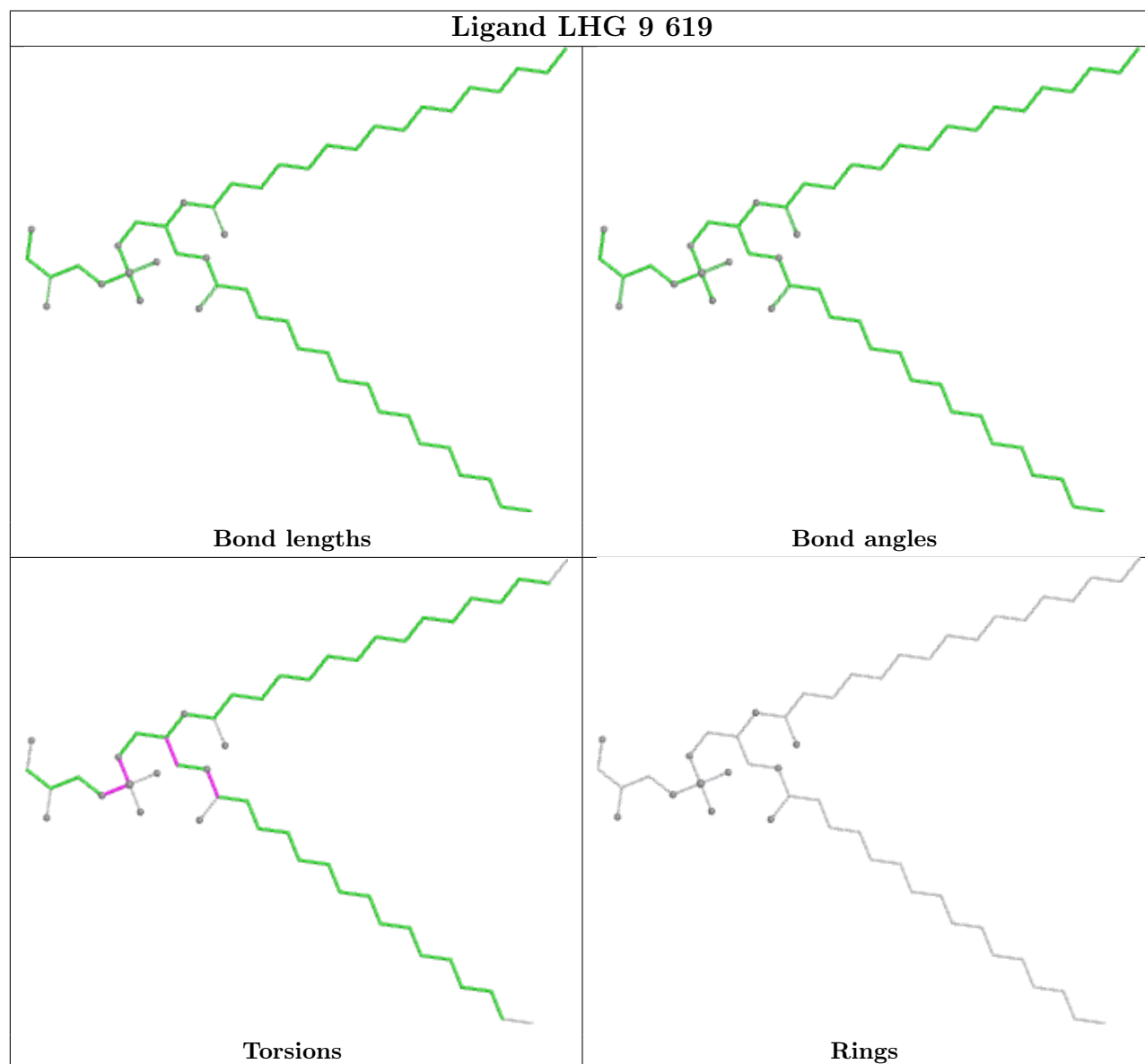
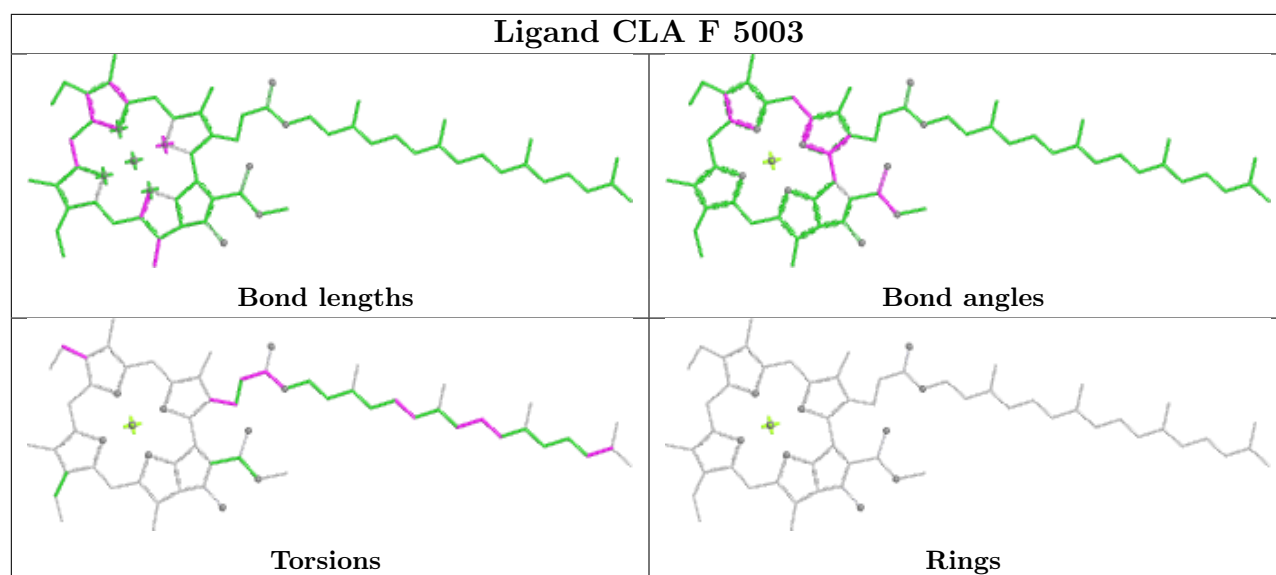
Ligand CLA B 818



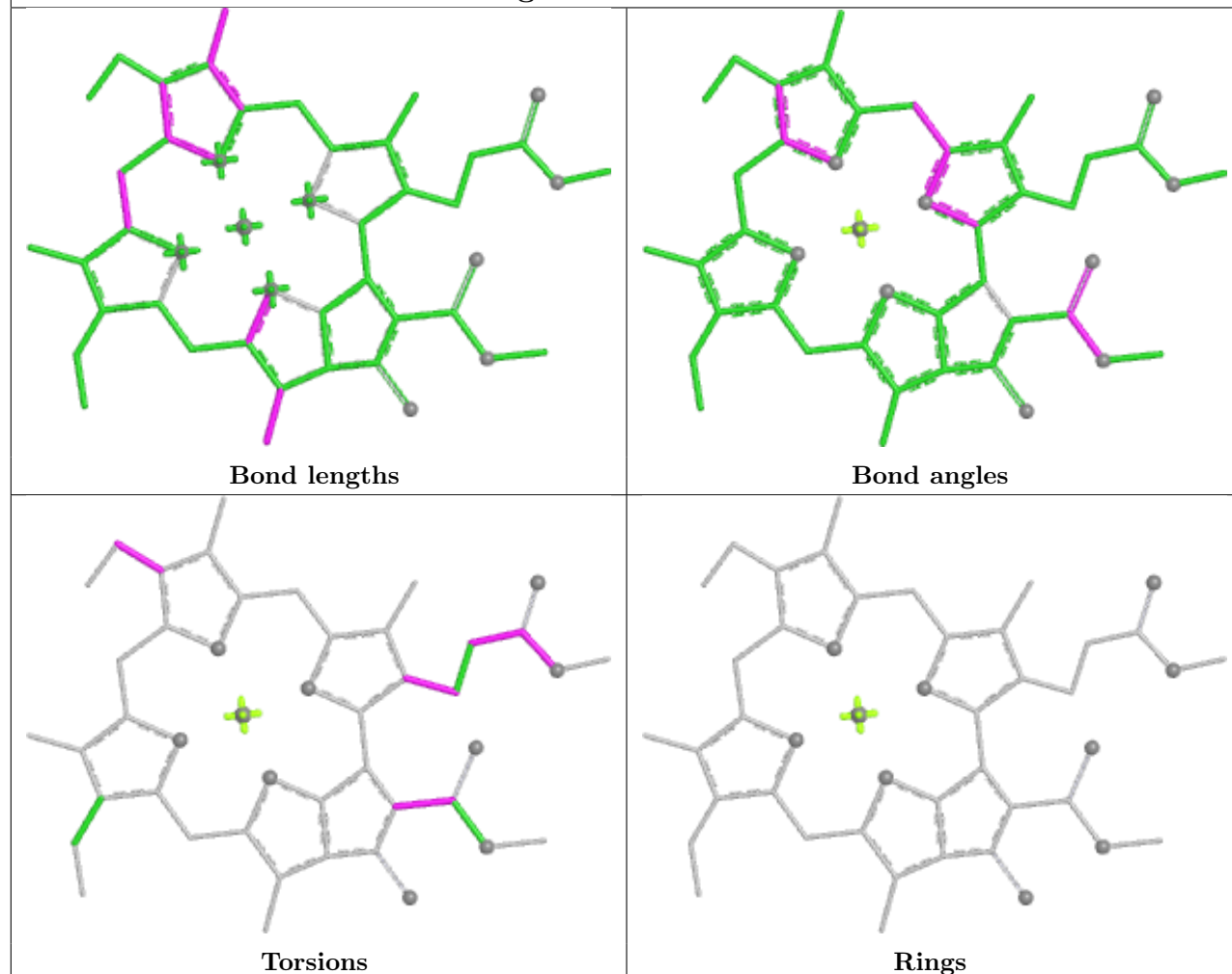
Ligand CLA 1 605



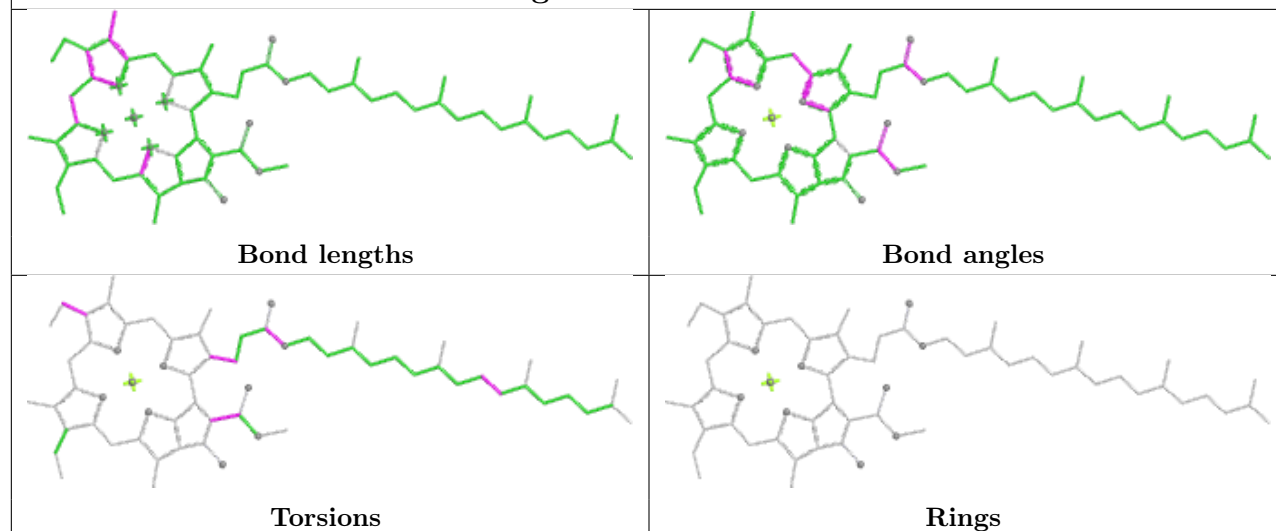




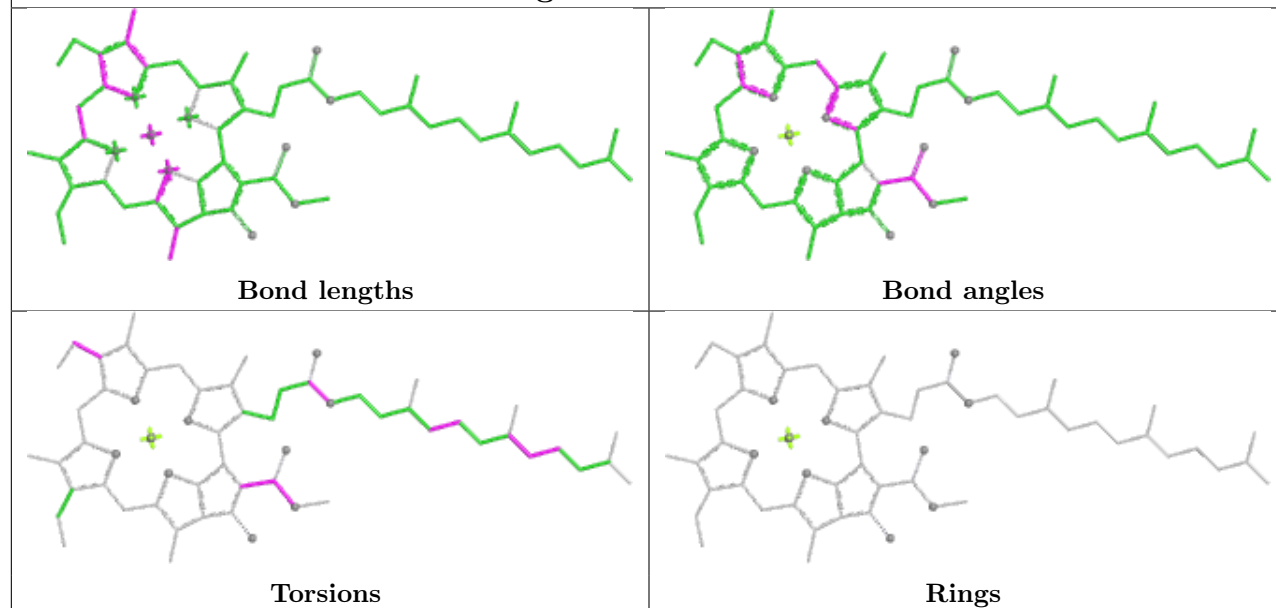
Ligand CLA 2 607



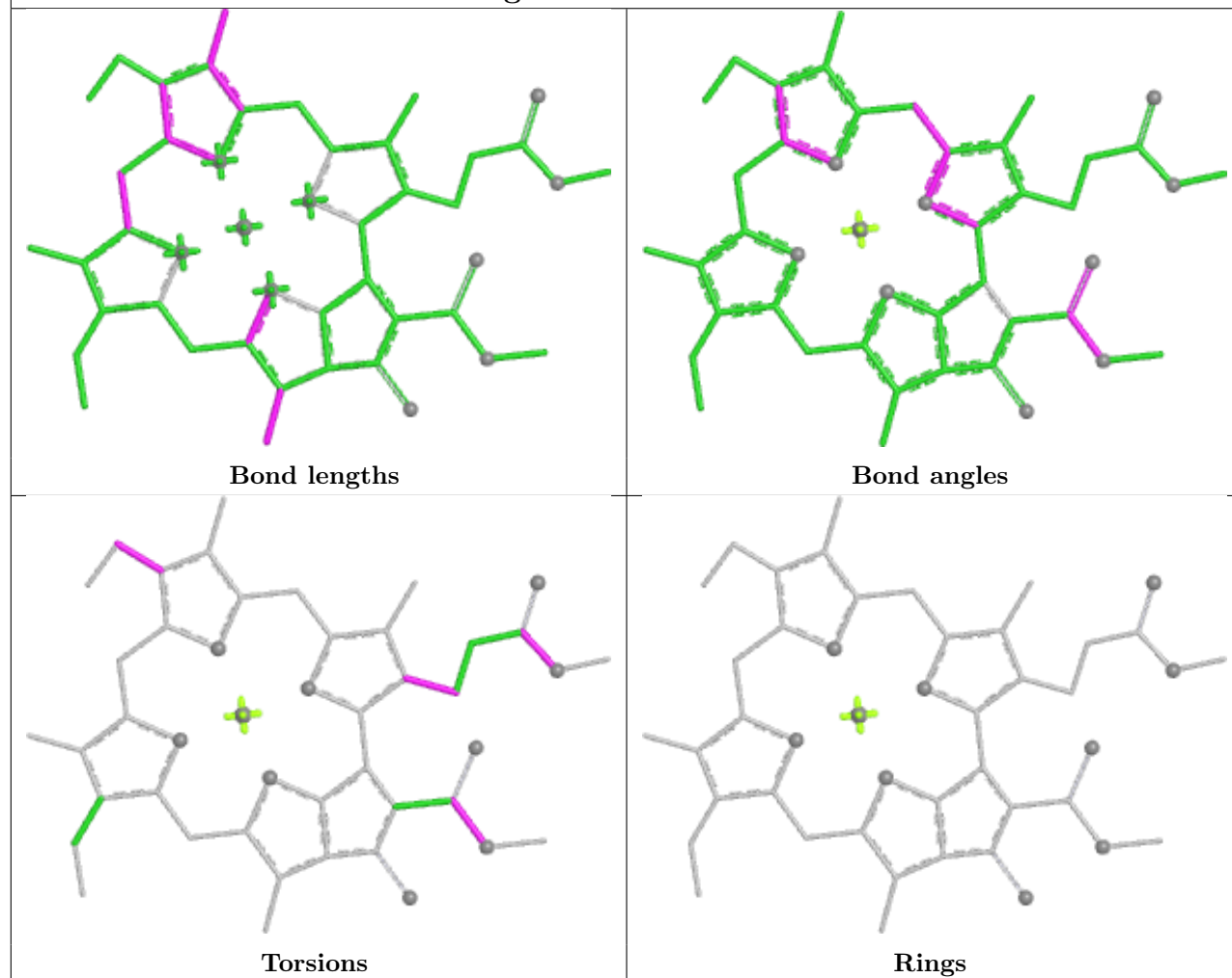
Ligand CLA A 807

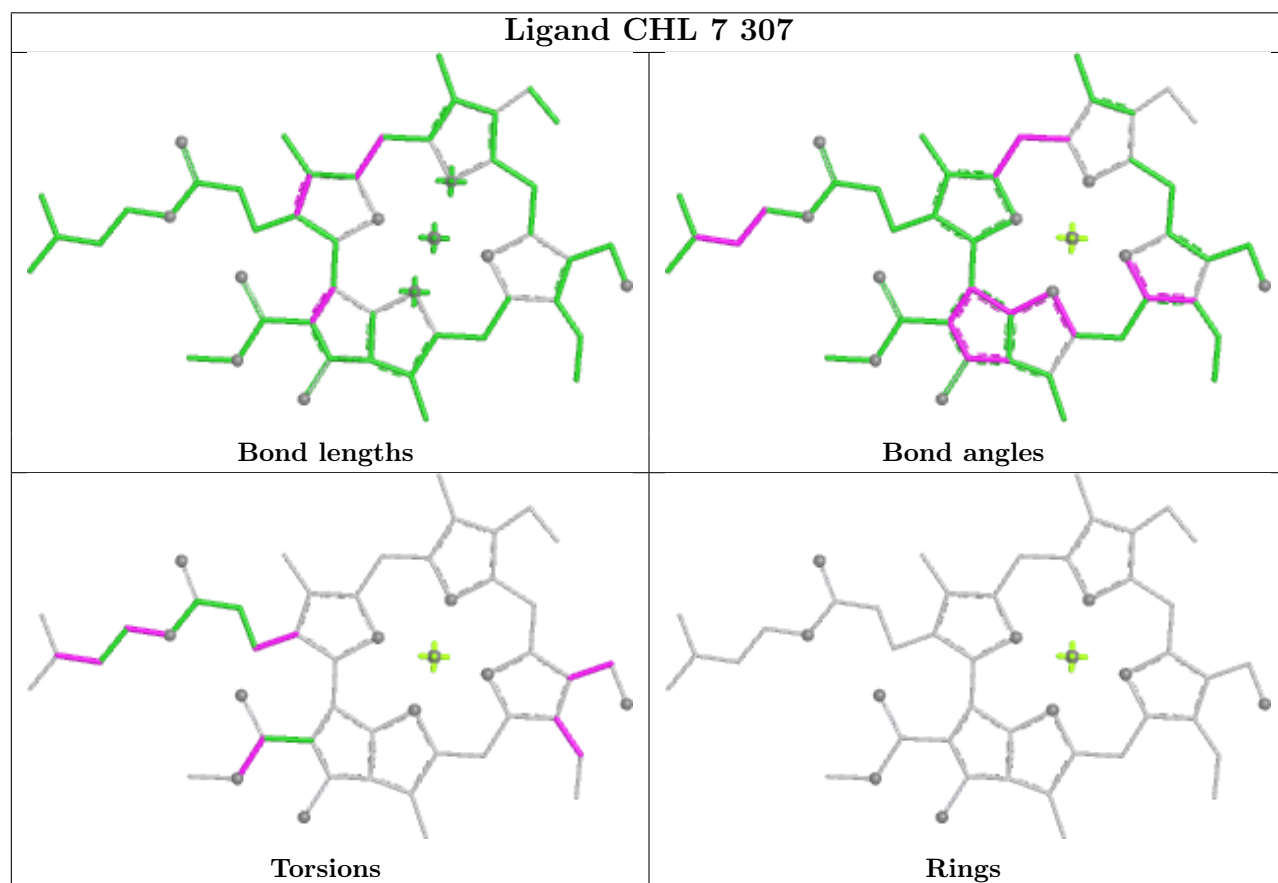
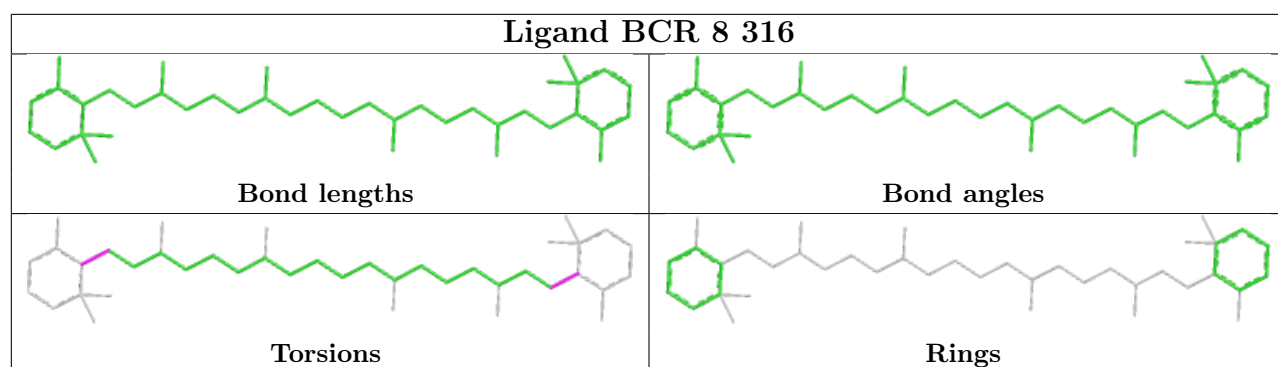


Ligand CLA 1 608

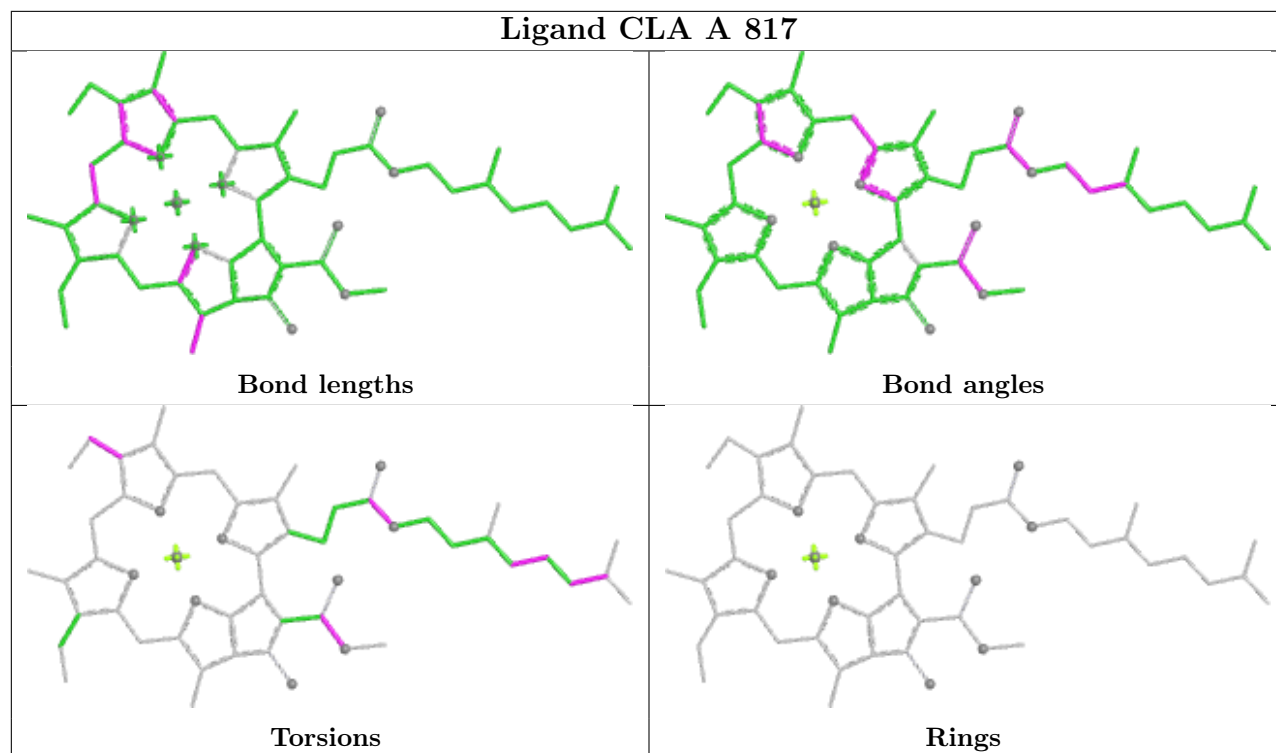


Ligand CLA G 4003

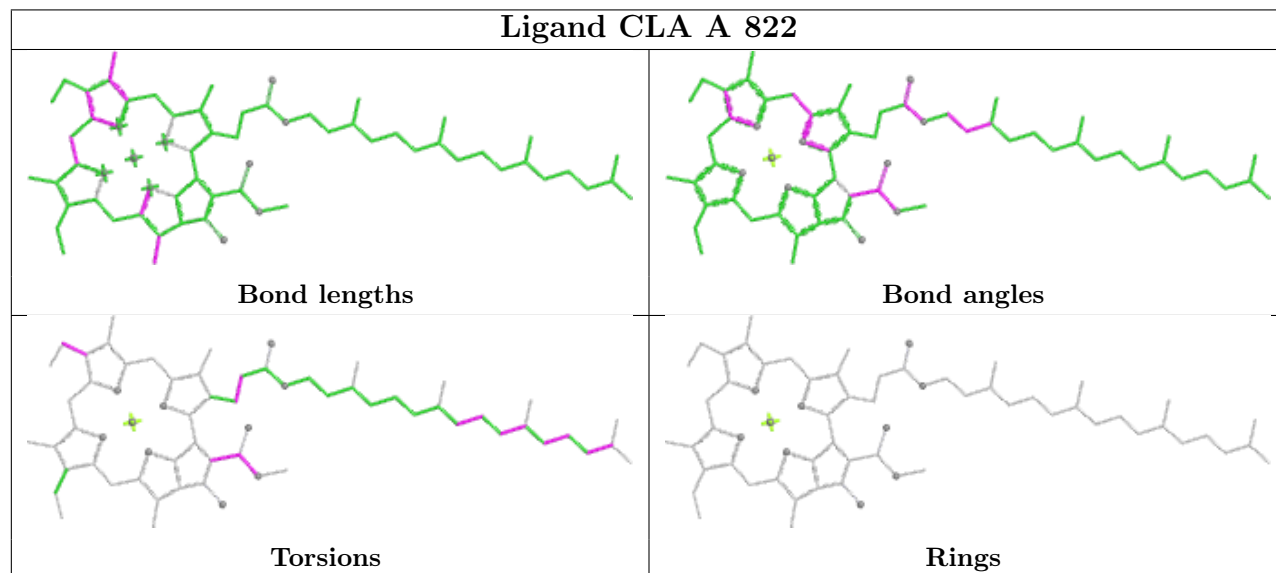


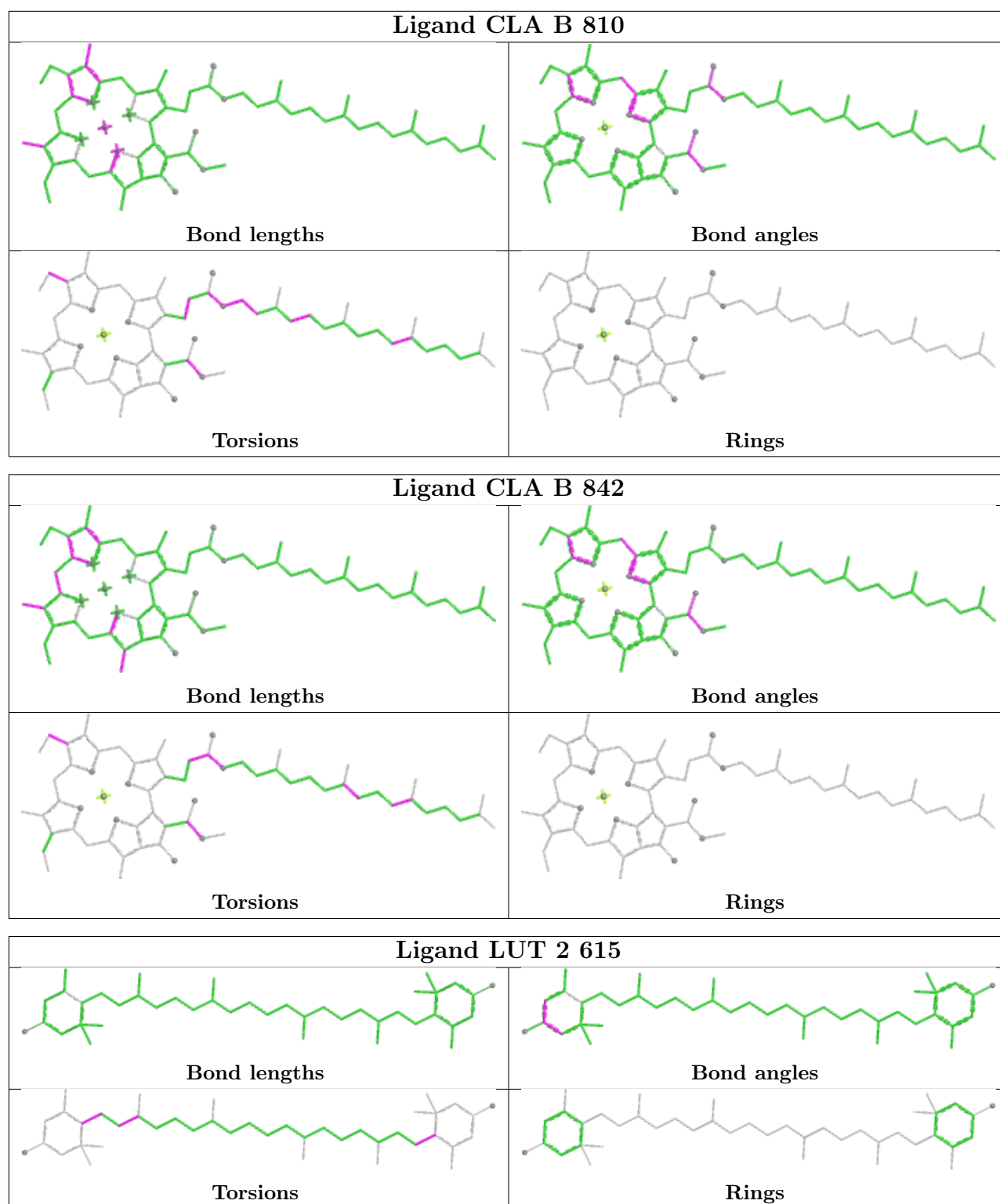


Ligand CLA A 817

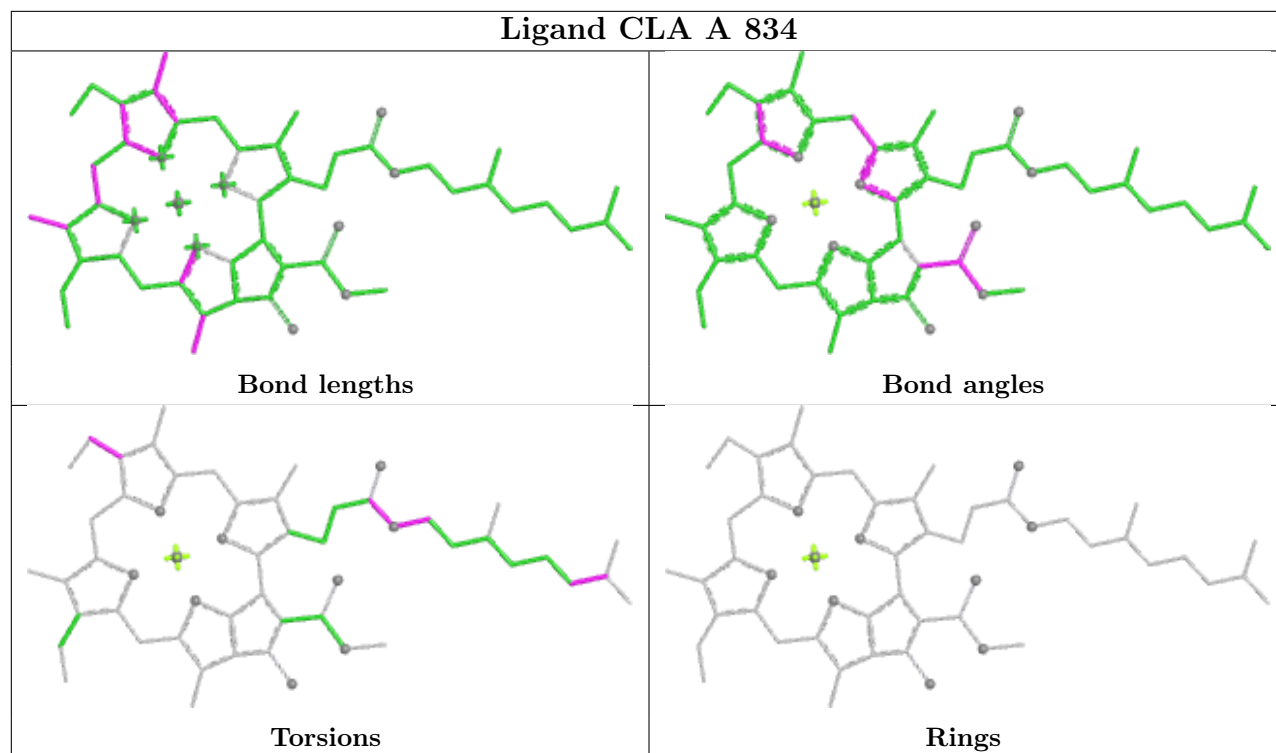


Ligand CLA A 822

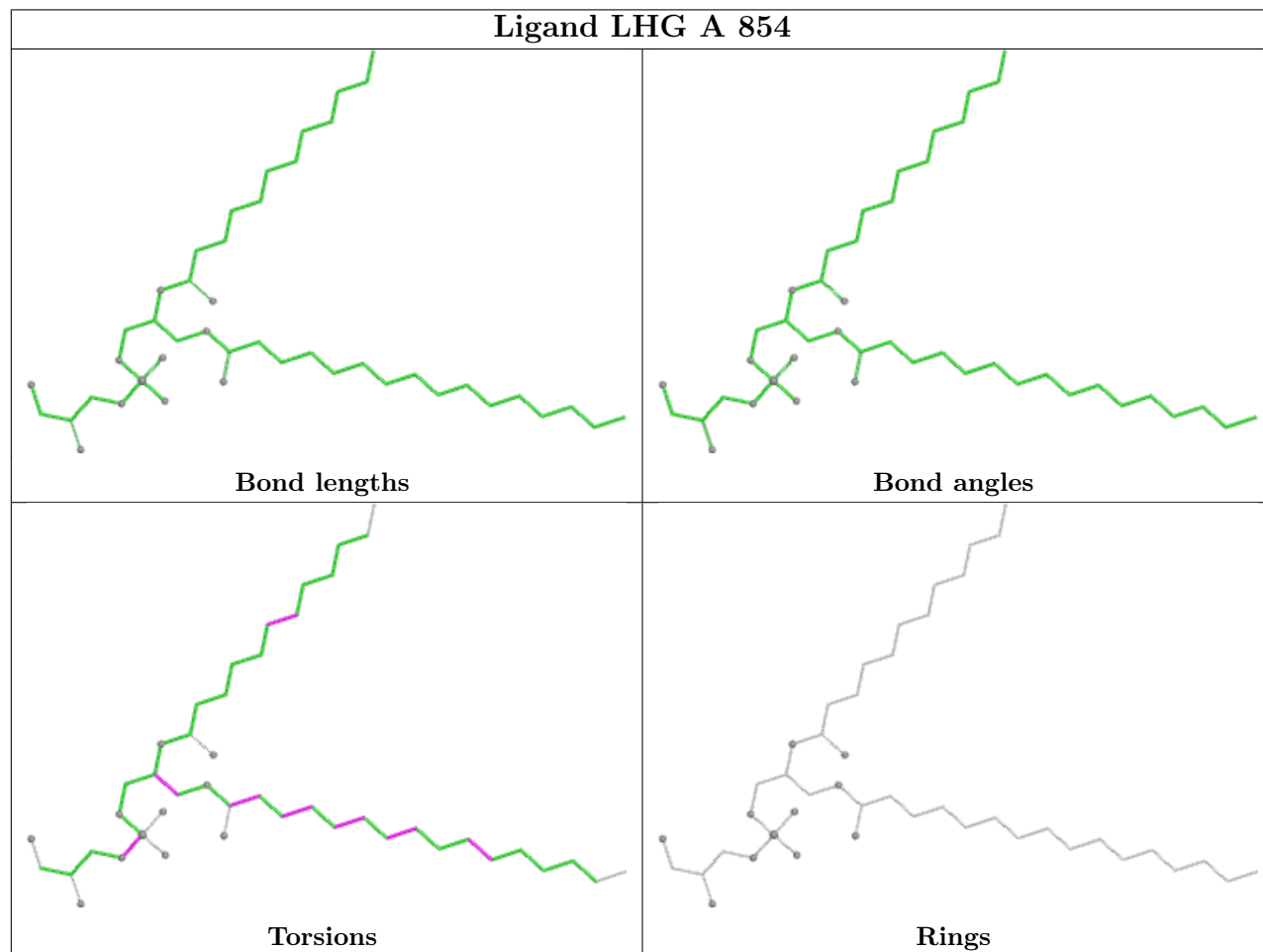


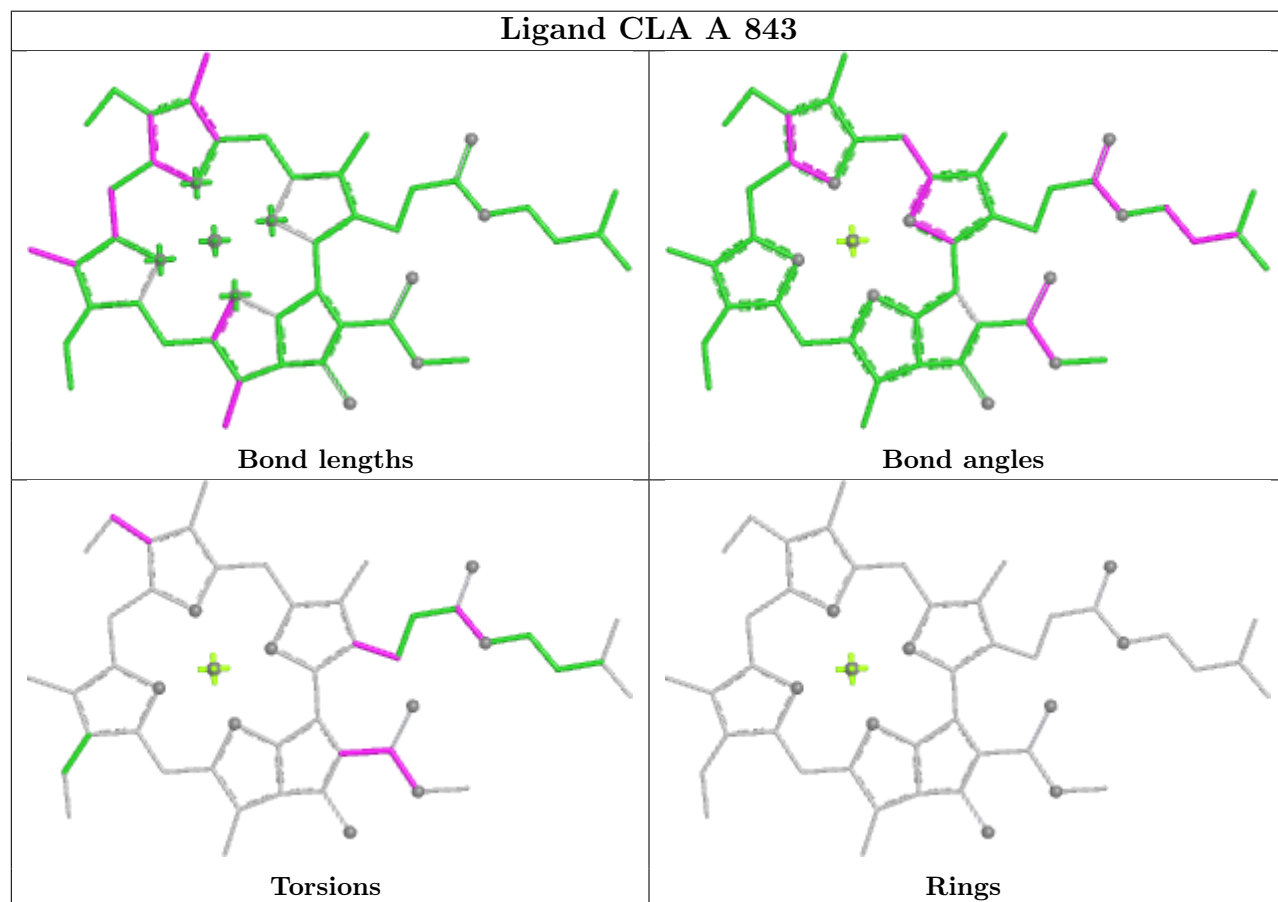
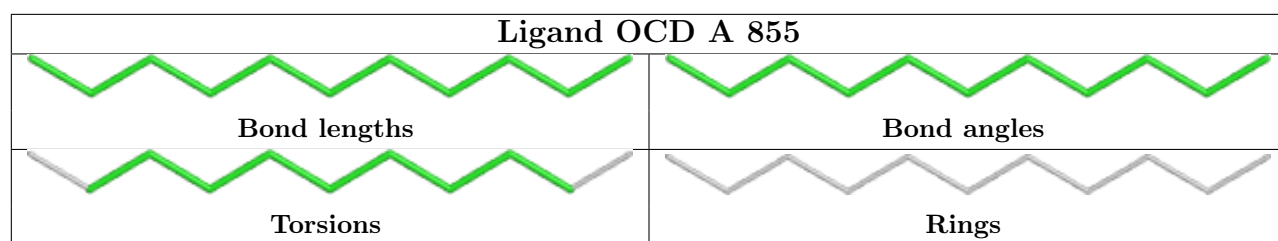


Ligand CLA A 834

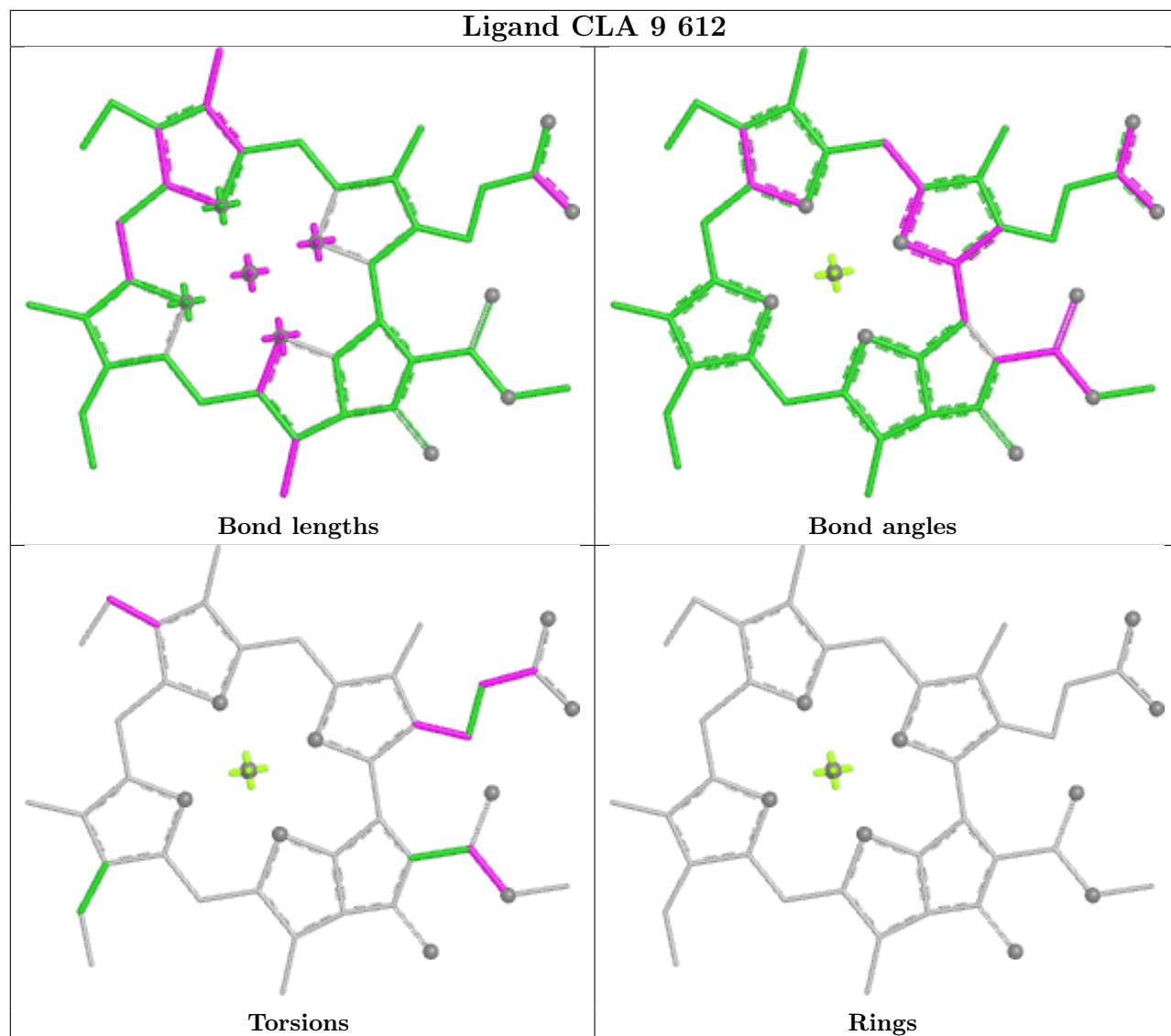


Ligand LHG A 854

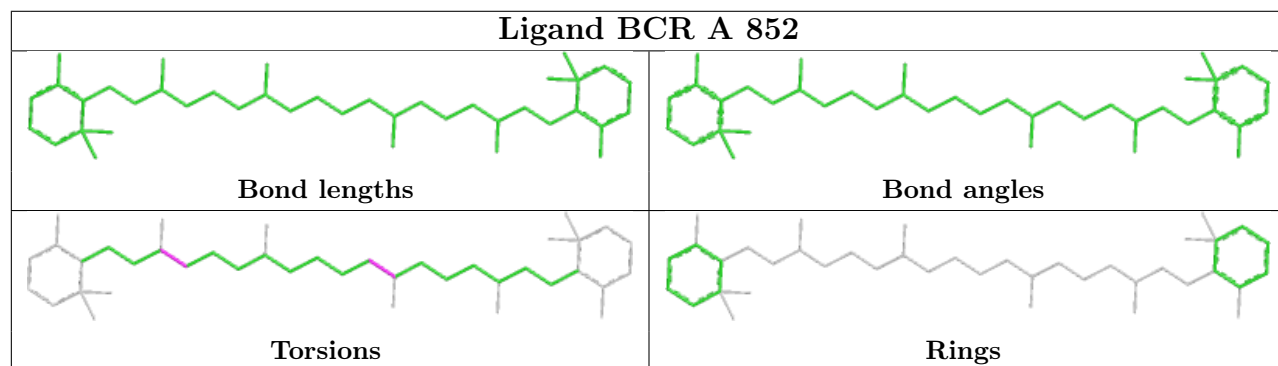


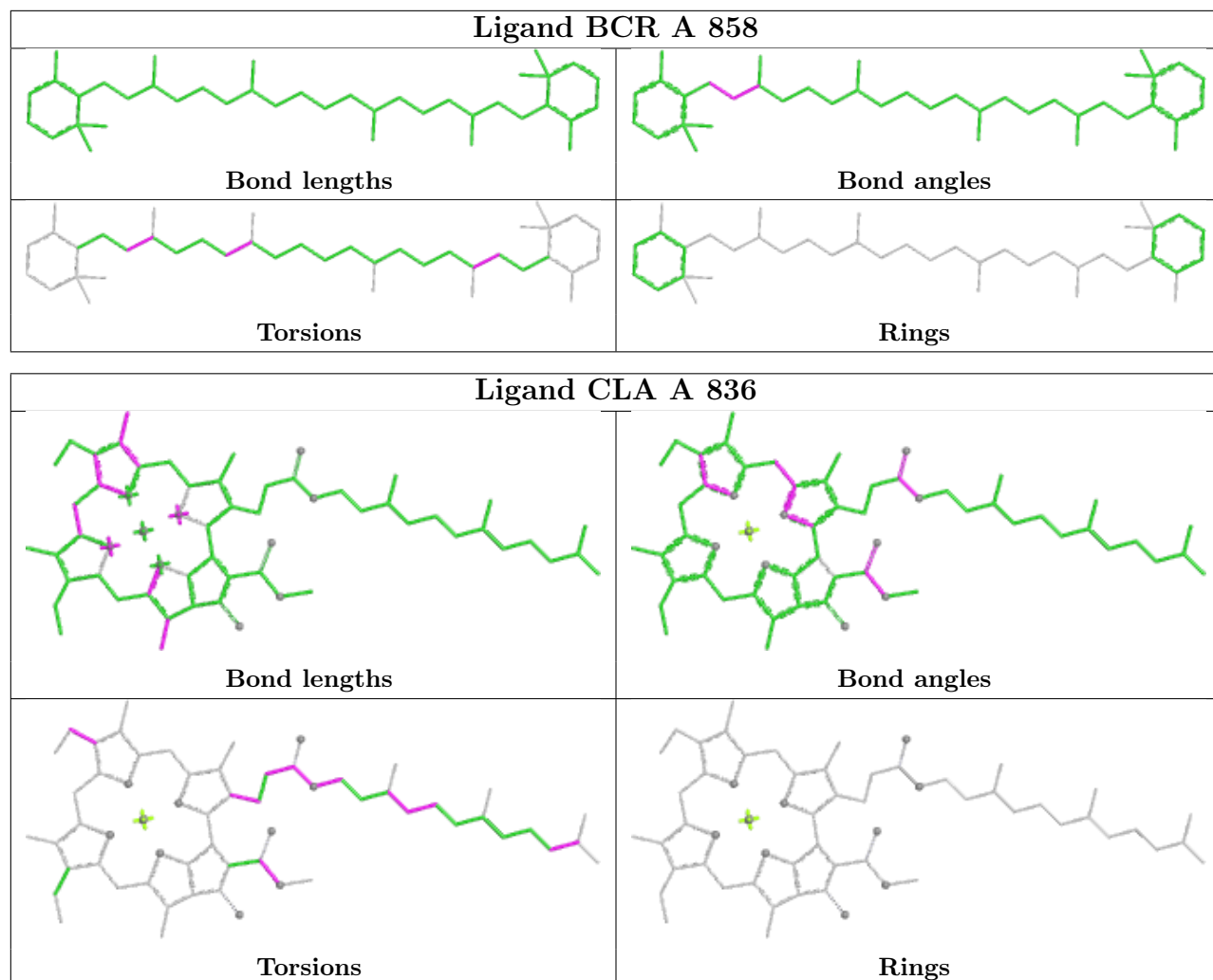


Ligand CLA 9 612

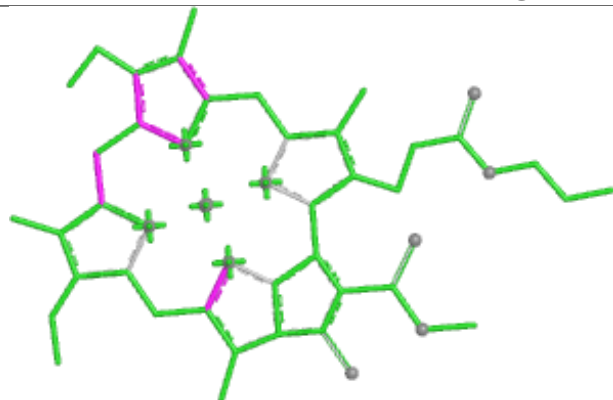


Ligand BCR A 852

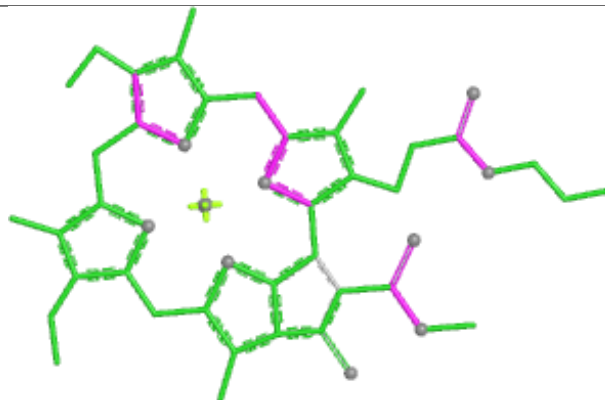




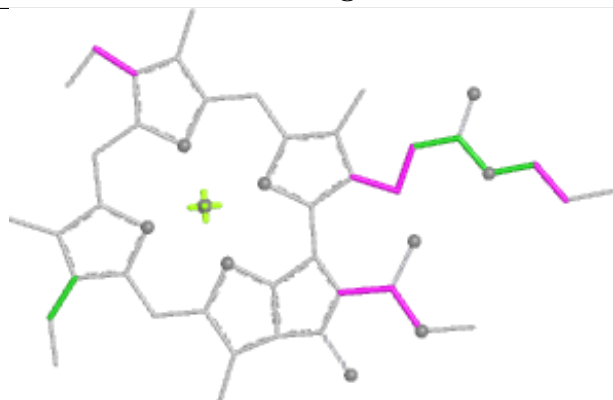
Ligand CLA K 204



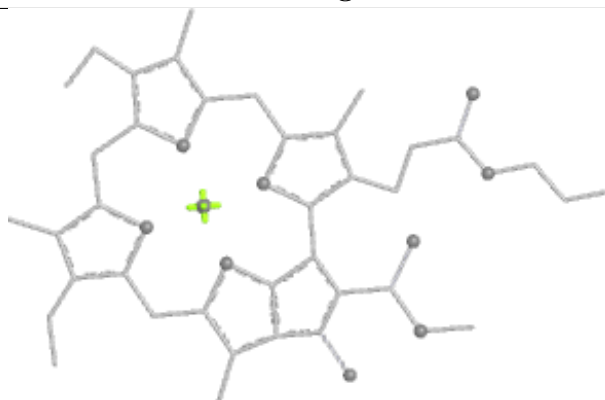
Bond lengths



Bond angles

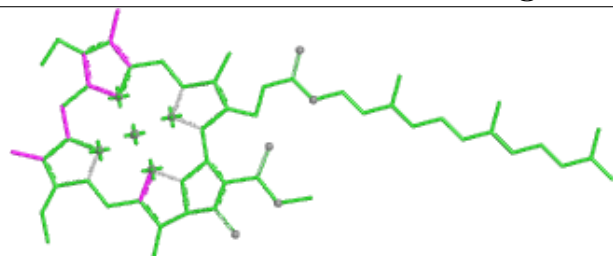


Torsions

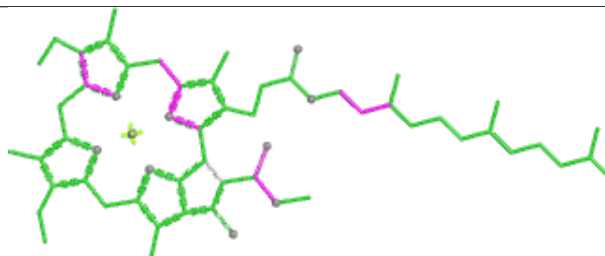


Rings

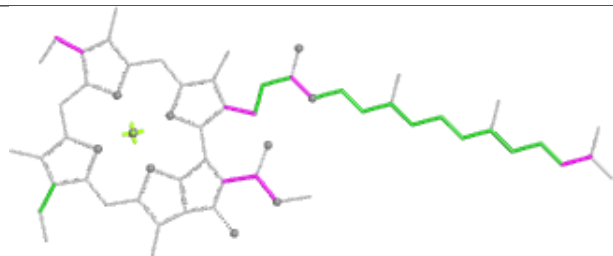
Ligand CLA 7 303



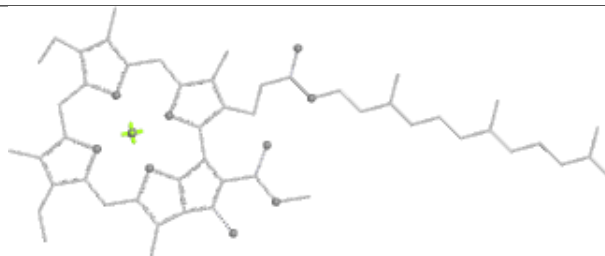
Bond lengths



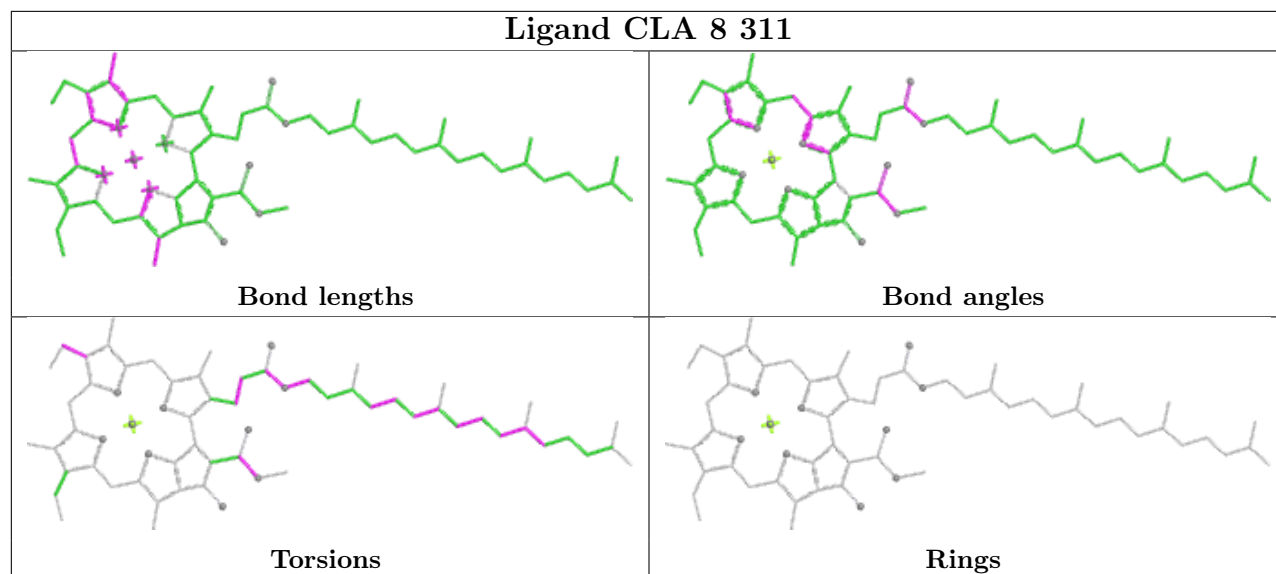
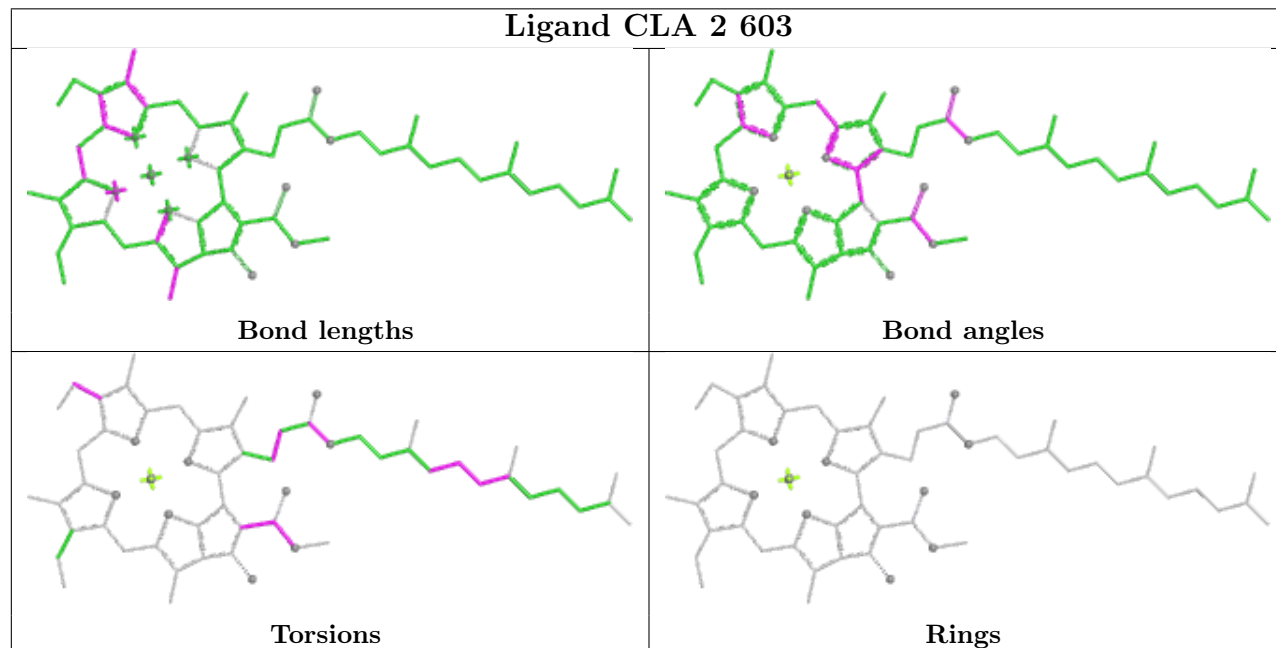
Bond angles



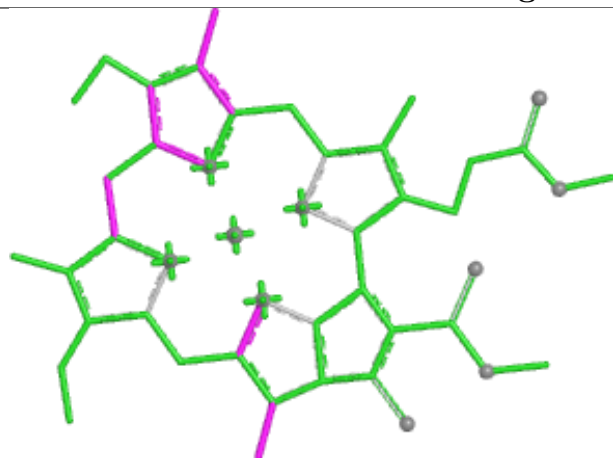
Torsions



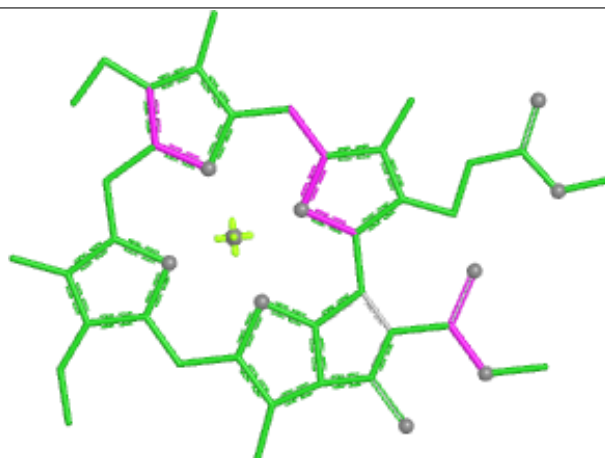
Rings

Ligand CLA 8 311**Ligand CLA 2 603**

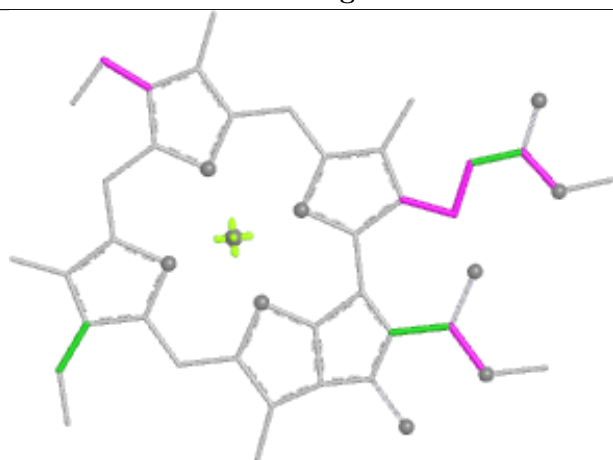
Ligand CLA 3 414



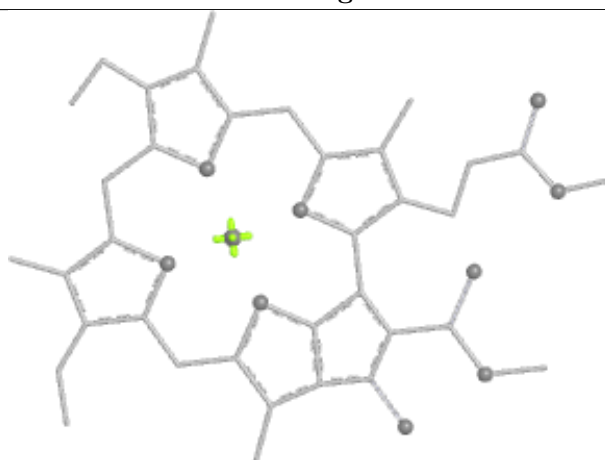
Bond lengths



Bond angles

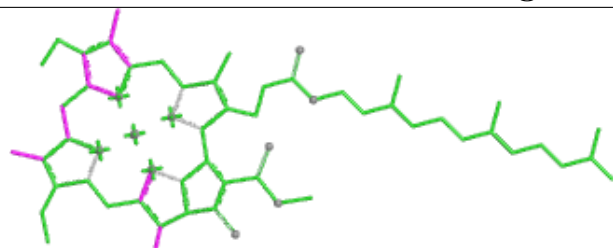


Torsions

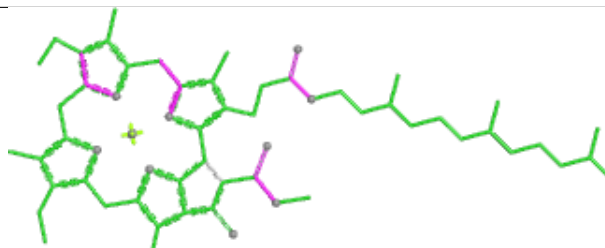


Rings

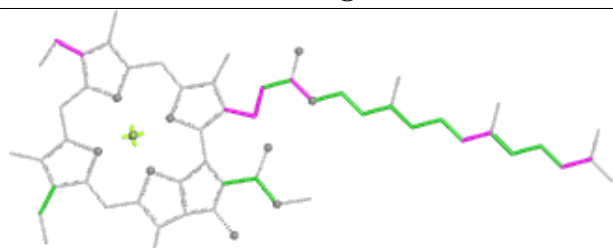
Ligand CLA 8 308



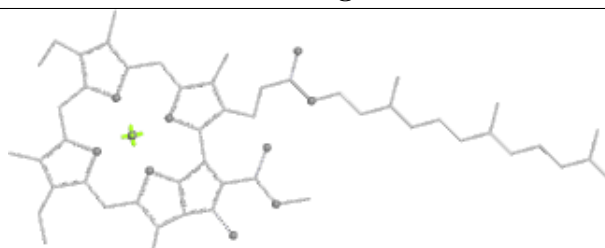
Bond lengths



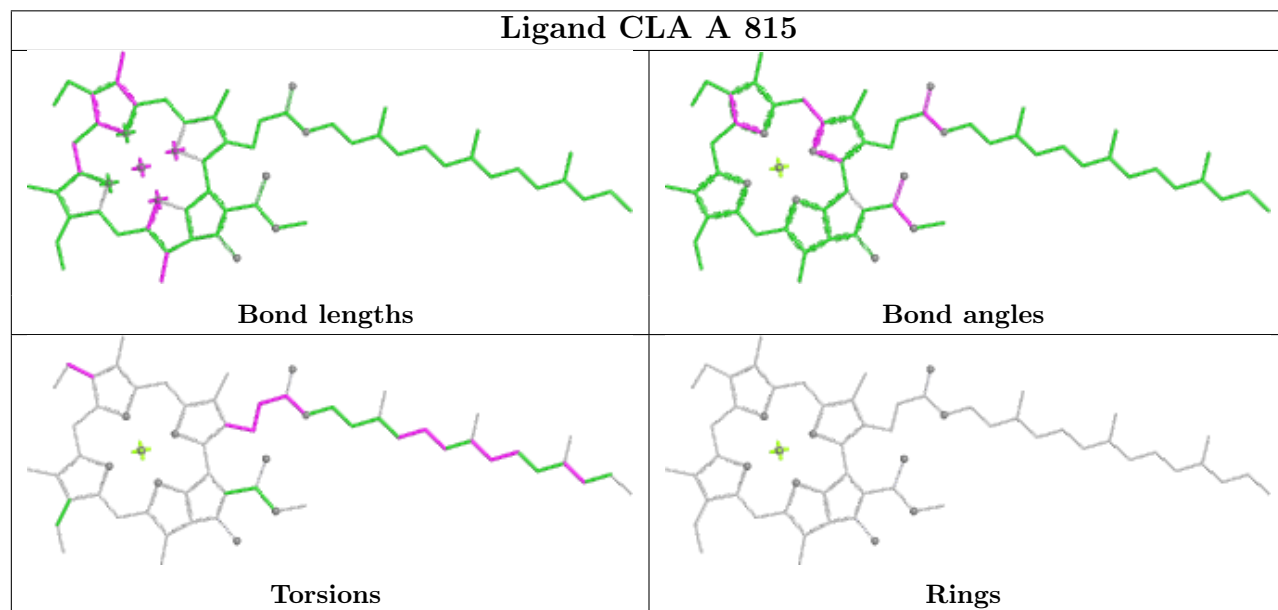
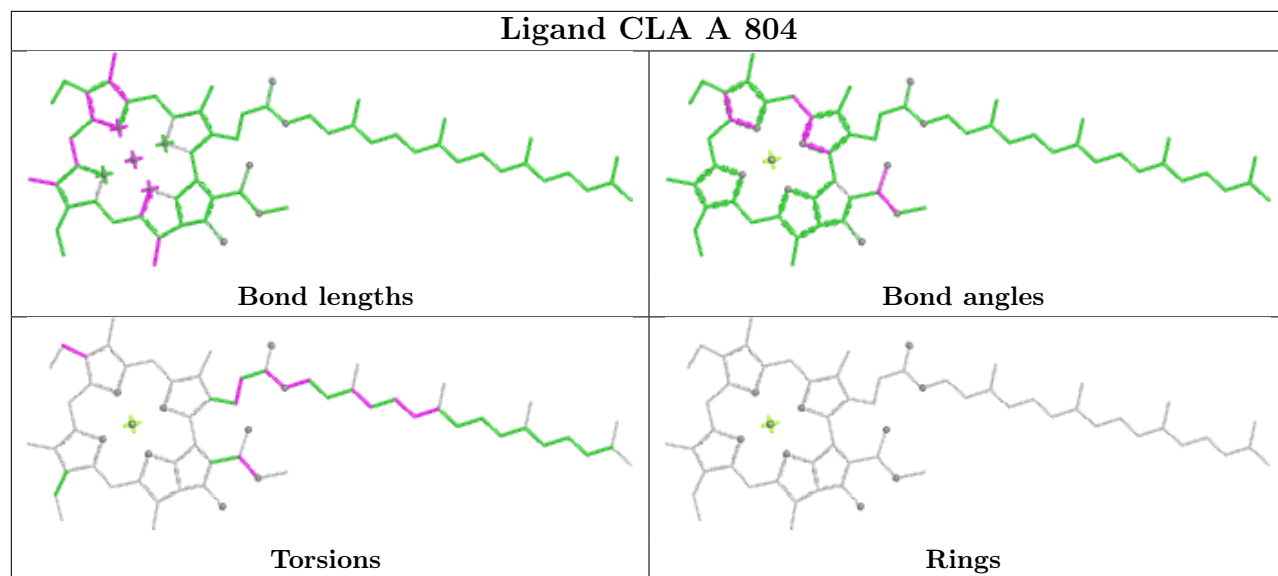
Bond angles



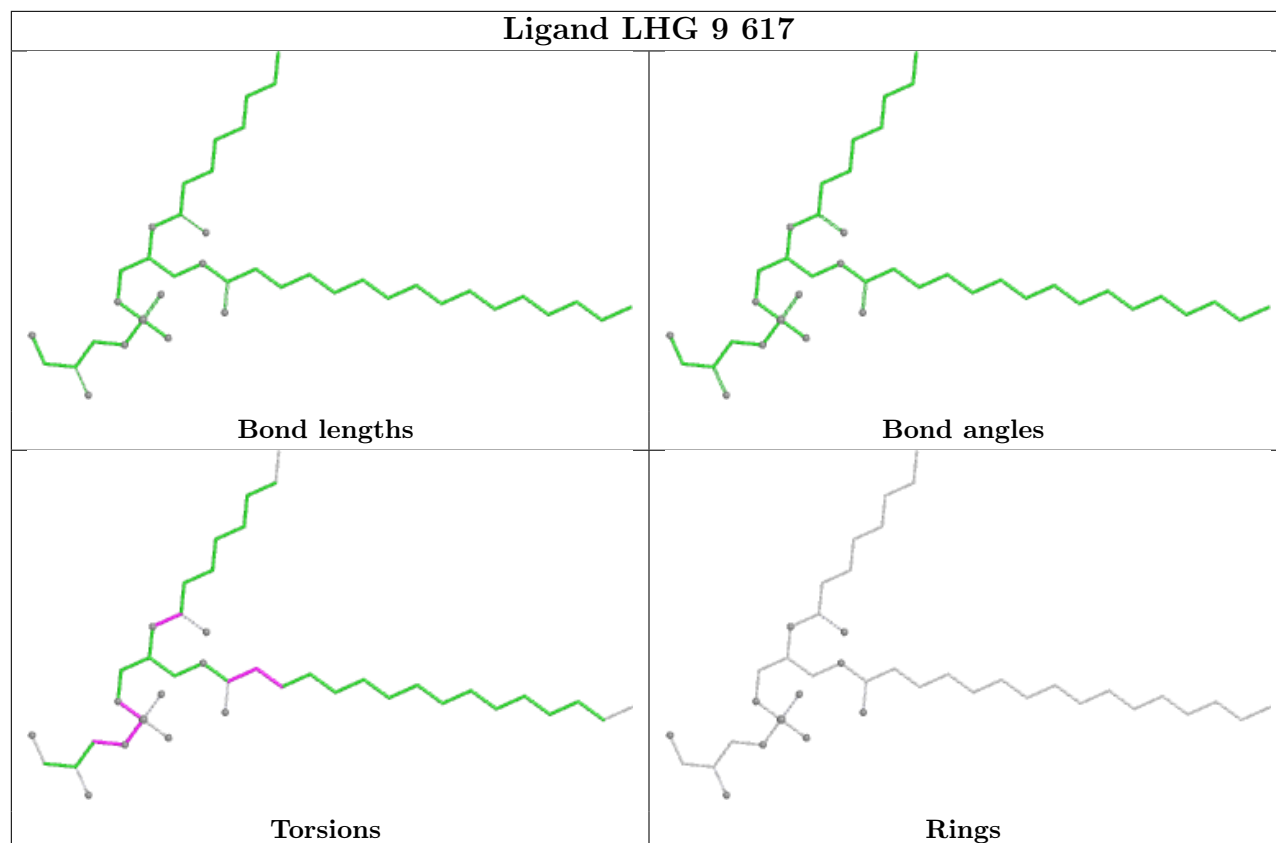
Torsions



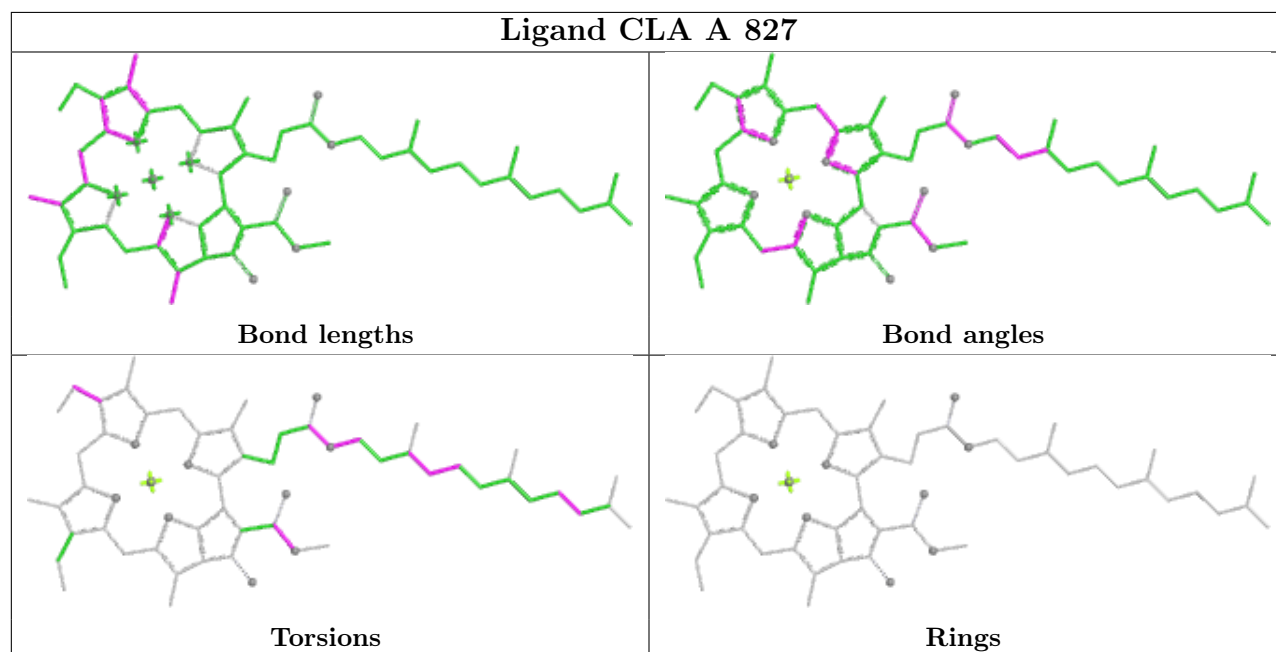
Rings

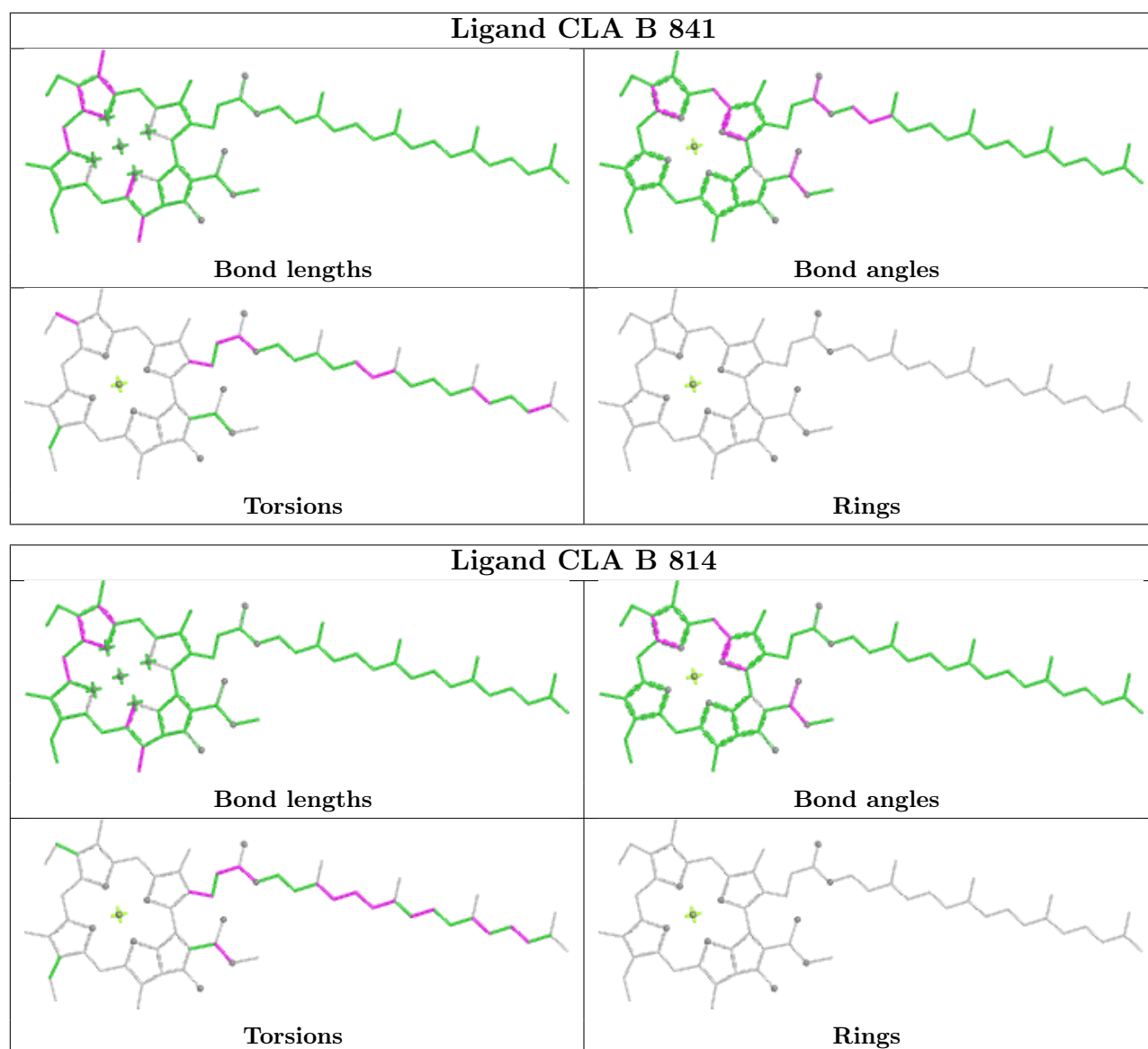


Ligand LHG 9 617

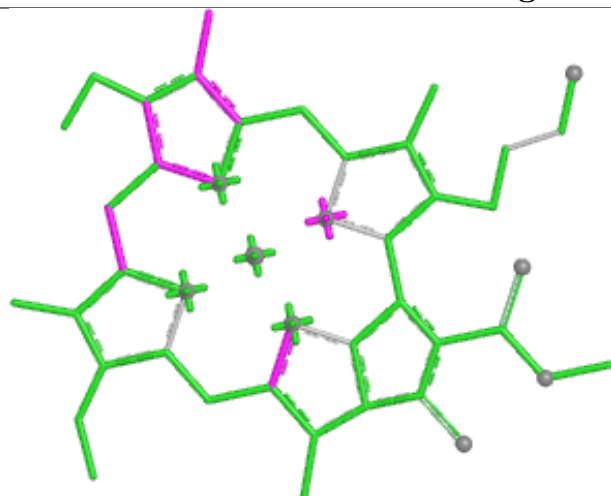


Ligand CLA A 827

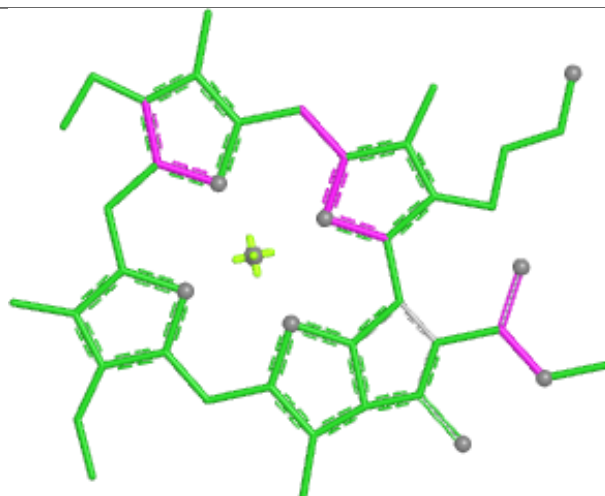




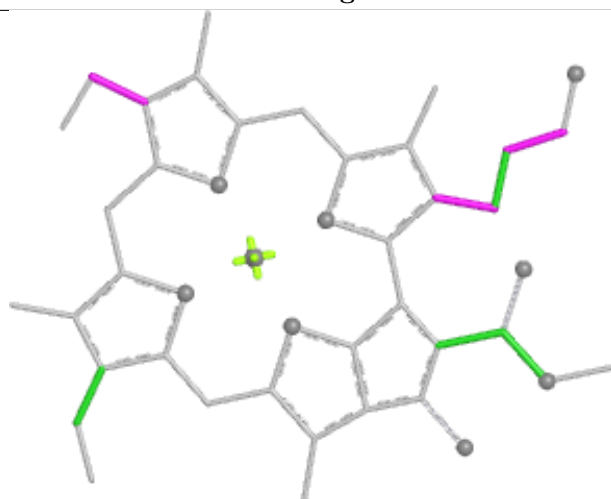
Ligand CLA 2 612



Bond lengths



Bond angles

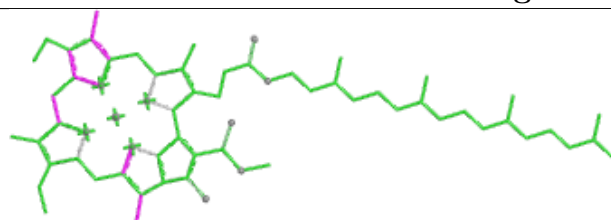


Torsions

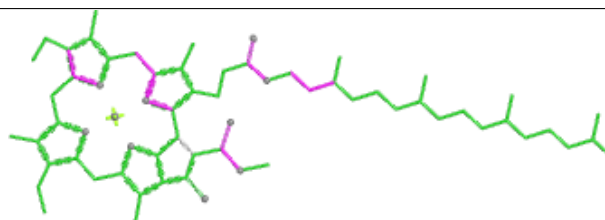


Rings

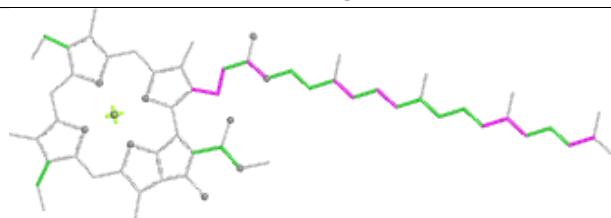
Ligand CLA A 818



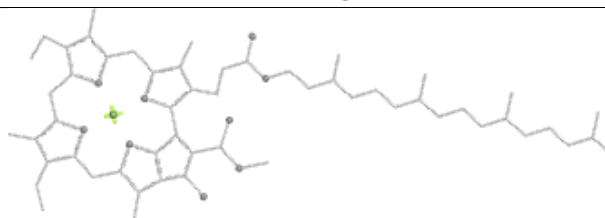
Bond lengths



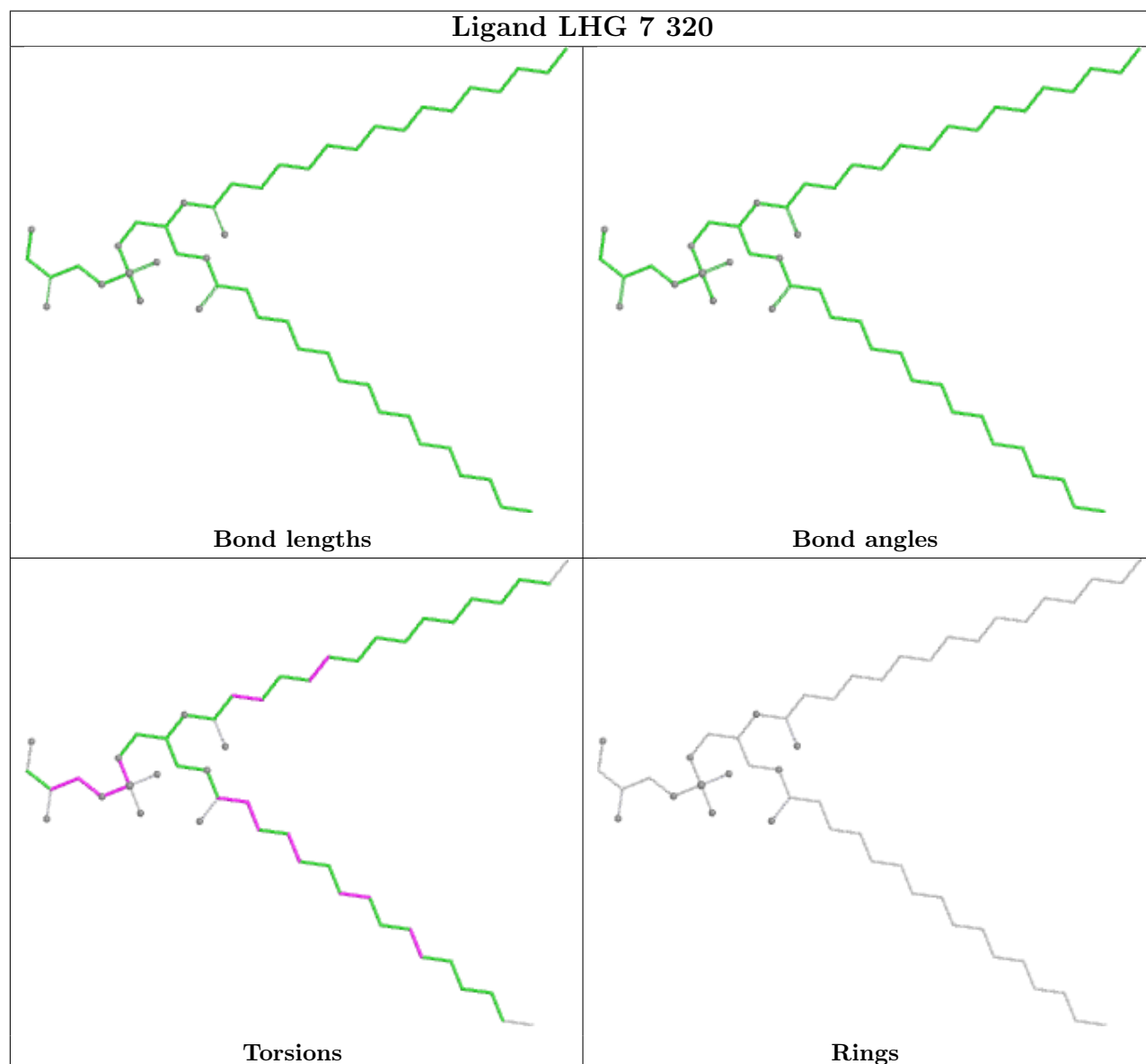
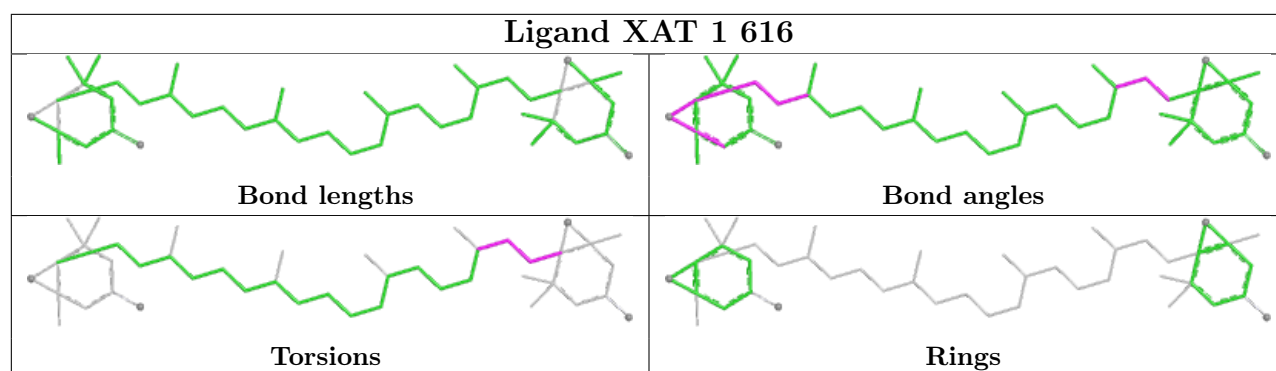
Bond angles



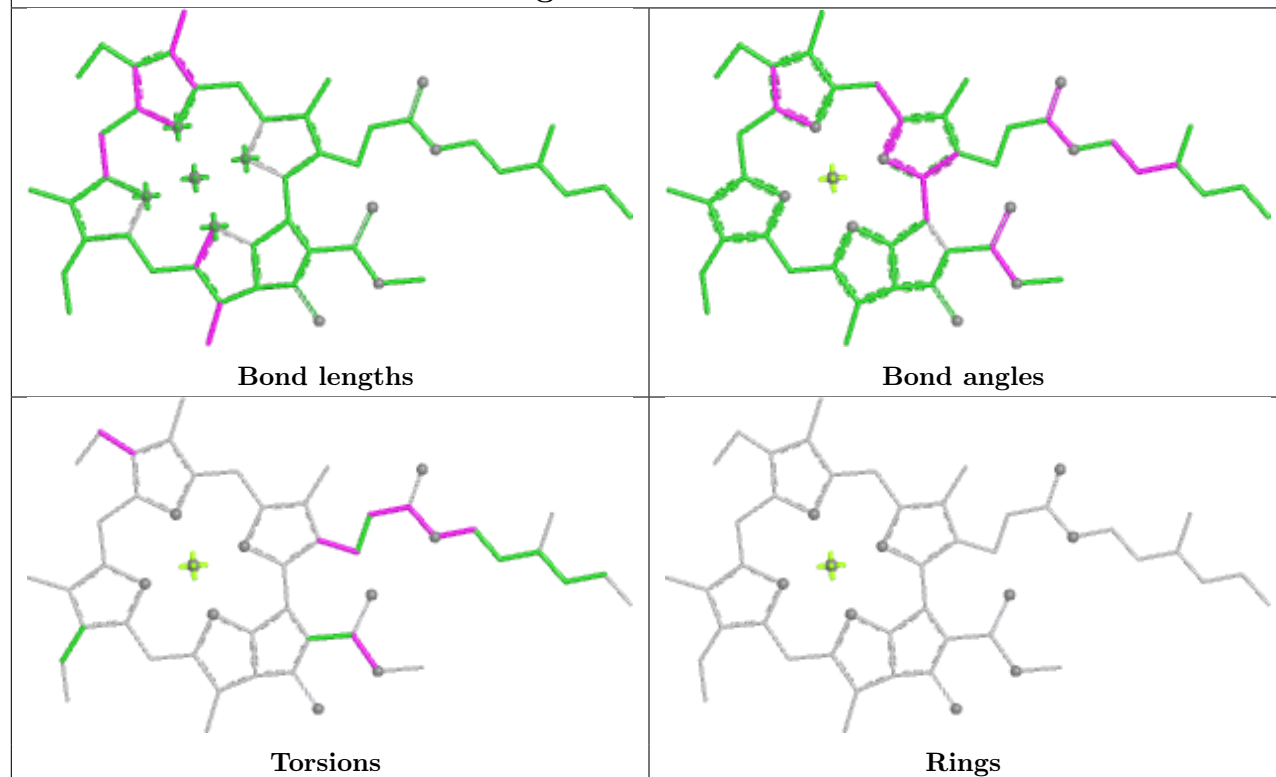
Torsions



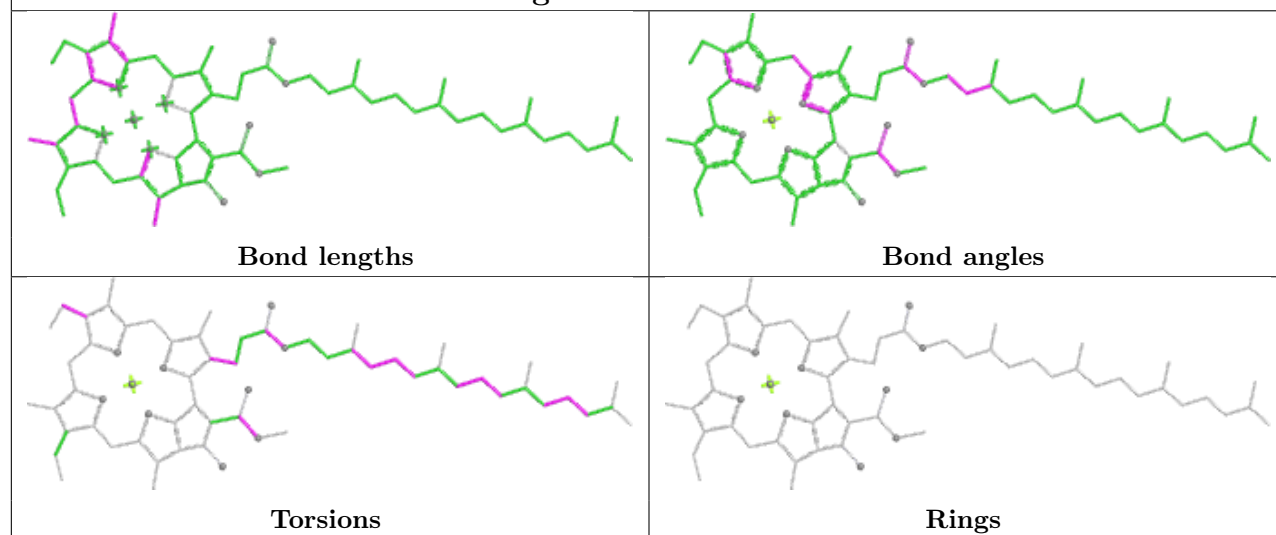
Rings



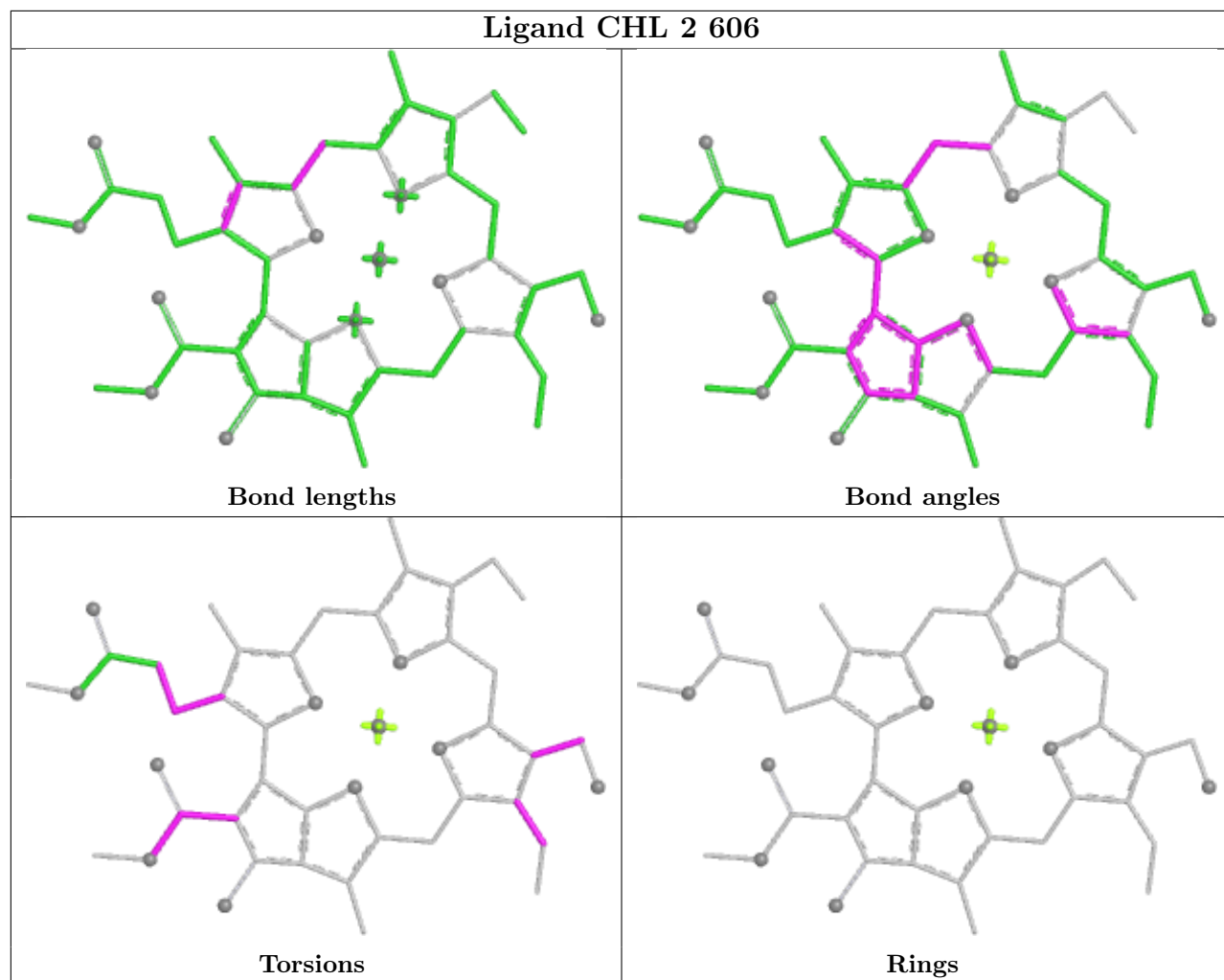
Ligand CLA 3 410



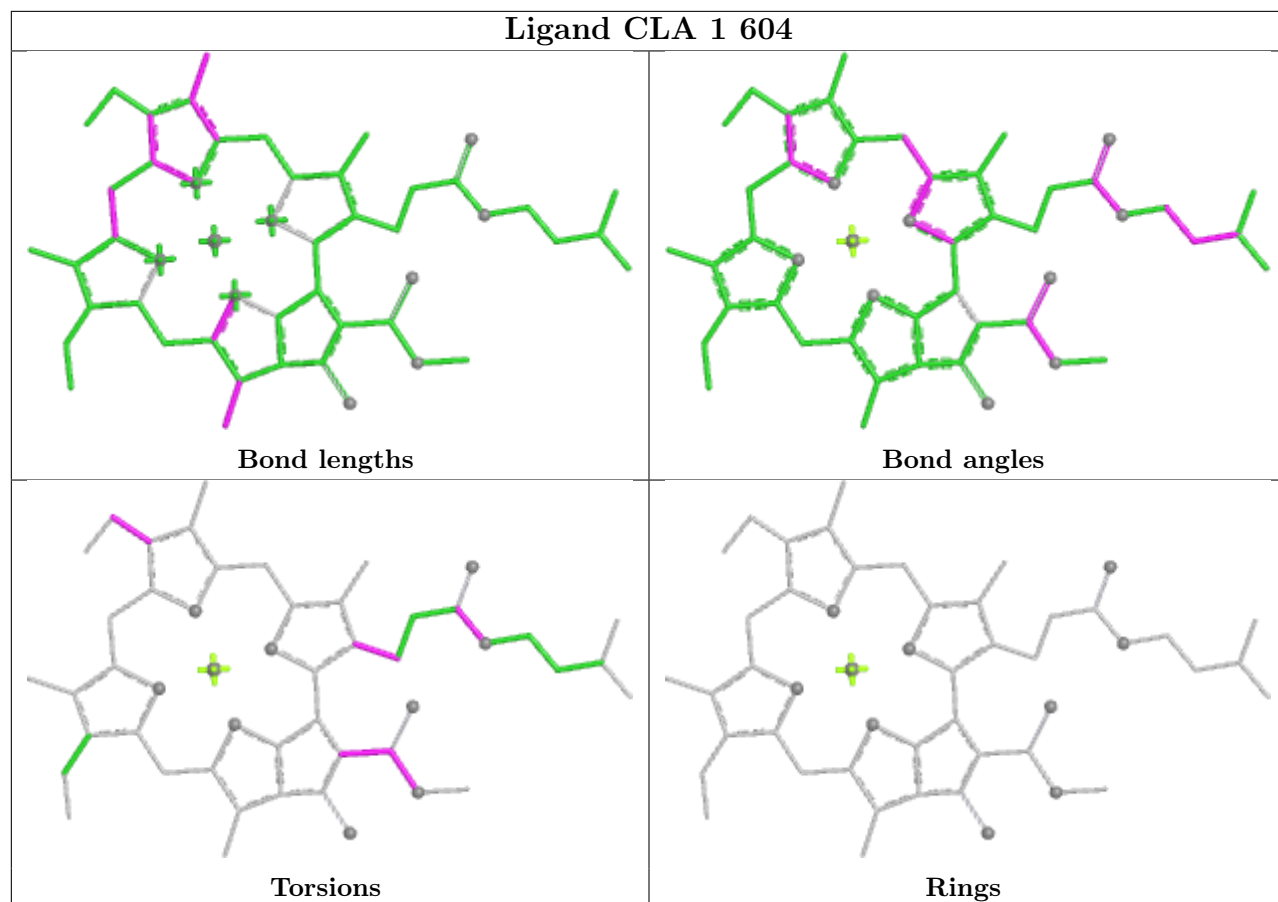
Ligand CLA B 823



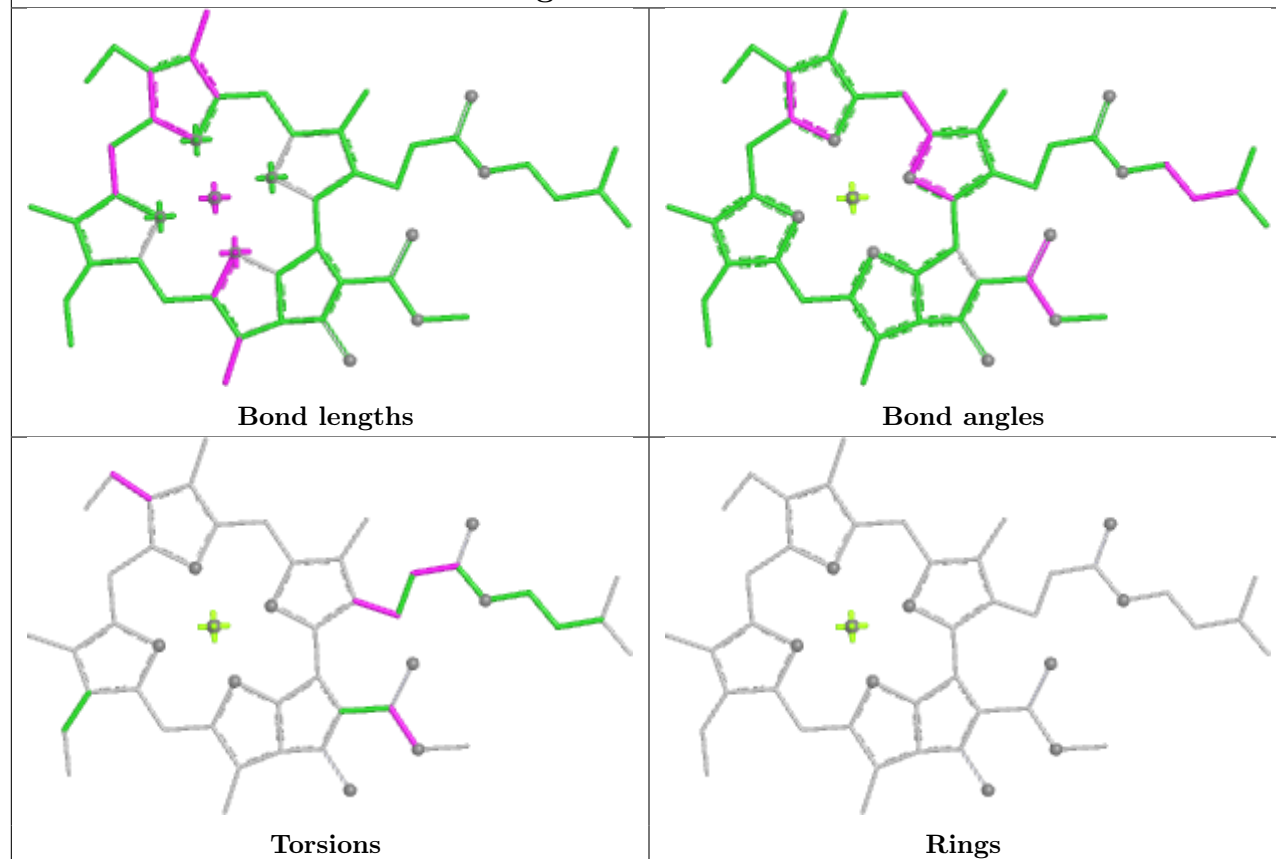
Ligand CHL 2 606



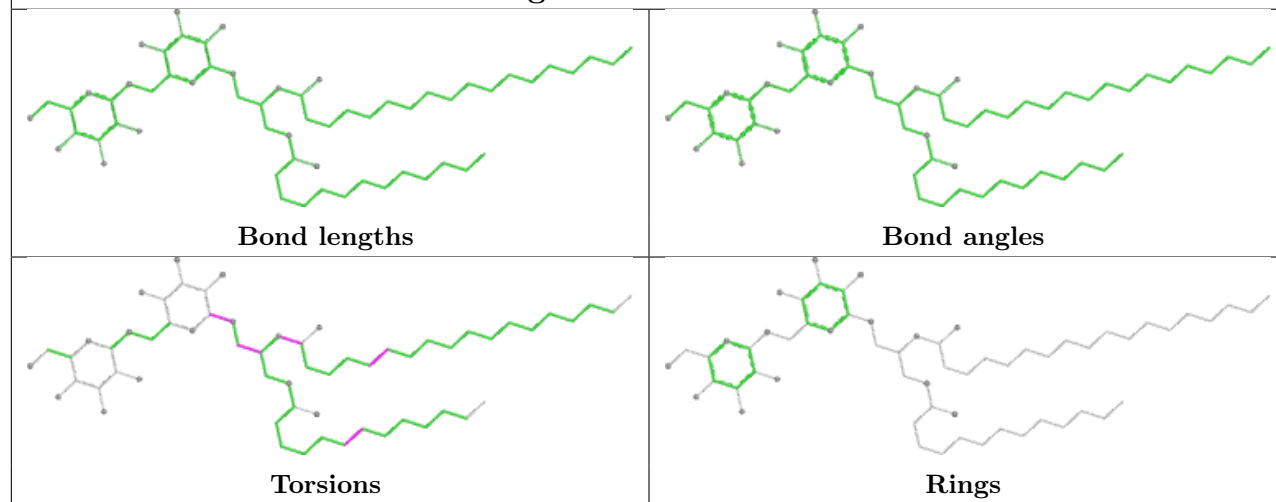
Ligand CLA 1 604

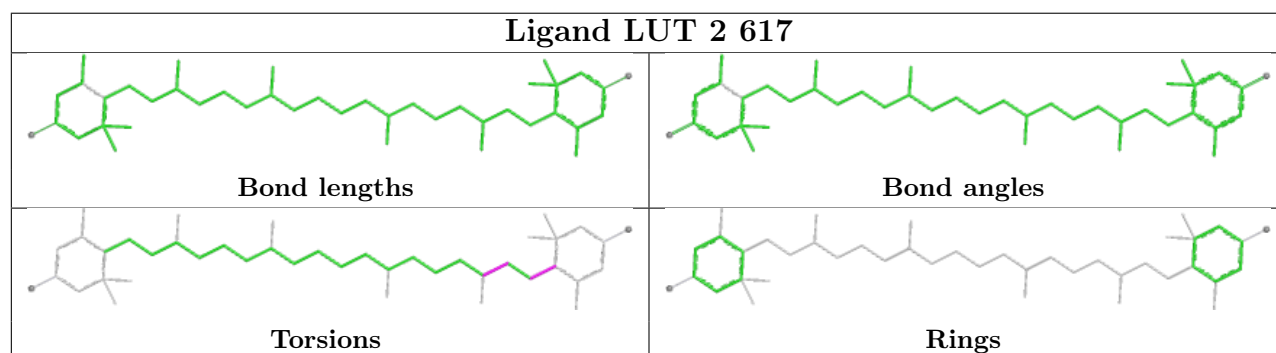
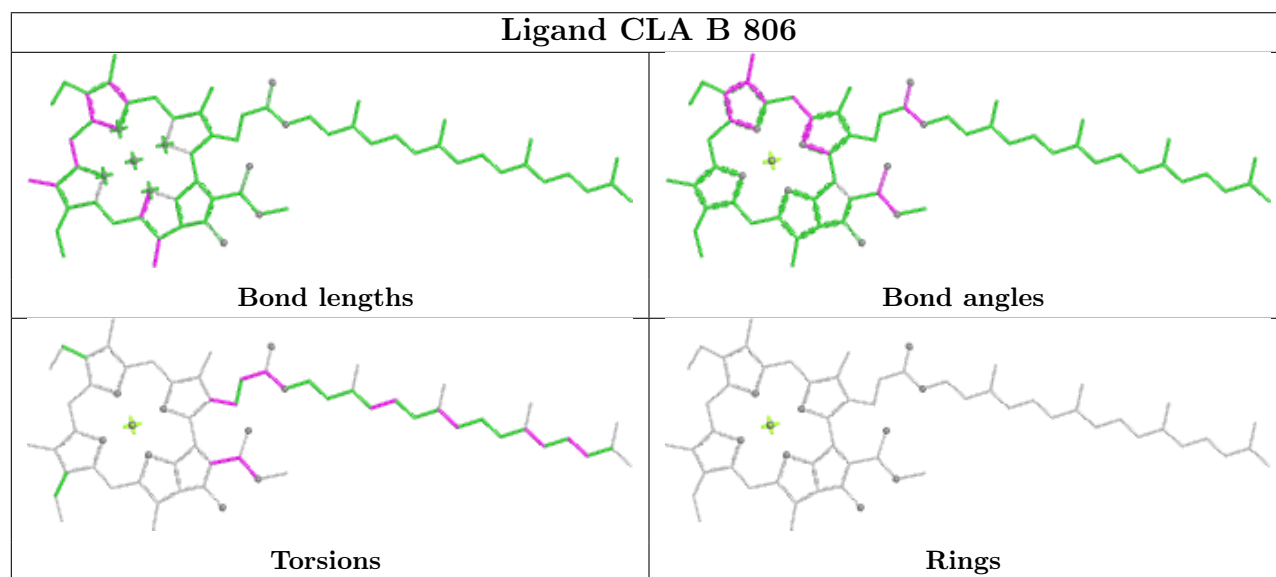
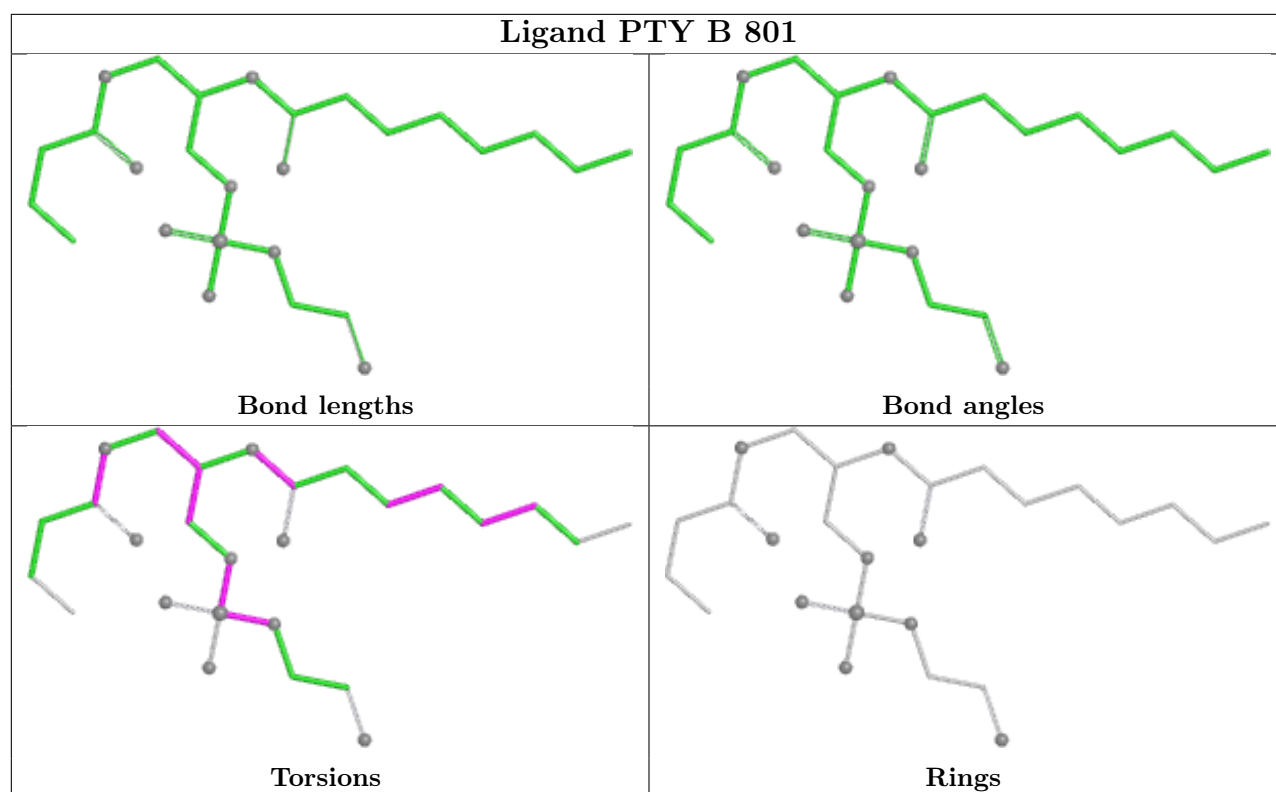


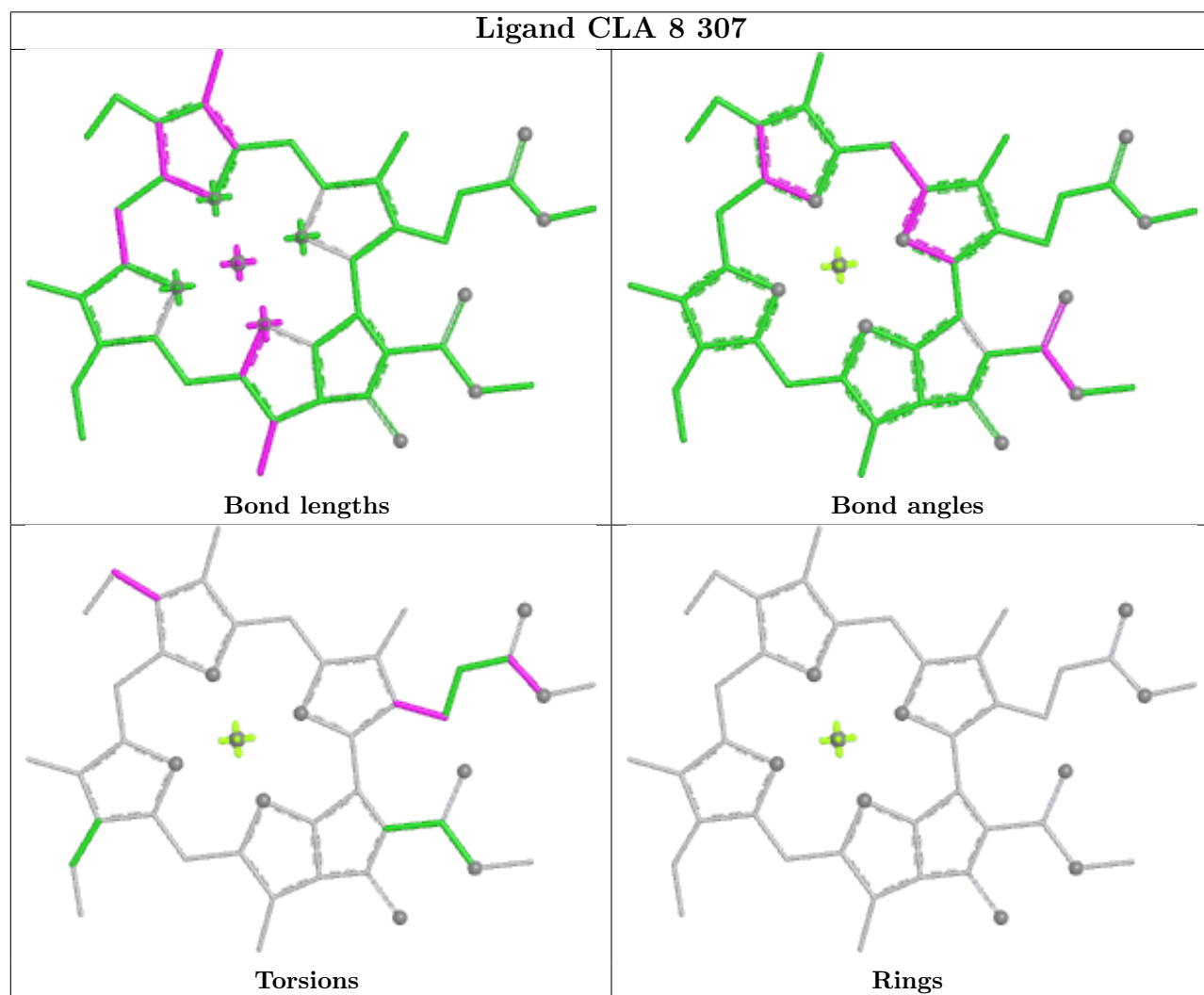
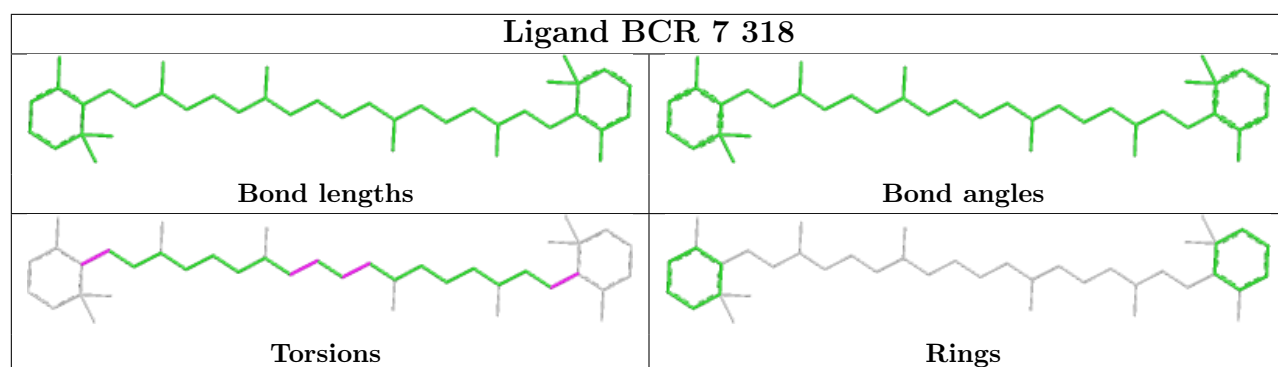
Ligand CLA 9 604



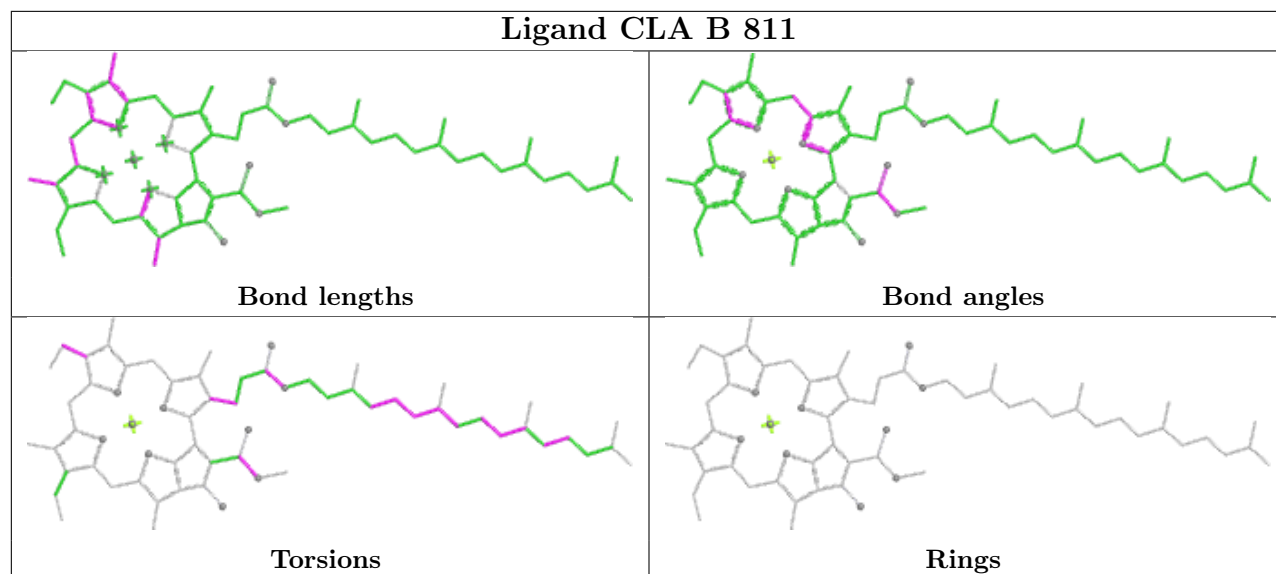
Ligand DGD B 850



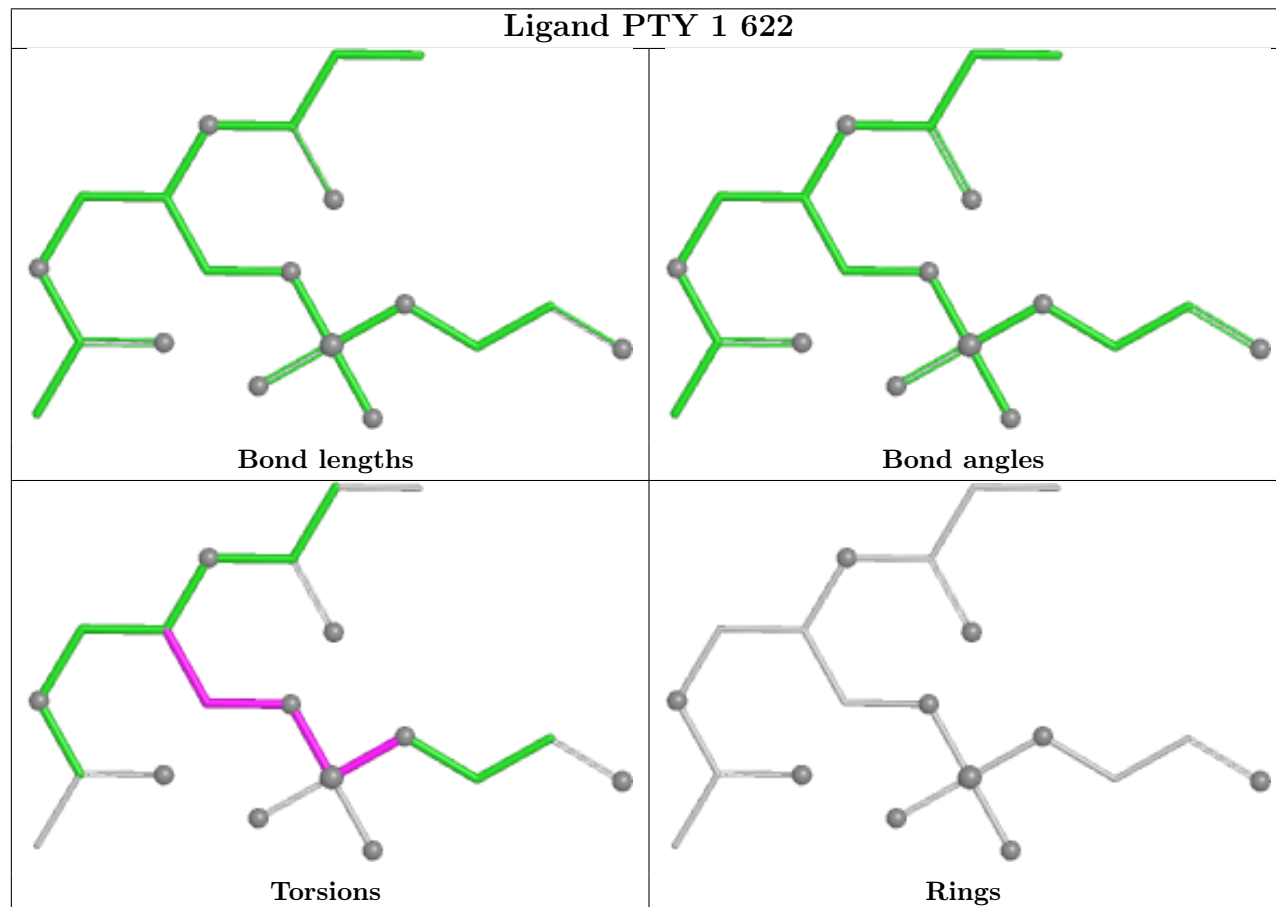




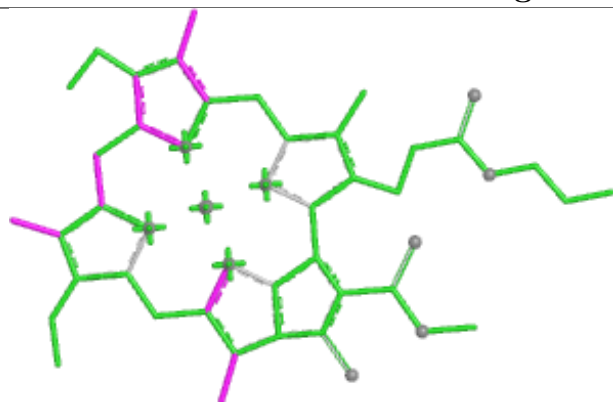
Ligand CLA B 811



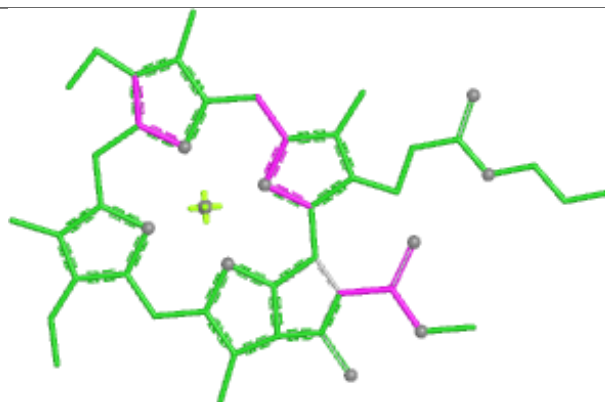
Ligand PTY 1 622



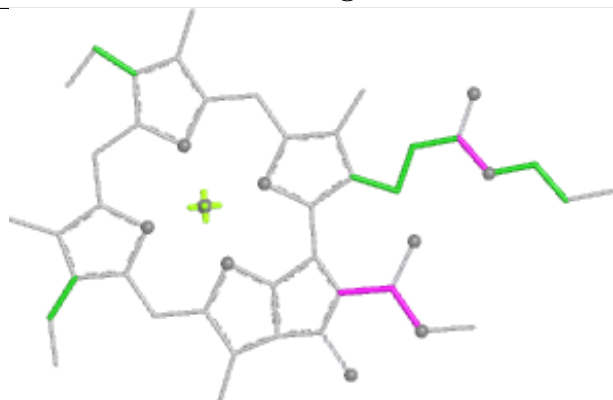
Ligand CLA B 805



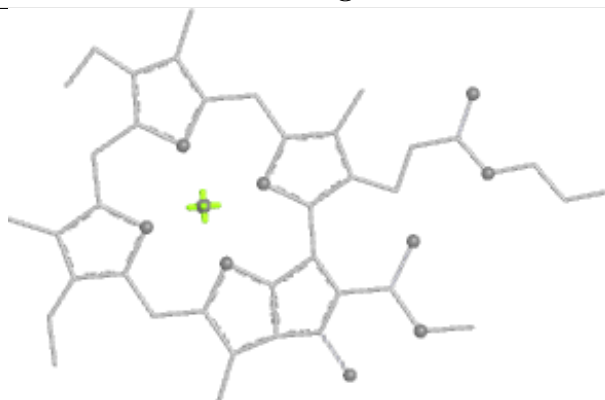
Bond lengths



Bond angles

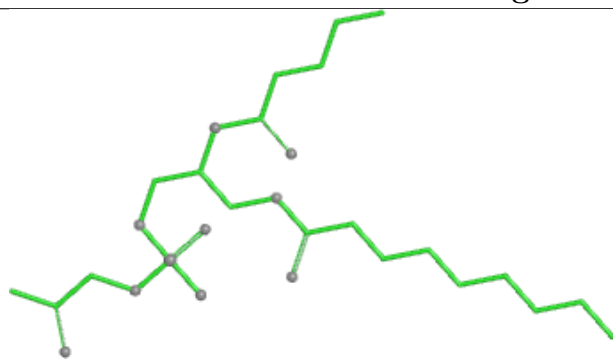


Torsions

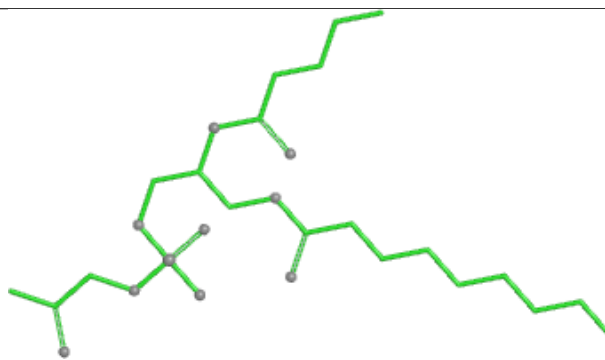


Rings

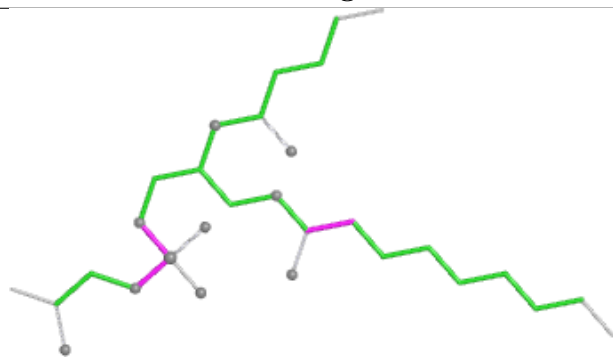
Ligand LHG A 853



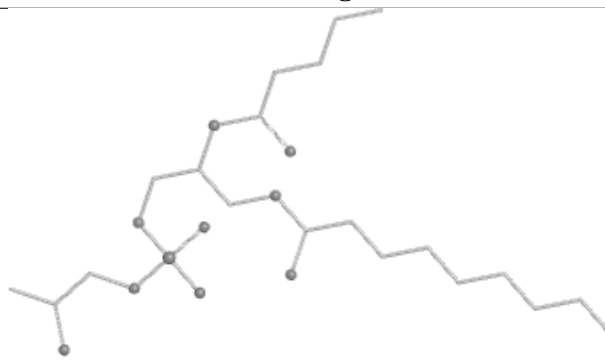
Bond lengths



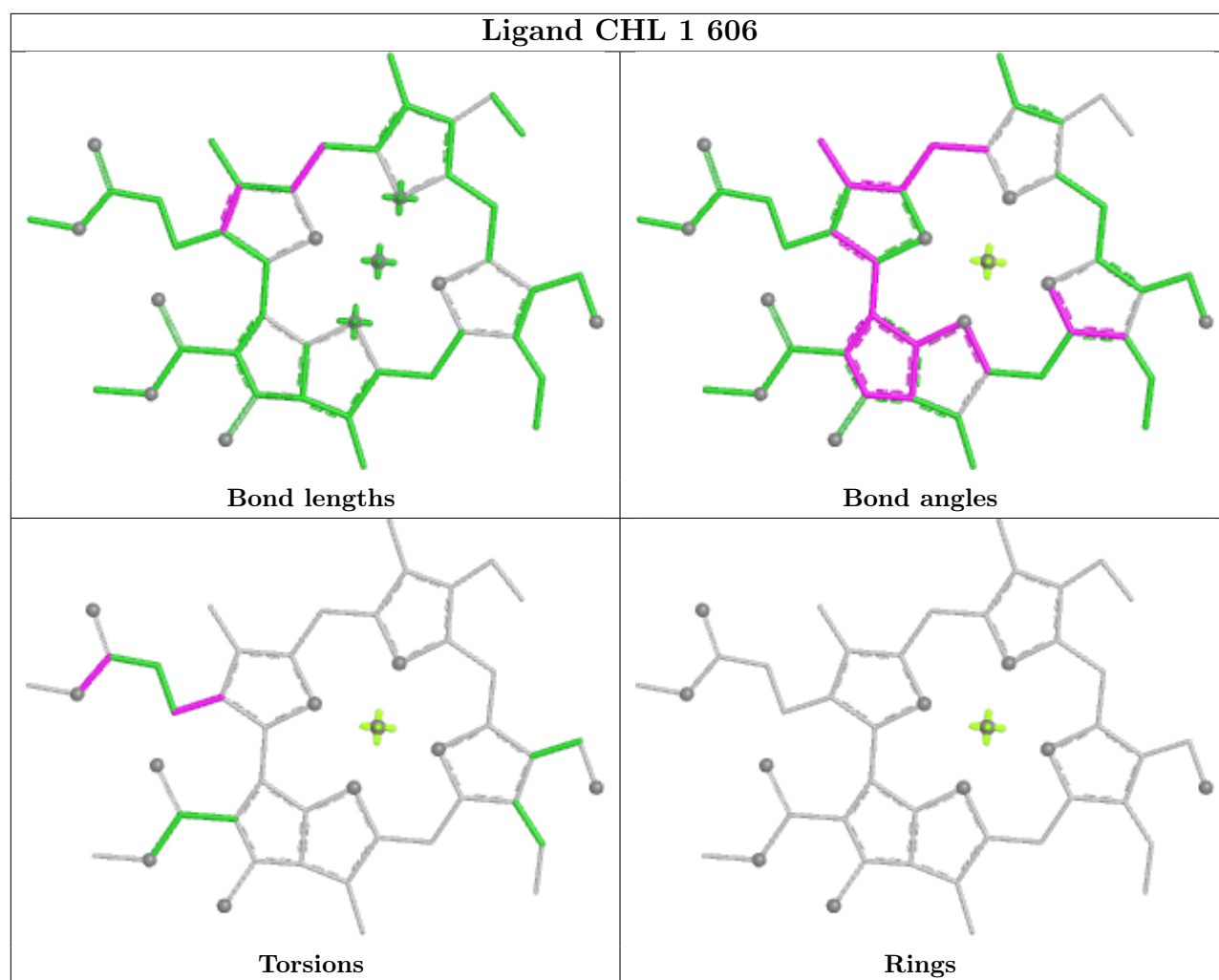
Bond angles



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.

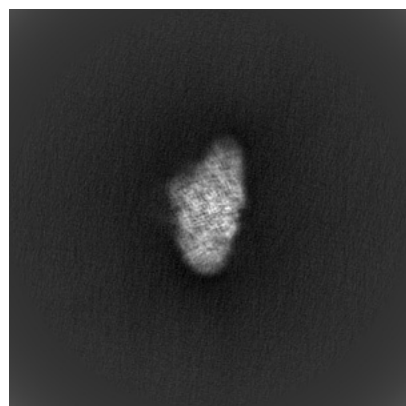
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48265. These allow visual inspection of the internal detail of the map and identification of artifacts.

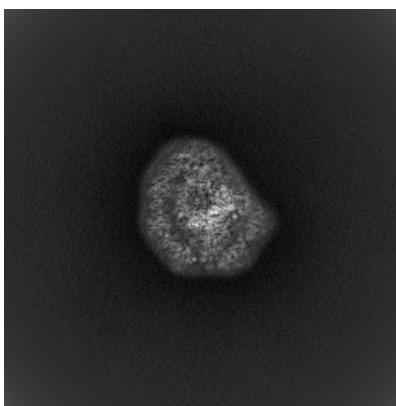
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

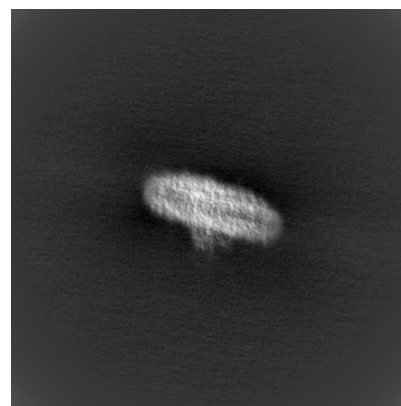
6.1.1 Primary map



X

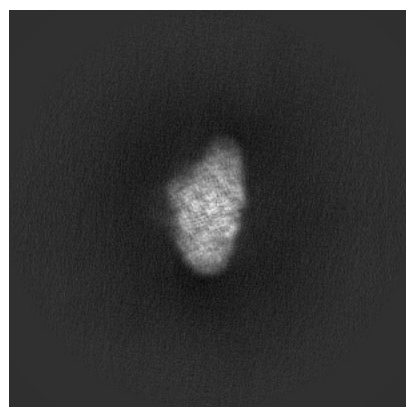


Y

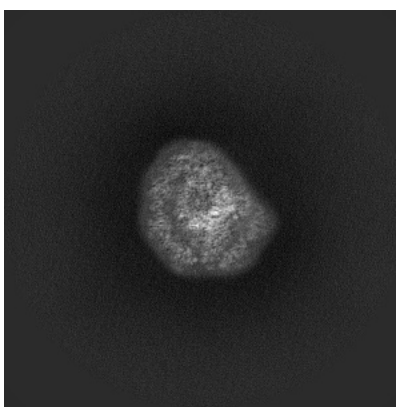


Z

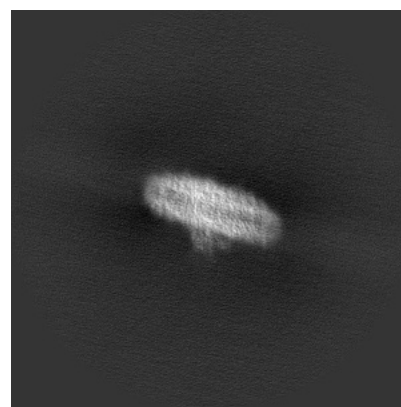
6.1.2 Raw map



X



Y

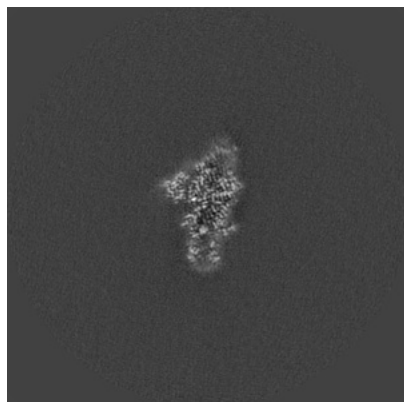


Z

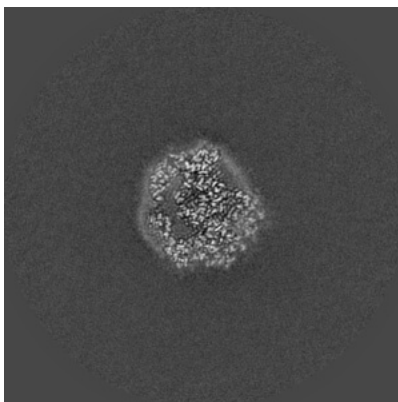
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

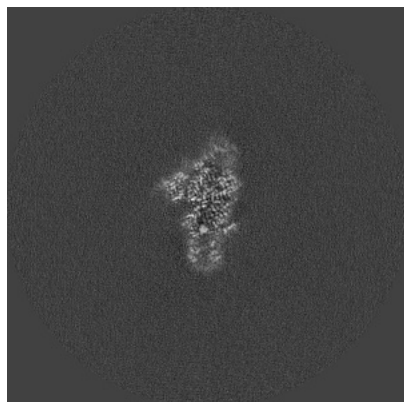


Y Index: 240

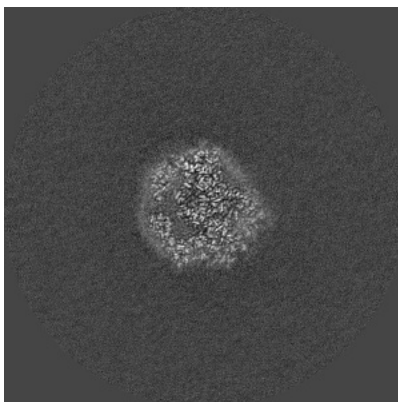


Z Index: 240

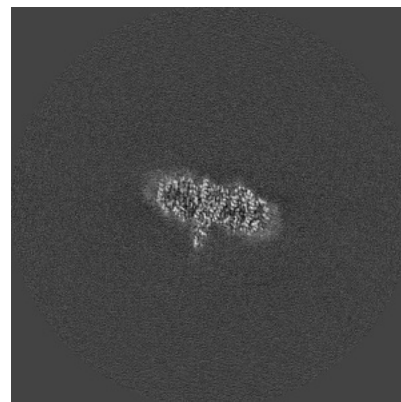
6.2.2 Raw map



X Index: 240



Y Index: 240

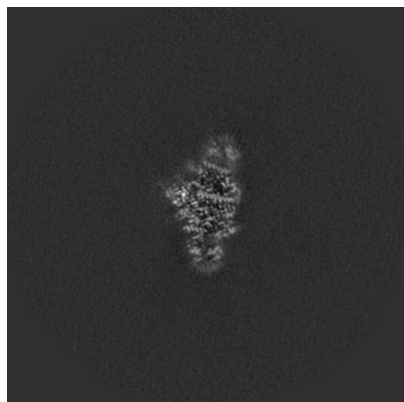


Z Index: 240

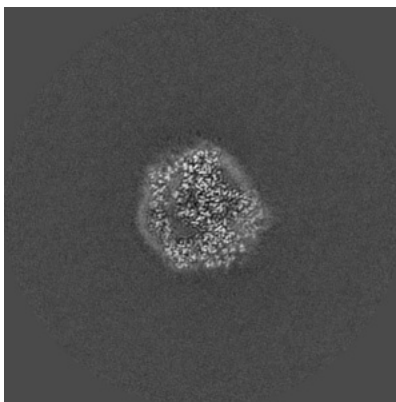
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

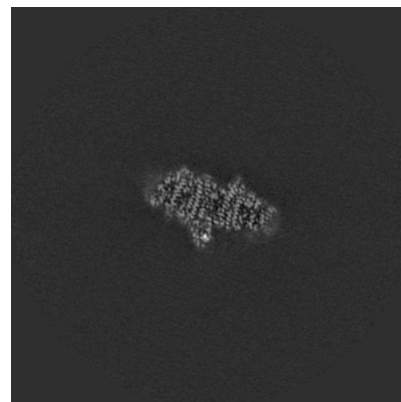
6.3.1 Primary map



X Index: 235

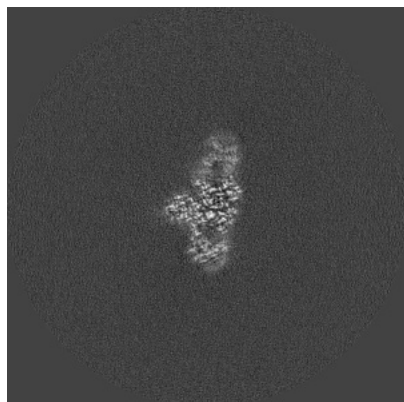


Y Index: 242

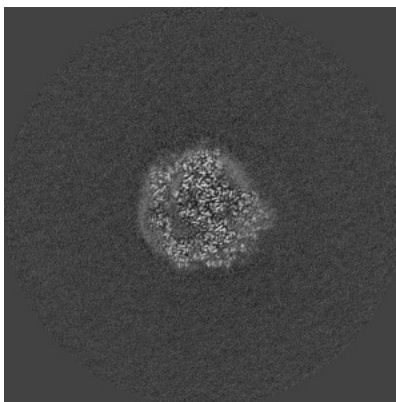


Z Index: 246

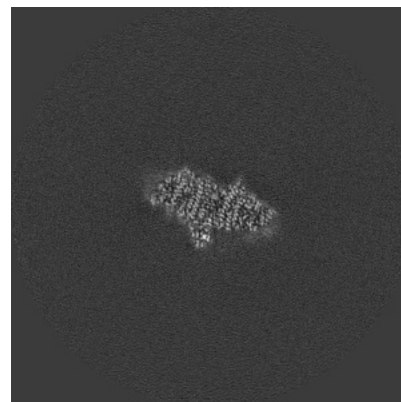
6.3.2 Raw map



X Index: 221



Y Index: 242

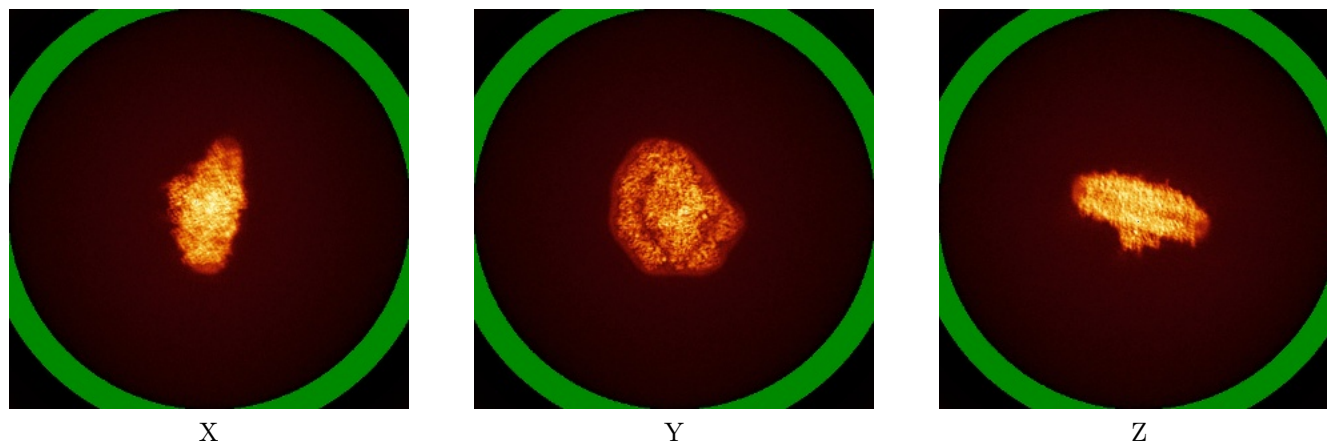


Z Index: 247

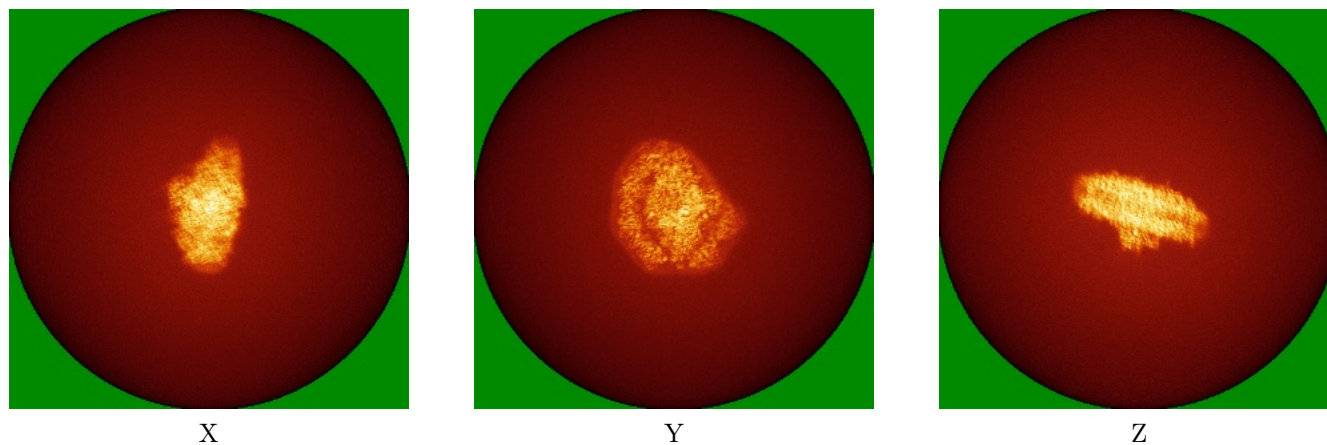
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



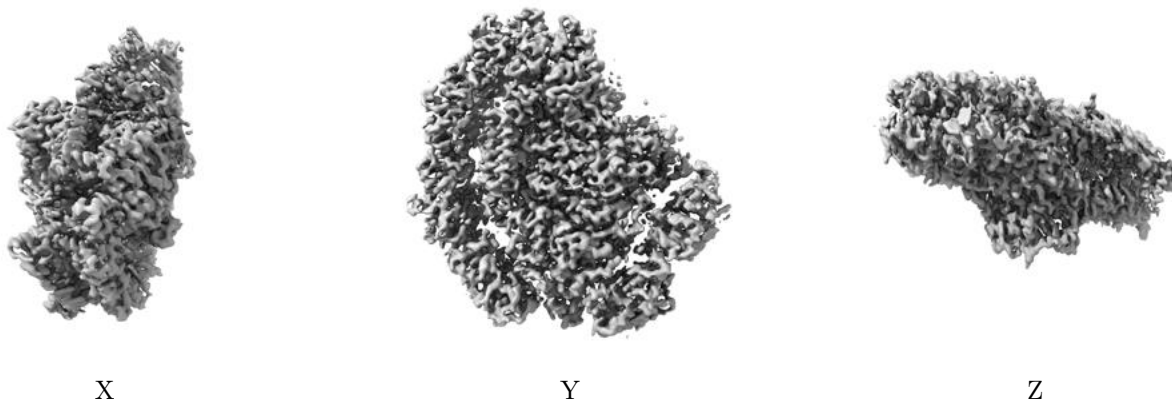
6.4.2 Raw map



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.

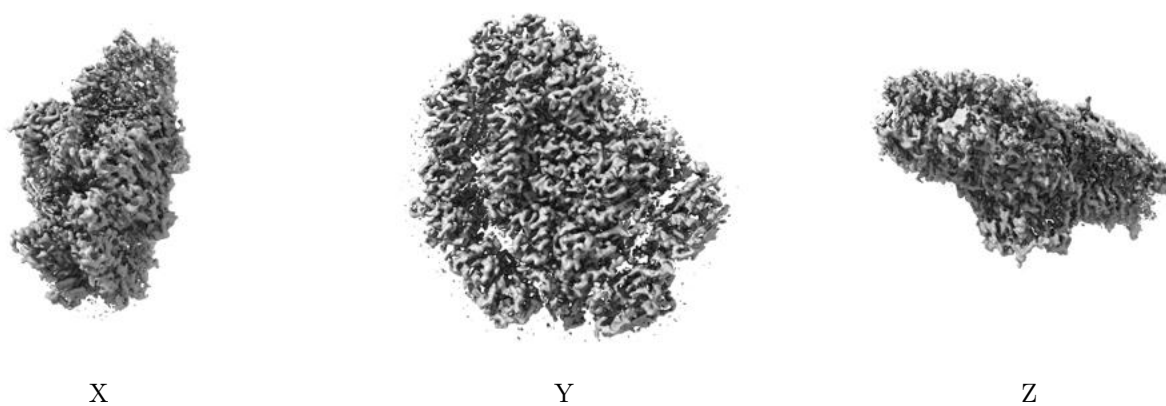
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0165. 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.

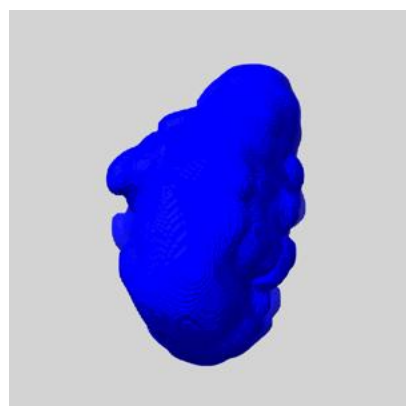
6.6 Mask visualisation [i](#)

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

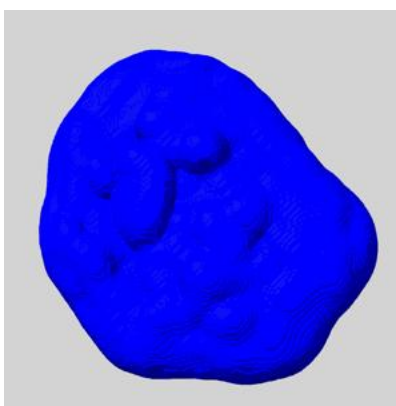
A mask typically either:

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

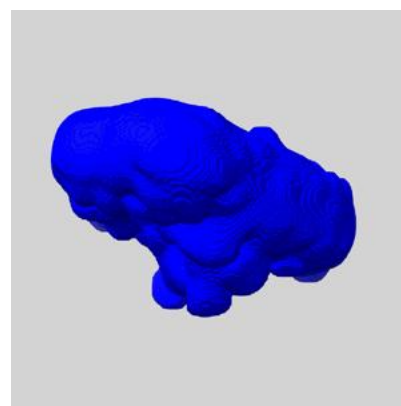
6.6.1 emd_48265_msk_1.map [i](#)



X



Y

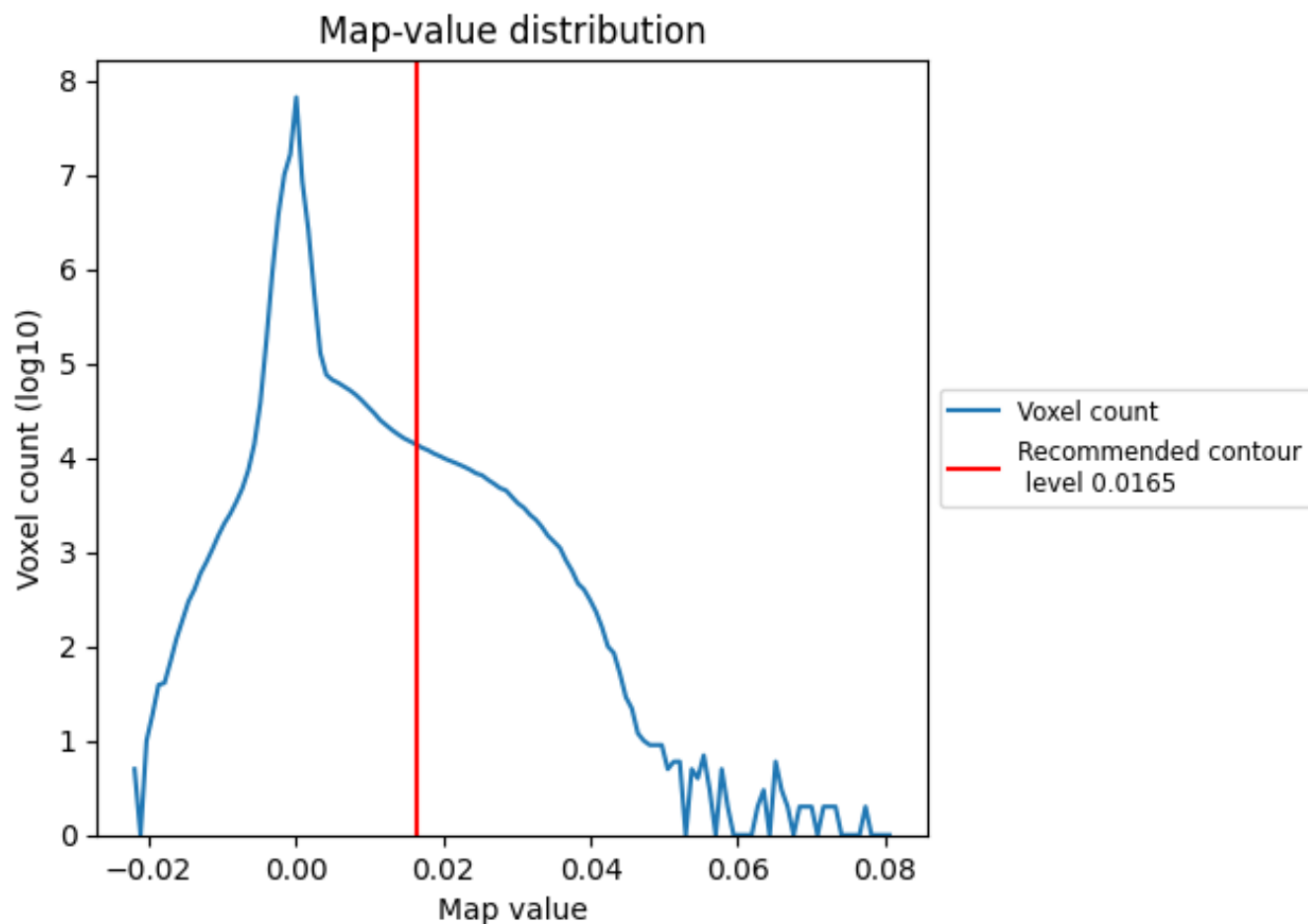


Z

7 Map analysis [i](#)

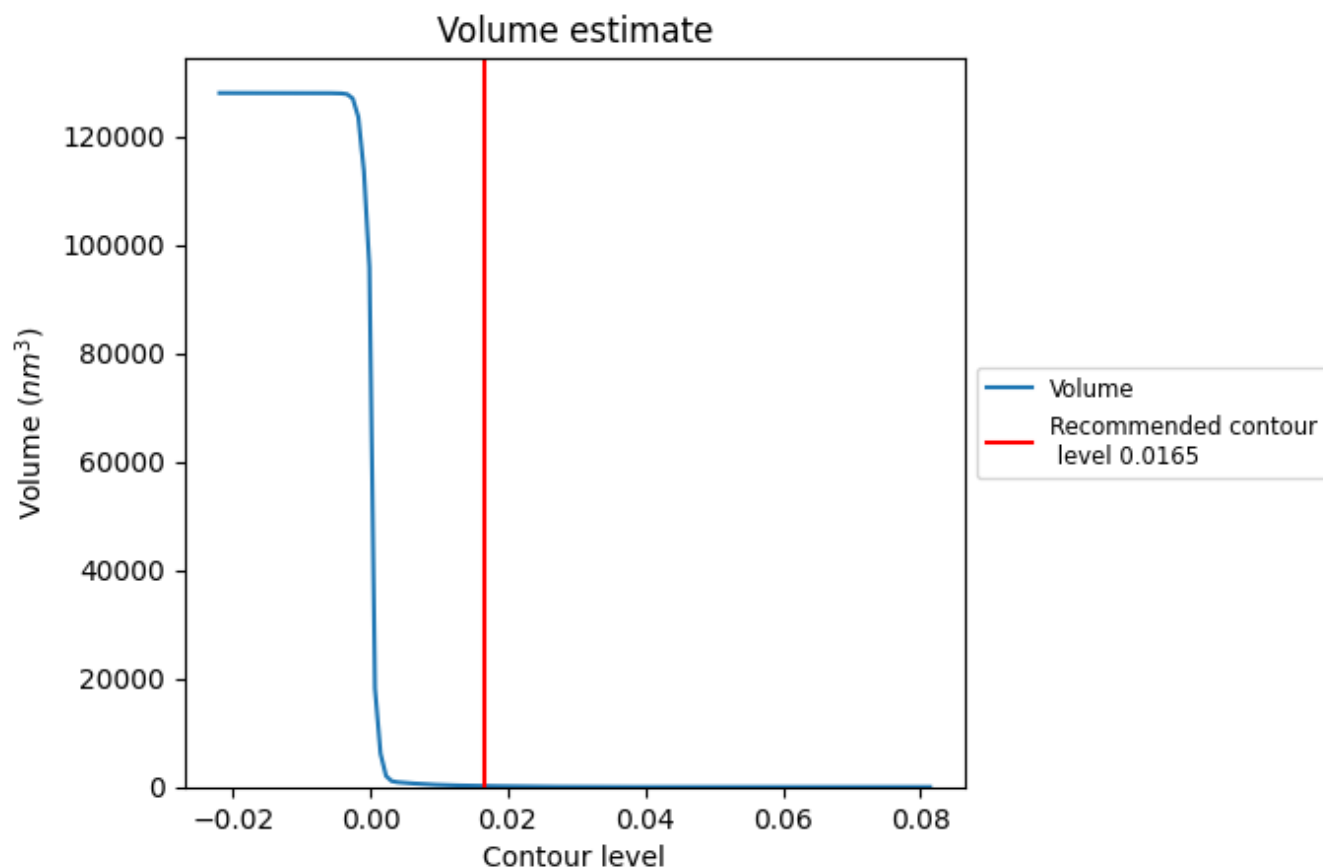
This section contains the results of statistical analysis of the map.

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.

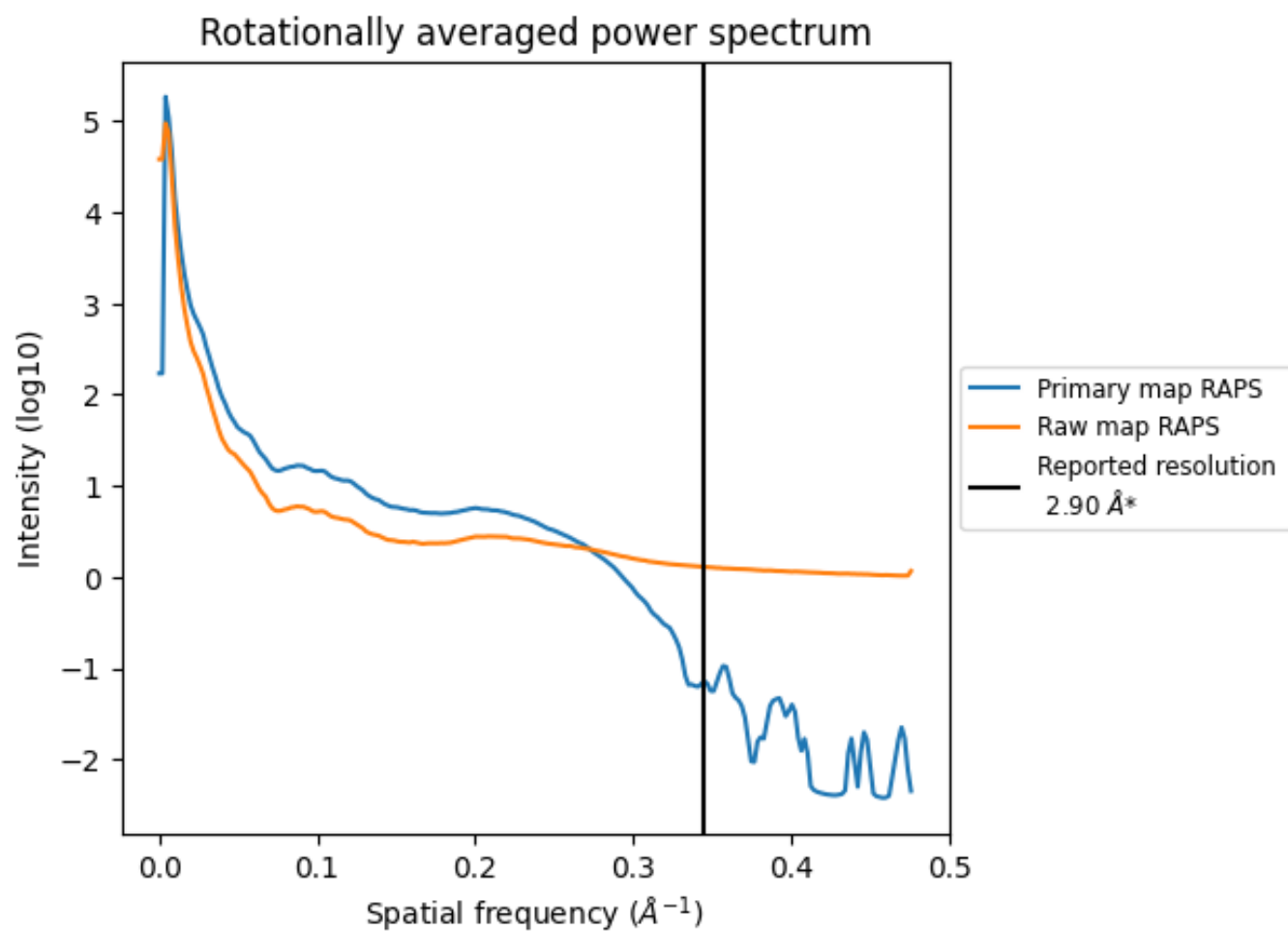
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm^3 ; this corresponds to an approximate mass of 165 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 ⓘ

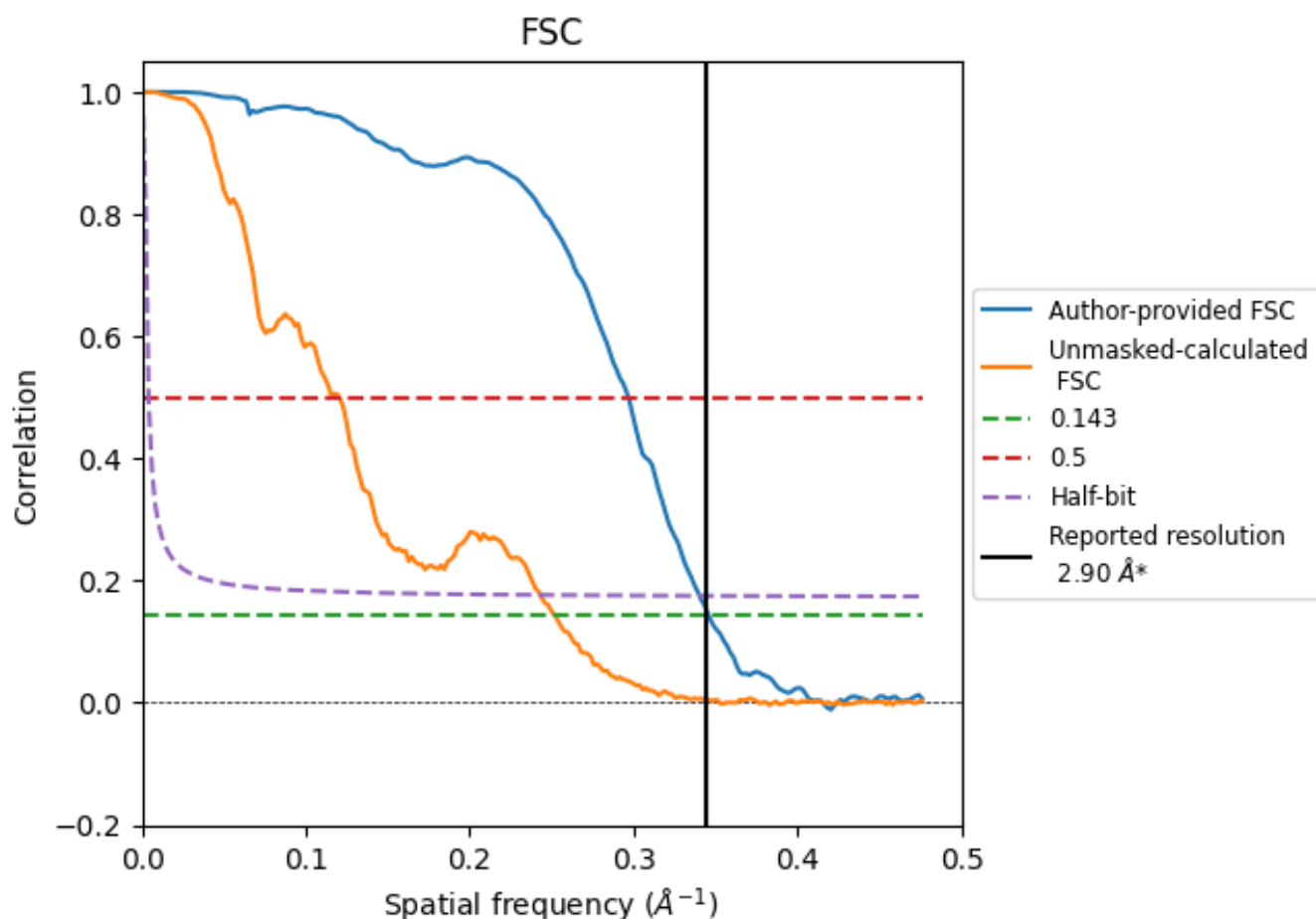


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

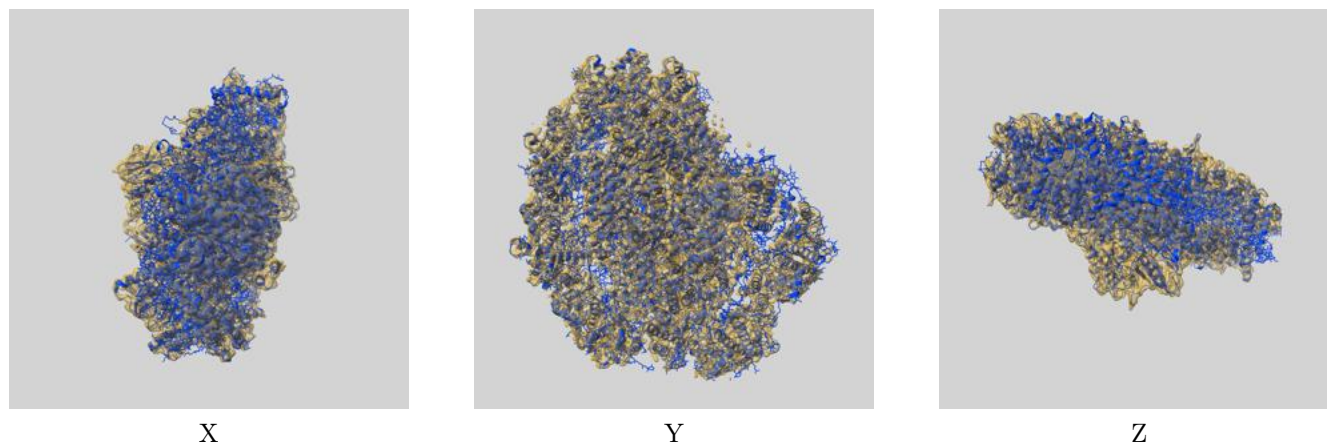
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.37	2.94
Unmasked-calculated*	3.97	8.32	4.11

*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 3.97 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

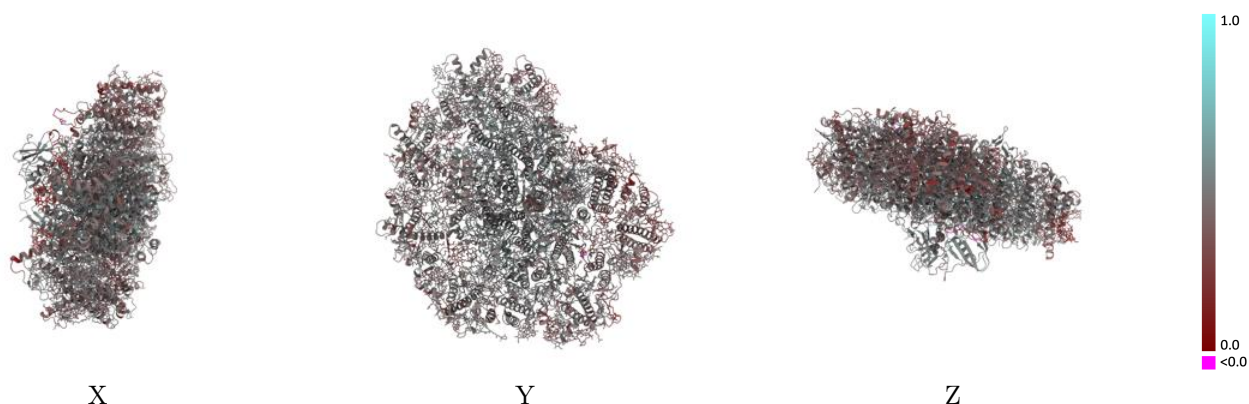
This section contains information regarding the fit between EMDB map EMD-48265 and PDB model 9MH0. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



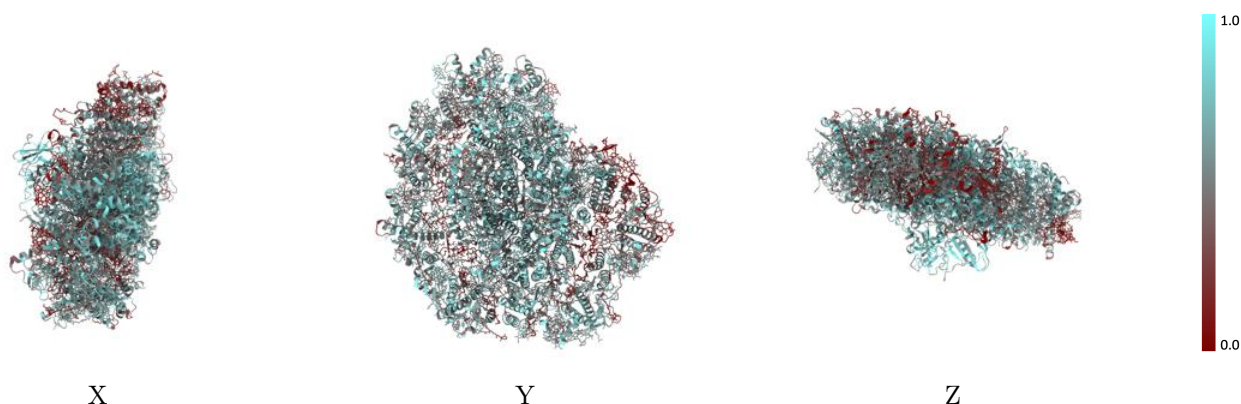
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



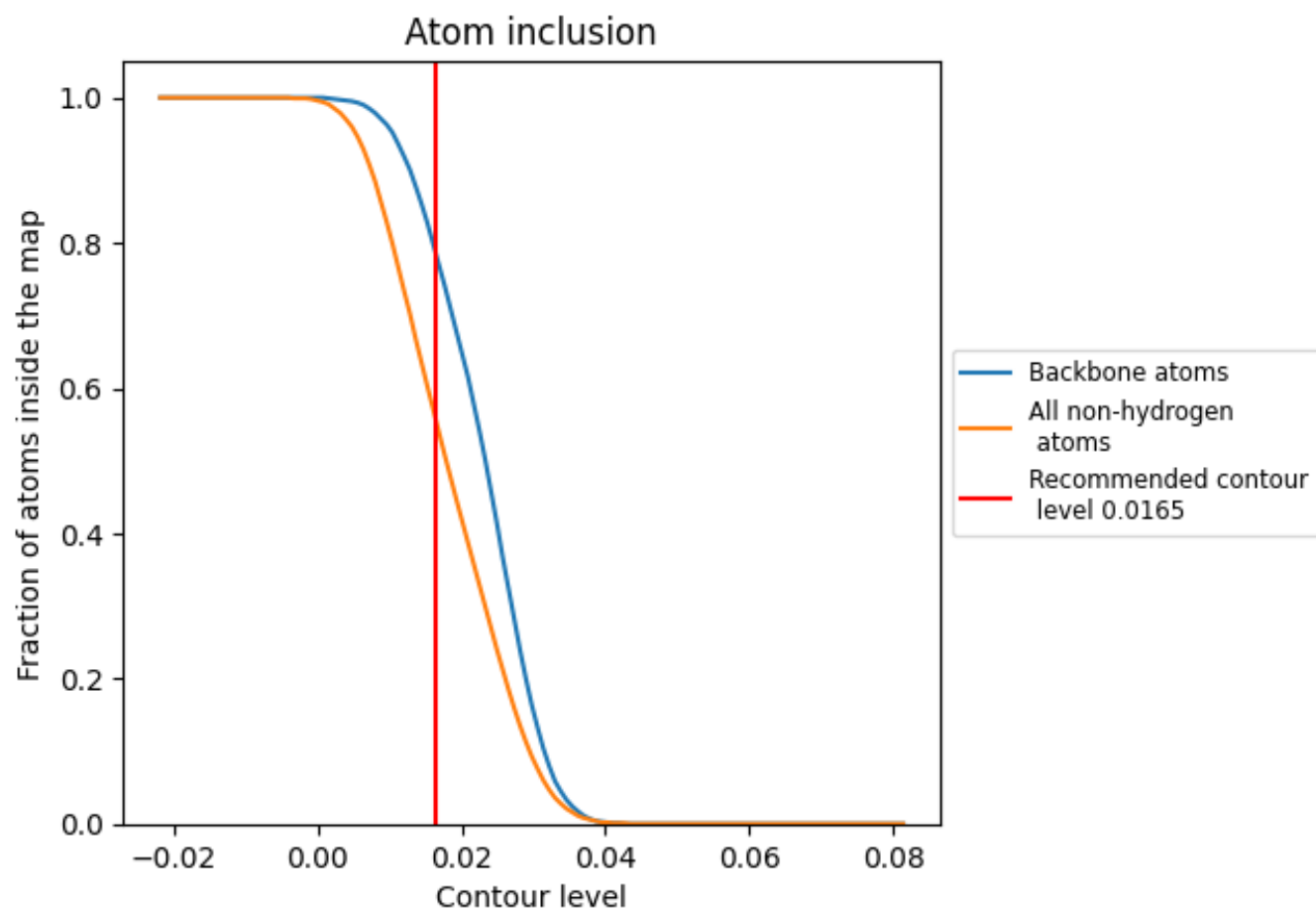
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 55% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5520	0.4360
1	0.5350	0.4200
2	0.3820	0.3660
3	0.5090	0.4240
7	0.5390	0.4240
8	0.5410	0.4220
9	0.5120	0.3960
A	0.6160	0.4740
B	0.6130	0.4740
C	0.7690	0.4800
D	0.7210	0.4760
E	0.6830	0.4800
F	0.5400	0.4330
G	0.5270	0.4380
H	0.2550	0.3310
I	0.4580	0.3700
J	0.4670	0.4080
K	0.3270	0.3070
L	0.4200	0.3670

