



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:11 PM UTC

PDB ID : 9GBI / pdb\_00009gbi  
EMDB ID : EMD-51219  
Title : Cryo-EM structure of Arabidopsis thaliana PSI-LHCI wild-type  
Authors : Capaldi, S.; Chaves-Sanjuan, A.; Bonnet, D.M.V.; Bassi, R.  
Deposited on : 2024-07-31  
Resolution : 3.13 Å(reported)  
Based on initial model : 7DKZ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

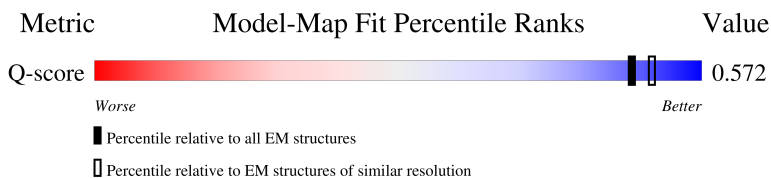
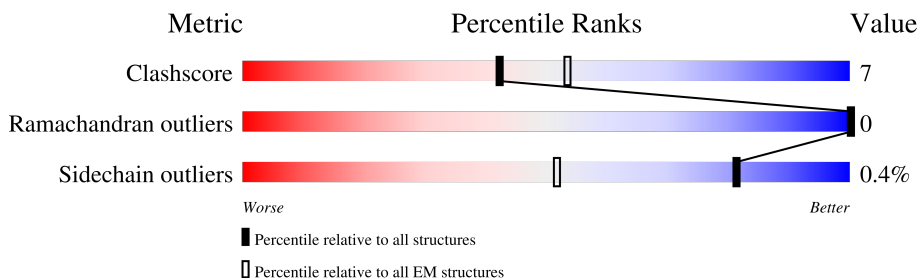
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 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.





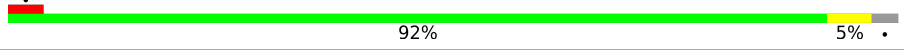
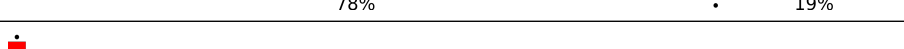

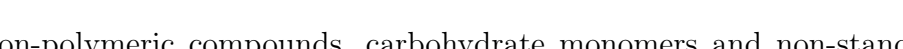

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 ( 2.63 - 3.63 )

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

Mol	Chain	Length	Quality of chain
1	1	206	 83% 11% 6%
2	2	214	 82% 13% 5%
3	3	234	 81% 12% 6%
4	4	199	 82% 17% 1%

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	160	
9	E	99	
10	F	154	
11	G	100	
12	H	95	
13	I	37	
14	J	44	
15	L	169	
16	K	84	
17	N	85	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CHL	1	301	X	-	-	-
18	CHL	1	306	X	-	-	-
18	CHL	2	301	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	307	X	-	-	-
18	CHL	2	314	X	-	-	-
18	CHL	3	307	X	-	-	-
18	CHL	4	304	X	-	-	-
18	CHL	4	305	X	-	-	-
18	CHL	4	306	X	-	-	-
18	CHL	4	314	X	-	-	-
19	CLA	1	302	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	305	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	1	321	X	-	-	-
19	CLA	2	302	X	-	-	-
19	CLA	2	303	X	-	-	-
19	CLA	2	304	X	-	-	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-
19	CLA	2	313	X	-	-	-
19	CLA	2	320	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	302	X	-	-	-
19	CLA	3	303	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	306	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	4	301	X	-	-	-
19	CLA	4	302	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	313	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	851	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	852	X	-	-	-
19	CLA	A	853	X	-	-	-
19	CLA	A	854	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	F	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	F	302	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	F	304	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	H	201	X	-	-	-
19	CLA	J	102	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	302	X	-	-	-
19	CLA	L	303	X	-	-	-

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 36064 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 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1501	978	249	269	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1582	1036	258	284	4		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	219	Total	C	N	O	S	0	0
			1678	1100	269	304	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5834	3821	991	1004	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5852	3840	1000	999	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			509	326	89	94		

- Molecule 10 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	152	Total	C	N	O	S	0	0
			1208	789	207	209	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	97	Total	C	N	O	0	0
			759	493	124	142		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	90	Total	C	N	O	0	0
			692	452	111	129		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			230	156	37	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	42	Total	C	N	O	S	0	0
			339	233	51	54	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	144	Total	C	N	O	S	0	0
			1076	710	172	192	2		

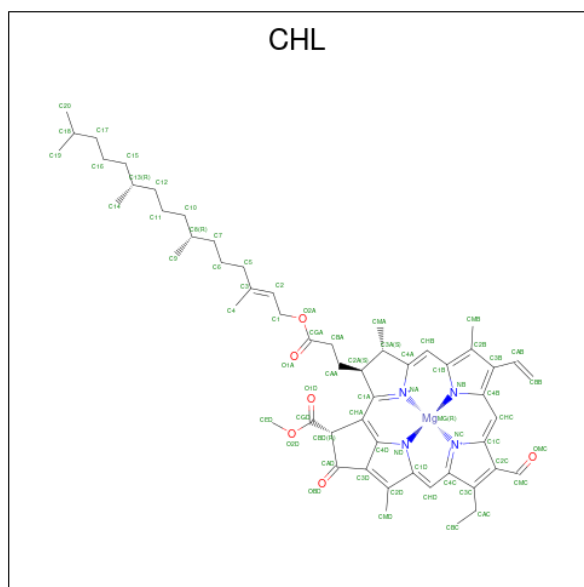
- Molecule 16 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	55	Total	C	N	O	S	0	0
			382	245	63	71	3		

- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	48	Total	C	N	O	S	0	0
			381	239	67	73	2		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



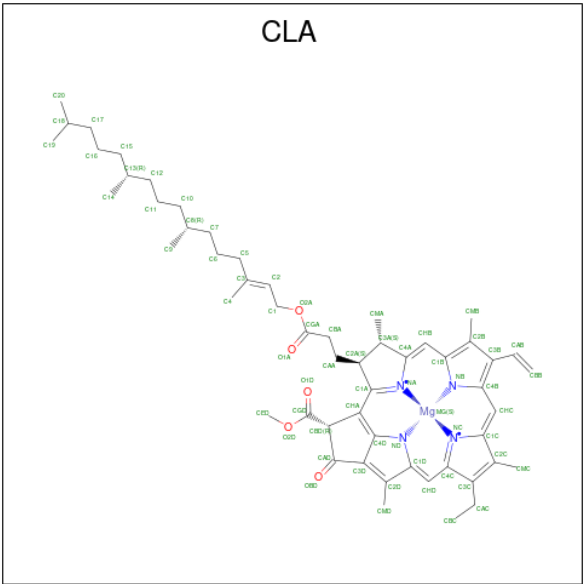
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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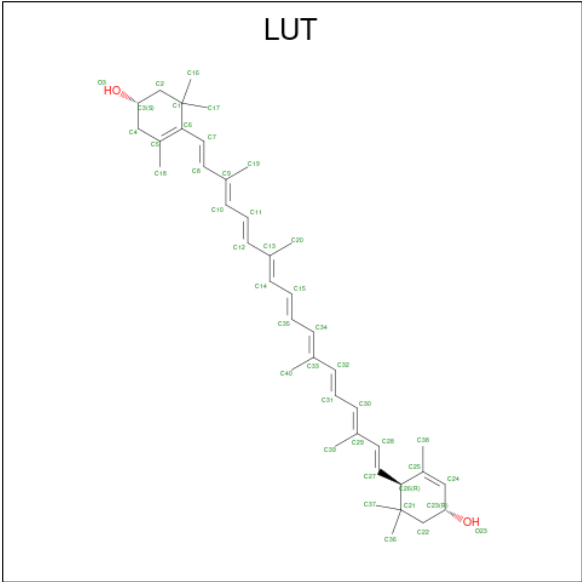
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total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

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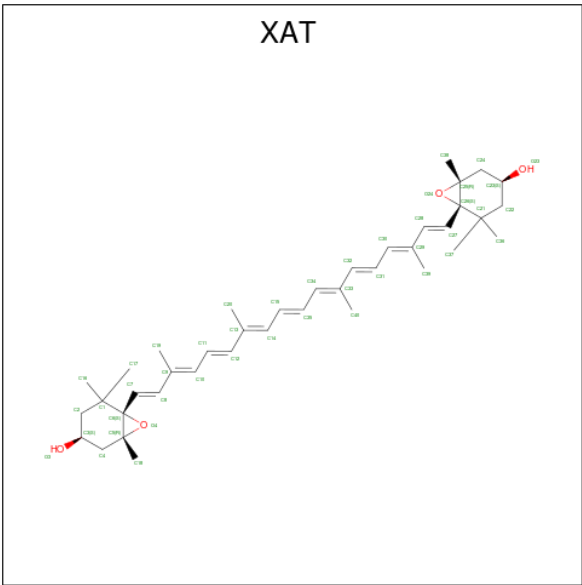
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	

- Molecule 20 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



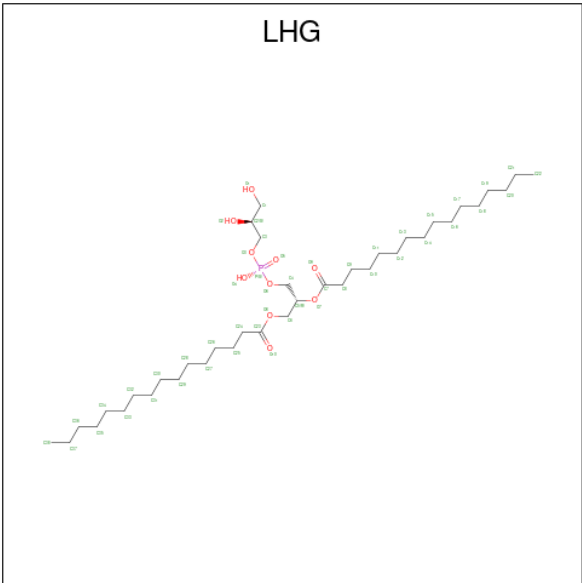
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			42	40	2	
20	1	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	4	1	Total	C	O	0
			42	40	2	

- Molecule 21 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

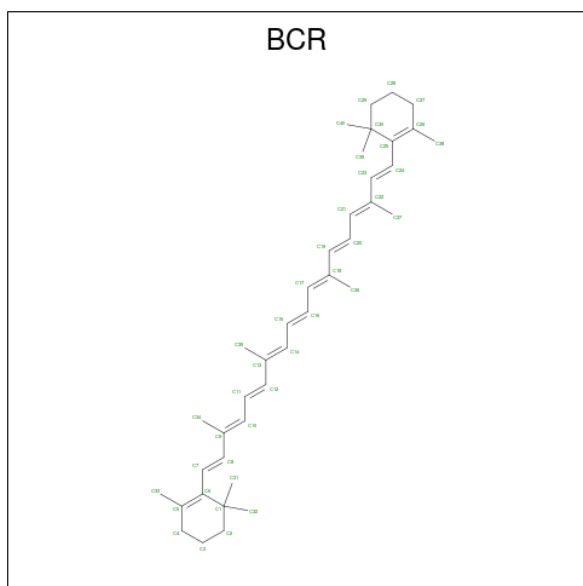
- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	2	1	Total	C	O	P	0
			37	26	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			45	34	10	1	

- 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	2	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	

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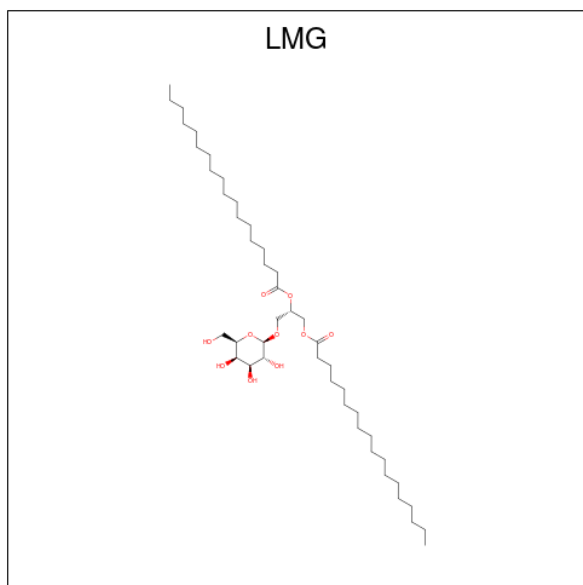
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 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	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

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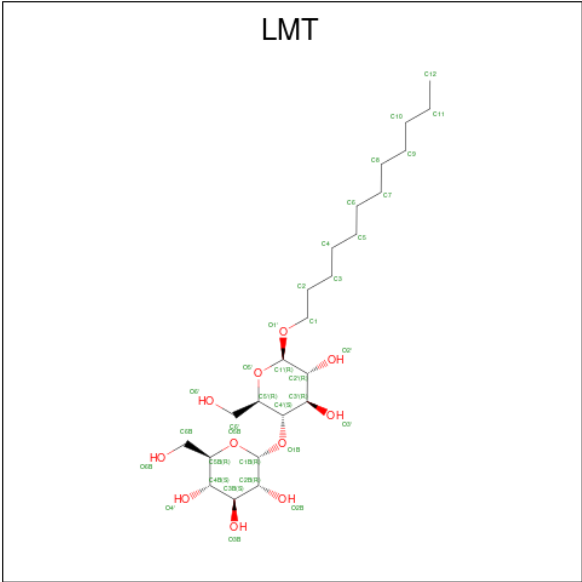
Mol	Chain	Residues	Atoms		AltConf
23	K	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



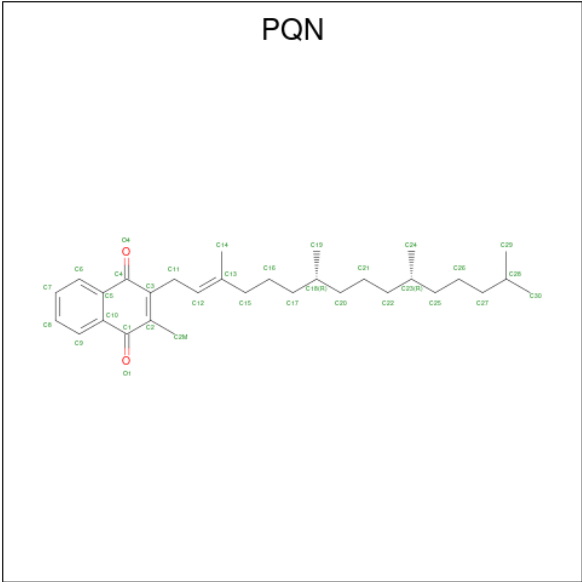
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			50	40	10	
24	4	1	Total	C	O	0
			36	26	10	
24	B	1	Total	C	O	0
			52	42	10	
24	F	1	Total	C	O	0
			30	20	10	

- Molecule 25 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



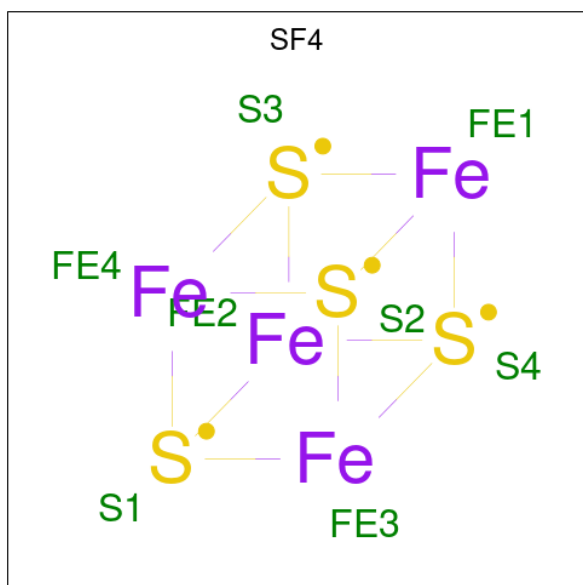
Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			35	24	11	
25	G	1	Total	C	O	0
			35	24	11	
25	N	1	Total	C	O	0
			35	24	11	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



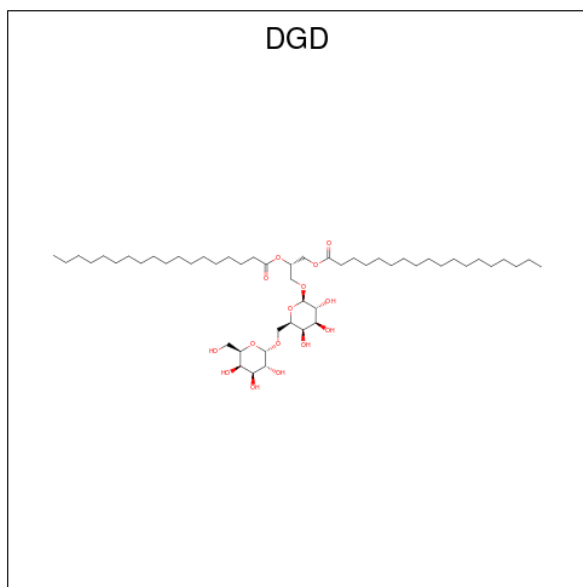
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ) (labeled as "Ligand of Interest" by depositor).

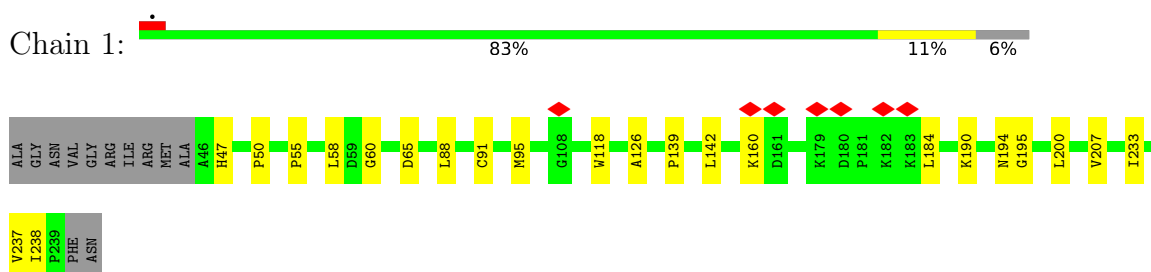


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B	1	66	51	15	0

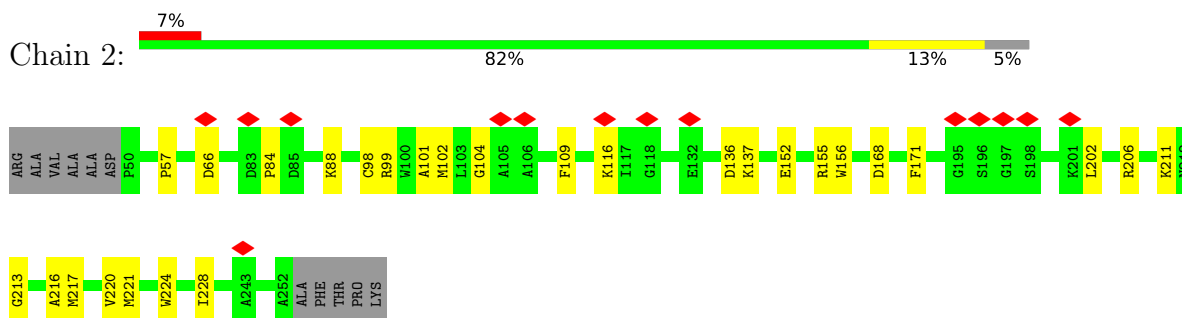
### 3 Residue-property plots [i](#)

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

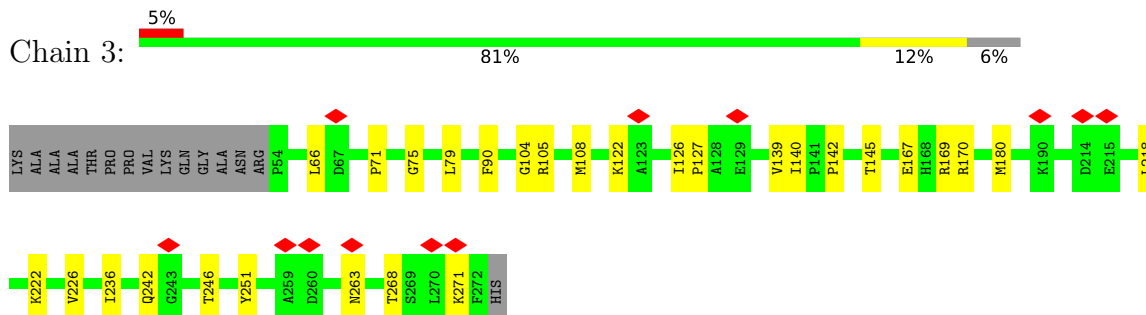
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



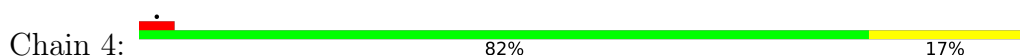
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

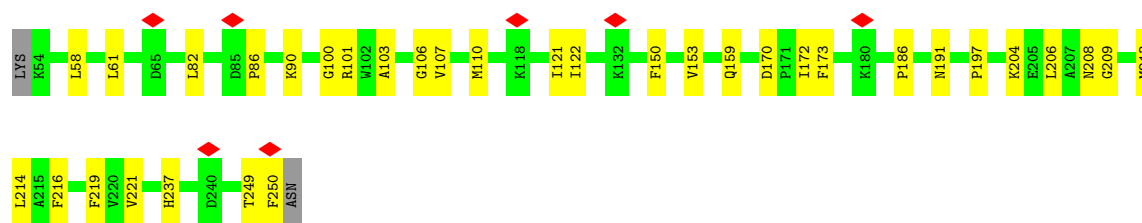


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



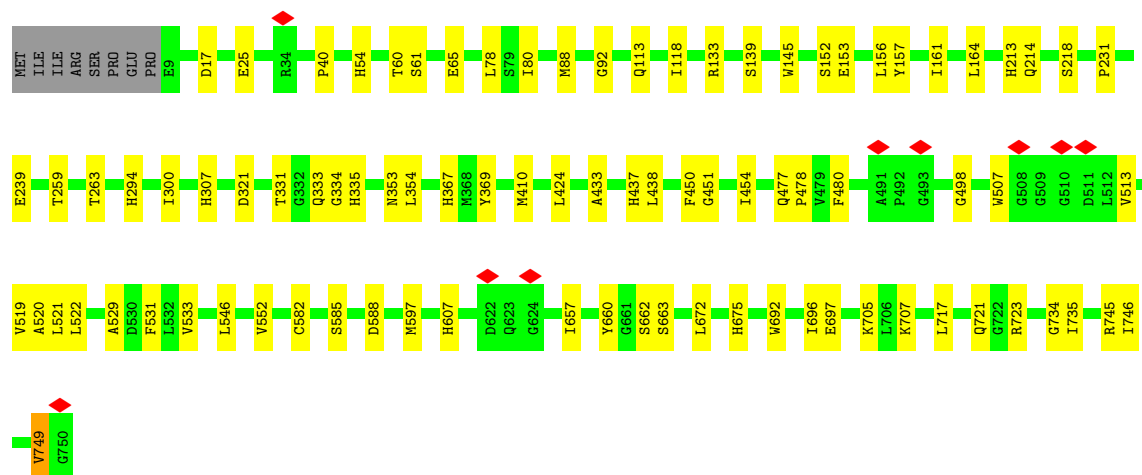
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic





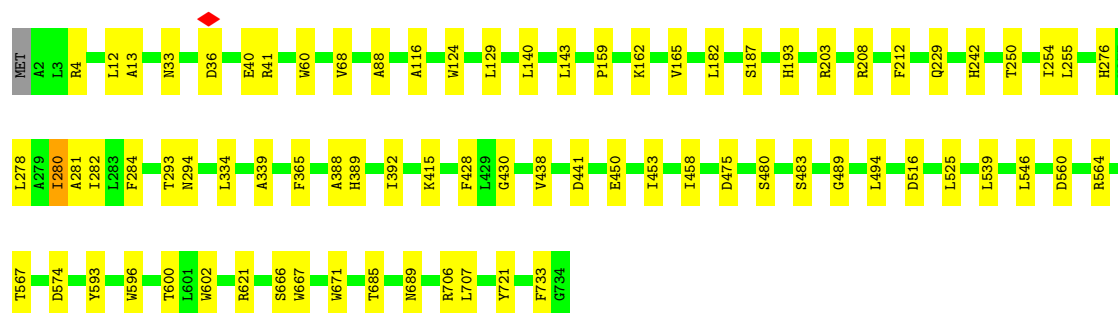
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 87% 12%



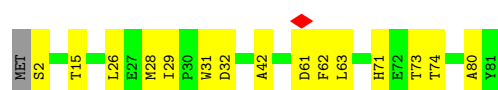
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 89% 10%



- Molecule 7: Photosystem I iron-sulfur center

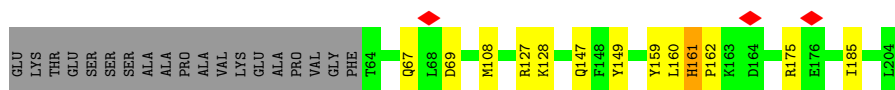
Chain C: 80% 19%



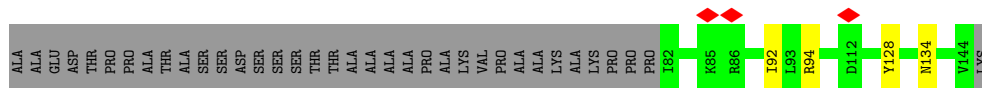
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D: 80% 8% 12%

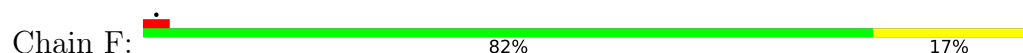




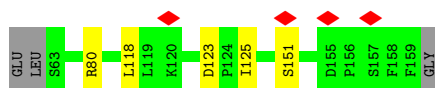
- Molecule 9: Photosystem I reaction center subunit IV B, chloroplastic



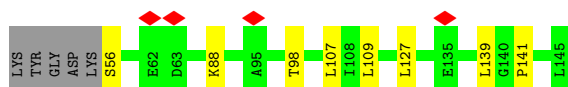
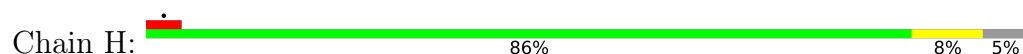
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



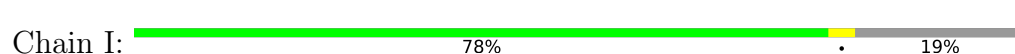
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



- Molecule 12: Photosystem I reaction center subunit VI-1, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII

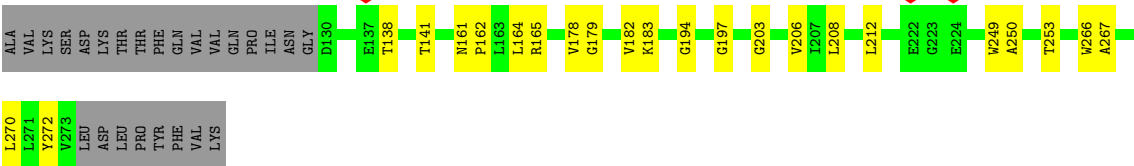


- Molecule 14: Photosystem I reaction center subunit IX



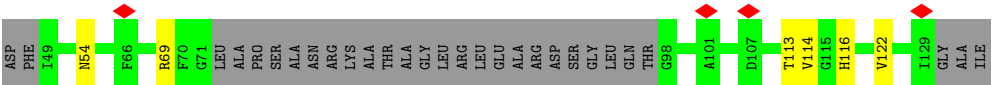
- Molecule 15: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 



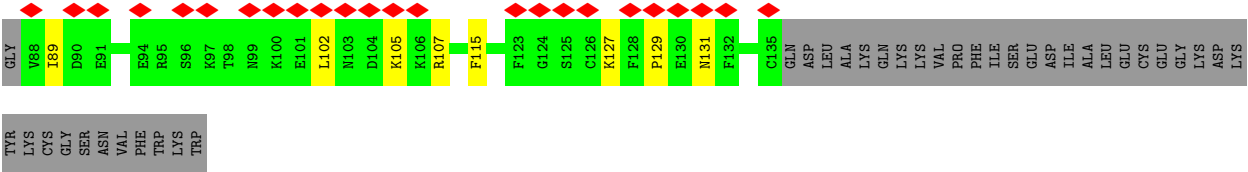
• Molecule 16: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 



• Molecule 17: Photosystem I reaction center subunit N, chloroplastic

Chain N: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.854	Depositor
Minimum map value	-1.833	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	398.272, 398.272, 398.272	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.889, 0.889, 0.889	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, SF4, XAT, PQN, LMG, LMT, CHL, CLA, LUT, LHG, 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	0.11	0/1551	0.28	0/2117
2	2	0.11	0/1639	0.25	0/2242
3	3	0.12	0/1730	0.26	0/2352
4	4	0.10	0/1611	0.31	0/2194
5	A	0.11	0/6031	0.24	0/8226
6	B	0.12	0/6063	0.27	0/8281
7	C	0.10	0/628	0.29	0/852
8	D	0.11	0/1140	0.28	0/1542
9	E	0.08	0/519	0.24	0/703
10	F	0.11	0/1238	0.26	0/1670
11	G	0.09	0/779	0.25	0/1056
12	H	0.10	0/712	0.27	0/968
13	I	0.11	0/236	0.26	0/322
14	J	0.10	0/349	0.24	0/476
15	L	0.12	0/1108	0.26	0/1512
16	K	0.08	0/385	0.19	0/520
17	N	0.10	0/387	0.31	0/517
All	All	0.11	0/26106	0.26	0/35550

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
8	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	161	HIS	Peptide

## 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	1501	0	1476	18	0
2	2	1582	0	1533	21	0
3	3	1678	0	1646	19	0
4	4	1562	0	1517	26	0
5	A	5834	0	5683	67	0
6	B	5852	0	5639	60	0
7	C	615	0	592	10	0
8	D	1112	0	1122	10	0
9	E	509	0	518	4	0
10	F	1208	0	1241	23	0
11	G	759	0	735	4	0
12	H	692	0	693	7	0
13	I	230	0	245	1	0
14	J	339	0	357	9	0
15	L	1076	0	1081	16	0
16	K	382	0	399	6	0
17	N	381	0	370	5	0
18	1	102	0	78	3	0
18	2	229	0	157	3	0
18	3	47	0	31	2	0
18	4	195	0	141	4	0
19	1	684	0	602	17	0
19	2	537	0	491	12	0
19	3	646	0	538	9	0
19	4	546	0	497	12	0
19	A	2599	0	2608	73	0
19	B	2262	0	2271	50	0
19	F	219	0	206	4	0
19	G	137	0	101	1	0
19	H	45	0	28	2	0
19	J	42	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	128	0	91	4	0
19	L	170	0	157	7	0
20	1	84	0	112	8	0
20	2	42	0	56	3	0
20	3	42	0	56	2	0
20	4	42	0	56	5	0
21	1	44	0	56	1	0
21	2	44	0	56	2	0
21	3	44	0	56	1	0
21	4	44	0	56	2	0
22	1	98	0	148	6	0
22	2	37	0	44	1	0
22	A	49	0	74	0	0
22	B	45	0	63	3	0
23	1	40	0	56	2	0
23	2	40	0	56	3	0
23	3	40	0	56	1	0
23	4	40	0	56	2	0
23	A	280	0	392	27	0
23	B	240	0	336	11	0
23	F	80	0	112	6	0
23	G	40	0	56	2	0
23	I	40	0	56	1	0
23	J	120	0	168	12	0
23	K	40	0	56	2	0
23	L	120	0	168	10	0
24	1	50	0	70	3	0
24	4	36	0	42	0	0
24	B	52	0	77	1	0
24	F	30	0	30	1	0
25	2	35	0	46	5	0
25	G	35	0	46	0	0
25	N	35	0	46	2	0
26	A	33	0	46	0	0
26	B	33	0	46	1	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	B	66	0	96	4	0
All	All	36064	0	35821	479	0

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

All (479) 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)
19:1:305:CLA:HBB1	18:1:306:CHL:HMC	1.60	0.84
7:C:61:ASP:HB3	9:E:134:ASN:HD21	1.44	0.82
4:4:121:ILE:HG22	4:4:122:ILE:HG12	1.62	0.81
20:1:315:LUT:H8	20:1:315:LUT:H171	1.64	0.80
20:2:315:LUT:H171	20:2:315:LUT:H8	1.64	0.80
17:N:127:LYS:HG3	17:N:129:PRO:HD2	1.67	0.77
23:L:305:BCR:H21C	23:L:305:BCR:H361	1.69	0.74
2:2:221:MET:HG2	21:2:316:XAT:H35	1.68	0.74
10:F:75:CYS:SG	10:F:130:CYS:N	2.61	0.73
19:A:827:CLA:H203	23:J:103:BCR:H17C	1.74	0.70
6:B:453:ILE:HD13	23:J:101:BCR:H20C	1.74	0.70
17:N:127:LYS:O	17:N:131:ASN:ND2	2.25	0.69
3:3:236:ILE:HG21	21:3:316:XAT:H12	1.76	0.68
20:1:320:LUT:H28	19:4:313:CLA:HBC3	1.75	0.67
19:F:302:CLA:HBD	19:F:302:CLA:HBA1	1.75	0.67
20:1:320:LUT:H171	20:1:320:LUT:H8	1.75	0.66
1:1:55:PRO:HG2	1:1:58:LEU:HD12	1.77	0.66
5:A:745:ARG:HH11	5:A:749:VAL:HG11	1.61	0.66
2:2:202:LEU:HD22	2:2:206:ARG:HE	1.61	0.65
3:3:167:GLU:OE1	3:3:170:ARG:NH2	2.26	0.65
5:A:353:ASN:ND2	19:A:804:CLA:OBD	2.28	0.64
23:A:844:BCR:H352	23:A:844:BCR:H10C	1.80	0.64
23:B:840:BCR:H362	23:G:205:BCR:H312	1.80	0.64
18:4:305:CHL:HBB1	21:4:316:XAT:H161	1.79	0.63
6:B:546:LEU:O	6:B:564:ARG:NH1	2.31	0.63
23:A:843:BCR:H10C	23:A:843:BCR:H352	1.81	0.63
6:B:339:ALA:HB2	23:B:844:BCR:H372	1.80	0.63
5:A:588:ASP:OD1	5:A:723:ARG:NH1	2.32	0.62
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.33	0.62
2:2:104:GLY:HA2	21:2:316:XAT:H181	1.81	0.62
19:A:806:CLA:OBD	25:N:201:LMT:O2B	2.17	0.62
5:A:531:PHE:HA	19:A:836:CLA:HED1	1.81	0.62
19:A:832:CLA:H152	19:L:302:CLA:HMB3	1.81	0.62
4:4:58:LEU:HD23	4:4:61:LEU:HB2	1.82	0.62
7:C:2:SER:N	7:C:71:HIS:O	2.32	0.62
19:A:809:CLA:HBB2	19:A:812:CLA:HMA3	1.83	0.61
19:4:302:CLA:H2	10:F:205:VAL:HG22	1.82	0.61
19:B:811:CLA:HBA2	19:B:811:CLA:H43	1.81	0.61
6:B:159:PRO:HA	6:B:162:LYS:HE3	1.82	0.61
1:1:50:PRO:O	4:4:159:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.83	0.61
23:1:318:BCR:H353	23:1:318:BCR:H10C	1.83	0.61
4:4:170:ASP:OD1	4:4:173:PHE:N	2.34	0.60
19:A:809:CLA:HBA2	19:A:812:CLA:H192	1.84	0.60
23:L:306:BCR:H10C	23:L:306:BCR:H352	1.83	0.60
6:B:182:LEU:HD13	19:B:812:CLA:HBB	1.84	0.60
6:B:203:ARG:HD3	6:B:250:THR:HB	1.84	0.60
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.67	0.59
19:A:807:CLA:HAB	23:J:103:BCR:H352	1.83	0.59
18:2:301:CHL:HHC	18:2:301:CHL:HBB1	1.85	0.59
6:B:707:LEU:HD11	28:B:846:DGD:HB81	1.85	0.59
19:B:813:CLA:C2C	23:B:842:BCR:H16C	2.33	0.58
5:A:367:HIS:ND1	19:A:817:CLA:OBD	2.32	0.58
22:B:848:LHG:H242	22:B:848:LHG:H102	1.84	0.58
6:B:458:ILE:HG21	10:F:141:ASN:HD21	1.69	0.58
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.68	0.58
19:L:302:CLA:H3A	23:L:305:BCR:H373	1.85	0.58
10:F:83:LYS:O	10:F:87:GLN:HG3	2.03	0.58
4:4:107:VAL:HG11	20:4:315:LUT:H12	1.86	0.57
6:B:721:TYR:HB2	19:B:801:CLA:HED2	1.86	0.57
4:4:106:GLY:O	4:4:110:MET:HG3	2.04	0.57
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.21	0.57
19:B:831:CLA:H51	23:F:306:BCR:H333	1.86	0.57
6:B:40:GLU:HG2	6:B:165:VAL:HG23	1.87	0.57
22:1:322:LHG:H132	19:B:821:CLA:H43	1.86	0.56
5:A:513:VAL:HG12	5:A:520:ALA:HB3	1.87	0.56
22:1:317:LHG:H162	19:4:313:CLA:HED1	1.86	0.56
23:L:305:BCR:H361	23:L:305:BCR:C21	2.32	0.56
14:J:12:PRO:HB2	23:J:104:BCR:H401	1.88	0.56
1:1:190:LYS:O	1:1:194:ASN:ND2	2.30	0.56
19:A:804:CLA:H143	23:A:845:BCR:H272	1.86	0.56
8:D:69:ASP:N	8:D:69:ASP:OD1	2.37	0.56
4:4:191:ASN:OD1	20:4:315:LUT:O23	2.24	0.55
5:A:65:GLU:N	5:A:65:GLU:OE2	2.38	0.55
1:1:190:LYS:HD3	19:1:311:CLA:HBD	1.88	0.55
5:A:707:LYS:HG3	10:F:218:ALA:HB2	1.88	0.55
6:B:36:ASP:O	6:B:41:ARG:NH1	2.39	0.55
25:2:318:LMT:H121	25:2:318:LMT:H3'	1.89	0.55
4:4:172:ILE:HD11	23:4:317:BCR:H323	1.88	0.55
3:3:79:LEU:HD23	19:A:811:CLA:H2	1.88	0.55
4:4:221:VAL:HG11	19:4:311:CLA:HAC2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.87	0.55
1:1:91:CYS:HB3	1:1:195:GLY:HA3	1.87	0.55
10:F:96:LEU:HA	10:F:109:LEU:HD13	1.89	0.55
19:A:823:CLA:H42	23:A:848:BCR:H363	1.88	0.55
5:A:433:ALA:O	5:A:437:HIS:ND1	2.40	0.54
10:F:68:ASP:N	10:F:72:LEU:O	2.41	0.54
6:B:33:ASN:HB3	28:B:846:DGD:HE62	1.89	0.54
16:K:54:ASN:ND2	19:K:202:CLA:O1D	2.40	0.54
19:A:853:CLA:H42	19:L:302:CLA:H102	1.89	0.54
19:1:308:CLA:HBA1	22:1:322:LHG:H141	1.89	0.54
10:F:190:VAL:HG21	24:F:307:LMG:H112	1.89	0.54
5:A:88:MET:HE1	19:A:807:CLA:HMA2	1.89	0.54
19:A:804:CLA:H61	23:A:846:BCR:H323	1.89	0.54
19:B:827:CLA:H202	23:B:841:BCR:H352	1.90	0.54
19:B:835:CLA:H152	23:F:305:BCR:H23C	1.89	0.54
10:F:103:SER:HB2	10:F:105:PRO:HD2	1.90	0.53
12:H:107:LEU:HD22	15:L:206:VAL:HG13	1.90	0.53
5:A:113:GLN:NE2	19:A:808:CLA:OBD	2.41	0.53
3:3:140:ILE:HG22	3:3:142:PRO:HG2	1.91	0.53
5:A:519:VAL:HG11	5:A:522:LEU:HD23	1.91	0.53
18:2:301:CHL:HMD1	23:3:317:BCR:HC21	1.91	0.53
19:A:826:CLA:HMB3	19:A:833:CLA:H11	1.90	0.53
19:B:813:CLA:HBA1	23:B:842:BCR:H332	1.90	0.53
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.42	0.52
4:4:110:MET:HE3	4:4:219:PHE:HD2	1.74	0.52
2:2:136:ASP:OD1	2:2:137:LYS:N	2.43	0.52
19:A:808:CLA:H71	25:N:201:LMT:H72	1.92	0.52
19:A:834:CLA:H52	6:B:438:VAL:HG13	1.92	0.52
15:L:162:PRO:HA	15:L:165:ARG:HD3	1.91	0.52
4:4:216:PHE:CD2	21:4:316:XAT:H14	2.45	0.52
19:B:822:CLA:H42	19:B:823:CLA:H112	1.92	0.52
19:B:828:CLA:HAA1	19:B:828:CLA:HBD	1.91	0.52
7:C:61:ASP:HB3	9:E:134:ASN:ND2	2.20	0.52
7:C:73:THR:OG1	7:C:74:THR:N	2.42	0.52
14:J:11:ALA:O	14:J:15:SER:OG	2.25	0.52
19:A:807:CLA:H192	19:A:854:CLA:H42	1.91	0.51
19:H:201:CLA:HAA1	19:H:201:CLA:HBD	1.91	0.51
14:J:28:GLU:OE1	14:J:31:ARG:NH1	2.43	0.51
19:3:304:CLA:CGA	19:3:304:CLA:HBD	2.39	0.51
4:4:82:LEU:HD13	19:4:301:CLA:H11	1.93	0.51
22:B:848:LHG:H272	22:B:848:LHG:H322	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:475:ASP:OD1	6:B:475:ASP:O	2.27	0.51
6:B:4:ARG:HB2	6:B:13:ALA:HB1	1.91	0.51
3:3:105:ARG:HB3	19:3:309:CLA:HBC3	1.93	0.51
23:J:101:BCR:H403	23:J:101:BCR:H23C	1.92	0.50
7:C:29:ILE:HG22	8:D:175:ARG:HB3	1.92	0.50
6:B:187:SER:HB2	6:B:281:ALA:HB2	1.92	0.50
2:2:216:ALA:O	2:2:220:VAL:HG23	2.12	0.50
19:A:801:CLA:HAA1	19:A:801:CLA:CGD	2.42	0.50
19:A:821:CLA:HBD	19:A:821:CLA:HAA1	1.94	0.50
7:C:80:ALA:HB2	8:D:127:ARG:HD2	1.93	0.50
4:4:249:THR:HG22	4:4:250:PHE:CD2	2.47	0.50
6:B:293:THR:HG22	6:B:294:ASN:H	1.77	0.49
6:B:489:GLY:C	6:B:494:LEU:HD12	2.37	0.49
8:D:161:HIS:CD2	8:D:162:PRO:HD3	2.47	0.49
2:2:84:PRO:O	2:2:88:LYS:HG2	2.11	0.49
10:F:89:ILE:HD12	10:F:113:ILE:HG23	1.94	0.49
1:1:95:MET:SD	19:1:309:CLA:HBB1	2.52	0.49
1:1:233:ILE:HG13	19:1:312:CLA:HMD2	1.95	0.49
19:A:834:CLA:H42	23:A:849:BCR:H362	1.93	0.49
23:2:319:BCR:C12	23:2:319:BCR:H341	2.43	0.49
6:B:685:THR:O	6:B:689:ASN:ND2	2.46	0.49
19:B:816:CLA:H42	19:B:825:CLA:HBB2	1.93	0.49
15:L:183:LYS:HG3	19:L:303:CLA:HBB	1.93	0.49
1:1:142:LEU:HD22	24:1:319:LMG:H142	1.94	0.49
2:2:57:PRO:HB2	3:3:180:MET:HE1	1.95	0.49
19:2:320:CLA:HBB2	19:4:301:CLA:HBC2	1.95	0.49
19:A:814:CLA:H12	23:A:844:BCR:HC31	1.94	0.49
6:B:284:PHE:HE1	19:B:818:CLA:HBB1	1.78	0.49
19:B:809:CLA:H143	15:L:203:GLY:HA2	1.94	0.49
23:L:305:BCR:H21C	23:L:305:BCR:C36	2.41	0.49
19:3:309:CLA:H2	20:3:315:LUT:H28	1.94	0.49
4:4:101:ARG:HB3	18:4:306:CHL:HED2	1.95	0.49
4:4:150:PHE:HA	4:4:153:VAL:HG22	1.95	0.49
6:B:596:TRP:O	6:B:600:THR:HG23	2.12	0.49
19:B:813:CLA:C1C	23:B:842:BCR:H15C	2.43	0.49
15:L:138:THR:H	15:L:141:THR:HG22	1.77	0.49
5:A:133:ARG:NH1	10:F:99:TYR:OH	2.45	0.49
10:F:100:ALA:O	10:F:103:SER:OG	2.30	0.49
3:3:139:VAL:HG13	3:3:140:ILE:HG13	1.94	0.49
5:A:660:TYR:OH	6:B:441:ASP:OD1	2.27	0.49
19:A:829:CLA:HAA1	19:A:829:CLA:HBD	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:193:HIS:HB2	19:B:813:CLA:C1C	2.43	0.48
19:B:823:CLA:H161	19:B:823:CLA:H122	1.57	0.48
19:B:813:CLA:C1B	23:B:842:BCR:H352	2.43	0.48
4:4:209:GLY:O	4:4:213:MET:HG3	2.13	0.48
4:4:197:PRO:HB3	19:4:308:CLA:HED3	1.94	0.48
19:A:853:CLA:H42	19:L:302:CLA:H122	1.95	0.48
1:1:238:ILE:O	1:1:238:ILE:HG13	2.14	0.48
24:1:319:LMG:HC8	24:1:319:LMG:H111	1.39	0.48
19:A:831:CLA:H61	19:B:837:CLA:H41	1.96	0.48
12:H:56:SER:O	12:H:56:SER:OG	2.28	0.48
23:J:101:BCR:H361	23:J:101:BCR:C21	2.43	0.48
23:1:318:BCR:H343	23:1:318:BCR:H311	1.96	0.48
15:L:212:LEU:HB3	15:L:253:THR:HG22	1.96	0.48
6:B:242:HIS:CE1	6:B:250:THR:HG22	2.49	0.48
6:B:480:SER:OG	6:B:483:SER:OG	2.27	0.48
4:4:186:PRO:HB3	18:4:306:CHL:HBC2	1.95	0.47
19:4:313:CLA:H202	22:B:848:LHG:H191	1.96	0.47
5:A:662:SER:OG	5:A:663:SER:N	2.47	0.47
19:A:826:CLA:H151	19:A:826:CLA:H111	1.71	0.47
19:A:840:CLA:HMA2	6:B:685:THR:HG21	1.96	0.47
23:A:843:BCR:H371	23:A:843:BCR:H393	1.96	0.47
10:F:133:ASP:OD1	10:F:133:ASP:N	2.34	0.47
8:D:161:HIS:CG	8:D:162:PRO:HD3	2.49	0.47
15:L:182:VAL:HG12	15:L:197:GLY:HA3	1.96	0.47
6:B:276:HIS:HB2	19:B:816:CLA:C1B	2.44	0.47
12:H:98:THR:O	15:L:250:ALA:HB1	2.14	0.47
19:A:854:CLA:H112	19:A:854:CLA:H152	1.58	0.47
6:B:666:SER:OG	6:B:671:TRP:NE1	2.36	0.47
8:D:67:GLN:NE2	8:D:147:GLN:OE1	2.47	0.47
15:L:194:GLY:HA3	15:L:272:TYR:CE2	2.50	0.47
6:B:458:ILE:HG21	10:F:141:ASN:ND2	2.29	0.47
26:B:839:PQN:H211	26:B:839:PQN:H252	1.77	0.47
5:A:531:PHE:HE2	23:A:843:BCR:H313	1.79	0.47
23:2:319:BCR:H341	23:2:319:BCR:H12C	1.95	0.47
19:3:308:CLA:H92	19:3:308:CLA:H2	1.96	0.47
5:A:139:SER:OG	19:A:807:CLA:OBD	2.32	0.47
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.50	0.47
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.96	0.47
3:3:104:GLY:O	3:3:108:MET:HG3	2.15	0.47
23:A:844:BCR:H10C	23:A:844:BCR:C35	2.43	0.47
19:A:852:CLA:H151	19:A:852:CLA:H112	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:102:LEU:HA	17:N:105:LYS:HB2	1.97	0.47
5:A:213:HIS:HB2	19:A:813:CLA:C1C	2.45	0.47
19:1:313:CLA:H3A	19:1:313:CLA:HBA2	1.60	0.46
18:4:304:CHL:CGA	23:4:317:BCR:H21C	2.46	0.46
15:L:178:VAL:HG21	15:L:267:ALA:HB3	1.97	0.46
19:A:817:CLA:H3A	19:A:817:CLA:HBA2	1.49	0.46
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.51	0.46
19:1:308:CLA:H3A	22:1:322:LHG:H122	1.98	0.46
4:4:249:THR:HG22	4:4:250:PHE:HD2	1.79	0.46
5:A:40:PRO:HG3	10:F:186:ILE:HD13	1.96	0.46
7:C:15:THR:HA	7:C:28:MET:HE3	1.96	0.46
5:A:354:LEU:HD21	19:A:829:CLA:HBB1	1.98	0.46
1:1:139:PRO:HB3	24:1:319:LMG:H112	1.97	0.46
19:A:810:CLA:H192	19:A:810:CLA:H161	1.76	0.46
6:B:428:PHE:CZ	23:J:101:BCR:H292	2.50	0.46
6:B:567:THR:O	6:B:567:THR:OG1	2.30	0.46
14:J:31:ARG:HD2	23:J:104:BCR:HC32	1.97	0.46
15:L:161:ASN:HD21	15:L:164:LEU:HG	1.80	0.46
19:1:309:CLA:H92	19:1:309:CLA:H61	1.78	0.46
5:A:153:GLU:HA	5:A:156:LEU:HD12	1.98	0.46
19:A:814:CLA:H3A	19:A:814:CLA:HBA2	1.46	0.46
23:A:847:BCR:H352	23:A:847:BCR:H10C	1.97	0.46
14:J:40:PRO:HD3	23:J:101:BCR:H10C	1.98	0.46
6:B:334:LEU:HD23	6:B:389:HIS:CE1	2.51	0.46
19:B:831:CLA:H91	19:F:303:CLA:HMA1	1.98	0.46
11:G:123:ASP:OD2	11:G:125:ILE:HG22	2.16	0.46
4:4:237:HIS:CD2	19:4:311:CLA:HAA2	2.50	0.46
19:B:808:CLA:HBA1	19:B:808:CLA:H3A	1.52	0.46
23:K:201:BCR:H24C	23:K:201:BCR:H371	1.83	0.46
25:2:318:LMT:O6'	25:2:318:LMT:O6B	2.28	0.46
3:3:66:LEU:HD13	3:3:75:GLY:HA2	1.97	0.46
5:A:735:ILE:HG21	19:A:827:CLA:HMC2	1.98	0.46
6:B:282:ILE:HG13	19:B:815:CLA:HBB1	1.97	0.46
20:4:315:LUT:C8	20:4:315:LUT:H181	2.46	0.45
5:A:531:PHE:CE2	23:A:843:BCR:H313	2.51	0.45
19:A:812:CLA:H41	19:A:812:CLA:H61	1.57	0.45
6:B:415:LYS:HB3	6:B:539:LEU:HD13	1.98	0.45
3:3:126:ILE:HG12	3:3:127:PRO:HD2	1.99	0.45
19:3:306:CLA:H3A	19:3:306:CLA:HBA2	1.63	0.45
5:A:152:SER:OG	5:A:153:GLU:N	2.49	0.45
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:734:GLY:O	19:A:801:CLA:HED1	2.16	0.45
1:1:200:LEU:HD21	19:1:312:CLA:H111	1.99	0.45
1:1:207:VAL:HG11	19:1:312:CLA:HAC2	1.99	0.45
19:2:320:CLA:HAA2	19:2:320:CLA:HBD	1.99	0.45
5:A:705:LYS:HE3	19:B:830:CLA:HED3	1.98	0.45
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.50	0.45
3:3:218:LEU:HG	3:3:222:LYS:HE3	1.99	0.45
5:A:231:PRO:HD2	17:N:107:ARG:HH21	1.82	0.45
6:B:60:TRP:HA	19:B:806:CLA:HBB2	1.97	0.45
19:1:312:CLA:C1B	20:1:315:LUT:H183	2.46	0.45
19:4:311:CLA:HAA1	19:4:311:CLA:HBD	1.98	0.45
19:A:801:CLA:H161	19:A:801:CLA:H122	1.59	0.45
19:B:818:CLA:HBC2	19:B:822:CLA:H71	1.98	0.45
6:B:733:PHE:HD2	12:H:141:PRO:HG2	1.82	0.45
19:1:302:CLA:CBB	21:1:316:XAT:H32	2.46	0.45
19:4:313:CLA:H3A	19:4:313:CLA:HBA2	1.56	0.45
19:A:825:CLA:HMB1	19:A:837:CLA:HBA1	1.97	0.45
19:B:826:CLA:H192	19:B:826:CLA:H161	1.82	0.45
19:B:832:CLA:H41	19:B:832:CLA:H61	1.68	0.45
14:J:28:GLU:HG3	19:J:102:CLA:C1B	2.47	0.45
16:K:122:VAL:HG12	19:K:203:CLA:HBB1	1.98	0.45
19:1:312:CLA:H11	19:1:312:CLA:HBA2	1.67	0.45
5:A:54:HIS:CD2	19:A:804:CLA:HBB2	2.51	0.45
5:A:214:GLN:HA	5:A:218:SER:HB3	1.99	0.45
23:A:844:BCR:H20C	23:A:844:BCR:H361	1.71	0.45
22:1:322:LHG:HC82	22:1:322:LHG:H131	2.00	0.45
23:F:306:BCR:H24C	23:F:306:BCR:H371	1.85	0.45
19:L:301:CLA:H102	19:L:301:CLA:H62	1.45	0.44
1:1:237:VAL:HG12	1:1:238:ILE:HG23	1.98	0.44
20:1:320:LUT:H7	20:1:320:LUT:H181	1.72	0.44
19:2:309:CLA:H61	19:2:309:CLA:H41	1.79	0.44
25:2:318:LMT:H41	25:2:318:LMT:H82	1.98	0.44
6:B:12:LEU:HG	28:B:846:DGD:HE1	1.99	0.44
19:2:304:CLA:H101	19:2:304:CLA:HBD	2.00	0.44
6:B:88:ALA:HB2	6:B:116:ALA:HB2	1.99	0.44
6:B:282:ILE:HD12	23:B:840:BCR:H361	2.00	0.44
18:1:301:CHL:HBA2	18:1:301:CHL:H3A	1.89	0.44
19:3:308:CLA:H92	19:3:308:CLA:H62	1.80	0.44
5:A:582:CYS:HB2	6:B:667:TRP:HB3	2.00	0.44
6:B:430:GLY:HA2	6:B:525:LEU:HD22	1.98	0.44
19:2:303:CLA:HBA1	19:2:303:CLA:H3A	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:333:GLN:HG2	5:A:334:GLY:N	2.32	0.44
19:B:816:CLA:H61	19:B:816:CLA:H101	1.47	0.44
22:2:317:LHG:HC62	22:2:317:LHG:H242	1.63	0.44
19:4:301:CLA:H91	19:4:302:CLA:H13	2.00	0.44
5:A:480:PHE:HE2	19:A:836:CLA:H2	1.83	0.44
6:B:280:ILE:HD13	6:B:280:ILE:HA	1.85	0.44
19:B:825:CLA:H152	23:B:844:BCR:H17C	1.99	0.44
2:2:224:TRP:O	2:2:228:ILE:HG22	2.18	0.43
5:A:450:PHE:O	5:A:454:ILE:HG12	2.18	0.43
19:B:811:CLA:H61	19:B:811:CLA:H92	1.73	0.43
10:F:179:LYS:HB2	10:F:179:LYS:HE2	1.82	0.43
19:K:202:CLA:HBA1	19:K:202:CLA:H3A	1.65	0.43
3:3:71:PRO:HB2	3:3:226:VAL:HG21	2.00	0.43
5:A:25:GLU:HG3	19:A:810:CLA:HMA2	2.00	0.43
4:4:100:GLY:HA2	4:4:103:ALA:HB3	2.00	0.43
5:A:80:ILE:HD11	19:A:810:CLA:H121	2.00	0.43
5:A:133:ARG:HB2	17:N:115:PHE:CE1	2.53	0.43
19:2:309:CLA:CBB	20:2:315:LUT:H32	2.48	0.43
5:A:294:HIS:HB2	19:A:817:CLA:C1B	2.48	0.43
19:B:838:CLA:H61	19:B:838:CLA:H41	1.81	0.43
14:J:38:ILE:O	14:J:40:PRO:HD3	2.19	0.43
3:3:122:LYS:HG3	3:3:251:TYR:HE2	1.84	0.43
5:A:585:SER:OG	5:A:588:ASP:OD2	2.36	0.43
6:B:143:LEU:HD12	6:B:143:LEU:HA	1.91	0.43
19:B:831:CLA:H61	19:B:831:CLA:H41	1.55	0.43
24:B:847:LMG:HC8	24:B:847:LMG:H111	1.38	0.43
7:C:31:TRP:CG	7:C:32:ASP:H	2.37	0.43
23:A:847:BCR:H20C	23:A:847:BCR:H361	1.81	0.43
6:B:278:LEU:O	6:B:282:ILE:HG12	2.19	0.43
19:B:805:CLA:H12	19:B:805:CLA:HED3	2.00	0.43
19:B:805:CLA:H151	19:B:827:CLA:HBB2	2.01	0.43
19:B:830:CLA:H2	23:F:305:BCR:H353	2.01	0.43
22:1:317:LHG:HC5	22:1:317:LHG:HC81	1.40	0.43
23:A:844:BCR:H24C	23:A:844:BCR:H371	1.73	0.43
4:4:219:PHE:HE1	20:4:315:LUT:H41	1.83	0.43
19:A:808:CLA:H121	23:J:103:BCR:HC41	2.00	0.43
8:D:128:LYS:HE3	8:D:160:LEU:HD13	2.00	0.43
2:2:99:ARG:NH1	18:2:307:CHL:OBD	2.50	0.43
19:A:823:CLA:HBA2	19:A:823:CLA:H3A	1.48	0.43
6:B:193:HIS:HB2	19:B:813:CLA:CHC	2.49	0.43
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:118:LEU:HD12	11:G:118:LEU:HA	1.89	0.43
23:L:305:BCR:H24C	23:L:305:BCR:H371	1.87	0.43
19:A:801:CLA:HBA1	19:A:801:CLA:H3A	1.77	0.42
19:A:805:CLA:HBB2	19:A:828:CLA:HMC1	2.01	0.42
19:A:839:CLA:H61	19:A:839:CLA:H41	1.54	0.42
1:1:118:TRP:CZ2	1:1:126:ALA:HB2	2.54	0.42
2:2:116:LYS:HD2	2:2:116:LYS:HA	1.76	0.42
5:A:477:GLN:HA	5:A:478:PRO:HD3	1.91	0.42
6:B:140:LEU:HD23	6:B:140:LEU:HA	1.93	0.42
19:B:805:CLA:H3A	19:B:828:CLA:HAB	2.01	0.42
19:B:810:CLA:H42	19:B:811:CLA:H51	2.01	0.42
1:1:160:LYS:HA	1:1:160:LYS:HD3	1.91	0.42
2:2:152:GLU:OE1	2:2:155:ARG:NH2	2.37	0.42
5:A:672:LEU:O	5:A:675:HIS:HB2	2.19	0.42
20:1:320:LUT:H11	20:1:320:LUT:H191	1.85	0.42
2:2:213:GLY:O	2:2:217:MET:HG3	2.18	0.42
5:A:507:TRP:CH2	19:A:826:CLA:HBC2	2.54	0.42
19:A:812:CLA:H61	19:A:812:CLA:H92	1.89	0.42
19:A:824:CLA:H93	19:A:824:CLA:H62	1.79	0.42
10:F:83:LYS:HB2	10:F:83:LYS:HE2	1.80	0.42
23:F:305:BCR:H24C	23:F:305:BCR:H371	1.85	0.42
19:1:321:CLA:H192	19:1:321:CLA:H162	1.82	0.42
2:2:168:ASP:HB3	2:2:171:PHE:O	2.19	0.42
2:2:211:LYS:NZ	19:2:310:CLA:O1D	2.46	0.42
5:A:60:THR:OG1	5:A:61:SER:N	2.53	0.42
23:A:844:BCR:C19	16:K:113:THR:HG21	2.49	0.42
19:B:813:CLA:H141	19:B:813:CLA:H162	1.88	0.42
11:G:80:ARG:NH2	11:G:123:ASP:OD1	2.50	0.42
25:2:318:LMT:H6'	25:2:318:LMT:H6B	1.57	0.42
5:A:529:ALA:O	5:A:533:VAL:HG23	2.19	0.42
6:B:124:TRP:HB3	6:B:129:LEU:HD12	2.01	0.42
23:I:101:BCR:H371	23:I:101:BCR:H24C	1.87	0.42
20:1:315:LUT:H7	20:1:315:LUT:H181	1.81	0.42
19:1:321:CLA:HED3	19:B:822:CLA:H3A	2.02	0.42
19:2:304:CLA:H92	19:2:304:CLA:H61	1.92	0.42
3:3:263:ASN:O	3:3:268:THR:OG1	2.29	0.42
3:3:271:LYS:HA	3:3:271:LYS:HD3	1.72	0.42
19:1:308:CLA:H92	19:1:308:CLA:H61	1.83	0.42
5:A:92:GLY:HA3	5:A:145:TRP:CH2	2.55	0.42
19:A:818:CLA:H3A	19:A:818:CLA:HBA2	1.63	0.42
6:B:254:ILE:HG13	6:B:255:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:88:LYS:HE3	12:H:88:LYS:HB3	1.89	0.42
23:2:319:BCR:HC8	23:2:319:BCR:H311	2.02	0.42
5:A:498:GLY:HA3	19:A:851:CLA:HED2	2.02	0.42
19:A:825:CLA:H102	19:A:825:CLA:H62	1.70	0.42
6:B:208:ARG:O	6:B:212:PHE:HB3	2.19	0.42
6:B:334:LEU:HD13	19:B:804:CLA:C2D	2.50	0.42
19:H:201:CLA:H3A	19:H:201:CLA:HBA2	1.55	0.42
14:J:25:LEU:HD23	14:J:26:LEU:HD23	2.01	0.42
19:3:308:CLA:H8	19:3:308:CLA:H121	1.80	0.42
5:A:164:LEU:HD23	5:A:164:LEU:HA	1.88	0.42
5:A:410:MET:HE1	5:A:424:LEU:HD11	2.02	0.42
5:A:746:ILE:HD12	5:A:746:ILE:HA	1.84	0.42
19:A:826:CLA:HED1	19:A:833:CLA:HAB	2.02	0.42
19:B:807:CLA:O1A	19:B:826:CLA:HBD	2.19	0.42
5:A:157:TYR:O	5:A:161:ILE:HG12	2.20	0.41
19:A:807:CLA:H3A	19:A:807:CLA:HBA2	1.71	0.41
19:A:832:CLA:HBA2	19:A:832:CLA:H3A	1.88	0.41
23:A:848:BCR:H24C	23:A:848:BCR:H371	1.86	0.41
19:B:818:CLA:H11	19:B:822:CLA:H12	2.02	0.41
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.91	0.41
19:F:304:CLA:HBA1	19:F:304:CLA:H3A	1.61	0.41
23:G:205:BCR:H24C	23:G:205:BCR:H371	1.83	0.41
2:2:109:PHE:CE1	20:2:315:LUT:H173	2.55	0.41
5:A:597:MET:HE3	5:A:597:MET:HB3	1.84	0.41
19:A:834:CLA:H192	19:A:834:CLA:H162	1.78	0.41
19:A:853:CLA:H61	19:A:853:CLA:H41	1.62	0.41
6:B:388:ALA:O	6:B:392:ILE:HG13	2.20	0.41
19:B:811:CLA:HAA1	19:B:811:CLA:HBD	2.03	0.41
9:E:92:ILE:HG22	9:E:94:ARG:H	1.85	0.41
10:F:68:ASP:N	10:F:68:ASP:OD1	2.53	0.41
10:F:163:TRP:CD1	10:F:200:GLY:HA3	2.56	0.41
15:L:266:TRP:HB2	23:L:305:BCR:H331	2.01	0.41
16:K:116:HIS:CE1	23:K:201:BCR:H14C	2.55	0.41
5:A:239:GLU:OE2	5:A:239:GLU:HA	2.19	0.41
5:A:697:GLU:OE2	9:E:128:TYR:OH	2.27	0.41
19:A:823:CLA:HMB1	23:A:847:BCR:H12C	2.02	0.41
19:A:836:CLA:H152	19:A:836:CLA:H18	1.83	0.41
23:A:847:BCR:H371	23:A:847:BCR:H24C	1.79	0.41
19:B:837:CLA:HBD	19:B:837:CLA:HAA1	2.02	0.41
8:D:149:TYR:HD2	8:D:159:TYR:HA	1.86	0.41
1:1:184:LEU:HD12	1:1:184:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:66:ASP:OD1	2:2:66:ASP:C	2.64	0.41
5:A:454:ILE:HG22	19:A:832:CLA:HBC2	2.03	0.41
19:A:824:CLA:H192	19:A:824:CLA:H161	1.73	0.41
15:L:179:GLY:O	15:L:182:VAL:HG22	2.21	0.41
19:L:302:CLA:H152	19:L:302:CLA:H111	1.78	0.41
3:3:105:ARG:NH1	18:3:307:CHL:OBD	2.54	0.41
5:A:451:GLY:HA3	19:A:832:CLA:CBB	2.50	0.41
12:H:127:LEU:HD23	12:H:127:LEU:HA	1.87	0.41
15:L:270:LEU:HD23	15:L:270:LEU:HA	1.85	0.41
1:1:88:LEU:HD23	1:1:88:LEU:HA	1.91	0.41
20:1:320:LUT:H171	20:1:320:LUT:C8	2.45	0.41
5:A:78:LEU:HD22	19:A:804:CLA:H92	2.02	0.41
5:A:300:ILE:HD11	23:A:844:BCR:H341	2.03	0.41
19:A:824:CLA:HBD	19:A:824:CLA:HAA2	2.02	0.41
19:F:302:CLA:H152	19:F:302:CLA:H112	1.53	0.41
12:H:139:LEU:HD23	12:H:139:LEU:HA	1.90	0.41
19:2:313:CLA:H62	19:2:313:CLA:H92	1.74	0.41
4:4:204:LYS:O	4:4:208:ASN:ND2	2.33	0.41
4:4:206:LEU:HD23	4:4:206:LEU:HA	1.90	0.41
5:A:533:VAL:HG11	5:A:607:HIS:CG	2.56	0.41
2:2:156:TRP:NE1	25:2:318:LMT:O1'	2.53	0.41
4:4:86:PRO:O	4:4:90:LYS:HG3	2.20	0.41
5:A:521:LEU:HD23	5:A:521:LEU:HA	1.91	0.41
19:A:834:CLA:C4B	19:A:852:CLA:HBB1	2.51	0.41
6:B:229:GLN:HA	11:G:151:SER:HB2	2.02	0.41
23:F:306:BCR:H20C	23:F:306:BCR:H361	1.90	0.41
2:2:221:MET:HE2	19:2:303:CLA:HBB2	2.02	0.41
3:3:90:PHE:HB3	19:3:302:CLA:H2	2.03	0.41
5:A:321:ASP:OD1	5:A:321:ASP:N	2.54	0.41
5:A:331:THR:HG21	5:A:335:HIS:HE1	1.85	0.41
5:A:692:TRP:O	5:A:696:ILE:HG13	2.21	0.41
19:A:822:CLA:HAA1	19:A:822:CLA:HBD	2.03	0.41
19:B:805:CLA:H192	19:B:805:CLA:H161	1.76	0.41
19:B:806:CLA:H92	19:B:806:CLA:H62	1.95	0.41
8:D:108:MET:HE3	8:D:108:MET:HB3	1.93	0.41
15:L:249:TRP:O	15:L:253:THR:HG23	2.20	0.41
23:L:306:BCR:H371	23:L:306:BCR:H24C	1.86	0.41
2:2:98:CYS:HB3	2:2:213:GLY:HA3	2.02	0.41
2:2:102:MET:SD	19:2:309:CLA:HBB1	2.61	0.41
19:3:302:CLA:H13	19:3:308:CLA:H93	2.03	0.41
4:4:214:LEU:HD23	4:4:214:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:844:BCR:H402	16:K:114:VAL:HG21	2.03	0.41
19:B:833:CLA:H3A	19:B:833:CLA:HBA2	1.54	0.41
23:J:104:BCR:H371	23:J:104:BCR:H24C	1.88	0.41
2:2:101:ALA:CB	2:2:217:MET:HG2	2.52	0.40
3:3:169:ARG:NH1	18:3:307:CHL:OMC	2.41	0.40
3:3:242:GLN:O	3:3:246:THR:OG1	2.37	0.40
23:A:843:BCR:H372	23:A:843:BCR:H361	2.02	0.40
23:B:840:BCR:H24C	23:B:840:BCR:H371	1.85	0.40
7:C:26:LEU:HD23	7:C:42:ALA:HB2	2.02	0.40
19:G:203:CLA:H3A	19:G:203:CLA:HBA2	1.48	0.40
20:3:315:LUT:H35	20:3:315:LUT:H401	1.90	0.40
5:A:307:HIS:NE2	23:A:844:BCR:H363	2.36	0.40
19:A:818:CLA:H192	19:A:818:CLA:H162	1.78	0.40
23:A:846:BCR:H371	23:A:846:BCR:H24C	1.85	0.40
10:F:96:LEU:HD13	10:F:109:LEU:HB2	2.03	0.40
13:I:31:ILE:HD11	23:L:304:BCR:H333	2.03	0.40
15:L:208:LEU:HD22	23:L:304:BCR:H401	2.02	0.40
20:4:315:LUT:H35	20:4:315:LUT:H401	1.92	0.40
5:A:552:VAL:HG21	23:A:848:BCR:HC31	2.03	0.40
6:B:428:PHE:HZ	23:J:101:BCR:H292	1.87	0.40
19:B:811:CLA:HBB1	19:B:819:CLA:HBC2	2.03	0.40
19:1:305:CLA:HBB2	18:1:306:CHL:CBB	2.50	0.40
19:2:312:CLA:H13	19:2:312:CLA:H172	1.93	0.40
23:A:846:BCR:H20C	23:A:846:BCR:H361	1.90	0.40
28:B:846:DGD:HBE1	28:B:846:DGD:HB82	1.97	0.40
16:K:69:ARG:HH21	19:K:204:CLA:C1D	2.34	0.40
1:1:60:GLY:HA2	1:1:65:ASP:HB3	2.02	0.40
5:A:259:THR:O	5:A:263:THR:OG1	2.33	0.40
23:A:845:BCR:H371	23:A:845:BCR:H24C	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/206 (93%)	186 (97%)	6 (3%)	0	100	100
2	2	201/214 (94%)	195 (97%)	6 (3%)	0	100	100
3	3	217/234 (93%)	210 (97%)	7 (3%)	0	100	100
4	4	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
5	A	740/750 (99%)	724 (98%)	16 (2%)	0	100	100
6	B	731/734 (100%)	717 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
8	D	139/160 (87%)	132 (95%)	7 (5%)	0	100	100
9	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
10	F	150/154 (97%)	149 (99%)	1 (1%)	0	100	100
11	G	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
12	H	88/95 (93%)	88 (100%)	0	0	100	100
13	I	28/37 (76%)	28 (100%)	0	0	100	100
14	J	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
15	L	142/169 (84%)	139 (98%)	3 (2%)	0	100	100
16	K	51/84 (61%)	50 (98%)	1 (2%)	0	100	100
17	N	46/85 (54%)	42 (91%)	4 (9%)	0	100	100
All	All	3194/3445 (93%)	3112 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/161 (95%)	152 (99%)	1 (1%)	76	79
2	2	164/171 (96%)	164 (100%)	0	100	100
3	3	169/179 (94%)	168 (99%)	1 (1%)	78	80
4	4	164/166 (99%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	601/609 (99%)	597 (99%)	4 (1%)	76	79
6	B	597/598 (100%)	596 (100%)	1 (0%)	87	87
7	C	70/71 (99%)	69 (99%)	1 (1%)	59	72
8	D	120/134 (90%)	120 (100%)	0	100	100
9	E	56/80 (70%)	56 (100%)	0	100	100
10	F	125/127 (98%)	125 (100%)	0	100	100
11	G	82/84 (98%)	82 (100%)	0	100	100
12	H	75/79 (95%)	74 (99%)	1 (1%)	61	73
13	I	26/33 (79%)	26 (100%)	0	100	100
14	J	36/38 (95%)	36 (100%)	0	100	100
15	L	111/134 (83%)	111 (100%)	0	100	100
16	K	41/61 (67%)	41 (100%)	0	100	100
17	N	41/73 (56%)	40 (98%)	1 (2%)	43	65
All	All	2631/2798 (94%)	2621 (100%)	10 (0%)	81	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	47	HIS
3	3	145	THR
5	A	17	ASP
5	A	118	ILE
5	A	369	TYR
5	A	749	VAL
6	B	280	ILE
7	C	63	LEU
12	H	109	LEU
17	N	89	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	116	GLN
1	1	154	HIS
1	1	208	GLN
1	1	209	GLN

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Mol	Chain	Res	Type
1	1	220	ASN
2	2	131	GLN
2	2	166	ASN
2	2	174	ASN
3	3	263	ASN
4	4	94	GLN
4	4	99	ASN
4	4	134	GLN
4	4	168	ASN
4	4	236	GLN
4	4	237	HIS
4	4	243	HIS
4	4	244	ASN
5	A	50	HIS
5	A	113	GLN
5	A	136	GLN
5	A	155	GLN
5	A	317	HIS
5	A	391	HIS
5	A	658	GLN
5	A	693	GLN
5	A	713	GLN
6	B	34	HIS
6	B	158	GLN
6	B	236	ASN
6	B	266	GLN
6	B	277	HIS
6	B	299	HIS
6	B	333	GLN
6	B	363	GLN
6	B	375	HIS
6	B	402	GLN
6	B	482	ASN
6	B	598	HIS
6	B	605	ASN
6	B	610	ASN
7	C	16	GLN
8	D	71	ASN
8	D	99	ASN
8	D	121	ASN
8	D	172	ASN
9	E	102	ASN

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Mol	Chain	Res	Type
9	E	134	ASN
10	F	110	ASN
11	G	85	ASN
11	G	90	ASN
11	G	99	GLN
11	G	140	HIS
12	H	134	GLN
13	I	34	ASN
15	L	161	ASN
16	K	128	ASN
17	N	99	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

210 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	$\# Z  > 2$
19	CLA	A	812	-	69,73,73	1.23	6 (8%)	82,113,113	1.69	8 (9%)
19	CLA	4	312	-	49,53,73	1.40	7 (14%)	58,89,113	1.77	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	A	843	-	41,41,41	0.19	0	56,56,56	0.70	2 (3%)
19	CLA	2	308	2	49,53,73	1.41	7 (14%)	58,89,113	1.76	6 (10%)
19	CLA	2	312	-	69,73,73	1.23	6 (8%)	82,113,113	1.63	8 (9%)
22	LHG	B	848	19	44,44,48	0.31	0	47,50,54	0.29	0
28	DGD	B	846	-	67,67,67	0.15	0	81,81,81	0.14	0
23	BCR	1	318	-	41,41,41	0.16	0	56,56,56	0.83	2 (3%)
23	BCR	B	840	-	41,41,41	0.13	0	56,56,56	0.28	0
23	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.72	1 (1%)
19	CLA	A	819	-	49,53,73	1.40	6 (12%)	58,89,113	1.80	6 (10%)
19	CLA	3	302	3	64,68,73	1.28	6 (9%)	76,107,113	1.68	10 (13%)
24	LMG	1	319	-	50,50,55	0.19	0	58,58,63	0.14	0
23	BCR	2	319	-	41,41,41	0.24	0	56,56,56	0.76	2 (3%)
19	CLA	B	817	-	64,68,73	1.28	6 (9%)	76,107,113	1.67	10 (13%)
20	LUT	2	315	-	42,43,43	1.28	8 (19%)	51,60,60	1.54	11 (21%)
19	CLA	1	304	-	55,59,73	1.37	7 (12%)	64,96,113	1.80	8 (12%)
19	CLA	1	312	-	64,68,73	1.28	6 (9%)	76,107,113	1.66	8 (10%)
23	BCR	4	317	-	41,41,41	0.14	0	56,56,56	0.33	0
19	CLA	H	201	12	49,53,73	1.41	7 (14%)	58,89,113	1.77	7 (12%)
24	LMG	4	318	-	36,36,55	0.19	0	44,44,63	0.13	0
19	CLA	B	805	6	69,73,73	1.24	7 (10%)	82,113,113	1.66	8 (9%)
19	CLA	2	313	-	62,66,73	1.31	8 (12%)	73,104,113	1.78	8 (10%)
19	CLA	B	801	-	69,73,73	1.23	6 (8%)	82,113,113	1.59	9 (10%)
23	BCR	B	844	-	41,41,41	0.11	0	56,56,56	0.33	0
19	CLA	B	808	6	69,73,73	1.23	7 (10%)	82,113,113	1.63	9 (10%)
19	CLA	A	808	5	66,70,73	1.27	7 (10%)	78,109,113	1.71	9 (11%)
19	CLA	1	307	-	49,53,73	1.41	7 (14%)	58,89,113	1.76	7 (12%)
23	BCR	J	103	-	41,41,41	0.13	0	56,56,56	0.22	0
18	CHL	1	301	1	50,64,74	2.09	12 (24%)	46,102,114	2.82	18 (39%)
19	CLA	A	804	-	69,73,73	1.23	7 (10%)	82,113,113	1.73	10 (12%)
19	CLA	B	815	-	59,63,73	1.33	7 (11%)	70,101,113	1.72	6 (8%)
19	CLA	A	815	-	49,53,73	1.41	6 (12%)	58,89,113	1.80	6 (10%)
19	CLA	B	811	-	59,63,73	1.34	7 (11%)	70,101,113	1.75	8 (11%)
22	LHG	1	322	-	48,48,48	0.30	0	51,54,54	0.27	0
19	CLA	A	816	-	67,72,73	1.24	7 (10%)	79,112,113	1.55	7 (8%)
20	LUT	1	315	-	42,43,43	1.28	8 (19%)	51,60,60	1.56	12 (23%)
19	CLA	B	819	-	54,58,73	1.38	7 (12%)	64,95,113	1.77	7 (10%)
24	LMG	F	307	-	30,30,55	0.20	0	38,38,63	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	813	-	69,73,73	1.24	7 (10%)	82,113,113	1.63	7 (8%)
19	CLA	B	807	-	69,73,73	1.23	6 (8%)	82,113,113	1.64	8 (9%)
19	CLA	B	836	-	51,55,73	1.38	7 (13%)	60,91,113	1.77	6 (10%)
19	CLA	A	854	-	69,73,73	1.23	7 (10%)	82,113,113	1.66	10 (12%)
19	CLA	A	807	5	69,73,73	1.23	6 (8%)	82,113,113	1.57	9 (10%)
19	CLA	3	309	3	54,58,73	1.38	7 (12%)	64,95,113	1.73	9 (14%)
21	XAT	2	316	-	41,47,47	0.16	0	54,74,74	0.71	1 (1%)
18	CHL	4	306	-	45,59,74	2.19	12 (26%)	40,96,114	3.00	18 (45%)
21	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.78	2 (3%)
20	LUT	4	315	-	42,43,43	1.30	8 (19%)	51,60,60	1.44	9 (17%)
19	CLA	A	840	-	69,73,73	1.23	7 (10%)	82,113,113	1.58	8 (9%)
19	CLA	4	303	-	49,53,73	1.41	6 (12%)	58,89,113	1.80	6 (10%)
19	CLA	B	837	-	69,73,73	1.24	6 (8%)	82,113,113	1.62	9 (10%)
19	CLA	F	304	10	49,53,73	1.41	6 (12%)	58,89,113	1.84	6 (10%)
19	CLA	3	311	-	49,53,73	1.42	7 (14%)	58,89,113	1.87	6 (10%)
19	CLA	G	203	-	54,58,73	1.38	7 (12%)	64,95,113	1.86	6 (9%)
21	XAT	4	316	-	41,47,47	0.13	0	54,74,74	0.73	1 (1%)
19	CLA	1	303	-	62,66,73	1.29	6 (9%)	73,104,113	1.69	7 (9%)
19	CLA	A	824	-	69,73,73	1.23	6 (8%)	82,113,113	1.60	10 (12%)
19	CLA	B	814	-	59,63,73	1.33	7 (11%)	70,101,113	1.76	7 (10%)
19	CLA	4	313	-	69,73,73	1.24	7 (10%)	82,113,113	1.64	8 (9%)
19	CLA	4	301	4	64,68,73	1.28	7 (10%)	76,107,113	1.70	8 (10%)
19	CLA	A	817	-	59,63,73	1.33	6 (10%)	70,101,113	1.69	7 (10%)
19	CLA	3	308	3	69,73,73	1.23	6 (8%)	82,113,113	1.62	7 (8%)
19	CLA	2	320	4	50,54,73	1.39	6 (12%)	59,90,113	1.83	5 (8%)
18	CHL	2	301	2	45,59,74	2.21	12 (26%)	40,96,114	3.06	18 (45%)
19	CLA	A	829	-	69,73,73	1.24	7 (10%)	82,113,113	1.66	8 (9%)
19	CLA	A	826	-	69,73,73	1.23	6 (8%)	82,113,113	1.70	8 (9%)
19	CLA	K	202	-	49,53,73	1.41	6 (12%)	58,89,113	1.79	7 (12%)
19	CLA	A	821	-	49,53,73	1.41	7 (14%)	58,89,113	1.82	6 (10%)
19	CLA	B	812	-	69,73,73	1.22	6 (8%)	82,113,113	1.70	9 (10%)
23	BCR	K	201	-	41,41,41	0.17	0	56,56,56	0.51	0
19	CLA	A	835	-	55,59,73	1.37	6 (10%)	64,96,113	1.86	7 (10%)
27	SF4	A	850	6,5	0,12,12	-	-	-	-	-
23	BCR	L	306	-	41,41,41	0.14	0	56,56,56	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LUT	3	315	-	42,43,43	1.30	8 (19%)	51,60,60	1.46	9 (17%)
19	CLA	B	832	-	69,73,73	1.24	8 (11%)	82,113,113	1.61	8 (9%)
23	BCR	A	844	-	41,41,41	0.25	0	56,56,56	0.87	3 (5%)
19	CLA	B	831	-	62,66,73	1.30	7 (11%)	73,104,113	1.68	7 (9%)
23	BCR	B	842	-	41,41,41	0.15	0	56,56,56	0.77	2 (3%)
19	CLA	F	303	-	49,53,73	1.41	7 (14%)	58,89,113	1.82	7 (12%)
19	CLA	2	309	2	61,65,73	1.31	7 (11%)	72,103,113	1.70	8 (11%)
19	CLA	3	305	-	46,50,73	1.41	7 (15%)	53,85,113	1.81	6 (11%)
19	CLA	A	839	-	69,73,73	1.24	7 (10%)	82,113,113	1.63	9 (10%)
19	CLA	1	311	1	49,53,73	1.41	7 (14%)	58,89,113	1.81	5 (8%)
19	CLA	B	804	-	69,73,73	1.24	7 (10%)	82,113,113	1.68	8 (9%)
19	CLA	B	824	-	64,68,73	1.29	7 (10%)	76,107,113	1.70	9 (11%)
19	CLA	A	814	-	54,58,73	1.38	7 (12%)	64,95,113	1.79	7 (10%)
19	CLA	3	301	3	64,68,73	1.28	7 (10%)	76,107,113	1.66	9 (11%)
18	CHL	4	304	-	50,64,74	2.12	12 (24%)	46,102,114	2.83	17 (36%)
19	CLA	4	302	-	64,68,73	1.29	7 (10%)	76,107,113	1.67	10 (13%)
19	CLA	2	311	2	49,53,73	1.41	7 (14%)	58,89,113	1.85	6 (10%)
19	CLA	A	809	-	63,67,73	1.29	7 (11%)	74,105,113	1.72	10 (13%)
19	CLA	3	306	3	49,53,73	1.41	7 (14%)	58,89,113	1.75	6 (10%)
19	CLA	G	204	11	50,54,73	1.39	6 (12%)	59,90,113	1.84	6 (10%)
19	CLA	A	825	-	69,73,73	1.24	7 (10%)	82,113,113	1.66	9 (10%)
19	CLA	4	307	4	54,58,73	1.39	6 (11%)	64,95,113	1.79	7 (10%)
19	CLA	B	803	-	49,53,73	1.41	6 (12%)	58,89,113	1.79	6 (10%)
19	CLA	A	806	-	54,58,73	1.39	7 (12%)	64,95,113	1.75	7 (10%)
19	CLA	4	309	-	64,68,73	1.28	7 (10%)	76,107,113	1.61	8 (10%)
19	CLA	B	828	-	69,73,73	1.24	7 (10%)	82,113,113	1.58	9 (10%)
19	CLA	A	820	-	69,73,73	1.23	7 (10%)	82,113,113	1.60	9 (10%)
19	CLA	A	833	-	54,58,73	1.39	7 (12%)	64,95,113	1.71	8 (12%)
19	CLA	B	835	-	69,73,73	1.22	7 (10%)	82,113,113	1.65	9 (10%)
19	CLA	4	310	4	49,53,73	1.41	7 (14%)	58,89,113	1.84	7 (12%)
18	CHL	4	314	4	36,50,74	2.31	10 (27%)	29,85,114	3.12	12 (41%)
19	CLA	B	827	-	69,73,73	1.23	7 (10%)	82,113,113	1.59	6 (7%)
23	BCR	I	101	-	41,41,41	0.11	0	56,56,56	0.21	0
25	LMT	2	318	-	36,36,36	0.14	0	47,47,47	0.17	0
18	CHL	3	307	-	41,55,74	2.23	11 (26%)	35,91,114	3.15	16 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	831	-	69,73,73	1.24	6 (8%)	82,113,113	1.63	7 (8%)
19	CLA	B	822	-	64,68,73	1.28	7 (10%)	76,107,113	1.62	8 (10%)
23	BCR	B	841	-	41,41,41	0.14	0	56,56,56	0.26	0
19	CLA	A	818	-	69,73,73	1.24	7 (10%)	82,113,113	1.60	10 (12%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
19	CLA	F	301	-	68,72,73	1.25	6 (8%)	80,111,113	1.72	9 (11%)
19	CLA	1	305	-	46,50,73	1.41	6 (13%)	53,85,113	1.82	6 (11%)
19	CLA	B	825	-	69,73,73	1.23	6 (8%)	82,113,113	1.72	8 (9%)
22	LHG	A	842	-	48,48,48	0.29	0	51,54,54	0.28	0
23	BCR	3	317	-	41,41,41	0.12	0	56,56,56	0.32	0
19	CLA	A	811	-	58,62,73	1.34	7 (12%)	68,99,113	1.74	7 (10%)
19	CLA	B	830	-	64,68,73	1.29	7 (10%)	76,107,113	1.70	8 (10%)
19	CLA	1	302	1	64,68,73	1.28	7 (10%)	76,107,113	1.68	9 (11%)
19	CLA	A	803	19	54,58,73	1.39	7 (12%)	64,95,113	1.74	7 (10%)
19	CLA	A	838	-	69,73,73	1.23	7 (10%)	82,113,113	1.64	9 (10%)
19	CLA	A	802	-	69,73,73	1.23	7 (10%)	82,113,113	1.55	10 (12%)
19	CLA	A	836	-	69,73,73	1.24	7 (10%)	82,113,113	1.60	7 (8%)
19	CLA	2	304	-	69,73,73	1.25	8 (11%)	82,113,113	1.62	9 (10%)
21	XAT	1	316	-	41,47,47	0.14	0	54,74,74	0.70	1 (1%)
24	LMG	B	847	-	52,52,55	0.18	0	60,60,63	0.16	0
19	CLA	A	801	-	69,73,73	1.23	7 (10%)	82,113,113	1.62	10 (12%)
23	BCR	L	305	-	41,41,41	0.22	0	56,56,56	0.86	2 (3%)
23	BCR	A	845	-	41,41,41	0.14	0	56,56,56	0.22	0
19	CLA	J	102	-	46,50,73	1.40	7 (15%)	53,85,113	1.79	5 (9%)
19	CLA	L	301	15	59,63,73	1.33	6 (10%)	70,101,113	1.70	8 (11%)
23	BCR	J	104	-	41,41,41	0.11	0	56,56,56	0.20	0
19	CLA	A	827	-	69,73,73	1.22	7 (10%)	82,113,113	1.62	9 (10%)
19	CLA	B	810	-	58,62,73	1.35	8 (13%)	71,100,113	1.97	11 (15%)
19	CLA	K	203	-	50,54,73	1.40	7 (14%)	59,90,113	1.80	5 (8%)
19	CLA	B	833	-	49,53,73	1.41	7 (14%)	58,89,113	1.84	6 (10%)
19	CLA	A	810	19	69,73,73	1.23	7 (10%)	82,113,113	1.62	10 (12%)
19	CLA	4	308	4	64,68,73	1.27	7 (10%)	76,107,113	1.69	9 (11%)
23	BCR	J	101	-	41,41,41	0.17	0	56,56,56	0.99	4 (7%)
27	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	B	821	-	59,63,73	1.33	6 (10%)	70,101,113	1.71	7 (10%)
20	LUT	1	320	-	42,43,43	1.28	8 (19%)	51,60,60	1.57	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	PQN	B	839	-	34,34,34	0.28	0	43,45,45	0.53	1 (2%)
23	BCR	F	305	-	41,41,41	0.11	0	56,56,56	0.24	0
23	BCR	A	848	-	41,41,41	0.12	0	56,56,56	0.18	0
19	CLA	A	822	-	55,59,73	1.37	6 (10%)	64,96,113	1.82	8 (12%)
19	CLA	B	806	-	58,62,73	1.34	7 (12%)	68,99,113	1.74	7 (10%)
23	BCR	G	205	-	41,41,41	0.10	0	56,56,56	0.33	0
19	CLA	3	314	-	50,54,73	1.40	7 (14%)	59,90,113	1.78	6 (10%)
23	BCR	F	306	-	41,41,41	0.13	0	56,56,56	0.29	0
18	CHL	2	307	-	40,54,74	2.31	12 (30%)	34,90,114	3.16	16 (47%)
19	CLA	A	832	-	69,73,73	1.23	6 (8%)	82,113,113	1.60	6 (7%)
19	CLA	B	809	-	69,73,73	1.23	7 (10%)	82,113,113	1.57	7 (8%)
19	CLA	B	816	-	63,67,73	1.28	6 (9%)	74,105,113	1.63	9 (12%)
19	CLA	2	302	2	69,73,73	1.23	7 (10%)	82,113,113	1.61	8 (9%)
18	CHL	1	306	-	40,54,74	2.33	12 (30%)	34,90,114	3.15	16 (47%)
22	LHG	1	317	19	48,48,48	0.29	0	51,54,54	0.29	0
19	CLA	A	852	-	69,73,73	1.23	7 (10%)	82,113,113	1.61	9 (10%)
19	CLA	3	304	-	51,55,73	1.38	6 (11%)	60,91,113	1.82	8 (13%)
18	CHL	2	305	-	37,51,74	2.31	11 (29%)	30,86,114	3.32	14 (46%)
22	LHG	2	317	19	36,36,48	0.34	0	39,42,54	0.31	0
18	CHL	2	314	2	37,51,74	2.32	11 (29%)	30,86,114	3.43	14 (46%)
19	CLA	G	202	-	45,49,73	1.44	7 (15%)	54,84,113	1.84	6 (11%)
26	PQN	A	841	-	34,34,34	0.29	0	43,45,45	0.53	1 (2%)
19	CLA	A	834	-	69,73,73	1.23	6 (8%)	82,113,113	1.54	10 (12%)
19	CLA	A	851	5	49,53,73	1.41	7 (14%)	58,89,113	1.80	6 (10%)
19	CLA	B	826	-	69,73,73	1.23	6 (8%)	82,113,113	1.58	9 (10%)
23	BCR	L	304	-	41,41,41	0.16	0	56,56,56	0.30	0
19	CLA	1	308	1	61,65,73	1.31	7 (11%)	72,103,113	1.74	9 (12%)
19	CLA	A	837	-	56,60,73	1.37	7 (12%)	65,97,113	1.75	8 (12%)
18	CHL	4	305	-	40,54,74	2.32	12 (30%)	34,90,114	3.15	16 (47%)
19	CLA	A	805	5	69,73,73	1.22	6 (8%)	82,113,113	1.66	9 (10%)
19	CLA	1	314	1	49,53,73	1.40	6 (12%)	58,89,113	1.77	5 (8%)
19	CLA	B	829	-	54,58,73	1.38	6 (11%)	64,95,113	1.72	7 (10%)
19	CLA	B	838	-	69,73,73	1.23	6 (8%)	82,113,113	1.58	9 (10%)
23	BCR	A	849	-	41,41,41	0.15	0	56,56,56	0.32	0
19	CLA	3	312	-	59,63,73	1.33	6 (10%)	70,101,113	1.71	5 (7%)
19	CLA	F	302	-	69,73,73	1.23	7 (10%)	82,113,113	1.63	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.21	0
19	CLA	4	311	-	60,64,73	1.31	6 (10%)	71,102,113	1.69	7 (9%)
19	CLA	1	321	22	69,73,73	1.23	7 (10%)	82,113,113	1.72	7 (8%)
19	CLA	1	309	1	60,64,73	1.32	7 (11%)	71,102,113	1.72	7 (9%)
23	BCR	A	846	-	41,41,41	0.12	0	56,56,56	0.17	0
19	CLA	3	313	-	49,53,73	1.41	7 (14%)	58,89,113	1.77	6 (10%)
19	CLA	B	834	-	59,63,73	1.33	6 (10%)	70,101,113	1.78	7 (10%)
23	BCR	B	845	-	41,41,41	0.11	0	56,56,56	0.23	0
19	CLA	L	303	-	54,58,73	1.38	6 (11%)	64,95,113	1.72	10 (15%)
19	CLA	1	313	-	49,53,73	1.40	7 (14%)	58,89,113	1.72	6 (10%)
19	CLA	A	830	-	54,58,73	1.39	7 (12%)	64,95,113	1.72	8 (12%)
19	CLA	B	802	-	69,73,73	1.23	6 (8%)	82,113,113	1.65	9 (10%)
18	CHL	2	306	-	40,54,74	2.32	13 (32%)	34,90,114	3.15	16 (47%)
19	CLA	2	310	22	45,49,73	1.44	7 (15%)	54,84,113	1.84	7 (12%)
19	CLA	B	818	-	64,68,73	1.29	7 (10%)	76,107,113	1.68	9 (11%)
19	CLA	B	820	-	59,63,73	1.33	6 (10%)	70,101,113	1.70	7 (10%)
19	CLA	L	302	-	69,73,73	1.24	7 (10%)	82,113,113	1.61	8 (9%)
19	CLA	3	310	-	45,49,73	1.44	7 (15%)	54,84,113	1.83	8 (14%)
23	BCR	B	843	-	41,41,41	0.12	0	56,56,56	0.31	0
19	CLA	2	303	-	54,58,73	1.38	6 (11%)	64,95,113	1.78	7 (10%)
19	CLA	A	828	-	69,73,73	1.24	7 (10%)	82,113,113	1.61	9 (10%)
25	LMT	N	201	-	36,36,36	0.10	0	47,47,47	0.26	0
19	CLA	B	823	-	69,73,73	1.23	6 (8%)	82,113,113	1.62	8 (9%)
19	CLA	A	813	-	49,53,73	1.41	7 (14%)	58,89,113	1.87	6 (10%)
19	CLA	3	303	-	49,53,73	1.41	6 (12%)	58,89,113	1.77	7 (12%)
19	CLA	A	823	-	59,63,73	1.33	7 (11%)	70,101,113	1.69	8 (11%)
19	CLA	1	310	22	59,63,73	1.34	7 (11%)	70,101,113	1.72	8 (11%)
19	CLA	K	204	16	41,45,73	1.53	8 (19%)	50,78,113	1.88	6 (12%)
19	CLA	A	853	-	64,68,73	1.28	6 (9%)	76,107,113	1.64	7 (9%)

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
19	CLA	A	812	-	1/1/15/20	25/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	312	-	1/1/11/20	3/15/91/115	-
23	BCR	A	843	-	-	11/29/63/63	0/2/2/2
19	CLA	2	308	2	1/1/11/20	5/15/91/115	-
19	CLA	2	312	-	1/1/15/20	20/39/115/115	-
22	LHG	B	848	19	-	9/49/49/53	-
28	DGD	B	846	-	-	8/55/95/95	0/2/2/2
23	BCR	1	318	-	-	8/29/63/63	0/2/2/2
23	BCR	B	840	-	-	0/29/63/63	0/2/2/2
23	BCR	A	847	-	-	3/29/63/63	0/2/2/2
19	CLA	A	819	-	1/1/11/20	0/15/91/115	-
19	CLA	3	302	3	1/1/14/20	8/33/109/115	-
24	LMG	1	319	-	-	12/45/65/70	0/1/1/1
23	BCR	2	319	-	-	9/29/63/63	0/2/2/2
19	CLA	B	817	-	1/1/14/20	15/33/109/115	-
20	LUT	2	315	-	-	0/29/67/67	0/2/2/2
19	CLA	1	304	-	1/1/12/20	10/23/99/115	-
19	CLA	1	312	-	1/1/14/20	13/33/109/115	-
23	BCR	4	317	-	-	2/29/63/63	0/2/2/2
19	CLA	H	201	12	1/1/11/20	11/15/91/115	-
24	LMG	4	318	-	-	5/31/51/70	0/1/1/1
19	CLA	B	805	6	1/1/15/20	13/39/115/115	-
19	CLA	2	313	-	1/1/13/20	8/31/107/115	-
19	CLA	B	801	-	1/1/15/20	11/39/115/115	-
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
19	CLA	B	808	6	1/1/15/20	12/39/115/115	-
19	CLA	A	808	5	1/1/14/20	14/36/112/115	-
19	CLA	1	307	-	1/1/11/20	5/15/91/115	-
23	BCR	J	103	-	-	0/29/63/63	0/2/2/2
18	CHL	1	301	1	3/3/18/26	8/27/125/137	-
19	CLA	A	804	-	1/1/15/20	18/39/115/115	-
19	CLA	B	815	-	1/1/13/20	4/27/103/115	-
19	CLA	A	815	-	1/1/11/20	3/15/91/115	-
19	CLA	B	811	-	1/1/13/20	10/27/103/115	-
22	LHG	1	322	-	-	9/53/53/53	-
19	CLA	A	816	-	1/1/15/20	13/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LUT	1	315	-	-	0/29/67/67	0/2/2/2
19	CLA	B	819	-	1/1/12/20	7/21/97/115	-
24	LMG	F	307	-	-	2/25/45/70	0/1/1/1
19	CLA	B	813	-	1/1/15/20	16/39/115/115	-
19	CLA	B	807	-	1/1/15/20	12/39/115/115	-
19	CLA	B	836	-	1/1/11/20	0/18/94/115	-
19	CLA	A	854	-	1/1/15/20	14/39/115/115	-
19	CLA	A	807	5	1/1/15/20	21/39/115/115	-
19	CLA	3	309	3	1/1/12/20	5/21/97/115	-
21	XAT	2	316	-	-	2/31/93/93	0/4/4/4
18	CHL	4	306	-	3/3/17/26	5/21/119/137	-
21	XAT	3	316	-	-	0/31/93/93	0/4/4/4
20	LUT	4	315	-	-	1/29/67/67	0/2/2/2
19	CLA	A	840	-	1/1/15/20	18/39/115/115	-
19	CLA	4	303	-	1/1/11/20	7/15/91/115	-
19	CLA	B	837	-	1/1/15/20	15/39/115/115	-
19	CLA	F	304	10	1/1/11/20	7/15/91/115	-
19	CLA	3	311	-	1/1/11/20	4/15/91/115	-
19	CLA	G	203	-	1/1/12/20	6/21/97/115	-
21	XAT	4	316	-	-	0/31/93/93	0/4/4/4
19	CLA	1	303	-	1/1/13/20	9/31/107/115	-
19	CLA	A	824	-	1/1/15/20	14/39/115/115	-
19	CLA	B	814	-	1/1/13/20	6/27/103/115	-
19	CLA	4	313	-	1/1/15/20	18/39/115/115	-
19	CLA	4	301	4	1/1/14/20	7/33/109/115	-
19	CLA	A	817	-	1/1/13/20	7/27/103/115	-
19	CLA	3	308	3	1/1/15/20	18/39/115/115	-
19	CLA	2	320	4	1/1/11/20	1/17/93/115	-
18	CHL	2	301	2	3/3/17/26	10/21/119/137	-
19	CLA	A	829	-	1/1/15/20	19/39/115/115	-
19	CLA	A	826	-	1/1/15/20	16/39/115/115	-
19	CLA	K	202	-	1/1/11/20	7/15/91/115	-
19	CLA	A	821	-	1/1/11/20	4/15/91/115	-
19	CLA	B	812	-	1/1/15/20	16/39/115/115	-
23	BCR	K	201	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	835	-	1/1/12/20	9/23/99/115	-
27	SF4	A	850	6,5	-	-	0/6/5/5
23	BCR	L	306	-	-	1/29/63/63	0/2/2/2
20	LUT	3	315	-	-	1/29/67/67	0/2/2/2
19	CLA	B	832	-	1/1/15/20	17/39/115/115	-
23	BCR	A	844	-	-	1/29/63/63	0/2/2/2
19	CLA	B	831	-	1/1/13/20	16/31/107/115	-
23	BCR	B	842	-	-	9/29/63/63	0/2/2/2
19	CLA	F	303	-	1/1/11/20	4/15/91/115	-
19	CLA	2	309	2	1/1/13/20	12/30/106/115	-
19	CLA	3	305	-	1/1/10/20	2/12/88/115	-
19	CLA	A	839	-	1/1/15/20	14/39/115/115	-
19	CLA	1	311	1	1/1/11/20	7/15/91/115	-
19	CLA	B	804	-	1/1/15/20	12/39/115/115	-
19	CLA	B	824	-	1/1/14/20	9/33/109/115	-
19	CLA	A	814	-	1/1/12/20	7/21/97/115	-
19	CLA	3	301	3	1/1/14/20	15/33/109/115	-
18	CHL	4	304	-	3/3/18/26	5/27/125/137	-
19	CLA	4	302	-	1/1/14/20	12/33/109/115	-
19	CLA	2	311	2	1/1/11/20	6/15/91/115	-
19	CLA	A	809	-	1/1/13/20	9/32/108/115	-
19	CLA	3	306	3	1/1/11/20	5/15/91/115	-
19	CLA	G	204	11	1/1/11/20	5/17/93/115	-
19	CLA	A	825	-	1/1/15/20	5/39/115/115	-
19	CLA	4	307	4	1/1/12/20	5/21/97/115	-
19	CLA	B	803	-	1/1/11/20	6/15/91/115	-
19	CLA	A	806	-	1/1/12/20	4/21/97/115	-
19	CLA	4	309	-	1/1/14/20	9/33/109/115	-
19	CLA	B	828	-	1/1/15/20	17/39/115/115	-
19	CLA	A	820	-	1/1/15/20	14/39/115/115	-
19	CLA	A	833	-	1/1/12/20	5/21/97/115	-
19	CLA	B	835	-	1/1/15/20	13/39/115/115	-
19	CLA	4	310	4	1/1/11/20	5/15/91/115	-
18	CHL	4	314	4	3/3/15/26	0/10/108/137	-
19	CLA	B	827	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	I	101	-	-	0/29/63/63	0/2/2/2
25	LMT	2	318	-	-	7/21/61/61	0/2/2/2
18	CHL	3	307	-	3/3/16/26	4/17/115/137	-
19	CLA	A	831	-	1/1/15/20	14/39/115/115	-
19	CLA	B	822	-	1/1/14/20	16/33/109/115	-
23	BCR	B	841	-	-	4/29/63/63	0/2/2/2
19	CLA	A	818	-	1/1/15/20	17/39/115/115	-
27	SF4	C	102	7	-	-	0/6/5/5
19	CLA	F	301	-	1/1/14/20	16/38/114/115	-
19	CLA	1	305	-	1/1/10/20	3/12/88/115	-
19	CLA	B	825	-	1/1/15/20	15/39/115/115	-
22	LHG	A	842	-	-	7/53/53/53	-
23	BCR	3	317	-	-	2/29/63/63	0/2/2/2
19	CLA	A	811	-	1/1/12/20	6/26/102/115	-
19	CLA	B	830	-	1/1/14/20	15/33/109/115	-
19	CLA	1	302	1	1/1/14/20	10/33/109/115	-
19	CLA	A	803	19	1/1/12/20	7/21/97/115	-
19	CLA	A	838	-	1/1/15/20	12/39/115/115	-
19	CLA	A	802	-	1/1/15/20	12/39/115/115	-
19	CLA	A	836	-	1/1/15/20	14/39/115/115	-
19	CLA	2	304	-	1/1/15/20	18/39/115/115	-
21	XAT	1	316	-	-	0/31/93/93	0/4/4/4
24	LMG	B	847	-	-	11/47/67/70	0/1/1/1
19	CLA	A	801	-	1/1/15/20	11/39/115/115	-
23	BCR	L	305	-	-	2/29/63/63	0/2/2/2
23	BCR	A	845	-	-	2/29/63/63	0/2/2/2
19	CLA	J	102	-	1/1/10/20	3/12/88/115	-
19	CLA	L	301	15	1/1/13/20	15/27/103/115	-
23	BCR	J	104	-	-	4/29/63/63	0/2/2/2
19	CLA	A	827	-	1/1/15/20	13/39/115/115	-
19	CLA	B	810	-	1/1/13/20	10/25/101/115	-
19	CLA	K	203	-	1/1/11/20	5/17/93/115	-
19	CLA	B	833	-	1/1/11/20	5/15/91/115	-
19	CLA	A	810	19	1/1/15/20	14/39/115/115	-
19	CLA	4	308	4	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	J	101	-	-	11/29/63/63	0/2/2/2
27	SF4	C	101	7	-	-	0/6/5/5
19	CLA	B	821	-	1/1/13/20	5/27/103/115	-
20	LUT	1	320	-	-	0/29/67/67	0/2/2/2
26	PQN	B	839	-	-	5/23/43/43	0/2/2/2
23	BCR	F	305	-	-	2/29/63/63	0/2/2/2
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
19	CLA	A	822	-	1/1/12/20	11/23/99/115	-
19	CLA	B	806	-	1/1/12/20	5/26/102/115	-
23	BCR	G	205	-	-	1/29/63/63	0/2/2/2
19	CLA	3	314	-	1/1/11/20	9/17/93/115	-
23	BCR	F	306	-	-	0/29/63/63	0/2/2/2
18	CHL	2	307	-	3/3/16/26	5/15/113/137	-
19	CLA	A	832	-	1/1/15/20	16/39/115/115	-
19	CLA	B	809	-	1/1/15/20	17/39/115/115	-
19	CLA	B	816	-	1/1/13/20	12/32/108/115	-
19	CLA	2	302	2	1/1/15/20	12/39/115/115	-
18	CHL	1	306	-	3/3/16/26	5/15/113/137	-
22	LHG	1	317	19	-	8/53/53/53	-
19	CLA	A	852	-	1/1/15/20	15/39/115/115	-
19	CLA	3	304	-	1/1/11/20	8/18/94/115	-
18	CHL	2	305	-	3/3/15/26	4/12/110/137	-
22	LHG	2	317	19	-	8/41/41/53	-
18	CHL	2	314	2	2/2/15/26	6/12/110/137	-
19	CLA	G	202	-	1/1/10/20	4/10/86/115	-
26	PQN	A	841	-	-	2/23/43/43	0/2/2/2
19	CLA	A	834	-	1/1/15/20	17/39/115/115	-
19	CLA	A	851	5	1/1/11/20	4/15/91/115	-
19	CLA	B	826	-	1/1/15/20	17/39/115/115	-
23	BCR	L	304	-	-	4/29/63/63	0/2/2/2
19	CLA	1	308	1	1/1/13/20	9/30/106/115	-
19	CLA	A	837	-	1/1/12/20	12/24/100/115	-
18	CHL	4	305	-	3/3/16/26	5/15/113/137	-
19	CLA	A	805	5	1/1/15/20	17/39/115/115	-
19	CLA	1	314	1	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	829	-	1/1/12/20	9/21/97/115	-
19	CLA	B	838	-	1/1/15/20	14/39/115/115	-
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
19	CLA	3	312	-	1/1/13/20	6/27/103/115	-
19	CLA	F	302	-	1/1/15/20	20/39/115/115	-
25	LMT	G	201	-	-	3/21/61/61	0/2/2/2
19	CLA	4	311	-	1/1/13/20	8/29/105/115	-
19	CLA	1	321	22	1/1/15/20	14/39/115/115	-
19	CLA	1	309	1	1/1/13/20	7/29/105/115	-
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
19	CLA	3	313	-	1/1/11/20	5/15/91/115	-
19	CLA	B	834	-	1/1/13/20	6/27/103/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
19	CLA	L	303	-	1/1/12/20	11/21/97/115	-
19	CLA	1	313	-	1/1/11/20	7/15/91/115	-
19	CLA	A	830	-	1/1/12/20	8/21/97/115	-
19	CLA	B	802	-	1/1/15/20	15/39/115/115	-
18	CHL	2	306	-	3/3/16/26	8/15/113/137	-
19	CLA	2	310	22	1/1/10/20	2/10/86/115	-
19	CLA	B	818	-	1/1/14/20	8/33/109/115	-
19	CLA	B	820	-	1/1/13/20	11/27/103/115	-
19	CLA	L	302	-	1/1/15/20	21/39/115/115	-
19	CLA	3	310	-	1/1/10/20	4/10/86/115	-
23	BCR	B	843	-	-	0/29/63/63	0/2/2/2
19	CLA	2	303	-	1/1/12/20	6/21/97/115	-
19	CLA	A	828	-	1/1/15/20	14/39/115/115	-
25	LMT	N	201	-	-	5/21/61/61	0/2/2/2
19	CLA	B	823	-	1/1/15/20	18/39/115/115	-
19	CLA	A	813	-	1/1/11/20	4/15/91/115	-
19	CLA	3	303	-	1/1/11/20	6/15/91/115	-
19	CLA	A	823	-	1/1/13/20	6/27/103/115	-
19	CLA	1	310	22	1/1/13/20	5/27/103/115	-
19	CLA	K	204	16	1/1/8/20	0/4/76/115	-
19	CLA	A	853	-	1/1/14/20	16/33/109/115	-

All (1135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	301	CHL	C3B-C4B	5.74	1.47	1.41
18	2	314	CHL	C3B-C4B	5.73	1.47	1.41
18	2	305	CHL	CMC-C2C	5.72	1.56	1.44
18	4	304	CHL	CMC-C2C	5.72	1.56	1.44
18	2	301	CHL	CMC-C2C	5.72	1.56	1.44
18	2	307	CHL	CMC-C2C	5.69	1.56	1.44
18	1	306	CHL	CMC-C2C	5.68	1.56	1.44
18	1	301	CHL	CMC-C2C	5.67	1.56	1.44
18	4	305	CHL	CMC-C2C	5.67	1.56	1.44
18	2	306	CHL	C3B-C4B	5.67	1.46	1.41
18	2	314	CHL	CMC-C2C	5.67	1.56	1.44
18	4	314	CHL	CMC-C2C	5.67	1.56	1.44
18	3	307	CHL	CMC-C2C	5.66	1.56	1.44
18	4	306	CHL	CMC-C2C	5.65	1.56	1.44
18	2	306	CHL	CMC-C2C	5.64	1.56	1.44
18	1	306	CHL	C3B-C4B	5.64	1.46	1.41
18	2	305	CHL	C3B-C4B	5.55	1.46	1.41
18	4	304	CHL	C3B-C4B	5.54	1.46	1.41
18	1	301	CHL	C3B-C4B	5.54	1.46	1.41
18	4	314	CHL	C3B-C4B	5.53	1.46	1.41
18	4	305	CHL	C3B-C4B	5.51	1.46	1.41
18	4	306	CHL	C3B-C4B	5.48	1.46	1.41
18	3	307	CHL	C3B-C4B	5.44	1.46	1.41
18	2	307	CHL	C3B-C4B	5.41	1.46	1.41
18	2	314	CHL	C1D-C2D	5.20	1.45	1.39
19	3	311	CLA	MG-NA	5.07	2.18	2.06
18	2	305	CHL	C1D-C2D	5.06	1.45	1.39
18	4	305	CHL	C1D-C2D	5.05	1.45	1.39
19	A	831	CLA	MG-NA	5.05	2.18	2.06
18	3	307	CHL	C1D-C2D	5.05	1.45	1.39
19	4	310	CLA	MG-NA	5.05	2.18	2.06
18	2	306	CHL	C1D-C2D	5.05	1.45	1.39
19	F	304	CLA	MG-NA	5.05	2.18	2.06
19	A	815	CLA	MG-NA	5.04	2.18	2.06
19	B	805	CLA	MG-NA	5.04	2.18	2.06
19	B	834	CLA	MG-NA	5.04	2.18	2.06
18	4	304	CHL	C1D-C2D	5.03	1.45	1.39
19	4	302	CLA	MG-NA	5.03	2.18	2.06
19	3	305	CLA	MG-NA	5.02	2.18	2.06
19	K	204	CLA	MG-NA	5.02	2.18	2.06
19	B	811	CLA	MG-NA	5.01	2.18	2.06
19	1	304	CLA	MG-NA	5.01	2.18	2.06
19	F	303	CLA	MG-NA	5.01	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	829	CLA	MG-NA	5.01	2.18	2.06
19	1	311	CLA	MG-NA	5.01	2.18	2.06
19	2	311	CLA	MG-NA	5.01	2.18	2.06
19	A	821	CLA	MG-NA	5.01	2.18	2.06
19	4	311	CLA	MG-NA	5.01	2.18	2.06
19	4	313	CLA	MG-NA	5.01	2.18	2.06
19	K	202	CLA	MG-NA	5.01	2.18	2.06
19	3	310	CLA	MG-NA	5.01	2.18	2.06
19	2	304	CLA	MG-NA	5.01	2.18	2.06
19	A	839	CLA	MG-NA	5.00	2.18	2.06
18	1	306	CHL	C1D-C2D	5.00	1.45	1.39
19	1	310	CLA	MG-NA	5.00	2.18	2.06
19	3	312	CLA	MG-NA	5.00	2.18	2.06
19	3	313	CLA	MG-NA	5.00	2.18	2.06
19	K	203	CLA	MG-NA	5.00	2.18	2.06
19	3	304	CLA	MG-NA	5.00	2.18	2.06
19	A	832	CLA	MG-NA	5.00	2.18	2.06
19	A	837	CLA	MG-NA	5.00	2.18	2.06
19	A	836	CLA	MG-NA	5.00	2.18	2.06
19	A	851	CLA	MG-NA	5.00	2.18	2.06
19	B	836	CLA	MG-NA	5.00	2.18	2.06
18	1	301	CHL	C1D-C2D	4.99	1.45	1.39
19	2	313	CLA	MG-NA	4.99	2.18	2.06
19	2	312	CLA	MG-NA	4.99	2.18	2.06
19	3	314	CLA	MG-NA	4.99	2.18	2.06
19	B	837	CLA	MG-NA	4.99	2.18	2.06
19	A	822	CLA	MG-NA	4.99	2.18	2.06
19	A	835	CLA	MG-NA	4.99	2.18	2.06
19	H	201	CLA	MG-NA	4.99	2.18	2.06
19	B	814	CLA	MG-NA	4.99	2.18	2.06
19	3	302	CLA	MG-NA	4.99	2.18	2.06
19	4	307	CLA	MG-NA	4.99	2.18	2.06
19	B	830	CLA	MG-NA	4.99	2.18	2.06
19	A	828	CLA	MG-NA	4.99	2.18	2.06
19	1	305	CLA	MG-NA	4.99	2.18	2.06
19	B	833	CLA	MG-NA	4.99	2.18	2.06
19	A	801	CLA	MG-NA	4.98	2.18	2.06
19	B	821	CLA	MG-NA	4.98	2.18	2.06
19	1	302	CLA	MG-NA	4.98	2.18	2.06
19	1	312	CLA	MG-NA	4.98	2.18	2.06
18	4	306	CHL	C1D-C2D	4.98	1.45	1.39
19	L	303	CLA	MG-NA	4.98	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	303	CLA	MG-NA	4.98	2.18	2.06
19	1	307	CLA	MG-NA	4.98	2.18	2.06
19	G	204	CLA	MG-NA	4.97	2.18	2.06
19	B	828	CLA	MG-NA	4.97	2.18	2.06
19	B	832	CLA	MG-NA	4.97	2.18	2.06
19	2	303	CLA	MG-NA	4.97	2.18	2.06
19	A	817	CLA	MG-NA	4.97	2.18	2.06
19	B	819	CLA	MG-NA	4.97	2.18	2.06
19	B	808	CLA	MG-NA	4.97	2.18	2.06
19	B	820	CLA	MG-NA	4.97	2.18	2.06
19	A	804	CLA	MG-NA	4.97	2.18	2.06
19	1	303	CLA	MG-NA	4.97	2.18	2.06
19	A	812	CLA	MG-NA	4.97	2.18	2.06
19	4	309	CLA	MG-NA	4.97	2.18	2.06
19	B	810	CLA	MG-NA	4.97	2.18	2.06
19	G	202	CLA	MG-NA	4.97	2.18	2.06
19	A	840	CLA	MG-NA	4.97	2.18	2.06
19	L	301	CLA	MG-NA	4.97	2.18	2.06
19	3	301	CLA	MG-NA	4.97	2.18	2.06
19	F	301	CLA	MG-NA	4.97	2.18	2.06
19	B	812	CLA	MG-NA	4.96	2.18	2.06
18	4	314	CHL	C1D-C2D	4.96	1.45	1.39
19	A	806	CLA	MG-NA	4.96	2.18	2.06
19	B	804	CLA	MG-NA	4.96	2.18	2.06
18	2	307	CHL	C1D-C2D	4.96	1.45	1.39
19	B	815	CLA	MG-NA	4.96	2.18	2.06
19	A	824	CLA	MG-NA	4.96	2.18	2.06
19	A	826	CLA	MG-NA	4.96	2.18	2.06
19	3	303	CLA	MG-NA	4.96	2.18	2.06
19	B	809	CLA	MG-NA	4.96	2.18	2.06
19	A	818	CLA	MG-NA	4.95	2.18	2.06
19	A	814	CLA	MG-NA	4.95	2.18	2.06
19	A	830	CLA	MG-NA	4.95	2.18	2.06
19	G	203	CLA	MG-NA	4.95	2.18	2.06
19	B	806	CLA	MG-NA	4.95	2.18	2.06
19	B	813	CLA	MG-NA	4.95	2.18	2.06
19	B	823	CLA	MG-NA	4.95	2.18	2.06
19	A	854	CLA	MG-NA	4.95	2.18	2.06
19	B	807	CLA	MG-NA	4.95	2.18	2.06
19	A	803	CLA	MG-NA	4.94	2.18	2.06
19	A	811	CLA	MG-NA	4.94	2.18	2.06
19	A	825	CLA	MG-NA	4.94	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	810	CLA	MG-NA	4.94	2.18	2.06
19	2	310	CLA	MG-NA	4.94	2.18	2.06
19	J	102	CLA	MG-NA	4.94	2.18	2.06
19	A	816	CLA	MG-NA	4.94	2.18	2.06
19	B	818	CLA	MG-NA	4.94	2.18	2.06
19	L	302	CLA	MG-NA	4.94	2.18	2.06
19	1	321	CLA	MG-NA	4.93	2.18	2.06
19	1	308	CLA	MG-NA	4.93	2.18	2.06
19	B	817	CLA	MG-NA	4.93	2.18	2.06
19	2	302	CLA	MG-NA	4.93	2.18	2.06
19	A	813	CLA	MG-NA	4.93	2.18	2.06
19	1	309	CLA	MG-NA	4.93	2.18	2.06
19	B	803	CLA	MG-NA	4.93	2.18	2.06
19	A	833	CLA	MG-NA	4.93	2.18	2.06
19	A	853	CLA	MG-NA	4.93	2.18	2.06
19	A	834	CLA	MG-NA	4.93	2.18	2.06
19	A	809	CLA	MG-NA	4.92	2.18	2.06
19	B	825	CLA	MG-NA	4.92	2.18	2.06
19	A	808	CLA	MG-NA	4.92	2.18	2.06
19	A	819	CLA	MG-NA	4.92	2.18	2.06
19	3	308	CLA	MG-NA	4.92	2.18	2.06
19	3	309	CLA	MG-NA	4.92	2.18	2.06
19	A	805	CLA	MG-NA	4.92	2.17	2.06
19	2	308	CLA	MG-NA	4.91	2.17	2.06
19	4	312	CLA	MG-NA	4.91	2.17	2.06
19	A	823	CLA	MG-NA	4.91	2.17	2.06
19	B	824	CLA	MG-NA	4.91	2.17	2.06
19	3	306	CLA	MG-NA	4.91	2.17	2.06
19	A	838	CLA	MG-NA	4.91	2.17	2.06
19	B	827	CLA	MG-NA	4.91	2.17	2.06
19	2	309	CLA	MG-NA	4.91	2.17	2.06
19	B	826	CLA	MG-NA	4.91	2.17	2.06
19	B	835	CLA	MG-NA	4.91	2.17	2.06
19	B	801	CLA	MG-NA	4.90	2.17	2.06
18	2	301	CHL	C1D-C2D	4.90	1.45	1.39
19	B	838	CLA	MG-NA	4.90	2.17	2.06
19	4	301	CLA	MG-NA	4.90	2.17	2.06
19	A	820	CLA	MG-NA	4.90	2.17	2.06
19	B	829	CLA	MG-NA	4.90	2.17	2.06
19	F	302	CLA	MG-NA	4.90	2.17	2.06
19	2	320	CLA	MG-NA	4.89	2.17	2.06
19	1	314	CLA	MG-NA	4.89	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	802	CLA	MG-NA	4.88	2.17	2.06
19	A	802	CLA	MG-NA	4.88	2.17	2.06
19	B	831	CLA	MG-NA	4.88	2.17	2.06
19	A	807	CLA	MG-NA	4.88	2.17	2.06
19	1	313	CLA	MG-NA	4.87	2.17	2.06
19	A	852	CLA	MG-NA	4.87	2.17	2.06
19	4	308	CLA	MG-NA	4.86	2.17	2.06
19	A	827	CLA	MG-NA	4.85	2.17	2.06
19	B	816	CLA	MG-NA	4.85	2.17	2.06
19	B	822	CLA	MG-NA	4.83	2.17	2.06
18	2	305	CHL	C1B-C2B	4.81	1.45	1.39
18	2	307	CHL	C1B-C2B	4.80	1.45	1.39
18	4	305	CHL	C1B-C2B	4.79	1.45	1.39
18	2	306	CHL	C1B-C2B	4.78	1.45	1.39
18	2	314	CHL	C1B-C2B	4.77	1.45	1.39
18	4	314	CHL	C1B-C2B	4.77	1.45	1.39
18	4	306	CHL	C1B-C2B	4.74	1.44	1.39
18	4	304	CHL	C1B-C2B	4.72	1.44	1.39
18	1	301	CHL	C1B-C2B	4.70	1.44	1.39
18	1	306	CHL	C1B-C2B	4.68	1.44	1.39
18	2	301	CHL	C1B-C2B	4.67	1.44	1.39
18	3	307	CHL	C1B-C2B	4.65	1.44	1.39
18	2	307	CHL	CHA-CBD	3.65	1.55	1.51
18	2	306	CHL	CHA-CBD	3.65	1.55	1.51
18	2	305	CHL	CHA-CBD	3.62	1.55	1.51
18	2	314	CHL	CHA-CBD	3.60	1.55	1.51
18	4	304	CHL	CHA-CBD	3.60	1.55	1.51
18	2	301	CHL	CHA-CBD	3.58	1.55	1.51
18	4	306	CHL	CHA-CBD	3.58	1.55	1.51
18	4	314	CHL	CHA-CBD	3.57	1.55	1.51
18	4	305	CHL	CHA-CBD	3.57	1.55	1.51
18	1	306	CHL	CHA-CBD	3.57	1.55	1.51
18	1	301	CHL	CHA-CBD	3.55	1.55	1.51
18	4	304	CHL	C3B-C2B	-3.54	1.35	1.40
18	3	307	CHL	C3B-C2B	-3.53	1.35	1.40
18	2	307	CHL	C3B-C2B	-3.52	1.35	1.40
18	3	307	CHL	CHA-CBD	3.49	1.55	1.51
18	4	314	CHL	O2D-CGD	3.46	1.41	1.30
18	4	314	CHL	C3B-C2B	-3.45	1.35	1.40
18	4	305	CHL	C3B-C2B	-3.45	1.35	1.40
18	2	306	CHL	O2D-CGD	3.45	1.41	1.33
18	2	314	CHL	O2D-CGD	3.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	306	CHL	C3B-C2B	-3.44	1.35	1.40
18	2	301	CHL	C3B-C2B	-3.44	1.35	1.40
18	2	301	CHL	O2D-CGD	3.44	1.41	1.33
18	4	306	CHL	C3B-C2B	-3.44	1.35	1.40
18	2	305	CHL	O2D-CGD	3.44	1.41	1.33
18	4	305	CHL	O2D-CGD	3.44	1.41	1.33
18	1	306	CHL	O2D-CGD	3.44	1.41	1.33
18	2	307	CHL	O2D-CGD	3.42	1.41	1.33
18	4	304	CHL	O2D-CGD	3.42	1.41	1.33
18	1	301	CHL	O2D-CGD	3.41	1.41	1.33
18	2	305	CHL	C3B-C2B	-3.41	1.35	1.40
18	1	306	CHL	O2A-CGA	3.40	1.42	1.30
18	4	305	CHL	O2A-CGA	3.39	1.42	1.30
18	4	306	CHL	O2D-CGD	3.39	1.41	1.33
18	2	307	CHL	O2A-CGA	3.39	1.42	1.30
18	2	306	CHL	O2A-CGA	3.38	1.42	1.30
18	3	307	CHL	O2D-CGD	3.38	1.41	1.33
18	2	306	CHL	C3B-C2B	-3.38	1.35	1.40
18	1	301	CHL	C3B-C2B	-3.35	1.35	1.40
18	2	314	CHL	C3B-C2B	-3.27	1.35	1.40
18	2	314	CHL	C1A-CHA	3.07	1.43	1.40
18	1	301	CHL	O2A-CGA	2.96	1.42	1.33
18	4	306	CHL	O2A-CGA	2.96	1.42	1.33
18	4	304	CHL	O2A-CGA	2.95	1.42	1.33
18	2	301	CHL	O2A-CGA	2.94	1.41	1.33
18	3	307	CHL	O2A-CGA	2.92	1.42	1.33
18	2	307	CHL	C1A-CHA	2.90	1.43	1.40
18	1	306	CHL	C1A-CHA	2.86	1.43	1.40
20	1	315	LUT	C8-C9	-2.85	1.39	1.46
18	3	307	CHL	C1A-CHA	2.84	1.43	1.40
20	1	320	LUT	C8-C9	-2.83	1.39	1.46
18	2	301	CHL	C1A-CHA	2.82	1.43	1.40
18	4	314	CHL	C1A-CHA	2.80	1.43	1.40
20	2	315	LUT	C8-C9	-2.80	1.40	1.46
18	2	306	CHL	C1A-CHA	2.80	1.43	1.40
20	3	315	LUT	C8-C9	-2.79	1.40	1.46
20	4	315	LUT	C8-C9	-2.79	1.40	1.46
18	4	304	CHL	C1A-CHA	2.78	1.43	1.40
18	2	305	CHL	C1A-CHA	2.75	1.43	1.40
18	4	306	CHL	C1A-CHA	2.74	1.43	1.40
18	4	305	CHL	C1A-CHA	2.74	1.43	1.40
18	1	301	CHL	C1A-CHA	2.72	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	304	CHL	C2C-C3C	2.63	1.38	1.36
19	A	808	CLA	C1D-ND	-2.62	1.34	1.37
18	1	306	CHL	C2C-C3C	2.62	1.38	1.36
19	A	804	CLA	C1D-ND	-2.60	1.34	1.37
18	2	305	CHL	MG-NB	2.59	2.10	2.05
19	B	822	CLA	CHC-C1C	2.59	1.43	1.38
19	B	822	CLA	C1D-ND	-2.59	1.34	1.37
18	4	304	CHL	C2-C3	2.58	1.39	1.33
19	1	308	CLA	C1D-ND	-2.57	1.34	1.37
18	1	301	CHL	C2-C3	2.57	1.39	1.33
18	4	305	CHL	MG-NB	2.57	2.10	2.05
18	2	305	CHL	C2C-C3C	2.56	1.38	1.36
18	4	306	CHL	MG-NB	2.56	2.10	2.05
19	A	806	CLA	C1D-ND	-2.56	1.34	1.37
19	A	834	CLA	C1D-ND	-2.56	1.34	1.37
18	4	304	CHL	MG-NB	2.56	2.10	2.05
19	A	852	CLA	C1D-ND	-2.56	1.34	1.37
19	B	824	CLA	C1D-ND	-2.56	1.34	1.37
19	B	820	CLA	C1D-ND	-2.55	1.34	1.37
19	B	801	CLA	C1D-ND	-2.55	1.34	1.37
19	B	802	CLA	C1D-ND	-2.55	1.34	1.37
19	B	829	CLA	C1D-ND	-2.55	1.34	1.37
19	B	831	CLA	C1D-ND	-2.55	1.34	1.37
19	A	825	CLA	C1D-ND	-2.54	1.34	1.37
19	A	803	CLA	C1D-ND	-2.54	1.34	1.37
19	L	302	CLA	C1D-ND	-2.54	1.34	1.37
19	A	808	CLA	CHC-C1C	2.54	1.43	1.38
19	A	833	CLA	C1D-ND	-2.53	1.34	1.37
19	B	816	CLA	C1D-ND	-2.53	1.34	1.37
18	4	314	CHL	MG-NB	2.53	2.10	2.05
19	F	302	CLA	CHC-C1C	2.53	1.43	1.38
19	3	308	CLA	C1D-ND	-2.53	1.34	1.37
19	B	827	CLA	C1D-ND	-2.53	1.34	1.37
19	B	804	CLA	C1D-ND	-2.53	1.34	1.37
19	A	807	CLA	C1D-ND	-2.52	1.34	1.37
19	A	820	CLA	C1D-ND	-2.52	1.34	1.37
19	B	809	CLA	C1D-ND	-2.52	1.34	1.37
19	4	313	CLA	C1D-ND	-2.52	1.34	1.37
19	A	827	CLA	C1D-ND	-2.52	1.34	1.37
19	B	828	CLA	C1D-ND	-2.52	1.34	1.37
19	B	833	CLA	C1D-ND	-2.52	1.34	1.37
19	A	811	CLA	C1D-ND	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	806	CLA	C1D-ND	-2.52	1.34	1.37
19	A	826	CLA	C1D-ND	-2.52	1.34	1.37
19	B	826	CLA	C1D-ND	-2.52	1.34	1.37
19	A	809	CLA	C1D-ND	-2.52	1.34	1.37
19	A	821	CLA	C1D-ND	-2.52	1.34	1.37
19	B	825	CLA	C1D-ND	-2.51	1.34	1.37
18	2	306	CHL	MG-NB	2.51	2.10	2.05
19	B	813	CLA	CHC-C1C	2.51	1.43	1.38
19	A	818	CLA	C1D-ND	-2.51	1.34	1.37
19	B	808	CLA	C1D-ND	-2.51	1.34	1.37
19	B	815	CLA	C1D-ND	-2.51	1.34	1.37
19	A	827	CLA	CHC-C1C	2.51	1.43	1.38
19	A	813	CLA	C1D-ND	-2.51	1.34	1.37
19	3	303	CLA	C1D-ND	-2.50	1.34	1.37
19	B	818	CLA	C1D-ND	-2.50	1.34	1.37
19	B	823	CLA	C1D-ND	-2.50	1.34	1.37
19	F	301	CLA	C1D-ND	-2.50	1.34	1.37
19	4	307	CLA	C1D-ND	-2.50	1.34	1.37
19	B	815	CLA	CHC-C1C	2.50	1.43	1.38
19	B	813	CLA	C1D-ND	-2.50	1.34	1.37
18	2	301	CHL	MG-NB	2.49	2.10	2.05
19	B	835	CLA	C1D-ND	-2.49	1.34	1.37
19	B	837	CLA	C1D-ND	-2.49	1.34	1.37
19	4	301	CLA	C1D-ND	-2.49	1.34	1.37
19	A	828	CLA	C1D-ND	-2.49	1.34	1.37
19	A	830	CLA	C1D-ND	-2.49	1.34	1.37
19	B	810	CLA	C1D-ND	-2.49	1.34	1.37
19	1	310	CLA	C1D-ND	-2.49	1.34	1.37
19	A	802	CLA	C1D-ND	-2.49	1.34	1.37
19	A	809	CLA	CHC-C1C	2.49	1.43	1.38
19	A	838	CLA	C1D-ND	-2.49	1.34	1.37
19	A	814	CLA	C1D-ND	-2.49	1.34	1.37
19	B	824	CLA	CHC-C1C	2.49	1.43	1.38
19	2	313	CLA	C1D-ND	-2.48	1.34	1.37
19	A	806	CLA	CHC-C1C	2.48	1.43	1.38
19	A	835	CLA	C1D-ND	-2.48	1.34	1.37
19	B	832	CLA	C1D-ND	-2.48	1.34	1.37
18	1	306	CHL	MG-NB	2.48	2.10	2.05
19	B	807	CLA	C1D-ND	-2.48	1.34	1.37
18	2	307	CHL	MG-NB	2.48	2.10	2.05
19	A	838	CLA	CHC-C1C	2.48	1.43	1.38
19	3	314	CLA	C1D-ND	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	817	CLA	C1D-ND	-2.48	1.34	1.37
19	B	814	CLA	C1D-ND	-2.48	1.34	1.37
19	L	302	CLA	CHC-C1C	2.48	1.43	1.38
19	3	301	CLA	C1D-ND	-2.48	1.34	1.37
19	A	837	CLA	C1D-ND	-2.47	1.34	1.37
19	F	302	CLA	C1D-ND	-2.47	1.34	1.37
19	F	303	CLA	C1D-ND	-2.47	1.34	1.37
18	3	307	CHL	MG-NB	2.47	2.10	2.05
19	A	816	CLA	C1D-ND	-2.47	1.34	1.37
19	A	840	CLA	C1D-ND	-2.47	1.34	1.37
19	A	837	CLA	CHC-C1C	2.47	1.43	1.38
19	A	823	CLA	C1D-ND	-2.47	1.34	1.37
19	2	302	CLA	CHC-C1C	2.47	1.43	1.38
19	2	304	CLA	C1D-ND	-2.47	1.34	1.37
19	1	309	CLA	CHC-C1C	2.47	1.43	1.38
19	2	310	CLA	C1D-ND	-2.47	1.34	1.37
19	3	311	CLA	C1D-ND	-2.47	1.34	1.37
18	1	301	CHL	MG-NB	2.47	2.10	2.05
19	B	828	CLA	CHC-C1C	2.47	1.43	1.38
19	B	812	CLA	C1D-ND	-2.47	1.34	1.37
19	1	302	CLA	C1D-ND	-2.47	1.34	1.37
19	A	836	CLA	C1D-ND	-2.47	1.34	1.37
19	B	817	CLA	C1D-ND	-2.47	1.34	1.37
19	A	839	CLA	C1D-ND	-2.47	1.34	1.37
19	A	853	CLA	C1D-ND	-2.46	1.34	1.37
19	B	838	CLA	C1D-ND	-2.46	1.34	1.37
19	4	308	CLA	CHC-C1C	2.46	1.43	1.38
19	2	320	CLA	C1D-ND	-2.46	1.34	1.37
19	B	821	CLA	C1D-ND	-2.46	1.34	1.37
19	2	308	CLA	C1D-ND	-2.46	1.34	1.37
19	4	301	CLA	CHC-C1C	2.46	1.43	1.38
19	2	309	CLA	CHC-C1C	2.46	1.43	1.38
19	A	831	CLA	C1D-ND	-2.46	1.34	1.37
19	3	306	CLA	C1D-ND	-2.46	1.34	1.37
19	2	302	CLA	C1D-ND	-2.46	1.34	1.37
19	3	312	CLA	C1D-ND	-2.46	1.34	1.37
19	L	303	CLA	C1D-ND	-2.46	1.34	1.37
19	A	816	CLA	CHC-C1C	2.46	1.43	1.38
19	A	852	CLA	CHC-C1C	2.46	1.43	1.38
19	G	202	CLA	C1D-ND	-2.46	1.34	1.37
19	B	818	CLA	CHC-C1C	2.46	1.43	1.38
19	A	828	CLA	CHC-C1C	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	308	CLA	C1D-ND	-2.45	1.34	1.37
19	L	301	CLA	C1D-ND	-2.45	1.34	1.37
19	3	301	CLA	CHC-C1C	2.45	1.43	1.38
19	A	803	CLA	CHC-C1C	2.45	1.43	1.38
19	1	303	CLA	C1D-ND	-2.45	1.34	1.37
19	B	819	CLA	C1D-ND	-2.45	1.34	1.37
19	A	811	CLA	CHC-C1C	2.45	1.43	1.38
19	A	833	CLA	CHC-C1C	2.45	1.43	1.38
19	1	309	CLA	C1D-ND	-2.45	1.34	1.37
19	A	825	CLA	CHC-C1C	2.45	1.43	1.38
18	2	307	CHL	CBA-CGA	2.45	1.56	1.50
19	A	823	CLA	CHC-C1C	2.45	1.43	1.38
19	B	803	CLA	C1D-ND	-2.45	1.34	1.37
19	A	812	CLA	C1D-ND	-2.45	1.34	1.37
19	B	836	CLA	C1D-ND	-2.45	1.34	1.37
19	3	309	CLA	CHC-C1C	2.45	1.43	1.38
19	B	825	CLA	CHC-C1C	2.44	1.43	1.38
19	A	804	CLA	CHC-C1C	2.44	1.43	1.38
19	A	810	CLA	CHC-C1C	2.44	1.43	1.38
19	A	801	CLA	C1D-ND	-2.44	1.34	1.37
19	A	801	CLA	CHC-C1C	2.44	1.43	1.38
19	B	814	CLA	CHC-C1C	2.44	1.43	1.38
19	1	312	CLA	C1D-ND	-2.44	1.34	1.37
19	A	818	CLA	CHC-C1C	2.44	1.43	1.38
19	B	830	CLA	C1D-ND	-2.44	1.34	1.37
18	2	306	CHL	CBA-CGA	2.44	1.56	1.50
19	3	305	CLA	C1D-ND	-2.44	1.34	1.37
19	A	824	CLA	C1D-ND	-2.44	1.34	1.37
19	A	829	CLA	C1D-ND	-2.44	1.34	1.37
19	B	805	CLA	C1D-ND	-2.44	1.34	1.37
19	2	303	CLA	CHC-C1C	2.44	1.43	1.38
19	A	814	CLA	CHC-C1C	2.44	1.43	1.38
18	1	306	CHL	CBA-CGA	2.44	1.56	1.50
19	4	303	CLA	C1D-ND	-2.44	1.34	1.37
19	4	312	CLA	C1D-ND	-2.44	1.34	1.37
19	2	308	CLA	CHC-C1C	2.44	1.43	1.38
19	B	801	CLA	CHC-C1C	2.44	1.43	1.38
19	B	820	CLA	CHC-C1C	2.44	1.43	1.38
19	B	831	CLA	CHC-C1C	2.44	1.43	1.38
19	3	304	CLA	CHC-C1C	2.44	1.43	1.38
19	A	834	CLA	CHC-C1C	2.43	1.43	1.38
19	B	811	CLA	CHC-C1C	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	309	CLA	C1D-ND	-2.43	1.34	1.37
19	B	804	CLA	CHC-C1C	2.43	1.43	1.38
19	A	805	CLA	CHC-C1C	2.43	1.43	1.38
19	A	813	CLA	CHC-C1C	2.43	1.43	1.38
19	B	817	CLA	CHC-C1C	2.43	1.43	1.38
19	A	853	CLA	CHC-C1C	2.43	1.43	1.38
19	1	313	CLA	C1D-ND	-2.43	1.34	1.37
19	A	805	CLA	C1D-ND	-2.43	1.34	1.37
19	4	313	CLA	CHC-C1C	2.43	1.43	1.38
19	B	805	CLA	CHC-C1C	2.43	1.43	1.38
19	B	809	CLA	CHC-C1C	2.43	1.43	1.38
19	H	201	CLA	CHC-C1C	2.43	1.43	1.38
19	B	833	CLA	CHC-C1C	2.43	1.43	1.38
19	J	102	CLA	C1D-ND	-2.43	1.34	1.37
19	1	313	CLA	CHC-C1C	2.42	1.43	1.38
19	A	829	CLA	CHC-C1C	2.42	1.43	1.38
19	3	306	CLA	CHC-C1C	2.42	1.43	1.38
19	3	303	CLA	CHC-C1C	2.42	1.43	1.38
19	2	303	CLA	C1D-ND	-2.42	1.34	1.37
19	3	304	CLA	C1D-ND	-2.42	1.34	1.37
19	A	854	CLA	CHC-C1C	2.42	1.43	1.38
19	1	307	CLA	C1D-ND	-2.42	1.34	1.37
18	4	305	CHL	CBA-CGA	2.42	1.56	1.50
19	B	811	CLA	C1D-ND	-2.42	1.34	1.37
19	B	835	CLA	CHC-C1C	2.42	1.43	1.38
19	B	837	CLA	CHC-C1C	2.42	1.43	1.38
19	B	816	CLA	CHC-C1C	2.42	1.43	1.38
19	1	314	CLA	CHC-C1C	2.42	1.43	1.38
19	A	820	CLA	CHC-C1C	2.42	1.43	1.38
19	A	802	CLA	CHC-C1C	2.42	1.43	1.38
19	G	203	CLA	C1D-ND	-2.42	1.34	1.37
19	L	303	CLA	MG-NB	2.41	2.10	2.05
19	A	807	CLA	CHC-C1C	2.41	1.43	1.38
19	A	832	CLA	C1D-ND	-2.41	1.34	1.37
19	G	203	CLA	CHC-C1C	2.41	1.43	1.38
19	3	308	CLA	CHC-C1C	2.41	1.43	1.38
19	B	806	CLA	CHC-C1C	2.41	1.43	1.38
19	B	832	CLA	CHC-C1C	2.41	1.43	1.38
19	A	830	CLA	CHC-C1C	2.41	1.43	1.38
19	F	301	CLA	CHC-C1C	2.41	1.43	1.38
19	G	204	CLA	C1D-ND	-2.41	1.34	1.37
19	A	821	CLA	CHC-C1C	2.41	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	310	CLA	CHC-C1C	2.41	1.43	1.38
19	1	311	CLA	C1D-ND	-2.41	1.34	1.37
19	3	309	CLA	C1D-ND	-2.41	1.34	1.37
19	A	851	CLA	C1D-ND	-2.41	1.34	1.37
19	B	802	CLA	CHC-C1C	2.41	1.43	1.38
19	4	302	CLA	C1D-ND	-2.41	1.34	1.37
19	3	313	CLA	C1D-ND	-2.41	1.34	1.37
19	J	102	CLA	CHC-C1C	2.41	1.43	1.38
19	1	321	CLA	CHC-C1C	2.41	1.43	1.38
19	1	305	CLA	C1D-ND	-2.40	1.34	1.37
19	K	203	CLA	CHC-C1C	2.40	1.43	1.38
19	3	310	CLA	C1D-ND	-2.40	1.34	1.37
19	B	810	CLA	CHC-C1C	2.40	1.43	1.38
19	4	309	CLA	C1D-ND	-2.40	1.34	1.37
19	B	803	CLA	CHC-C1C	2.40	1.43	1.38
19	1	314	CLA	C1D-ND	-2.40	1.34	1.37
19	B	830	CLA	CHC-C1C	2.40	1.43	1.38
19	1	302	CLA	CHC-C1C	2.40	1.43	1.38
19	2	312	CLA	C1D-ND	-2.40	1.34	1.37
19	1	304	CLA	C1D-ND	-2.40	1.34	1.37
19	H	201	CLA	C1D-ND	-2.40	1.34	1.37
19	3	313	CLA	CHC-C1C	2.40	1.43	1.38
19	4	303	CLA	CHC-C1C	2.40	1.43	1.38
19	4	310	CLA	MG-NB	2.40	2.10	2.05
19	2	304	CLA	CHC-C1C	2.40	1.43	1.38
19	A	835	CLA	CHC-C1C	2.39	1.43	1.38
19	3	314	CLA	CHC-C1C	2.39	1.43	1.38
19	A	826	CLA	CHC-C1C	2.39	1.43	1.38
19	A	815	CLA	C1D-ND	-2.39	1.34	1.37
19	A	854	CLA	C1D-ND	-2.39	1.34	1.37
19	F	304	CLA	C1D-ND	-2.39	1.34	1.37
19	4	302	CLA	MG-NB	2.39	2.10	2.05
19	A	851	CLA	CHC-C1C	2.39	1.43	1.38
19	B	838	CLA	CHC-C1C	2.39	1.43	1.38
19	1	303	CLA	CHC-C1C	2.39	1.43	1.38
19	K	204	CLA	CHC-C1C	2.39	1.43	1.38
19	A	810	CLA	C1D-ND	-2.39	1.34	1.37
19	A	836	CLA	CHC-C1C	2.39	1.43	1.38
19	B	834	CLA	CHC-C1C	2.39	1.43	1.38
19	4	311	CLA	C1D-ND	-2.39	1.34	1.37
19	B	819	CLA	CHC-C1C	2.39	1.43	1.38
19	3	310	CLA	CHC-C1C	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	307	CLA	CHC-C1C	2.39	1.43	1.38
19	B	836	CLA	CHC-C1C	2.39	1.43	1.38
19	2	313	CLA	CHC-C1C	2.39	1.43	1.38
19	K	202	CLA	MG-NB	2.39	2.10	2.05
19	3	302	CLA	C1D-ND	-2.39	1.34	1.37
19	1	312	CLA	CHC-C1C	2.39	1.43	1.38
19	2	311	CLA	MG-NB	2.39	2.10	2.05
18	2	306	CHL	C2C-C3C	2.38	1.38	1.36
19	2	310	CLA	CHC-C1C	2.38	1.43	1.38
19	A	839	CLA	CHC-C1C	2.38	1.43	1.38
19	B	834	CLA	C1D-ND	-2.38	1.34	1.37
19	F	304	CLA	MG-NB	2.38	2.10	2.05
19	1	304	CLA	CHC-C1C	2.38	1.43	1.38
20	1	315	LUT	C32-C33	-2.38	1.40	1.46
19	B	826	CLA	CHC-C1C	2.38	1.43	1.38
19	G	204	CLA	CHC-C1C	2.38	1.43	1.38
19	K	203	CLA	C1D-ND	-2.38	1.34	1.37
19	3	302	CLA	MG-NB	2.38	2.10	2.05
19	A	822	CLA	C1D-ND	-2.38	1.34	1.37
19	B	827	CLA	CHC-C1C	2.38	1.43	1.38
19	1	321	CLA	C1D-ND	-2.38	1.34	1.37
19	A	817	CLA	CHC-C1C	2.38	1.43	1.38
19	3	311	CLA	CHC-C1C	2.38	1.43	1.38
19	K	202	CLA	C1D-ND	-2.38	1.34	1.37
19	B	821	CLA	CHC-C1C	2.38	1.43	1.38
19	4	310	CLA	C1D-ND	-2.37	1.34	1.37
19	F	303	CLA	CHC-C1C	2.37	1.43	1.38
19	4	309	CLA	CHC-C1C	2.37	1.43	1.38
19	A	819	CLA	C1D-ND	-2.37	1.34	1.37
19	1	311	CLA	CHC-C1C	2.37	1.43	1.38
19	1	308	CLA	CHC-C1C	2.37	1.43	1.38
19	B	807	CLA	CHC-C1C	2.37	1.43	1.38
19	G	202	CLA	CHC-C1C	2.37	1.43	1.38
19	L	301	CLA	CHC-C1C	2.37	1.43	1.38
19	K	203	CLA	MG-NB	2.37	2.10	2.05
19	2	311	CLA	CHC-C1C	2.37	1.43	1.38
19	3	305	CLA	CHC-C1C	2.37	1.43	1.38
20	1	315	LUT	C12-C13	-2.37	1.40	1.46
19	K	202	CLA	CHC-C1C	2.37	1.43	1.38
19	A	822	CLA	MG-NB	2.37	2.10	2.05
19	4	309	CLA	MG-NB	2.36	2.10	2.05
19	1	307	CLA	CHC-C1C	2.36	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	312	CLA	CHC-C1C	2.36	1.43	1.38
19	3	312	CLA	CHC-C1C	2.36	1.43	1.38
19	2	320	CLA	CHC-C1C	2.36	1.43	1.38
19	4	312	CLA	MG-NB	2.36	2.10	2.05
19	2	311	CLA	C1D-ND	-2.36	1.34	1.37
19	A	851	CLA	MG-NB	2.36	2.10	2.05
19	4	310	CLA	CHC-C1C	2.36	1.43	1.38
19	J	102	CLA	MG-NB	2.36	2.10	2.05
19	K	204	CLA	MG-NB	2.36	2.10	2.05
19	4	307	CLA	MG-NB	2.36	2.10	2.05
19	3	302	CLA	CHC-C1C	2.36	1.43	1.38
19	3	301	CLA	MG-NB	2.36	2.10	2.05
19	A	832	CLA	MG-NB	2.36	2.10	2.05
19	B	829	CLA	CHC-C1C	2.36	1.43	1.38
19	1	305	CLA	MG-NB	2.36	2.10	2.05
19	A	822	CLA	CHC-C1C	2.36	1.43	1.38
19	B	812	CLA	CHC-C1C	2.36	1.43	1.38
19	A	831	CLA	MG-NB	2.35	2.10	2.05
19	4	312	CLA	CHC-C1C	2.35	1.43	1.38
19	B	823	CLA	CHC-C1C	2.35	1.43	1.38
19	L	303	CLA	CHC-C1C	2.35	1.43	1.38
19	B	808	CLA	CHC-C1C	2.35	1.43	1.38
19	A	828	CLA	MG-NB	2.35	2.10	2.05
19	B	830	CLA	MG-NB	2.35	2.10	2.05
20	3	315	LUT	C12-C13	-2.35	1.40	1.46
19	A	840	CLA	CHC-C1C	2.35	1.43	1.38
19	4	303	CLA	MG-NB	2.35	2.10	2.05
19	B	823	CLA	MG-NB	2.35	2.10	2.05
19	4	302	CLA	CHC-C1C	2.35	1.43	1.38
19	2	308	CLA	MG-NB	2.35	2.10	2.05
19	A	819	CLA	MG-NB	2.35	2.10	2.05
19	2	309	CLA	MG-NB	2.35	2.10	2.05
19	1	307	CLA	MG-NB	2.35	2.10	2.05
19	1	311	CLA	MG-NB	2.35	2.10	2.05
19	G	202	CLA	MG-NB	2.34	2.10	2.05
19	A	819	CLA	CHC-C1C	2.34	1.43	1.38
19	4	311	CLA	MG-NB	2.34	2.10	2.05
20	4	315	LUT	C34-C33	2.34	1.41	1.35
19	B	834	CLA	MG-NB	2.34	2.10	2.05
20	4	315	LUT	C14-C13	2.34	1.41	1.35
19	1	309	CLA	MG-NB	2.34	2.10	2.05
19	A	824	CLA	MG-NB	2.34	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	827	CLA	MG-NB	2.33	2.10	2.05
19	A	836	CLA	MG-NB	2.33	2.10	2.05
19	B	807	CLA	MG-NB	2.33	2.10	2.05
19	A	815	CLA	MG-NB	2.33	2.10	2.05
20	1	320	LUT	C32-C33	-2.33	1.41	1.46
19	3	311	CLA	MG-NB	2.33	2.10	2.05
19	A	824	CLA	CHC-C1C	2.33	1.43	1.38
19	A	829	CLA	MG-NB	2.33	2.10	2.05
19	K	204	CLA	C1D-ND	-2.33	1.34	1.37
19	F	302	CLA	MG-NB	2.33	2.10	2.05
19	F	303	CLA	MG-NB	2.33	2.10	2.05
18	4	305	CHL	C2C-C3C	2.33	1.38	1.36
19	3	305	CLA	MG-NB	2.33	2.10	2.05
19	B	805	CLA	MG-NB	2.33	2.10	2.05
19	1	304	CLA	MG-NB	2.33	2.10	2.05
20	3	315	LUT	C32-C33	-2.33	1.41	1.46
19	B	821	CLA	MG-NB	2.33	2.10	2.05
19	3	309	CLA	MG-NB	2.33	2.10	2.05
19	B	810	CLA	C4B-C3B	2.33	1.48	1.43
19	A	815	CLA	CHC-C1C	2.32	1.43	1.38
20	2	315	LUT	C32-C33	-2.32	1.41	1.46
20	2	315	LUT	C12-C13	-2.32	1.41	1.46
19	3	313	CLA	MG-NB	2.32	2.10	2.05
20	4	315	LUT	C30-C29	2.32	1.41	1.35
19	B	802	CLA	MG-NB	2.32	2.10	2.05
19	F	304	CLA	CHC-C1C	2.32	1.43	1.38
19	1	305	CLA	CHC-C1C	2.32	1.43	1.38
20	3	315	LUT	C28-C29	-2.32	1.41	1.46
19	A	812	CLA	CHC-C1C	2.32	1.43	1.38
20	2	315	LUT	C34-C33	2.32	1.41	1.35
20	3	315	LUT	C34-C33	2.32	1.41	1.35
20	4	315	LUT	C12-C13	-2.32	1.41	1.46
19	B	801	CLA	MG-NB	2.31	2.10	2.05
19	B	833	CLA	MG-NB	2.31	2.10	2.05
19	G	204	CLA	MG-NB	2.31	2.10	2.05
19	A	839	CLA	MG-NB	2.31	2.10	2.05
19	2	310	CLA	MG-NB	2.31	2.10	2.05
19	1	310	CLA	MG-NB	2.31	2.10	2.05
19	3	310	CLA	MG-NB	2.31	2.10	2.05
19	1	311	CLA	CHB-C1B	-2.31	1.34	1.39
19	3	311	CLA	CHB-C1B	-2.31	1.34	1.39
19	2	302	CLA	MG-NB	2.31	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	854	CLA	MG-NB	2.31	2.10	2.05
19	1	321	CLA	MG-NB	2.31	2.10	2.05
19	4	301	CLA	MG-NB	2.31	2.10	2.05
20	1	320	LUT	C12-C13	-2.31	1.41	1.46
19	3	314	CLA	MG-NB	2.31	2.10	2.05
19	3	305	CLA	CHB-C1B	-2.31	1.34	1.39
19	A	840	CLA	CHB-C1B	-2.31	1.34	1.39
19	1	313	CLA	MG-NB	2.31	2.10	2.05
19	2	304	CLA	MG-NB	2.31	2.10	2.05
19	B	813	CLA	MG-NB	2.31	2.10	2.05
19	A	831	CLA	CHB-C1B	-2.31	1.34	1.39
19	B	836	CLA	MG-NB	2.31	2.10	2.05
19	3	306	CLA	MG-NB	2.30	2.10	2.05
20	1	315	LUT	C28-C29	-2.30	1.41	1.46
19	A	831	CLA	CHC-C1C	2.30	1.43	1.38
19	A	832	CLA	CHC-C1C	2.30	1.43	1.38
19	3	304	CLA	MG-NB	2.30	2.10	2.05
19	B	826	CLA	MG-NB	2.30	2.10	2.05
19	A	803	CLA	CHB-C1B	-2.30	1.34	1.39
19	A	802	CLA	MG-NB	2.30	2.10	2.05
19	A	812	CLA	CHB-C1B	-2.30	1.34	1.39
19	B	837	CLA	CHB-C1B	-2.30	1.34	1.39
20	4	315	LUT	C10-C9	2.29	1.41	1.35
19	B	803	CLA	MG-NB	2.29	2.10	2.05
20	2	315	LUT	C14-C13	2.29	1.41	1.35
19	A	812	CLA	MG-NB	2.29	2.10	2.05
18	2	307	CHL	C2C-C3C	2.29	1.38	1.36
18	4	314	CHL	C2C-C3C	2.29	1.38	1.36
19	A	817	CLA	MG-NB	2.29	2.10	2.05
19	A	840	CLA	MG-NB	2.29	2.10	2.05
19	B	835	CLA	MG-NB	2.29	2.10	2.05
19	B	805	CLA	CHB-C1B	-2.29	1.34	1.39
19	B	814	CLA	MG-NB	2.29	2.10	2.05
19	A	810	CLA	MG-NB	2.29	2.10	2.05
19	A	829	CLA	CHB-C1B	-2.29	1.34	1.39
19	B	818	CLA	MG-NB	2.29	2.10	2.05
19	A	805	CLA	CHB-C1B	-2.29	1.34	1.39
19	A	820	CLA	MG-NB	2.29	2.10	2.05
20	1	315	LUT	C34-C33	2.29	1.41	1.35
19	A	818	CLA	MG-NB	2.29	2.10	2.05
19	B	812	CLA	CHB-C1B	-2.29	1.34	1.39
19	A	815	CLA	CHB-C1B	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	810	CLA	MG-NB	2.28	2.10	2.05
19	A	834	CLA	MG-NB	2.28	2.10	2.05
19	L	302	CLA	MG-NB	2.28	2.10	2.05
19	2	313	CLA	MG-NB	2.28	2.10	2.05
19	1	310	CLA	CHB-C1B	-2.28	1.34	1.39
19	2	313	CLA	CHB-C1B	-2.28	1.34	1.39
19	3	312	CLA	MG-NB	2.28	2.10	2.05
19	A	830	CLA	CHB-C1B	-2.28	1.34	1.39
18	1	301	CHL	C2C-C3C	2.28	1.38	1.36
19	3	314	CLA	CHB-C1B	-2.28	1.34	1.39
19	H	201	CLA	CHB-C1B	-2.28	1.34	1.39
19	4	309	CLA	CHB-C1B	-2.28	1.34	1.39
19	A	837	CLA	MG-NB	2.28	2.10	2.05
19	B	811	CLA	CHB-C1B	-2.28	1.34	1.39
20	3	315	LUT	C10-C9	2.28	1.41	1.35
19	B	823	CLA	CHB-C1B	-2.27	1.34	1.39
19	A	805	CLA	MG-NB	2.27	2.10	2.05
19	F	304	CLA	CHB-C1B	-2.27	1.34	1.39
19	1	302	CLA	CHB-C1B	-2.27	1.34	1.39
19	4	303	CLA	CHB-C1B	-2.27	1.34	1.39
19	1	305	CLA	CHB-C1B	-2.27	1.34	1.39
19	B	814	CLA	CHB-C1B	-2.27	1.34	1.39
19	A	835	CLA	MG-NB	2.27	2.10	2.05
19	B	819	CLA	MG-NB	2.27	2.10	2.05
19	B	828	CLA	CHB-C1B	-2.27	1.34	1.39
20	1	315	LUT	C14-C13	2.27	1.41	1.35
19	G	203	CLA	MG-NB	2.27	2.10	2.05
19	A	803	CLA	MG-NB	2.27	2.10	2.05
19	L	301	CLA	MG-NB	2.27	2.10	2.05
20	4	315	LUT	C32-C33	-2.27	1.41	1.46
19	K	204	CLA	CHB-C1B	-2.27	1.34	1.39
20	1	320	LUT	C28-C29	-2.27	1.41	1.46
19	4	308	CLA	MG-NB	2.26	2.10	2.05
19	2	312	CLA	MG-NB	2.26	2.10	2.05
19	B	832	CLA	MG-NB	2.26	2.10	2.05
19	4	302	CLA	CHB-C1B	-2.26	1.34	1.39
18	2	301	CHL	C2C-C3C	2.26	1.38	1.36
19	A	832	CLA	CHB-C1B	-2.26	1.34	1.39
19	1	302	CLA	MG-NB	2.26	2.10	2.05
19	1	314	CLA	MG-NB	2.26	2.10	2.05
19	B	838	CLA	MG-NB	2.26	2.10	2.05
19	4	310	CLA	CHB-C1B	-2.26	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	826	CLA	MG-NB	2.26	2.10	2.05
19	B	830	CLA	CHB-C1B	-2.26	1.34	1.39
19	B	825	CLA	MG-NB	2.26	2.10	2.05
19	3	302	CLA	CHB-C1B	-2.26	1.34	1.39
19	A	822	CLA	CHB-C1B	-2.26	1.34	1.39
19	B	834	CLA	CHB-C1B	-2.26	1.34	1.39
18	2	314	CHL	MG-NB	2.26	2.10	2.05
19	2	304	CLA	CHB-C1B	-2.26	1.34	1.39
19	A	828	CLA	CHB-C1B	-2.26	1.34	1.39
20	3	315	LUT	C14-C13	2.26	1.41	1.35
19	A	837	CLA	CHB-C1B	-2.26	1.34	1.39
20	2	315	LUT	C28-C29	-2.26	1.41	1.46
19	B	808	CLA	MG-NB	2.26	2.10	2.05
20	1	320	LUT	C34-C33	2.26	1.41	1.35
19	B	808	CLA	CHB-C1B	-2.26	1.34	1.39
19	4	311	CLA	CHC-C1C	2.26	1.43	1.38
19	B	803	CLA	CHB-C1B	-2.26	1.34	1.39
20	4	315	LUT	C28-C29	-2.26	1.41	1.46
19	K	203	CLA	CHB-C1B	-2.26	1.34	1.39
19	4	302	CLA	MG-NC	2.26	2.11	2.06
19	2	311	CLA	CHB-C1B	-2.26	1.34	1.39
19	A	827	CLA	MG-NB	2.26	2.10	2.05
19	F	301	CLA	MG-NB	2.26	2.10	2.05
19	2	309	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	854	CLA	CHB-C1B	-2.25	1.34	1.39
20	1	320	LUT	C14-C13	2.25	1.41	1.35
20	2	315	LUT	C30-C29	2.25	1.41	1.35
19	3	301	CLA	CHB-C1B	-2.25	1.34	1.39
19	B	806	CLA	MG-NB	2.25	2.10	2.05
19	B	818	CLA	CHB-C1B	-2.25	1.34	1.39
19	G	202	CLA	CHB-C1B	-2.25	1.34	1.39
19	1	304	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	853	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	831	CLA	MG-NC	2.25	2.11	2.06
19	2	320	CLA	CHB-C1B	-2.25	1.34	1.39
19	4	312	CLA	CHB-C1B	-2.25	1.34	1.39
19	1	312	CLA	MG-NB	2.25	2.10	2.05
19	1	312	CLA	CHB-C1B	-2.25	1.34	1.39
19	G	204	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	806	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	852	CLA	CHB-C1B	-2.25	1.34	1.39
19	F	304	CLA	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	MG-NB	2.25	2.10	2.05
19	A	835	CLA	CHB-C1B	-2.25	1.34	1.39
19	3	308	CLA	MG-NB	2.25	2.10	2.05
19	B	807	CLA	CHB-C1B	-2.25	1.34	1.39
19	A	807	CLA	MG-NB	2.25	2.10	2.05
19	B	813	CLA	CHB-C1B	-2.25	1.34	1.39
19	F	303	CLA	CHB-C1B	-2.25	1.34	1.39
19	L	303	CLA	CHB-C1B	-2.25	1.34	1.39
20	1	320	LUT	C30-C29	2.25	1.41	1.35
20	3	315	LUT	C30-C29	2.24	1.41	1.35
19	3	309	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	833	CLA	CHB-C1B	-2.24	1.34	1.39
20	1	320	LUT	C10-C9	2.24	1.41	1.35
19	B	821	CLA	CHB-C1B	-2.24	1.34	1.39
19	F	301	CLA	CHB-C1B	-2.24	1.34	1.39
19	B	834	CLA	MG-NC	2.24	2.11	2.06
19	B	815	CLA	CHB-C1B	-2.24	1.34	1.39
19	4	311	CLA	MG-NC	2.24	2.11	2.06
19	L	302	CLA	CHB-C1B	-2.24	1.34	1.39
19	1	321	CLA	CHB-C1B	-2.24	1.34	1.39
19	1	308	CLA	MG-NB	2.24	2.10	2.05
19	B	824	CLA	MG-NB	2.24	2.10	2.05
19	A	821	CLA	CHB-C1B	-2.24	1.34	1.39
19	3	311	CLA	MG-NC	2.24	2.11	2.06
19	4	313	CLA	MG-NB	2.24	2.10	2.05
19	B	811	CLA	MG-NB	2.24	2.10	2.05
19	3	306	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	817	CLA	CHB-C1B	-2.24	1.34	1.39
19	G	203	CLA	CHB-C1B	-2.24	1.34	1.39
19	2	303	CLA	MG-NB	2.24	2.10	2.05
19	2	308	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	836	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	801	CLA	MG-NB	2.24	2.10	2.05
19	A	822	CLA	MG-NC	2.24	2.11	2.06
19	A	811	CLA	MG-NB	2.24	2.10	2.05
19	A	819	CLA	CHB-C1B	-2.24	1.34	1.39
20	2	315	LUT	C10-C9	2.24	1.41	1.35
19	B	810	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	852	CLA	MG-NB	2.24	2.10	2.05
19	1	309	CLA	CHB-C1B	-2.24	1.34	1.39
19	A	839	CLA	CHB-C1B	-2.24	1.34	1.39
19	B	836	CLA	CHB-C1B	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	814	CLA	MG-NB	2.24	2.10	2.05
19	A	813	CLA	MG-NB	2.24	2.10	2.05
19	1	303	CLA	MG-NB	2.23	2.10	2.05
19	B	806	CLA	CHB-C1B	-2.23	1.34	1.39
19	A	853	CLA	MG-NB	2.23	2.10	2.05
19	4	311	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	825	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	833	CLA	CHB-C1B	-2.23	1.34	1.39
19	A	816	CLA	MG-NB	2.23	2.10	2.05
19	4	301	CLA	CHB-C1B	-2.23	1.34	1.39
19	K	203	CLA	MG-NC	2.23	2.11	2.06
19	A	814	CLA	CHB-C1B	-2.23	1.34	1.39
19	2	311	CLA	MG-NC	2.23	2.11	2.06
19	1	311	CLA	MG-NC	2.23	2.11	2.06
19	A	825	CLA	MG-NB	2.23	2.10	2.05
19	L	301	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	838	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	837	CLA	MG-NB	2.23	2.10	2.05
19	A	809	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	826	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	827	CLA	CHB-C1B	-2.23	1.34	1.39
19	A	816	CLA	CHB-C1B	-2.23	1.34	1.39
19	B	802	CLA	CHB-C1B	-2.23	1.34	1.39
19	A	807	CLA	CHB-C1B	-2.23	1.34	1.39
19	2	302	CLA	CHB-C1B	-2.23	1.34	1.39
19	H	201	CLA	MG-NB	2.23	2.10	2.05
19	B	832	CLA	CHB-C1B	-2.23	1.34	1.39
19	1	307	CLA	CHB-C1B	-2.22	1.34	1.39
19	3	313	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	823	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	824	CLA	CHB-C1B	-2.22	1.34	1.39
19	B	817	CLA	CHB-C1B	-2.22	1.34	1.39
18	2	314	CHL	C2C-C3C	2.22	1.38	1.36
19	1	308	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	818	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	835	CLA	MG-NC	2.22	2.11	2.06
19	B	817	CLA	MG-NB	2.22	2.10	2.05
19	4	313	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	804	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	826	CLA	CHB-C1B	-2.22	1.34	1.39
19	K	202	CLA	CHB-C1B	-2.22	1.34	1.39
19	K	204	CLA	MG-NC	2.22	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	304	CLA	CHB-C1B	-2.22	1.34	1.39
19	3	308	CLA	CHB-C1B	-2.22	1.34	1.39
19	B	816	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	838	CLA	CHB-C1B	-2.22	1.34	1.39
19	B	816	CLA	MG-NB	2.22	2.10	2.05
20	1	315	LUT	C30-C29	2.22	1.40	1.35
19	A	811	CLA	CHB-C1B	-2.22	1.34	1.39
19	1	304	CLA	MG-NC	2.22	2.11	2.06
19	A	815	CLA	MG-NC	2.22	2.11	2.06
19	A	809	CLA	MG-NB	2.22	2.10	2.05
19	A	834	CLA	CHB-C1B	-2.22	1.34	1.39
19	B	835	CLA	CHB-C1B	-2.22	1.34	1.39
19	B	819	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	810	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	851	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	829	CLA	MG-NC	2.22	2.11	2.06
19	4	307	CLA	CHB-C1B	-2.22	1.34	1.39
19	A	808	CLA	CHB-C1B	-2.21	1.34	1.39
19	B	804	CLA	CHB-C1B	-2.21	1.34	1.39
19	1	303	CLA	CHB-C1B	-2.21	1.34	1.39
19	B	822	CLA	MG-NB	2.21	2.10	2.05
19	4	307	CLA	MG-NC	2.21	2.11	2.06
19	B	812	CLA	MG-NB	2.21	2.10	2.05
19	2	303	CLA	CHB-C1B	-2.21	1.34	1.39
19	A	813	CLA	CHB-C1B	-2.21	1.34	1.39
19	A	825	CLA	CHB-C1B	-2.21	1.34	1.39
19	1	305	CLA	MG-NC	2.21	2.11	2.06
19	2	312	CLA	MG-NC	2.21	2.11	2.06
19	2	310	CLA	CHB-C1B	-2.21	1.34	1.39
19	3	303	CLA	MG-NB	2.21	2.10	2.05
19	B	820	CLA	CHB-C1B	-2.21	1.34	1.39
19	1	310	CLA	MG-NC	2.21	2.11	2.06
19	4	310	CLA	MG-NC	2.21	2.11	2.06
19	B	828	CLA	MG-NB	2.21	2.10	2.05
19	2	313	CLA	MG-NC	2.21	2.11	2.06
19	A	839	CLA	MG-NC	2.21	2.11	2.06
19	A	828	CLA	MG-NC	2.21	2.11	2.06
19	F	303	CLA	MG-NC	2.21	2.11	2.06
19	3	313	CLA	MG-NC	2.21	2.11	2.06
19	4	308	CLA	CHB-C1B	-2.21	1.34	1.39
19	3	310	CLA	CHB-C1B	-2.21	1.34	1.39
19	3	312	CLA	CHB-C1B	-2.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	802	CLA	CHB-C1B	-2.21	1.34	1.39
19	3	314	CLA	MG-NC	2.21	2.11	2.06
19	A	824	CLA	MG-NC	2.21	2.11	2.06
19	A	832	CLA	MG-NC	2.21	2.11	2.06
19	B	805	CLA	MG-NC	2.21	2.11	2.06
19	B	804	CLA	MG-NB	2.21	2.10	2.05
19	A	833	CLA	MG-NB	2.21	2.10	2.05
19	B	809	CLA	MG-NB	2.21	2.10	2.05
19	3	303	CLA	CHB-C1B	-2.20	1.34	1.39
19	B	809	CLA	CHB-C1B	-2.20	1.34	1.39
19	J	102	CLA	CHB-C1B	-2.20	1.34	1.39
19	A	851	CLA	MG-NC	2.20	2.11	2.06
19	B	815	CLA	MG-NB	2.20	2.10	2.05
19	B	830	CLA	MG-NC	2.20	2.11	2.06
19	A	823	CLA	MG-NB	2.20	2.10	2.05
19	1	313	CLA	CHB-C1B	-2.20	1.34	1.39
19	1	314	CLA	CHB-C1B	-2.20	1.34	1.39
19	3	305	CLA	MG-NC	2.20	2.11	2.06
19	A	836	CLA	MG-NC	2.20	2.11	2.06
19	A	820	CLA	CHB-C1B	-2.20	1.34	1.39
19	3	304	CLA	MG-NC	2.20	2.11	2.06
19	3	302	CLA	MG-NC	2.20	2.11	2.06
19	3	310	CLA	MG-NC	2.20	2.11	2.06
19	2	304	CLA	MG-NC	2.20	2.11	2.06
19	B	825	CLA	MG-NC	2.20	2.11	2.06
19	B	836	CLA	MG-NC	2.20	2.11	2.06
19	B	801	CLA	CHB-C1B	-2.20	1.34	1.39
19	B	829	CLA	CHB-C1B	-2.20	1.34	1.39
19	A	830	CLA	MG-NB	2.20	2.10	2.05
19	4	309	CLA	MG-NC	2.19	2.11	2.06
18	2	301	CHL	C2-C3	2.19	1.39	1.32
19	2	312	CLA	CHB-C1B	-2.19	1.34	1.39
19	B	822	CLA	CHB-C1B	-2.19	1.34	1.39
19	A	817	CLA	MG-NC	2.19	2.11	2.06
19	A	837	CLA	MG-NC	2.19	2.11	2.06
19	2	320	CLA	MG-NB	2.19	2.10	2.05
19	B	837	CLA	MG-NC	2.19	2.11	2.06
19	G	204	CLA	MG-NC	2.19	2.11	2.06
19	2	303	CLA	MG-NC	2.19	2.11	2.06
19	B	824	CLA	CHB-C1B	-2.19	1.34	1.39
19	G	202	CLA	MG-NC	2.19	2.11	2.06
19	B	821	CLA	MG-NC	2.19	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	831	CLA	MG-NB	2.19	2.10	2.05
19	B	812	CLA	MG-NC	2.19	2.11	2.06
19	H	201	CLA	MG-NC	2.19	2.11	2.06
19	3	312	CLA	MG-NC	2.19	2.11	2.06
20	1	315	LUT	C10-C9	2.19	1.40	1.35
19	B	823	CLA	MG-NC	2.19	2.11	2.06
19	F	302	CLA	CHB-C1B	-2.19	1.34	1.39
19	B	811	CLA	MG-NC	2.19	2.11	2.06
19	A	804	CLA	MG-NB	2.19	2.10	2.05
19	4	303	CLA	MG-NC	2.19	2.11	2.06
19	F	301	CLA	MG-NC	2.19	2.11	2.06
19	J	102	CLA	MG-NC	2.18	2.11	2.06
19	B	833	CLA	MG-NC	2.18	2.11	2.06
18	4	306	CHL	C2-C3	2.18	1.39	1.32
19	L	303	CLA	MG-NC	2.18	2.11	2.06
19	B	813	CLA	MG-NC	2.18	2.11	2.06
19	1	307	CLA	MG-NC	2.18	2.11	2.06
19	A	834	CLA	MG-NC	2.18	2.11	2.06
19	A	840	CLA	MG-NC	2.18	2.11	2.06
19	4	313	CLA	MG-NC	2.18	2.11	2.06
19	G	203	CLA	MG-NC	2.18	2.11	2.06
19	K	202	CLA	MG-NC	2.18	2.11	2.06
19	A	819	CLA	MG-NC	2.18	2.11	2.06
19	B	820	CLA	MG-NB	2.18	2.10	2.05
19	1	312	CLA	MG-NC	2.18	2.11	2.06
19	A	820	CLA	MG-NC	2.18	2.11	2.06
19	B	826	CLA	MG-NC	2.18	2.11	2.06
19	B	818	CLA	MG-NC	2.18	2.11	2.06
19	L	302	CLA	MG-NC	2.18	2.11	2.06
19	B	819	CLA	MG-NC	2.17	2.11	2.06
19	A	812	CLA	MG-NC	2.17	2.11	2.06
19	3	301	CLA	MG-NC	2.17	2.11	2.06
19	2	302	CLA	MG-NC	2.17	2.11	2.06
19	A	801	CLA	CHB-C1B	-2.17	1.34	1.39
19	B	808	CLA	MG-NC	2.17	2.11	2.06
19	B	807	CLA	MG-NC	2.17	2.11	2.06
19	A	808	CLA	C1B-NB	-2.17	1.35	1.37
19	B	803	CLA	MG-NC	2.17	2.11	2.06
19	3	303	CLA	MG-NC	2.17	2.11	2.06
19	B	814	CLA	MG-NC	2.17	2.11	2.06
19	2	320	CLA	MG-NC	2.17	2.11	2.06
19	B	827	CLA	MG-NC	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	829	CLA	MG-NB	2.16	2.10	2.05
19	L	301	CLA	MG-NC	2.16	2.11	2.06
19	A	853	CLA	MG-NC	2.16	2.11	2.06
19	A	821	CLA	MG-NC	2.16	2.11	2.06
19	A	825	CLA	MG-NC	2.16	2.11	2.06
19	B	809	CLA	MG-NC	2.16	2.11	2.06
19	2	309	CLA	MG-NC	2.16	2.11	2.06
19	1	321	CLA	MG-NC	2.16	2.11	2.06
19	B	832	CLA	MG-NC	2.16	2.11	2.06
19	A	827	CLA	CHB-C1B	-2.16	1.34	1.39
19	A	838	CLA	MG-NB	2.16	2.10	2.05
19	1	303	CLA	MG-NC	2.16	2.11	2.06
19	2	308	CLA	MG-NC	2.16	2.11	2.06
19	A	811	CLA	MG-NC	2.16	2.11	2.06
19	A	818	CLA	MG-NC	2.16	2.11	2.06
19	B	806	CLA	MG-NC	2.15	2.11	2.06
19	A	813	CLA	MG-NC	2.15	2.11	2.06
19	A	854	CLA	MG-NC	2.15	2.11	2.06
19	A	816	CLA	MG-NC	2.15	2.11	2.06
19	3	308	CLA	MG-NC	2.15	2.11	2.06
19	A	803	CLA	MG-NC	2.15	2.11	2.06
19	B	828	CLA	MG-NC	2.15	2.11	2.06
19	A	802	CLA	MG-NC	2.15	2.11	2.06
19	A	830	CLA	MG-NC	2.15	2.11	2.06
19	3	306	CLA	MG-NC	2.15	2.11	2.06
19	4	312	CLA	MG-NC	2.15	2.11	2.06
19	B	801	CLA	MG-NC	2.15	2.11	2.06
19	1	309	CLA	MG-NC	2.15	2.11	2.06
19	B	817	CLA	MG-NC	2.15	2.11	2.06
19	2	310	CLA	MG-NC	2.15	2.11	2.06
19	3	309	CLA	MG-NC	2.15	2.11	2.06
19	A	826	CLA	MG-NC	2.15	2.11	2.06
19	1	308	CLA	MG-NC	2.15	2.11	2.06
19	B	810	CLA	MG-NC	2.14	2.11	2.06
19	1	302	CLA	MG-NC	2.14	2.11	2.06
19	A	814	CLA	MG-NC	2.14	2.11	2.06
19	F	302	CLA	MG-NC	2.14	2.11	2.06
19	F	302	CLA	C3B-C4B	2.14	1.49	1.42
19	A	805	CLA	MG-NC	2.14	2.11	2.06
19	A	810	CLA	MG-NC	2.14	2.11	2.06
19	1	313	CLA	MG-NC	2.14	2.11	2.06
19	1	314	CLA	MG-NC	2.14	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	831	CLA	CHB-C1B	-2.13	1.34	1.39
19	A	806	CLA	MG-NB	2.13	2.10	2.05
19	A	807	CLA	MG-NC	2.13	2.11	2.06
19	A	801	CLA	MG-NC	2.13	2.11	2.06
19	B	820	CLA	MG-NC	2.13	2.11	2.06
19	A	806	CLA	MG-NC	2.13	2.11	2.06
19	B	815	CLA	MG-NC	2.13	2.11	2.06
19	B	802	CLA	MG-NC	2.12	2.11	2.06
18	4	306	CHL	C2C-C3C	2.12	1.38	1.36
19	B	829	CLA	MG-NC	2.12	2.11	2.06
19	A	833	CLA	MG-NC	2.12	2.11	2.06
19	B	824	CLA	MG-NC	2.12	2.11	2.06
19	A	808	CLA	MG-NC	2.12	2.11	2.06
19	A	838	CLA	MG-NC	2.12	2.11	2.06
19	A	809	CLA	MG-NC	2.12	2.11	2.06
19	B	810	CLA	C3B-C2B	-2.11	1.36	1.44
19	4	301	CLA	MG-NC	2.11	2.11	2.06
19	A	852	CLA	MG-NC	2.11	2.11	2.06
19	B	804	CLA	MG-NC	2.11	2.11	2.06
19	A	827	CLA	MG-NC	2.11	2.11	2.06
19	B	838	CLA	MG-NC	2.11	2.11	2.06
19	A	804	CLA	MG-NC	2.11	2.11	2.06
19	B	816	CLA	MG-NC	2.10	2.11	2.06
19	B	835	CLA	MG-NC	2.10	2.11	2.06
19	1	309	CLA	C3B-C4B	2.10	1.48	1.42
19	4	308	CLA	MG-NC	2.09	2.11	2.06
19	B	831	CLA	MG-NC	2.09	2.11	2.06
19	2	309	CLA	C3B-C4B	2.09	1.48	1.42
19	2	313	CLA	CAA-C2A	2.08	1.57	1.54
19	A	823	CLA	MG-NC	2.08	2.11	2.06
19	B	822	CLA	C3B-C4B	2.08	1.48	1.42
19	3	301	CLA	C3B-C4B	2.07	1.48	1.42
19	A	808	CLA	C3B-C4B	2.07	1.48	1.42
19	B	822	CLA	MG-NC	2.07	2.11	2.06
19	B	815	CLA	C3B-C4B	2.06	1.48	1.42
19	3	309	CLA	C3B-C4B	2.06	1.48	1.42
19	K	204	CLA	CAA-C2A	2.06	1.57	1.53
19	B	818	CLA	C3B-C4B	2.06	1.48	1.42
19	2	304	CLA	CAA-C2A	2.06	1.57	1.54
19	B	833	CLA	C3B-C4B	2.06	1.48	1.42
19	A	838	CLA	C3B-C4B	2.06	1.48	1.42
19	2	302	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	301	CLA	C3B-C4B	2.06	1.48	1.42
19	A	828	CLA	C3B-C4B	2.05	1.48	1.42
19	4	308	CLA	C3B-C4B	2.05	1.48	1.42
19	A	825	CLA	C3B-C4B	2.05	1.48	1.42
19	A	803	CLA	C3B-C4B	2.05	1.48	1.42
19	B	832	CLA	CAA-C2A	2.04	1.57	1.54
19	B	813	CLA	C3B-C4B	2.04	1.48	1.42
19	L	302	CLA	C3B-C4B	2.04	1.48	1.42
19	3	314	CLA	C3B-C4B	2.04	1.48	1.42
19	A	816	CLA	C3B-C4B	2.04	1.48	1.42
19	1	302	CLA	C3B-C4B	2.04	1.48	1.42
19	3	310	CLA	CAA-C2A	2.04	1.57	1.53
19	A	827	CLA	C3B-C4B	2.04	1.48	1.42
19	A	854	CLA	C3B-C4B	2.04	1.48	1.42
19	B	824	CLA	C3B-C4B	2.04	1.48	1.42
19	A	852	CLA	C3B-C4B	2.03	1.48	1.42
19	B	832	CLA	C3B-C4B	2.03	1.48	1.42
19	A	851	CLA	C3B-C4B	2.03	1.48	1.42
19	B	814	CLA	C3B-C4B	2.03	1.48	1.42
19	K	203	CLA	C3B-C4B	2.03	1.48	1.42
19	A	809	CLA	C3B-C4B	2.03	1.48	1.42
19	A	813	CLA	C3B-C4B	2.03	1.48	1.42
19	2	304	CLA	C3B-C4B	2.03	1.48	1.42
19	A	814	CLA	C3B-C4B	2.03	1.48	1.42
19	B	831	CLA	C3B-C4B	2.03	1.48	1.42
19	G	202	CLA	CAA-C2A	2.03	1.57	1.53
19	3	306	CLA	C3B-C4B	2.02	1.48	1.42
19	A	820	CLA	C3B-C4B	2.02	1.48	1.42
19	B	809	CLA	C3B-C4B	2.02	1.48	1.42
19	A	810	CLA	C3B-C4B	2.02	1.48	1.42
19	1	313	CLA	C3B-C4B	2.02	1.48	1.42
19	2	311	CLA	C3B-C4B	2.02	1.48	1.42
19	3	311	CLA	C3B-C4B	2.02	1.48	1.42
19	2	313	CLA	C3B-C4B	2.02	1.48	1.42
19	3	305	CLA	C3B-C4B	2.02	1.48	1.42
19	B	835	CLA	C3B-C4B	2.02	1.48	1.42
19	A	829	CLA	C3B-C4B	2.02	1.48	1.42
19	A	818	CLA	C3B-C4B	2.02	1.48	1.42
19	1	310	CLA	C3B-C4B	2.02	1.48	1.42
19	B	811	CLA	C3B-C4B	2.02	1.48	1.42
19	J	102	CLA	C3B-C4B	2.02	1.48	1.42
19	4	313	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	307	CLA	C3B-C4B	2.02	1.48	1.42
19	3	313	CLA	C3B-C4B	2.02	1.48	1.42
19	4	302	CLA	C3B-C4B	2.02	1.48	1.42
19	A	837	CLA	C3B-C4B	2.02	1.48	1.42
19	B	804	CLA	C3B-C4B	2.01	1.48	1.42
19	G	203	CLA	C3B-C4B	2.01	1.48	1.42
18	3	307	CHL	O1D-CGD	2.01	1.26	1.21
19	H	201	CLA	C3B-C4B	2.01	1.48	1.42
19	2	308	CLA	C3B-C4B	2.01	1.48	1.42
19	B	828	CLA	C3B-C4B	2.01	1.48	1.42
19	1	311	CLA	C3B-C4B	2.01	1.48	1.42
19	2	310	CLA	C3B-C4B	2.01	1.48	1.42
19	A	840	CLA	C3B-C4B	2.01	1.48	1.42
19	B	836	CLA	C3B-C4B	2.01	1.48	1.42
19	4	310	CLA	C3B-C4B	2.01	1.48	1.42
19	K	204	CLA	C3B-C4B	2.01	1.48	1.42
19	4	309	CLA	C3B-C4B	2.01	1.48	1.42
19	4	312	CLA	C3B-C4B	2.01	1.48	1.42
19	A	823	CLA	C3B-C4B	2.01	1.48	1.42
19	A	806	CLA	C3B-C4B	2.01	1.48	1.42
19	A	833	CLA	C3B-C4B	2.01	1.48	1.42
18	2	305	CHL	O1D-CGD	2.01	1.26	1.21
19	A	804	CLA	C3B-C4B	2.01	1.48	1.42
19	A	802	CLA	C3B-C4B	2.01	1.48	1.42
19	A	830	CLA	C3B-C4B	2.01	1.48	1.42
19	B	805	CLA	C3B-C4B	2.01	1.48	1.42
19	A	811	CLA	C3B-C4B	2.01	1.48	1.42
19	1	321	CLA	C3B-C4B	2.01	1.48	1.42
19	B	830	CLA	C3B-C4B	2.00	1.48	1.42
19	1	308	CLA	C3B-C4B	2.00	1.48	1.42
19	B	806	CLA	C3B-C4B	2.00	1.48	1.42
19	B	827	CLA	C3B-C4B	2.00	1.48	1.42
18	2	314	CHL	O1D-CGD	2.00	1.26	1.21
19	A	801	CLA	C3B-C4B	2.00	1.48	1.42
19	A	821	CLA	C3B-C4B	2.00	1.48	1.42
18	2	306	CHL	O1D-CGD	2.00	1.26	1.21
19	A	839	CLA	C3B-C4B	2.00	1.48	1.42
19	A	836	CLA	C3B-C4B	2.00	1.48	1.42
19	B	819	CLA	C3B-C4B	2.00	1.48	1.42
19	1	304	CLA	C3B-C4B	2.00	1.48	1.42
19	B	808	CLA	C3B-C4B	2.00	1.48	1.42
19	F	303	CLA	C3B-C4B	2.00	1.48	1.42

All (1368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	314	CHL	C1B-CHB-C4A	12.72	129.51	121.32
18	2	305	CHL	C1B-CHB-C4A	12.22	129.18	121.32
18	4	314	CHL	C1B-CHB-C4A	12.15	129.14	121.32
18	2	301	CHL	C1B-CHB-C4A	12.11	129.12	121.32
18	4	304	CHL	C1B-CHB-C4A	12.06	129.08	121.32
18	1	301	CHL	C1B-CHB-C4A	11.94	129.00	121.32
18	4	306	CHL	C1B-CHB-C4A	11.86	128.95	121.32
18	3	307	CHL	C1B-CHB-C4A	11.80	128.91	121.32
18	2	306	CHL	C1B-CHB-C4A	11.73	128.87	121.32
18	2	307	CHL	C1B-CHB-C4A	11.68	128.83	121.32
18	1	306	CHL	C1B-CHB-C4A	11.56	128.76	121.32
18	4	305	CHL	C1B-CHB-C4A	11.49	128.71	121.32
19	1	321	CLA	C4A-NA-C1A	10.83	111.62	106.68
19	A	804	CLA	C4A-NA-C1A	10.79	111.60	106.68
19	G	203	CLA	C4A-NA-C1A	10.78	111.59	106.68
19	B	825	CLA	C4A-NA-C1A	10.73	111.57	106.68
19	B	812	CLA	C4A-NA-C1A	10.60	111.52	106.68
19	A	812	CLA	C4A-NA-C1A	10.56	111.50	106.68
19	A	826	CLA	C4A-NA-C1A	10.55	111.49	106.68
19	2	311	CLA	C4A-NA-C1A	10.53	111.48	106.68
19	2	313	CLA	C4A-NA-C1A	10.51	111.47	106.68
19	B	834	CLA	C4A-NA-C1A	10.50	111.47	106.68
19	G	204	CLA	C4A-NA-C1A	10.48	111.46	106.68
19	F	301	CLA	C4A-NA-C1A	10.46	111.45	106.68
19	3	311	CLA	C4A-NA-C1A	10.45	111.45	106.68
19	K	204	CLA	C4A-NA-C1A	10.39	111.42	106.68
19	A	813	CLA	C4A-NA-C1A	10.38	111.42	106.68
19	B	804	CLA	C4A-NA-C1A	10.37	111.41	106.68
19	F	304	CLA	C4A-NA-C1A	10.32	111.39	106.68
19	2	320	CLA	C4A-NA-C1A	10.30	111.38	106.68
19	A	835	CLA	C4A-NA-C1A	10.28	111.37	106.68
19	4	310	CLA	C4A-NA-C1A	10.27	111.36	106.68
19	B	805	CLA	C4A-NA-C1A	10.26	111.36	106.68
19	B	814	CLA	C4A-NA-C1A	10.17	111.32	106.68
19	A	805	CLA	C4A-NA-C1A	10.12	111.29	106.68
19	K	203	CLA	C4A-NA-C1A	10.09	111.28	106.68
19	1	311	CLA	C4A-NA-C1A	10.08	111.28	106.68
19	A	821	CLA	C4A-NA-C1A	10.08	111.28	106.68
19	A	822	CLA	C4A-NA-C1A	10.07	111.27	106.68
19	B	802	CLA	C4A-NA-C1A	10.05	111.26	106.68
19	B	807	CLA	C4A-NA-C1A	10.05	111.26	106.68
19	A	808	CLA	C4A-NA-C1A	10.04	111.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	811	CLA	C4A-NA-C1A	10.04	111.26	106.68
19	B	833	CLA	C4A-NA-C1A	10.04	111.26	106.68
19	A	825	CLA	C4A-NA-C1A	10.02	111.25	106.68
19	F	303	CLA	C4A-NA-C1A	10.02	111.25	106.68
19	3	312	CLA	C4A-NA-C1A	9.98	111.23	106.68
19	A	829	CLA	C4A-NA-C1A	9.96	111.22	106.68
19	4	307	CLA	C4A-NA-C1A	9.94	111.22	106.68
19	1	309	CLA	C4A-NA-C1A	9.94	111.21	106.68
19	A	819	CLA	C4A-NA-C1A	9.94	111.21	106.68
19	4	301	CLA	C4A-NA-C1A	9.93	111.21	106.68
19	B	835	CLA	C4A-NA-C1A	9.93	111.21	106.68
19	3	304	CLA	C4A-NA-C1A	9.92	111.21	106.68
19	A	854	CLA	C4A-NA-C1A	9.92	111.21	106.68
19	B	810	CLA	C4A-NA-C1A	9.92	111.21	106.68
19	1	308	CLA	C4A-NA-C1A	9.90	111.20	106.68
19	1	305	CLA	C4A-NA-C1A	9.90	111.19	106.68
19	A	815	CLA	C4A-NA-C1A	9.89	111.19	106.68
19	4	311	CLA	C4A-NA-C1A	9.87	111.18	106.68
19	A	838	CLA	C4A-NA-C1A	9.86	111.18	106.68
19	A	831	CLA	C4A-NA-C1A	9.85	111.17	106.68
19	3	302	CLA	C4A-NA-C1A	9.84	111.17	106.68
19	B	830	CLA	C4A-NA-C1A	9.83	111.16	106.68
19	4	303	CLA	C4A-NA-C1A	9.83	111.16	106.68
19	2	312	CLA	C4A-NA-C1A	9.82	111.16	106.68
19	A	851	CLA	C4A-NA-C1A	9.80	111.15	106.68
19	A	809	CLA	C4A-NA-C1A	9.78	111.14	106.68
19	A	839	CLA	C4A-NA-C1A	9.78	111.14	106.68
19	B	813	CLA	C4A-NA-C1A	9.76	111.13	106.68
19	B	803	CLA	C4A-NA-C1A	9.76	111.13	106.68
19	B	821	CLA	C4A-NA-C1A	9.75	111.13	106.68
19	4	308	CLA	C4A-NA-C1A	9.75	111.13	106.68
19	4	313	CLA	C4A-NA-C1A	9.75	111.13	106.68
19	A	832	CLA	C4A-NA-C1A	9.75	111.13	106.68
19	A	811	CLA	C4A-NA-C1A	9.75	111.12	106.68
19	B	808	CLA	C4A-NA-C1A	9.75	111.12	106.68
19	K	202	CLA	C4A-NA-C1A	9.73	111.12	106.68
19	1	302	CLA	C4A-NA-C1A	9.73	111.12	106.68
19	1	310	CLA	C4A-NA-C1A	9.72	111.11	106.68
19	2	303	CLA	C4A-NA-C1A	9.72	111.11	106.68
19	G	202	CLA	C4A-NA-C1A	9.72	111.11	106.68
19	A	814	CLA	C4A-NA-C1A	9.68	111.10	106.68
19	3	314	CLA	C4A-NA-C1A	9.68	111.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	C4A-NA-C1A	9.65	111.08	106.68
19	B	824	CLA	C4A-NA-C1A	9.65	111.08	106.68
19	1	312	CLA	C4A-NA-C1A	9.63	111.07	106.68
19	H	201	CLA	C4A-NA-C1A	9.61	111.06	106.68
19	3	308	CLA	C4A-NA-C1A	9.59	111.05	106.68
19	1	304	CLA	C4A-NA-C1A	9.58	111.05	106.68
19	B	819	CLA	C4A-NA-C1A	9.58	111.05	106.68
19	2	302	CLA	C4A-NA-C1A	9.56	111.04	106.68
19	4	312	CLA	C4A-NA-C1A	9.56	111.04	106.68
19	1	303	CLA	C4A-NA-C1A	9.55	111.04	106.68
19	3	305	CLA	C4A-NA-C1A	9.55	111.03	106.68
19	A	817	CLA	C4A-NA-C1A	9.53	111.03	106.68
19	B	820	CLA	C4A-NA-C1A	9.53	111.03	106.68
19	3	301	CLA	C4A-NA-C1A	9.52	111.02	106.68
19	1	314	CLA	C4A-NA-C1A	9.52	111.02	106.68
19	B	806	CLA	C4A-NA-C1A	9.52	111.02	106.68
19	2	309	CLA	C4A-NA-C1A	9.51	111.02	106.68
19	3	303	CLA	C4A-NA-C1A	9.50	111.01	106.68
19	B	815	CLA	C4A-NA-C1A	9.49	111.01	106.68
19	A	828	CLA	C4A-NA-C1A	9.49	111.01	106.68
19	A	836	CLA	C4A-NA-C1A	9.49	111.01	106.68
19	2	310	CLA	C4A-NA-C1A	9.48	111.01	106.68
19	A	852	CLA	C4A-NA-C1A	9.48	111.00	106.68
19	A	810	CLA	C4A-NA-C1A	9.47	111.00	106.68
19	3	309	CLA	C4A-NA-C1A	9.46	111.00	106.68
19	L	301	CLA	C4A-NA-C1A	9.46	111.00	106.68
19	A	827	CLA	C4A-NA-C1A	9.45	110.99	106.68
19	A	806	CLA	C4A-NA-C1A	9.44	110.99	106.68
19	B	827	CLA	C4A-NA-C1A	9.44	110.99	106.68
19	2	308	CLA	C4A-NA-C1A	9.44	110.98	106.68
19	1	307	CLA	C4A-NA-C1A	9.43	110.98	106.68
19	B	836	CLA	C4A-NA-C1A	9.41	110.97	106.68
19	J	102	CLA	C4A-NA-C1A	9.41	110.97	106.68
19	3	313	CLA	C4A-NA-C1A	9.40	110.97	106.68
19	A	840	CLA	C4A-NA-C1A	9.40	110.97	106.68
19	B	823	CLA	C4A-NA-C1A	9.39	110.97	106.68
19	4	302	CLA	C4A-NA-C1A	9.39	110.96	106.68
19	B	832	CLA	C4A-NA-C1A	9.37	110.96	106.68
19	B	817	CLA	C4A-NA-C1A	9.37	110.95	106.68
19	A	820	CLA	C4A-NA-C1A	9.36	110.95	106.68
19	B	801	CLA	C4A-NA-C1A	9.35	110.94	106.68
19	L	302	CLA	C4A-NA-C1A	9.34	110.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	C4A-NA-C1A	9.34	110.94	106.68
19	A	818	CLA	C4A-NA-C1A	9.34	110.94	106.68
19	B	831	CLA	C4A-NA-C1A	9.32	110.93	106.68
19	F	302	CLA	C4A-NA-C1A	9.32	110.93	106.68
19	L	303	CLA	C4A-NA-C1A	9.31	110.93	106.68
19	A	824	CLA	C4A-NA-C1A	9.31	110.93	106.68
19	A	837	CLA	C4A-NA-C1A	9.29	110.92	106.68
19	A	853	CLA	C4A-NA-C1A	9.29	110.92	106.68
19	B	837	CLA	C4A-NA-C1A	9.28	110.92	106.68
19	A	803	CLA	C4A-NA-C1A	9.27	110.91	106.68
19	3	306	CLA	C4A-NA-C1A	9.25	110.90	106.68
19	A	833	CLA	C4A-NA-C1A	9.21	110.88	106.68
19	2	304	CLA	C4A-NA-C1A	9.20	110.88	106.68
19	B	829	CLA	C4A-NA-C1A	9.19	110.87	106.68
19	3	310	CLA	C4A-NA-C1A	9.16	110.86	106.68
19	B	826	CLA	C4A-NA-C1A	9.13	110.84	106.68
19	A	823	CLA	C4A-NA-C1A	9.11	110.83	106.68
19	B	838	CLA	C4A-NA-C1A	9.10	110.83	106.68
19	A	830	CLA	C4A-NA-C1A	9.05	110.81	106.68
19	4	309	CLA	C4A-NA-C1A	9.04	110.81	106.68
19	1	313	CLA	C4A-NA-C1A	9.03	110.80	106.68
19	B	828	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	A	807	CLA	C4A-NA-C1A	8.97	110.77	106.68
19	B	809	CLA	C4A-NA-C1A	8.92	110.75	106.68
19	A	801	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	B	822	CLA	C4A-NA-C1A	8.71	110.65	106.68
19	B	816	CLA	C4A-NA-C1A	8.60	110.60	106.68
19	A	802	CLA	C4A-NA-C1A	8.44	110.53	106.68
19	A	834	CLA	C4A-NA-C1A	8.35	110.49	106.68
19	B	810	CLA	CAB-C3B-C4B	7.80	137.29	125.42
18	4	304	CHL	O2D-CGD-CBD	6.87	118.50	110.95
18	2	301	CHL	O2D-CGD-CBD	6.69	118.30	110.95
18	4	305	CHL	O2D-CGD-CBD	6.64	118.25	110.95
18	2	307	CHL	O2D-CGD-CBD	6.59	118.19	110.95
18	2	305	CHL	O2D-CGD-CBD	6.58	118.18	110.95
18	1	301	CHL	O2D-CGD-CBD	6.57	118.16	110.95
18	3	307	CHL	O2D-CGD-CBD	6.54	118.14	110.95
18	4	306	CHL	O2D-CGD-CBD	6.51	118.10	110.95
18	2	314	CHL	O2D-CGD-CBD	6.46	118.04	110.95
18	1	306	CHL	O2D-CGD-CBD	6.37	117.95	110.95
18	2	306	CHL	O2D-CGD-CBD	6.37	117.95	110.95
18	2	314	CHL	C4D-CHA-CBD	-4.96	103.97	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	314	CHL	C3D-C4D-CHA	4.72	115.72	108.54
18	2	307	CHL	C4D-CHA-CBD	-4.66	104.27	108.97
18	1	306	CHL	C3D-C4D-CHA	4.59	115.51	108.54
18	1	301	CHL	C3D-C4D-CHA	4.59	115.51	108.54
18	3	307	CHL	C3D-C4D-CHA	4.58	115.50	108.54
18	4	314	CHL	C3D-C4D-CHA	4.58	115.50	108.54
18	2	307	CHL	C3D-C4D-CHA	4.55	115.46	108.54
18	2	301	CHL	C3D-C4D-CHA	4.54	115.44	108.54
18	2	305	CHL	C3D-C4D-CHA	4.53	115.43	108.54
18	2	301	CHL	C4D-CHA-CBD	-4.52	104.41	108.97
19	A	829	CLA	O2D-CGD-CBD	4.51	119.11	111.23
19	A	801	CLA	O2D-CGD-CBD	4.50	119.10	111.23
18	2	306	CHL	C3D-C4D-CHA	4.50	115.38	108.54
18	4	306	CHL	C3D-C4D-CHA	4.50	115.38	108.54
18	4	304	CHL	C3D-C4D-CHA	4.49	115.37	108.54
18	4	306	CHL	C4D-CHA-CBD	-4.43	104.50	108.97
18	3	307	CHL	CBC-CAC-C3C	-4.43	106.54	112.87
18	4	305	CHL	C3D-C4D-CHA	4.42	115.26	108.54
18	2	306	CHL	C4D-CHA-CBD	-4.40	104.53	108.97
19	B	835	CLA	O2D-CGD-CBD	4.39	118.90	111.23
19	A	826	CLA	O2D-CGD-CBD	4.35	118.83	111.23
18	3	307	CHL	C4D-CHA-CBD	-4.34	104.59	108.97
18	1	306	CHL	C4D-CHA-CBD	-4.32	104.61	108.97
18	4	314	CHL	C4D-CHA-CBD	-4.32	104.62	108.97
19	B	806	CLA	O2D-CGD-CBD	4.30	118.75	111.23
18	1	301	CHL	C4D-CHA-CBD	-4.30	104.63	108.97
20	1	320	LUT	C35-C15-C14	4.30	132.32	123.52
18	4	305	CHL	C4D-CHA-CBD	-4.29	104.64	108.97
19	3	310	CLA	O2D-CGD-CBD	4.28	118.71	111.23
19	B	819	CLA	O2D-CGD-CBD	4.26	118.67	111.23
19	B	813	CLA	O2D-CGD-CBD	4.25	118.65	111.23
18	2	305	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
19	2	320	CLA	O2D-CGD-CBD	4.24	118.65	111.23
18	4	304	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
19	3	312	CLA	O2D-CGD-CBD	4.23	118.63	111.23
19	A	827	CLA	O2D-CGD-CBD	4.23	118.63	111.23
19	1	321	CLA	O2D-CGD-CBD	4.23	118.62	111.23
19	A	803	CLA	O2D-CGD-CBD	4.21	118.59	111.23
19	A	814	CLA	O2D-CGD-CBD	4.21	118.59	111.23
19	B	827	CLA	O2D-CGD-CBD	4.20	118.57	111.23
19	B	812	CLA	O2D-CGD-CBD	4.19	118.56	111.23
19	A	836	CLA	O2D-CGD-CBD	4.18	118.54	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	836	CLA	O2D-CGD-CBD	4.18	118.54	111.23
19	4	309	CLA	O2D-CGD-CBD	4.17	118.52	111.23
19	1	309	CLA	O2D-CGD-CBD	4.17	118.51	111.23
19	B	834	CLA	O2D-CGD-CBD	4.16	118.51	111.23
19	3	314	CLA	O2D-CGD-CBD	4.16	118.50	111.23
19	A	854	CLA	O2D-CGD-CBD	4.15	118.48	111.23
20	1	315	LUT	C15-C35-C34	4.15	132.00	123.52
19	A	853	CLA	O2D-CGD-CBD	4.13	118.46	111.23
19	4	307	CLA	O2D-CGD-CBD	4.13	118.46	111.23
19	B	809	CLA	O2D-CGD-CBD	4.12	118.44	111.23
19	A	825	CLA	O2D-CGD-CBD	4.12	118.44	111.23
19	1	303	CLA	O2D-CGD-CBD	4.12	118.43	111.23
19	B	815	CLA	O2D-CGD-CBD	4.12	118.43	111.23
19	B	825	CLA	O2D-CGD-CBD	4.12	118.43	111.23
19	B	832	CLA	O2D-CGD-CBD	4.11	118.42	111.23
19	G	203	CLA	O2D-CGD-CBD	4.11	118.42	111.23
19	A	819	CLA	O2D-CGD-CBD	4.11	118.41	111.23
19	J	102	CLA	O2D-CGD-CBD	4.11	118.41	111.23
19	A	804	CLA	O2D-CGD-CBD	4.11	118.41	111.23
19	1	312	CLA	O2D-CGD-CBD	4.11	118.41	111.23
19	A	822	CLA	O2D-CGD-CBD	4.11	118.41	111.23
19	B	810	CLA	O2D-CGD-CBD	4.10	118.39	111.23
19	A	812	CLA	O2D-CGD-CBD	4.09	118.39	111.23
19	B	817	CLA	O2D-CGD-CBD	4.09	118.38	111.23
19	B	821	CLA	O2D-CGD-CBD	4.08	118.36	111.23
19	2	303	CLA	O2D-CGD-CBD	4.08	118.36	111.23
19	A	840	CLA	O2D-CGD-CBD	4.07	118.35	111.23
19	3	308	CLA	O2D-CGD-CBD	4.07	118.35	111.23
19	B	816	CLA	O2D-CGD-CBD	4.06	118.33	111.23
19	B	829	CLA	O2D-CGD-CBD	4.06	118.32	111.23
19	2	309	CLA	O2D-CGD-CBD	4.06	118.32	111.23
19	4	311	CLA	O2D-CGD-CBD	4.05	118.31	111.23
19	B	823	CLA	O2D-CGD-CBD	4.05	118.31	111.23
20	2	315	LUT	C15-C35-C34	4.05	131.80	123.52
19	K	202	CLA	O2D-CGD-CBD	4.05	118.30	111.23
19	B	833	CLA	O2D-CGD-CBD	4.04	118.30	111.23
19	3	303	CLA	O2D-CGD-CBD	4.04	118.29	111.23
19	A	811	CLA	O2D-CGD-CBD	4.04	118.29	111.23
19	A	824	CLA	O2D-CGD-CBD	4.04	118.29	111.23
19	1	307	CLA	O2D-CGD-CBD	4.04	118.28	111.23
19	K	203	CLA	O2D-CGD-CBD	4.03	118.28	111.23
19	A	802	CLA	O2D-CGD-CBD	4.03	118.27	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	302	CLA	O2D-CGD-CBD	4.03	118.27	111.23
19	B	804	CLA	O2D-CGD-CBD	4.02	118.27	111.23
19	2	313	CLA	O2D-CGD-CBD	4.02	118.26	111.23
19	2	304	CLA	O2D-CGD-CBD	4.02	118.26	111.23
19	A	818	CLA	O2D-CGD-CBD	4.02	118.26	111.23
19	B	808	CLA	O2D-CGD-CBD	4.02	118.26	111.23
19	A	835	CLA	O2D-CGD-CBD	4.02	118.25	111.23
19	A	839	CLA	O2D-CGD-CBD	4.01	118.25	111.23
19	B	803	CLA	O2D-CGD-CBD	4.01	118.25	111.23
19	L	301	CLA	O2D-CGD-CBD	4.01	118.25	111.23
19	B	805	CLA	O2D-CGD-CBD	4.01	118.25	111.23
19	A	852	CLA	O2D-CGD-CBD	4.01	118.24	111.23
19	B	838	CLA	O2D-CGD-CBD	4.01	118.24	111.23
19	4	308	CLA	O2D-CGD-CBD	4.00	118.23	111.23
19	A	851	CLA	O2D-CGD-CBD	4.00	118.22	111.23
19	A	805	CLA	O2D-CGD-CBD	4.00	118.22	111.23
19	4	301	CLA	O2D-CGD-CBD	3.99	118.21	111.23
19	F	304	CLA	O2D-CGD-CBD	3.99	118.21	111.23
19	4	313	CLA	O2D-CGD-CBD	3.99	118.21	111.23
19	A	820	CLA	O2D-CGD-CBD	3.99	118.21	111.23
19	4	303	CLA	O2D-CGD-CBD	3.99	118.21	111.23
19	A	831	CLA	O2D-CGD-CBD	3.99	118.20	111.23
19	A	838	CLA	O2D-CGD-CBD	3.98	118.20	111.23
19	A	828	CLA	O2D-CGD-CBD	3.98	118.19	111.23
19	A	807	CLA	O2D-CGD-CBD	3.98	118.18	111.23
19	A	808	CLA	C3B-C4B-NB	-3.97	106.98	110.53
19	F	301	CLA	O2D-CGD-CBD	3.97	118.17	111.23
19	1	304	CLA	O2D-CGD-CBD	3.97	118.17	111.23
19	2	310	CLA	O2D-CGD-CBD	3.97	118.17	111.23
19	1	311	CLA	O2D-CGD-CBD	3.97	118.16	111.23
19	1	314	CLA	O2D-CGD-CBD	3.96	118.16	111.23
19	A	837	CLA	O2D-CGD-CBD	3.96	118.15	111.23
19	A	806	CLA	O2D-CGD-CBD	3.95	118.14	111.23
19	F	303	CLA	O2D-CGD-CBD	3.95	118.14	111.23
19	2	311	CLA	O2D-CGD-CBD	3.95	118.14	111.23
19	3	313	CLA	O2D-CGD-CBD	3.95	118.14	111.23
19	B	814	CLA	O2D-CGD-CBD	3.95	118.13	111.23
19	4	312	CLA	O2D-CGD-CBD	3.94	118.12	111.23
19	4	302	CLA	O2D-CGD-CBD	3.94	118.12	111.23
19	B	831	CLA	O2D-CGD-CBD	3.94	118.12	111.23
19	1	313	CLA	O2D-CGD-CBD	3.94	118.12	111.23
19	3	305	CLA	O2D-CGD-CBD	3.94	118.12	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	306	CLA	O2D-CGD-CBD	3.94	118.12	111.23
19	B	826	CLA	O2D-CGD-CBD	3.93	118.11	111.23
19	3	311	CLA	O2D-CGD-CBD	3.93	118.10	111.23
19	1	308	CLA	O2D-CGD-CBD	3.93	118.10	111.23
19	A	830	CLA	O2D-CGD-CBD	3.92	118.08	111.23
19	B	802	CLA	O2D-CGD-CBD	3.92	118.08	111.23
19	L	302	CLA	O2D-CGD-CBD	3.92	118.08	111.23
19	A	808	CLA	O2D-CGD-CBD	3.92	118.08	111.23
19	B	818	CLA	O2D-CGD-CBD	3.91	118.07	111.23
19	A	833	CLA	O2D-CGD-CBD	3.91	118.06	111.23
19	B	837	CLA	O2D-CGD-CBD	3.91	118.06	111.23
19	A	815	CLA	O2D-CGD-CBD	3.90	118.05	111.23
19	A	823	CLA	O2D-CGD-CBD	3.90	118.05	111.23
19	G	202	CLA	O2D-CGD-CBD	3.89	118.04	111.23
19	2	308	CLA	O2D-CGD-CBD	3.89	118.04	111.23
19	B	811	CLA	O2D-CGD-CBD	3.89	118.03	111.23
19	B	830	CLA	O2D-CGD-CBD	3.89	118.03	111.23
19	A	813	CLA	O2D-CGD-CBD	3.88	118.02	111.23
19	B	807	CLA	O2D-CGD-CBD	3.88	118.02	111.23
19	L	303	CLA	O2D-CGD-CBD	3.88	118.01	111.23
19	A	817	CLA	O2D-CGD-CBD	3.88	118.01	111.23
19	F	302	CLA	O2D-CGD-CBD	3.87	118.00	111.23
19	A	809	CLA	O2D-CGD-CBD	3.87	118.00	111.23
19	A	834	CLA	O2D-CGD-CBD	3.86	117.98	111.23
19	1	302	CLA	O2D-CGD-CBD	3.86	117.98	111.23
19	4	310	CLA	O2D-CGD-CBD	3.85	117.96	111.23
19	B	820	CLA	O2D-CGD-CBD	3.85	117.96	111.23
19	2	312	CLA	O2D-CGD-CBD	3.85	117.96	111.23
19	A	810	CLA	O2D-CGD-CBD	3.84	117.94	111.23
19	1	305	CLA	O2D-CGD-CBD	3.83	117.92	111.23
19	3	304	CLA	O2D-CGD-CBD	3.83	117.92	111.23
19	3	301	CLA	O2D-CGD-CBD	3.82	117.91	111.23
19	B	822	CLA	C3B-C4B-NB	-3.82	107.12	110.53
23	B	842	BCR	C16-C15-C14	3.81	131.31	123.52
19	A	832	CLA	O2D-CGD-CBD	3.81	117.88	111.23
18	4	305	CHL	CBC-CAC-C3C	-3.80	107.43	112.87
19	A	821	CLA	O2D-CGD-CBD	3.80	117.87	111.23
19	B	828	CLA	O2D-CGD-CBD	3.80	117.86	111.23
19	3	302	CLA	O2D-CGD-CBD	3.78	117.84	111.23
19	B	822	CLA	O2D-CGD-CBD	3.78	117.83	111.23
18	4	305	CHL	CMA-C3A-C4A	-3.78	106.47	114.61
18	2	305	CHL	CBC-CAC-C3C	-3.77	107.48	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	309	CLA	O2D-CGD-CBD	3.77	117.82	111.23
18	4	304	CHL	CBC-CAC-C3C	-3.76	107.49	112.87
19	A	835	CLA	C4-C3-C5	-3.73	111.74	116.13
19	A	838	CLA	C3B-C4B-NB	-3.72	107.21	110.53
19	1	310	CLA	O2D-CGD-CBD	3.71	117.72	111.23
18	4	314	CHL	CBC-CAC-C3C	-3.70	107.58	112.87
19	B	801	CLA	O2D-CGD-CBD	3.70	117.69	111.23
19	B	815	CLA	C3B-C4B-NB	-3.69	107.24	110.53
20	3	315	LUT	C15-C35-C34	3.66	131.00	123.52
23	J	101	BCR	C21-C20-C19	3.65	133.78	123.20
18	2	301	CHL	CBC-CAC-C3C	-3.65	107.65	112.87
19	B	824	CLA	O2D-CGD-CBD	3.65	117.60	111.23
19	G	204	CLA	O2D-CGD-CBD	3.64	117.60	111.23
19	A	827	CLA	C3B-C4B-NB	-3.64	107.28	110.53
19	A	825	CLA	C3B-C4B-NB	-3.62	107.30	110.53
19	A	806	CLA	C3B-C4B-NB	-3.62	107.30	110.53
23	1	318	BCR	C8-C7-C6	3.58	136.56	127.00
19	B	824	CLA	C3B-C4B-NB	-3.58	107.34	110.53
19	A	823	CLA	C3B-C4B-NB	-3.57	107.34	110.53
19	A	809	CLA	C3B-C4B-NB	-3.57	107.34	110.53
18	2	305	CHL	CMA-C3A-C4A	-3.56	106.94	114.61
19	A	804	CLA	C3B-C4B-NB	-3.56	107.35	110.53
19	B	809	CLA	C3B-C4B-NB	-3.56	107.35	110.53
19	A	816	CLA	C3B-C4B-NB	-3.55	107.36	110.53
19	H	201	CLA	O2D-CGD-CBD	3.55	117.44	111.23
23	B	842	BCR	C15-C16-C17	3.55	130.78	123.52
19	A	814	CLA	C3B-C4B-NB	-3.55	107.36	110.53
18	4	306	CHL	CBC-CAC-C3C	-3.55	107.80	112.87
20	1	320	LUT	C19-C9-C10	-3.55	117.07	122.82
23	1	318	BCR	C7-C8-C9	3.53	131.46	126.23
18	1	301	CHL	CBC-CAC-C3C	-3.53	107.82	112.87
19	A	803	CLA	C3B-C4B-NB	-3.53	107.38	110.53
19	B	828	CLA	C3B-C4B-NB	-3.52	107.39	110.53
18	2	306	CHL	CBC-CAC-C3C	-3.52	107.84	112.87
19	B	818	CLA	C3B-C4B-NB	-3.51	107.39	110.53
19	B	820	CLA	C3B-C4B-NB	-3.51	107.39	110.53
19	A	802	CLA	C3B-C4B-NB	-3.51	107.40	110.53
18	4	304	CHL	CMA-C3A-C4A	-3.50	107.06	114.61
19	A	813	CLA	C3B-C4B-NB	-3.50	107.40	110.53
19	B	831	CLA	C3B-C4B-NB	-3.50	107.40	110.53
19	B	806	CLA	C3B-C4B-NB	-3.50	107.41	110.53
19	A	801	CLA	C3B-C4B-NB	-3.49	107.41	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	833	CLA	C3B-C4B-NB	-3.49	107.41	110.53
19	A	853	CLA	C3B-C4B-NB	-3.49	107.42	110.53
19	L	302	CLA	C3B-C4B-NB	-3.49	107.42	110.53
19	B	837	CLA	C3B-C4B-NB	-3.48	107.42	110.53
19	A	833	CLA	C3B-C4B-NB	-3.48	107.42	110.53
18	1	301	CHL	CAA-C2A-C3A	-3.48	103.59	113.00
19	B	813	CLA	C3B-C4B-NB	-3.48	107.42	110.53
23	J	101	BCR	C16-C15-C14	3.48	130.63	123.52
19	B	817	CLA	C3B-C4B-NB	-3.48	107.43	110.53
18	4	305	CHL	CAA-C2A-C3A	-3.48	103.61	113.00
19	4	301	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	A	811	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	A	852	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	2	303	CLA	C3B-C4B-NB	-3.47	107.43	110.53
18	1	306	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
19	A	820	CLA	C3B-C4B-NB	-3.47	107.44	110.53
19	3	303	CLA	C3B-C4B-NB	-3.47	107.44	110.53
19	3	308	CLA	C3B-C4B-NB	-3.46	107.44	110.53
19	A	830	CLA	C3B-C4B-NB	-3.46	107.44	110.53
18	4	314	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
19	2	309	CLA	C3B-C4B-NB	-3.45	107.45	110.53
19	4	308	CLA	C3B-C4B-NB	-3.45	107.45	110.53
19	F	301	CLA	C3B-C4B-NB	-3.45	107.45	110.53
20	4	315	LUT	C15-C35-C34	3.45	130.57	123.52
19	B	816	CLA	C3B-C4B-NB	-3.44	107.45	110.53
18	3	307	CHL	CMA-C3A-C4A	-3.44	107.19	114.61
18	2	307	CHL	CBC-CAC-C3C	-3.44	107.95	112.87
18	2	306	CHL	CMA-C3A-C4A	-3.43	107.21	114.61
19	2	302	CLA	C3B-C4B-NB	-3.43	107.47	110.53
18	2	314	CHL	CMA-C3A-C4A	-3.43	107.22	114.61
19	A	810	CLA	C3B-C4B-NB	-3.43	107.47	110.53
19	A	837	CLA	C3B-C4B-NB	-3.43	107.47	110.53
19	1	309	CLA	C3B-C4B-NB	-3.43	107.47	110.53
19	B	835	CLA	C3B-C4B-NB	-3.43	107.47	110.53
18	2	307	CHL	CAA-C2A-C3A	-3.42	103.75	113.00
19	B	801	CLA	C3B-C4B-NB	-3.42	107.47	110.53
19	3	314	CLA	C3B-C4B-NB	-3.42	107.48	110.53
18	2	314	CHL	CBC-CAC-C3C	-3.42	107.98	112.87
18	1	301	CHL	C1-C2-C3	3.42	131.80	126.20
19	3	309	CLA	C3B-C4B-NB	-3.42	107.48	110.53
18	2	301	CHL	CMA-C3A-C4A	-3.41	107.25	114.61
19	1	313	CLA	C3B-C4B-NB	-3.41	107.48	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	804	CLA	C3B-C4B-NB	-3.41	107.48	110.53
19	B	825	CLA	C3B-C4B-NB	-3.41	107.48	110.53
18	1	306	CHL	CBC-CAC-C3C	-3.41	107.99	112.87
19	1	304	CLA	C4-C3-C5	-3.41	112.12	116.13
19	B	803	CLA	C3B-C4B-NB	-3.40	107.49	110.53
18	1	301	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
19	A	807	CLA	C3B-C4B-NB	-3.40	107.49	110.53
19	H	201	CLA	C3B-C4B-NB	-3.40	107.49	110.53
18	2	307	CHL	CMA-C3A-C4A	-3.40	107.29	114.61
19	A	829	CLA	C3B-C4B-NB	-3.40	107.50	110.53
19	4	313	CLA	C3B-C4B-NB	-3.39	107.50	110.53
19	A	821	CLA	C3B-C4B-NB	-3.39	107.50	110.53
19	B	814	CLA	C3B-C4B-NB	-3.39	107.50	110.53
18	4	306	CHL	CMA-C3A-C4A	-3.39	107.31	114.61
19	L	301	CLA	O2A-CGA-CBA	3.39	122.16	111.83
19	2	308	CLA	C3B-C4B-NB	-3.39	107.51	110.53
19	A	826	CLA	O2A-CGA-CBA	3.38	122.16	111.83
19	B	811	CLA	C3B-C4B-NB	-3.38	107.51	110.53
19	A	828	CLA	C3B-C4B-NB	-3.38	107.51	110.53
19	3	301	CLA	C3B-C4B-NB	-3.38	107.51	110.53
19	A	834	CLA	C3B-C4B-NB	-3.38	107.51	110.53
19	B	832	CLA	C3B-C4B-NB	-3.38	107.52	110.53
18	2	301	CHL	CAA-C2A-C3A	-3.37	103.89	113.00
19	B	819	CLA	C3B-C4B-NB	-3.37	107.52	110.53
19	G	203	CLA	C3B-C4B-NB	-3.37	107.52	110.53
19	3	306	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	2	320	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	2	304	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	B	829	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	A	818	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	1	309	CLA	O2A-CGA-CBA	3.36	122.07	111.83
19	B	812	CLA	C3B-C4B-NB	-3.35	107.54	110.53
18	2	306	CHL	CAA-C2A-C3A	-3.35	103.94	113.00
20	3	315	LUT	C19-C9-C10	-3.35	117.39	122.82
19	1	312	CLA	C3B-C4B-NB	-3.34	107.54	110.53
19	A	805	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	1	308	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	J	102	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	A	835	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	B	838	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	A	817	CLA	C3B-C4B-NB	-3.34	107.55	110.53
19	A	834	CLA	O2A-CGA-CBA	3.34	122.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	307	CLA	C3B-C4B-NB	-3.33	107.55	110.53
19	1	304	CLA	O2A-CGA-CBA	3.33	121.99	111.83
19	1	310	CLA	C3B-C4B-NB	-3.33	107.56	110.53
19	A	839	CLA	C3B-C4B-NB	-3.33	107.56	110.53
19	A	854	CLA	C3B-C4B-NB	-3.33	107.56	110.53
20	2	315	LUT	C39-C29-C30	-3.33	117.43	122.82
19	B	808	CLA	C3B-C4B-NB	-3.32	107.56	110.53
19	A	807	CLA	O2A-CGA-CBA	3.32	121.96	111.83
19	1	314	CLA	C3B-C4B-NB	-3.32	107.56	110.53
19	B	827	CLA	O2A-CGA-CBA	3.32	121.96	111.83
19	B	838	CLA	O2A-CGA-CBA	3.32	121.96	111.83
18	4	306	CHL	CAA-C2A-C3A	-3.32	104.03	113.00
19	B	836	CLA	O2A-CGA-CBA	3.32	121.95	111.83
19	2	313	CLA	C3B-C4B-NB	-3.32	107.57	110.53
19	1	310	CLA	O2A-CGA-CBA	3.32	121.95	111.83
20	4	315	LUT	C35-C15-C14	3.32	130.30	123.52
19	3	308	CLA	O2A-CGA-CBA	3.31	121.94	111.83
19	3	304	CLA	C3B-C4B-NB	-3.31	107.57	110.53
19	2	309	CLA	O2A-CGA-CBA	3.31	121.94	111.83
19	A	835	CLA	O2A-CGA-CBA	3.31	121.94	111.83
19	B	807	CLA	C3B-C4B-NB	-3.31	107.57	110.53
19	A	806	CLA	O2A-CGA-CBA	3.31	121.93	111.83
19	B	836	CLA	C3B-C4B-NB	-3.31	107.58	110.53
19	A	836	CLA	C3B-C4B-NB	-3.31	107.58	110.53
19	A	826	CLA	C3B-C4B-NB	-3.30	107.58	110.53
19	4	308	CLA	O2A-CGA-CBA	3.30	121.90	111.83
18	4	304	CHL	C1-C2-C3	3.30	131.60	126.20
19	1	303	CLA	C3B-C4B-NB	-3.30	107.59	110.53
19	2	304	CLA	C1-C2-C3	3.30	131.60	126.20
18	4	304	CHL	CAA-C2A-C3A	-3.29	104.10	113.00
19	B	830	CLA	O2A-CGA-CBA	3.29	121.87	111.83
19	A	810	CLA	O2A-CGA-CBA	3.29	121.87	111.83
19	B	807	CLA	O2A-CGA-CBA	3.29	121.86	111.83
19	F	303	CLA	C3B-C4B-NB	-3.29	107.59	110.53
19	A	840	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	B	834	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	3	313	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	B	837	CLA	O2A-CGA-CBA	3.28	121.85	111.83
19	2	310	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	4	303	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	2	302	CLA	O2A-CGA-CBA	3.28	121.84	111.83
18	1	306	CHL	CAA-C2A-C3A	-3.28	104.13	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	315	LUT	C35-C15-C14	3.28	130.22	123.52
19	A	808	CLA	O2A-CGA-CBA	3.28	121.82	111.83
20	3	315	LUT	C39-C29-C30	-3.28	117.51	122.82
20	4	315	LUT	C19-C9-C10	-3.27	117.51	122.82
19	B	801	CLA	O2A-CGA-CBA	3.27	121.82	111.83
19	2	312	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	B	805	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	B	825	CLA	O2A-CGA-CBA	3.27	121.81	111.83
19	B	802	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	L	301	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	F	302	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	F	301	CLA	O2A-CGA-CBA	3.27	121.80	111.83
19	B	830	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	A	836	CLA	O2A-CGA-CBA	3.26	121.78	111.83
19	A	851	CLA	C3B-C4B-NB	-3.26	107.62	110.53
19	B	828	CLA	O2A-CGA-CBA	3.26	121.77	111.83
19	3	310	CLA	C3B-C4B-NB	-3.26	107.62	110.53
19	B	820	CLA	O2A-CGA-CBA	3.26	121.76	111.83
21	3	316	XAT	C7-C8-C9	3.25	130.58	125.53
19	B	826	CLA	C3B-C4B-NB	-3.25	107.62	110.53
19	A	832	CLA	O2A-CGA-CBA	3.25	121.76	111.83
20	1	320	LUT	C39-C29-C30	-3.25	117.55	122.82
20	1	315	LUT	C39-C29-C30	-3.25	117.55	122.82
19	B	814	CLA	O2A-CGA-CBA	3.25	121.75	111.83
18	3	307	CHL	CAA-C2A-C3A	-3.25	104.22	113.00
19	B	821	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	B	804	CLA	O2A-CGA-CBA	3.24	121.72	111.83
20	4	315	LUT	C39-C29-C30	-3.24	117.56	122.82
19	4	311	CLA	O2A-CGA-CBA	3.24	121.71	111.83
19	B	823	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	1	307	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	B	827	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	B	818	CLA	O2A-CGA-CBA	3.23	121.70	111.83
19	L	302	CLA	O2A-CGA-CBA	3.23	121.69	111.83
19	K	203	CLA	C3B-C4B-NB	-3.23	107.64	110.53
19	1	321	CLA	C3B-C4B-NB	-3.23	107.64	110.53
19	1	312	CLA	O2A-CGA-CBA	3.23	121.68	111.83
19	A	838	CLA	O2A-CGA-CBA	3.22	121.67	111.83
19	1	302	CLA	C3B-C4B-NB	-3.22	107.65	110.53
19	4	309	CLA	C3B-C4B-NB	-3.22	107.65	110.53
19	3	311	CLA	C3B-C4B-NB	-3.22	107.65	110.53
19	A	831	CLA	C3B-C4B-NB	-3.22	107.65	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	304	CLA	C3B-C4B-NB	-3.22	107.66	110.53
19	1	311	CLA	C3B-C4B-NB	-3.22	107.66	110.53
19	3	304	CLA	O2A-CGA-CBA	3.22	121.65	111.83
19	B	806	CLA	O2A-CGA-CBA	3.22	121.65	111.83
19	B	822	CLA	O2A-CGA-CBA	3.22	121.64	111.83
20	2	315	LUT	C19-C9-C10	-3.22	117.61	122.82
19	B	829	CLA	O2A-CGA-CBA	3.21	121.63	111.83
19	3	312	CLA	C3B-C4B-NB	-3.21	107.66	110.53
19	A	823	CLA	O2A-CGA-CBA	3.20	121.61	111.83
19	B	815	CLA	O2A-CGA-CBA	3.20	121.60	111.83
19	2	312	CLA	O2A-CGA-CBA	3.20	121.59	111.83
19	K	204	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	G	202	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	B	823	CLA	O2A-CGA-CBA	3.20	121.58	111.83
19	A	831	CLA	O2A-CGA-CBA	3.19	121.56	111.83
19	B	824	CLA	O2A-CGA-CBA	3.19	121.56	111.83
19	3	305	CLA	C3B-C4B-NB	-3.19	107.69	110.53
19	4	307	CLA	O2A-CGA-CBA	3.19	121.55	111.83
19	A	829	CLA	O2A-CGA-CBA	3.19	121.55	111.83
19	B	831	CLA	O2A-CGA-CBA	3.18	121.55	111.83
19	A	819	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	A	822	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	B	808	CLA	O2A-CGA-CBA	3.17	121.52	111.83
19	1	305	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	4	312	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	1	302	CLA	O2A-CGA-CBA	3.17	121.50	111.83
19	4	302	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	1	321	CLA	O2A-CGA-CBA	3.17	121.50	111.83
19	G	204	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	L	303	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	2	313	CLA	O2A-CGA-CBA	3.16	121.46	111.83
19	G	203	CLA	O2A-CGA-CBA	3.16	121.46	111.83
19	3	302	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	A	815	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	B	809	CLA	O2A-CGA-CBA	3.15	121.44	111.83
20	1	315	LUT	C19-C9-C10	-3.15	117.71	122.82
19	3	309	CLA	O2A-CGA-CBA	3.15	121.44	111.83
19	A	833	CLA	O2A-CGA-CBA	3.15	121.44	111.83
19	A	824	CLA	O2A-CGA-CBA	3.15	121.44	111.83
19	A	811	CLA	O2A-CGA-CBA	3.15	121.43	111.83
19	A	801	CLA	O2A-CGA-CBA	3.14	121.42	111.83
19	3	312	CLA	O2A-CGA-CBA	3.14	121.41	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	C3B-C4B-NB	-3.13	107.74	110.53
19	A	814	CLA	O2A-CGA-CBA	3.12	121.36	111.83
19	A	803	CLA	O2A-CGA-CBA	3.12	121.34	111.83
19	L	303	CLA	O2A-CGA-CBA	3.12	121.34	111.83
19	A	832	CLA	C3B-C4B-NB	-3.12	107.75	110.53
19	1	308	CLA	O2A-CGA-CBA	3.11	121.33	111.83
19	K	202	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	4	301	CLA	O2A-CGA-CBA	3.11	121.31	111.83
19	A	818	CLA	O2A-CGA-CBA	3.10	121.29	111.83
19	A	812	CLA	C3B-C4B-NB	-3.10	107.76	110.53
19	B	826	CLA	O2A-CGA-CBA	3.09	121.27	111.83
19	A	804	CLA	O2A-CGA-CBA	3.09	121.27	111.83
19	A	812	CLA	O2A-CGA-CBA	3.09	121.27	111.83
19	A	802	CLA	O2A-CGA-CBA	3.09	121.27	111.83
19	B	832	CLA	O2A-CGA-CBA	3.09	121.26	111.83
19	2	311	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	B	834	CLA	O2A-CGA-CBA	3.09	121.25	111.83
19	4	310	CLA	C3B-C4B-NB	-3.09	107.77	110.53
18	2	314	CHL	C1A-CHA-C4D	3.09	124.13	118.98
23	L	305	BCR	C16-C15-C14	3.09	129.83	123.52
19	A	839	CLA	O2A-CGA-CBA	3.08	121.24	111.83
19	4	313	CLA	O2A-CGA-CBA	3.08	121.23	111.83
19	B	812	CLA	O2A-CGA-CBA	3.08	121.22	111.83
19	F	304	CLA	C3B-C4B-NB	-3.08	107.78	110.53
19	1	303	CLA	O2A-CGA-CBA	3.08	121.22	111.83
19	A	840	CLA	O2A-CGA-CBA	3.08	121.22	111.83
19	A	820	CLA	O2A-CGA-CBA	3.08	121.21	111.83
26	A	841	PQN	C11-C3-C4	-3.07	115.34	118.58
19	2	303	CLA	O2A-CGA-CBA	3.07	121.21	111.83
19	B	805	CLA	O2A-CGA-CBA	3.07	121.19	111.83
19	B	816	CLA	C12-C11-C10	-3.07	102.05	113.62
26	B	839	PQN	C11-C3-C4	-3.06	115.35	118.58
19	B	819	CLA	O2A-CGA-CBA	3.06	121.17	111.83
18	4	306	CHL	C1-C2-C3	3.06	131.72	126.76
18	2	301	CHL	C1-C2-C3	3.06	131.71	126.76
19	B	835	CLA	O2A-CGA-CBA	3.05	121.15	111.83
19	4	302	CLA	O2A-CGA-CBA	3.05	121.14	111.83
19	F	302	CLA	O2A-CGA-CBA	3.04	121.11	111.83
19	A	854	CLA	O2A-CGA-CBA	3.04	121.11	111.83
19	A	830	CLA	O2A-CGA-CBA	3.03	121.09	111.83
19	B	811	CLA	O2A-CGA-CBA	3.03	121.08	111.83
19	A	822	CLA	C4-C3-C5	-3.03	112.56	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	830	CLA	C1-C2-C3	3.03	131.17	126.20
20	1	320	LUT	C12-C13-C14	3.03	123.77	119.01
19	4	311	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	2	304	CLA	O2A-CGA-CBA	3.03	121.06	111.83
19	A	828	CLA	O2A-CGA-CBA	3.02	121.03	111.83
18	2	314	CHL	OBD-CAD-CBD	-3.02	121.40	125.82
18	2	301	CHL	O2A-CGA-CBA	3.01	121.01	111.83
18	1	306	CHL	C1A-CHA-C4D	3.01	124.00	118.98
21	4	316	XAT	C7-C8-C9	3.01	130.20	125.53
19	A	822	CLA	O2A-CGA-CBA	3.01	121.00	111.83
19	A	825	CLA	O2A-CGA-CBA	3.01	121.00	111.83
19	A	817	CLA	O2A-CGA-CBA	3.00	121.00	111.83
19	A	837	CLA	O2A-CGA-CBA	3.00	120.99	111.83
19	B	813	CLA	O2A-CGA-CBA	3.00	120.99	111.83
19	A	809	CLA	O2A-CGA-CBA	3.00	120.99	111.83
19	A	853	CLA	O2A-CGA-CBA	3.00	120.98	111.83
19	B	816	CLA	O2A-CGA-CBA	3.00	120.98	111.83
19	B	810	CLA	O2A-CGA-CBA	3.00	120.97	111.83
19	B	817	CLA	O2A-CGA-CBA	3.00	120.97	111.83
19	3	301	CLA	O2A-CGA-CBA	2.99	120.96	111.83
19	4	301	CLA	C1-C2-C3	2.99	131.10	126.20
19	A	852	CLA	O2A-CGA-CBA	2.99	120.94	111.83
18	1	301	CHL	OBD-CAD-CBD	-2.98	121.45	125.82
18	3	307	CHL	C1A-CHA-C4D	2.98	123.95	118.98
19	B	821	CLA	O2A-CGA-CBA	2.98	120.91	111.83
18	4	306	CHL	O2A-CGA-CBA	2.97	120.90	111.83
19	A	816	CLA	O2A-CGA-CBA	2.96	120.86	111.83
19	A	827	CLA	O2A-CGA-CBA	2.96	120.85	111.83
19	B	802	CLA	O2A-CGA-CBA	2.95	120.83	111.83
18	1	301	CHL	O2A-CGA-CBA	2.94	120.81	111.83
19	A	809	CLA	C12-C11-C10	-2.94	102.54	113.62
18	4	304	CHL	OBD-CAD-CBD	-2.92	121.53	125.82
19	2	313	CLA	C1-C2-C3	2.92	130.98	126.20
18	4	304	CHL	O2A-CGA-CBA	2.91	120.70	111.83
19	4	309	CLA	O2A-CGA-CBA	2.90	120.69	111.83
20	1	320	LUT	C20-C13-C14	-2.90	118.12	122.82
18	4	305	CHL	OBD-CAD-CBD	-2.88	121.60	125.82
19	A	816	CLA	C1-C2-C3	2.88	130.91	126.20
18	2	307	CHL	OBD-CAD-CBD	-2.87	121.61	125.82
18	4	314	CHL	C1A-CHA-C4D	2.87	123.78	118.98
20	1	315	LUT	C19-C9-C8	2.87	122.47	118.09
18	2	301	CHL	OBD-CAD-CBD	-2.87	121.61	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	302	CLA	O2A-CGA-CBA	2.87	120.59	111.83
19	A	825	CLA	C1-C2-C3	2.86	130.89	126.20
19	B	828	CLA	C1-C2-C3	2.86	130.88	126.20
18	1	306	CHL	OBD-CAD-CBD	-2.86	121.63	125.82
23	L	305	BCR	C15-C16-C17	2.86	129.37	123.52
19	A	805	CLA	O2A-CGA-CBA	2.86	120.54	111.83
19	2	310	CLA	CMA-C3A-C2A	-2.85	109.68	116.23
18	4	314	CHL	OBD-CAD-CBD	-2.85	121.64	125.82
18	2	306	CHL	C1A-CHA-C4D	2.84	123.72	118.98
18	2	301	CHL	C1A-CHA-C4D	2.84	123.72	118.98
19	1	304	CLA	C1-C2-C3	2.84	130.85	126.20
18	4	306	CHL	CHA-C1A-C2A	-2.84	126.64	133.31
23	J	101	BCR	C15-C16-C17	-2.84	117.72	123.52
18	2	301	CHL	CHA-C1A-C2A	-2.83	126.65	133.31
19	L	301	CLA	C1-C2-C3	2.83	130.83	126.20
18	2	301	CHL	O1D-CGD-CBD	-2.83	120.44	124.72
18	2	301	CHL	C1C-CHC-C4B	2.82	126.16	116.07
19	4	302	CLA	C1-C2-C3	2.82	130.81	126.20
18	2	314	CHL	CHA-C1A-C2A	-2.81	126.71	133.31
18	4	306	CHL	OBD-CAD-CBD	-2.81	121.71	125.82
19	B	837	CLA	C1-C2-C3	2.81	130.79	126.20
19	B	806	CLA	C1-C2-C3	2.80	130.79	126.20
23	A	844	BCR	C15-C16-C17	2.80	129.25	123.52
19	3	308	CLA	C1-C2-C3	2.79	130.77	126.20
18	2	306	CHL	C1C-CHC-C4B	2.79	126.06	116.07
19	B	810	CLA	CAB-C3B-C2B	-2.79	116.12	123.53
19	A	805	CLA	C1-C2-C3	2.78	130.75	126.20
18	1	306	CHL	CHA-C1A-C2A	-2.78	126.79	133.31
18	2	314	CHL	C1C-CHC-C4B	2.77	125.99	116.07
18	1	306	CHL	C1C-CHC-C4B	2.77	125.98	116.07
19	B	812	CLA	C1-C2-C3	2.76	130.72	126.20
18	2	314	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
18	4	305	CHL	C1A-CHA-C4D	2.76	123.58	118.98
18	1	301	CHL	C1C-CHC-C4B	2.75	125.93	116.07
18	4	304	CHL	C1A-CHA-C4D	2.75	123.58	118.98
19	B	824	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
18	1	306	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
19	A	802	CLA	C1-C2-C3	2.75	130.70	126.20
19	B	811	CLA	C1-C2-C3	2.75	130.70	126.20
19	A	811	CLA	C1-C2-C3	2.75	130.70	126.20
19	G	202	CLA	CMA-C3A-C2A	-2.74	109.94	116.23
19	B	809	CLA	C1-C2-C3	2.74	130.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	307	CHL	C1C-CHC-C4B	2.74	125.88	116.07
23	2	319	BCR	C16-C15-C14	2.74	129.12	123.52
18	4	314	CHL	C1C-CHC-C4B	2.74	125.87	116.07
18	2	305	CHL	C1A-CHA-C4D	2.74	123.55	118.98
18	2	306	CHL	O1D-CGD-CBD	-2.74	120.57	124.72
20	2	315	LUT	C35-C15-C14	2.73	129.11	123.52
18	4	305	CHL	C1C-CHC-C4B	2.73	125.85	116.07
18	3	307	CHL	C1C-CHC-C4B	2.73	125.84	116.07
18	4	306	CHL	O1D-CGD-CBD	-2.73	120.59	124.72
19	B	815	CLA	C1-C2-C3	2.73	130.66	126.20
19	1	310	CLA	C1-C2-C3	2.73	130.66	126.20
19	B	831	CLA	C1-C2-C3	2.72	130.66	126.20
19	A	812	CLA	C1-C2-C3	2.72	130.65	126.20
19	K	204	CLA	CMA-C3A-C2A	-2.72	110.00	116.23
19	A	829	CLA	C1-C2-C3	2.72	130.65	126.20
19	A	823	CLA	C1-C2-C3	2.71	130.64	126.20
20	1	315	LUT	C40-C33-C34	-2.71	118.43	122.82
19	A	801	CLA	C1-C2-C3	2.70	130.63	126.20
19	3	310	CLA	CMA-C3A-C2A	-2.70	110.03	116.23
18	2	314	CHL	C4C-CHD-C1D	2.70	125.73	116.07
20	2	315	LUT	C40-C33-C34	-2.70	118.44	122.82
19	F	301	CLA	C1-C2-C3	2.70	130.61	126.20
18	1	301	CHL	C4C-CHD-C1D	2.69	125.68	116.07
18	4	306	CHL	C1A-CHA-C4D	2.69	123.46	118.98
18	2	305	CHL	C4C-CHD-C1D	2.68	125.67	116.07
18	4	304	CHL	C4C-CHD-C1D	2.68	125.65	116.07
19	B	822	CLA	C1-C2-C3	2.68	130.58	126.20
18	4	314	CHL	C4C-CHD-C1D	2.67	125.62	116.07
19	B	816	CLA	C1-C2-C3	2.67	130.56	126.20
18	4	306	CHL	C4C-CHD-C1D	2.66	125.60	116.07
20	3	315	LUT	C40-C33-C34	-2.66	118.50	122.82
18	1	301	CHL	C1A-CHA-C4D	2.66	123.42	118.98
19	B	804	CLA	C1-C2-C3	2.66	130.55	126.20
18	2	305	CHL	C1C-CHC-C4B	2.65	125.56	116.07
18	2	305	CHL	OBD-CAD-CBD	-2.65	121.94	125.82
18	4	305	CHL	O1D-CGD-CBD	-2.64	120.71	124.72
18	3	307	CHL	OBD-CAD-CBD	-2.64	121.95	125.82
20	2	315	LUT	C32-C33-C34	2.64	123.17	119.01
18	4	306	CHL	C1C-CHC-C4B	2.64	125.51	116.07
19	B	832	CLA	C1-C2-C3	2.64	130.52	126.20
20	3	315	LUT	C20-C13-C14	-2.64	118.55	122.82
19	A	839	CLA	C1-C2-C3	2.64	130.51	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	301	CHL	C4C-CHD-C1D	2.63	125.50	116.07
18	2	307	CHL	C4C-CHD-C1D	2.63	125.50	116.07
18	2	307	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
21	1	316	XAT	C7-C8-C9	2.63	129.61	125.53
20	1	315	LUT	C32-C33-C34	2.63	123.14	119.01
19	B	810	CLA	C3B-C4B-NB	-2.62	107.61	110.33
18	4	304	CHL	C1C-CHC-C4B	2.62	125.45	116.07
20	4	315	LUT	C40-C33-C34	-2.62	118.57	122.82
20	1	320	LUT	C15-C35-C34	2.62	128.88	123.52
19	A	832	CLA	C1-C2-C3	2.62	130.49	126.20
19	B	824	CLA	C1-C2-C3	2.62	130.49	126.20
18	2	306	CHL	OBD-CAD-CBD	-2.61	121.99	125.82
19	4	313	CLA	C1-C2-C3	2.61	130.47	126.20
19	1	308	CLA	C1-C2-C3	2.61	130.47	126.20
18	3	307	CHL	C3C-C4C-NC	-2.60	108.29	114.65
18	3	307	CHL	C4C-CHD-C1D	2.60	125.36	116.07
21	2	316	XAT	O4-C5-C4	-2.60	111.06	113.49
19	B	821	CLA	C1-C2-C3	2.59	130.45	126.20
18	2	306	CHL	CHA-C1A-C2A	-2.59	127.22	133.31
19	B	820	CLA	C1-C2-C3	2.59	130.44	126.20
19	K	203	CLA	O2A-CGA-CBA	2.59	121.91	112.14
18	2	305	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
20	2	315	LUT	C19-C9-C8	2.58	122.02	118.09
19	2	302	CLA	C1-C2-C3	2.57	130.41	126.20
19	A	820	CLA	C1-C2-C3	2.57	130.41	126.20
19	4	309	CLA	C1-C2-C3	2.56	130.39	126.20
20	3	315	LUT	C32-C33-C34	2.56	123.03	119.01
19	B	823	CLA	C1-C2-C3	2.56	130.39	126.20
19	3	301	CLA	C12-C11-C10	-2.56	101.82	113.28
18	2	307	CHL	CHA-C1A-C2A	-2.56	127.31	133.31
18	4	305	CHL	C4C-CHD-C1D	2.55	125.21	116.07
19	A	810	CLA	C1-C2-C3	2.55	130.38	126.20
19	A	836	CLA	C1-C2-C3	2.55	130.38	126.20
18	2	305	CHL	CHA-C1A-C2A	-2.55	127.31	133.31
19	B	824	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
19	A	831	CLA	C1-C2-C3	2.55	130.38	126.20
20	4	315	LUT	C20-C13-C14	-2.54	118.70	122.82
19	A	805	CLA	C12-C11-C10	-2.54	101.90	113.28
19	B	838	CLA	C1-C2-C3	2.54	130.36	126.20
19	A	822	CLA	C1-C2-C3	2.54	130.35	126.20
19	3	312	CLA	C1-C2-C3	2.54	130.35	126.20
19	B	813	CLA	C1-C2-C3	2.53	130.35	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	814	CLA	C1-C2-C3	2.53	130.86	126.76
19	3	314	CLA	O2A-CGA-CBA	2.53	121.68	112.14
19	A	808	CLA	C1-C2-C3	2.53	130.34	126.20
19	B	835	CLA	C1-C2-C3	2.52	130.33	126.20
20	1	320	LUT	C40-C33-C34	-2.52	118.73	122.82
19	B	818	CLA	C1-C2-C3	2.52	130.33	126.20
19	2	312	CLA	C1-C2-C3	2.52	130.32	126.20
19	1	310	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
19	B	814	CLA	C1-C2-C3	2.52	130.32	126.20
19	4	307	CLA	C1-C2-C3	2.52	130.83	126.76
19	A	827	CLA	C12-C11-C10	-2.52	102.01	113.28
18	3	307	CHL	CHA-C1A-C2A	-2.51	127.40	133.31
19	A	818	CLA	C12-C11-C10	-2.51	102.03	113.28
18	2	314	CHL	C3C-C4C-NC	-2.51	108.52	114.65
20	1	320	LUT	C39-C29-C28	2.51	121.92	118.09
20	1	315	LUT	C39-C29-C28	2.50	121.91	118.09
19	B	826	CLA	C1-C2-C3	2.50	130.30	126.20
18	1	306	CHL	C4C-CHD-C1D	2.50	125.02	116.07
20	1	315	LUT	C35-C15-C14	2.50	128.63	123.52
20	3	315	LUT	C12-C13-C14	2.50	122.93	119.01
18	4	314	CHL	C3C-C4C-NC	-2.49	108.55	114.65
19	A	818	CLA	C1-C2-C3	2.49	130.28	126.20
18	4	306	CHL	C3C-C4C-NC	-2.49	108.56	114.65
19	F	302	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	2	307	CHL	C1A-CHA-C4D	2.49	123.13	118.98
19	B	825	CLA	C1-C2-C3	2.49	130.27	126.20
19	F	302	CLA	C12-C11-C10	-2.49	102.14	113.28
19	B	812	CLA	C12-C11-C10	-2.49	102.14	113.28
18	4	314	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
18	2	307	CHL	C3C-C4C-NC	-2.48	108.59	114.65
19	1	307	CLA	O2A-CGA-CBA	2.48	121.84	114.00
18	4	305	CHL	C3C-C4C-NC	-2.48	108.59	114.65
18	2	306	CHL	C4C-CHD-C1D	2.48	124.94	116.07
20	2	315	LUT	C20-C13-C14	-2.48	118.80	122.82
18	1	301	CHL	C3C-C4C-NC	-2.48	108.60	114.65
19	B	830	CLA	C12-C11-C10	-2.47	102.19	113.28
19	F	302	CLA	C4-C3-C5	-2.47	110.93	115.23
19	A	853	CLA	C1-C2-C3	2.47	130.25	126.20
19	A	838	CLA	C1-C2-C3	2.47	130.24	126.20
19	2	304	CLA	C12-C11-C10	-2.46	102.24	113.28
19	4	308	CLA	C1-C2-C3	2.46	130.23	126.20
19	2	308	CLA	O2A-CGA-CBA	2.46	121.78	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	320	LUT	C8-C9-C10	2.46	122.88	119.01
19	L	302	CLA	C1-C2-C3	2.46	130.23	126.20
18	2	301	CHL	C3C-C4C-NC	-2.46	108.64	114.65
19	B	802	CLA	C12-C11-C10	-2.46	102.27	113.28
18	1	306	CHL	C3C-C4C-NC	-2.46	108.65	114.65
18	4	304	CHL	O1D-CGD-CBD	-2.45	121.00	124.72
19	3	306	CLA	O2A-CGA-CBA	2.45	121.74	114.00
19	4	308	CLA	C12-C11-C10	-2.45	102.31	113.28
19	A	810	CLA	C12-C11-C10	-2.45	102.31	113.28
18	2	306	CHL	C3C-C4C-NC	-2.45	108.67	114.65
19	B	825	CLA	C12-C11-C10	-2.45	102.31	113.28
18	2	305	CHL	C3C-C4C-NC	-2.45	108.67	114.65
19	B	808	CLA	C1-C2-C3	2.45	130.20	126.20
19	4	310	CLA	O2A-CGA-CBA	2.44	121.72	114.00
18	4	304	CHL	C3C-C4C-NC	-2.44	108.68	114.65
19	B	817	CLA	C1-C2-C3	2.44	130.19	126.20
19	A	824	CLA	C1-C2-C3	2.44	130.19	126.20
20	4	315	LUT	C32-C33-C34	2.44	122.84	119.01
19	A	854	CLA	C1-C2-C3	2.44	130.19	126.20
19	A	854	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
19	A	804	CLA	C4-C3-C5	-2.44	111.00	115.23
19	B	802	CLA	C1-C2-C3	2.43	130.19	126.20
19	A	808	CLA	C12-C11-C10	-2.43	102.37	113.28
19	B	809	CLA	C12-C11-C10	-2.43	102.37	113.28
18	2	306	CHL	OMC-CMC-C2C	-2.43	120.89	125.12
19	A	807	CLA	C1-C2-C3	2.43	130.18	126.20
19	B	823	CLA	C12-C11-C10	-2.43	102.38	113.28
19	B	817	CLA	C12-C11-C10	-2.43	102.38	113.28
19	A	827	CLA	CHD-C1D-ND	-2.43	121.39	124.80
18	3	307	CHL	O2A-CGA-CBA	2.43	121.31	112.14
19	K	204	CLA	OBD-CAD-CBD	-2.43	121.07	125.94
19	2	320	CLA	O2A-CGA-CBA	2.43	121.31	112.14
19	B	810	CLA	C1-C2-C3	2.42	130.16	126.20
19	1	321	CLA	C12-C11-C10	-2.42	102.43	113.28
19	B	808	CLA	C12-C11-C10	-2.42	102.43	113.28
19	2	309	CLA	C1-C2-C3	2.42	130.16	126.20
19	A	840	CLA	C12-C11-C10	-2.42	102.44	113.28
19	A	802	CLA	CHD-C1D-ND	-2.42	121.40	124.80
19	A	830	CLA	C1-C2-C3	2.42	130.68	126.76
19	A	809	CLA	C1-C2-C3	2.42	130.16	126.20
19	1	313	CLA	O2A-CGA-CBA	2.42	121.63	114.00
19	B	834	CLA	C1-C2-C3	2.41	130.15	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	303	CLA	C1-C2-C3	2.41	130.15	126.20
19	B	824	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	1	311	CLA	O2A-CGA-CBA	2.41	121.62	114.00
19	A	816	CLA	C12-C11-C10	-2.41	102.47	113.28
19	B	832	CLA	C12-C11-C10	-2.41	102.48	113.28
19	L	302	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
19	A	837	CLA	C1-C2-C3	2.41	130.15	126.20
19	A	828	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
19	4	303	CLA	O2A-CGA-CBA	2.41	121.61	114.00
23	J	101	BCR	C20-C19-C18	2.41	132.96	126.36
19	F	301	CLA	C12-C11-C10	-2.41	102.49	113.28
19	1	312	CLA	C12-C11-C10	-2.41	102.50	113.28
19	4	301	CLA	C12-C11-C10	-2.41	102.50	113.28
19	B	817	CLA	C4-C3-C5	-2.40	111.05	115.23
19	A	829	CLA	C12-C11-C10	-2.40	102.51	113.28
19	3	302	CLA	C12-C11-C10	-2.40	102.51	113.28
19	B	837	CLA	C12-C11-C10	-2.40	102.51	113.28
19	1	302	CLA	C1-C2-C3	2.40	130.13	126.20
19	1	302	CLA	C12-C11-C10	-2.40	102.51	113.28
19	2	312	CLA	C12-C11-C10	-2.40	102.52	113.28
19	A	836	CLA	C12-C11-C10	-2.40	102.52	113.28
19	3	308	CLA	C12-C11-C10	-2.40	102.52	113.28
19	A	852	CLA	C12-C11-C10	-2.40	102.52	113.28
19	A	801	CLA	CHD-C1D-ND	-2.40	121.43	124.80
20	3	315	LUT	C39-C29-C28	2.40	121.75	118.09
19	L	303	CLA	C1-C2-C3	2.40	130.64	126.76
19	3	311	CLA	CHD-C1D-ND	-2.40	121.43	124.80
20	1	315	LUT	C20-C13-C14	-2.40	118.94	122.82
19	B	804	CLA	C12-C11-C10	-2.40	102.55	113.28
19	2	313	CLA	C4-C3-C5	-2.39	111.07	115.23
19	1	321	CLA	C1-C2-C3	2.39	130.12	126.20
19	A	839	CLA	C12-C11-C10	-2.39	102.56	113.28
19	A	835	CLA	C1-C2-C3	2.39	130.11	126.20
19	4	309	CLA	C12-C11-C10	-2.39	102.58	113.28
19	B	822	CLA	C12-C11-C10	-2.39	102.58	113.28
19	A	853	CLA	C12-C11-C10	-2.39	102.58	113.28
19	B	805	CLA	C12-C11-C10	-2.39	102.59	113.28
18	4	305	CHL	CHA-C1A-C2A	-2.38	127.71	133.31
19	4	302	CLA	C12-C11-C10	-2.38	102.59	113.28
18	4	304	CHL	CHA-C1A-C2A	-2.38	127.71	133.31
19	B	801	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
19	F	303	CLA	O2A-CGA-CBA	2.38	121.53	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	826	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
19	3	311	CLA	O2A-CGA-CBA	2.38	121.52	114.00
19	A	834	CLA	C12-C11-C10	-2.38	102.61	113.28
19	A	817	CLA	C1-C2-C3	2.38	130.09	126.20
19	B	807	CLA	C12-C11-C10	-2.38	102.62	113.28
19	B	824	CLA	C12-C11-C10	-2.38	102.62	113.28
19	G	204	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
18	1	306	CHL	OMC-CMC-C2C	-2.37	121.00	125.12
19	A	824	CLA	C12-C11-C10	-2.37	102.64	113.28
19	B	826	CLA	C12-C11-C10	-2.37	102.65	113.28
19	B	803	CLA	O2A-CGA-CBA	2.37	121.49	114.00
19	K	202	CLA	O2A-CGA-CBA	2.37	121.49	114.00
19	A	802	CLA	C12-C11-C10	-2.37	102.65	113.28
19	A	851	CLA	O2A-CGA-CBA	2.37	121.49	114.00
19	B	827	CLA	C12-C11-C10	-2.37	102.66	113.28
19	A	814	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	3	307	CHL	O1D-CGD-CBD	-2.37	121.13	124.72
19	B	818	CLA	C12-C11-C10	-2.37	102.66	113.28
23	A	843	BCR	C23-C24-C25	2.37	133.33	127.00
19	F	304	CLA	O2A-CGA-CBA	2.37	121.48	114.00
23	A	844	BCR	C16-C15-C14	2.37	128.36	123.52
20	4	315	LUT	C39-C29-C28	2.37	121.70	118.09
19	B	828	CLA	CMD-C2D-C1D	2.37	128.90	124.73
19	A	820	CLA	C12-C11-C10	-2.36	102.68	113.28
19	A	823	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	A	821	CLA	O2A-CGA-CBA	2.36	121.46	114.00
19	B	813	CLA	C12-C11-C10	-2.36	102.71	113.28
19	A	819	CLA	O2A-CGA-CBA	2.36	121.45	114.00
19	A	801	CLA	C12-C11-C10	-2.36	102.72	113.28
19	A	831	CLA	C12-C11-C10	-2.36	102.72	113.28
19	B	822	CLA	CHD-C1D-ND	-2.36	121.49	124.80
19	1	314	CLA	O2A-CGA-CBA	2.35	121.44	114.00
19	A	813	CLA	O2A-CGA-CBA	2.35	121.44	114.00
19	L	302	CLA	C12-C11-C10	-2.35	102.73	113.28
19	B	837	CLA	C4-C3-C5	-2.35	111.15	115.23
23	A	843	BCR	C24-C23-C22	2.35	129.71	126.23
19	4	312	CLA	O2A-CGA-CBA	2.35	121.41	114.00
19	A	854	CLA	C12-C11-C10	-2.35	102.77	113.28
19	3	306	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
19	A	827	CLA	C1-C2-C3	2.34	130.04	126.20
19	4	313	CLA	C12-C11-C10	-2.34	102.77	113.28
19	3	313	CLA	O2A-CGA-CBA	2.34	121.40	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	820	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
19	A	815	CLA	O2A-CGA-CBA	2.34	121.39	114.00
19	1	312	CLA	C1-C2-C3	2.34	130.03	126.20
19	2	302	CLA	C12-C11-C10	-2.34	102.81	113.28
19	B	828	CLA	C12-C11-C10	-2.34	102.81	113.28
19	4	308	CLA	CHD-C1D-ND	-2.34	121.52	124.80
18	4	306	CHL	OMC-CMC-C2C	-2.34	121.06	125.12
19	A	804	CLA	C12-C11-C10	-2.33	102.82	113.28
19	A	807	CLA	C12-C11-C10	-2.33	102.83	113.28
19	B	811	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
19	3	302	CLA	C1-C2-C3	2.33	130.01	126.20
19	A	826	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	A	838	CLA	C12-C11-C10	-2.33	102.85	113.28
19	B	838	CLA	C12-C11-C10	-2.33	102.85	113.28
19	G	204	CLA	O2A-CGA-CBA	2.33	120.93	112.14
19	H	201	CLA	O2A-CGA-CBA	2.32	120.92	112.14
19	A	824	CLA	C4-C3-C5	-2.32	111.20	115.23
19	2	303	CLA	C1-C2-C3	2.32	130.52	126.76
18	1	301	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
19	2	311	CLA	O2A-CGA-CBA	2.32	121.33	114.00
19	B	801	CLA	C12-C11-C10	-2.32	102.89	113.28
19	A	825	CLA	C12-C11-C10	-2.32	102.89	113.28
19	1	308	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	A	828	CLA	C12-C11-C10	-2.32	102.89	113.28
19	A	804	CLA	C1-C2-C3	2.32	129.99	126.20
19	A	810	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	823	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
18	4	314	CHL	OMC-CMC-C2C	-2.31	121.11	125.12
19	B	833	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	801	CLA	C1-C2-C3	2.31	129.98	126.20
20	2	315	LUT	C1-C6-C7	2.30	121.90	115.65
19	3	309	CLA	C1-C2-C3	2.30	130.49	126.76
20	2	315	LUT	C39-C29-C28	2.30	121.60	118.09
19	A	826	CLA	C12-C11-C10	-2.30	102.97	113.28
19	G	202	CLA	CAA-C2A-C3A	-2.30	110.96	116.23
19	A	803	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	B	835	CLA	C12-C11-C10	-2.30	102.99	113.28
19	4	302	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
19	4	311	CLA	C1-C2-C3	2.29	129.96	126.20
19	A	832	CLA	C12-C11-C10	-2.29	103.00	113.28
20	1	315	LUT	C1-C6-C7	2.29	121.87	115.65
19	A	825	CLA	CHD-C1D-ND	-2.29	121.58	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	852	CLA	C1-C2-C3	2.29	129.95	126.20
18	2	306	CHL	O2A-CGA-CBA	2.29	121.23	114.00
20	4	315	LUT	C12-C13-C14	2.28	122.60	119.01
19	A	834	CLA	C4-C3-C5	-2.28	111.26	115.23
19	B	838	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
19	B	829	CLA	C1-C2-C3	2.28	130.46	126.76
19	A	837	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
19	4	313	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
19	A	812	CLA	C12-C11-C10	-2.28	103.07	113.28
19	A	834	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
19	3	309	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
19	1	309	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	2	310	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
19	B	835	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	F	302	CLA	C1-C2-C3	2.27	129.92	126.20
19	L	301	CLA	C4-C3-C5	-2.27	111.29	115.23
19	A	813	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	3	301	CLA	C1-C2-C3	2.27	129.91	126.20
18	1	306	CHL	O2A-CGA-CBA	2.27	121.16	114.00
19	B	814	CLA	CHD-C1D-ND	-2.27	121.61	124.80
18	1	301	CHL	CHA-C1A-C2A	-2.27	127.98	133.31
19	F	301	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	A	852	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
20	1	320	LUT	C1-C6-C7	2.26	121.78	115.65
19	B	837	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
19	2	309	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	2	310	CLA	CHD-C1D-ND	-2.26	121.63	124.80
18	4	305	CHL	OMC-CMC-C2C	-2.25	121.20	125.12
19	2	310	CLA	CAA-C2A-C3A	-2.25	111.06	116.23
19	A	806	CLA	O1D-CGD-CBD	-2.25	120.07	124.52
18	4	304	CHL	O2A-CGA-O1A	-2.25	117.99	123.63
19	A	830	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	1	301	CHL	O2A-CGA-O1A	-2.25	117.99	123.63
19	4	313	CLA	CHD-C1D-ND	-2.25	121.63	124.80
19	B	819	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	3	308	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	A	826	CLA	C1-C2-C3	2.24	129.88	126.20
19	3	303	CLA	O2A-CGA-CBA	2.24	121.09	114.00
19	A	828	CLA	C1-C2-C3	2.24	129.87	126.20
18	2	307	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
19	A	834	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	A	852	CLA	CHD-C1D-ND	-2.24	121.65	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	817	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
19	A	810	CLA	CMD-C2D-C1D	2.24	128.67	124.73
19	2	308	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	B	833	CLA	O2A-CGA-CBA	2.24	121.08	114.00
18	1	301	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
20	1	320	LUT	C32-C33-C34	2.24	122.53	119.01
19	A	804	CLA	CHD-C1D-ND	-2.24	121.65	124.80
18	4	305	CHL	O2A-CGA-CBA	2.24	121.07	114.00
19	A	820	CLA	CHD-C1D-ND	-2.24	121.66	124.80
19	B	802	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	1	302	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
19	A	838	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	B	828	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
19	B	806	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	4	303	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	L	302	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	A	839	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
19	A	824	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	H	201	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	3	301	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
19	A	806	CLA	C1-C2-C3	2.22	130.36	126.76
19	L	301	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
19	1	308	CLA	C12-C11-C10	-2.22	102.46	113.23
19	3	310	CLA	CAA-C2A-C3A	-2.22	111.14	116.23
19	4	301	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
19	B	807	CLA	CHD-C1D-ND	-2.22	121.68	124.80
19	B	815	CLA	CHD-C1D-ND	-2.22	121.68	124.80
19	B	818	CLA	CHD-C1D-ND	-2.22	121.68	124.80
19	2	309	CLA	C12-C11-C10	-2.22	102.48	113.23
19	B	802	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
19	A	807	CLA	C4-C3-C5	-2.21	111.38	115.23
19	3	304	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	2	312	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
19	A	808	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
19	B	822	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
19	F	302	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
19	B	817	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	A	821	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
19	A	813	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
19	4	310	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	B	819	CLA	C1-C2-C3	2.20	130.33	126.76
19	A	809	CLA	CHD-C1D-ND	-2.20	121.70	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	304	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
19	A	851	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	J	102	CLA	CHD-C1D-ND	-2.20	121.71	124.80
18	2	307	CHL	O2A-CGA-CBA	2.20	120.95	114.00
19	2	304	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	B	823	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	B	837	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	F	303	CLA	CHD-C1D-ND	-2.20	121.71	124.80
23	2	319	BCR	C15-C16-C17	2.20	128.02	123.52
19	1	313	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
18	2	301	CHL	O2A-CGA-O1A	-2.20	118.14	123.63
19	B	831	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
19	B	831	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	K	204	CLA	C2A-C3A-C4A	2.19	104.16	101.59
18	2	314	CHL	OMC-CMC-C2C	-2.19	121.31	125.12
19	A	823	CLA	CMD-C2D-C1D	2.19	128.59	124.73
19	A	837	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	B	832	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	A	815	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
19	3	313	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
19	B	829	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
19	K	204	CLA	CAA-C2A-C3A	-2.19	111.22	116.23
19	G	203	CLA	C1-C2-C3	2.19	130.30	126.76
19	1	302	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	3	304	CLA	CMD-C2D-C1D	2.18	128.57	124.73
19	2	303	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	4	307	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	2	302	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
19	A	830	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
19	B	830	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
19	3	310	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
19	A	811	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
19	B	807	CLA	C1-C2-C3	2.17	129.76	126.20
19	1	313	CLA	CHD-C1D-ND	-2.17	121.74	124.80
21	3	316	XAT	O24-C25-C24	-2.17	111.45	113.49
19	A	807	CLA	CHD-C1D-ND	-2.17	121.74	124.80
19	A	805	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	A	820	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	1	312	CLA	C4-C3-C5	-2.17	111.46	115.23
19	B	801	CLA	CHD-C1D-ND	-2.17	121.75	124.80
19	B	833	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
19	1	307	CLA	CHD-C1D-ND	-2.17	121.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	803	CLA	C1-C2-C3	2.17	130.27	126.76
19	A	825	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
19	A	837	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	A	808	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	B	825	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	A	828	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	A	836	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	B	810	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	B	801	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
19	3	309	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	A	825	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
19	A	838	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
19	A	840	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
19	A	838	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
18	2	305	CHL	OMC-CMC-C2C	-2.15	121.38	125.12
18	3	307	CHL	OMC-CMC-C2C	-2.15	121.38	125.12
19	4	308	CLA	CMD-C2D-C1D	2.15	128.52	124.73
19	4	302	CLA	CHD-C1D-ND	-2.15	121.77	124.80
19	B	834	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
19	3	301	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
19	1	310	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
19	K	202	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	A	818	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
19	A	807	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
19	A	824	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
19	F	301	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
19	3	313	CLA	CHD-C1D-ND	-2.14	121.78	124.80
19	B	816	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
19	1	303	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
19	A	851	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
19	B	804	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
19	B	814	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
23	A	847	BCR	C10-C11-C12	2.14	129.41	123.20
19	3	310	CLA	C2A-C3A-C4A	2.14	104.10	101.59
19	3	302	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	4	309	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	A	840	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	4	312	CLA	CHD-C1D-ND	-2.14	121.80	124.80
19	B	803	CLA	CHD-C1D-ND	-2.14	121.80	124.80
20	2	315	LUT	C12-C13-C14	2.14	122.37	119.01
19	1	309	CLA	C1-C2-C3	2.14	129.70	126.20
19	3	305	CLA	O1D-CGD-CBD	-2.14	120.31	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
19	A	823	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
19	B	825	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
19	B	817	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	A	839	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	A	804	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
19	2	302	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	A	816	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	2	313	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
19	A	833	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	A	820	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	B	809	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	B	836	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	B	808	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	A	801	CLA	C4D-C3D-CAD	-2.13	105.80	108.11
19	A	810	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
19	A	802	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
19	B	821	CLA	CHD-C1D-ND	-2.12	121.81	124.80
19	F	303	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
19	B	805	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	A	801	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
19	A	816	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	3	311	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
19	3	306	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	A	809	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
19	A	809	CLA	C4-C3-C5	-2.12	111.55	115.23
19	2	304	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	A	852	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	L	303	CLA	CHD-C1D-ND	-2.12	121.82	124.80
18	4	306	CHL	O2A-CGA-O1A	-2.12	118.33	123.63
19	A	833	CLA	C1-C2-C3	2.12	130.19	126.76
19	G	202	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	B	805	CLA	C4-C3-C5	-2.12	111.56	115.23
19	A	812	CLA	CHD-C1D-ND	-2.12	121.83	124.80
19	2	320	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
19	A	854	CLA	CHD-C1D-ND	-2.11	121.83	124.80
19	1	305	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
19	A	804	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
19	3	305	CLA	CHD-C1D-ND	-2.11	121.83	124.80
19	4	312	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
19	B	836	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
19	B	812	CLA	CHD-C1D-ND	-2.11	121.84	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	832	CLA	CMD-C2D-C1D	2.10	128.43	124.73
19	K	202	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
19	A	829	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
19	B	817	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
19	H	201	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
19	A	822	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
19	A	826	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
19	J	102	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
19	A	806	CLA	CHD-C1D-ND	-2.09	121.86	124.80
19	B	811	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
19	B	813	CLA	CHD-C1D-ND	-2.09	121.86	124.80
19	B	838	CLA	CHD-C1D-ND	-2.09	121.86	124.80
19	A	805	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
19	3	305	CLA	CMD-C2D-C1D	2.09	128.41	124.73
19	3	302	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
19	A	821	CLA	CHD-C1D-ND	-2.09	121.87	124.80
20	1	315	LUT	C11-C10-C9	2.09	130.20	127.28
18	2	301	CHL	OMC-CMC-C2C	-2.09	121.50	125.12
19	A	835	CLA	O1D-CGD-CBD	-2.09	120.41	124.52
19	B	808	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
23	A	844	BCR	C23-C24-C25	2.08	132.56	127.00
19	3	314	CLA	CHD-C1D-ND	-2.08	121.87	124.80
19	B	804	CLA	CHD-C1D-ND	-2.08	121.87	124.80
19	1	303	CLA	CHD-C1D-ND	-2.08	121.87	124.80
19	1	307	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	A	812	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	B	821	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	A	819	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	3	309	CLA	CMD-C2D-C1D	2.08	128.39	124.73
19	B	803	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
19	4	301	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	1	308	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
19	F	301	CLA	C4-C3-C5	-2.08	111.62	115.23
19	B	826	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	3	310	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	A	831	CLA	CHD-C1D-ND	-2.07	121.88	124.80
19	F	304	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
19	1	307	CLA	CMD-C2D-C1D	2.07	128.38	124.73
19	F	304	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	H	201	CLA	CMD-C2D-C1D	2.07	128.38	124.73
19	4	302	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	1	310	CLA	CHD-C1D-ND	-2.07	121.89	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	303	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	B	812	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	1	304	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	A	803	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	A	815	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	4	311	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	1	305	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	B	828	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	F	302	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
19	3	303	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	B	810	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	B	816	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	2	304	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	A	822	CLA	CHD-C1D-ND	-2.07	121.90	124.80
19	A	827	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
19	1	314	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	A	833	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	3	303	CLA	CMD-C2D-C1D	2.06	128.36	124.73
19	B	810	CLA	C4-C3-C5	-2.06	111.64	115.23
19	3	309	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	A	811	CLA	CHD-C1D-ND	-2.06	121.90	124.80
19	B	830	CLA	CHD-C1D-ND	-2.06	121.90	124.80
19	B	802	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
19	1	311	CLA	CHD-C1D-ND	-2.06	121.90	124.80
19	2	308	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
19	A	839	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	B	810	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	B	826	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	B	829	CLA	CHD-C1D-ND	-2.06	121.91	124.80
19	1	304	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
19	3	302	CLA	CMD-C2D-C1D	2.06	128.35	124.73
19	G	203	CLA	CHD-C1D-ND	-2.06	121.91	124.80
19	4	307	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
19	B	805	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
19	A	818	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	A	818	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	B	838	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	A	824	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	A	818	CLA	C4-C3-C5	-2.05	111.67	115.23
19	A	833	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
19	B	806	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
19	L	303	CLA	O1D-CGD-CBD	-2.04	120.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	303	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
19	2	303	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	2	309	CLA	CMD-C2D-C1D	2.04	128.33	124.73
19	2	311	CLA	CMD-C2D-C1D	2.04	128.33	124.73
19	4	310	CLA	CMD-C2D-C1D	2.04	128.33	124.73
19	A	801	CLA	CMD-C2D-C1D	2.04	128.33	124.73
19	B	816	CLA	CHD-C1D-ND	-2.04	121.93	124.80
19	1	302	CLA	CMD-C2D-C1D	2.04	128.32	124.73
19	4	308	CLA	CED-O2D-CGD	2.04	120.55	115.92
19	3	314	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
19	A	810	CLA	C4-C3-C5	-2.04	111.69	115.23
19	B	818	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	B	812	CLA	CMD-C2D-C1D	2.04	128.32	124.73
19	1	309	CLA	CMD-C2D-C1D	2.04	128.32	124.73
19	A	830	CLA	CMD-C2D-C1D	2.04	128.32	124.73
19	B	827	CLA	CHD-C1D-ND	-2.04	121.94	124.80
19	B	819	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
19	A	819	CLA	CHD-C1D-ND	-2.04	121.94	124.80
19	3	301	CLA	CHD-C1D-ND	-2.04	121.94	124.80
19	4	309	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
19	B	820	CLA	CHD-C1D-ND	-2.03	121.94	124.80
19	L	303	CLA	CMD-C2D-C1D	2.03	128.31	124.73
19	2	312	CLA	CHD-C1D-ND	-2.03	121.94	124.80
19	L	301	CLA	CHD-C1D-ND	-2.03	121.94	124.80
19	A	840	CLA	CMD-C2D-C1D	2.03	128.31	124.73
19	A	809	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
19	A	828	CLA	CHD-C1D-ND	-2.03	121.95	124.80
19	B	835	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
19	A	854	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	4	312	CLA	CMD-C2D-C1D	2.03	128.30	124.73
19	A	817	CLA	CHD-C1D-ND	-2.03	121.95	124.80
19	4	302	CLA	CMD-C2D-C1D	2.03	128.29	124.73
19	1	305	CLA	CMD-C2D-C1D	2.02	128.29	124.73
19	A	854	CLA	CMD-C2D-C1D	2.02	128.29	124.73
19	A	802	CLA	CMD-C2D-C1D	2.02	128.29	124.73
19	L	303	CLA	CED-O2D-CGD	2.02	120.50	115.92
19	A	814	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	A	853	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	1	308	CLA	C4-C3-C5	-2.02	111.72	115.23
19	2	311	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	1	312	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	A	829	CLA	CHD-C1D-ND	-2.02	121.96	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	805	CLA	C4-C3-C5	-2.02	111.72	115.23
19	A	808	CLA	C4D-CHA-C1A	2.02	123.65	121.24
19	4	311	CLA	CHD-C1D-ND	-2.02	121.97	124.80
19	G	204	CLA	CMD-C2D-C1D	2.01	128.28	124.73
19	F	302	CLA	CMD-C2D-C1D	2.01	128.27	124.73
19	4	303	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
19	A	834	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
19	1	321	CLA	CHD-C1D-ND	-2.01	121.97	124.80
19	A	827	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
19	B	834	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
19	K	203	CLA	CHD-C1D-ND	-2.01	121.97	124.80
19	3	302	CLA	CED-O2D-CGD	2.01	120.47	115.92
19	A	834	CLA	C1-C2-C3	2.01	129.49	126.20
19	A	802	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
19	F	303	CLA	CMD-C2D-C1D	2.01	128.26	124.73
19	K	202	CLA	CMD-C2D-C1D	2.01	128.26	124.73
19	4	310	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
19	B	807	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
19	2	313	CLA	CHD-C1D-ND	-2.00	121.98	124.80
19	B	811	CLA	CHD-C1D-ND	-2.00	121.98	124.80
19	3	304	CLA	CED-O2D-CGD	2.00	120.46	115.92
19	B	808	CLA	C4-C3-C5	-2.00	111.75	115.23
19	B	835	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	1	315	LUT	C12-C13-C14	2.00	122.16	119.01

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	1	301	CHL	NA
18	1	301	CHL	ND
18	1	301	CHL	NC
18	1	306	CHL	NA
18	1	306	CHL	ND
18	1	306	CHL	NC
18	2	301	CHL	NA
18	2	301	CHL	ND
18	2	301	CHL	NC
18	2	305	CHL	NA
18	2	305	CHL	ND
18	2	305	CHL	NC
18	2	306	CHL	NA
18	2	306	CHL	ND

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Mol	Chain	Res	Type	Atom
18	2	306	CHL	NC
18	2	307	CHL	NA
18	2	307	CHL	ND
18	2	307	CHL	NC
18	2	314	CHL	ND
18	2	314	CHL	NC
18	3	307	CHL	NA
18	3	307	CHL	ND
18	3	307	CHL	NC
18	4	304	CHL	NA
18	4	304	CHL	ND
18	4	304	CHL	NC
18	4	305	CHL	NA
18	4	305	CHL	ND
18	4	305	CHL	NC
18	4	306	CHL	NA
18	4	306	CHL	ND
18	4	306	CHL	NC
18	4	314	CHL	NA
18	4	314	CHL	ND
18	4	314	CHL	NC
19	1	302	CLA	ND
19	1	303	CLA	ND
19	1	304	CLA	ND
19	1	305	CLA	ND
19	1	307	CLA	ND
19	1	308	CLA	ND
19	1	309	CLA	ND
19	1	310	CLA	ND
19	1	311	CLA	ND
19	1	312	CLA	ND
19	1	313	CLA	ND
19	1	314	CLA	ND
19	1	321	CLA	ND
19	2	302	CLA	ND
19	2	303	CLA	ND
19	2	304	CLA	ND
19	2	308	CLA	ND
19	2	309	CLA	ND
19	2	310	CLA	ND
19	2	311	CLA	ND
19	2	312	CLA	ND

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Mol	Chain	Res	Type	Atom
19	2	313	CLA	ND
19	2	320	CLA	ND
19	3	301	CLA	ND
19	3	302	CLA	ND
19	3	303	CLA	ND
19	3	304	CLA	ND
19	3	305	CLA	ND
19	3	306	CLA	ND
19	3	308	CLA	ND
19	3	309	CLA	ND
19	3	310	CLA	ND
19	3	311	CLA	ND
19	3	312	CLA	ND
19	3	313	CLA	ND
19	3	314	CLA	ND
19	4	301	CLA	ND
19	4	302	CLA	ND
19	4	303	CLA	ND
19	4	307	CLA	ND
19	4	308	CLA	ND
19	4	309	CLA	ND
19	4	310	CLA	ND
19	4	311	CLA	ND
19	4	312	CLA	ND
19	4	313	CLA	ND
19	A	801	CLA	ND
19	A	802	CLA	ND
19	A	803	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND
19	A	811	CLA	ND
19	A	812	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	817	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	818	CLA	ND
19	A	819	CLA	ND
19	A	820	CLA	ND
19	A	821	CLA	ND
19	A	822	CLA	ND
19	A	823	CLA	ND
19	A	824	CLA	ND
19	A	825	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	831	CLA	ND
19	A	832	CLA	ND
19	A	833	CLA	ND
19	A	834	CLA	ND
19	A	835	CLA	ND
19	A	836	CLA	ND
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	851	CLA	ND
19	A	852	CLA	ND
19	A	853	CLA	ND
19	A	854	CLA	ND
19	B	801	CLA	ND
19	B	802	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	805	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	816	CLA	ND
19	B	817	CLA	ND
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	820	CLA	ND
19	B	821	CLA	ND
19	B	822	CLA	ND
19	B	823	CLA	ND
19	B	824	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND
19	B	827	CLA	ND
19	B	828	CLA	ND
19	B	829	CLA	ND
19	B	830	CLA	ND
19	B	831	CLA	ND
19	B	832	CLA	ND
19	B	833	CLA	ND
19	B	834	CLA	ND
19	B	835	CLA	ND
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	838	CLA	ND
19	F	301	CLA	ND
19	F	302	CLA	ND
19	F	303	CLA	ND
19	F	304	CLA	ND
19	G	202	CLA	ND
19	G	203	CLA	ND
19	G	204	CLA	ND
19	H	201	CLA	ND
19	J	102	CLA	ND
19	L	301	CLA	ND
19	L	302	CLA	ND
19	L	303	CLA	ND
19	K	202	CLA	ND
19	K	203	CLA	ND
19	K	204	CLA	ND

All (1724) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
18	1	301	CHL	CBD-CGD-O2D-CED
18	1	301	CHL	O1D-CGD-O2D-CED
18	1	306	CHL	C1C-C2C-CMC-OMC
18	2	301	CHL	C1-C2-C3-C4
18	2	301	CHL	C1-C2-C3-C5
18	2	305	CHL	C1C-C2C-CMC-OMC
18	2	305	CHL	C3C-C2C-CMC-OMC
18	2	306	CHL	C1C-C2C-CMC-OMC
18	2	306	CHL	C3C-C2C-CMC-OMC
18	2	306	CHL	CBD-CGD-O2D-CED
18	2	307	CHL	C1A-C2A-CAA-CBA
18	2	314	CHL	C1A-C2A-CAA-CBA
18	2	314	CHL	C3A-C2A-CAA-CBA
18	2	314	CHL	CBD-CGD-O2D-CED
18	4	305	CHL	C1A-C2A-CAA-CBA
18	4	305	CHL	CBD-CGD-O2D-CED
19	1	302	CLA	C2B-C3B-CAB-CBB
19	1	302	CLA	C4B-C3B-CAB-CBB
19	1	302	CLA	CHA-CBD-CGD-O1D
19	1	302	CLA	CHA-CBD-CGD-O2D
19	1	304	CLA	CBD-CGD-O2D-CED
19	1	304	CLA	C2-C3-C5-C6
19	1	305	CLA	C1A-C2A-CAA-CBA
19	1	305	CLA	C3A-C2A-CAA-CBA
19	1	308	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C1-C2-C3-C5
19	1	311	CLA	CBD-CGD-O2D-CED
19	1	312	CLA	CBA-CGA-O2A-C1
19	1	312	CLA	O1A-CGA-O2A-C1
19	1	313	CLA	C1A-C2A-CAA-CBA
19	1	313	CLA	C3A-C2A-CAA-CBA
19	1	313	CLA	CHA-CBD-CGD-O1D
19	1	313	CLA	CHA-CBD-CGD-O2D
19	1	314	CLA	C1A-C2A-CAA-CBA
19	1	314	CLA	C2B-C3B-CAB-CBB
19	1	314	CLA	C4B-C3B-CAB-CBB
19	1	321	CLA	C1A-C2A-CAA-CBA
19	1	321	CLA	CAD-CBD-CGD-O1D
19	1	321	CLA	CAD-CBD-CGD-O2D
19	2	303	CLA	C2B-C3B-CAB-CBB
19	2	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	2	304	CLA	C1A-C2A-CAA-CBA
19	2	304	CLA	C3A-C2A-CAA-CBA
19	2	308	CLA	C1A-C2A-CAA-CBA
19	2	308	CLA	C3A-C2A-CAA-CBA
19	2	309	CLA	C1A-C2A-CAA-CBA
19	2	312	CLA	CBD-CGD-O2D-CED
19	2	313	CLA	C1A-C2A-CAA-CBA
19	2	313	CLA	C1-C2-C3-C4
19	2	313	CLA	C1-C2-C3-C5
19	3	301	CLA	CHA-CBD-CGD-O2D
19	3	301	CLA	CBD-CGD-O2D-CED
19	3	302	CLA	O1A-CGA-O2A-C1
19	3	303	CLA	C1A-C2A-CAA-CBA
19	3	303	CLA	C3A-C2A-CAA-CBA
19	3	303	CLA	CHA-CBD-CGD-O2D
19	3	304	CLA	C2B-C3B-CAB-CBB
19	3	304	CLA	C4B-C3B-CAB-CBB
19	3	306	CLA	C1A-C2A-CAA-CBA
19	3	306	CLA	C3A-C2A-CAA-CBA
19	3	308	CLA	C1A-C2A-CAA-CBA
19	3	308	CLA	C3A-C2A-CAA-CBA
19	3	308	CLA	C1-C2-C3-C5
19	3	310	CLA	CHA-CBD-CGD-O1D
19	3	310	CLA	CHA-CBD-CGD-O2D
19	3	314	CLA	CBA-CGA-O2A-C1
19	3	314	CLA	C2B-C3B-CAB-CBB
19	3	314	CLA	C4B-C3B-CAB-CBB
19	4	301	CLA	CHA-CBD-CGD-O2D
19	4	303	CLA	CHA-CBD-CGD-O2D
19	4	307	CLA	C1A-C2A-CAA-CBA
19	4	307	CLA	C3A-C2A-CAA-CBA
19	4	308	CLA	C2B-C3B-CAB-CBB
19	4	308	CLA	C4B-C3B-CAB-CBB
19	4	312	CLA	C1A-C2A-CAA-CBA
19	4	312	CLA	C3A-C2A-CAA-CBA
19	4	313	CLA	C3A-C2A-CAA-CBA
19	A	801	CLA	C1A-C2A-CAA-CBA
19	A	801	CLA	C3A-C2A-CAA-CBA
19	A	801	CLA	C4-C3-C5-C6
19	A	802	CLA	C11-C12-C13-C14
19	A	803	CLA	C1A-C2A-CAA-CBA
19	A	803	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	803	CLA	C1-C2-C3-C5
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	804	CLA	CAD-CBD-CGD-O1D
19	A	804	CLA	CAD-CBD-CGD-O2D
19	A	804	CLA	C1-C2-C3-C4
19	A	804	CLA	C1-C2-C3-C5
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C2B-C3B-CAB-CBB
19	A	806	CLA	C4B-C3B-CAB-CBB
19	A	807	CLA	CHA-CBD-CGD-O1D
19	A	807	CLA	CHA-CBD-CGD-O2D
19	A	807	CLA	C1-C2-C3-C5
19	A	808	CLA	C6-C7-C8-C9
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C3A-C2A-CAA-CBA
19	A	810	CLA	C1-C2-C3-C5
19	A	812	CLA	C2B-C3B-CAB-CBB
19	A	812	CLA	C4B-C3B-CAB-CBB
19	A	812	CLA	CAD-CBD-CGD-O2D
19	A	814	CLA	C1A-C2A-CAA-CBA
19	A	814	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	C1-C2-C3-C4
19	A	816	CLA	C1-C2-C3-C5
19	A	817	CLA	C3A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C14-C13-C15-C16
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	CHA-CBD-CGD-O1D
19	A	821	CLA	CHA-CBD-CGD-O2D
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	C4-C3-C5-C6
19	A	823	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	C2B-C3B-CAB-CBB
19	A	824	CLA	C4B-C3B-CAB-CBB
19	A	824	CLA	C1-C2-C3-C5
19	A	826	CLA	C2B-C3B-CAB-CBB
19	A	826	CLA	C4B-C3B-CAB-CBB
19	A	827	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	828	CLA	C2B-C3B-CAB-CBB
19	A	828	CLA	C4B-C3B-CAB-CBB
19	A	829	CLA	CHA-CBD-CGD-O1D
19	A	829	CLA	CHA-CBD-CGD-O2D
19	A	830	CLA	C1A-C2A-CAA-CBA
19	A	830	CLA	C3A-C2A-CAA-CBA
19	A	831	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	C3A-C2A-CAA-CBA
19	A	832	CLA	C11-C10-C8-C9
19	A	833	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	C1-C2-C3-C4
19	A	833	CLA	C1-C2-C3-C5
19	A	834	CLA	C2B-C3B-CAB-CBB
19	A	834	CLA	C4B-C3B-CAB-CBB
19	A	834	CLA	CAD-CBD-CGD-O2D
19	A	835	CLA	C1-C2-C3-C4
19	A	835	CLA	C1-C2-C3-C5
19	A	839	CLA	C14-C13-C15-C16
19	A	840	CLA	C1-C2-C3-C4
19	A	840	CLA	C1-C2-C3-C5
19	A	852	CLA	C2B-C3B-CAB-CBB
19	A	852	CLA	C4B-C3B-CAB-CBB
19	A	853	CLA	C1A-C2A-CAA-CBA
19	A	853	CLA	C3A-C2A-CAA-CBA
19	A	854	CLA	C1A-C2A-CAA-CBA
19	A	854	CLA	C3A-C2A-CAA-CBA
19	A	854	CLA	CHA-CBD-CGD-O1D
19	A	854	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	C2B-C3B-CAB-CBB
19	B	802	CLA	C4B-C3B-CAB-CBB
19	B	803	CLA	C1A-C2A-CAA-CBA
19	B	803	CLA	C3A-C2A-CAA-CBA
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	804	CLA	C14-C13-C15-C16
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	808	CLA	C1A-C2A-CAA-CBA
19	B	808	CLA	C3A-C2A-CAA-CBA
19	B	809	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	809	CLA	C1-C2-C3-C4
19	B	809	CLA	C1-C2-C3-C5
19	B	810	CLA	C1A-C2A-CAA-CBA
19	B	810	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	CHA-CBD-CGD-O1D
19	B	810	CLA	CHA-CBD-CGD-O2D
19	B	812	CLA	C2B-C3B-CAB-CBB
19	B	812	CLA	C4B-C3B-CAB-CBB
19	B	812	CLA	C14-C13-C15-C16
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B	817	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	C1-C2-C3-C5
19	B	819	CLA	C1-C2-C3-C4
19	B	819	CLA	C1-C2-C3-C5
19	B	820	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C1-C2-C3-C5
19	B	823	CLA	C1A-C2A-CAA-CBA
19	B	823	CLA	C2B-C3B-CAB-CBB
19	B	823	CLA	C4B-C3B-CAB-CBB
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C3A-C2A-CAA-CBA
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	C2B-C3B-CAB-CBB
19	B	826	CLA	C4B-C3B-CAB-CBB
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C3A-C2A-CAA-CBA
19	B	828	CLA	CHA-CBD-CGD-O1D
19	B	828	CLA	CHA-CBD-CGD-O2D
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	C2B-C3B-CAB-CBB
19	B	829	CLA	C4B-C3B-CAB-CBB
19	B	829	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	830	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C3A-C2A-CAA-CBA
19	B	831	CLA	CHA-CBD-CGD-O1D
19	B	831	CLA	CHA-CBD-CGD-O2D
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C3A-C2A-CAA-CBA
19	B	834	CLA	C1-C2-C3-C4
19	B	837	CLA	C1-C2-C3-C4
19	B	837	CLA	C1-C2-C3-C5
19	F	302	CLA	C1-C2-C3-C5
19	F	304	CLA	C1A-C2A-CAA-CBA
19	F	304	CLA	C3A-C2A-CAA-CBA
19	F	304	CLA	C2B-C3B-CAB-CBB
19	F	304	CLA	C4B-C3B-CAB-CBB
19	G	202	CLA	CHA-CBD-CGD-O1D
19	G	202	CLA	CHA-CBD-CGD-O2D
19	G	203	CLA	C1A-C2A-CAA-CBA
19	G	203	CLA	C3A-C2A-CAA-CBA
19	G	203	CLA	CBA-CGA-O2A-C1
19	G	203	CLA	C1-C2-C3-C5
19	G	204	CLA	CBD-CGD-O2D-CED
19	H	201	CLA	C1A-C2A-CAA-CBA
19	H	201	CLA	C3A-C2A-CAA-CBA
19	H	201	CLA	C2B-C3B-CAB-CBB
19	H	201	CLA	C4B-C3B-CAB-CBB
19	H	201	CLA	CBD-CGD-O2D-CED
19	J	102	CLA	CAD-CBD-CGD-O1D
19	J	102	CLA	CAD-CBD-CGD-O2D
19	L	301	CLA	C1A-C2A-CAA-CBA
19	L	301	CLA	C3A-C2A-CAA-CBA
19	L	301	CLA	CBA-CGA-O2A-C1
19	L	301	CLA	O1A-CGA-O2A-C1
19	L	301	CLA	C1-C2-C3-C4
19	L	301	CLA	C1-C2-C3-C5
19	L	303	CLA	C1-C2-C3-C5
19	K	202	CLA	C1A-C2A-CAA-CBA
19	K	202	CLA	C3A-C2A-CAA-CBA
19	K	202	CLA	CHA-CBD-CGD-O1D
19	K	202	CLA	CHA-CBD-CGD-O2D
19	K	203	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	1	317	LHG	C4-O6-P-O3
22	1	317	LHG	C4-O6-P-O4
22	1	317	LHG	C4-O6-P-O5
22	1	317	LHG	O9-C7-O7-C5
22	1	317	LHG	C8-C7-O7-C5
22	1	322	LHG	O10-C23-O8-C6
22	1	322	LHG	C24-C23-O8-C6
22	2	317	LHG	C3-O3-P-O4
22	2	317	LHG	C3-O3-P-O5
22	2	317	LHG	C3-O3-P-O6
22	2	317	LHG	O10-C23-O8-C6
22	2	317	LHG	C24-C23-O8-C6
22	A	842	LHG	C3-O3-P-O6
22	B	848	LHG	C3-O3-P-O4
22	B	848	LHG	C3-O3-P-O5
22	B	848	LHG	C4-O6-P-O3
22	B	848	LHG	C4-O6-P-O4
23	1	318	BCR	C11-C12-C13-C14
23	1	318	BCR	C11-C12-C13-C35
23	2	319	BCR	C1-C6-C7-C8
23	2	319	BCR	C5-C6-C7-C8
23	2	319	BCR	C13-C14-C15-C16
23	2	319	BCR	C21-C22-C23-C24
23	A	843	BCR	C11-C12-C13-C14
23	A	843	BCR	C11-C12-C13-C35
23	A	843	BCR	C17-C18-C19-C20
23	A	843	BCR	C36-C18-C19-C20
23	A	843	BCR	C21-C22-C23-C24
23	A	845	BCR	C5-C6-C7-C8
23	A	847	BCR	C11-C12-C13-C14
23	A	847	BCR	C11-C12-C13-C35
23	B	842	BCR	C11-C12-C13-C14
23	J	101	BCR	C11-C12-C13-C14
23	J	101	BCR	C23-C24-C25-C26
23	J	101	BCR	C23-C24-C25-C30
23	J	104	BCR	C23-C24-C25-C26
23	L	304	BCR	C23-C24-C25-C26
23	L	304	BCR	C23-C24-C25-C30
24	1	319	LMG	O6-C1-O1-C7
24	1	319	LMG	O9-C10-O7-C8
24	1	319	LMG	C11-C10-O7-C8
24	1	319	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
24	1	319	LMG	C29-C28-O8-C9
24	B	847	LMG	O9-C10-O7-C8
24	B	847	LMG	C11-C10-O7-C8
24	B	847	LMG	O10-C28-O8-C9
24	B	847	LMG	C29-C28-O8-C9
25	2	318	LMT	C2'-C1'-O1'-C1
25	2	318	LMT	O5'-C1'-O1'-C1
18	2	305	CHL	O1D-CGD-O2D-CED
18	4	305	CHL	O1D-CGD-O2D-CED
19	4	302	CLA	O1D-CGD-O2D-CED
18	2	306	CHL	O1D-CGD-O2D-CED
19	H	201	CLA	O1D-CGD-O2D-CED
18	2	305	CHL	CBD-CGD-O2D-CED
19	1	314	CLA	CBD-CGD-O2D-CED
19	2	302	CLA	CBD-CGD-O2D-CED
19	2	311	CLA	CBD-CGD-O2D-CED
19	3	304	CLA	CBD-CGD-O2D-CED
19	3	309	CLA	CBD-CGD-O2D-CED
19	4	302	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	A	851	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	CBD-CGD-O2D-CED
19	G	202	CLA	CBD-CGD-O2D-CED
19	K	202	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	O1A-CGA-O2A-C1
19	4	313	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	O1A-CGA-O2A-C1
19	A	833	CLA	O1A-CGA-O2A-C1
19	A	837	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1
19	G	203	CLA	O1A-CGA-O2A-C1
19	3	314	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	CBA-CGA-O2A-C1
19	1	308	CLA	O1D-CGD-O2D-CED
19	1	311	CLA	O1D-CGD-O2D-CED
19	3	302	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	814	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	O1A-CGA-O2A-C1
19	A	814	CLA	O1A-CGA-O2A-C1
19	A	818	CLA	O1A-CGA-O2A-C1
19	A	822	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	O1A-CGA-O2A-C1
19	B	819	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	L	303	CLA	O1A-CGA-O2A-C1
18	2	314	CHL	O1D-CGD-O2D-CED
19	B	809	CLA	O1D-CGD-O2D-CED
19	2	311	CLA	O1D-CGD-O2D-CED
19	3	304	CLA	O1D-CGD-O2D-CED
19	3	309	CLA	O1D-CGD-O2D-CED
19	B	802	CLA	O1D-CGD-O2D-CED
19	B	813	CLA	O1D-CGD-O2D-CED
19	G	202	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1A-CGA-O2A-C1
19	3	308	CLA	C3-C5-C6-C7
19	A	816	CLA	C3-C5-C6-C7
19	A	838	CLA	C3-C5-C6-C7
19	B	810	CLA	C3-C5-C6-C7
19	B	822	CLA	C3-C5-C6-C7
19	A	811	CLA	CBA-CGA-O2A-C1
19	A	812	CLA	CBA-CGA-O2A-C1
19	A	816	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBA-CGA-O2A-C1
25	G	201	LMT	C3'-C4'-O1B-C1B
18	1	306	CHL	CBD-CGD-O2D-CED
18	2	301	CHL	CBD-CGD-O2D-CED
19	1	302	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	CBD-CGD-O2D-CED
19	2	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	305	CLA	CBD-CGD-O2D-CED
19	3	313	CLA	CBD-CGD-O2D-CED
19	4	313	CLA	CBD-CGD-O2D-CED
19	A	805	CLA	CBD-CGD-O2D-CED
19	A	818	CLA	CBD-CGD-O2D-CED
19	A	837	CLA	CBD-CGD-O2D-CED
19	A	840	CLA	CBD-CGD-O2D-CED
19	B	824	CLA	CBD-CGD-O2D-CED
19	B	830	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	F	304	CLA	CBD-CGD-O2D-CED
19	1	314	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	O1A-CGA-O2A-C1
19	1	309	CLA	C4-C3-C5-C6
19	A	839	CLA	C4-C3-C5-C6
19	A	853	CLA	C4-C3-C5-C6
19	B	831	CLA	C4-C3-C5-C6
19	B	838	CLA	C4-C3-C5-C6
19	1	309	CLA	C2-C3-C5-C6
19	2	309	CLA	C2-C3-C5-C6
19	A	812	CLA	C2-C3-C5-C6
19	A	829	CLA	C2-C3-C5-C6
19	A	839	CLA	C2-C3-C5-C6
19	B	832	CLA	C2-C3-C5-C6
19	B	838	CLA	C2-C3-C5-C6
18	3	307	CHL	CBA-CGA-O2A-C1
19	H	201	CLA	CBA-CGA-O2A-C1
19	1	311	CLA	C2A-CAA-CBA-CGA
19	3	314	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	C2A-CAA-CBA-CGA
19	A	854	CLA	C2A-CAA-CBA-CGA
19	B	811	CLA	C2A-CAA-CBA-CGA
19	B	823	CLA	C2A-CAA-CBA-CGA
19	B	827	CLA	C2A-CAA-CBA-CGA
19	L	303	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	O1A-CGA-O2A-C1
19	2	304	CLA	CBA-CGA-O2A-C1
19	3	312	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	818	CLA	CBA-CGA-O2A-C1
19	A	822	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	836	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	CBA-CGA-O2A-C1
19	B	819	CLA	CBA-CGA-O2A-C1
19	L	303	CLA	CBA-CGA-O2A-C1
23	2	319	BCR	C19-C20-C21-C22
23	J	101	BCR	C13-C14-C15-C16
19	3	312	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
19	B	832	CLA	O1A-CGA-O2A-C1
18	3	307	CHL	O1A-CGA-O2A-C1
19	1	304	CLA	O1D-CGD-O2D-CED
19	L	302	CLA	C3-C5-C6-C7
19	2	309	CLA	CBD-CGD-O2D-CED
19	4	301	CLA	CBD-CGD-O2D-CED
19	4	311	CLA	CBD-CGD-O2D-CED
19	L	302	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	O1D-CGD-O2D-CED
19	F	304	CLA	O1D-CGD-O2D-CED
19	G	204	CLA	O1D-CGD-O2D-CED
19	4	313	CLA	CBA-CGA-O2A-C1
19	A	835	CLA	CBA-CGA-O2A-C1
19	A	837	CLA	CBA-CGA-O2A-C1
19	B	811	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	CBA-CGA-O2A-C1
19	4	302	CLA	O1A-CGA-O2A-C1
19	B	805	CLA	O1A-CGA-O2A-C1
19	3	310	CLA	CBD-CGD-O2D-CED
19	F	302	CLA	CBD-CGD-O2D-CED
19	F	303	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	814	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	CBA-CGA-O2A-C1
19	B	809	CLA	CBA-CGA-O2A-C1
19	A	812	CLA	C4-C3-C5-C6
19	B	822	CLA	C4-C3-C5-C6
19	A	834	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	2	312	CLA	O1A-CGA-O2A-C1
19	B	835	CLA	O1A-CGA-O2A-C1
19	3	311	CLA	CBD-CGD-O2D-CED
19	4	303	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	C2A-CAA-CBA-CGA
19	A	834	CLA	C2A-CAA-CBA-CGA
19	A	840	CLA	C2A-CAA-CBA-CGA
19	3	301	CLA	O1D-CGD-O2D-CED
18	2	301	CHL	O1A-CGA-O2A-C1
28	B	846	DGD	O6D-C1D-O3G-C3G
18	2	301	CHL	CBA-CGA-O2A-C1
19	A	817	CLA	CBA-CGA-O2A-C1
19	B	801	CLA	CBA-CGA-O2A-C1
19	F	301	CLA	CBA-CGA-O2A-C1
19	2	304	CLA	CBD-CGD-O2D-CED
19	2	308	CLA	CBD-CGD-O2D-CED
19	A	803	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	O1A-CGA-O2A-C1
19	B	817	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	CBD-CGD-O2D-CED
23	J	101	BCR	C19-C20-C21-C22
19	A	835	CLA	O1A-CGA-O2A-C1
19	2	312	CLA	CBA-CGA-O2A-C1
19	4	302	CLA	CBA-CGA-O2A-C1
19	A	801	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	B	804	CLA	CBA-CGA-O2A-C1
19	B	805	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	B	835	CLA	CBA-CGA-O2A-C1
18	2	307	CHL	CBD-CGD-O2D-CED
19	A	812	CLA	O1D-CGD-O2D-CED
19	B	818	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	A	853	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	B	831	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	812	CLA	C3-C5-C6-C7
19	A	834	CLA	C3-C5-C6-C7
19	B	837	CLA	C3-C5-C6-C7
19	A	808	CLA	CBD-CGD-O2D-CED
19	1	312	CLA	C6-C7-C8-C9
19	1	321	CLA	C14-C13-C15-C16
19	2	302	CLA	C11-C12-C13-C14
19	2	309	CLA	C11-C10-C8-C9
19	2	312	CLA	C11-C10-C8-C9
19	2	312	CLA	C11-C12-C13-C14
19	4	308	CLA	C11-C10-C8-C9
19	A	805	CLA	C6-C7-C8-C9
19	A	807	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C10-C8-C9
19	A	826	CLA	C14-C13-C15-C16
19	A	829	CLA	C11-C12-C13-C14
19	A	836	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C10-C8-C9
19	A	852	CLA	C14-C13-C15-C16
19	A	853	CLA	C11-C10-C8-C9
19	B	802	CLA	C11-C12-C13-C14
19	B	807	CLA	C11-C12-C13-C14
19	B	807	CLA	C14-C13-C15-C16
19	B	809	CLA	C14-C13-C15-C16
19	B	813	CLA	C11-C10-C8-C9
19	B	813	CLA	C14-C13-C15-C16
19	B	816	CLA	C11-C10-C8-C9
19	B	824	CLA	C11-C10-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B	827	CLA	C14-C13-C15-C16
19	B	828	CLA	C11-C12-C13-C14
19	B	830	CLA	C6-C7-C8-C9
19	B	831	CLA	C11-C10-C8-C9
19	B	837	CLA	C11-C10-C8-C9
19	B	838	CLA	C11-C10-C8-C9
19	F	301	CLA	C11-C10-C8-C9
19	L	302	CLA	C11-C10-C8-C9
28	B	846	DGD	C2D-C1D-O3G-C3G
19	B	801	CLA	O1A-CGA-O2A-C1
19	J	102	CLA	CBD-CGD-O2D-CED
23	2	319	BCR	C36-C18-C19-C20
23	A	843	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	K	201	BCR	C36-C18-C19-C20
23	2	319	BCR	C17-C18-C19-C20
23	K	201	BCR	C17-C18-C19-C20
19	A	807	CLA	C2A-CAA-CBA-CGA
19	B	819	CLA	C2A-CAA-CBA-CGA
19	G	203	CLA	C2A-CAA-CBA-CGA
19	H	201	CLA	C2A-CAA-CBA-CGA
25	N	201	LMT	O5B-C1B-O1B-C4'
19	2	312	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	CBA-CGA-O2A-C1
19	4	313	CLA	C15-C16-C17-C18
19	4	313	CLA	C2-C1-O2A-CGA
18	2	307	CHL	O1D-CGD-O2D-CED
19	1	302	CLA	C10-C11-C12-C13
19	A	812	CLA	C5-C6-C7-C8
19	H	201	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	C11-C12-C13-C15
19	A	818	CLA	C12-C13-C15-C16
19	A	836	CLA	C11-C12-C13-C15
19	A	852	CLA	C11-C12-C13-C15
19	A	854	CLA	C11-C12-C13-C15
19	B	801	CLA	C12-C13-C15-C16
19	B	823	CLA	C12-C13-C15-C16
19	F	302	CLA	C11-C12-C13-C15
19	L	302	CLA	C11-C12-C13-C15
23	A	843	BCR	C19-C20-C21-C22
23	K	201	BCR	C15-C16-C17-C18
19	A	810	CLA	C10-C11-C12-C13
19	A	817	CLA	O1A-CGA-O2A-C1
19	B	804	CLA	O1A-CGA-O2A-C1
19	B	824	CLA	O1A-CGA-O2A-C1
19	3	314	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	CBD-CGD-O2D-CED
19	1	321	CLA	C13-C15-C16-C17
19	2	302	CLA	C10-C11-C12-C13
19	4	302	CLA	C10-C11-C12-C13
19	A	801	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	816	CLA	C10-C11-C12-C13
19	A	818	CLA	C15-C16-C17-C18
19	A	824	CLA	C5-C6-C7-C8
19	A	825	CLA	C10-C11-C12-C13
19	A	825	CLA	C15-C16-C17-C18
19	A	839	CLA	C10-C11-C12-C13
19	B	804	CLA	C15-C16-C17-C18
19	B	807	CLA	C10-C11-C12-C13
19	B	813	CLA	C15-C16-C17-C18
19	B	823	CLA	C8-C10-C11-C12
19	B	826	CLA	C10-C11-C12-C13
19	B	832	CLA	C10-C11-C12-C13
19	B	835	CLA	C15-C16-C17-C18
19	L	302	CLA	C15-C16-C17-C18
19	1	313	CLA	C2A-CAA-CBA-CGA
19	3	304	CLA	C2A-CAA-CBA-CGA
19	3	306	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	A	811	CLA	C2A-CAA-CBA-CGA
19	A	812	CLA	C2A-CAA-CBA-CGA
19	A	823	CLA	C2A-CAA-CBA-CGA
19	A	831	CLA	C2A-CAA-CBA-CGA
19	A	836	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	B	816	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
19	2	304	CLA	C5-C6-C7-C8
19	3	301	CLA	C10-C11-C12-C13
19	3	312	CLA	C5-C6-C7-C8
19	4	308	CLA	C10-C11-C12-C13
19	A	834	CLA	C15-C16-C17-C18
19	A	838	CLA	C15-C16-C17-C18
19	A	840	CLA	C5-C6-C7-C8
19	B	809	CLA	C15-C16-C17-C18
19	B	827	CLA	C15-C16-C17-C18
19	B	834	CLA	C5-C6-C7-C8
19	A	815	CLA	O1D-CGD-O2D-CED
19	2	303	CLA	O1A-CGA-O2A-C1
19	2	304	CLA	O1A-CGA-O2A-C1
19	A	803	CLA	O1A-CGA-O2A-C1
19	B	807	CLA	C3-C5-C6-C7
23	1	318	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	2	312	CLA	C5-C6-C7-C8
19	2	312	CLA	C10-C11-C12-C13
19	3	302	CLA	C10-C11-C12-C13
19	4	311	CLA	C5-C6-C7-C8
19	A	805	CLA	C5-C6-C7-C8
19	A	828	CLA	C15-C16-C17-C18
19	A	834	CLA	C10-C11-C12-C13
19	A	854	CLA	C10-C11-C12-C13
19	B	801	CLA	C15-C16-C17-C18
19	B	804	CLA	C10-C11-C12-C13
19	B	805	CLA	C5-C6-C7-C8
19	B	809	CLA	C10-C11-C12-C13
19	B	811	CLA	C5-C6-C7-C8
19	B	813	CLA	C10-C11-C12-C13
19	B	813	CLA	C13-C15-C16-C17
19	B	822	CLA	C8-C10-C11-C12
19	B	837	CLA	C10-C11-C12-C13
19	B	838	CLA	C10-C11-C12-C13
19	B	820	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	CBA-CGA-O2A-C1
19	3	304	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	O1A-CGA-O2A-C1
19	3	302	CLA	C5-C6-C7-C8
19	A	826	CLA	C8-C10-C11-C12
19	A	831	CLA	C10-C11-C12-C13
19	B	805	CLA	C15-C16-C17-C18
19	B	808	CLA	C10-C11-C12-C13
19	B	822	CLA	C10-C11-C12-C13
19	A	810	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	C3-C5-C6-C7
19	B	808	CLA	C3-C5-C6-C7
19	B	832	CLA	O1D-CGD-O2D-CED
19	1	312	CLA	C5-C6-C7-C8
19	3	308	CLA	C15-C16-C17-C18
19	A	838	CLA	C10-C11-C12-C13
19	B	837	CLA	C15-C16-C17-C18
19	B	827	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	C5-C6-C7-C8
19	B	805	CLA	C10-C11-C12-C13
19	B	812	CLA	C10-C11-C12-C13
19	B	817	CLA	C10-C11-C12-C13
19	B	823	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	F	302	CLA	C15-C16-C17-C18
19	B	808	CLA	CBD-CGD-O2D-CED
19	K	203	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	O1D-CGD-O2D-CED
19	2	309	CLA	C8-C10-C11-C12
19	1	321	CLA	C10-C11-C12-C13
19	A	808	CLA	C5-C6-C7-C8
18	4	306	CHL	C2A-CAA-CBA-CGA
19	2	312	CLA	C2A-CAA-CBA-CGA
19	3	312	CLA	C2A-CAA-CBA-CGA
19	A	802	CLA	C2A-CAA-CBA-CGA
19	A	814	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	C2A-CAA-CBA-CGA
19	B	832	CLA	C2A-CAA-CBA-CGA
19	K	202	CLA	C2A-CAA-CBA-CGA
18	4	306	CHL	CBA-CGA-O2A-C1
19	3	304	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	CBA-CGA-O2A-C1
19	2	304	CLA	C10-C11-C12-C13
19	2	312	CLA	C13-C15-C16-C17
19	4	313	CLA	C10-C11-C12-C13
19	A	804	CLA	C15-C16-C17-C18
19	A	824	CLA	C15-C16-C17-C18
19	A	836	CLA	C10-C11-C12-C13
19	A	854	CLA	C15-C16-C17-C18
19	B	825	CLA	C10-C11-C12-C13
25	N	201	LMT	C2B-C1B-O1B-C4'
19	K	202	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	C10-C11-C12-C13
19	B	817	CLA	C5-C6-C7-C8
19	B	828	CLA	C10-C11-C12-C13
19	A	851	CLA	O1D-CGD-O2D-CED
19	4	302	CLA	C5-C6-C7-C8
19	A	807	CLA	C15-C16-C17-C18
19	A	818	CLA	C10-C11-C12-C13
19	A	829	CLA	C5-C6-C7-C8
19	A	852	CLA	C10-C11-C12-C13
19	A	853	CLA	C8-C10-C11-C12
19	B	816	CLA	C5-C6-C7-C8
19	B	830	CLA	C10-C11-C12-C13
19	F	302	CLA	C10-C11-C12-C13
19	B	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	C4-C3-C5-C6
19	A	802	CLA	C15-C16-C17-C18
19	A	806	CLA	C1-C2-C3-C5
19	A	808	CLA	C14-C13-C15-C16
24	B	847	LMG	C2-C1-O1-C7
19	3	308	CLA	C10-C11-C12-C13
19	B	827	CLA	C10-C11-C12-C13
19	B	832	CLA	C15-C16-C17-C18
19	F	301	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	C2A-CAA-CBA-CGA
19	1	314	CLA	C2A-CAA-CBA-CGA
19	2	309	CLA	C2A-CAA-CBA-CGA
19	4	303	CLA	C2A-CAA-CBA-CGA
19	A	808	CLA	C2A-CAA-CBA-CGA
19	A	839	CLA	C2A-CAA-CBA-CGA
19	A	853	CLA	C2A-CAA-CBA-CGA
19	A	805	CLA	C10-C11-C12-C13
19	B	807	CLA	C15-C16-C17-C18
19	B	822	CLA	C5-C6-C7-C8
19	F	301	CLA	C10-C11-C12-C13
18	4	304	CHL	C6-C7-C8-C10
19	B	817	CLA	C11-C12-C13-C14
19	B	834	CLA	C6-C7-C8-C10
19	2	302	CLA	O1D-CGD-O2D-CED
18	1	301	CHL	C3-C5-C6-C7
23	B	842	BCR	C12-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C19
23	J	101	BCR	C12-C13-C14-C15
23	J	101	BCR	C20-C21-C22-C23
19	A	814	CLA	O1D-CGD-O2D-CED
19	A	803	CLA	CBA-CGA-O2A-C1
19	A	812	CLA	C13-C15-C16-C17
19	A	829	CLA	C13-C15-C16-C17
18	1	301	CHL	C6-C7-C8-C9
19	1	312	CLA	C11-C12-C13-C15
19	4	309	CLA	C11-C12-C13-C14
19	A	823	CLA	O1A-CGA-O2A-C1
19	B	820	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	C13-C15-C16-C17
19	B	828	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	C5-C6-C7-C8
19	A	807	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	848	LHG	C29-C30-C31-C32
25	2	318	LMT	C2-C1-O1'-C1'
19	B	828	CLA	C4B-C3B-CAB-CBB
19	F	302	CLA	C4B-C3B-CAB-CBB
19	1	310	CLA	C6-C7-C8-C9
19	1	310	CLA	C6-C7-C8-C10
19	B	818	CLA	C11-C12-C13-C15
19	B	830	CLA	C11-C12-C13-C14
19	B	822	CLA	O1D-CGD-O2D-CED
19	A	801	CLA	C12-C13-C15-C16
19	A	812	CLA	C12-C13-C15-C16
19	A	820	CLA	C15-C16-C17-C18
19	A	810	CLA	C3-C5-C6-C7
18	2	307	CHL	C3A-C2A-CAA-CBA
18	4	305	CHL	C3A-C2A-CAA-CBA
19	1	311	CLA	C3A-C2A-CAA-CBA
19	1	321	CLA	C3A-C2A-CAA-CBA
19	2	313	CLA	C3A-C2A-CAA-CBA
19	3	302	CLA	C3A-C2A-CAA-CBA
19	3	314	CLA	C3A-C2A-CAA-CBA
19	4	302	CLA	C3A-C2A-CAA-CBA
19	4	309	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	831	CLA	C3A-C2A-CAA-CBA
19	A	835	CLA	C3A-C2A-CAA-CBA
19	B	801	CLA	C3A-C2A-CAA-CBA
19	B	823	CLA	C3A-C2A-CAA-CBA
19	B	830	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	L	303	CLA	C3A-C2A-CAA-CBA
19	K	203	CLA	C3A-C2A-CAA-CBA
19	2	309	CLA	O1D-CGD-O2D-CED
19	B	816	CLA	C10-C11-C12-C13
19	A	808	CLA	C10-C11-C12-C13
18	4	304	CHL	C6-C7-C8-C9
19	B	822	CLA	C11-C12-C13-C15
19	B	834	CLA	C6-C7-C8-C9
19	2	303	CLA	CBA-CGA-O2A-C1
19	B	817	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	O1A-CGA-O2A-C1
19	B	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	4	318	LMG	C11-C12-C13-C14
19	3	301	CLA	C11-C12-C13-C14
19	B	806	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	C2B-C3B-CAB-CBB
23	A	843	BCR	C1-C6-C7-C8
23	A	843	BCR	C5-C6-C7-C8
23	A	845	BCR	C1-C6-C7-C8
23	B	841	BCR	C1-C6-C7-C8
23	J	101	BCR	C1-C6-C7-C8
23	J	101	BCR	C5-C6-C7-C8
23	J	104	BCR	C1-C6-C7-C8
23	J	104	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C30
19	A	809	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	C15-C16-C17-C18
19	A	831	CLA	C5-C6-C7-C8
19	A	853	CLA	C5-C6-C7-C8
19	F	301	CLA	C15-C16-C17-C18
19	A	832	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	C2A-CAA-CBA-CGA
19	B	803	CLA	C2A-CAA-CBA-CGA
19	B	809	CLA	C2A-CAA-CBA-CGA
19	1	310	CLA	O1A-CGA-O2A-C1
19	A	830	CLA	O1A-CGA-O2A-C1
19	L	301	CLA	C11-C10-C8-C7
18	4	304	CHL	C2-C3-C5-C6
19	A	808	CLA	C2-C3-C5-C6
19	A	805	CLA	C3-C5-C6-C7
19	4	313	CLA	C11-C12-C13-C14
19	A	828	CLA	C11-C10-C8-C9
19	B	835	CLA	C11-C12-C13-C14
19	B	802	CLA	C15-C16-C17-C18
24	B	847	LMG	O6-C1-O1-C7
25	N	201	LMT	C2'-C1'-O1'-C1
18	4	306	CHL	CBD-CGD-O2D-CED
19	1	309	CLA	C5-C6-C7-C8
19	A	805	CLA	C15-C16-C17-C18
19	B	817	CLA	C8-C10-C11-C12
19	F	301	CLA	C5-C6-C7-C8
19	B	826	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	C13-C15-C16-C17
19	B	828	CLA	C8-C10-C11-C12
19	B	824	CLA	C3-C5-C6-C7
19	A	838	CLA	CBA-CGA-O2A-C1
19	B	813	CLA	C2A-CAA-CBA-CGA
19	L	301	CLA	C2A-CAA-CBA-CGA
19	3	301	CLA	C11-C12-C13-C15
19	A	810	CLA	C16-C17-C18-C20
19	A	828	CLA	C16-C17-C18-C19
19	A	828	CLA	C16-C17-C18-C20
19	B	810	CLA	C6-C7-C8-C10
19	B	811	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	C4-C3-C5-C6
24	B	847	LMG	C21-C22-C23-C24
19	B	826	CLA	C5-C6-C7-C8
19	B	827	CLA	C13-C15-C16-C17
19	A	831	CLA	C3-C5-C6-C7
19	A	812	CLA	C10-C11-C12-C13
19	A	832	CLA	C10-C11-C12-C13
19	A	840	CLA	C15-C16-C17-C18
24	B	847	LMG	O6-C5-C6-O5
25	2	318	LMT	O5'-C5'-C6'-O6'
19	4	309	CLA	C10-C11-C12-C13
18	1	301	CHL	C6-C7-C8-C10
19	1	312	CLA	C11-C12-C13-C14
19	B	817	CLA	C11-C12-C13-C15
24	1	319	LMG	C18-C19-C20-C21
19	3	308	CLA	C5-C6-C7-C8
19	A	826	CLA	C10-C11-C12-C13
19	2	304	CLA	C3-C5-C6-C7
19	A	823	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	C10-C11-C12-C13
22	1	322	LHG	C11-C10-C9-C8
19	B	823	CLA	C13-C15-C16-C17
24	1	319	LMG	O6-C5-C6-O5
19	4	309	CLA	C11-C12-C13-C15
19	B	810	CLA	C6-C7-C8-C9
19	B	830	CLA	C11-C12-C13-C15
19	B	826	CLA	C2-C3-C5-C6
22	A	842	LHG	C24-C25-C26-C27
18	3	307	CHL	C2A-CAA-CBA-CGA
19	B	805	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	B	834	CLA	CBA-CGA-O2A-C1
24	4	318	LMG	O6-C5-C6-O5
19	3	313	CLA	O1D-CGD-O2D-CED
19	A	818	CLA	O1D-CGD-O2D-CED
19	B	824	CLA	C10-C11-C12-C13
19	A	801	CLA	O1A-CGA-O2A-C1
19	A	834	CLA	O1A-CGA-O2A-C1
19	1	307	CLA	C1A-C2A-CAA-CBA
19	1	311	CLA	C1A-C2A-CAA-CBA
19	3	302	CLA	C1A-C2A-CAA-CBA
19	3	314	CLA	C1A-C2A-CAA-CBA
19	4	302	CLA	C1A-C2A-CAA-CBA
19	4	303	CLA	C1A-C2A-CAA-CBA
19	4	313	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	831	CLA	C1A-C2A-CAA-CBA
19	A	832	CLA	C1A-C2A-CAA-CBA
19	A	835	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	817	CLA	C1A-C2A-CAA-CBA
19	L	303	CLA	C1A-C2A-CAA-CBA
19	2	304	CLA	C13-C15-C16-C17
19	1	302	CLA	C11-C10-C8-C7
19	1	303	CLA	C6-C7-C8-C10
19	2	304	CLA	C12-C13-C15-C16
19	2	312	CLA	C12-C13-C15-C16
19	3	301	CLA	C11-C10-C8-C7
19	A	808	CLA	C11-C10-C8-C7
19	A	809	CLA	C11-C10-C8-C7
19	A	812	CLA	C11-C12-C13-C15
19	A	816	CLA	C11-C10-C8-C7
19	A	820	CLA	C12-C13-C15-C16
19	A	826	CLA	C11-C12-C13-C15
19	A	829	CLA	C12-C13-C15-C16
19	A	836	CLA	C6-C7-C8-C10
19	B	809	CLA	C6-C7-C8-C10
19	B	812	CLA	C11-C10-C8-C7
19	B	812	CLA	C11-C12-C13-C15
19	B	823	CLA	C11-C10-C8-C7
19	F	301	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	F	302	CLA	C12-C13-C15-C16
19	L	301	CLA	C6-C7-C8-C10
26	A	841	PQN	C21-C22-C23-C25
26	B	839	PQN	C16-C17-C18-C20
19	A	840	CLA	C16-C17-C18-C20
19	1	307	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	C13-C15-C16-C17
19	A	837	CLA	C4-C3-C5-C6
19	4	311	CLA	C2-C3-C5-C6
19	A	826	CLA	C2-C3-C5-C6
19	A	838	CLA	C2-C3-C5-C6
19	B	807	CLA	C2-C3-C5-C6
19	B	805	CLA	C3-C5-C6-C7
19	A	813	CLA	CBD-CGD-O2D-CED
19	2	313	CLA	C2A-CAA-CBA-CGA
19	3	313	CLA	C2A-CAA-CBA-CGA
19	4	307	CLA	C2A-CAA-CBA-CGA
19	L	302	CLA	C2A-CAA-CBA-CGA
19	3	301	CLA	C11-C10-C8-C9
19	3	308	CLA	C14-C13-C15-C16
19	A	807	CLA	C11-C12-C13-C14
19	A	818	CLA	C11-C12-C13-C14
19	A	829	CLA	C14-C13-C15-C16
19	A	836	CLA	C6-C7-C8-C9
19	B	804	CLA	C11-C12-C13-C14
19	B	809	CLA	C6-C7-C8-C9
19	B	812	CLA	C11-C10-C8-C9
19	B	812	CLA	C11-C12-C13-C14
19	B	823	CLA	C11-C10-C8-C9
19	B	825	CLA	C11-C12-C13-C14
19	B	826	CLA	C11-C10-C8-C9
19	B	822	CLA	C11-C12-C13-C14
19	1	310	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
19	L	302	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	O1D-CGD-O2D-CED
24	1	319	LMG	C2-C1-O1-C7
19	4	313	CLA	O1D-CGD-O2D-CED
24	B	847	LMG	O1-C7-C8-C9
19	A	853	CLA	C10-C11-C12-C13
19	A	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	827	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	CBA-CGA-O2A-C1
19	B	828	CLA	CBA-CGA-O2A-C1
19	4	302	CLA	C11-C12-C13-C15
19	A	840	CLA	C16-C17-C18-C19
18	2	314	CHL	CHA-CBD-CGD-O2D
22	1	322	LHG	C24-C25-C26-C27
19	A	838	CLA	C4-C3-C5-C6
19	B	817	CLA	C4-C3-C5-C6
19	L	301	CLA	CBD-CGD-O2D-CED
19	2	304	CLA	C2-C3-C5-C6
19	2	312	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	L	302	CLA	C10-C11-C12-C13
23	L	304	BCR	C21-C22-C23-C24
19	B	813	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	C8-C10-C11-C12
19	A	832	CLA	C5-C6-C7-C8
19	B	826	CLA	C15-C16-C17-C18
19	L	302	CLA	C5-C6-C7-C8
18	2	306	CHL	C2A-CAA-CBA-CGA
19	B	830	CLA	C5-C6-C7-C8
19	B	816	CLA	O2A-C1-C2-C3
19	B	819	CLA	O2A-C1-C2-C3
19	B	829	CLA	O2A-C1-C2-C3
19	F	302	CLA	O2A-C1-C2-C3
18	1	306	CHL	C3C-C2C-CMC-OMC
19	3	305	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	C4-C3-C5-C6
19	A	820	CLA	C2-C3-C5-C6
19	A	809	CLA	C10-C11-C12-C13
19	A	811	CLA	C5-C6-C7-C8
22	A	842	LHG	O7-C5-C6-O8
19	2	313	CLA	C10-C11-C12-C13
22	1	322	LHG	C10-C11-C12-C13
18	1	306	CHL	C2A-CAA-CBA-CGA
19	1	303	CLA	C10-C11-C12-C13
19	B	816	CLA	C11-C12-C13-C14
19	1	304	CLA	CBA-CGA-O2A-C1
19	A	853	CLA	CBA-CGA-O2A-C1
19	B	822	CLA	CBA-CGA-O2A-C1
23	K	201	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	4	301	CLA	C11-C12-C13-C15
19	A	804	CLA	C4-C3-C5-C6
19	A	832	CLA	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	L	301	CLA	C5-C6-C7-C8
25	G	201	LMT	C2-C1-O1'-C1'
25	N	201	LMT	C2-C1-O1'-C1'
19	2	304	CLA	C14-C13-C15-C16
19	2	312	CLA	C14-C13-C15-C16
19	2	313	CLA	C6-C7-C8-C9
19	A	807	CLA	C11-C10-C8-C9
19	A	809	CLA	C11-C10-C8-C9
19	A	812	CLA	C11-C10-C8-C9
19	A	812	CLA	C14-C13-C15-C16
19	A	818	CLA	C14-C13-C15-C16
19	A	852	CLA	C11-C10-C8-C9
19	A	853	CLA	C6-C7-C8-C9
19	B	825	CLA	C6-C7-C8-C9
19	B	832	CLA	C6-C7-C8-C9
19	B	838	CLA	C6-C7-C8-C9
19	F	301	CLA	C6-C7-C8-C9
19	F	302	CLA	C11-C10-C8-C9
19	F	302	CLA	C14-C13-C15-C16
19	L	302	CLA	C11-C12-C13-C14
26	B	839	PQN	C16-C17-C18-C19
22	2	317	LHG	C2-C3-O3-P
19	1	321	CLA	CAA-CBA-CGA-O2A
19	B	838	CLA	CAA-CBA-CGA-O2A
22	1	322	LHG	C28-C29-C30-C31
19	A	834	CLA	C8-C10-C11-C12
19	B	833	CLA	C2A-CAA-CBA-CGA
19	A	809	CLA	C11-C12-C13-C14
19	1	321	CLA	C12-C13-C15-C16
19	3	308	CLA	C12-C13-C15-C16
19	A	802	CLA	C11-C12-C13-C15
19	A	802	CLA	C12-C13-C15-C16
19	A	805	CLA	C6-C7-C8-C10
19	A	807	CLA	C11-C10-C8-C7
19	A	818	CLA	C11-C12-C13-C15
19	A	832	CLA	C11-C10-C8-C7
19	A	836	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C12-C13-C15-C16
19	A	852	CLA	C11-C10-C8-C7
19	A	853	CLA	C6-C7-C8-C10
19	A	853	CLA	C11-C10-C8-C7
19	B	804	CLA	C11-C12-C13-C15
19	B	807	CLA	C11-C12-C13-C15
19	B	812	CLA	C12-C13-C15-C16
19	B	813	CLA	C12-C13-C15-C16
19	B	818	CLA	C11-C10-C8-C7
19	B	825	CLA	C6-C7-C8-C10
19	B	825	CLA	C11-C12-C13-C15
19	B	826	CLA	C11-C10-C8-C7
19	B	832	CLA	C6-C7-C8-C10
19	B	838	CLA	C6-C7-C8-C10
26	B	839	PQN	C22-C23-C25-C26
19	3	308	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	O1D-CGD-O2D-CED
19	A	839	CLA	O1A-CGA-O2A-C1
19	B	816	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	C3-C5-C6-C7
18	1	301	CHL	C4-C3-C5-C6
18	3	307	CHL	C3A-C2A-CAA-CBA
19	4	303	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	A	831	CLA	C4-C3-C5-C6
19	B	812	CLA	C3A-C2A-CAA-CBA
19	B	822	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	C4-C3-C5-C6
19	L	302	CLA	C3A-C2A-CAA-CBA
19	2	320	CLA	CAA-CBA-CGA-O2A
19	A	837	CLA	C2-C3-C5-C6
19	1	305	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	C5-C6-C7-C8
23	2	319	BCR	C9-C10-C11-C12
23	K	201	BCR	C19-C20-C21-C22
19	A	839	CLA	C3-C5-C6-C7
19	B	802	CLA	O1A-CGA-O2A-C1
19	4	313	CLA	C5-C6-C7-C8
23	J	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	A	837	CLA	C2A-CAA-CBA-CGA
19	B	821	CLA	C2A-CAA-CBA-CGA
24	1	319	LMG	C7-C8-C9-O8
19	1	308	CLA	C1-C2-C3-C4
19	1	312	CLA	C1-C2-C3-C4
19	B	801	CLA	C1-C2-C3-C4
19	A	852	CLA	C15-C16-C17-C18
19	4	313	CLA	C4-C3-C5-C6
19	B	817	CLA	C2-C3-C5-C6
19	F	302	CLA	C2-C3-C5-C6
19	4	313	CLA	C3-C5-C6-C7
19	L	301	CLA	C3-C5-C6-C7
20	3	315	LUT	C1-C6-C7-C8
23	1	318	BCR	C23-C24-C25-C30
23	K	201	BCR	C23-C24-C25-C30
19	L	301	CLA	C11-C10-C8-C9
19	F	301	CLA	C16-C17-C18-C19
19	A	852	CLA	C8-C10-C11-C12
19	A	810	CLA	C16-C17-C18-C19
19	4	309	CLA	CAA-CBA-CGA-O2A
19	1	304	CLA	C2A-CAA-CBA-CGA
19	2	308	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2A-CAA-CBA-CGA
19	A	838	CLA	C2A-CAA-CBA-CGA
24	B	847	LMG	O1-C7-C8-O7
19	1	304	CLA	C1-C2-C3-C5
19	1	321	CLA	C1-C2-C3-C5
19	2	309	CLA	C1-C2-C3-C5
19	A	801	CLA	C1-C2-C3-C5
19	A	802	CLA	C1-C2-C3-C5
19	A	809	CLA	C1-C2-C3-C5
19	A	812	CLA	C1-C2-C3-C5
19	A	827	CLA	C1-C2-C3-C5
19	A	832	CLA	C1-C2-C3-C5
19	A	834	CLA	C1-C2-C3-C5
19	A	837	CLA	C1-C2-C3-C5
19	B	808	CLA	C1-C2-C3-C5
19	B	815	CLA	C1-C2-C3-C5
19	B	816	CLA	C1-C2-C3-C5
19	B	824	CLA	C1-C2-C3-C5
19	B	831	CLA	C1-C2-C3-C5
19	F	301	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
19	B	818	CLA	C11-C12-C13-C14
19	A	833	CLA	O1D-CGD-O2D-CED
19	A	803	CLA	C1-C2-C3-C4
19	L	303	CLA	C1-C2-C3-C4
19	A	832	CLA	C6-C7-C8-C9
19	A	838	CLA	C6-C7-C8-C9
19	B	802	CLA	C6-C7-C8-C9
19	F	302	CLA	C6-C7-C8-C9
19	A	854	CLA	C16-C17-C18-C19
26	A	841	PQN	C25-C26-C27-C28
19	1	303	CLA	C2-C3-C5-C6
19	4	302	CLA	C11-C12-C13-C14
19	A	839	CLA	C15-C16-C17-C18
19	L	302	CLA	C13-C15-C16-C17
19	2	312	CLA	C3-C5-C6-C7
19	4	301	CLA	C11-C12-C13-C14
19	B	801	CLA	C10-C11-C12-C13
19	B	820	CLA	C5-C6-C7-C8
19	A	808	CLA	C6-C7-C8-C10
19	A	825	CLA	C11-C12-C13-C15
19	A	832	CLA	C6-C7-C8-C10
19	A	838	CLA	C6-C7-C8-C10
19	A	839	CLA	C6-C7-C8-C10
19	A	852	CLA	C12-C13-C15-C16
19	A	854	CLA	C12-C13-C15-C16
19	B	802	CLA	C6-C7-C8-C10
19	B	805	CLA	C11-C12-C13-C15
19	B	816	CLA	C11-C10-C8-C7
19	B	822	CLA	C6-C7-C8-C10
19	B	830	CLA	C6-C7-C8-C10
19	B	832	CLA	C12-C13-C15-C16
19	F	302	CLA	C6-C7-C8-C10
19	L	302	CLA	C11-C10-C8-C7
25	G	201	LMT	C5'-C4'-O1B-C1B
19	B	812	CLA	C15-C16-C17-C18
19	1	321	CLA	O1A-CGA-O2A-C1
19	B	826	CLA	C2A-CAA-CBA-CGA
19	A	837	CLA	O1D-CGD-O2D-CED
19	2	304	CLA	C4-C3-C5-C6
19	B	809	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	L	301	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	4	307	CLA	O2A-C1-C2-C3
19	A	825	CLA	O2A-C1-C2-C3
19	B	830	CLA	O2A-C1-C2-C3
19	A	854	CLA	C16-C17-C18-C20
24	B	847	LMG	C12-C13-C14-C15
19	A	808	CLA	C8-C10-C11-C12
19	A	830	CLA	CAA-CBA-CGA-O2A
19	4	301	CLA	C3-C5-C6-C7
19	B	821	CLA	C4-C3-C5-C6
19	B	801	CLA	C2A-CAA-CBA-CGA
19	A	831	CLA	C2-C3-C5-C6
19	B	821	CLA	C2-C3-C5-C6
24	1	319	LMG	O7-C8-C9-O8
19	B	805	CLA	C11-C12-C13-C14
19	B	808	CLA	C16-C17-C18-C20
19	A	826	CLA	C15-C16-C17-C18
22	2	317	LHG	C23-C24-C25-C26
19	A	820	CLA	C16-C17-C18-C19
19	2	309	CLA	C5-C6-C7-C8
19	4	309	CLA	C3-C5-C6-C7
19	A	852	CLA	C2-C3-C5-C6
19	A	827	CLA	C13-C15-C16-C17
19	B	835	CLA	C5-C6-C7-C8
19	3	311	CLA	C2A-CAA-CBA-CGA
19	B	806	CLA	C2A-CAA-CBA-CGA
19	L	302	CLA	O1A-CGA-O2A-C1
19	2	303	CLA	O1D-CGD-O2D-CED
19	B	808	CLA	C16-C17-C18-C19
18	4	306	CHL	O1A-CGA-O2A-C1
19	A	801	CLA	C3-C5-C6-C7
28	B	846	DGD	CAA-CBA-CCA-CDA
19	3	301	CLA	C4B-C3B-CAB-CBB
19	4	309	CLA	C1A-C2A-CAA-CBA
19	A	802	CLA	C4B-C3B-CAB-CBB
19	A	838	CLA	C4B-C3B-CAB-CBB
19	B	812	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C1A-C2A-CAA-CBA
19	F	301	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C1A-C2A-CAA-CBA
19	L	302	CLA	C4B-C3B-CAB-CBB
19	A	805	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	2	319	BCR	C11-C12-C13-C14
22	B	848	LHG	C14-C15-C16-C17
19	A	804	CLA	C2A-CAA-CBA-CGA
28	B	846	DGD	C7B-C8B-C9B-CAB
19	A	822	CLA	C2-C3-C5-C6
18	2	301	CHL	O1D-CGD-O2D-CED
19	1	312	CLA	C11-C10-C8-C7
19	2	302	CLA	C11-C10-C8-C7
19	2	302	CLA	C11-C12-C13-C15
19	2	312	CLA	C11-C10-C8-C7
19	4	309	CLA	C11-C10-C8-C7
19	A	805	CLA	C11-C12-C13-C15
19	A	810	CLA	C11-C12-C13-C15
19	A	827	CLA	C11-C10-C8-C7
19	B	802	CLA	C11-C12-C13-C15
19	B	825	CLA	C12-C13-C15-C16
19	B	826	CLA	C11-C12-C13-C15
19	B	831	CLA	C6-C7-C8-C10
19	B	835	CLA	C12-C13-C15-C16
19	B	837	CLA	C12-C13-C15-C16
19	F	301	CLA	C11-C10-C8-C7
19	B	804	CLA	C13-C15-C16-C17
23	B	842	BCR	C14-C15-C16-C17
19	1	312	CLA	C11-C10-C8-C9
19	2	302	CLA	C11-C10-C8-C9
19	A	802	CLA	C14-C13-C15-C16
19	A	839	CLA	C6-C7-C8-C9
19	A	854	CLA	C14-C13-C15-C16
19	B	818	CLA	C11-C10-C8-C9
19	B	822	CLA	C6-C7-C8-C9
19	B	832	CLA	C14-C13-C15-C16
26	B	839	PQN	C24-C23-C25-C26
18	1	306	CHL	O1D-CGD-O2D-CED
19	A	820	CLA	C16-C17-C18-C20
19	A	824	CLA	C16-C17-C18-C19
19	B	812	CLA	C16-C17-C18-C19
19	B	830	CLA	O1D-CGD-O2D-CED
19	3	301	CLA	C2-C3-C5-C6
19	B	835	CLA	CAD-CBD-CGD-O2D
19	A	812	CLA	C8-C10-C11-C12
19	B	837	CLA	C13-C15-C16-C17
19	3	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	C15-C16-C17-C18
19	B	802	CLA	C10-C11-C12-C13
19	A	834	CLA	C16-C17-C18-C19
19	B	805	CLA	C16-C17-C18-C19
19	B	828	CLA	C16-C17-C18-C19
22	1	317	LHG	C25-C26-C27-C28
19	4	302	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	C2A-CAA-CBA-CGA
19	B	835	CLA	C2A-CAA-CBA-CGA
19	B	826	CLA	C8-C10-C11-C12
19	A	805	CLA	O1A-CGA-O2A-C1
19	1	303	CLA	CHA-CBD-CGD-O1D
19	3	314	CLA	CHA-CBD-CGD-O1D
19	4	303	CLA	CHA-CBD-CGD-O1D
19	A	805	CLA	CHA-CBD-CGD-O1D
19	A	812	CLA	CAD-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O1D
19	A	830	CLA	CAD-CBD-CGD-O1D
19	A	831	CLA	CAD-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	834	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	829	CLA	CHA-CBD-CGD-O1D
19	B	835	CLA	CAD-CBD-CGD-O1D
19	B	838	CLA	CAD-CBD-CGD-O1D
22	A	842	LHG	C3-O3-P-O5
22	A	842	LHG	C4-O6-P-O5
22	B	848	LHG	C3-O3-P-O6
23	B	842	BCR	C13-C14-C15-C16
19	3	301	CLA	C2B-C3B-CAB-CBB
19	A	829	CLA	C2B-C3B-CAB-CBB
19	F	302	CLA	C2B-C3B-CAB-CBB
20	4	315	LUT	C1-C6-C7-C8
23	B	841	BCR	C5-C6-C7-C8
19	3	312	CLA	C2-C3-C5-C6
19	A	836	CLA	C13-C15-C16-C17
19	B	812	CLA	CBD-CGD-O2D-CED
19	1	309	CLA	C11-C10-C8-C7
19	B	825	CLA	C3-C5-C6-C7
23	1	318	BCR	C10-C11-C12-C13
23	A	843	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	A	843	BCR	C18-C19-C20-C21
23	A	844	BCR	C10-C11-C12-C13
23	A	847	BCR	C10-C11-C12-C13
23	J	101	BCR	C18-C19-C20-C21
23	L	305	BCR	C18-C19-C20-C21
23	L	306	BCR	C10-C11-C12-C13
19	B	822	CLA	C2-C3-C5-C6
24	F	307	LMG	C10-C11-C12-C13
19	1	302	CLA	C11-C10-C8-C9
19	1	303	CLA	C6-C7-C8-C9
19	2	304	CLA	C11-C12-C13-C14
19	A	825	CLA	C11-C12-C13-C14
19	A	828	CLA	C11-C12-C13-C14
19	A	832	CLA	C14-C13-C15-C16
19	A	836	CLA	C11-C12-C13-C14
19	A	852	CLA	C11-C12-C13-C14
19	B	826	CLA	C11-C12-C13-C14
19	B	828	CLA	C6-C7-C8-C9
19	F	302	CLA	C11-C12-C13-C14
19	2	312	CLA	C11-C12-C13-C15
19	B	816	CLA	C6-C7-C8-C10
19	A	827	CLA	C10-C11-C12-C13
19	A	826	CLA	O1A-CGA-O2A-C1
19	3	301	CLA	CBA-CGA-O2A-C1
19	A	802	CLA	O1A-CGA-O2A-C1
19	3	310	CLA	O1D-CGD-O2D-CED
19	A	832	CLA	C13-C15-C16-C17
19	A	826	CLA	CBA-CGA-O2A-C1
19	1	321	CLA	C2A-CAA-CBA-CGA
19	3	302	CLA	C2A-CAA-CBA-CGA
19	B	815	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	CBD-CGD-O2D-CED
19	2	304	CLA	C2-C1-O2A-CGA
19	A	840	CLA	C4-C3-C5-C6
19	A	826	CLA	C5-C6-C7-C8
19	A	804	CLA	CAA-CBA-CGA-O2A
19	A	816	CLA	C5-C6-C7-C8
28	B	846	DGD	C5B-C6B-C7B-C8B
19	B	811	CLA	C6-C7-C8-C9
25	2	318	LMT	C1-C2-C3-C4
19	2	310	CLA	O1D-CGD-O2D-CED
19	3	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	4	313	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
25	N	201	LMT	O5'-C1'-O1'-C1
19	4	303	CLA	O1D-CGD-O2D-CED
19	A	818	CLA	C16-C17-C18-C19
19	4	309	CLA	C11-C10-C8-C9
19	A	801	CLA	C14-C13-C15-C16
19	A	805	CLA	C11-C12-C13-C14
19	A	827	CLA	C11-C10-C8-C9
19	B	808	CLA	C11-C12-C13-C14
19	B	831	CLA	C6-C7-C8-C9
19	B	837	CLA	C14-C13-C15-C16
19	A	829	CLA	C4B-C3B-CAB-CBB
28	B	846	DGD	O6D-C5D-C6D-O5D
19	1	303	CLA	CBA-CGA-O2A-C1
19	1	313	CLA	CAA-CBA-CGA-O2A
19	3	301	CLA	C4-C3-C5-C6
19	A	818	CLA	C4-C3-C5-C6
19	1	304	CLA	O1A-CGA-O2A-C1
19	1	302	CLA	C11-C12-C13-C14
19	B	804	CLA	CAA-CBA-CGA-O2A
19	A	804	CLA	C6-C7-C8-C10
19	A	818	CLA	C6-C7-C8-C10
19	A	820	CLA	C11-C12-C13-C15
19	B	813	CLA	C11-C10-C8-C7
19	B	827	CLA	C11-C10-C8-C7
19	B	837	CLA	C11-C10-C8-C7
19	A	828	CLA	C10-C11-C12-C13
19	B	818	CLA	C10-C11-C12-C13
19	1	308	CLA	C5-C6-C7-C8
19	B	801	CLA	C8-C10-C11-C12
19	1	314	CLA	C3A-C2A-CAA-CBA
19	A	813	CLA	C3A-C2A-CAA-CBA
19	B	828	CLA	C4-C3-C5-C6
19	F	301	CLA	C3A-C2A-CAA-CBA
19	3	309	CLA	C2C-C3C-CAC-CBC
19	1	307	CLA	CAA-CBA-CGA-O1A
21	2	316	XAT	C20-C13-C14-C15
23	1	318	BCR	C11-C10-C9-C34
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C16-C17-C18-C36
23	B	841	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	B	842	BCR	C11-C10-C9-C34
23	B	842	BCR	C20-C21-C22-C37
23	F	305	BCR	C35-C13-C14-C15
19	A	834	CLA	C2-C1-O2A-CGA
19	B	813	CLA	C16-C17-C18-C19
23	L	304	BCR	C37-C22-C23-C24
19	1	304	CLA	C4-C3-C5-C6
19	A	820	CLA	C5-C6-C7-C8
19	2	302	CLA	C15-C16-C17-C18
19	K	203	CLA	C2A-CAA-CBA-CGA
19	3	311	CLA	CAA-CBA-CGA-O2A
19	A	851	CLA	CAA-CBA-CGA-O1A
19	1	308	CLA	C6-C7-C8-C9
19	1	308	CLA	C11-C10-C8-C9
19	3	308	CLA	C11-C12-C13-C14
19	4	313	CLA	C14-C13-C15-C16
19	A	810	CLA	C14-C13-C15-C16
19	A	834	CLA	C11-C12-C13-C14
19	B	805	CLA	C14-C13-C15-C16
19	B	823	CLA	C14-C13-C15-C16
19	B	827	CLA	C11-C10-C8-C9
19	B	835	CLA	C14-C13-C15-C16
19	4	312	CLA	O1D-CGD-O2D-CED
19	B	835	CLA	C13-C15-C16-C17
18	2	301	CHL	C1A-C2A-CAA-CBA
18	2	306	CHL	C1A-C2A-CAA-CBA
19	2	304	CLA	C1-C2-C3-C4
19	A	810	CLA	C1-C2-C3-C4
19	B	820	CLA	C1-C2-C3-C4
19	A	854	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	C5-C6-C7-C8
19	F	304	CLA	C2A-CAA-CBA-CGA
19	4	308	CLA	C5-C6-C7-C8
19	3	304	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	B	819	CLA	C1A-C2A-CAA-CBA
19	B	822	CLA	C1A-C2A-CAA-CBA
19	L	302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	2	316	XAT	C12-C13-C14-C15
23	1	318	BCR	C11-C10-C9-C8
23	A	849	BCR	C11-C10-C9-C8
23	A	849	BCR	C16-C17-C18-C19
23	B	841	BCR	C11-C10-C9-C8
23	B	842	BCR	C11-C10-C9-C8
23	B	842	BCR	C20-C21-C22-C23
23	F	305	BCR	C12-C13-C14-C15
19	A	812	CLA	C16-C17-C18-C20
19	3	311	CLA	CAA-CBA-CGA-O1A
19	B	824	CLA	C5-C6-C7-C8
19	B	809	CLA	C13-C15-C16-C17
19	A	802	CLA	C2B-C3B-CAB-CBB
19	A	837	CLA	C2B-C3B-CAB-CBB
19	A	838	CLA	C2B-C3B-CAB-CBB
19	L	302	CLA	C2B-C3B-CAB-CBB
23	1	318	BCR	C23-C24-C25-C26
23	3	317	BCR	C23-C24-C25-C30
23	4	317	BCR	C23-C24-C25-C30
23	B	844	BCR	C23-C24-C25-C30
23	B	845	BCR	C1-C6-C7-C8
23	K	201	BCR	C1-C6-C7-C8
23	K	201	BCR	C23-C24-C25-C26
19	1	313	CLA	CAA-CBA-CGA-O1A
19	2	311	CLA	CAA-CBA-CGA-O1A
19	3	303	CLA	CAA-CBA-CGA-O1A
19	1	309	CLA	C11-C10-C8-C9
19	B	825	CLA	C15-C16-C17-C18
19	F	302	CLA	C13-C15-C16-C17
19	A	851	CLA	CAA-CBA-CGA-O2A
19	A	809	CLA	C4-C3-C5-C6
19	L	301	CLA	C4-C3-C5-C6
18	1	301	CHL	C2-C3-C5-C6
19	A	827	CLA	C11-C12-C13-C15
19	A	828	CLA	C11-C12-C13-C15
19	A	829	CLA	C11-C12-C13-C15
19	B	809	CLA	C12-C13-C15-C16
19	L	302	CLA	C12-C13-C15-C16
19	3	308	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	C16-C17-C18-C20
19	B	827	CLA	C16-C17-C18-C20
19	B	832	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	2	306	CHL	CAA-CBA-CGA-O2A
19	1	307	CLA	CAA-CBA-CGA-O2A
19	F	303	CLA	CAA-CBA-CGA-O2A
19	1	321	CLA	C15-C16-C17-C18
19	3	306	CLA	CAA-CBA-CGA-O2A
19	1	303	CLA	C5-C6-C7-C8
19	B	835	CLA	C10-C11-C12-C13
19	A	804	CLA	C2-C3-C5-C6
19	1	312	CLA	C1-C2-C3-C5
19	2	304	CLA	C1-C2-C3-C5
19	A	811	CLA	C2-C1-O2A-CGA
19	B	801	CLA	C1-C2-C3-C5
19	2	311	CLA	CAA-CBA-CGA-O2A
19	3	308	CLA	C16-C17-C18-C19
19	4	310	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	C6-C7-C8-C9
19	A	854	CLA	C11-C12-C13-C14
19	L	302	CLA	C6-C7-C8-C9
19	A	836	CLA	C8-C10-C11-C12
19	A	824	CLA	C4-C3-C5-C6
19	F	302	CLA	C4-C3-C5-C6
19	3	301	CLA	C8-C10-C11-C12
19	2	302	CLA	C2-C3-C5-C6
19	B	835	CLA	C2-C3-C5-C6
19	B	833	CLA	CAA-CBA-CGA-O2A
19	3	309	CLA	O1A-CGA-O2A-C1
25	2	318	LMT	C4-C5-C6-C7
19	4	307	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	C2A-CAA-CBA-CGA
19	A	818	CLA	C2A-CAA-CBA-CGA
18	4	304	CHL	O1A-CGA-O2A-C1
19	1	311	CLA	CAA-CBA-CGA-O2A
19	A	817	CLA	CAA-CBA-CGA-O2A
19	F	302	CLA	C5-C6-C7-C8
19	1	309	CLA	C4B-C3B-CAB-CBB
19	A	837	CLA	C4B-C3B-CAB-CBB
19	3	313	CLA	CAA-CBA-CGA-O2A
18	2	307	CHL	CHA-CBD-CGD-O2D
18	2	314	CHL	CHA-CBD-CGD-O1D
19	B	806	CLA	C3-C5-C6-C7
18	2	306	CHL	CAA-CBA-CGA-O1A
19	3	306	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	2	304	CLA	C15-C16-C17-C18
19	A	852	CLA	C16-C17-C18-C19
19	3	303	CLA	CAA-CBA-CGA-O2A
19	1	312	CLA	C6-C7-C8-C10
19	A	807	CLA	C6-C7-C8-C10
19	A	827	CLA	C12-C13-C15-C16
19	B	807	CLA	C12-C13-C15-C16
19	B	838	CLA	C11-C12-C13-C15
19	L	302	CLA	C6-C7-C8-C10
19	B	803	CLA	CAA-CBA-CGA-O2A
19	A	805	CLA	C11-C10-C8-C9
19	A	828	CLA	C6-C7-C8-C9
19	B	837	CLA	C11-C12-C13-C14
19	A	852	CLA	C2A-CAA-CBA-CGA
19	B	812	CLA	C2A-CAA-CBA-CGA
19	3	308	CLA	C2-C1-O2A-CGA
19	A	812	CLA	C2-C1-O2A-CGA
19	A	826	CLA	C2-C1-O2A-CGA
19	A	837	CLA	C2-C1-O2A-CGA
19	A	852	CLA	C2-C1-O2A-CGA
19	B	811	CLA	C2-C1-O2A-CGA
19	B	828	CLA	C2-C1-O2A-CGA
19	L	303	CLA	C2-C1-O2A-CGA
22	1	322	LHG	C27-C28-C29-C30
19	B	832	CLA	C16-C17-C18-C20
19	1	304	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	C3A-C2A-CAA-CBA
19	B	814	CLA	C3A-C2A-CAA-CBA
19	B	838	CLA	C3A-C2A-CAA-CBA
19	B	806	CLA	C5-C6-C7-C8
19	A	839	CLA	O2A-C1-C2-C3
19	B	820	CLA	O2A-C1-C2-C3
19	B	831	CLA	O2A-C1-C2-C3
19	3	308	CLA	C16-C17-C18-C20
19	3	309	CLA	C4C-C3C-CAC-CBC
19	B	825	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C4-C3-C5-C6
19	A	805	CLA	C4-C3-C5-C6
19	A	831	CLA	C15-C16-C17-C18
19	4	310	CLA	CAA-CBA-CGA-O1A
19	4	310	CLA	O1D-CGD-O2D-CED
22	1	317	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
22	A	842	LHG	C4-C5-C6-O8
19	3	303	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	C2-C3-C5-C6
19	A	840	CLA	C2-C3-C5-C6
19	A	853	CLA	C11-C12-C13-C14
19	2	313	CLA	C5-C6-C7-C8
19	F	303	CLA	CAA-CBA-CGA-O1A
19	1	311	CLA	CAA-CBA-CGA-O1A
19	A	804	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C12-C13-C14
19	A	810	CLA	C11-C12-C13-C14
19	B	813	CLA	C6-C7-C8-C9
19	1	303	CLA	CAA-CBA-CGA-O2A
19	4	301	CLA	O1D-CGD-O2D-CED
19	A	807	CLA	CAA-CBA-CGA-O2A
18	2	301	CHL	C2A-CAA-CBA-CGA
19	2	302	CLA	C12-C13-C15-C16
19	3	308	CLA	C11-C10-C8-C7
19	3	308	CLA	C11-C12-C13-C15
19	4	313	CLA	C12-C13-C15-C16
19	A	805	CLA	C11-C10-C8-C7
19	A	826	CLA	C12-C13-C15-C16
19	A	828	CLA	C6-C7-C8-C10
19	A	840	CLA	C6-C7-C8-C10
19	A	840	CLA	C11-C12-C13-C15
19	B	805	CLA	C12-C13-C15-C16
19	B	838	CLA	C11-C10-C8-C7
26	B	839	PQN	C21-C22-C23-C25
19	1	309	CLA	C2B-C3B-CAB-CBB
23	3	317	BCR	C23-C24-C25-C26
23	4	317	BCR	C23-C24-C25-C26
23	B	844	BCR	C23-C24-C25-C26
23	B	845	BCR	C5-C6-C7-C8
23	G	205	BCR	C1-C6-C7-C8
23	K	201	BCR	C5-C6-C7-C8
19	B	823	CLA	CBD-CGD-O2D-CED
19	2	309	CLA	C2-C1-O2A-CGA
19	3	312	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA
19	A	806	CLA	C2-C1-O2A-CGA
19	A	810	CLA	C2-C1-O2A-CGA
19	3	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	827	CLA	C2A-CAA-CBA-CGA
19	4	302	CLA	CAA-CBA-CGA-O2A
19	A	835	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
19	A	804	CLA	CAA-CBA-CGA-O1A
19	2	312	CLA	C4-C3-C5-C6
22	B	848	LHG	C15-C16-C17-C18
19	A	816	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	CAA-CBA-CGA-O2A
24	4	318	LMG	O7-C10-C11-C12
19	4	308	CLA	C2-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	F	303	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	C16-C17-C18-C19
19	G	204	CLA	C2A-CAA-CBA-CGA
19	B	833	CLA	CAA-CBA-CGA-O1A
19	2	312	CLA	C6-C7-C8-C9
19	B	817	CLA	C11-C10-C8-C9
22	2	317	LHG	C4-C5-C6-O8
19	A	813	CLA	C4B-C3B-CAB-CBB
19	B	838	CLA	C1A-C2A-CAA-CBA
19	L	303	CLA	C4B-C3B-CAB-CBB
18	4	304	CHL	C4-C3-C5-C6
18	1	301	CHL	CAA-CBA-CGA-O2A
19	2	309	CLA	CAA-CBA-CGA-O2A
19	A	853	CLA	CAA-CBA-CGA-O2A
22	1	322	LHG	O8-C23-C24-C25
19	A	811	CLA	C2-C3-C5-C6
24	F	307	LMG	O1-C7-C8-O7
23	L	305	BCR	C17-C18-C19-C20
19	A	822	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
19	B	823	CLA	CAA-CBA-CGA-O2A
19	A	815	CLA	CAA-CBA-CGA-O2A
19	B	802	CLA	CAA-CBA-CGA-O2A
19	A	801	CLA	C5-C6-C7-C8
19	1	321	CLA	C4-C3-C5-C6
19	1	304	CLA	C2-C1-O2A-CGA
19	A	822	CLA	C2-C1-O2A-CGA
19	A	836	CLA	C2-C1-O2A-CGA
19	2	312	CLA	C6-C7-C8-C10
19	4	308	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C11-C10-C8-C7
19	B	804	CLA	C12-C13-C15-C16
19	B	813	CLA	C6-C7-C8-C10
19	B	828	CLA	C11-C12-C13-C15
19	B	837	CLA	C11-C12-C13-C15
19	A	828	CLA	C8-C10-C11-C12
19	A	827	CLA	C16-C17-C18-C19
18	2	301	CHL	O2A-C1-C2-C3
19	A	837	CLA	O2A-C1-C2-C3
22	A	842	LHG	O7-C7-C8-C9
19	A	807	CLA	C10-C11-C12-C13
19	F	302	CLA	C3-C5-C6-C7
19	A	835	CLA	CAA-CBA-CGA-O1A
19	A	835	CLA	C2A-CAA-CBA-CGA
19	B	830	CLA	C2A-CAA-CBA-CGA
19	1	302	CLA	O1D-CGD-O2D-CED
25	2	318	LMT	C5-C6-C7-C8
19	A	820	CLA	C8-C10-C11-C12
19	B	838	CLA	C15-C16-C17-C18
19	2	309	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CAA-CBA-CGA-O1A
19	L	303	CLA	CAA-CBA-CGA-O1A
18	4	305	CHL	CAA-CBA-CGA-O2A
19	2	308	CLA	CAA-CBA-CGA-O2A
24	1	319	LMG	C29-C30-C31-C32
19	B	823	CLA	CAA-CBA-CGA-O1A
19	A	808	CLA	CAA-CBA-CGA-O1A
18	4	306	CHL	C1-C2-C3-C5
28	B	846	DGD	C2B-C3B-C4B-C5B
19	B	818	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	C11-C12-C13-C14
19	A	840	CLA	C14-C13-C15-C16
19	B	838	CLA	C11-C12-C13-C14
19	L	302	CLA	C14-C13-C15-C16
22	1	317	LHG	C27-C28-C29-C30
19	A	853	CLA	C3-C5-C6-C7
19	A	840	CLA	C8-C10-C11-C12
19	B	805	CLA	C8-C10-C11-C12
19	A	836	CLA	C4-C3-C5-C6
19	B	820	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	840	CLA	C13-C15-C16-C17
19	A	807	CLA	CAA-CBA-CGA-O1A
24	4	318	LMG	O9-C10-C11-C12
24	1	319	LMG	C8-C7-O1-C1
19	3	313	CLA	CAA-CBA-CGA-O1A
19	B	827	CLA	CAA-CBA-CGA-O1A
22	1	322	LHG	O10-C23-C24-C25
19	2	303	CLA	C2A-CAA-CBA-CGA
19	2	311	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	C2A-CAA-CBA-CGA
19	B	827	CLA	C16-C17-C18-C19
19	1	303	CLA	CAA-CBA-CGA-O1A
28	B	846	DGD	C5A-C6A-C7A-C8A
18	2	301	CHL	CAA-CBA-CGA-O2A
19	A	808	CLA	CAA-CBA-CGA-O2A
19	F	301	CLA	CAA-CBA-CGA-O1A
19	A	829	CLA	C16-C17-C18-C20
19	2	311	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	H	201	CLA	CAD-CBD-CGD-O2D
19	L	303	CLA	CAA-CBA-CGA-O2A
19	A	804	CLA	C13-C15-C16-C17
19	B	802	CLA	C2-C1-O2A-CGA
19	A	807	CLA	C1-C2-C3-C4
19	A	827	CLA	C1-C2-C3-C4
19	B	817	CLA	C1-C2-C3-C4
19	B	830	CLA	C1-C2-C3-C4
19	2	302	CLA	C2A-CAA-CBA-CGA
22	B	848	LHG	C27-C28-C29-C30
19	4	313	CLA	CAA-CBA-CGA-O1A
19	1	312	CLA	C10-C11-C12-C13
19	2	312	CLA	C15-C16-C17-C18
19	B	824	CLA	C11-C10-C8-C7
19	2	302	CLA	CAA-CBA-CGA-O2A
19	B	809	CLA	CAA-CBA-CGA-O2A
19	H	201	CLA	CAA-CBA-CGA-O2A
19	B	823	CLA	C10-C11-C12-C13
19	1	314	CLA	CAA-CBA-CGA-O1A
19	A	826	CLA	C16-C17-C18-C19
19	4	301	CLA	CAA-CBA-CGA-O1A
19	4	313	CLA	CAA-CBA-CGA-O2A
19	B	827	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	K	203	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	CAA-CBA-CGA-O1A
24	4	318	LMG	C29-C30-C31-C32

There are no ring outliers.

156 monomers are involved in 290 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	812	CLA	4	0
23	A	843	BCR	5	0
19	2	312	CLA	1	0
22	B	848	LHG	3	0
28	B	846	DGD	4	0
23	1	318	BCR	2	0
23	B	840	BCR	3	0
23	A	847	BCR	4	0
19	3	302	CLA	2	0
24	1	319	LMG	3	0
23	2	319	BCR	3	0
20	2	315	LUT	3	0
19	1	312	CLA	5	0
23	4	317	BCR	2	0
19	H	201	CLA	2	0
19	B	805	CLA	4	0
19	2	313	CLA	1	0
19	B	801	CLA	1	0
23	B	844	BCR	2	0
19	B	808	CLA	1	0
19	A	808	CLA	3	0
23	J	103	BCR	3	0
18	1	301	CHL	1	0
19	A	804	CLA	5	0
19	B	815	CLA	1	0
19	B	811	CLA	5	0
22	1	322	LHG	4	0
20	1	315	LUT	3	0
19	B	819	CLA	1	0
24	F	307	LMG	1	0
19	B	813	CLA	7	0
19	B	807	CLA	1	0
19	A	854	CLA	2	0
19	A	807	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	309	CLA	2	0
21	2	316	XAT	2	0
18	4	306	CHL	2	0
21	3	316	XAT	1	0
20	4	315	LUT	5	0
19	A	840	CLA	1	0
19	B	837	CLA	2	0
19	F	304	CLA	1	0
19	G	203	CLA	1	0
21	4	316	XAT	2	0
19	A	824	CLA	3	0
19	4	313	CLA	4	0
19	4	301	CLA	3	0
19	A	817	CLA	3	0
19	3	308	CLA	4	0
19	2	320	CLA	2	0
18	2	301	CHL	2	0
19	A	829	CLA	2	0
19	A	826	CLA	4	0
19	K	202	CLA	2	0
19	A	821	CLA	1	0
19	B	812	CLA	1	0
23	K	201	BCR	2	0
23	L	306	BCR	2	0
20	3	315	LUT	2	0
19	B	832	CLA	1	0
23	A	844	BCR	9	0
19	B	831	CLA	3	0
23	B	842	BCR	4	0
19	F	303	CLA	1	0
19	2	309	CLA	3	0
19	A	839	CLA	1	0
19	1	311	CLA	1	0
19	B	804	CLA	1	0
19	A	814	CLA	2	0
18	4	304	CHL	1	0
19	4	302	CLA	2	0
19	A	809	CLA	2	0
19	3	306	CLA	1	0
19	A	825	CLA	2	0
19	A	806	CLA	1	0
19	B	828	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	833	CLA	2	0
19	B	835	CLA	1	0
19	B	827	CLA	2	0
23	I	101	BCR	1	0
25	2	318	LMT	5	0
18	3	307	CHL	2	0
19	A	831	CLA	1	0
19	B	822	CLA	4	0
23	B	841	BCR	1	0
19	A	818	CLA	2	0
19	1	305	CLA	2	0
19	B	825	CLA	2	0
23	3	317	BCR	1	0
19	A	811	CLA	1	0
19	B	830	CLA	2	0
19	1	302	CLA	1	0
19	A	836	CLA	3	0
19	2	304	CLA	2	0
21	1	316	XAT	1	0
24	B	847	LMG	1	0
19	A	801	CLA	4	0
23	L	305	BCR	6	0
23	A	845	BCR	2	0
19	J	102	CLA	1	0
19	L	301	CLA	1	0
23	J	104	BCR	3	0
19	A	827	CLA	2	0
19	B	810	CLA	1	0
19	K	203	CLA	1	0
19	B	833	CLA	1	0
19	A	810	CLA	3	0
19	4	308	CLA	1	0
23	J	101	BCR	6	0
19	B	821	CLA	1	0
20	1	320	LUT	5	0
26	B	839	PQN	1	0
23	F	305	BCR	3	0
23	A	848	BCR	3	0
19	A	822	CLA	1	0
19	B	806	CLA	2	0
23	G	205	BCR	2	0
23	F	306	BCR	3	0

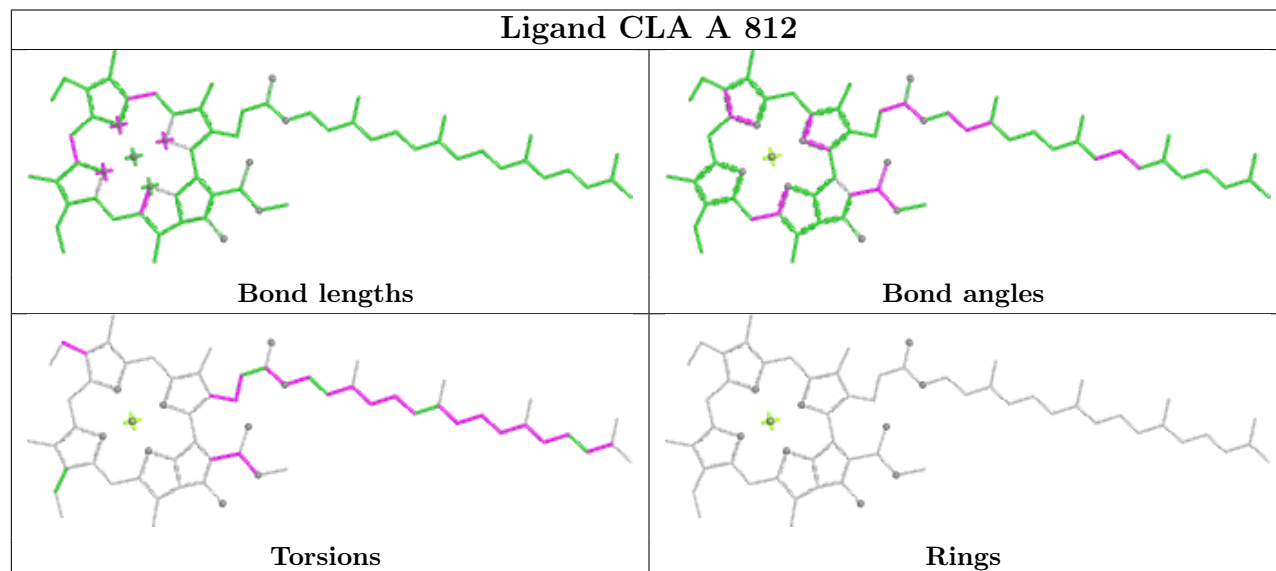
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	307	CHL	1	0
19	A	832	CLA	4	0
19	B	809	CLA	1	0
19	B	816	CLA	3	0
18	1	306	CHL	2	0
22	1	317	LHG	2	0
19	A	852	CLA	2	0
19	3	304	CLA	1	0
22	2	317	LHG	1	0
19	A	834	CLA	4	0
19	A	851	CLA	1	0
19	B	826	CLA	2	0
23	L	304	BCR	2	0
19	1	308	CLA	3	0
19	A	837	CLA	1	0
18	4	305	CHL	1	0
19	A	805	CLA	1	0
19	B	838	CLA	1	0
23	A	849	BCR	1	0
19	F	302	CLA	2	0
19	4	311	CLA	3	0
19	1	321	CLA	2	0
19	1	309	CLA	2	0
23	A	846	BCR	3	0
19	L	303	CLA	1	0
19	1	313	CLA	1	0
19	2	310	CLA	1	0
19	B	818	CLA	3	0
19	L	302	CLA	5	0
23	B	843	BCR	1	0
19	2	303	CLA	2	0
19	A	828	CLA	1	0
25	N	201	LMT	2	0
19	B	823	CLA	2	0
19	A	813	CLA	1	0
19	A	823	CLA	3	0
19	K	204	CLA	1	0
19	A	853	CLA	3	0

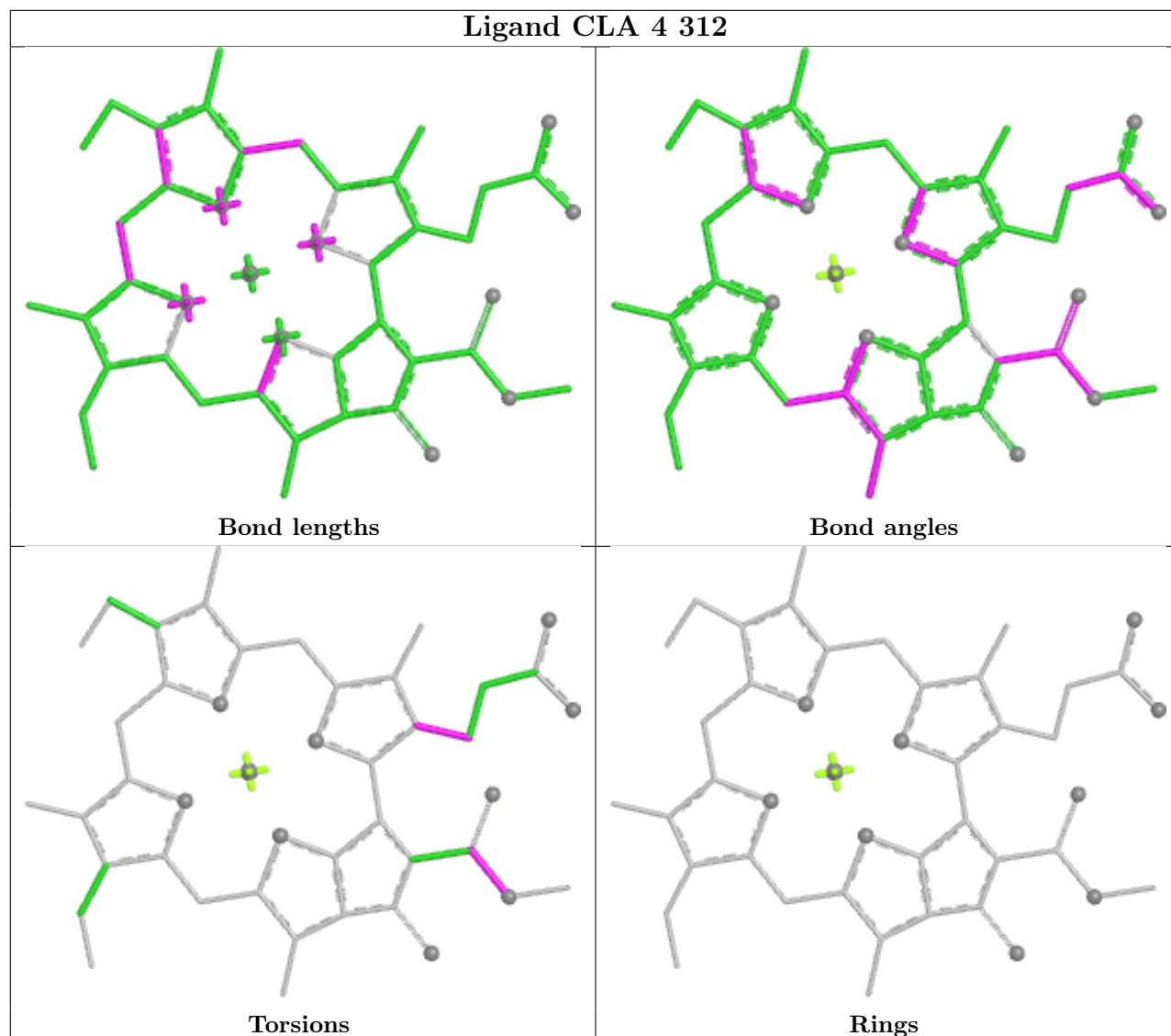
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

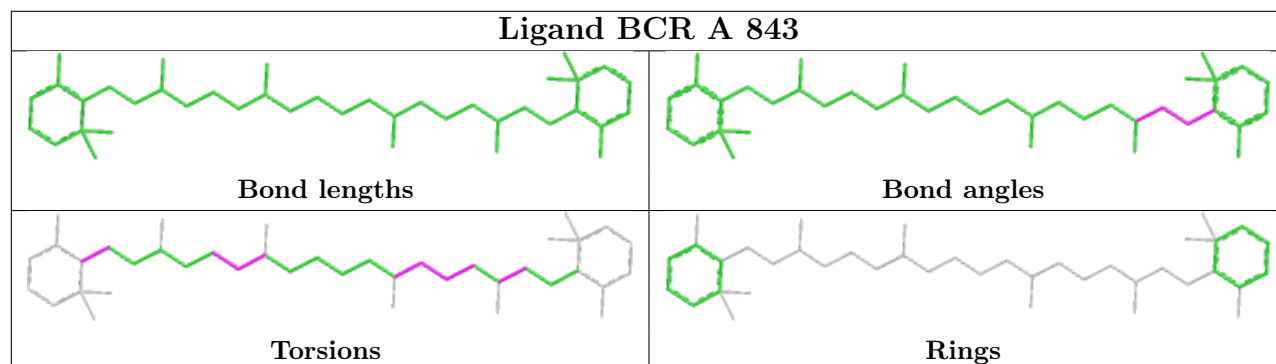




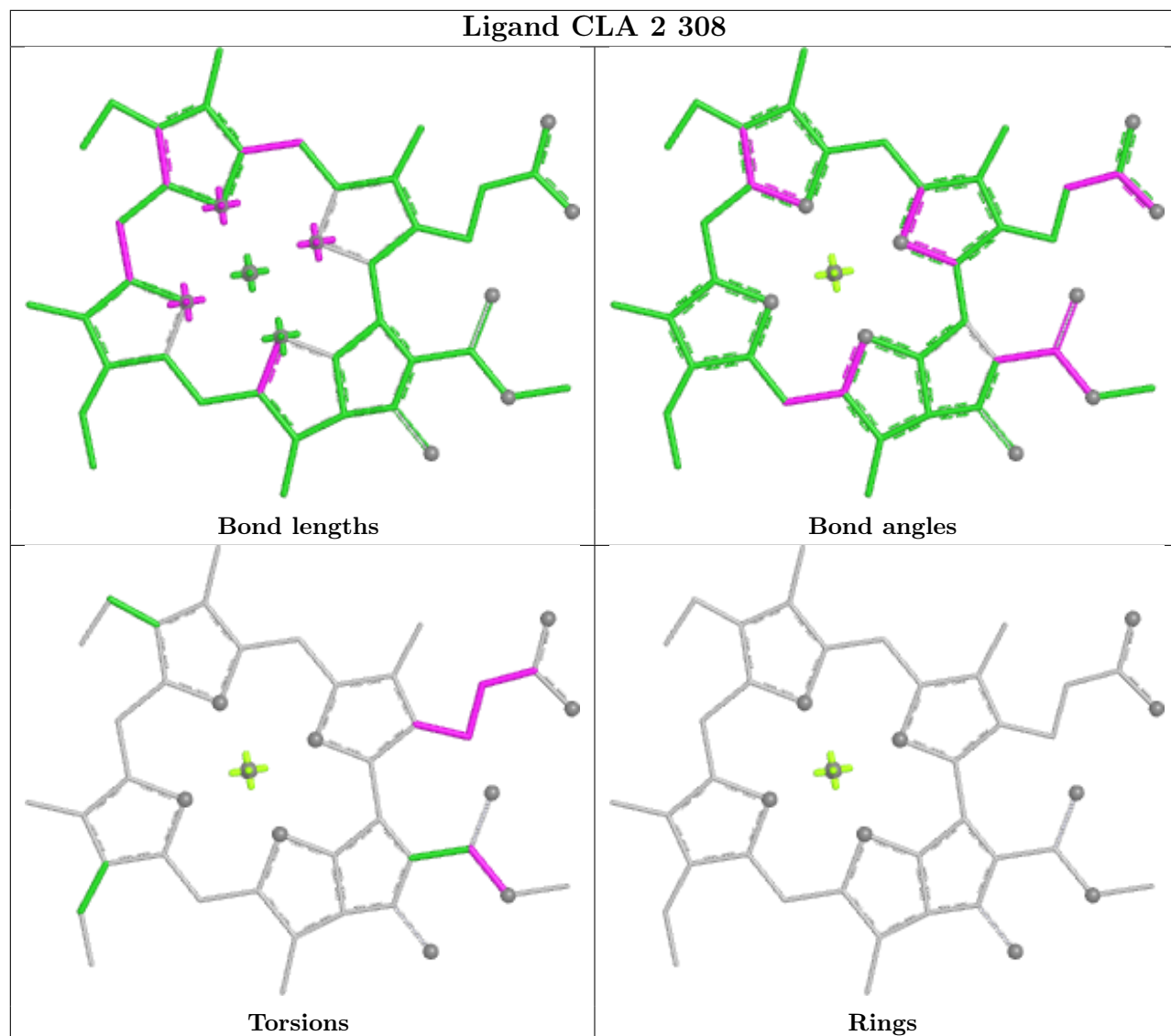
## Ligand CLA 4 312



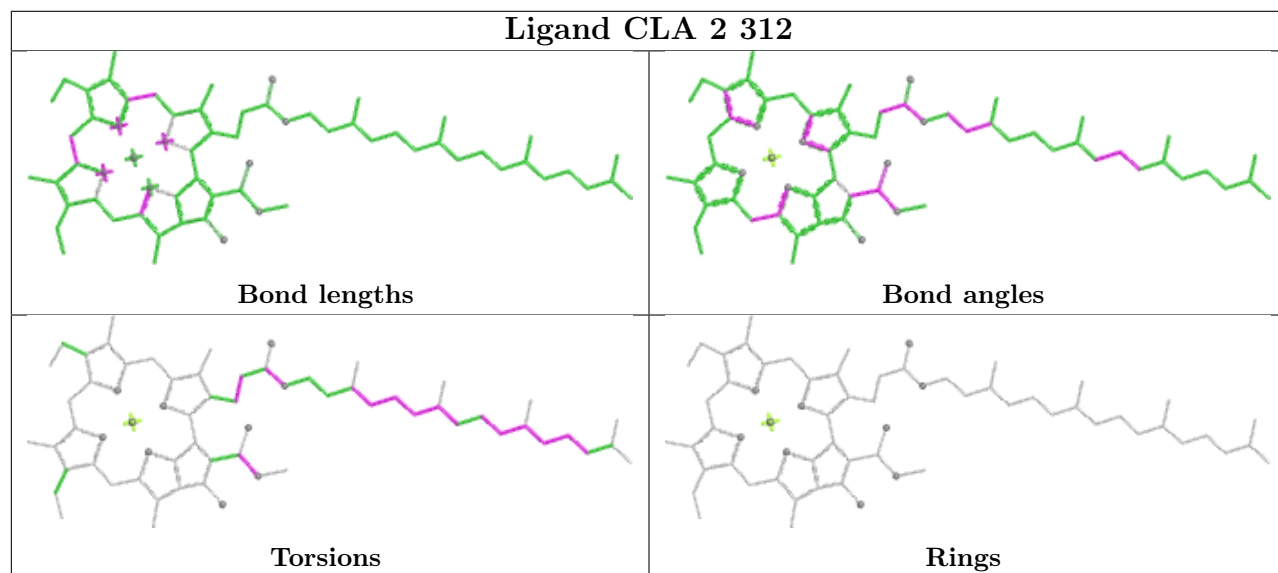
## Ligand BCR A 843

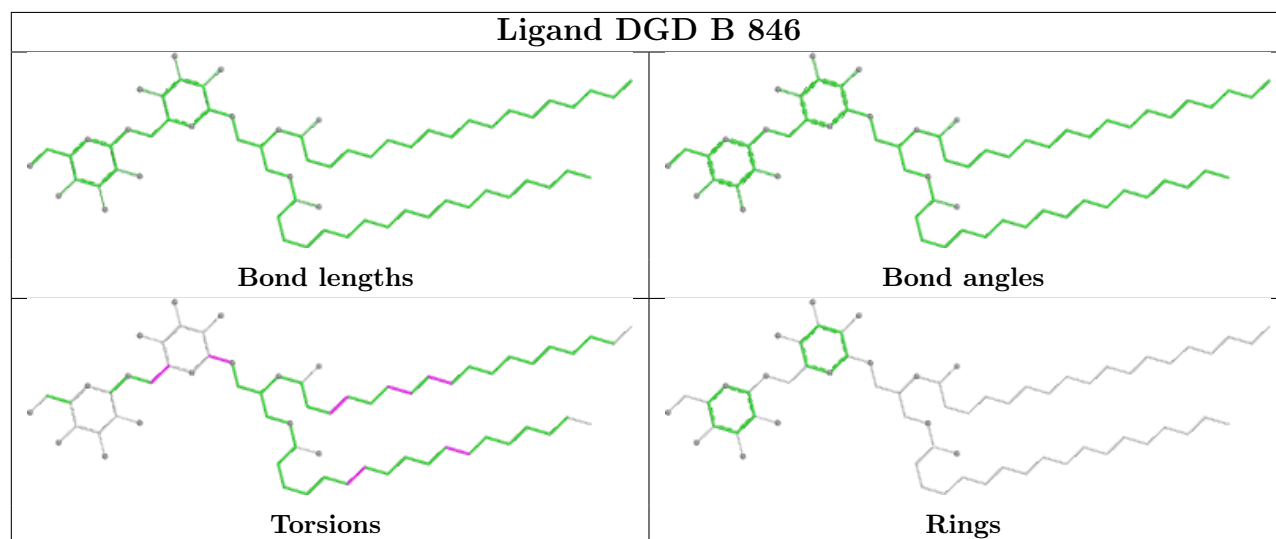
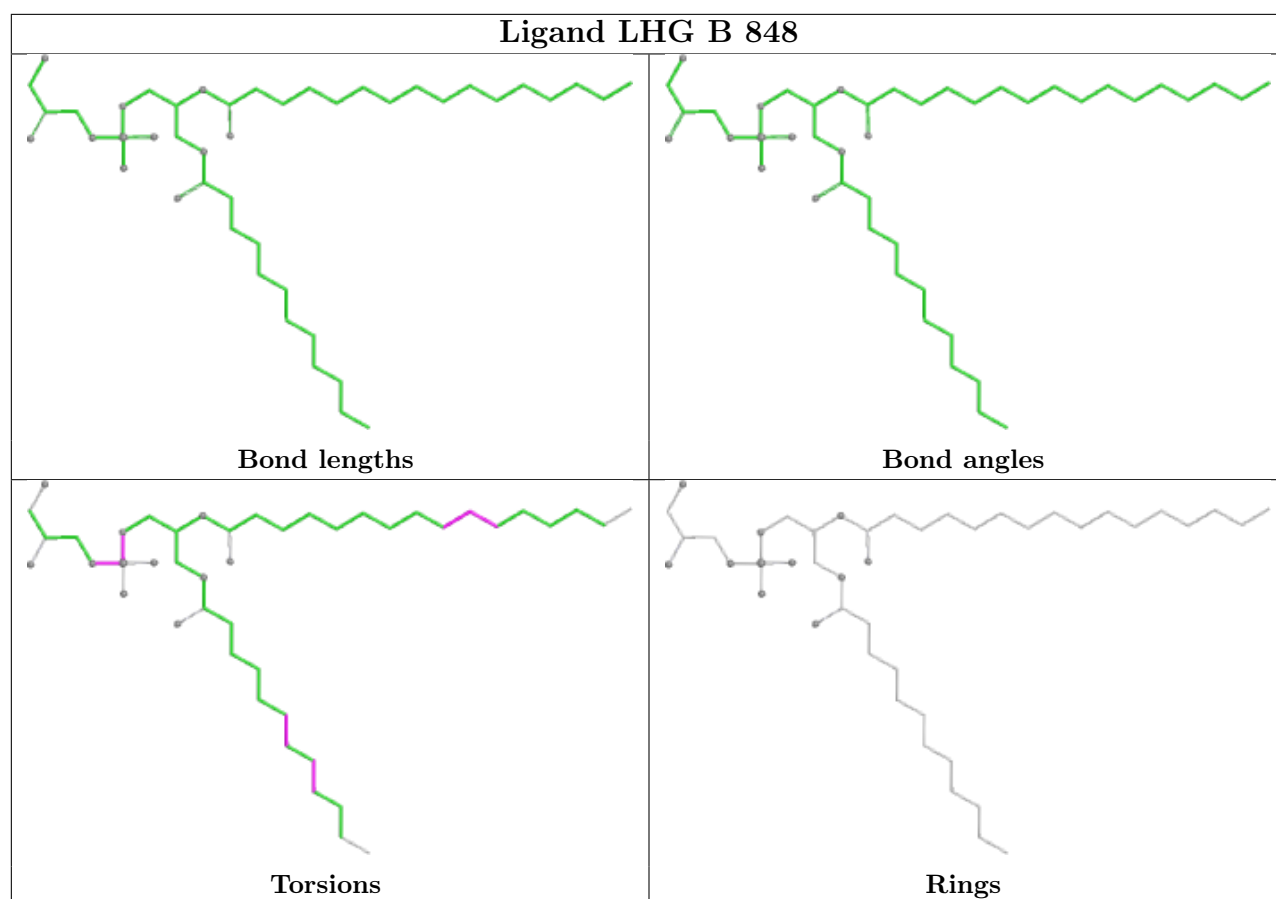


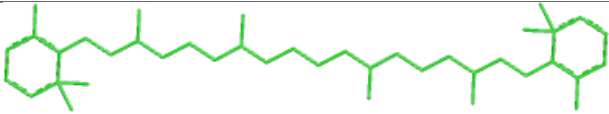
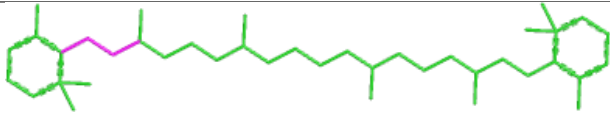
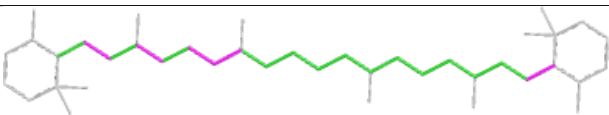
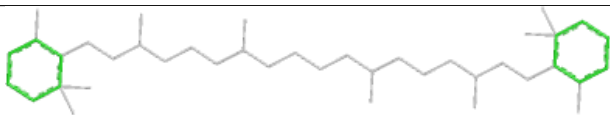
## Ligand CLA 2 308



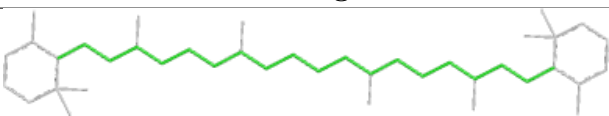
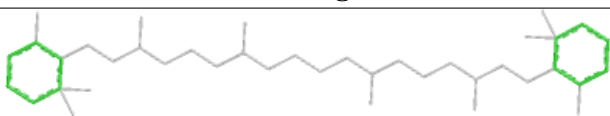


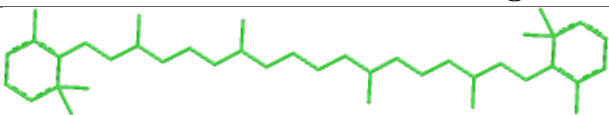
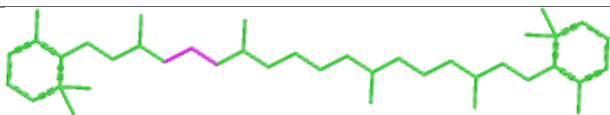
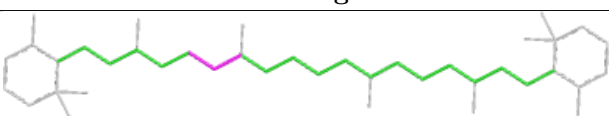
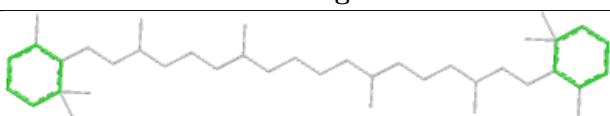
## Ligand CLA 2 312



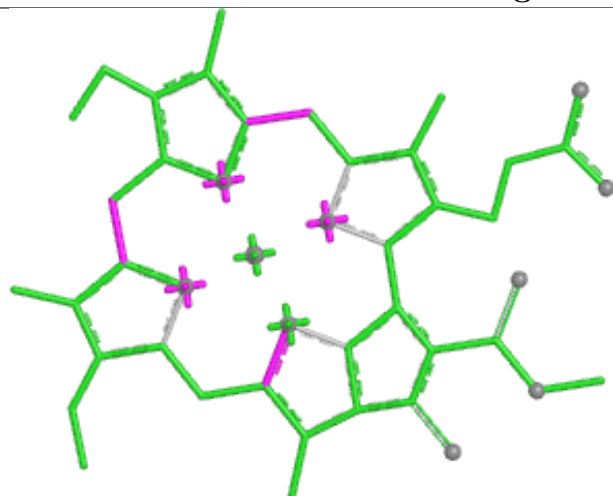


Ligand BCR 1 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

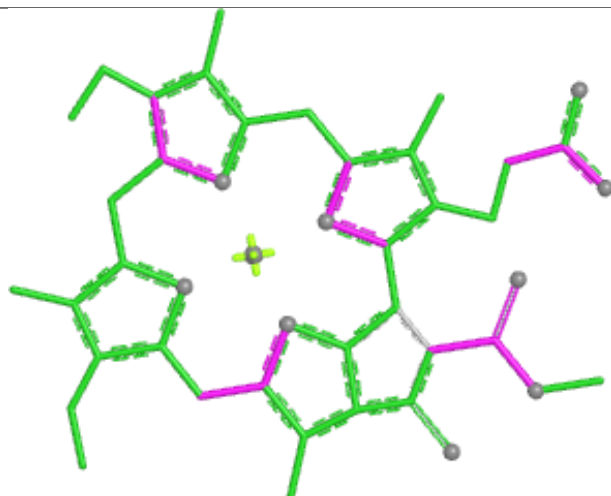
Ligand BCR B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

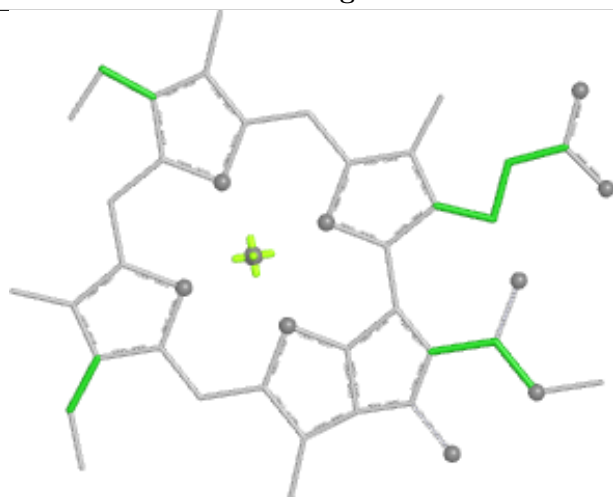
## Ligand CLA A 819



Bond lengths



Bond angles

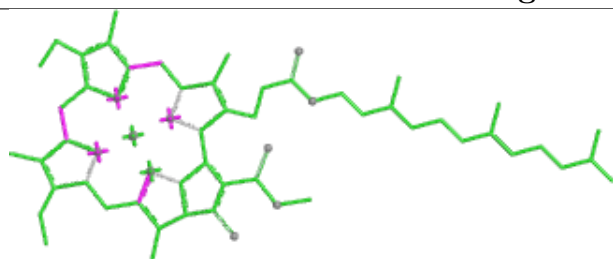


Torsions

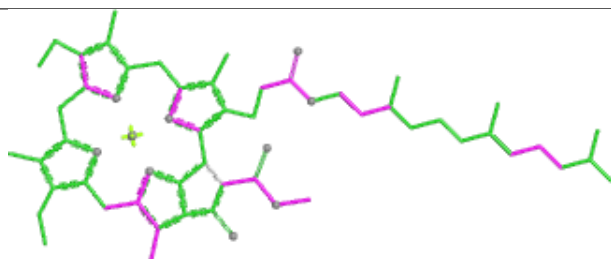


Rings

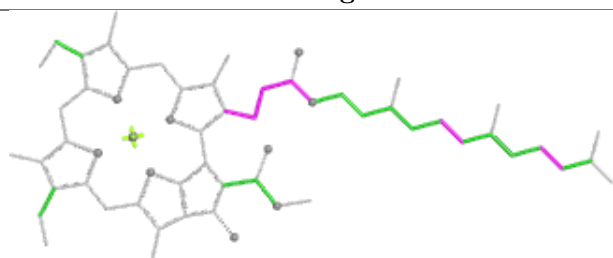
## Ligand CLA 3 302



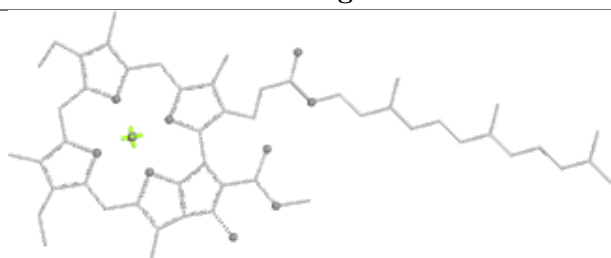
Bond lengths



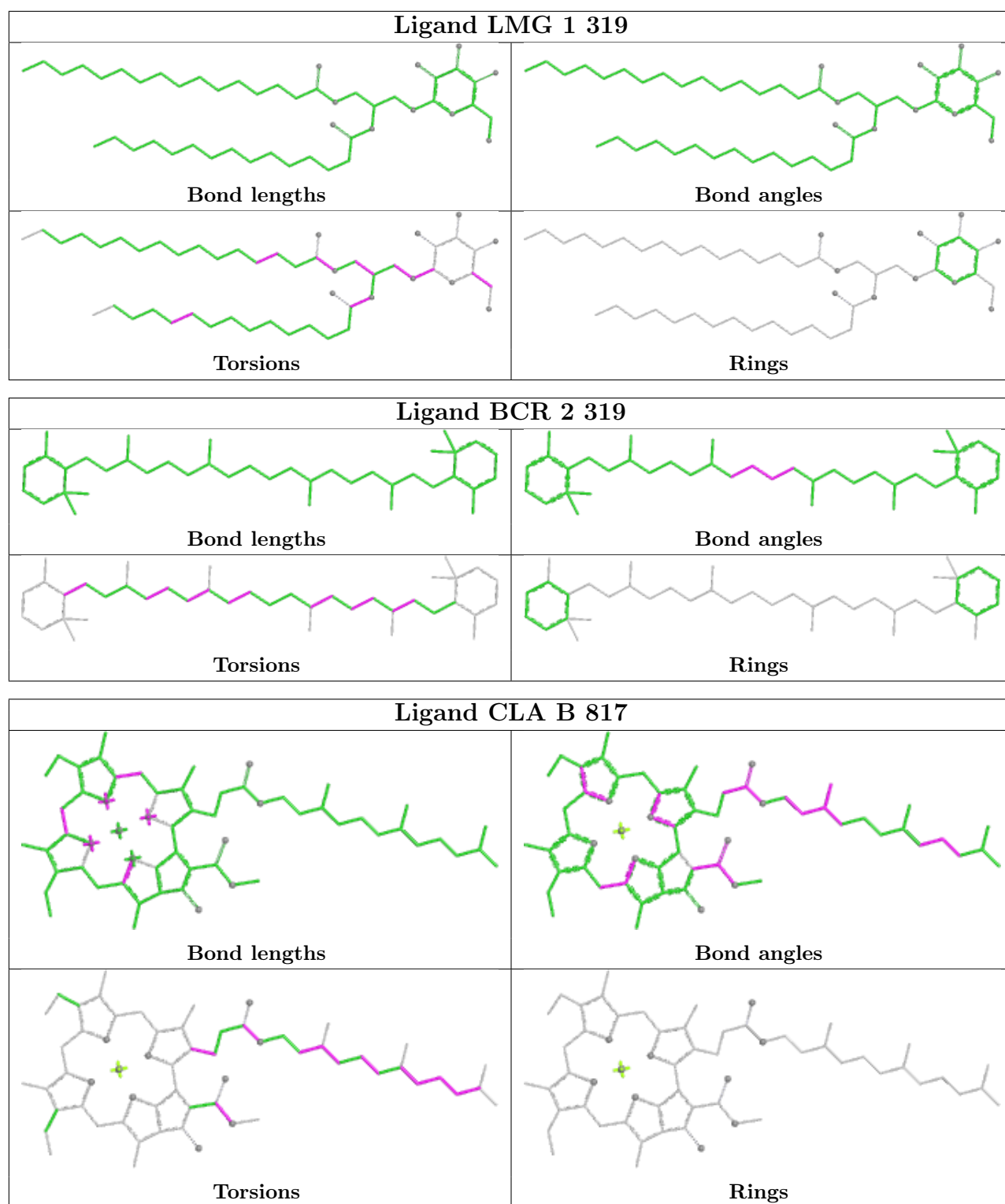
Bond angles

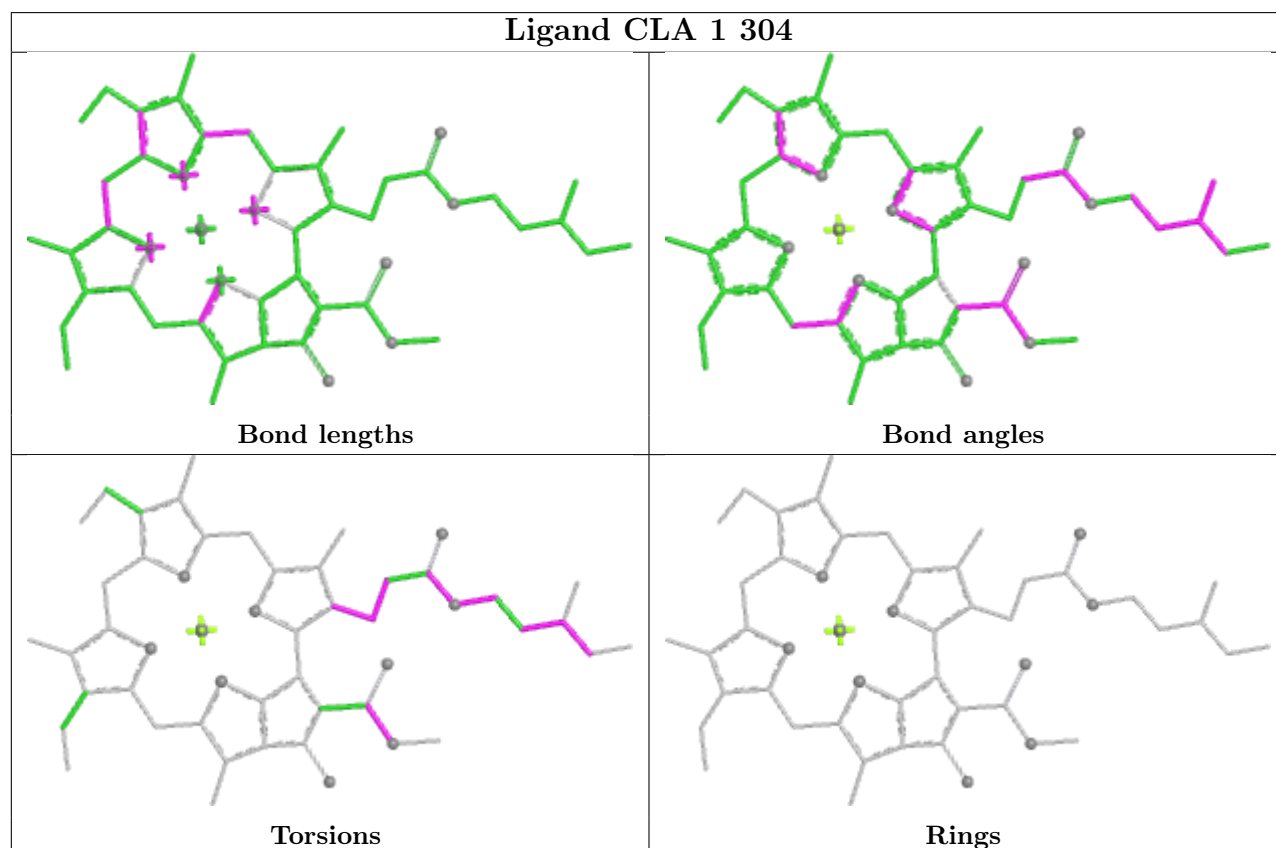
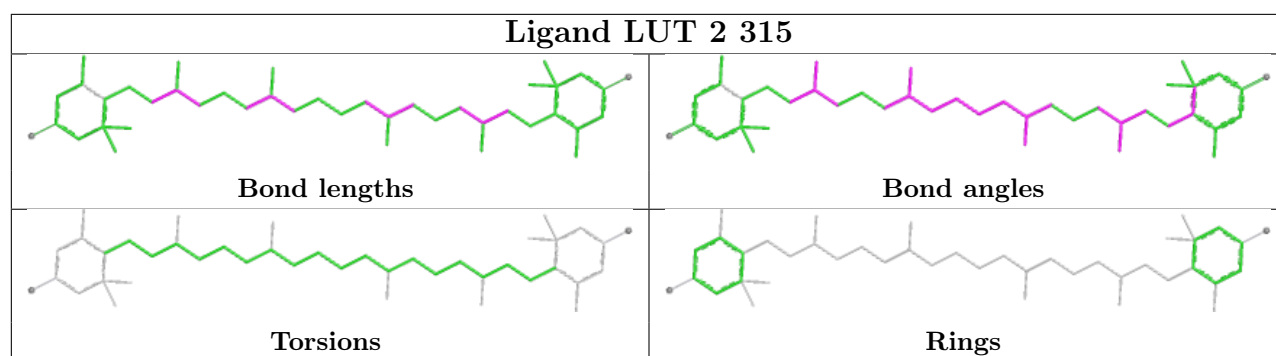


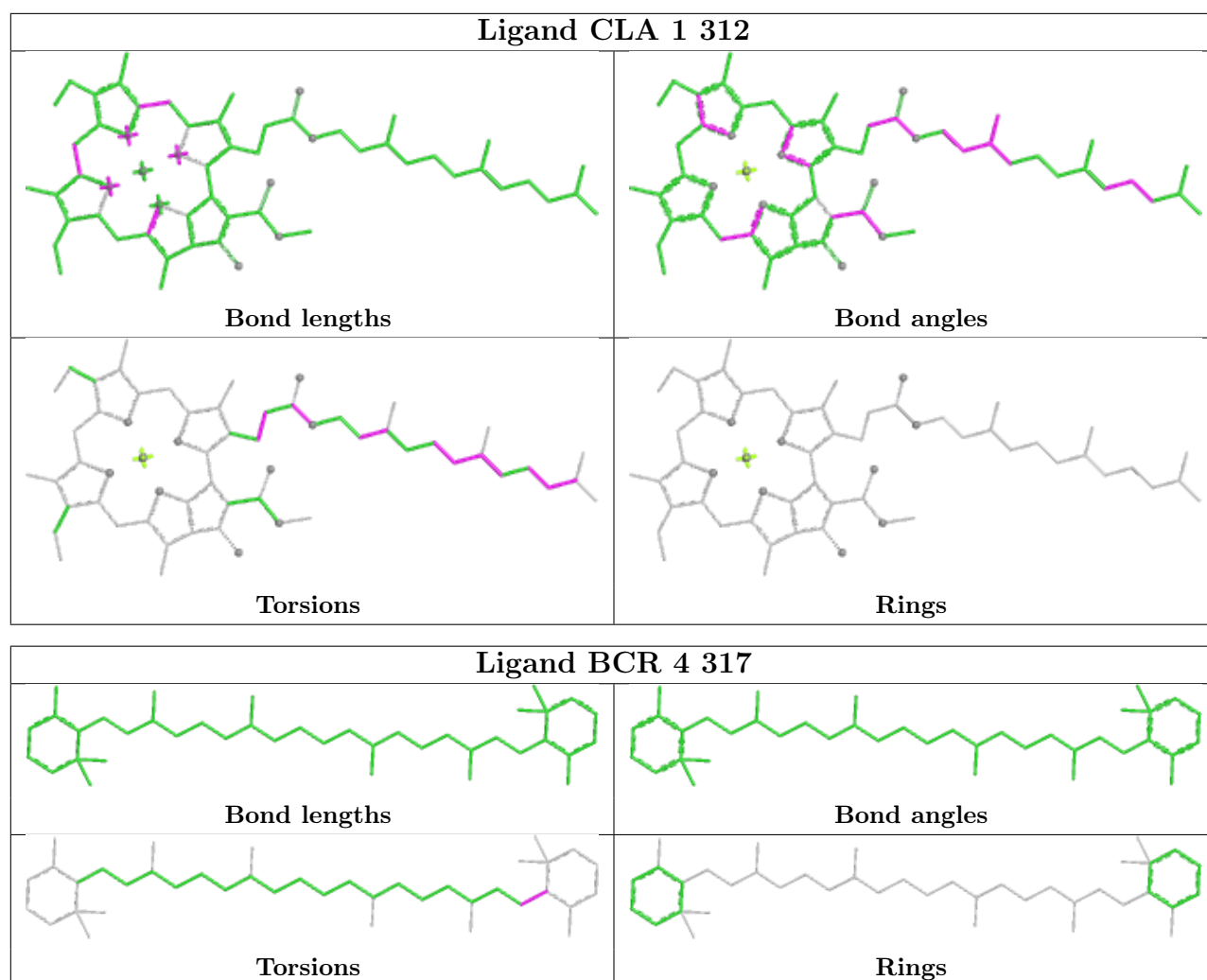
Torsions



Rings

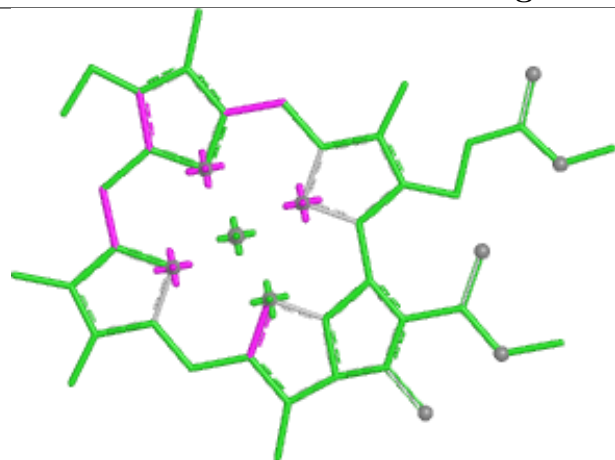




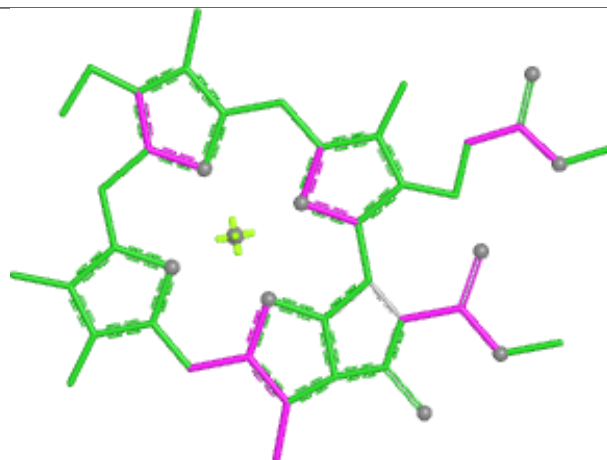




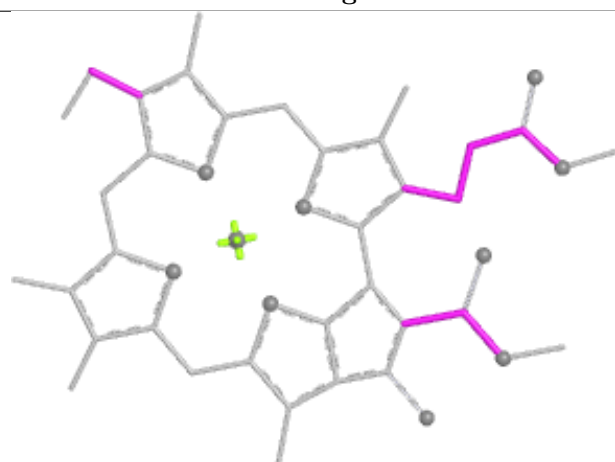
## Ligand CLA H 201



Bond lengths



Bond angles

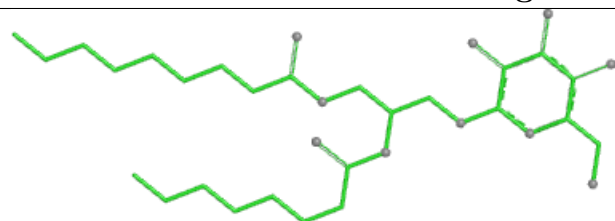


Torsions

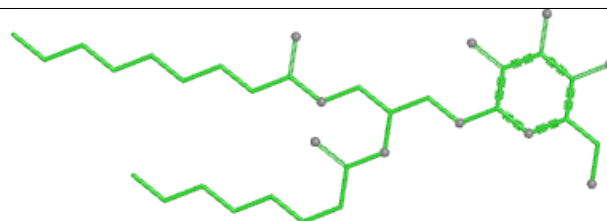


Rings

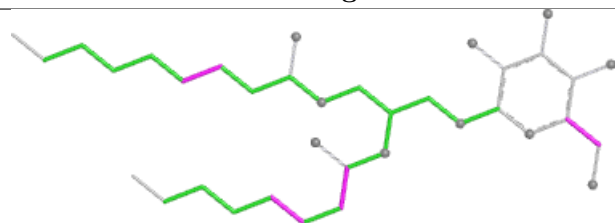
## Ligand LMG 4 318



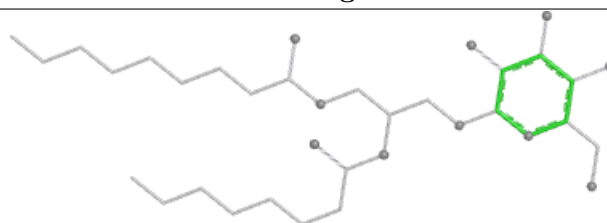
Bond lengths



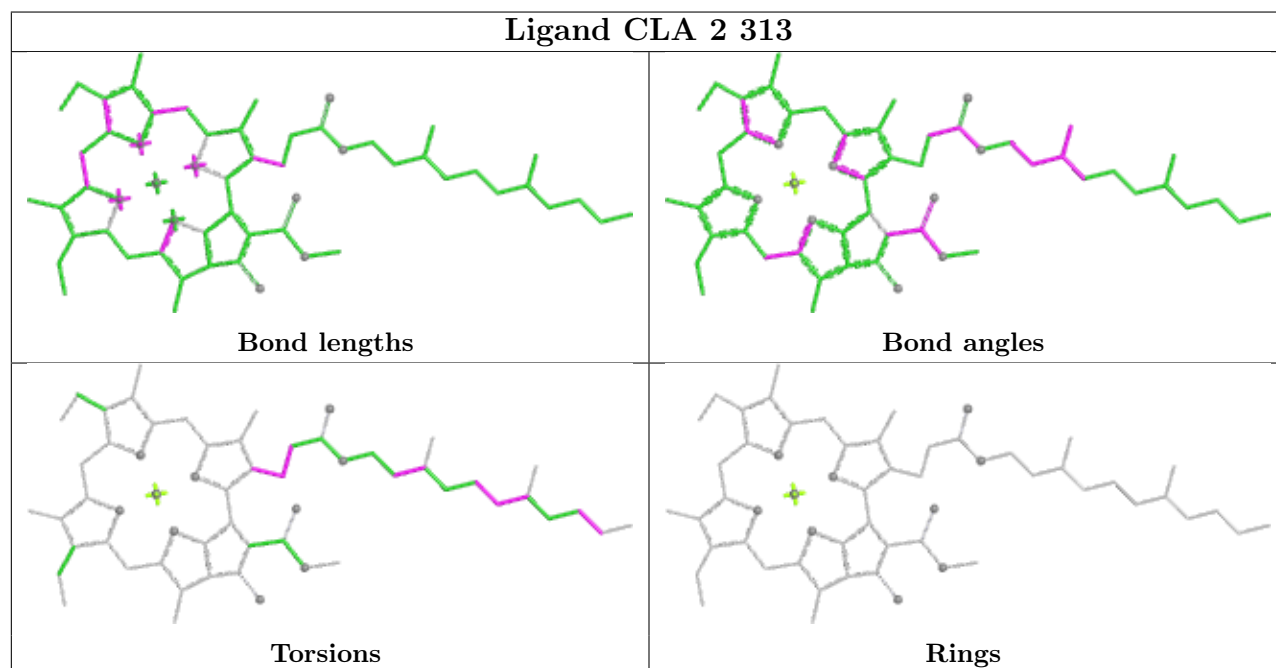
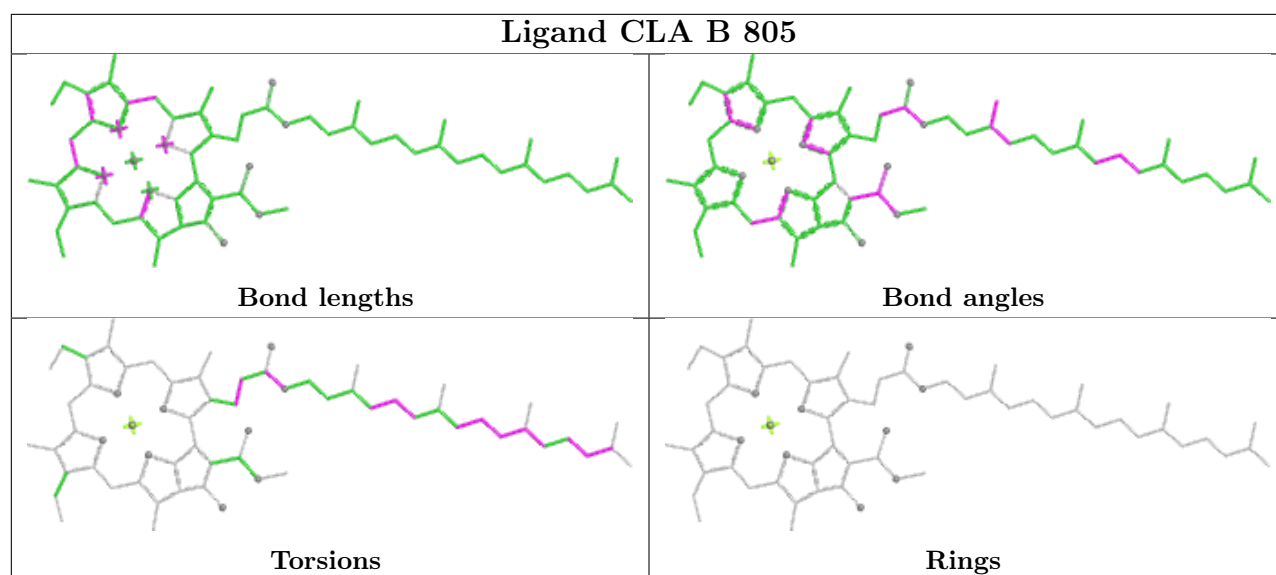
Bond angles

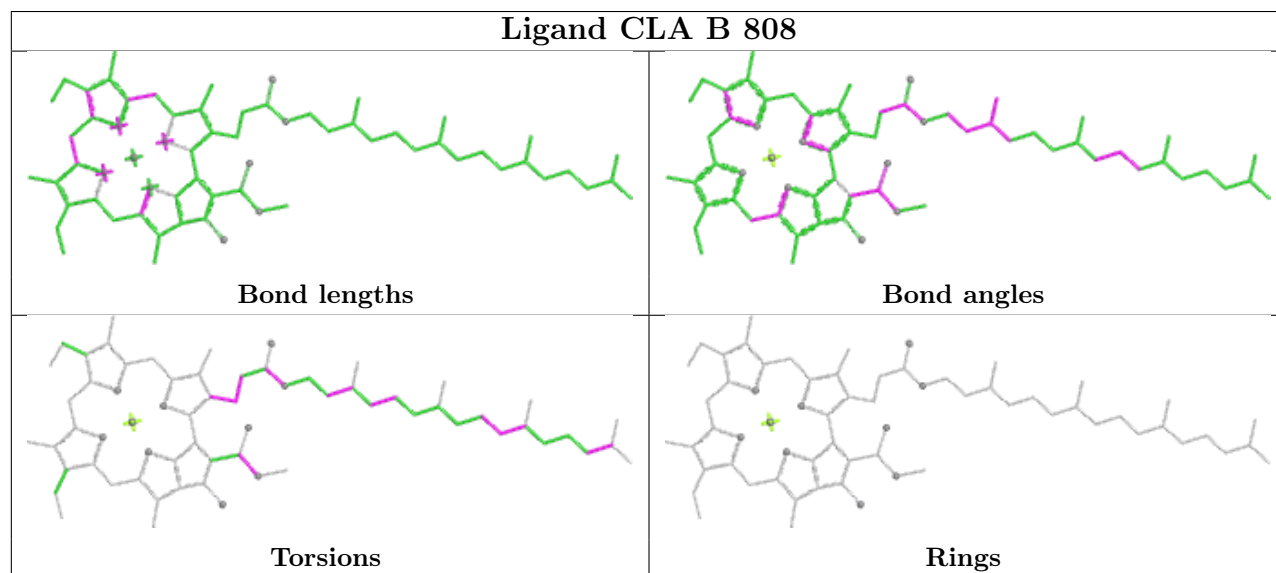
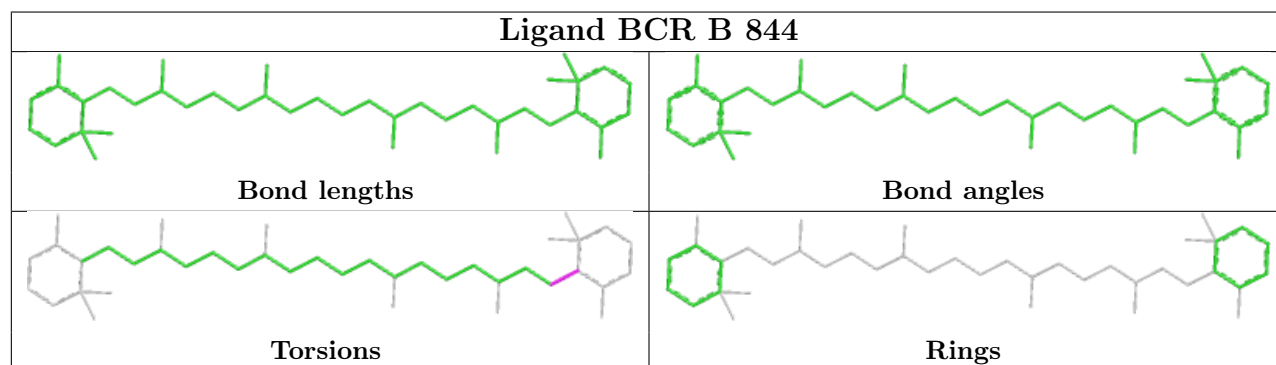
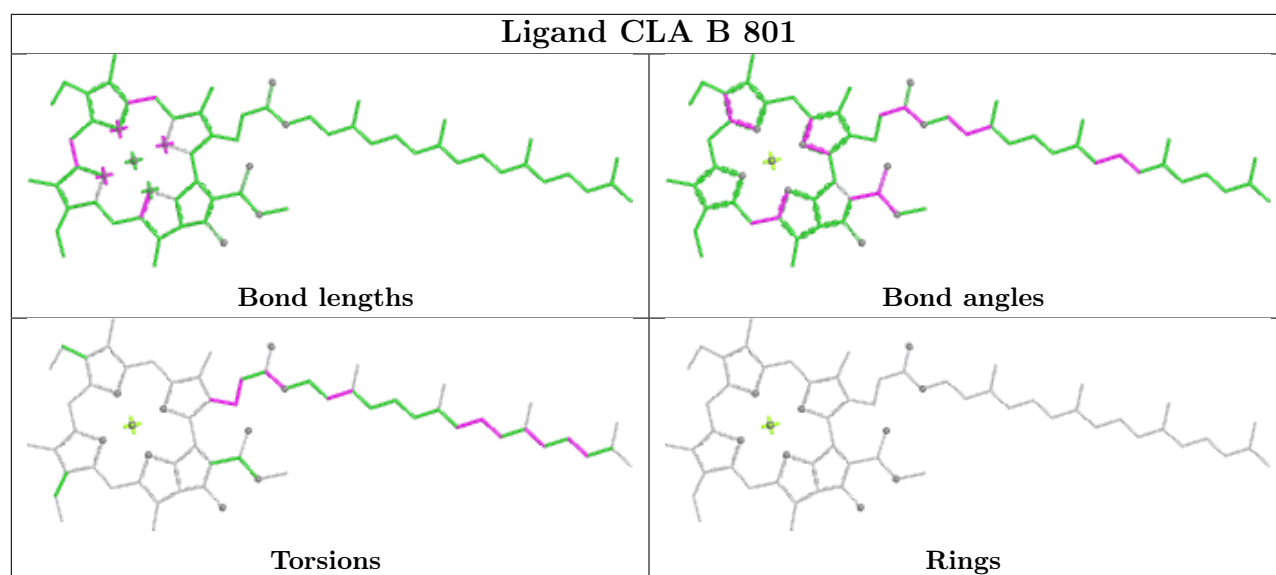


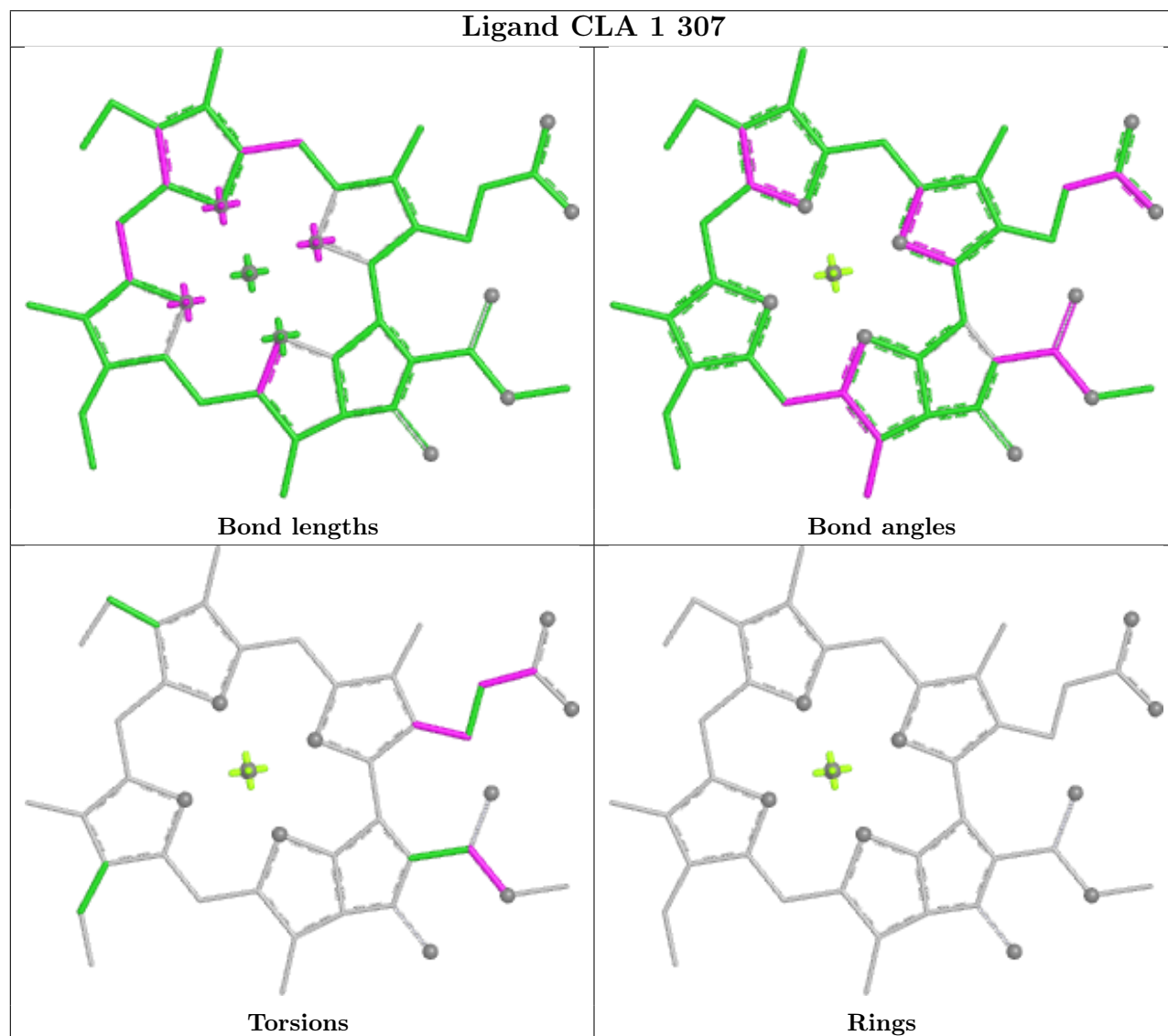
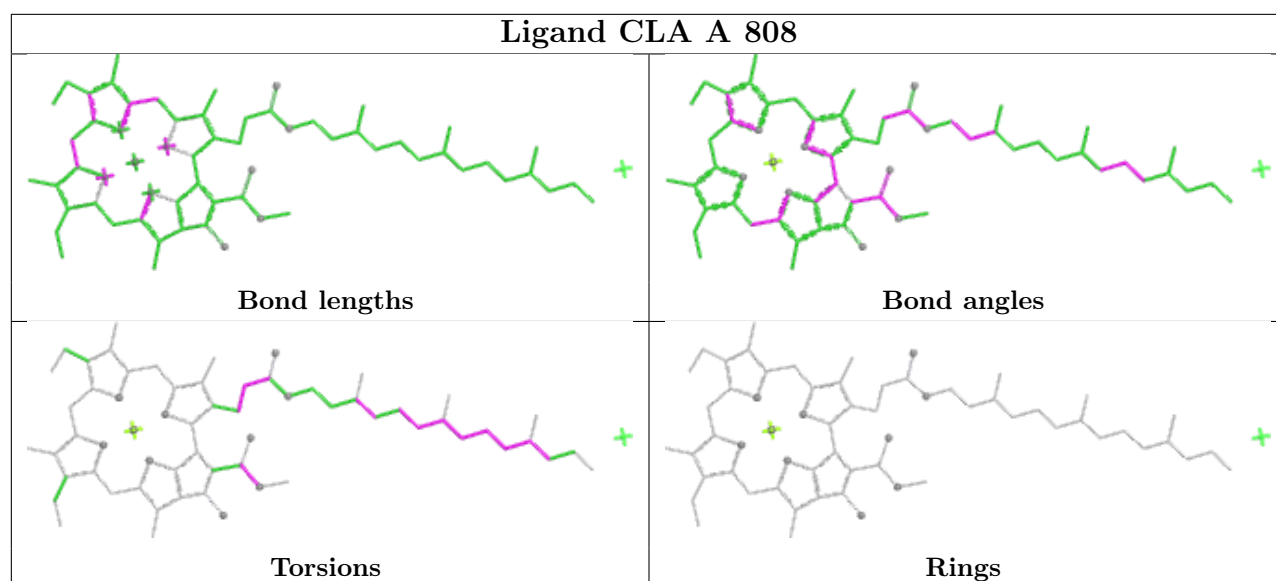
Torsions

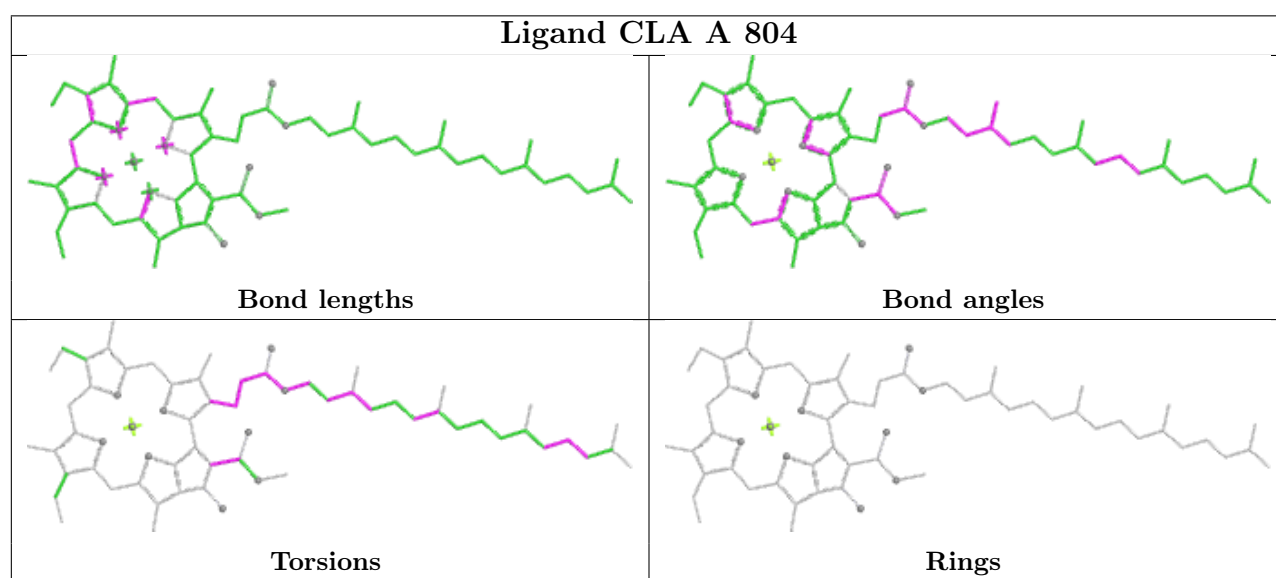
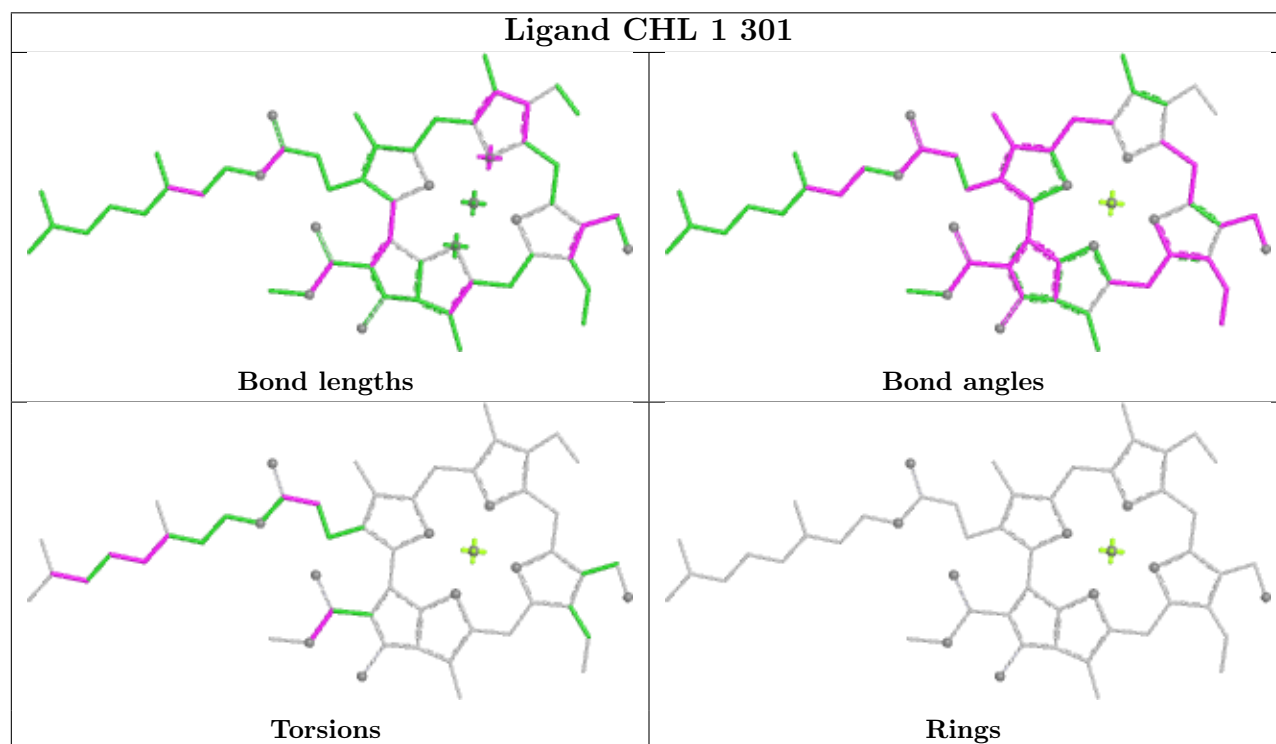
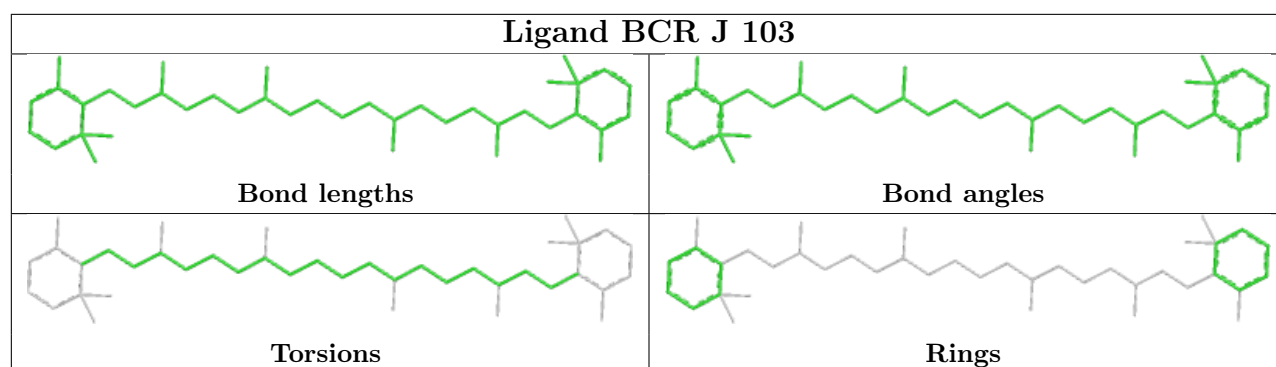


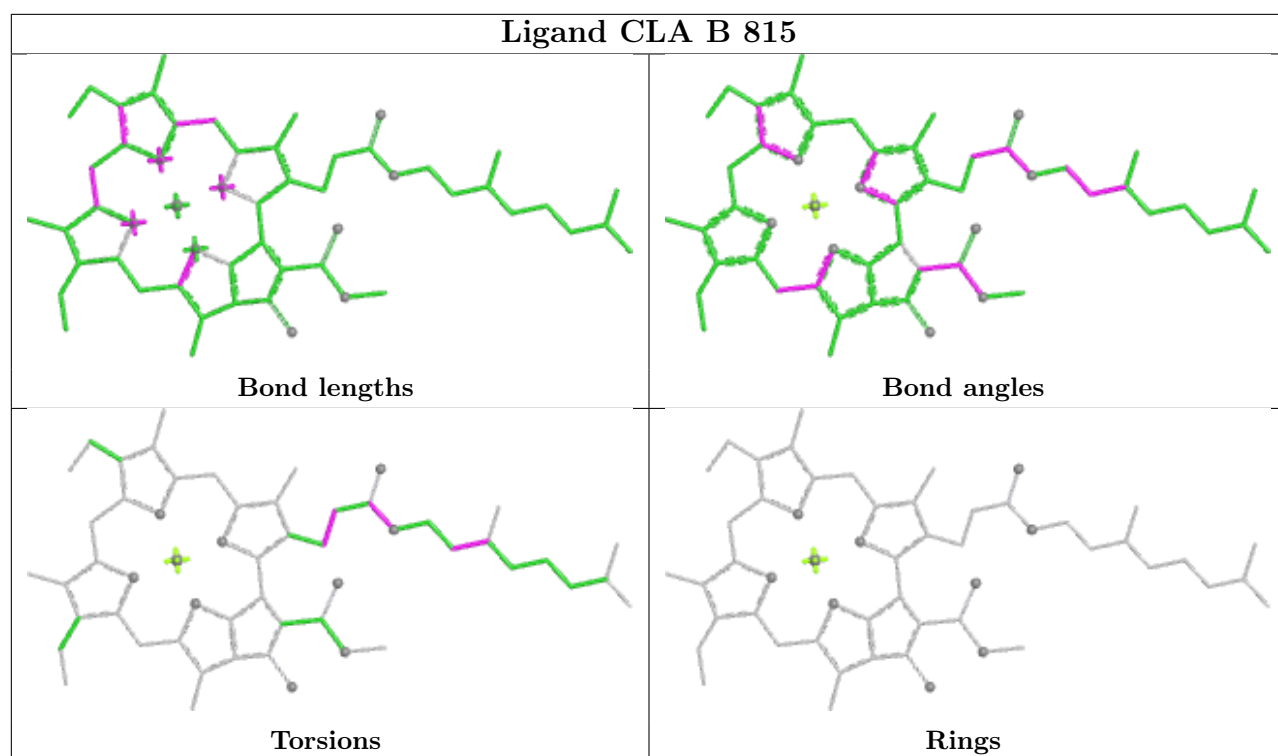
Rings



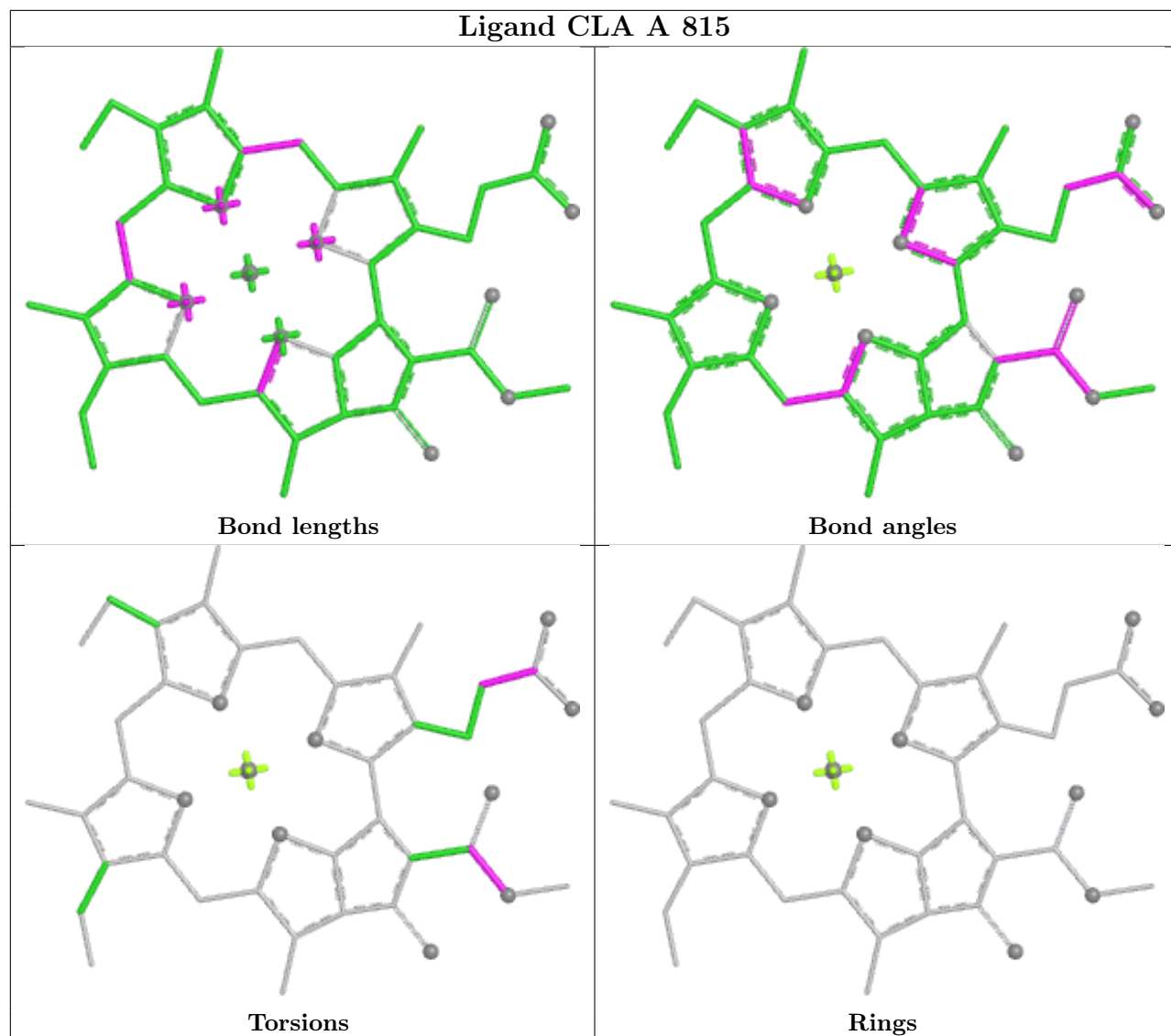


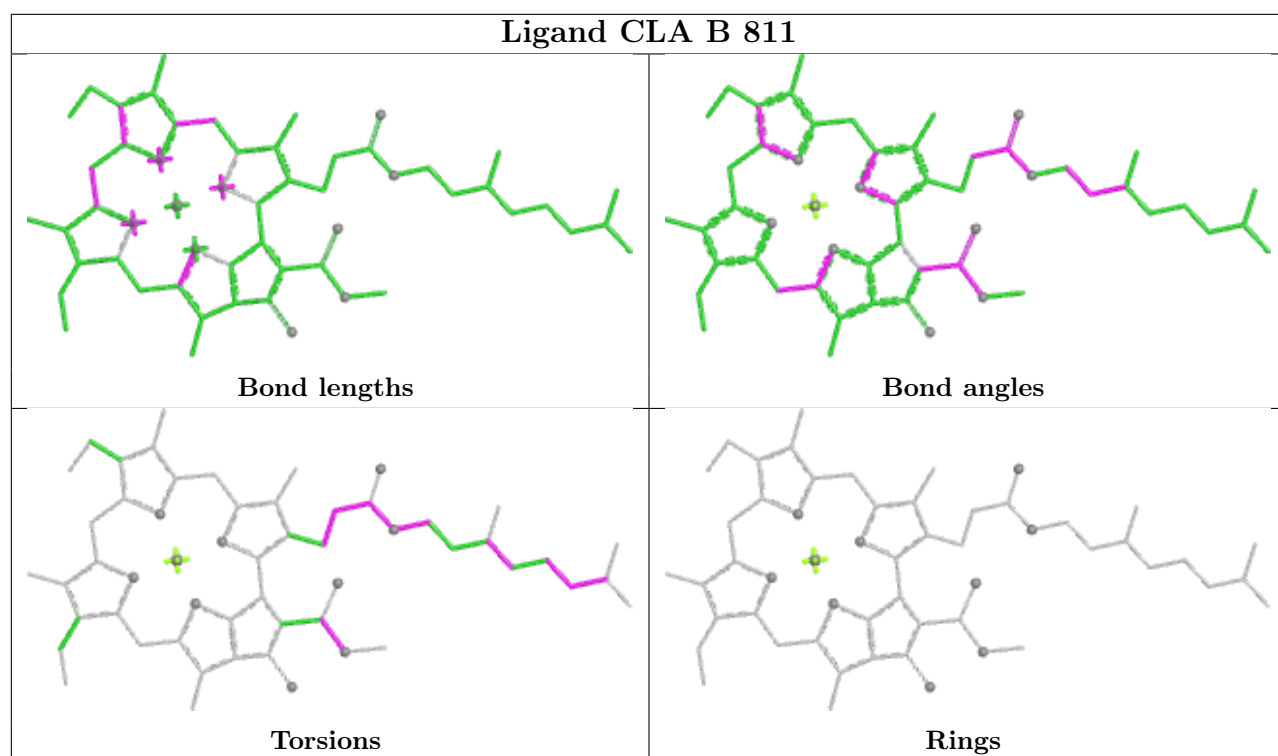




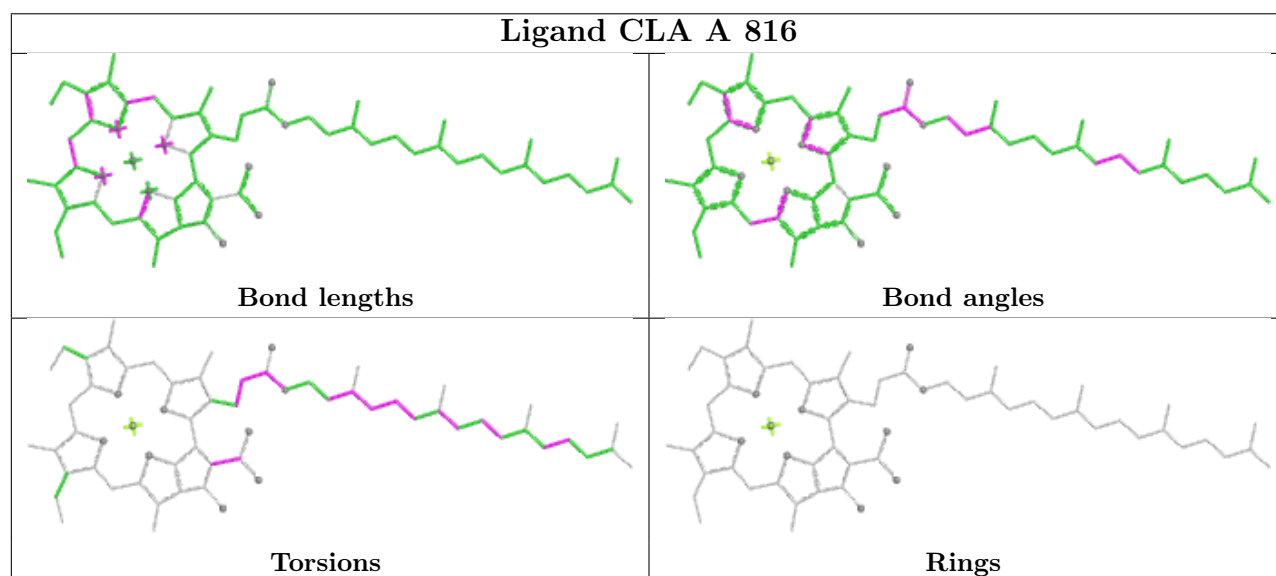
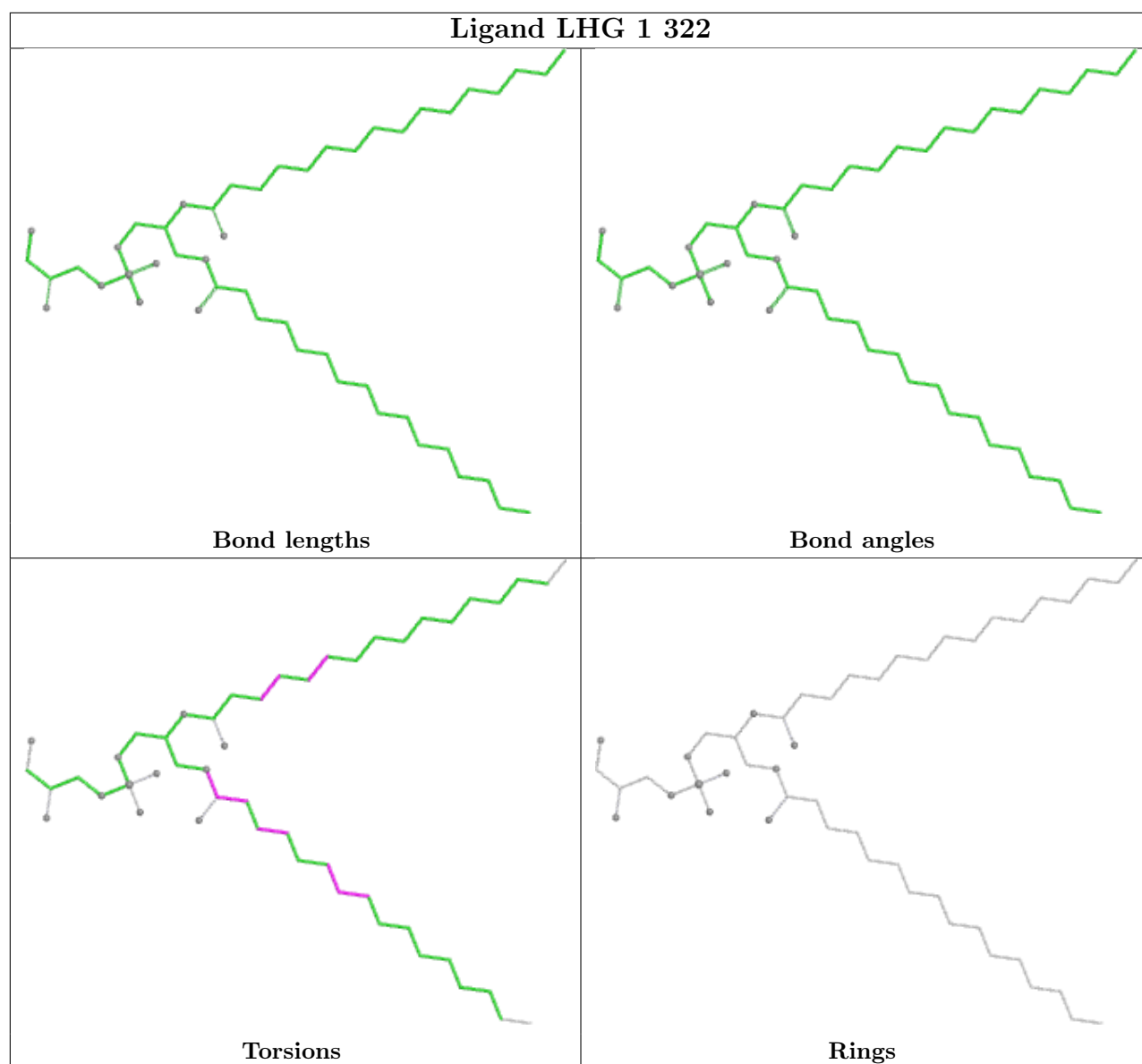


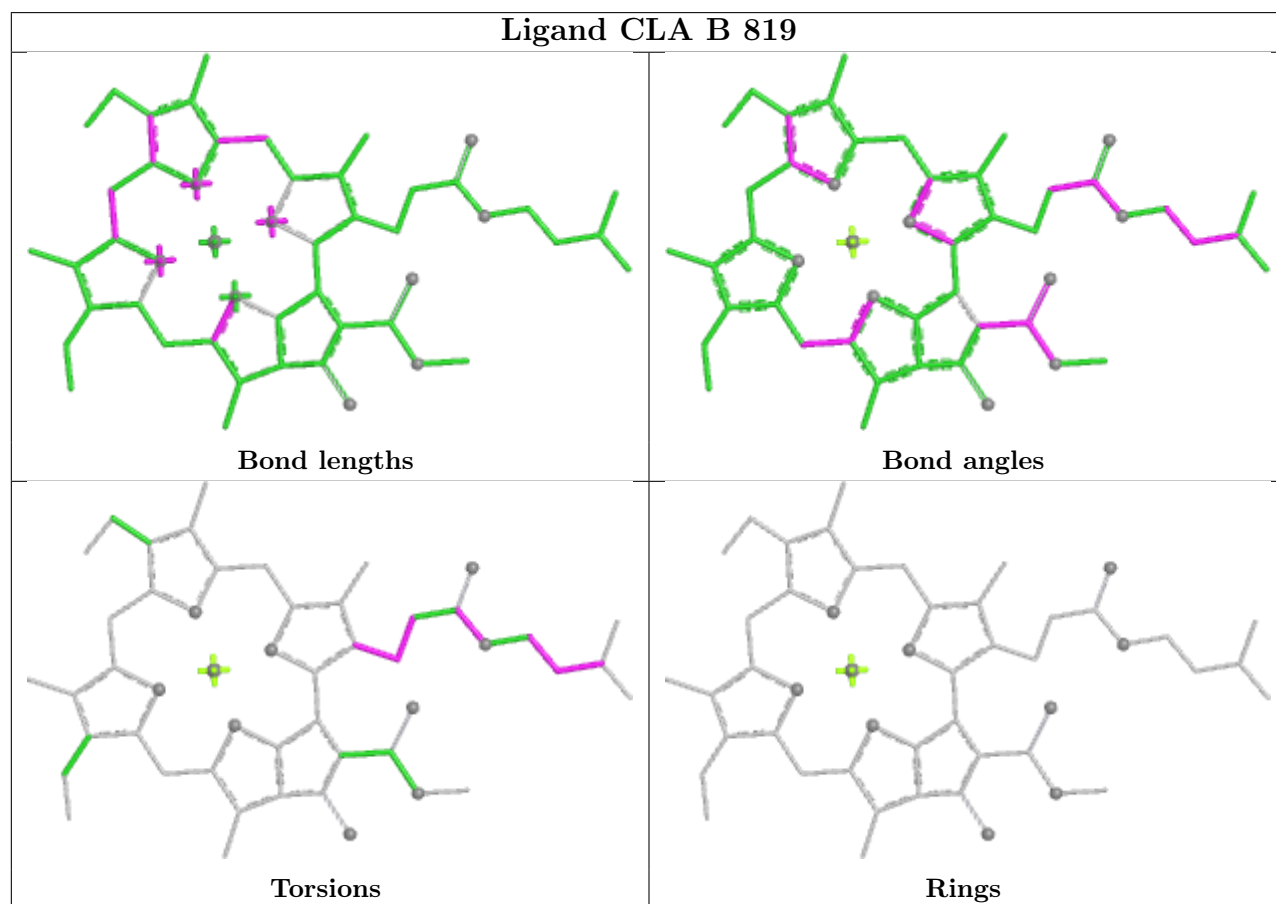
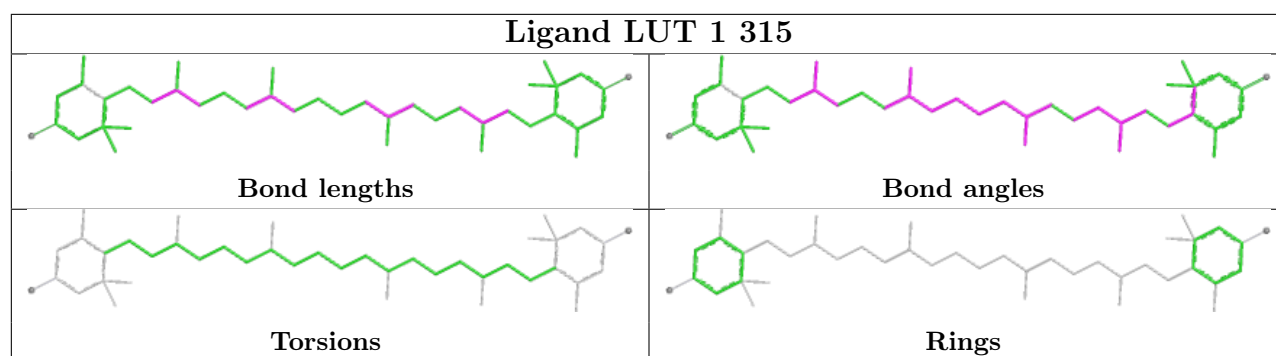
## Ligand CLA A 815

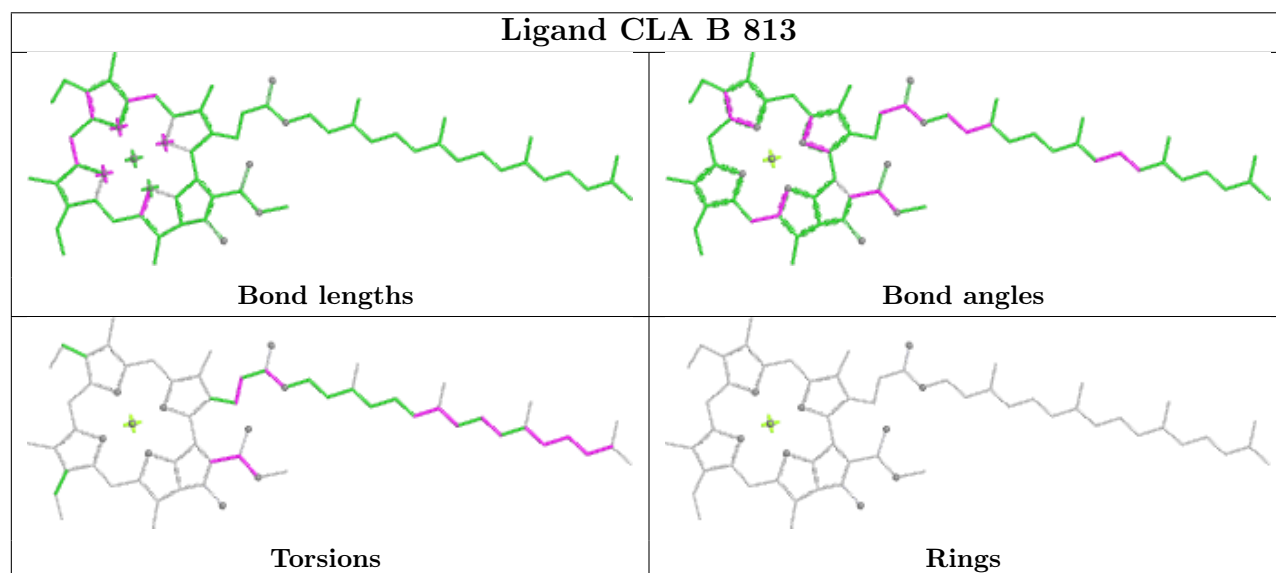
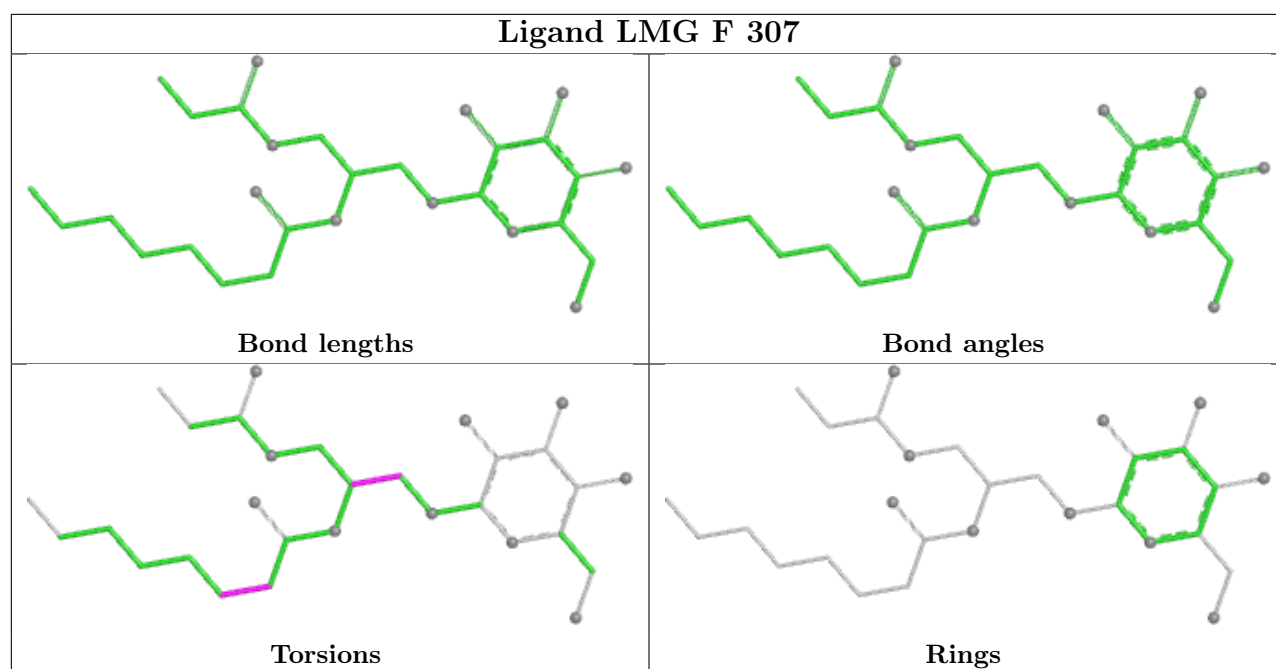




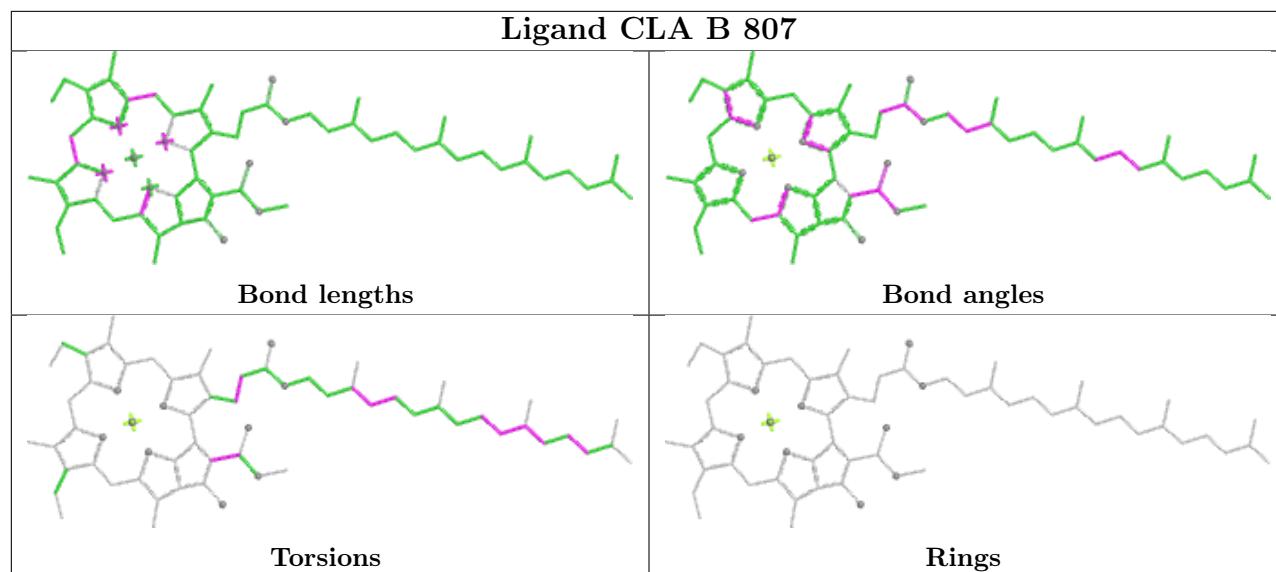




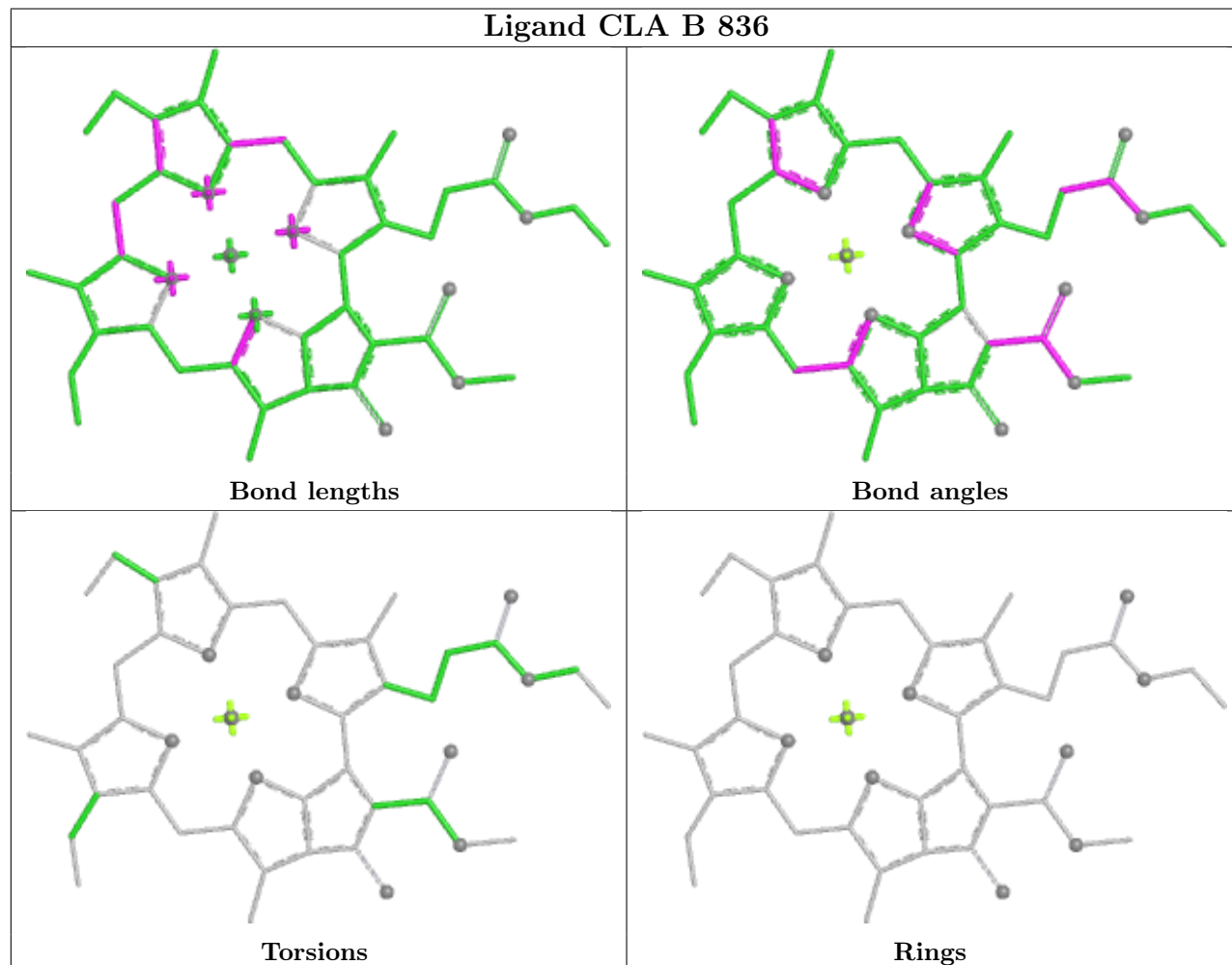


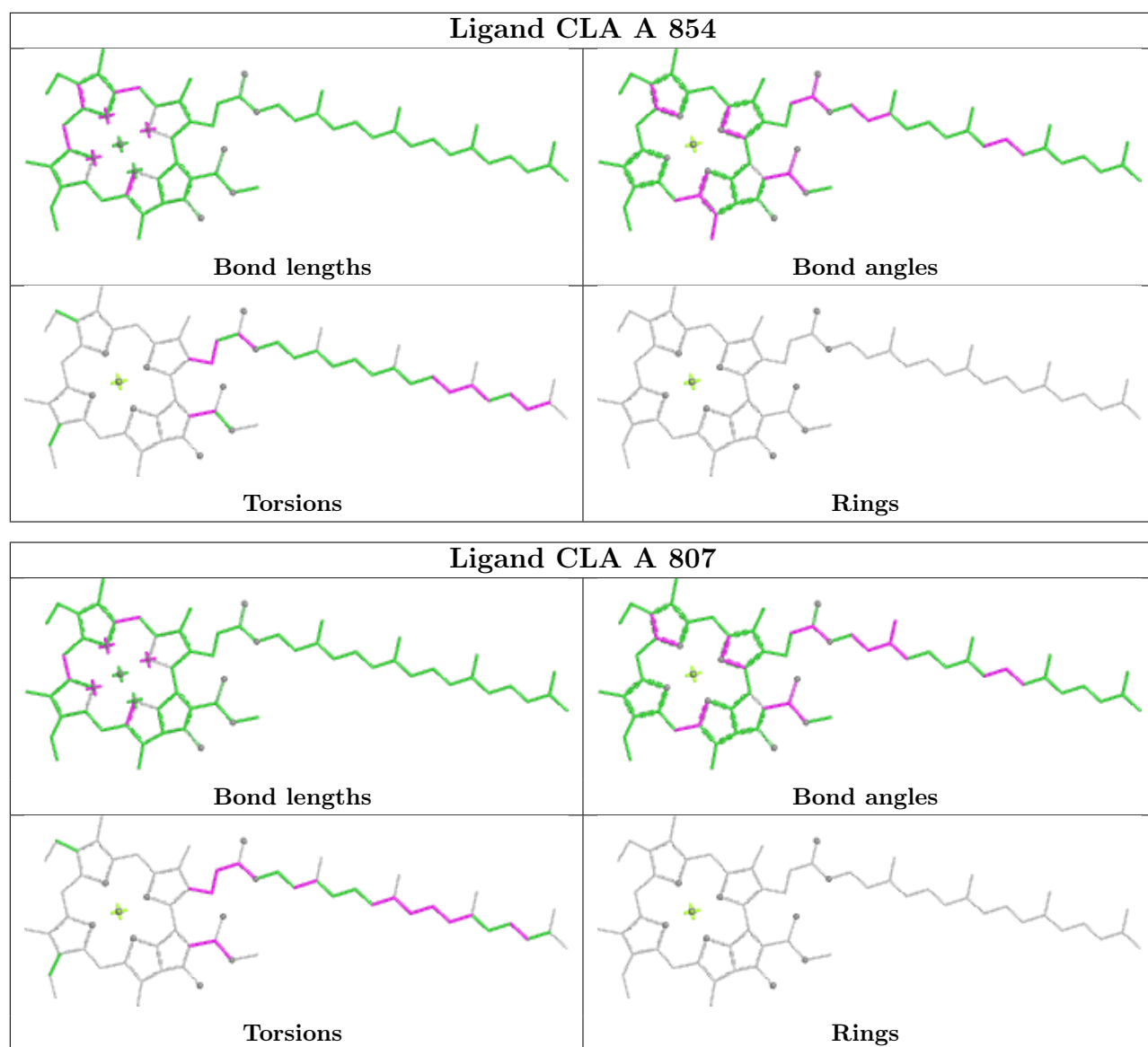


## Ligand CLA B 807

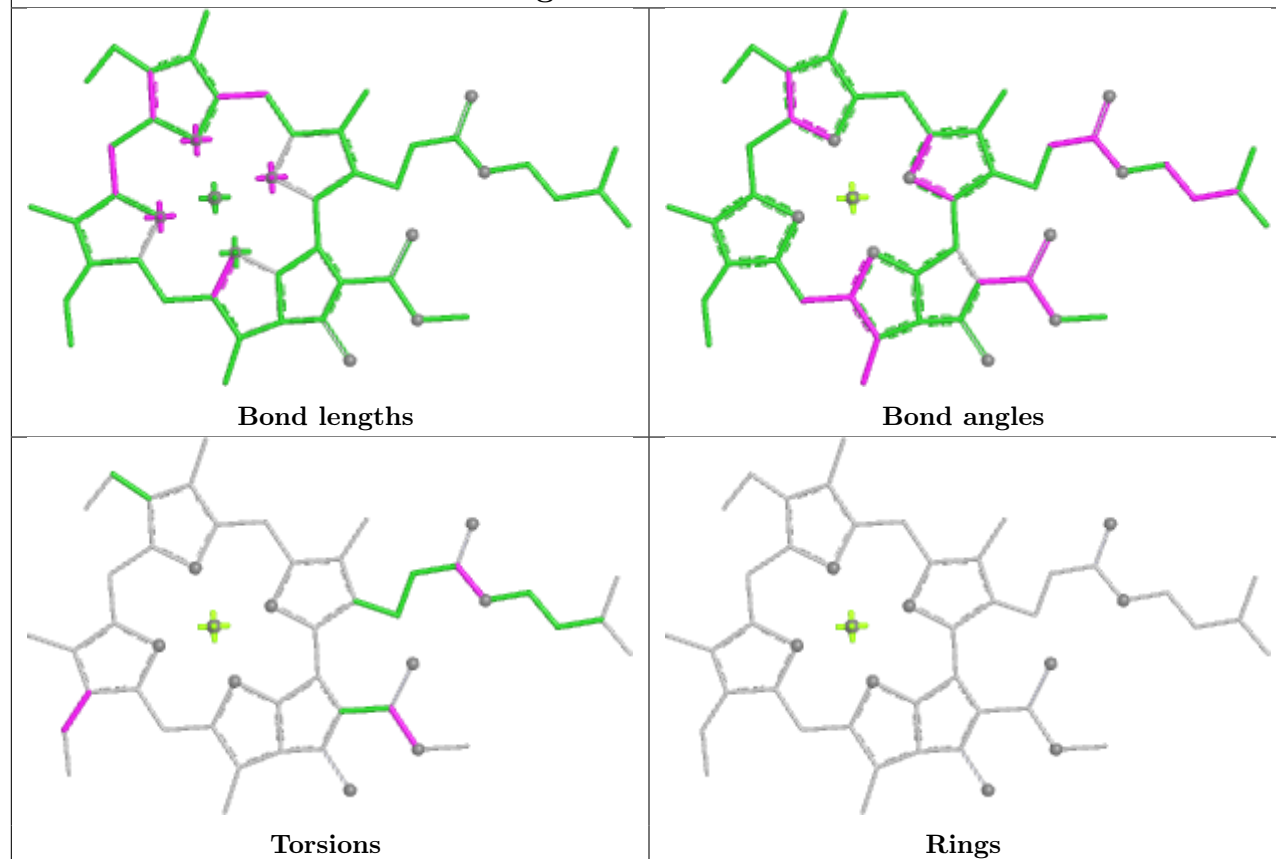


## Ligand CLA B 836

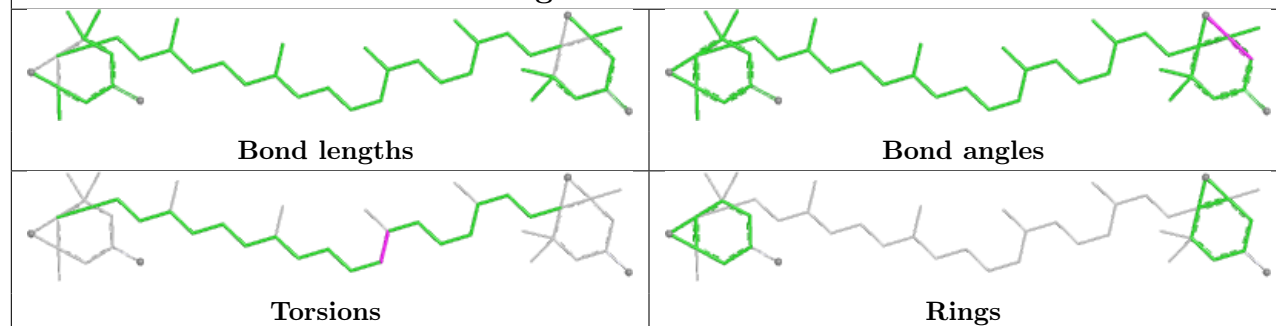


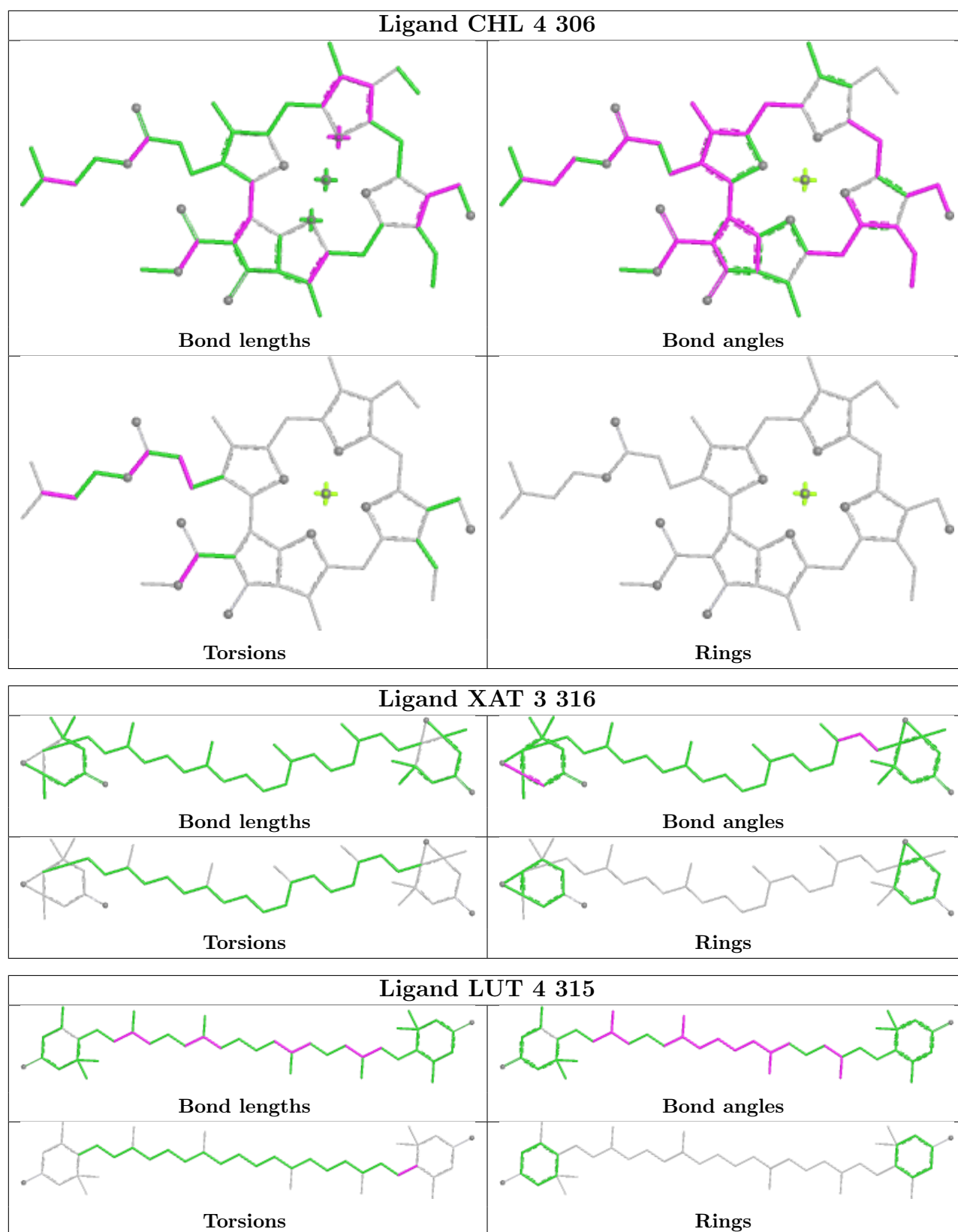


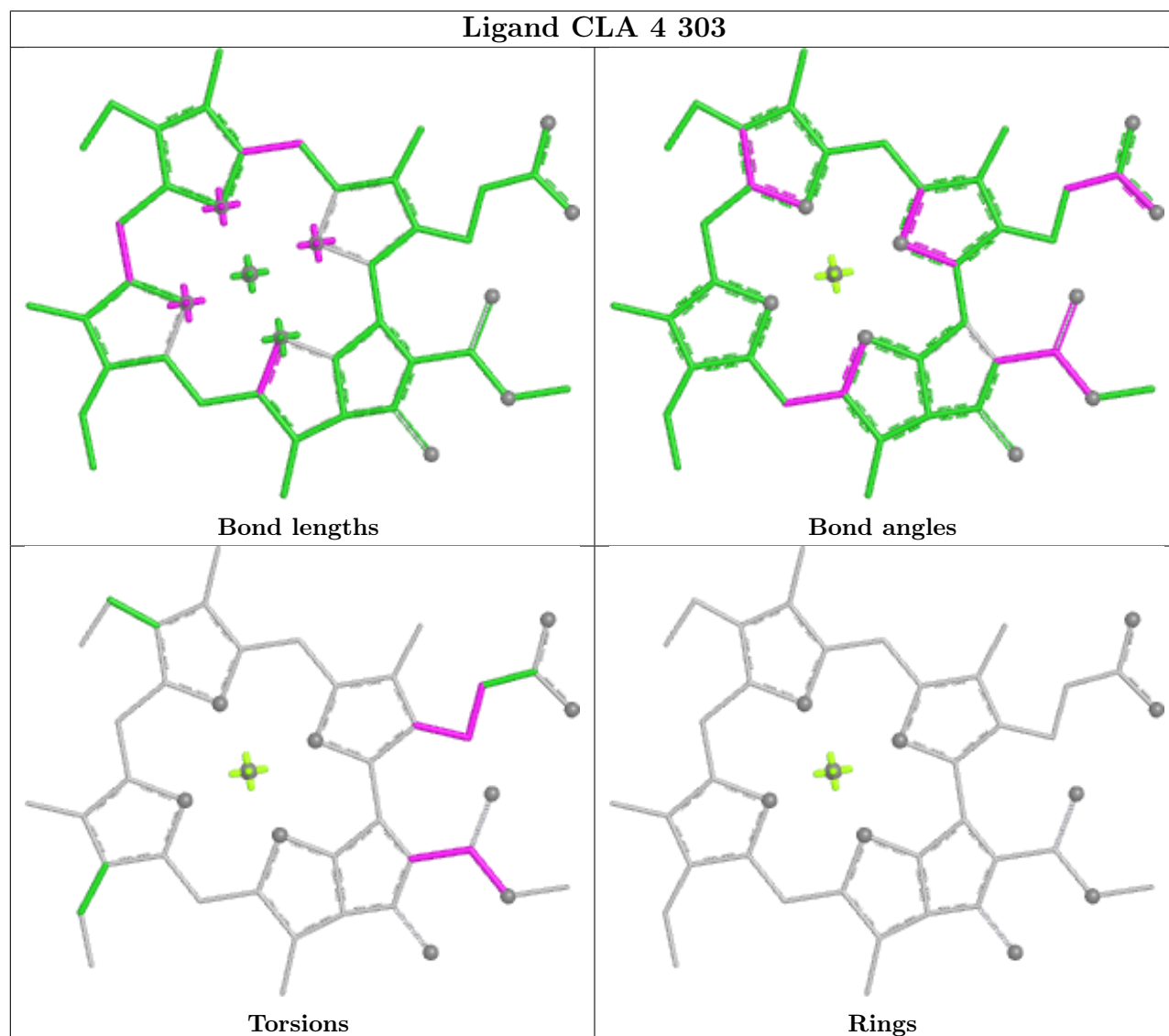
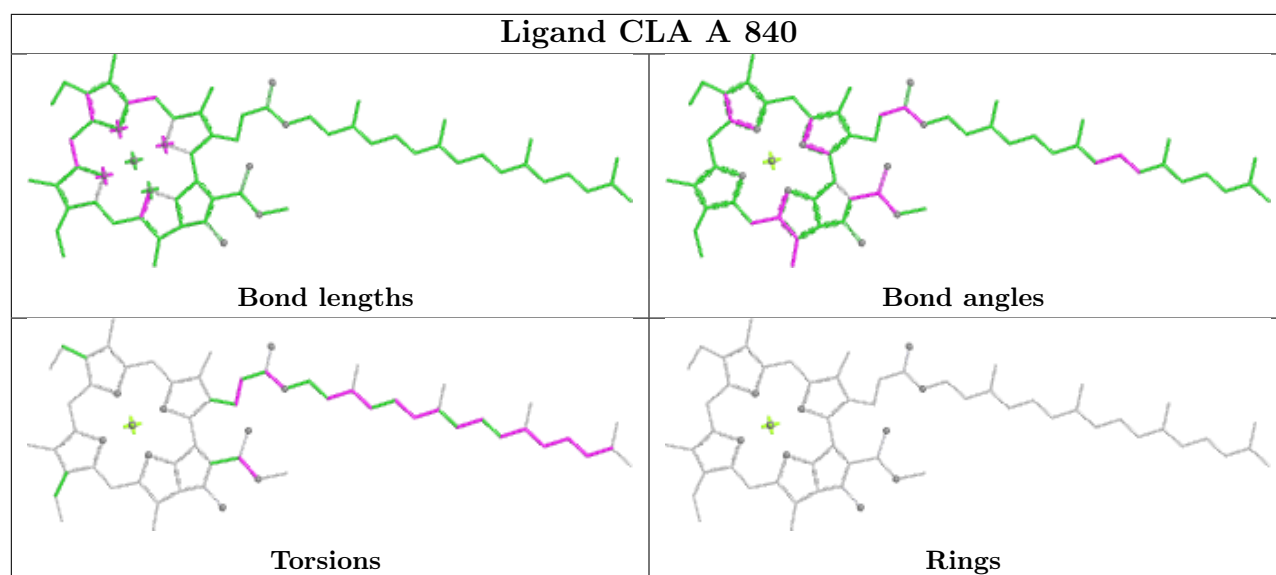
## Ligand CLA 3 309



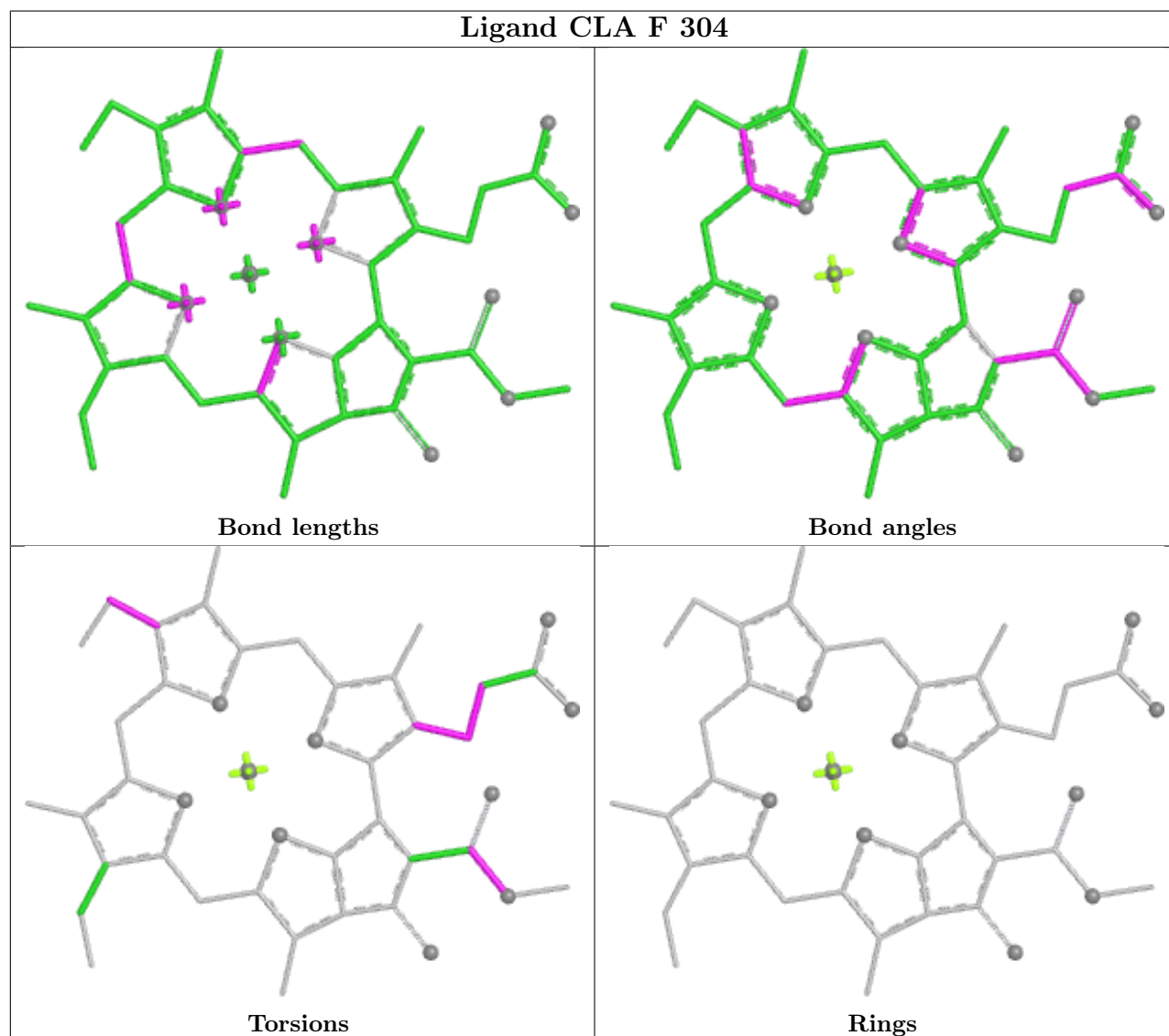
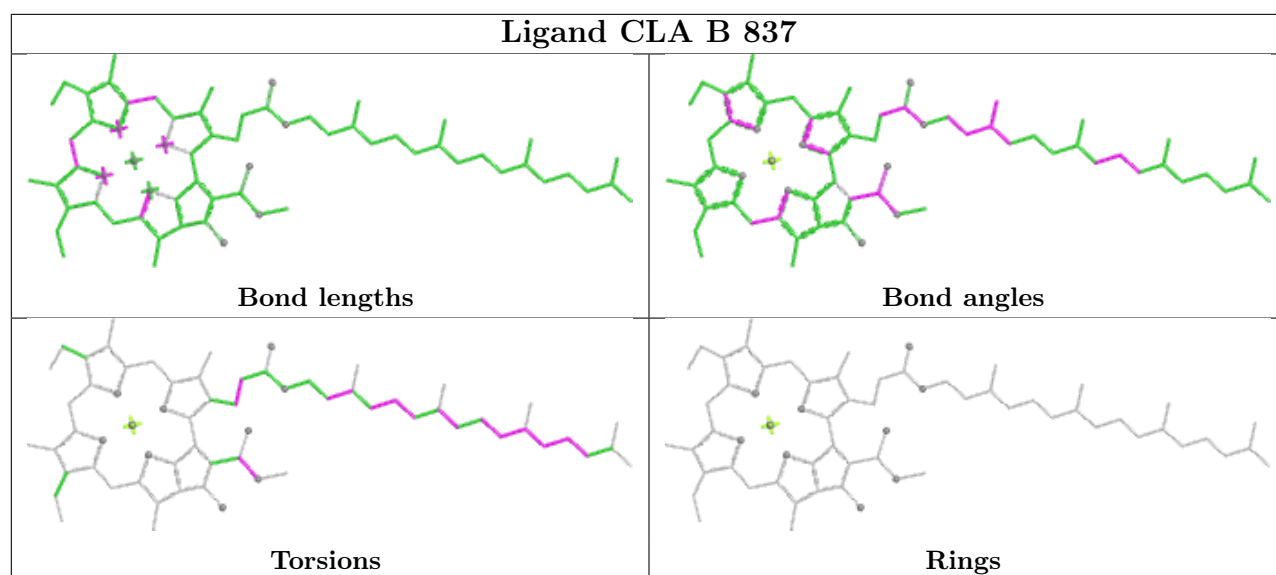
## Ligand XAT 2 316



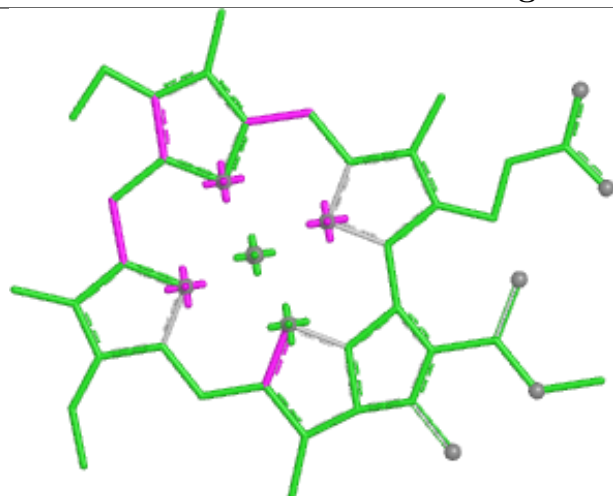




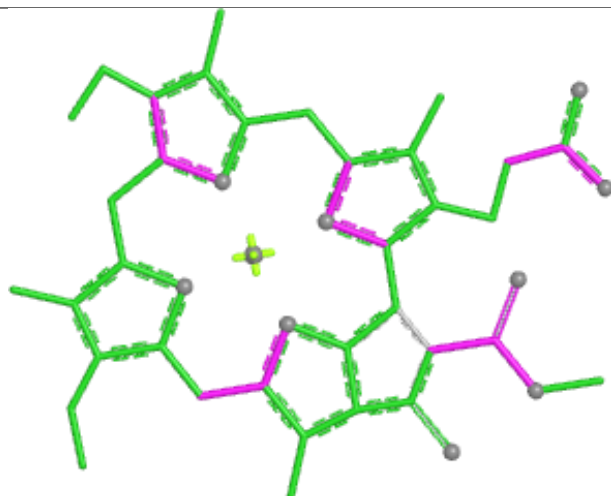




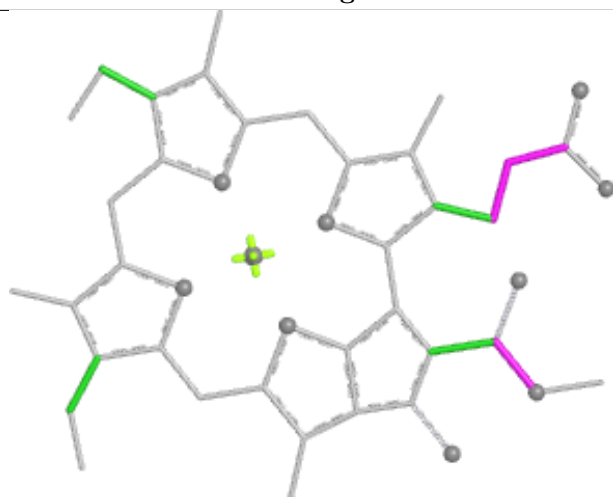
## Ligand CLA 3 311



Bond lengths



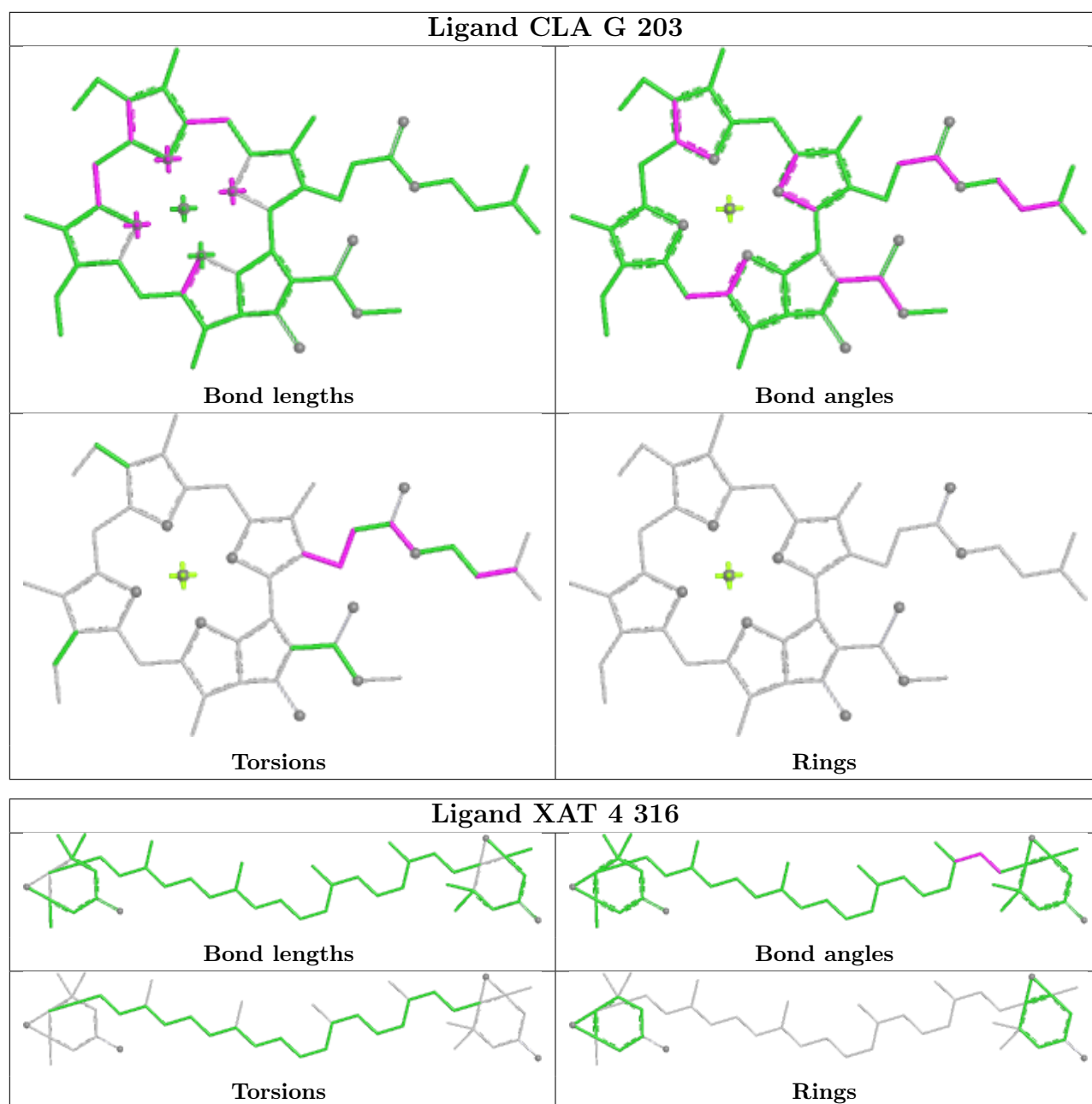
Bond angles

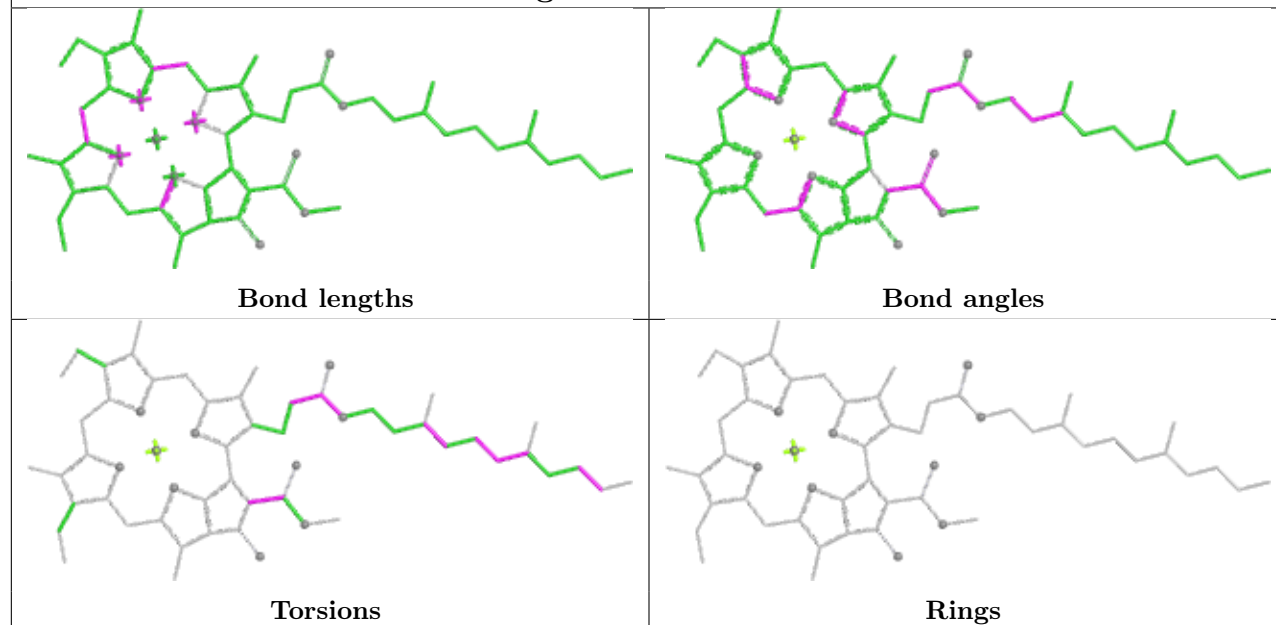
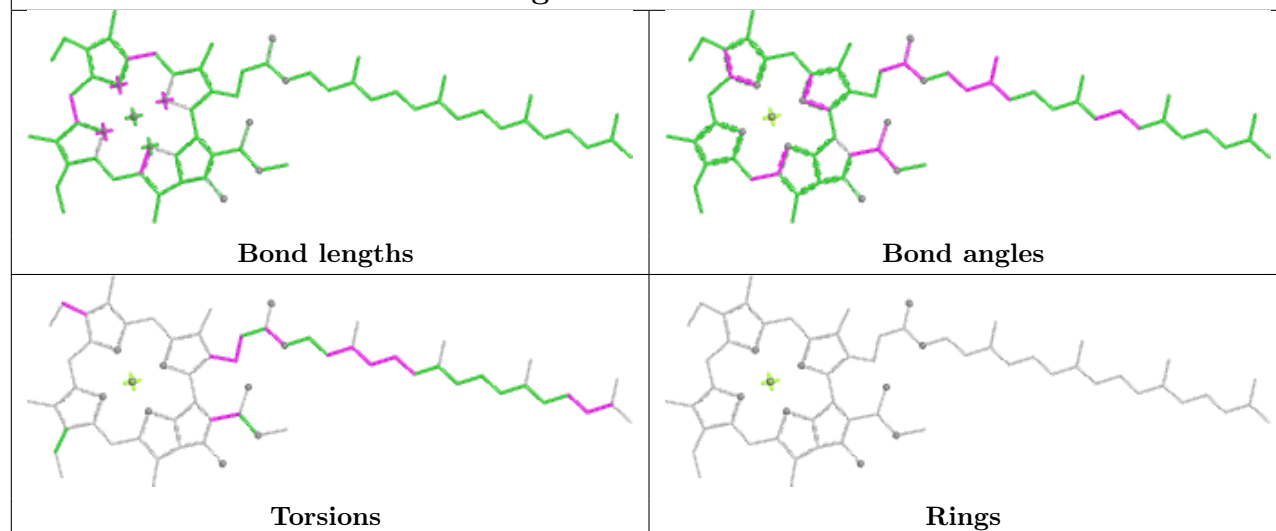


Torsions

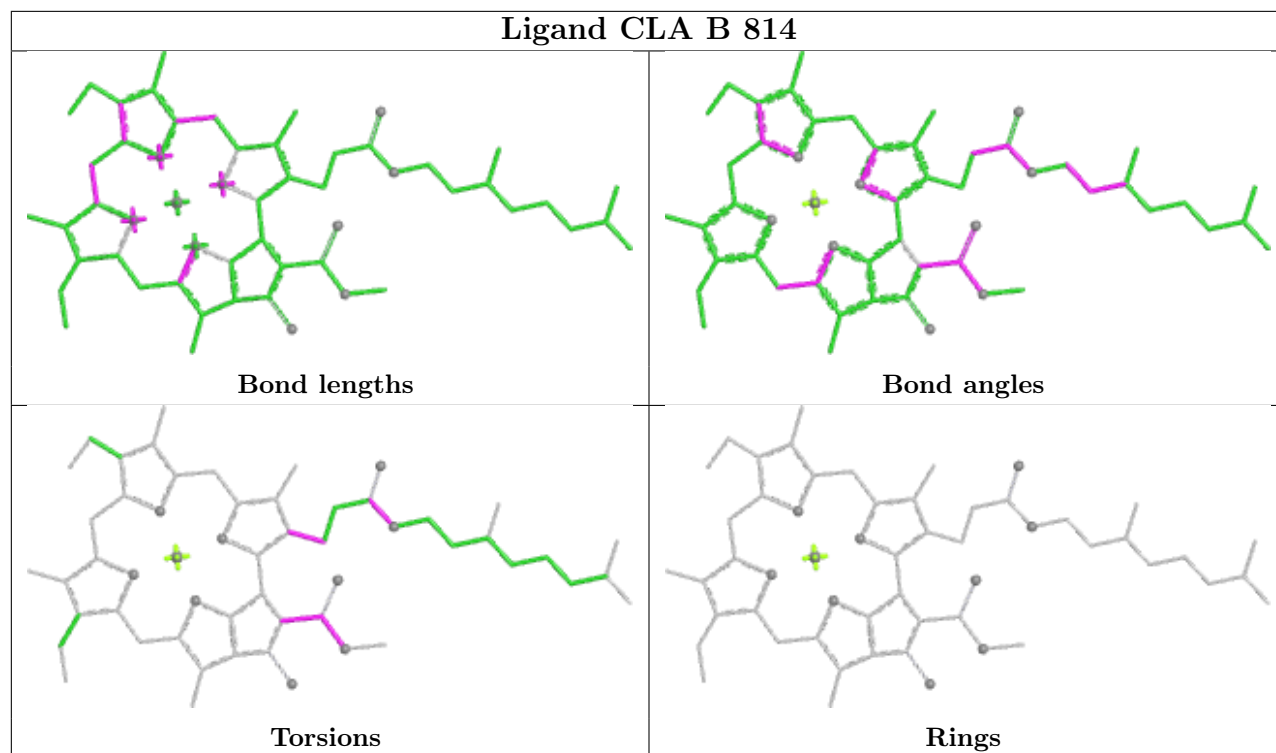


Rings

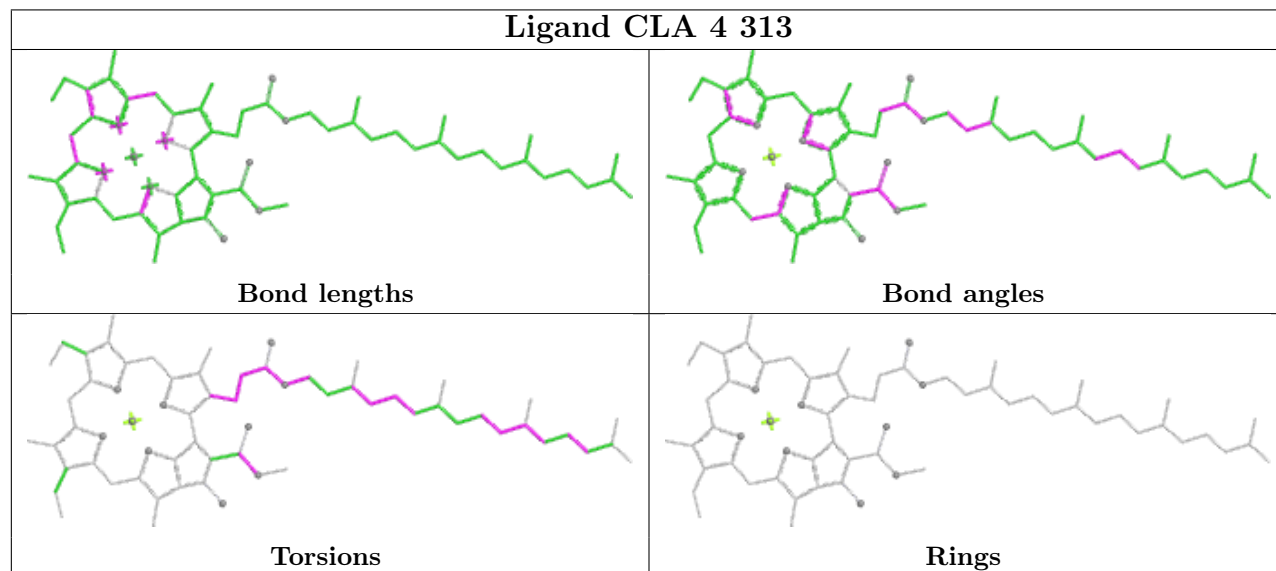


**Ligand CLA 1 303****Ligand CLA A 824**

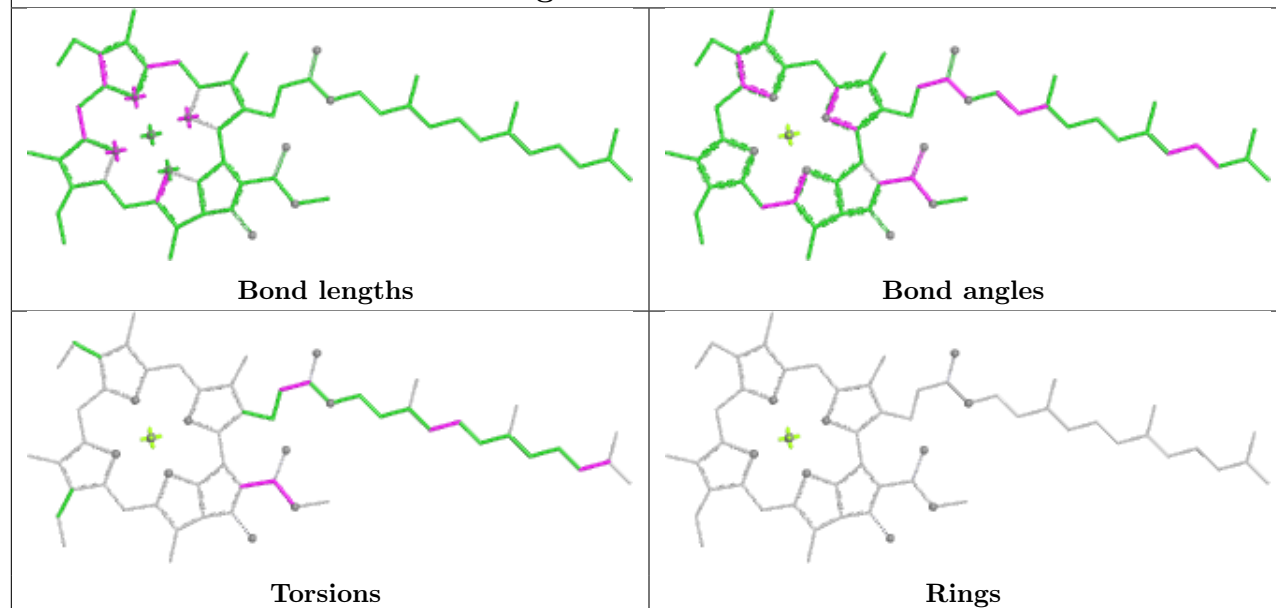
## Ligand CLA B 814



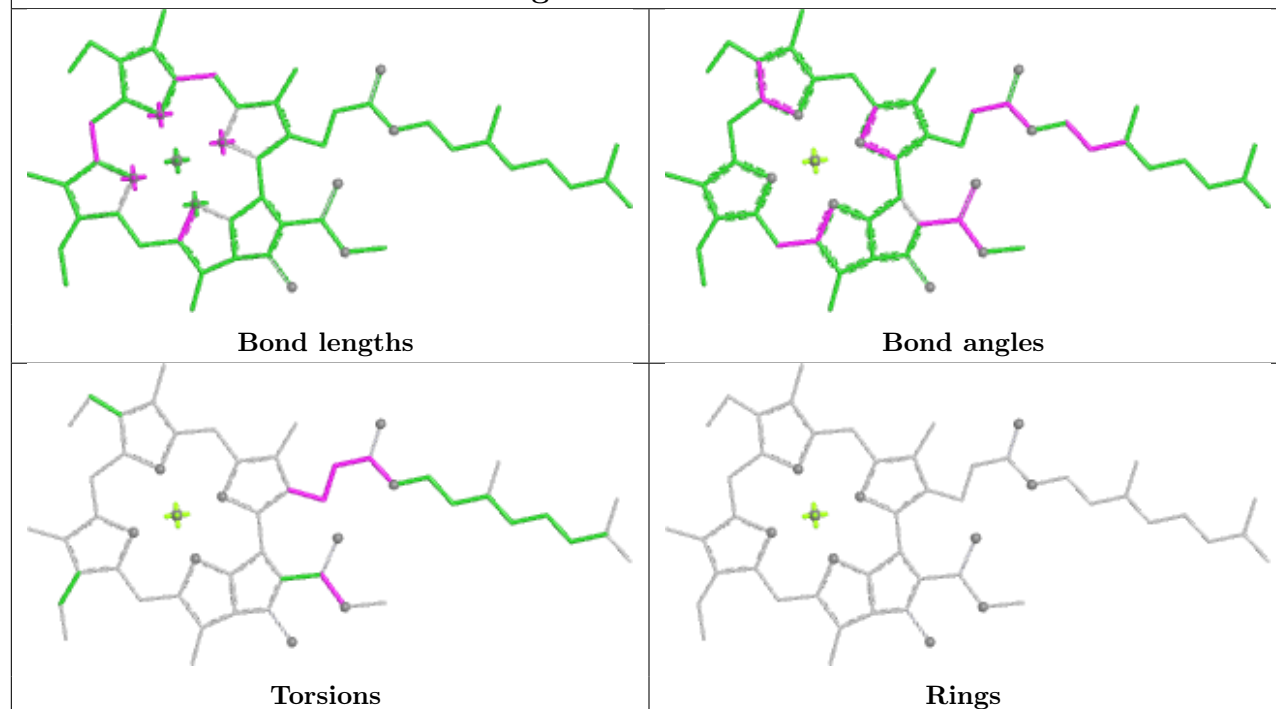
## Ligand CLA 4 313



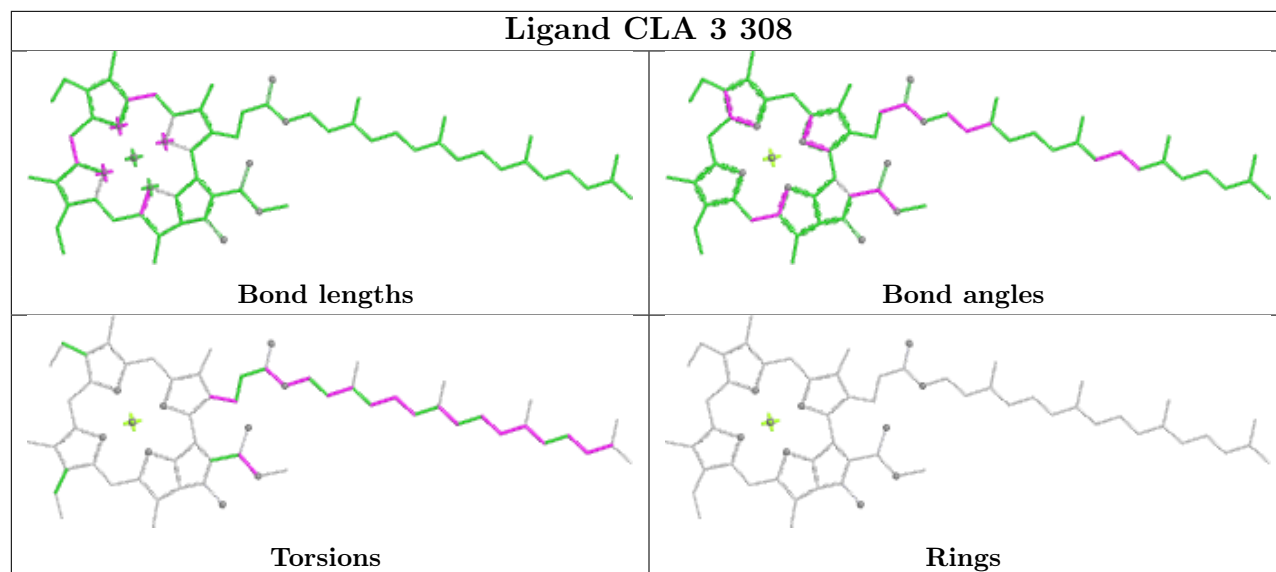
## Ligand CLA 4 301



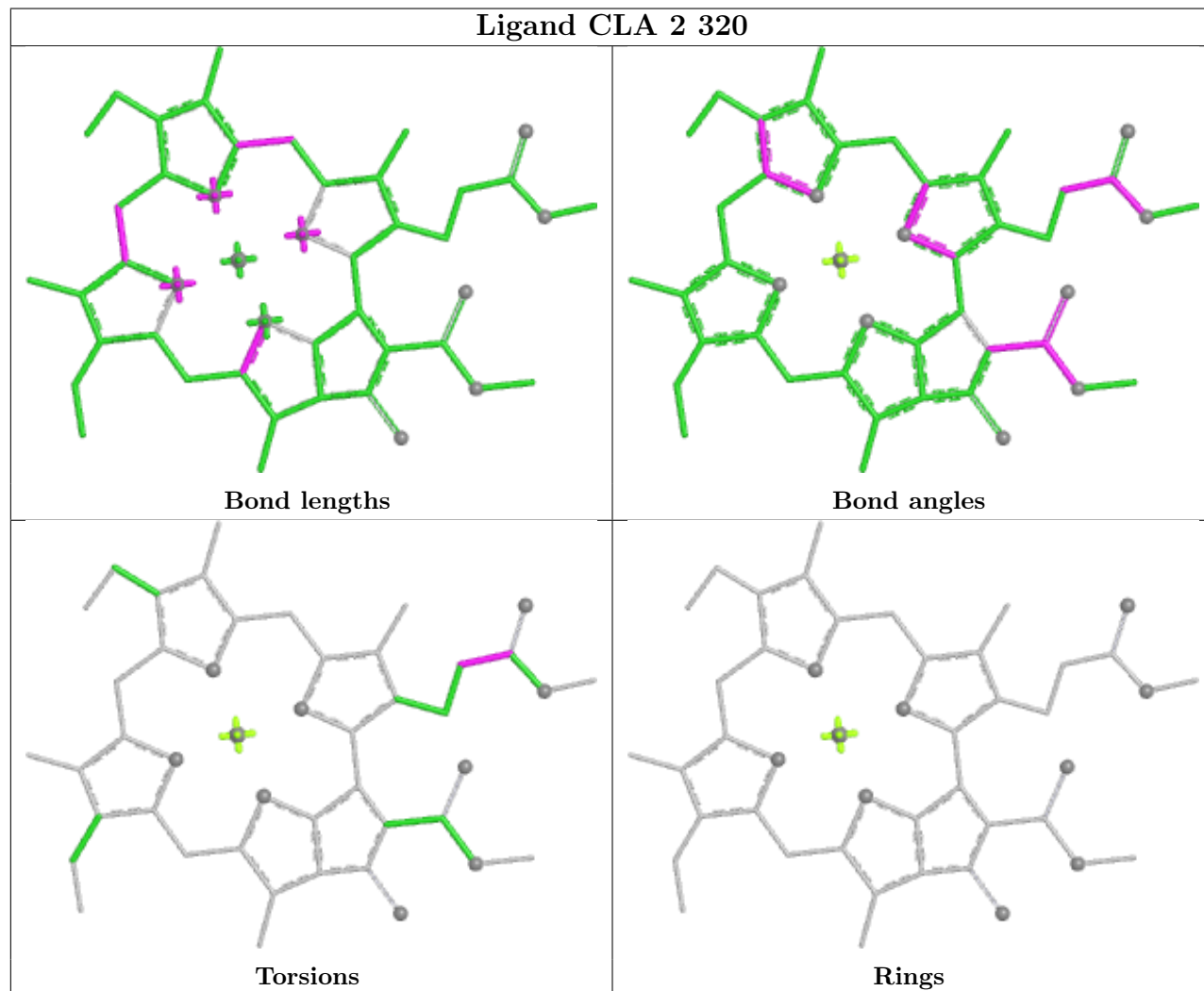
## Ligand CLA A 817



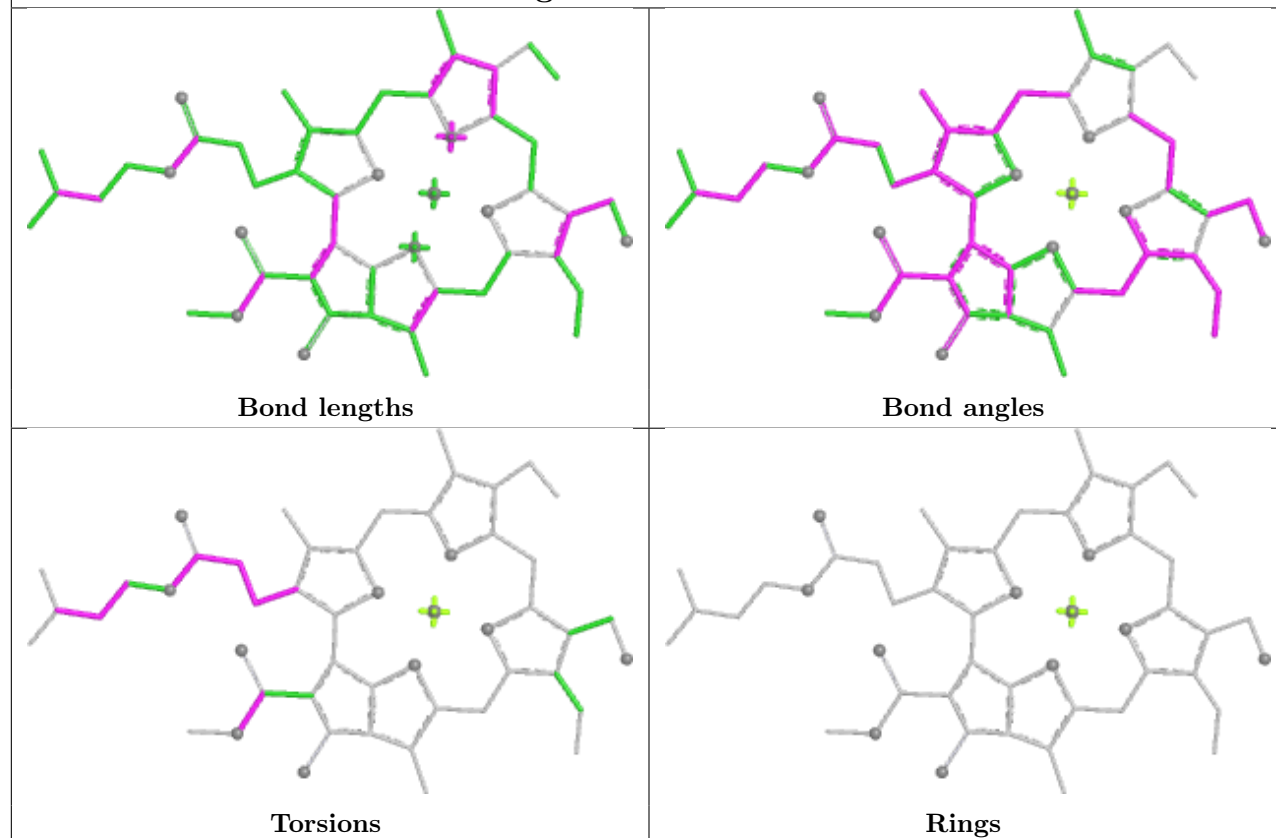
## Ligand CLA 3 308



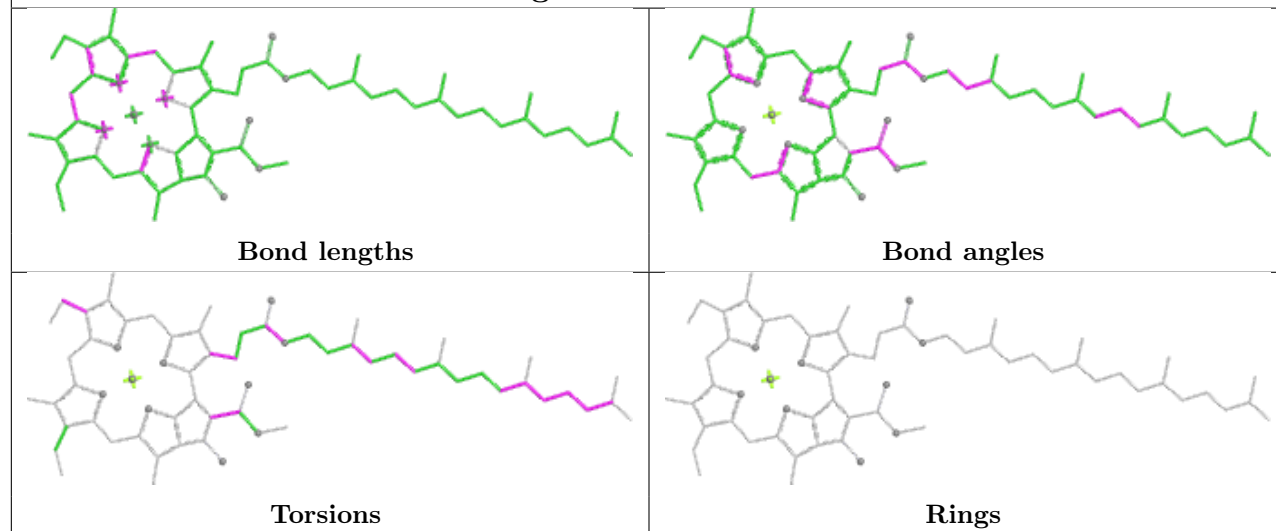
## Ligand CLA 2 320



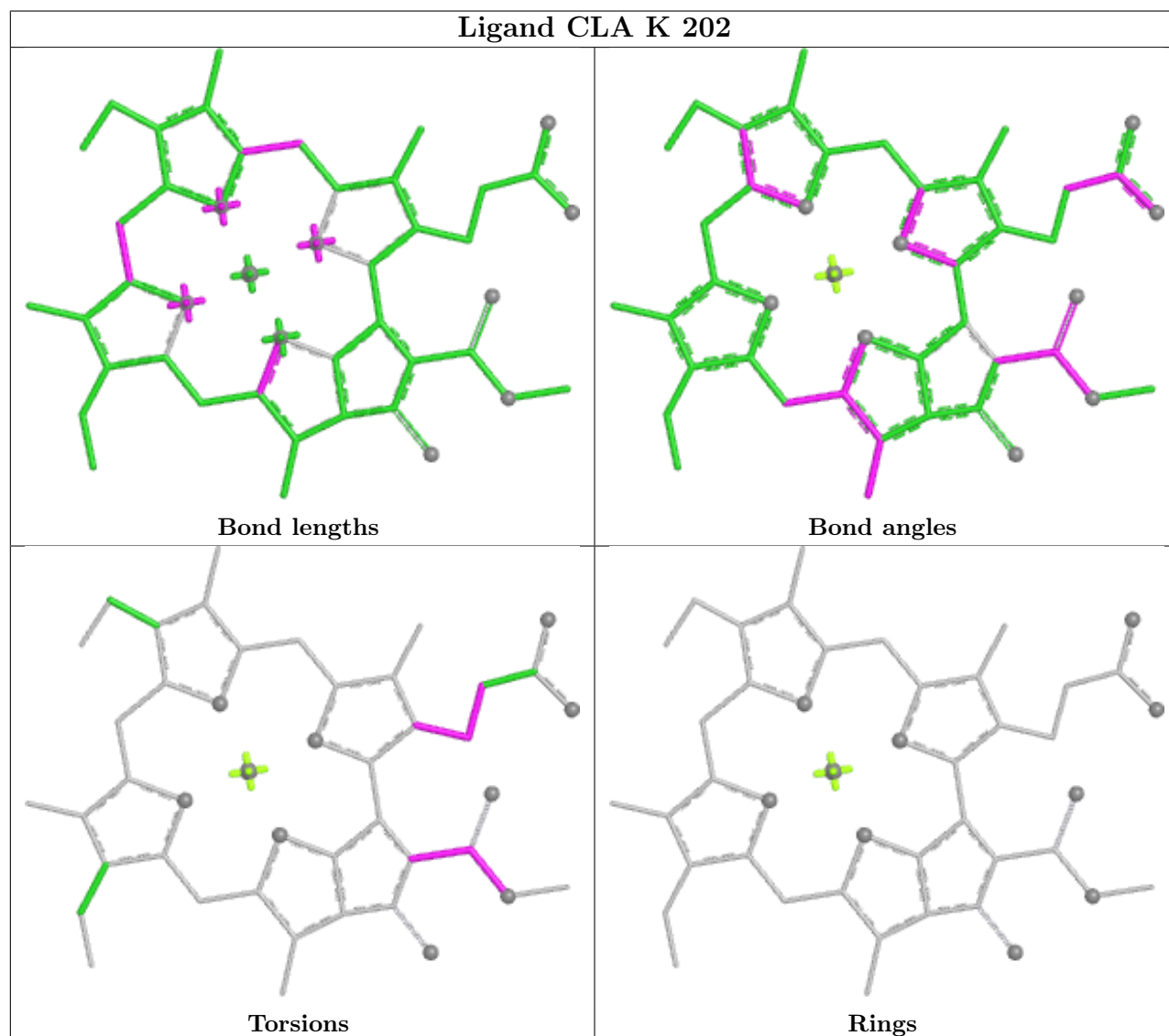
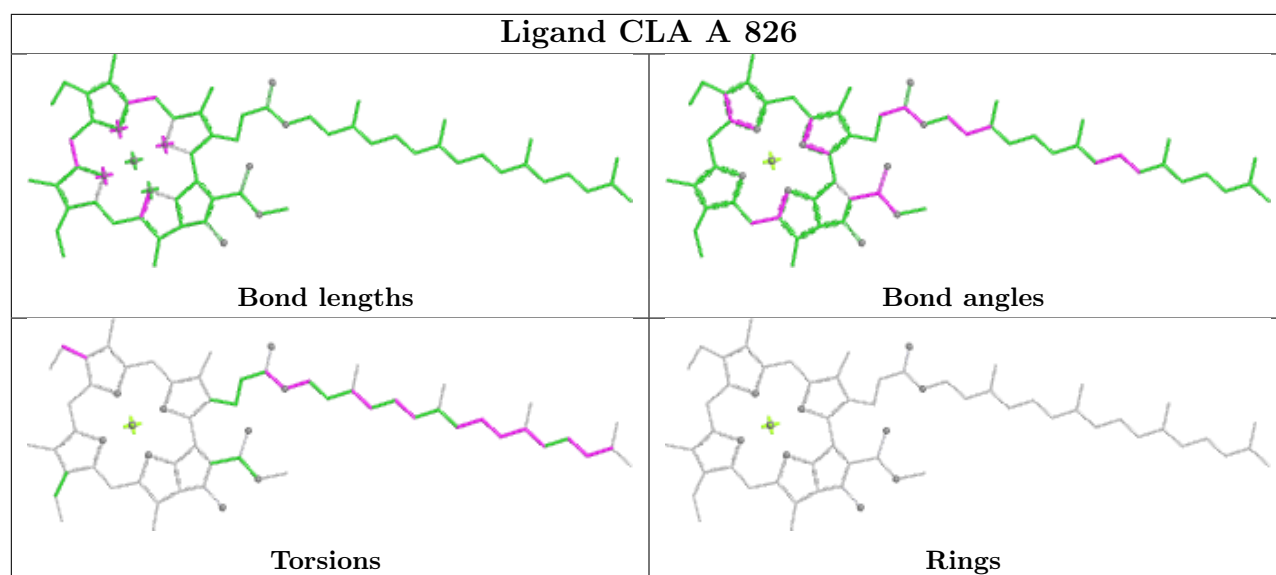
## Ligand CHL 2 301



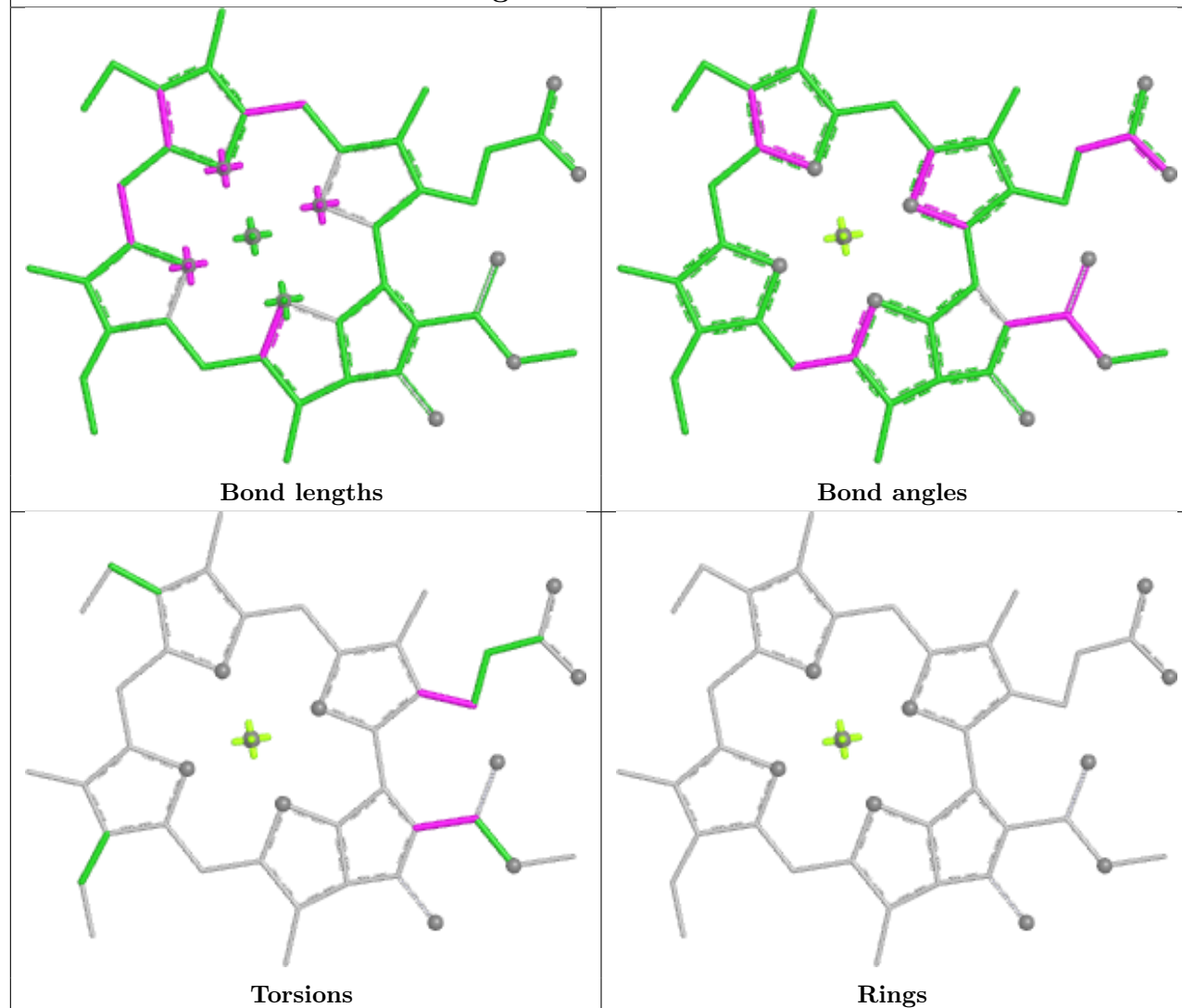
## Ligand CLA A 829



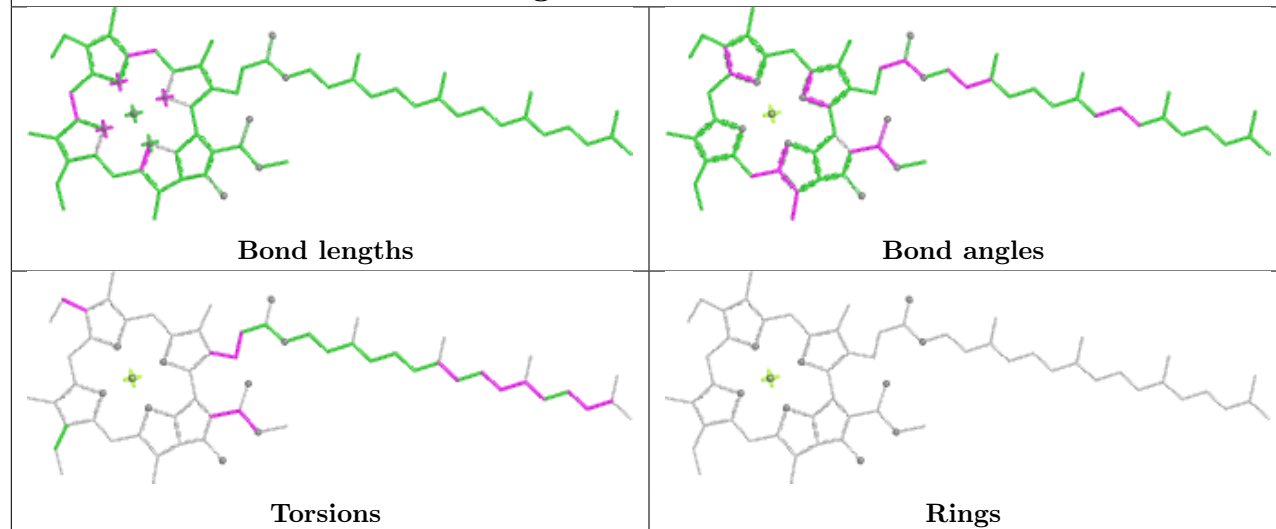


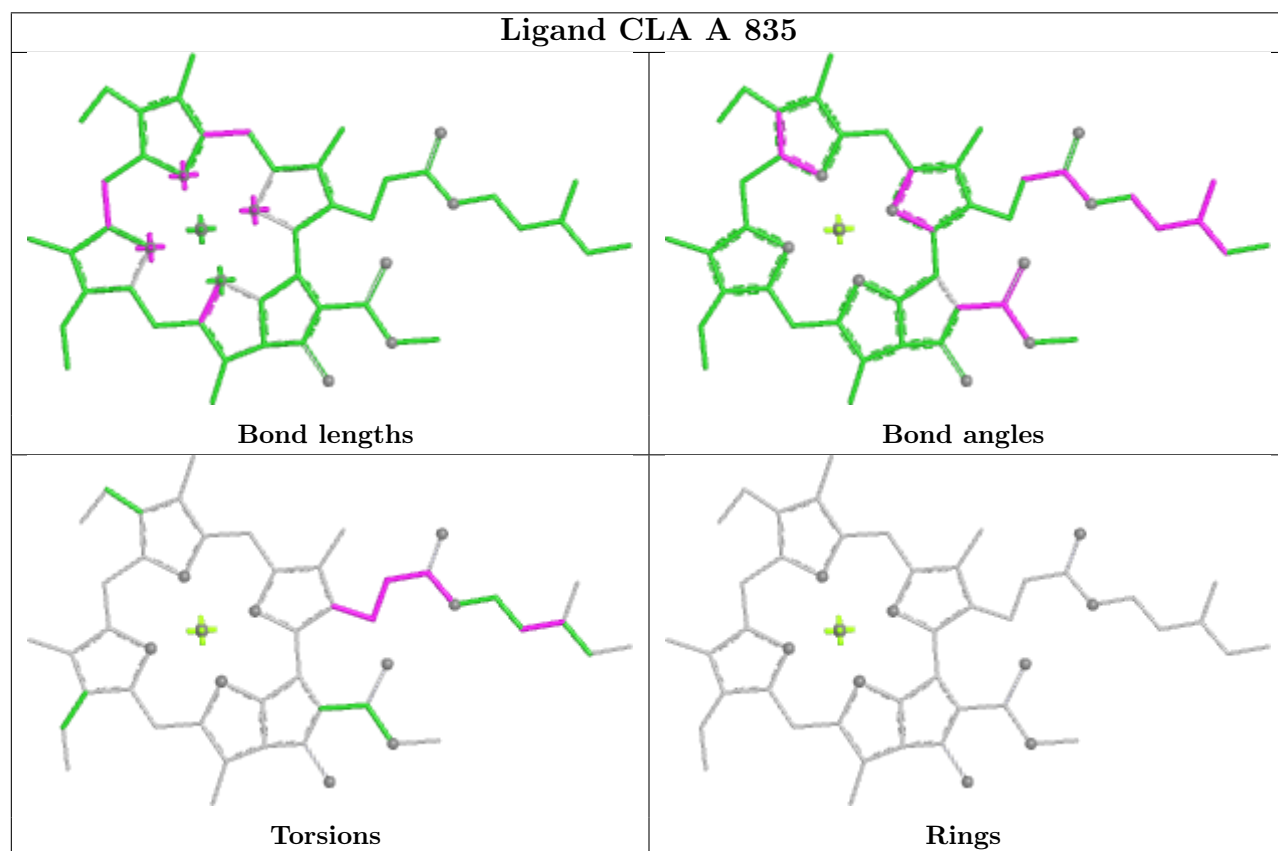
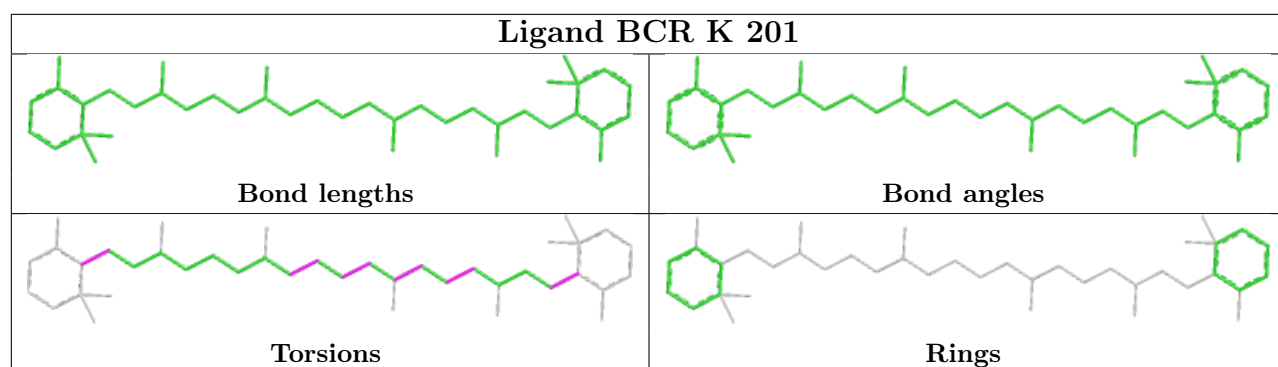


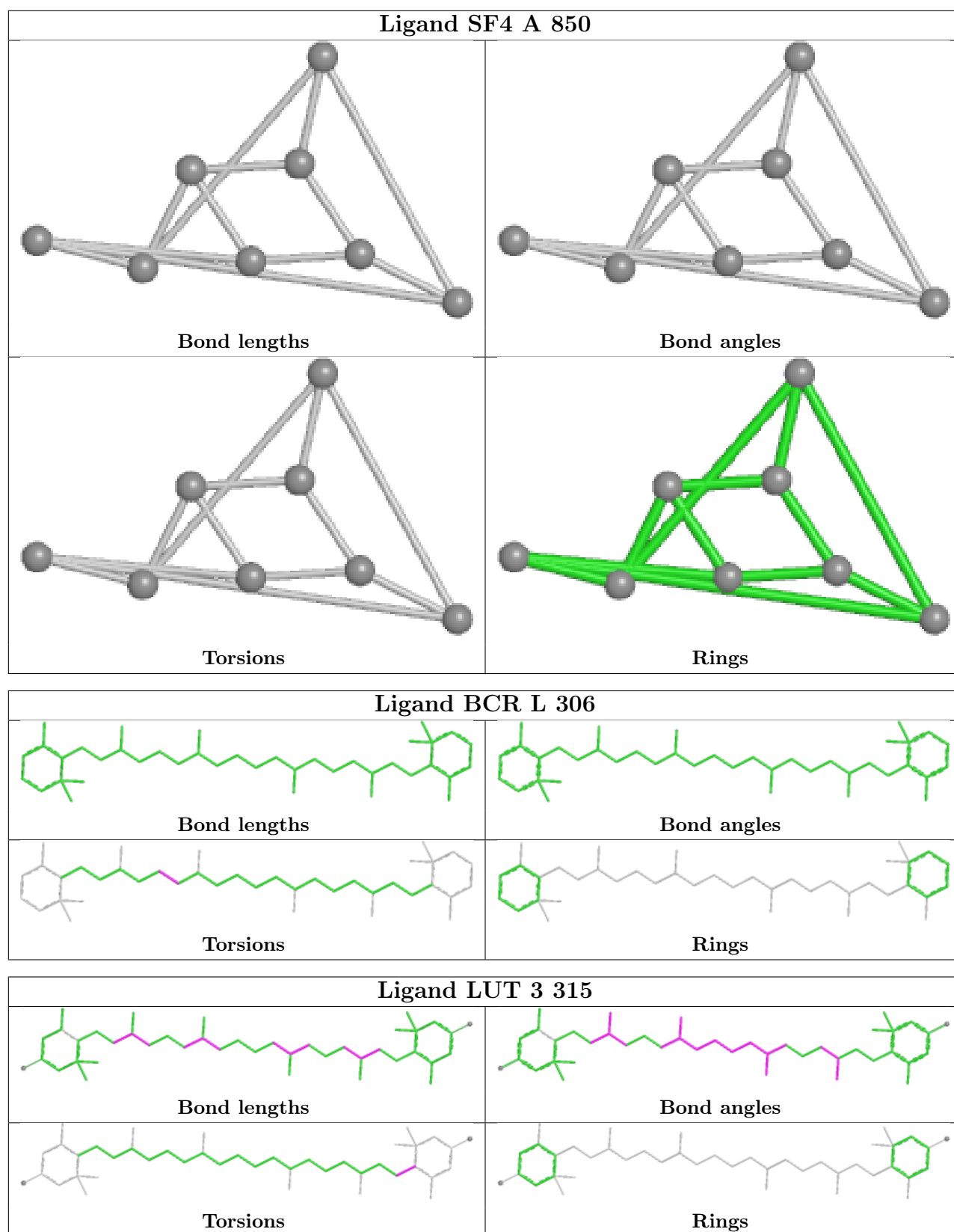
## Ligand CLA A 821

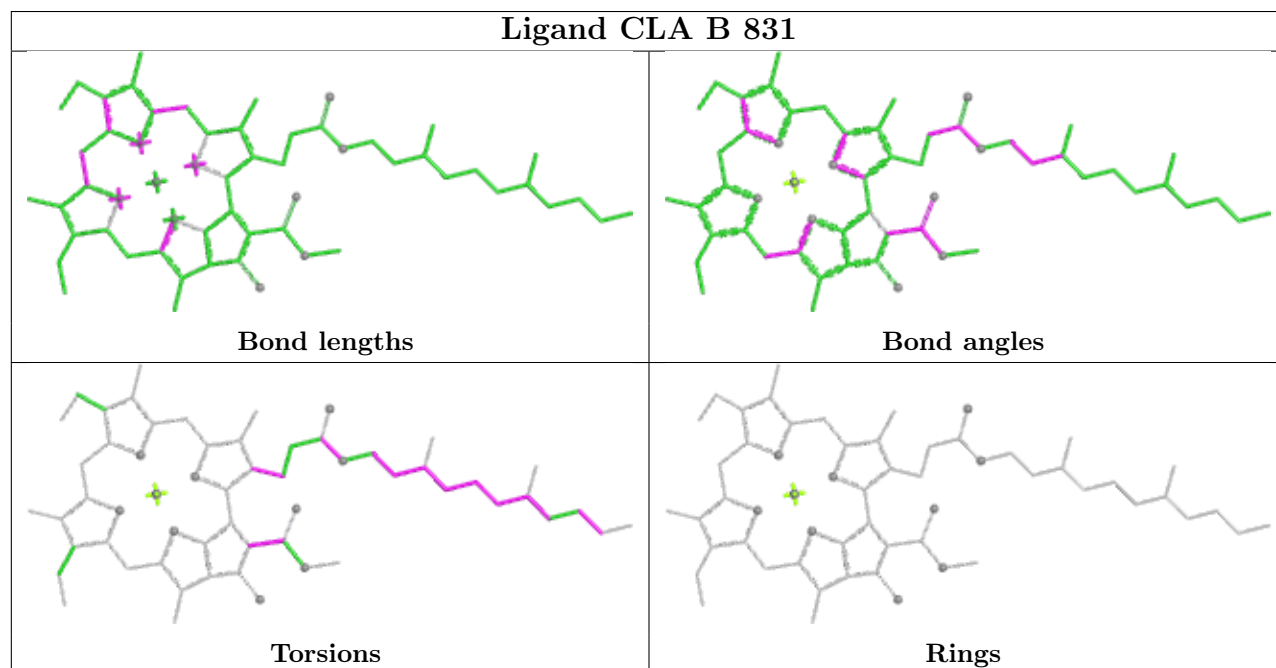
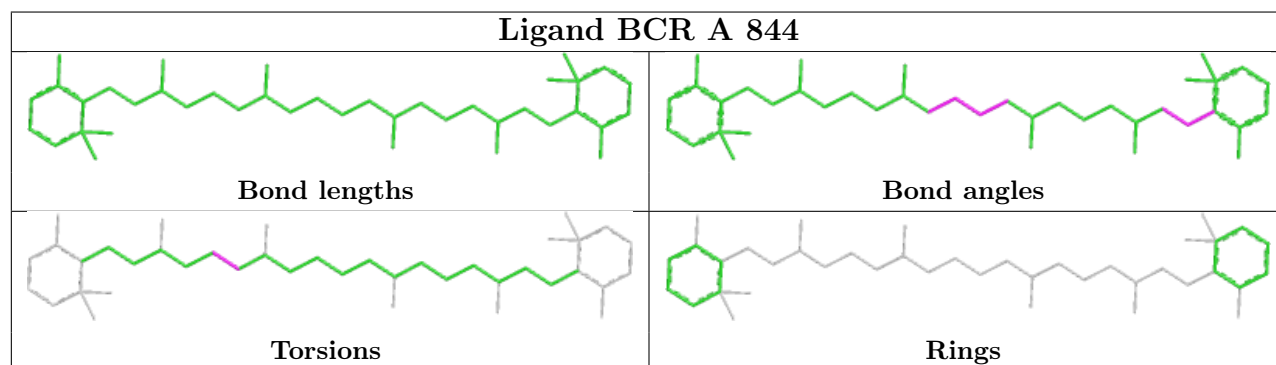
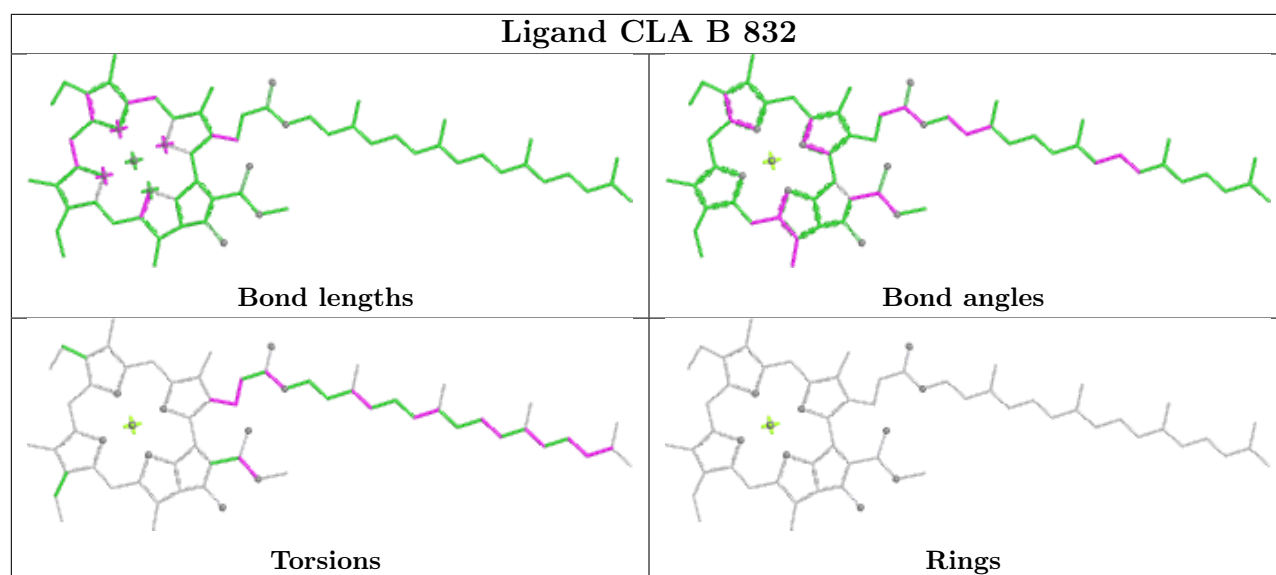


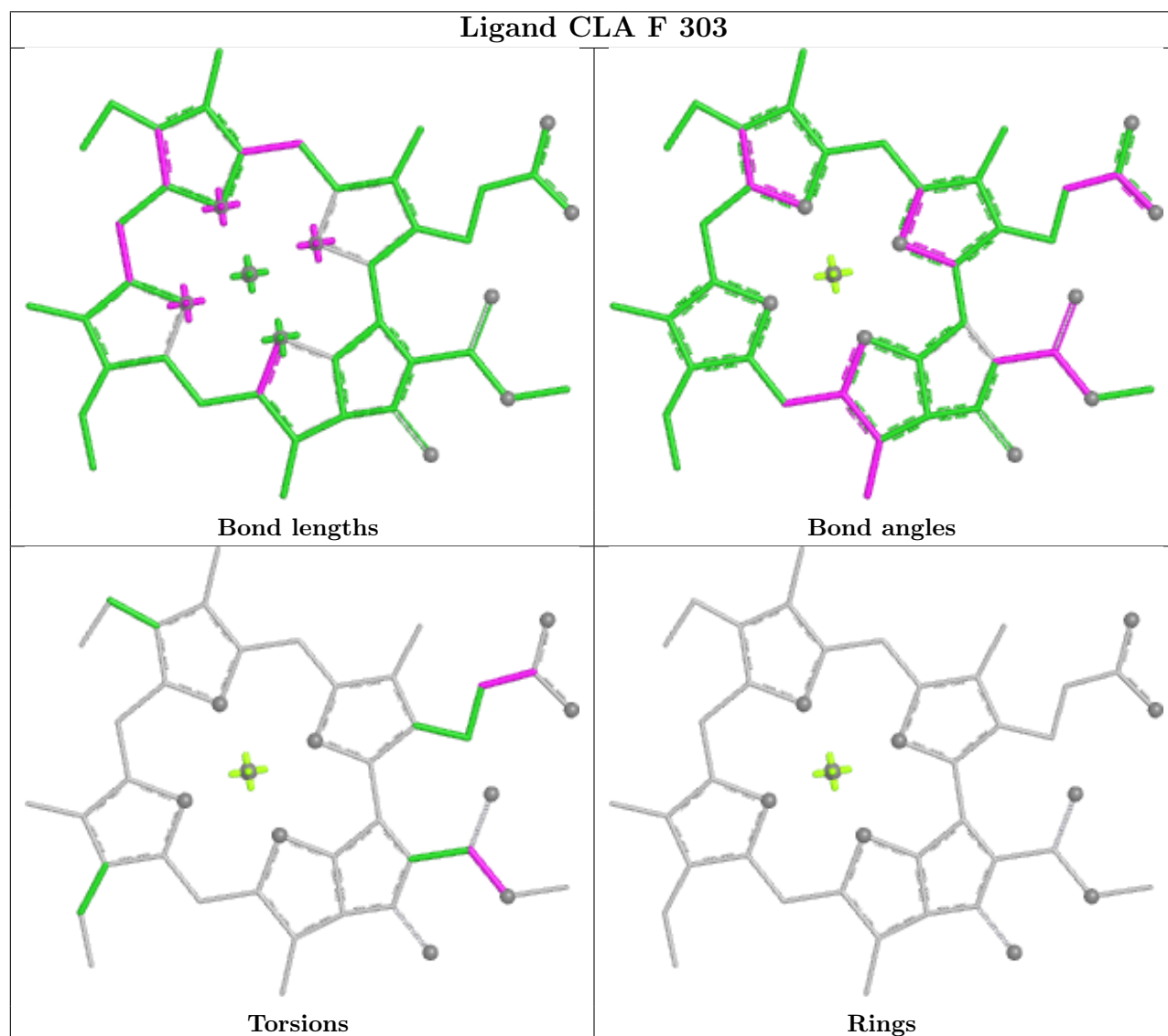
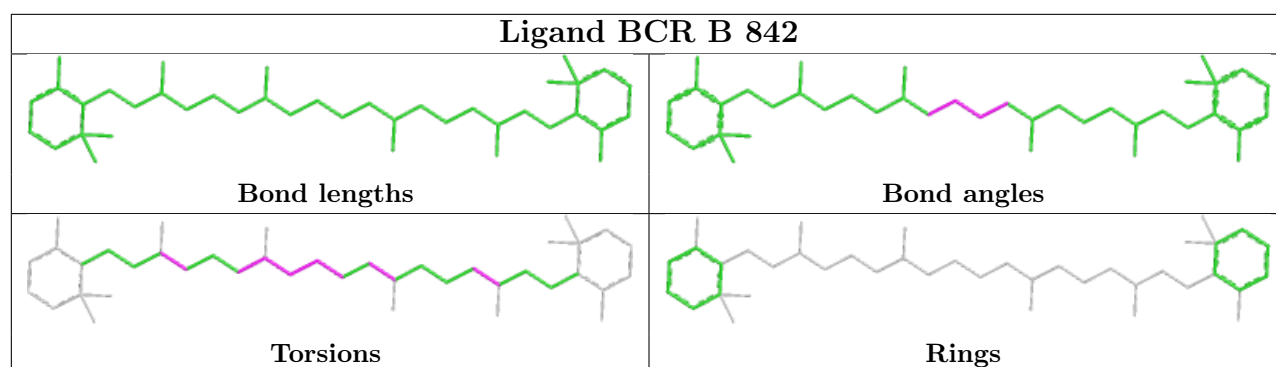
## Ligand CLA B 812

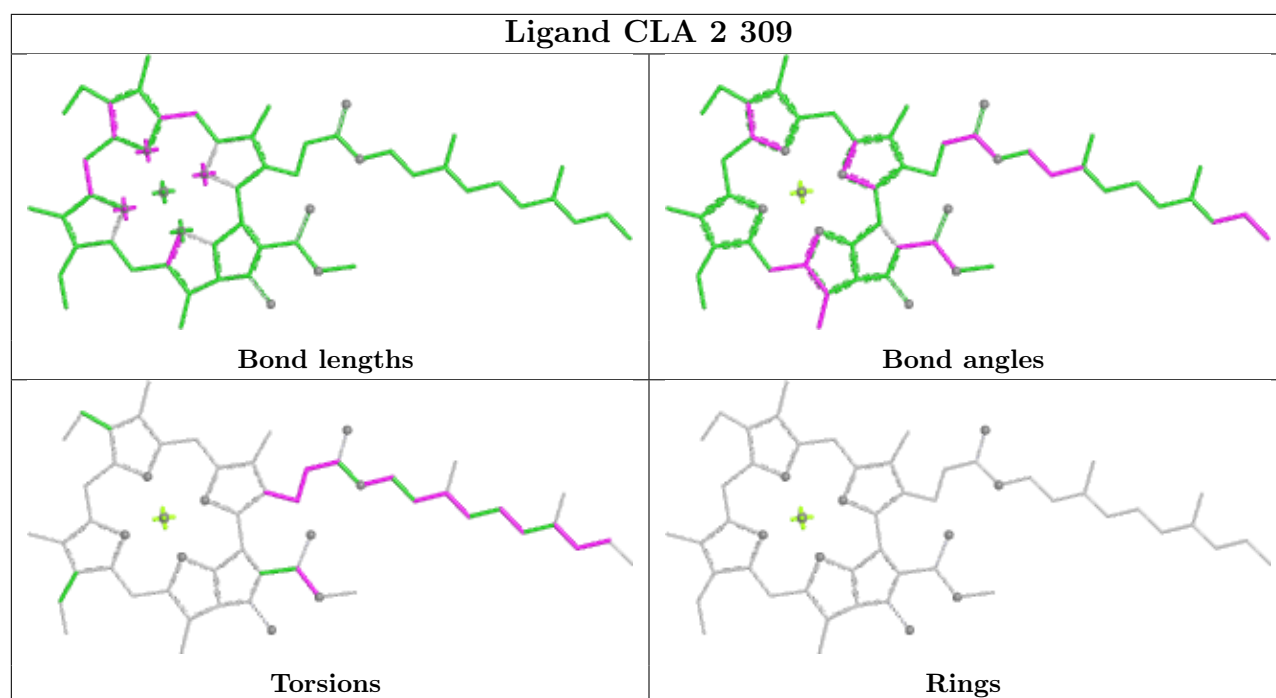




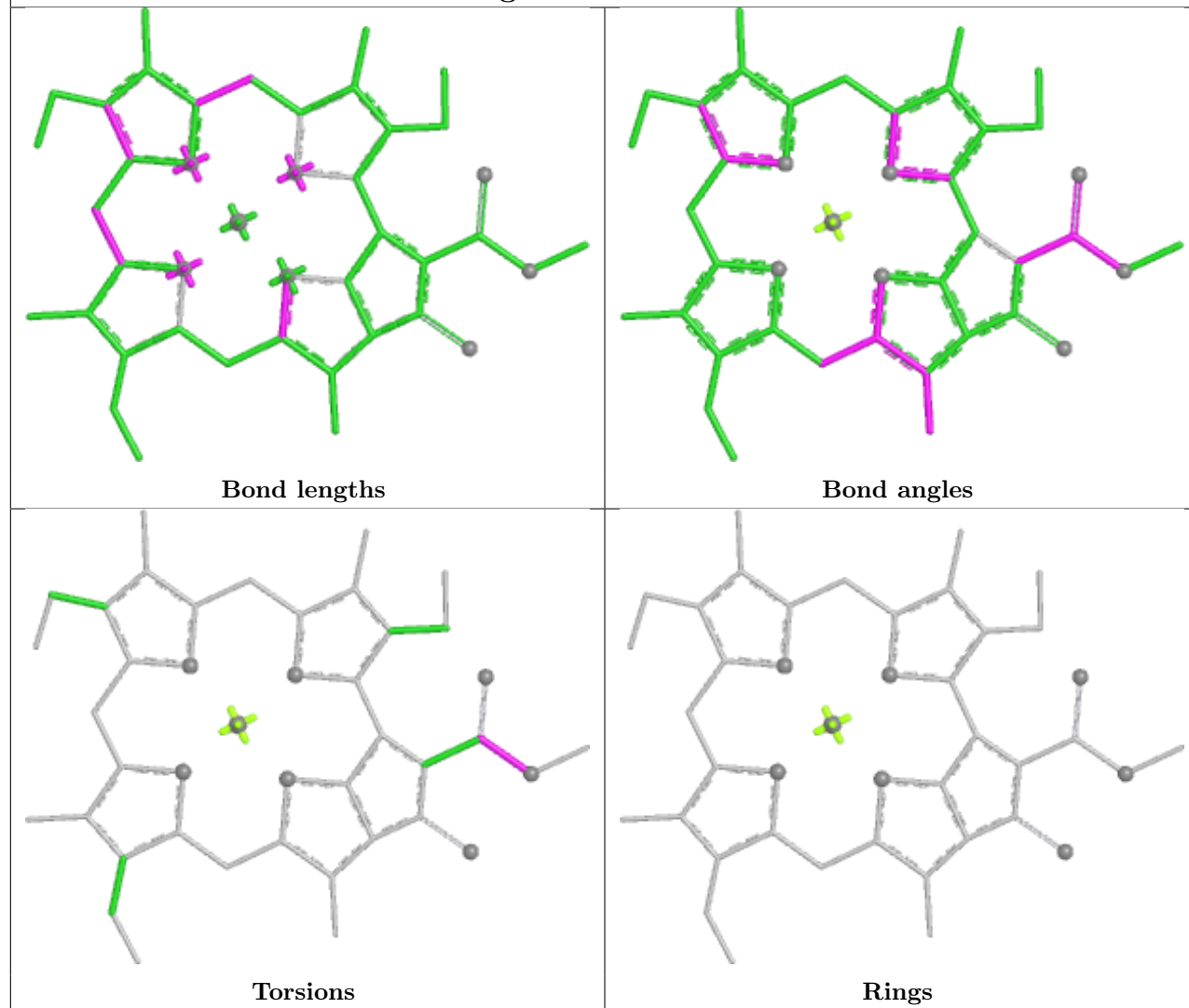




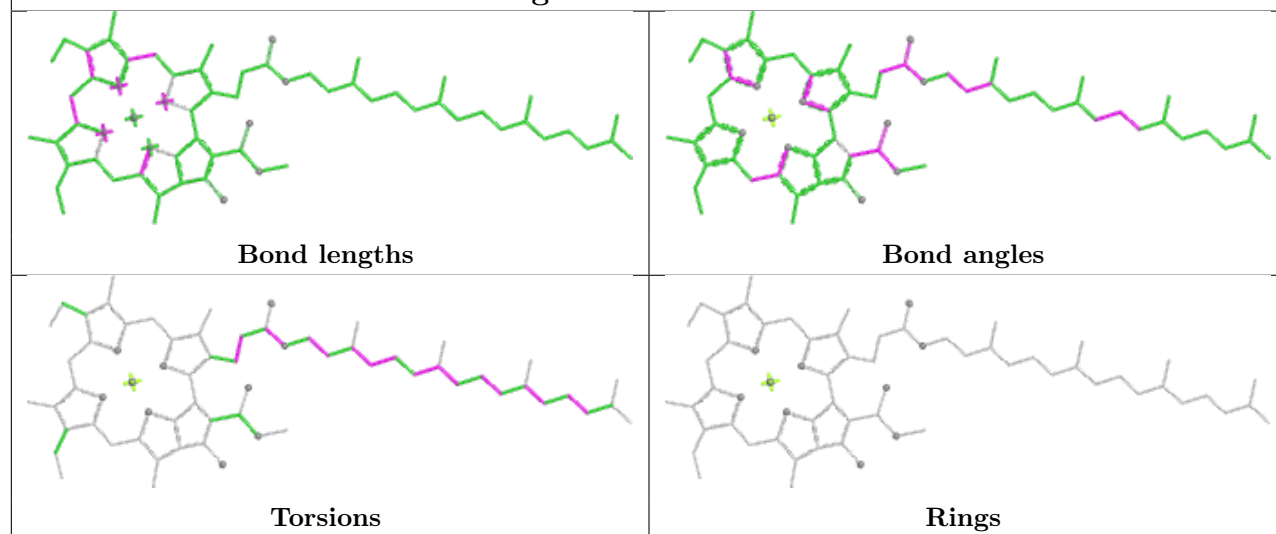




## Ligand CLA 3 305

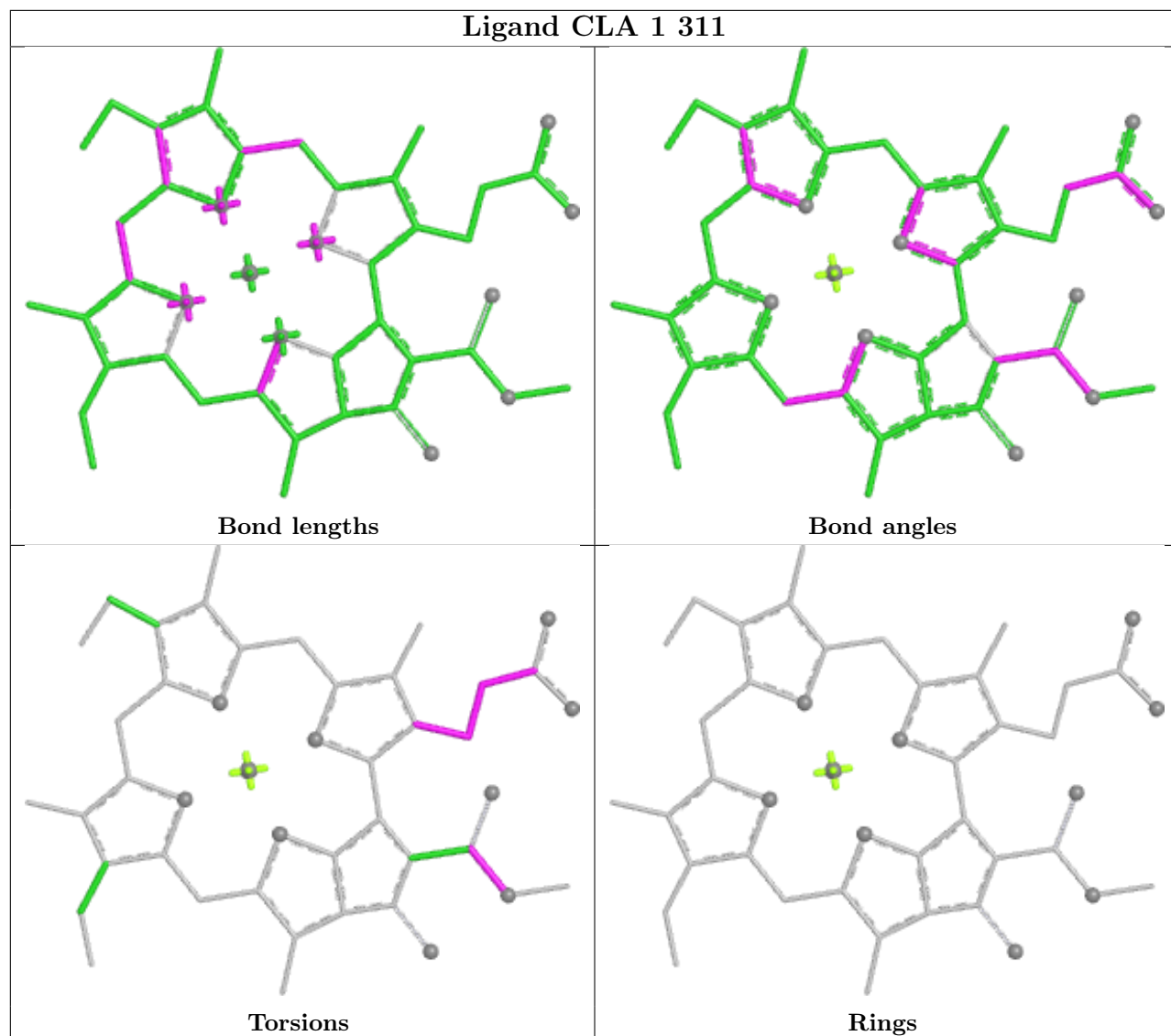


## Ligand CLA A 839

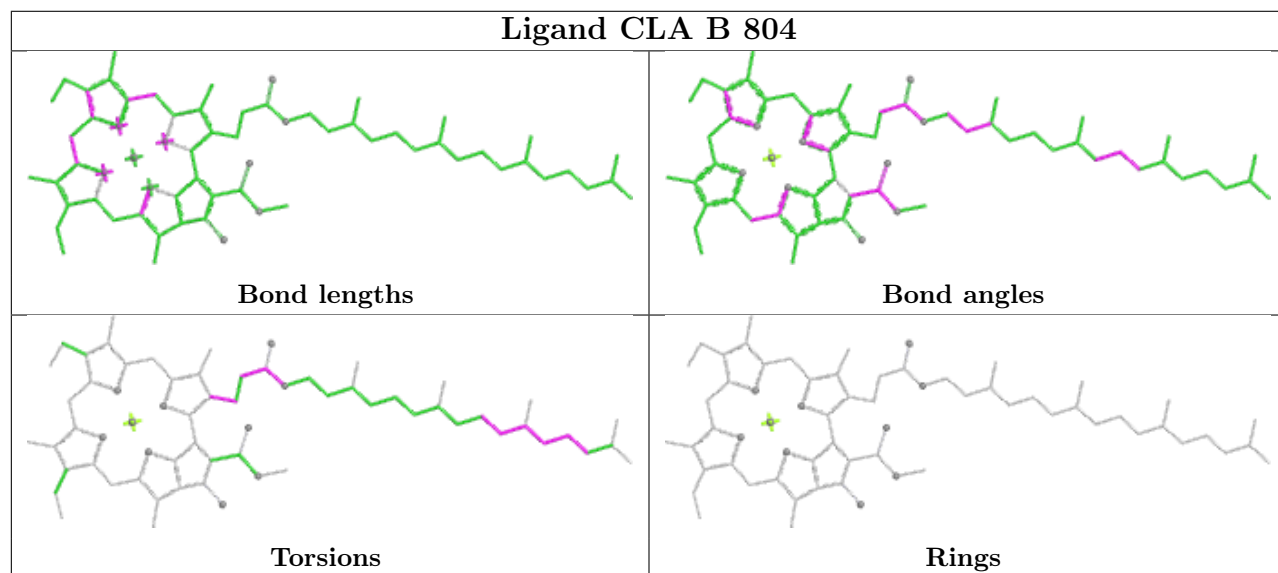


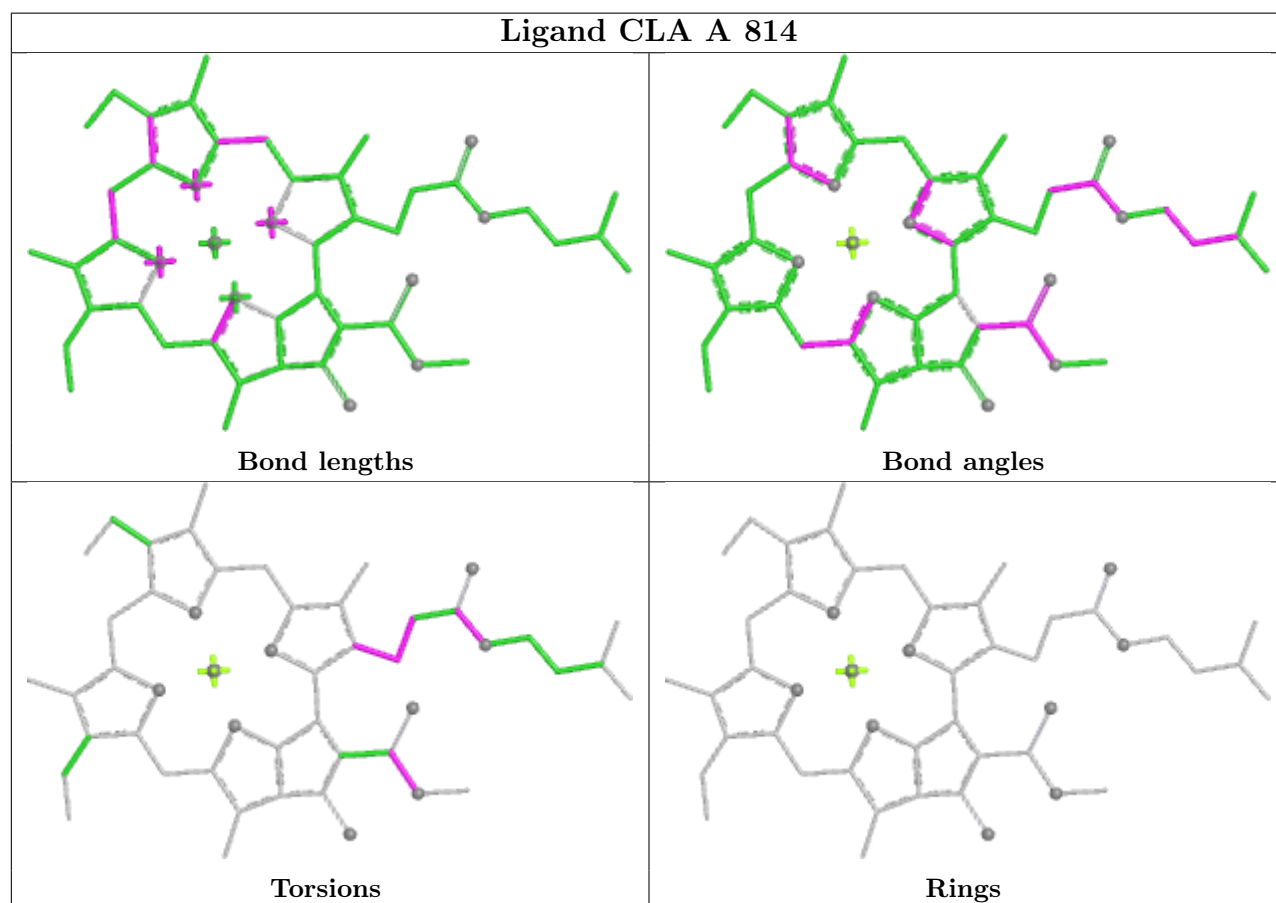
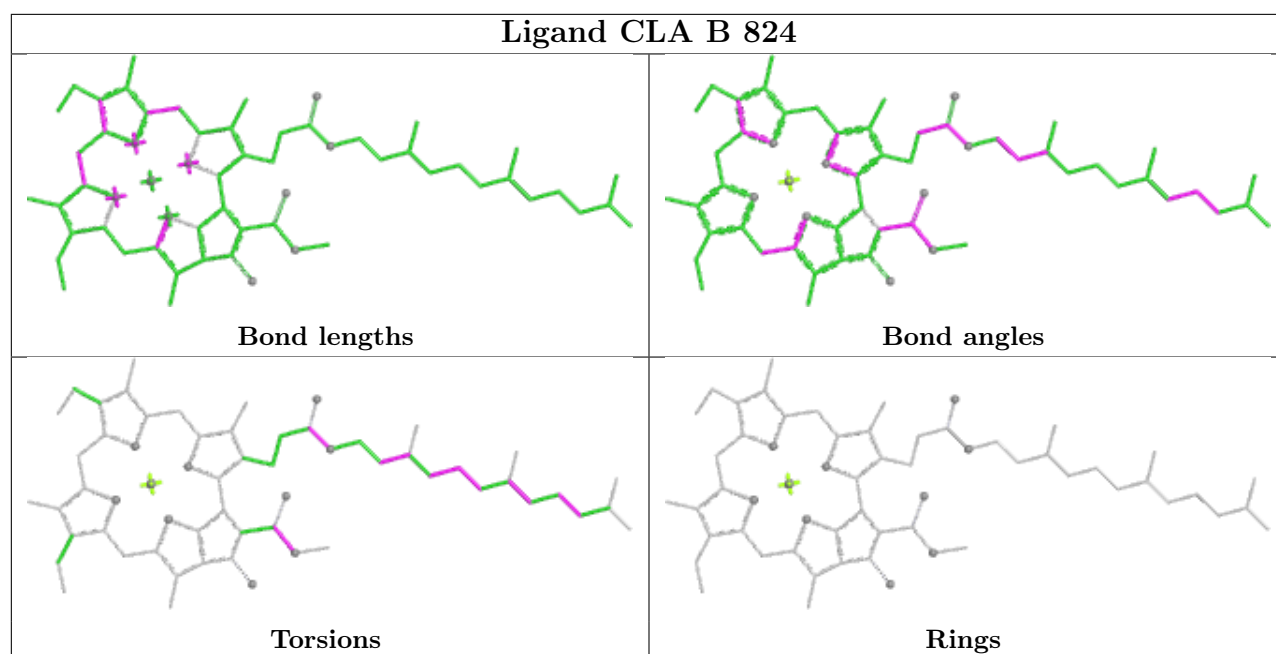


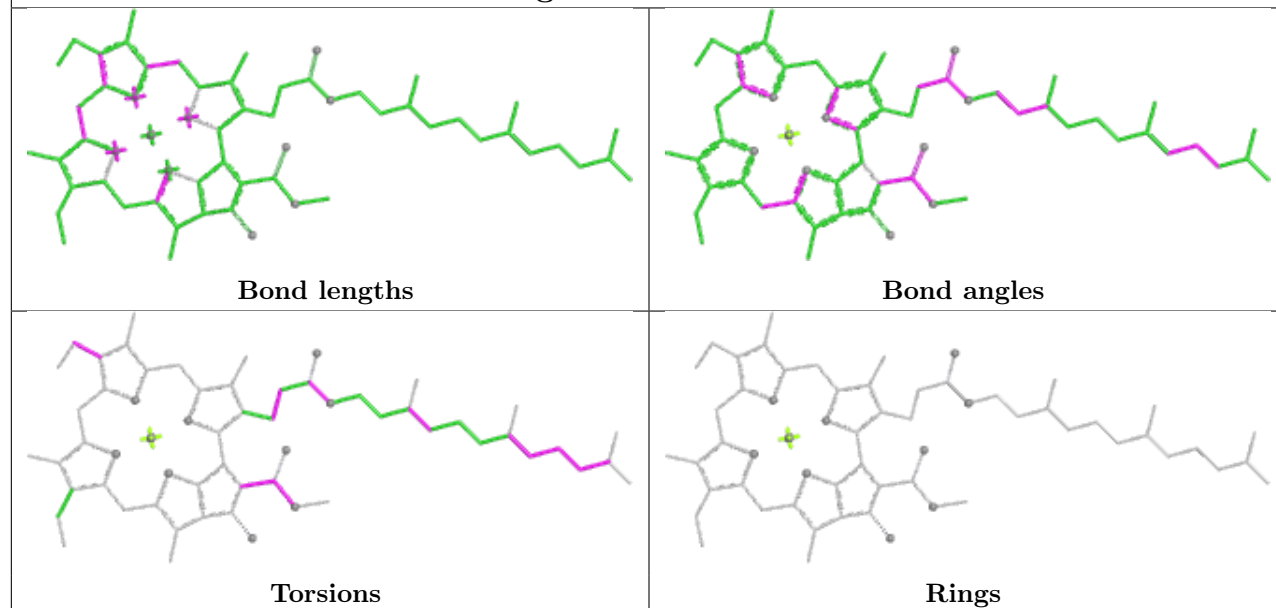
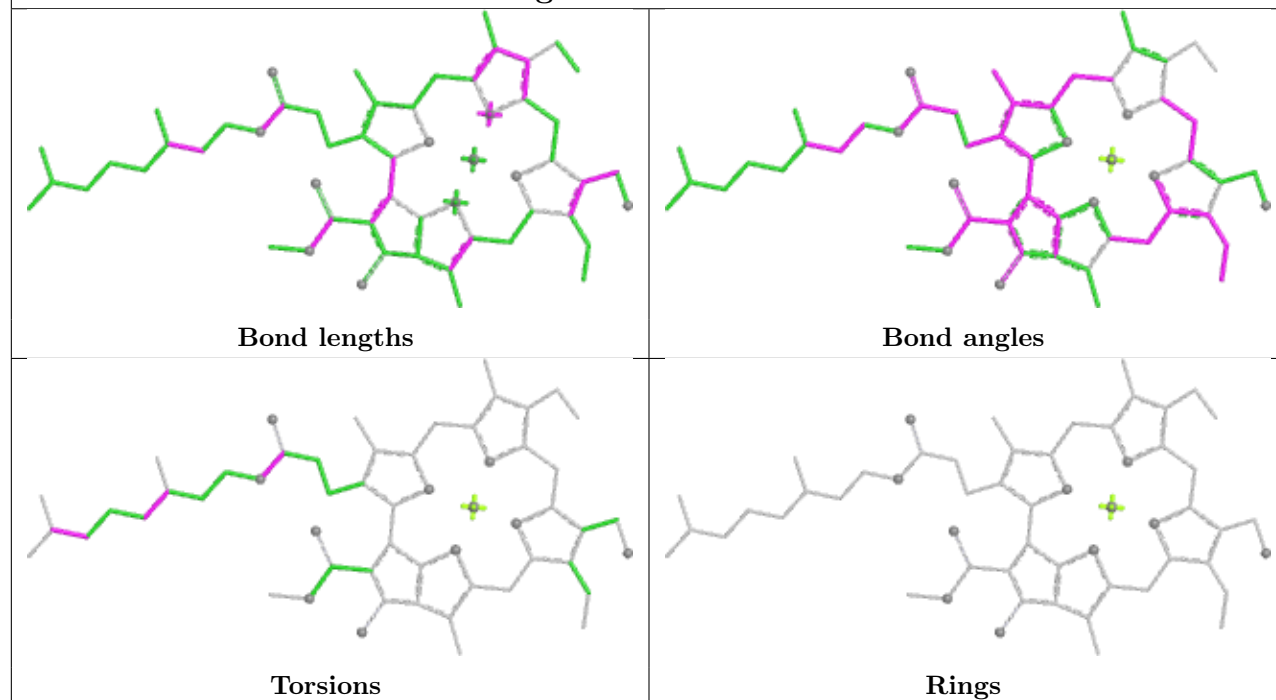
## Ligand CLA 1 311



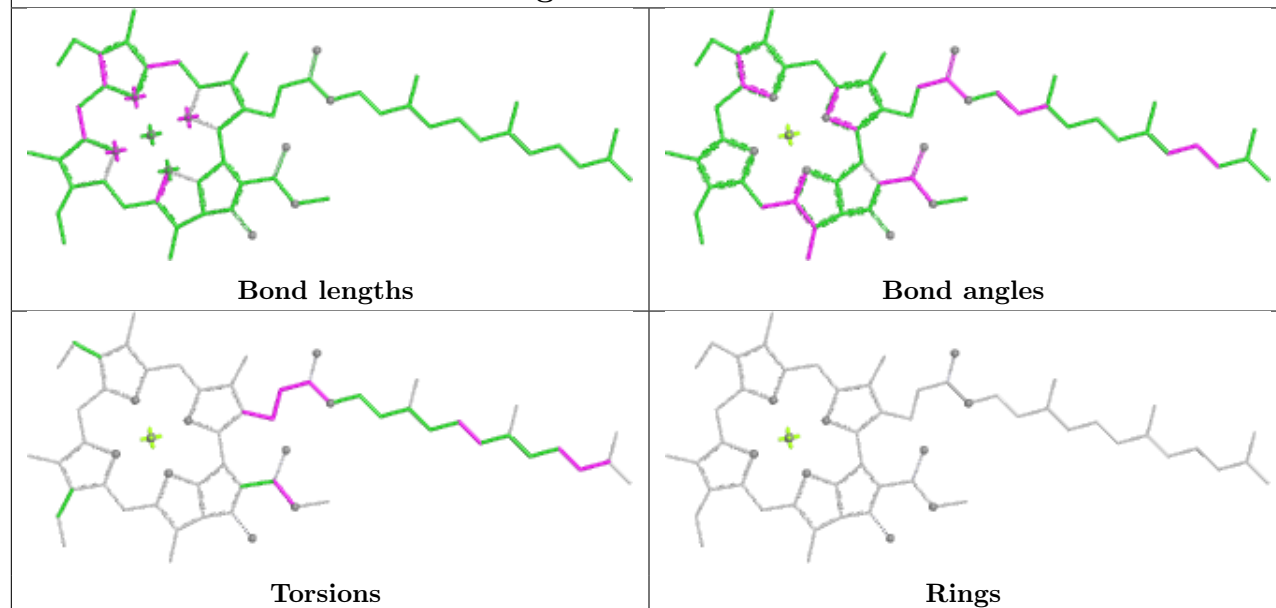
## Ligand CLA B 804



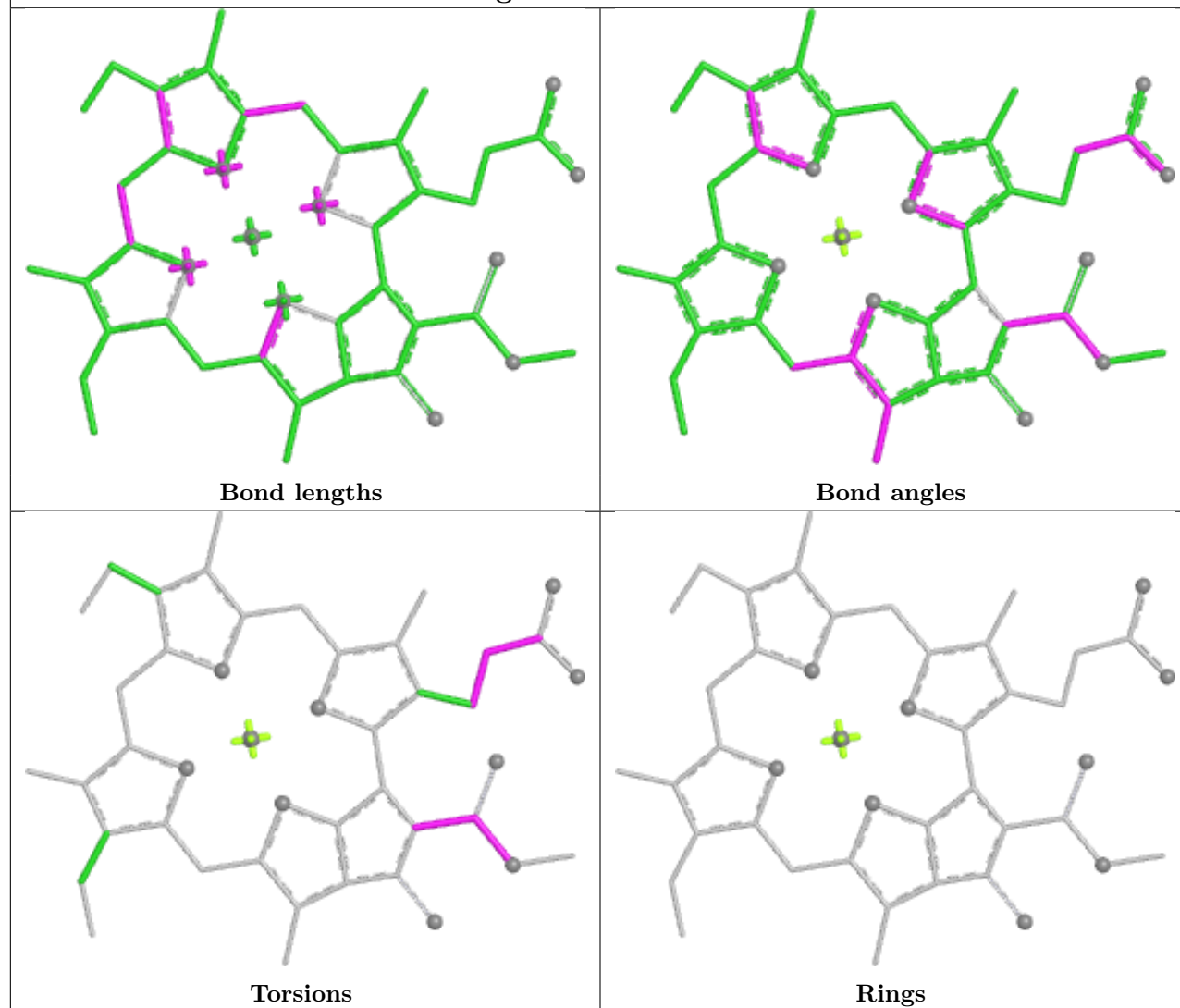


**Ligand CLA 3 301****Ligand CHL 4 304**

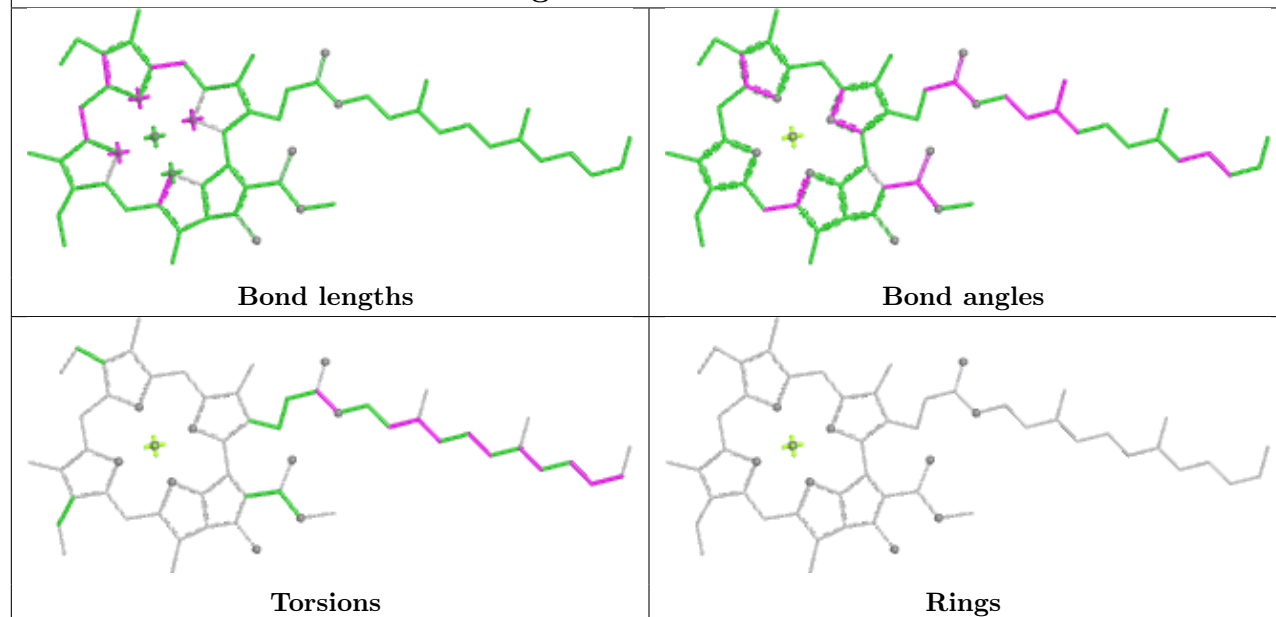
## Ligand CLA 4 302



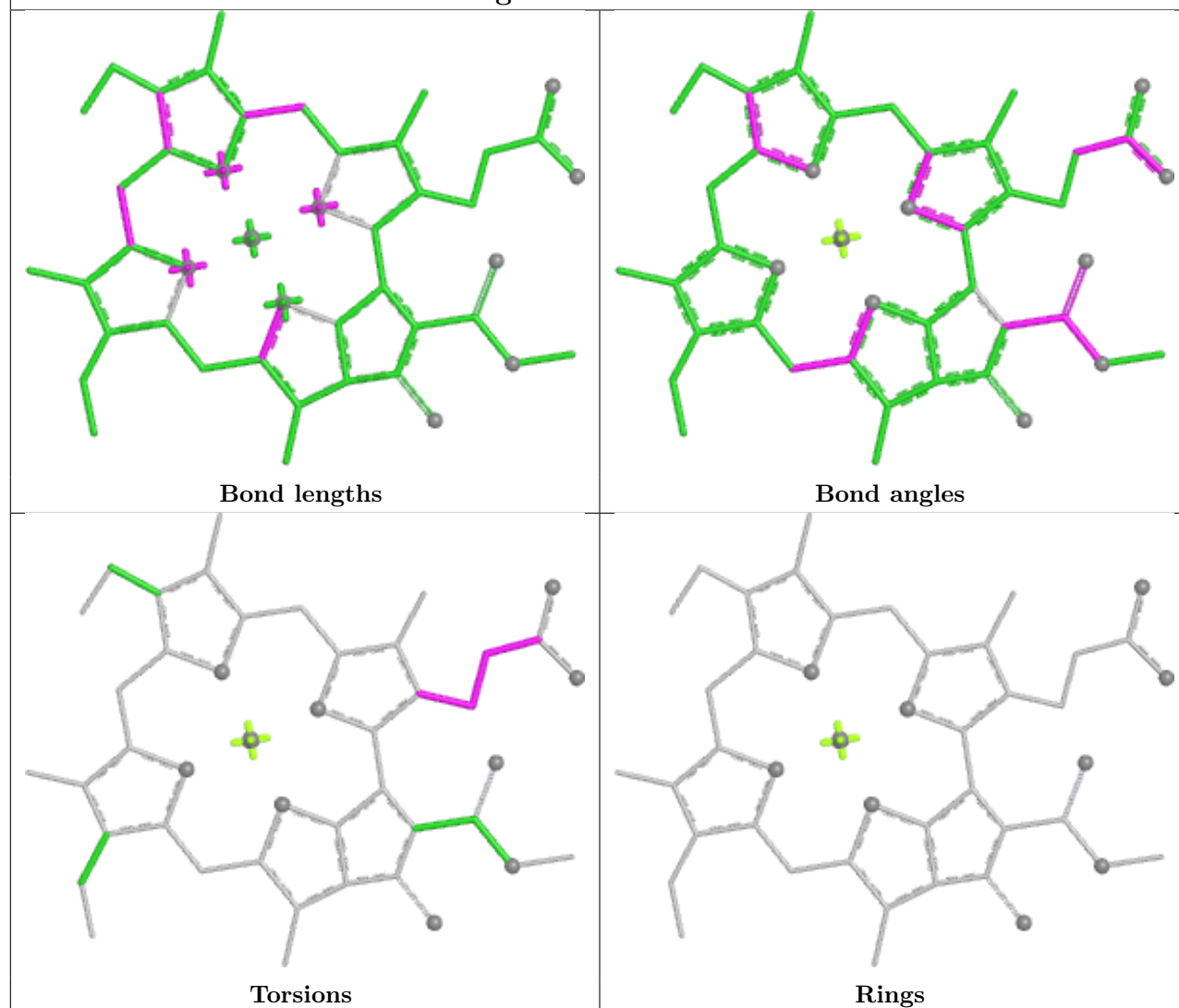
## Ligand CLA 2 311



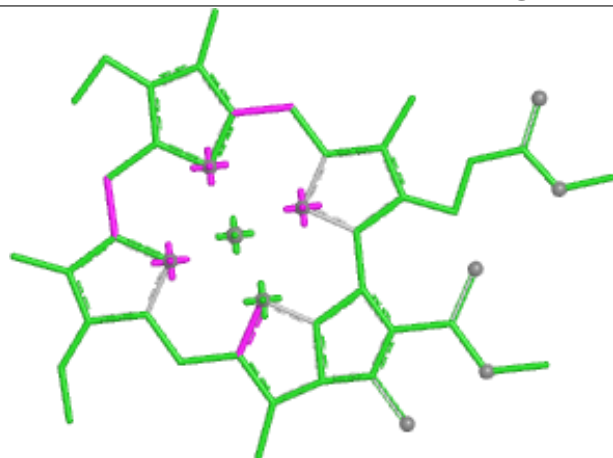
## Ligand CLA A 809



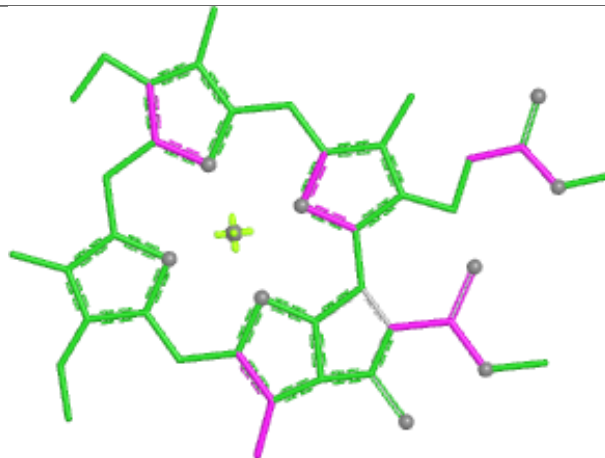
## Ligand CLA 3 306



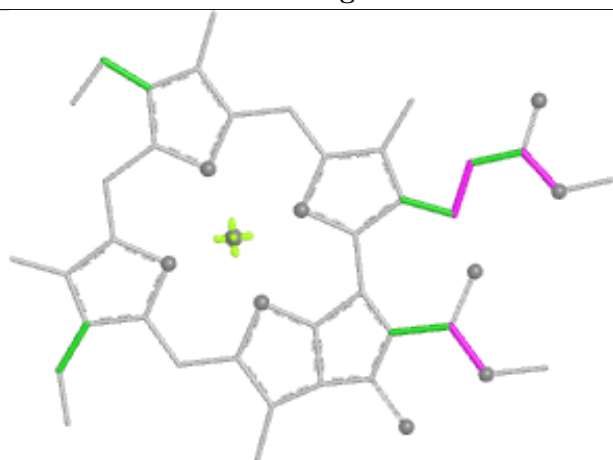
## Ligand CLA G 204



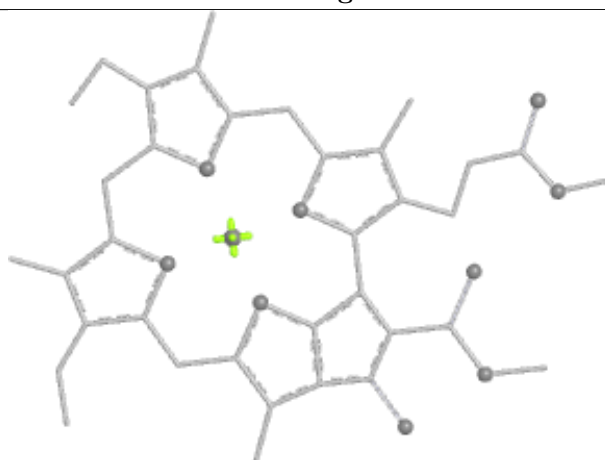
Bond lengths



Bond angles

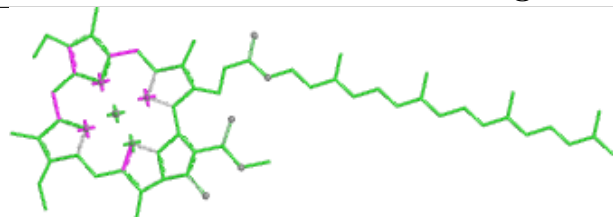


Torsions

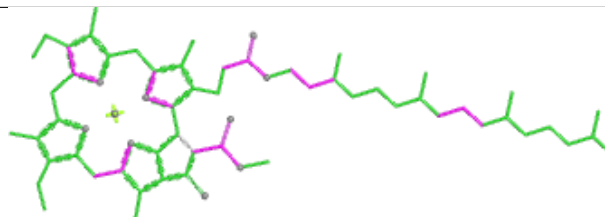


Rings

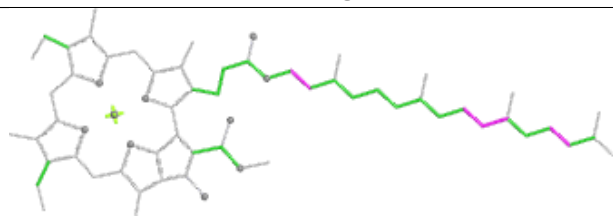
## Ligand CLA A 825



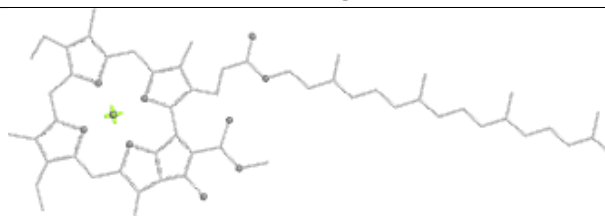
Bond lengths



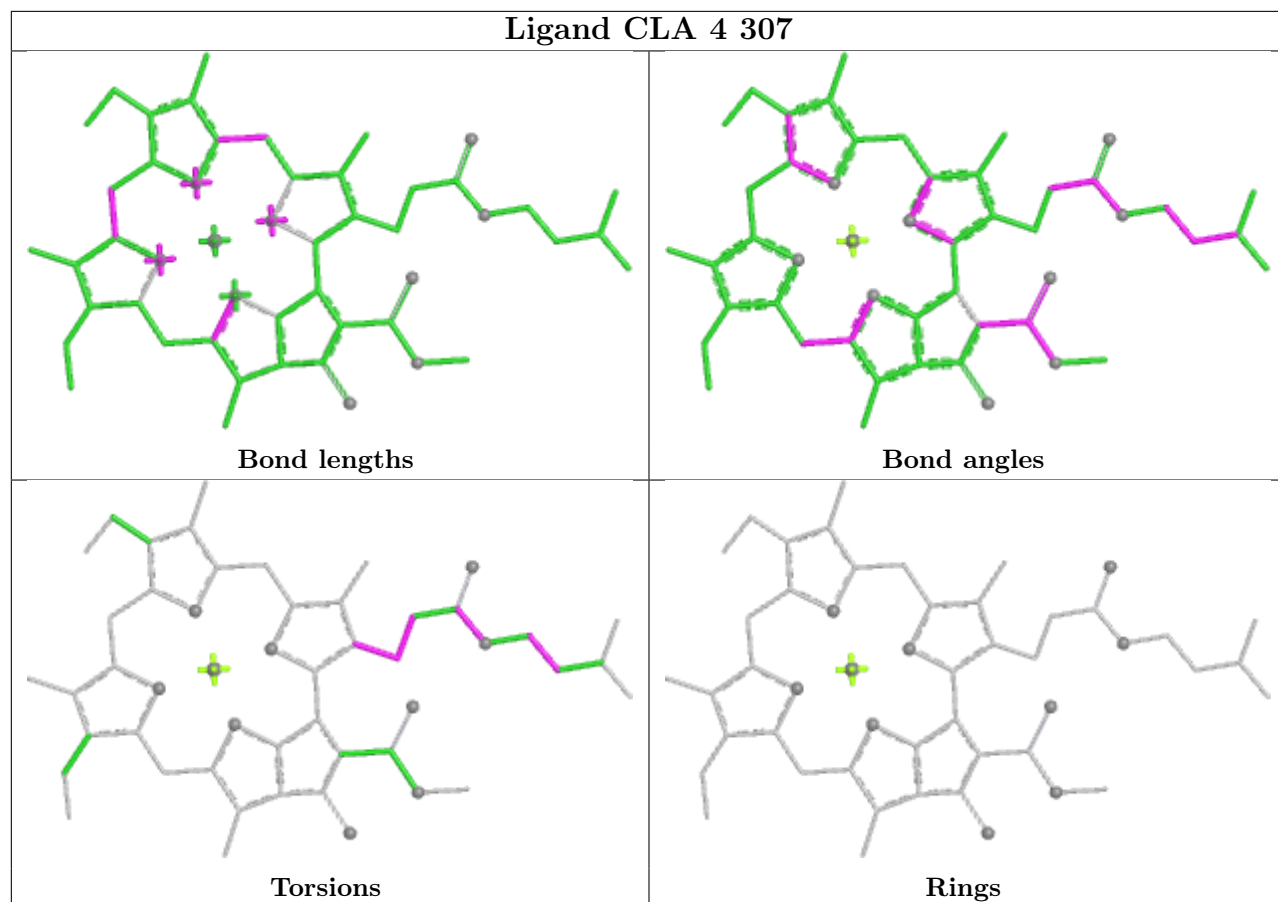
Bond angles

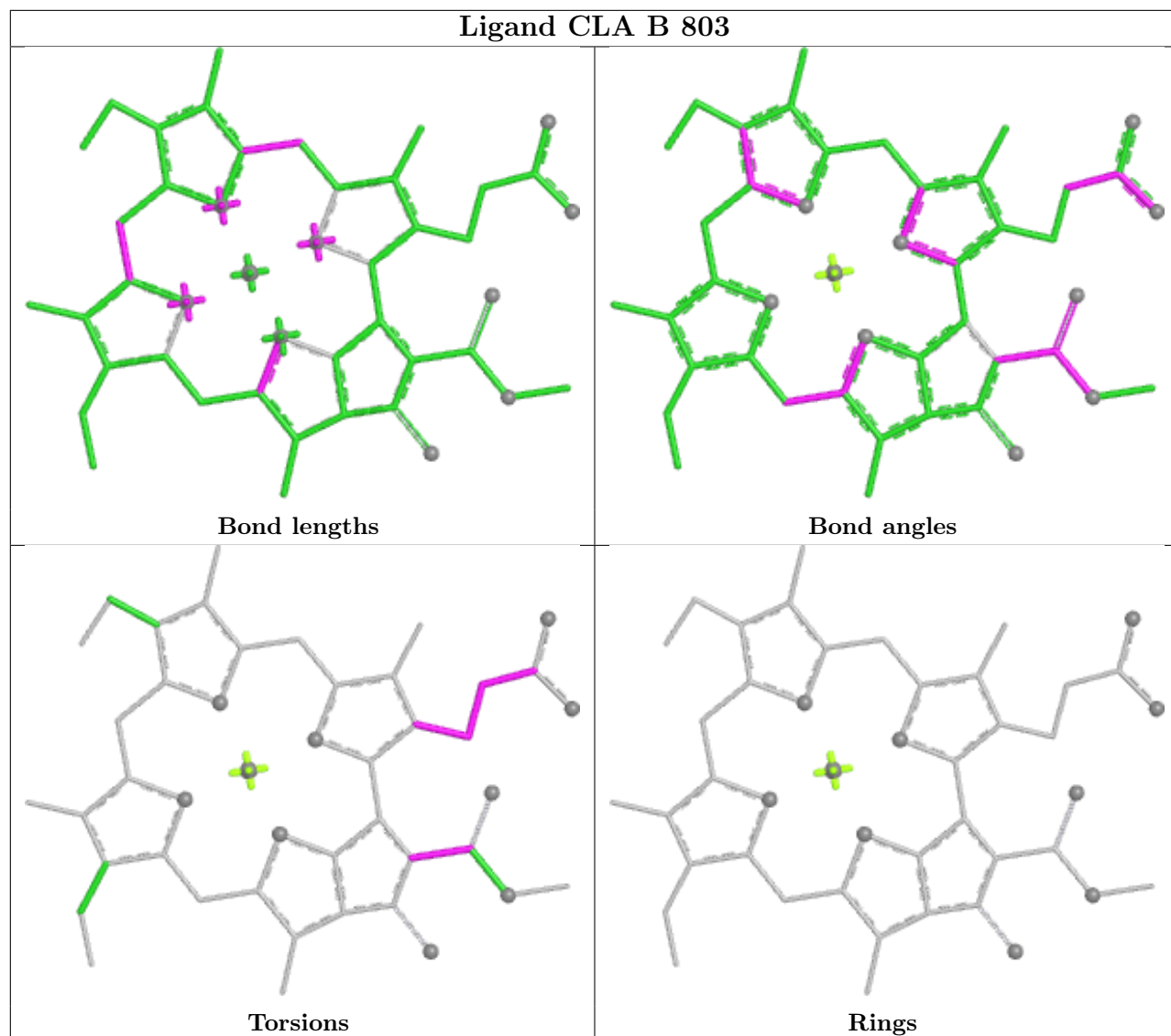


Torsions



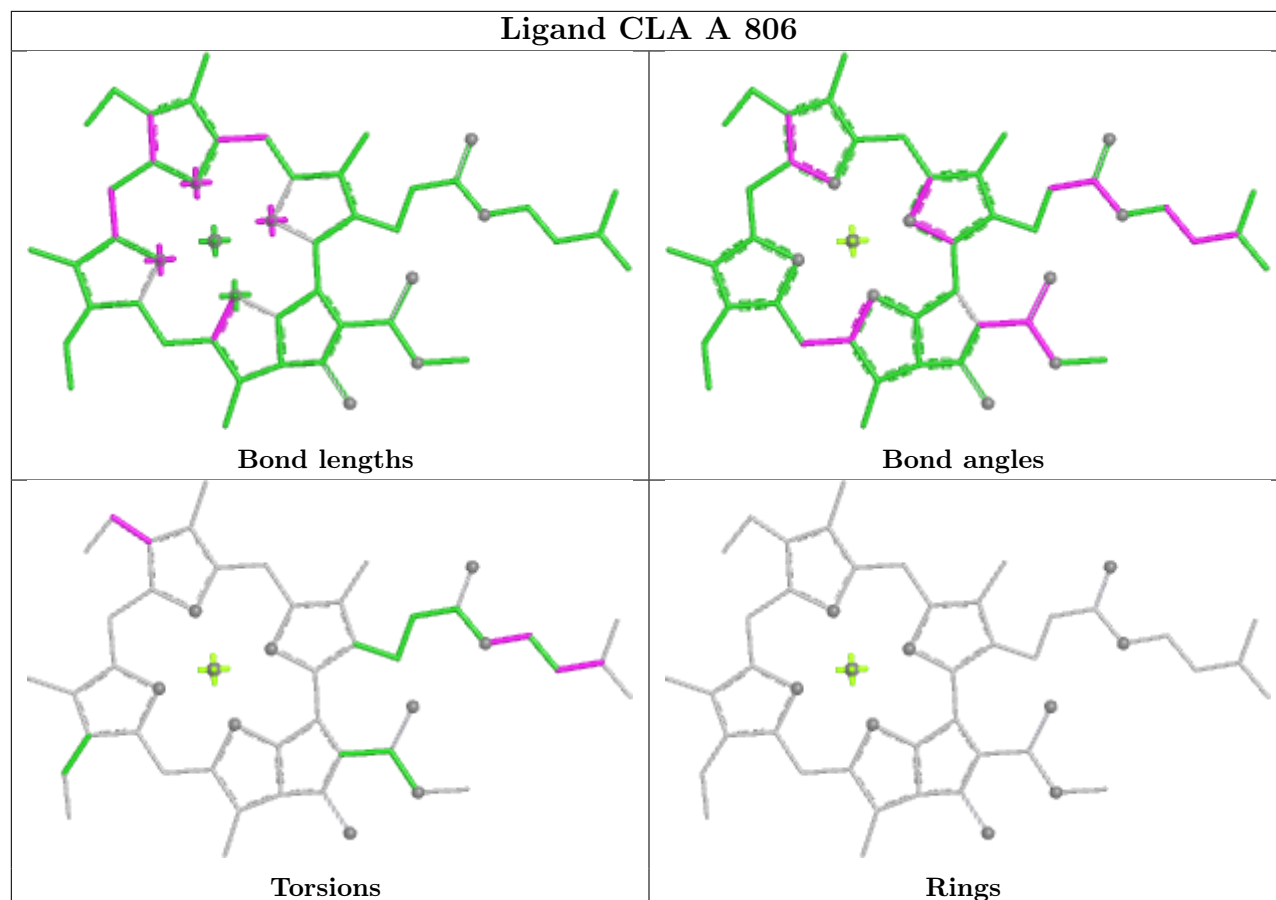
Rings



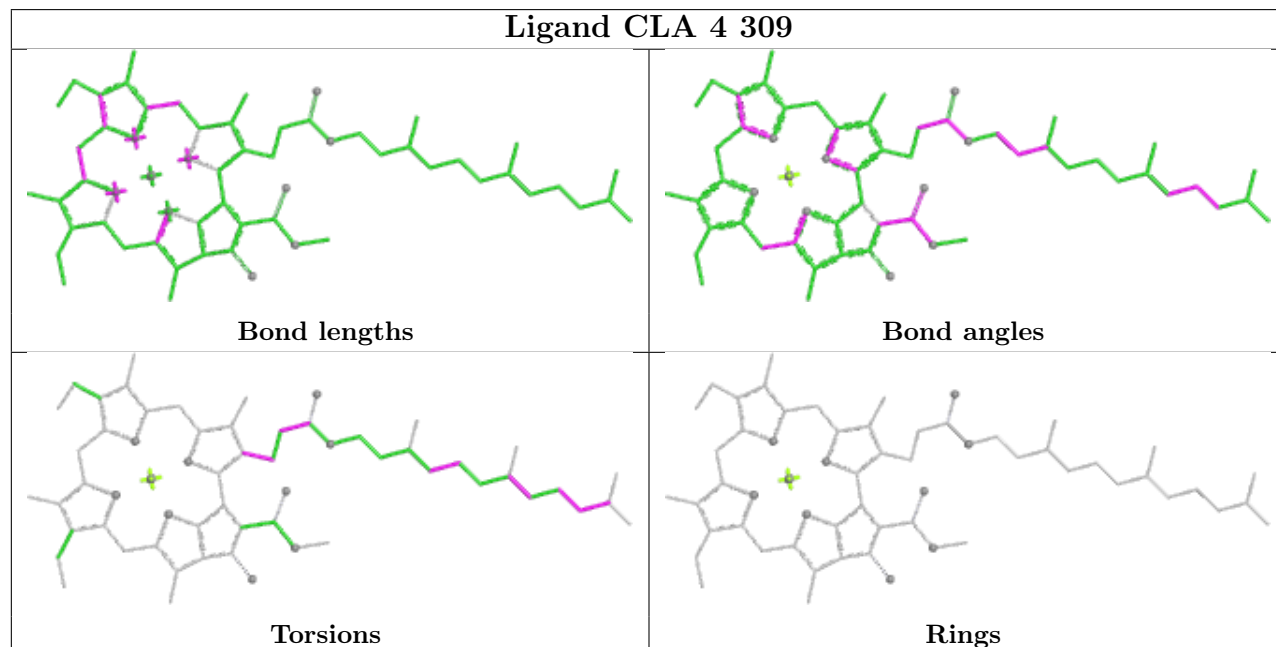


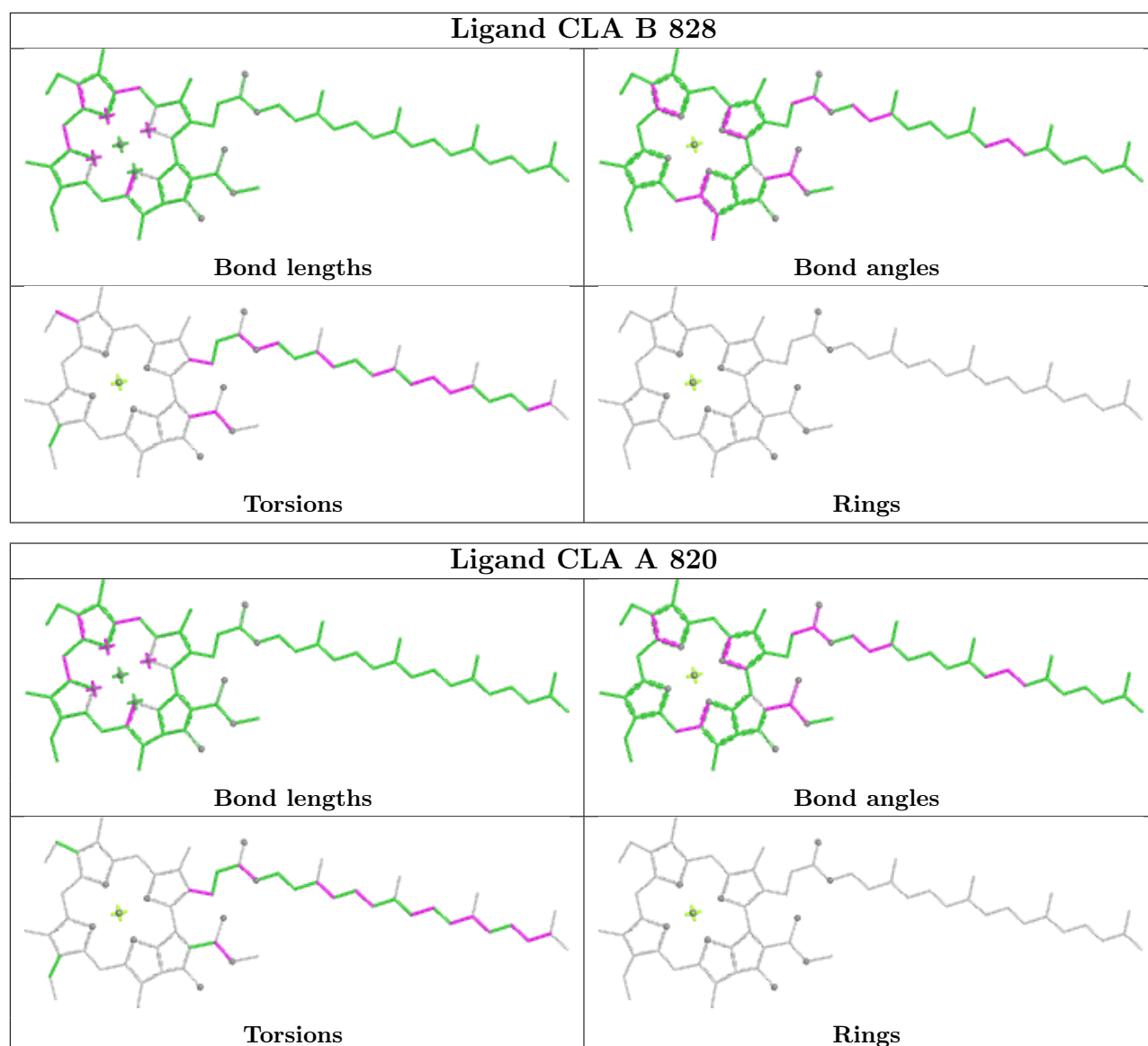


## Ligand CLA A 806

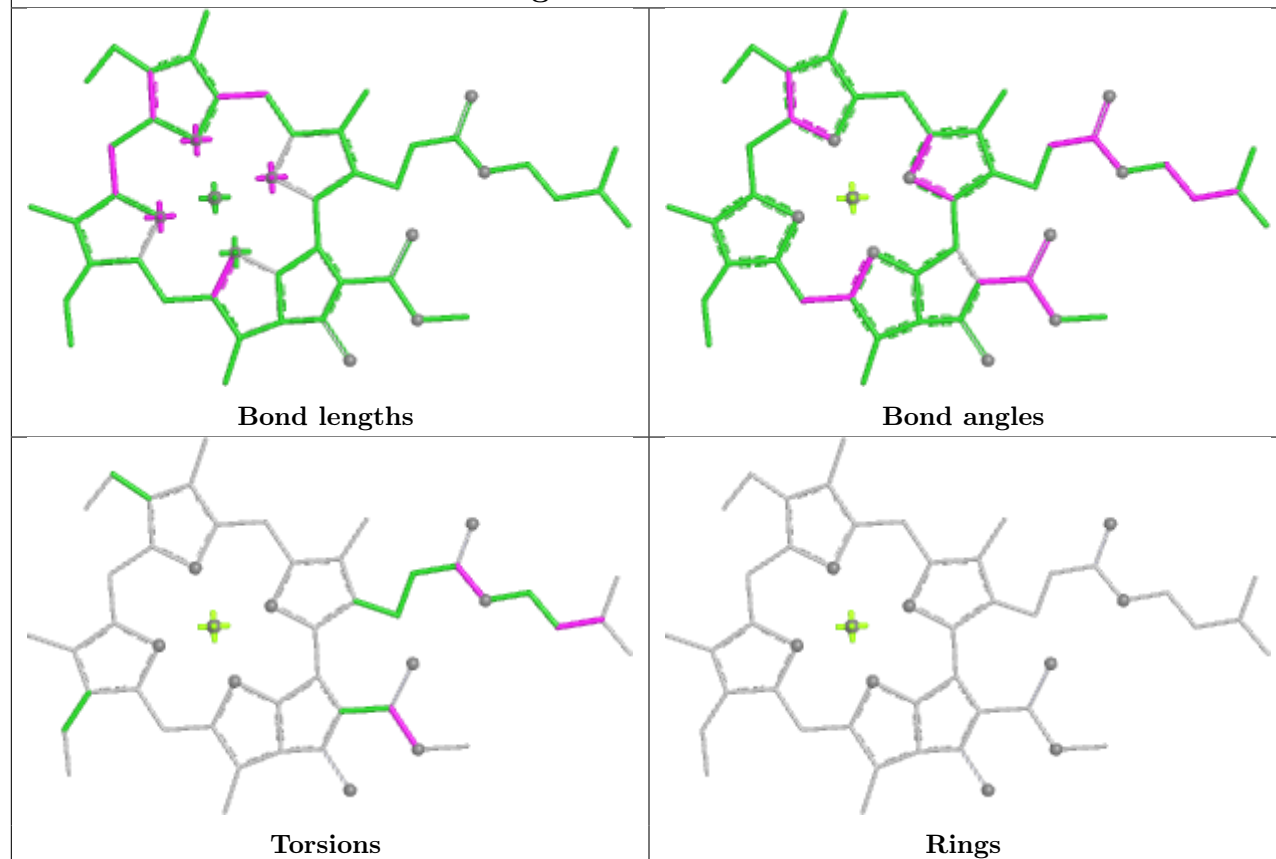


## Ligand CLA 4 309

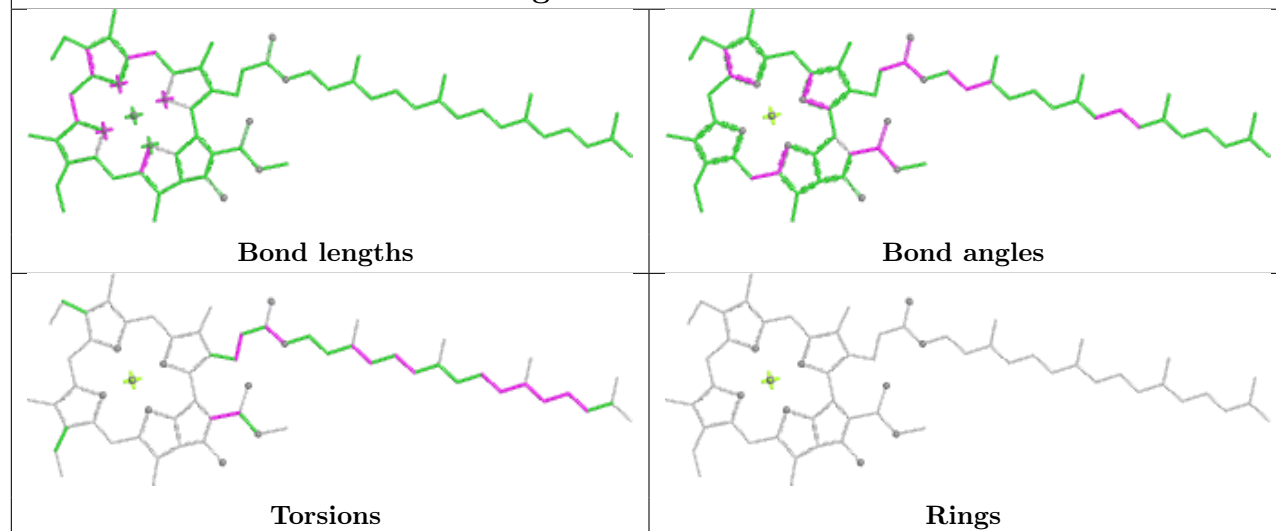




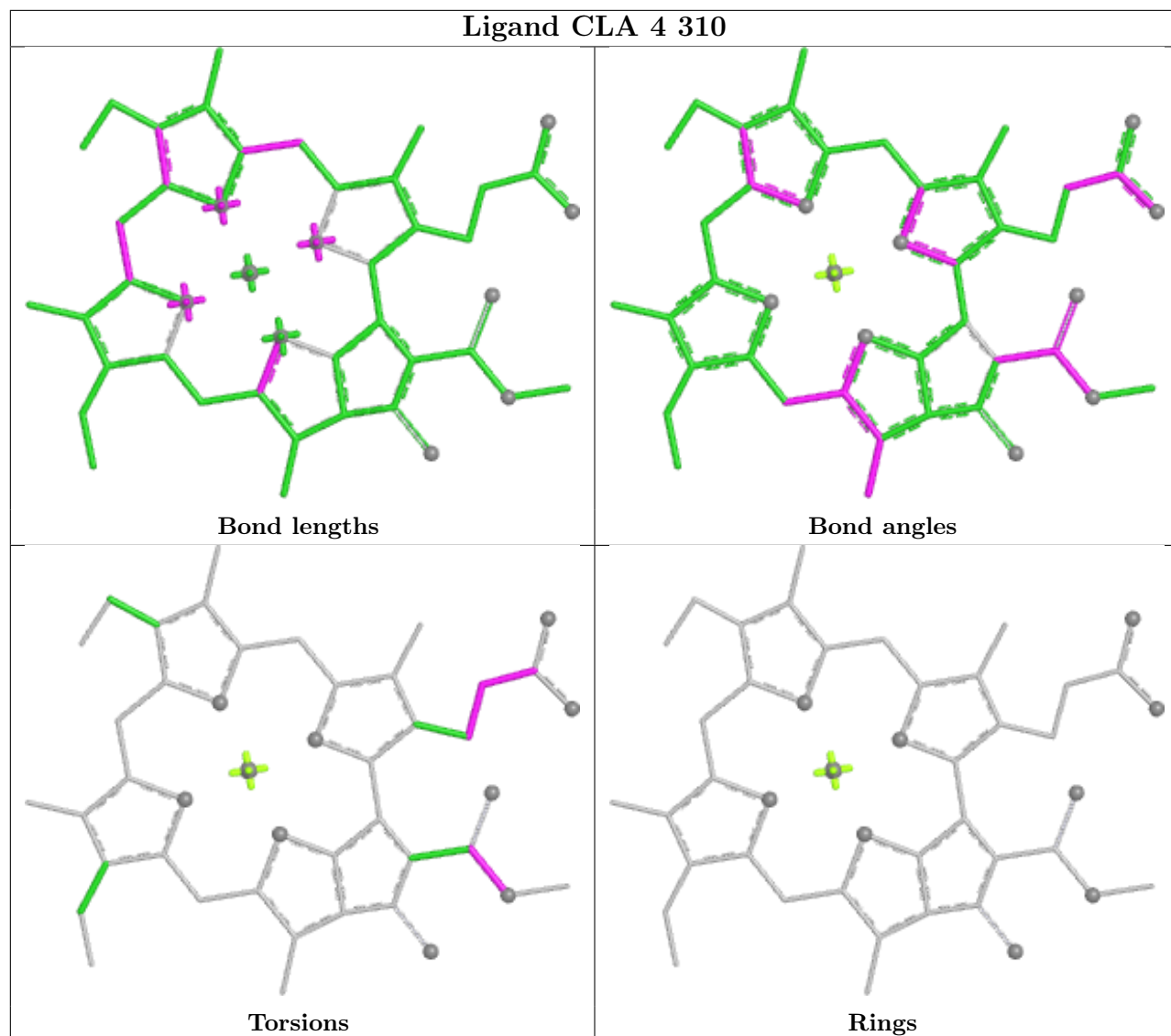
## Ligand CLA A 833



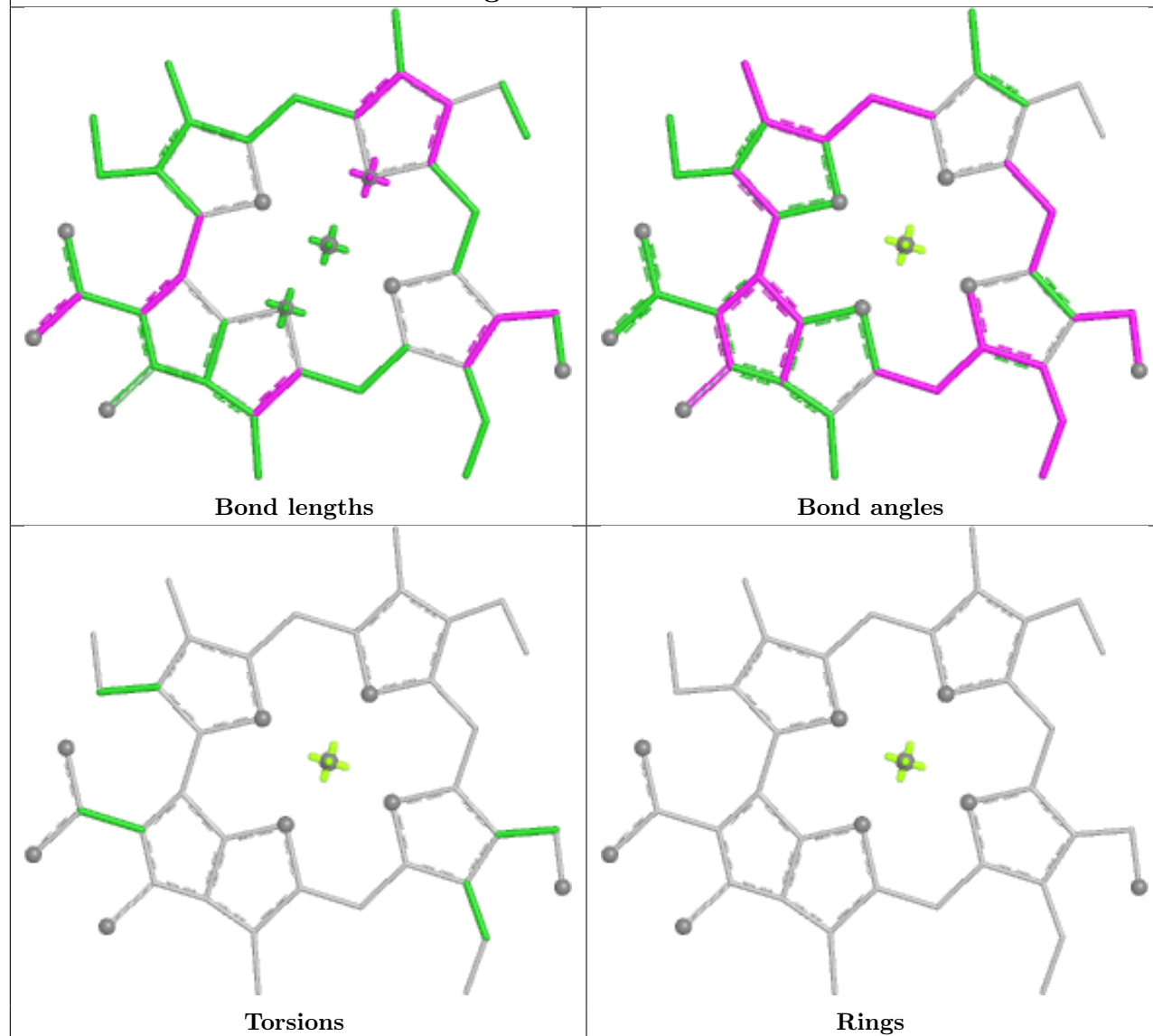
## Ligand CLA B 835



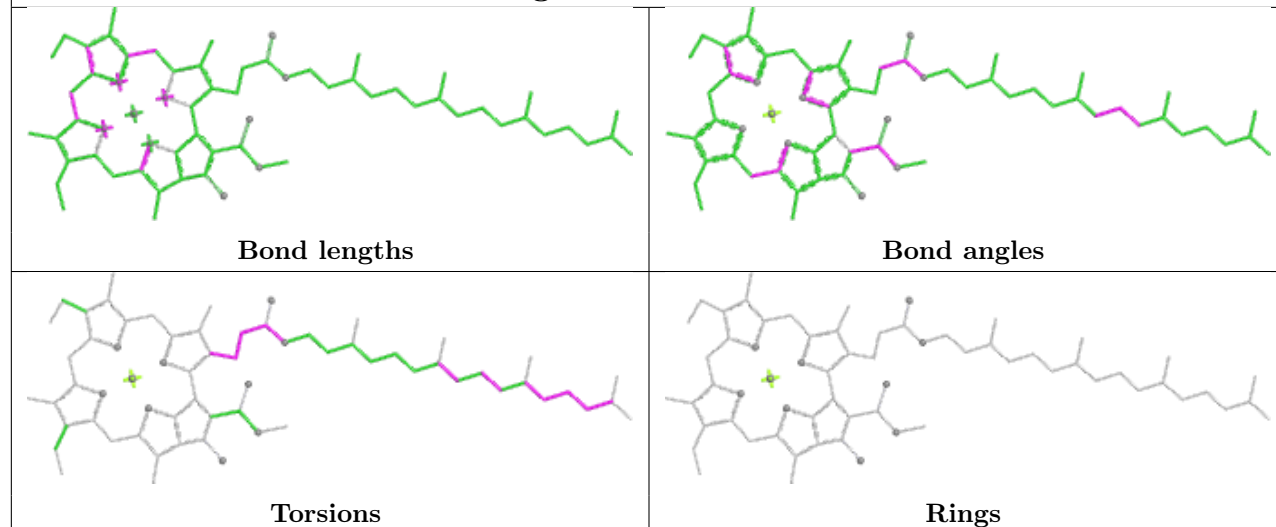
## Ligand CLA 4 310

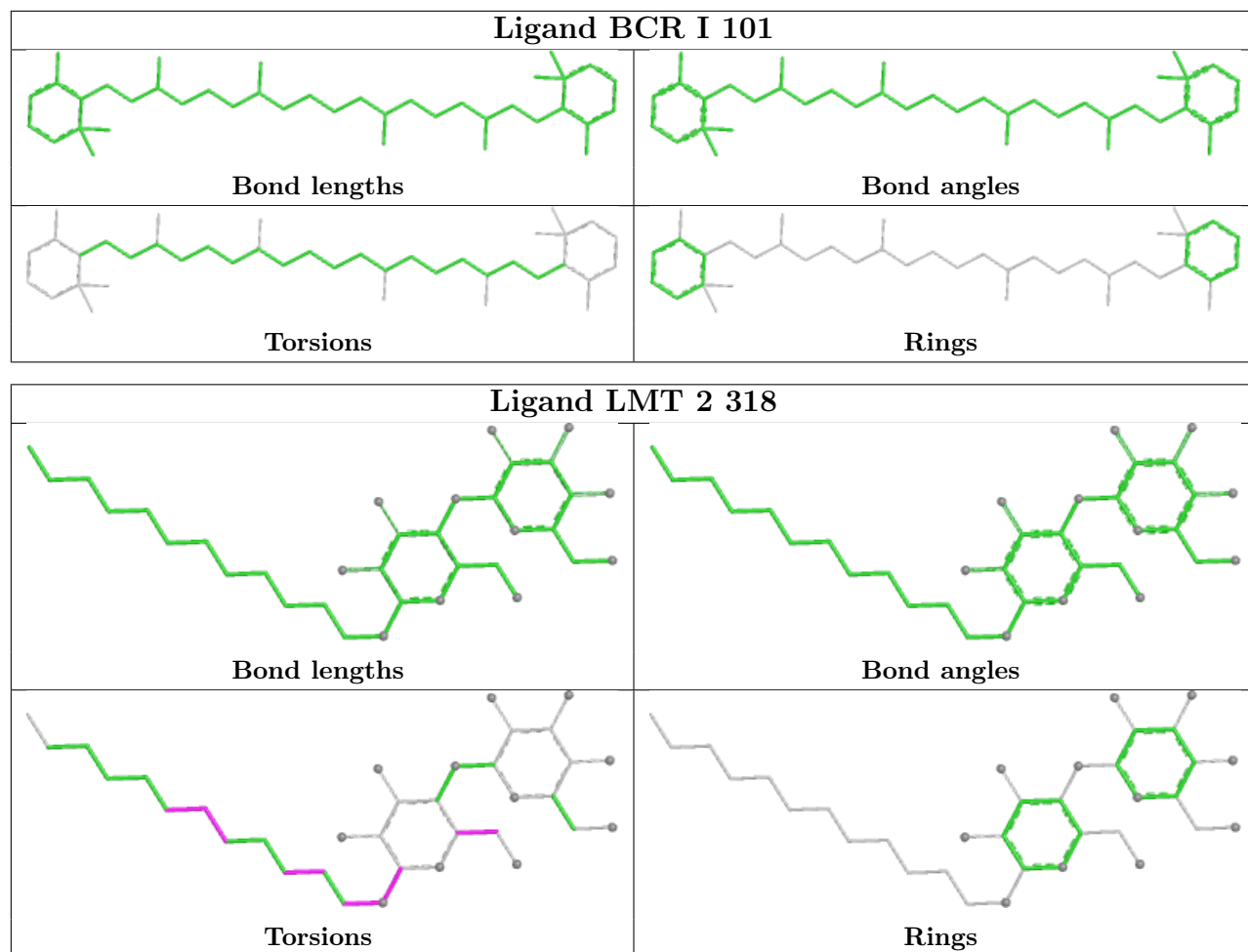


## Ligand CHL 4 314

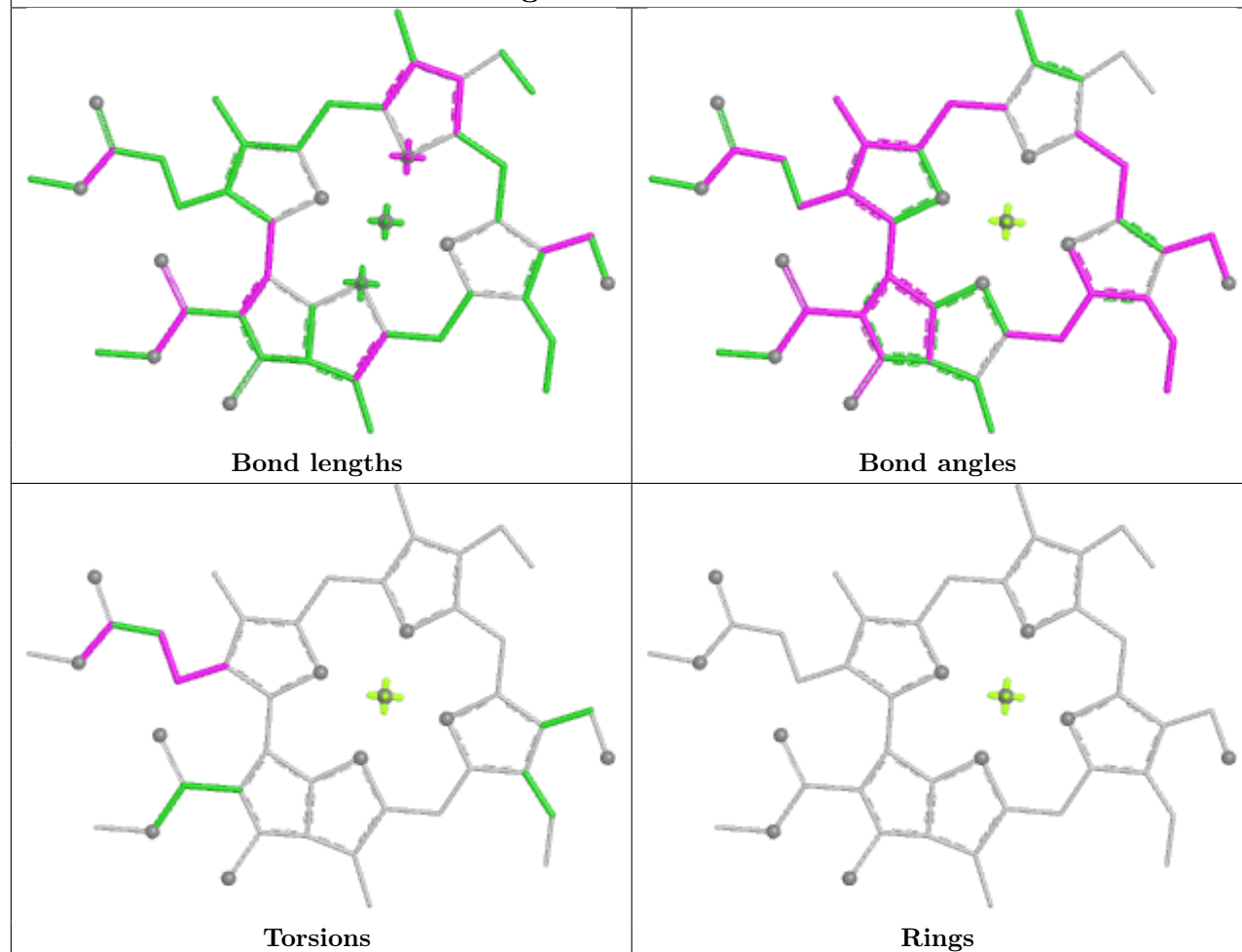


## Ligand CLA B 827

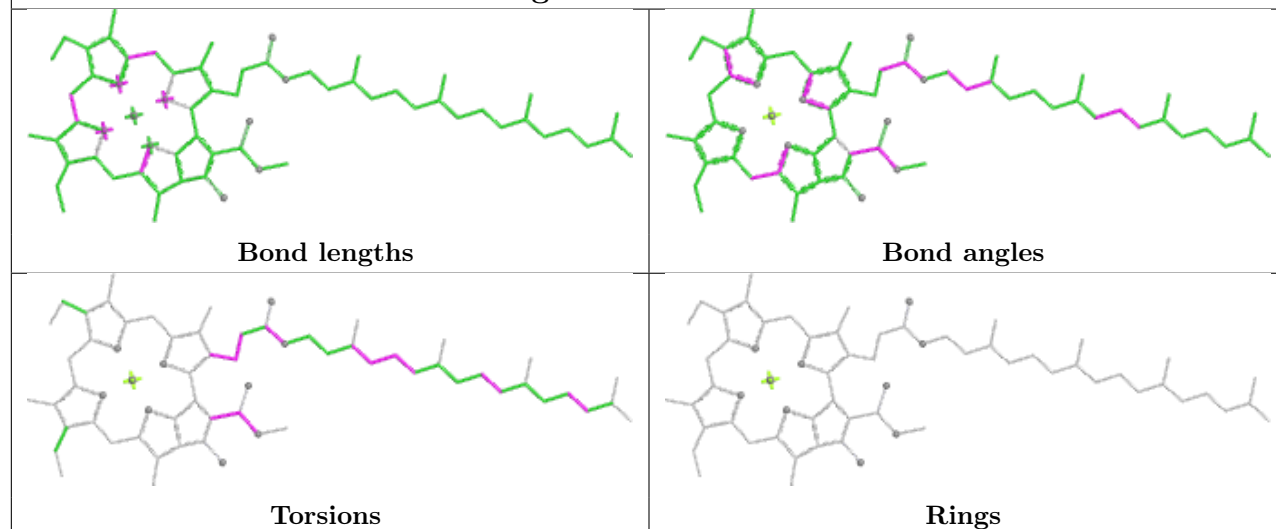


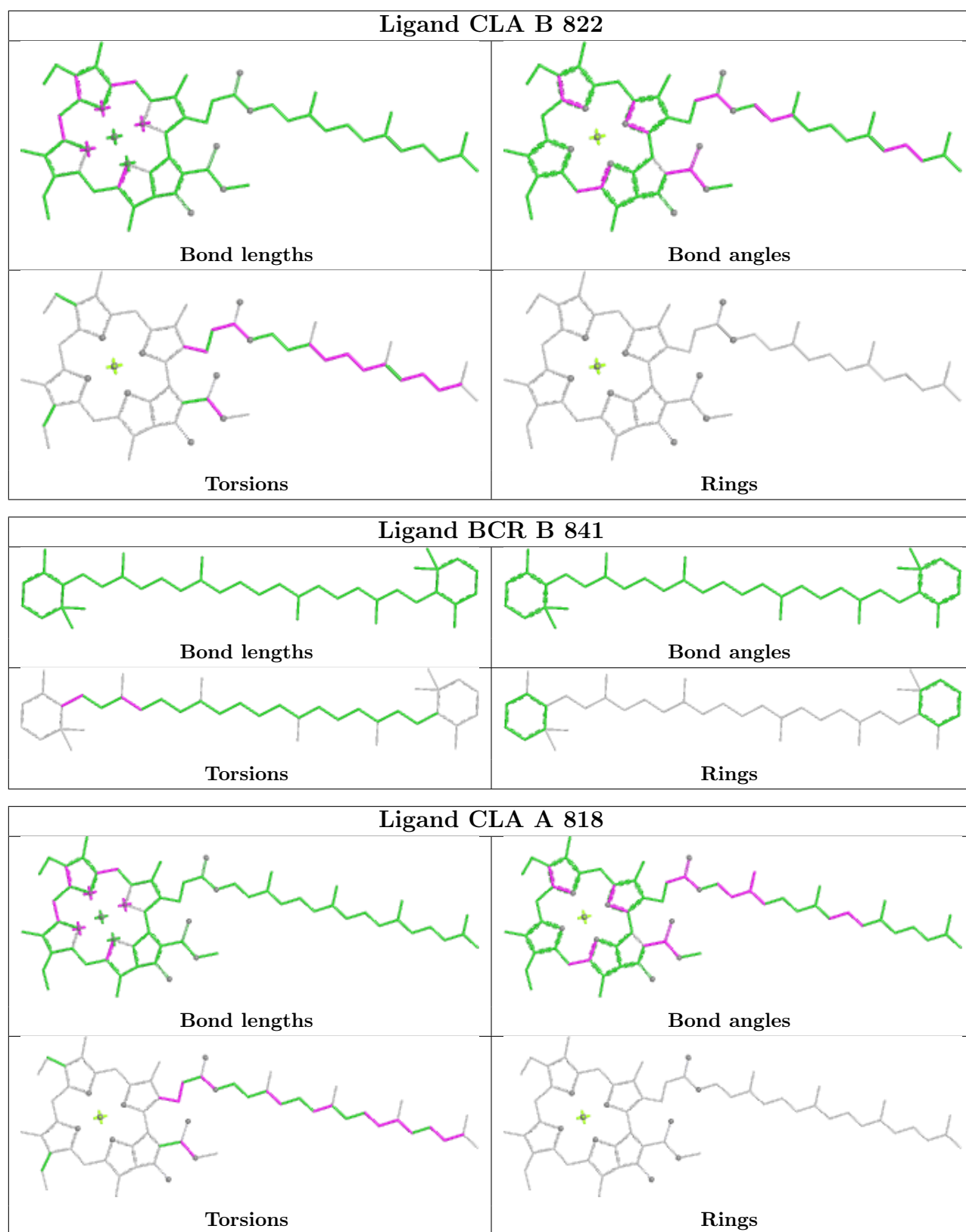


## Ligand CHL 3 307

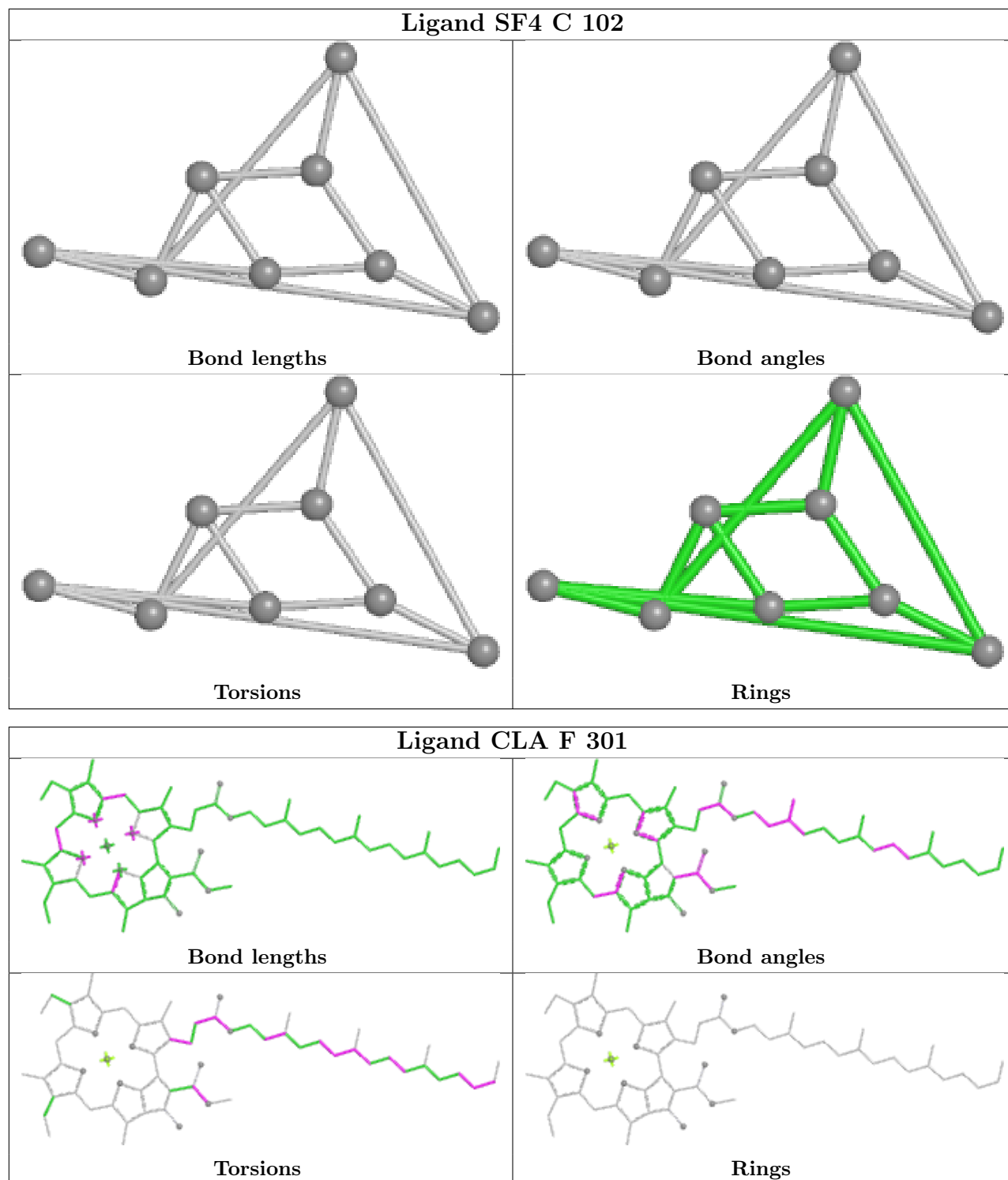


## Ligand CLA A 831

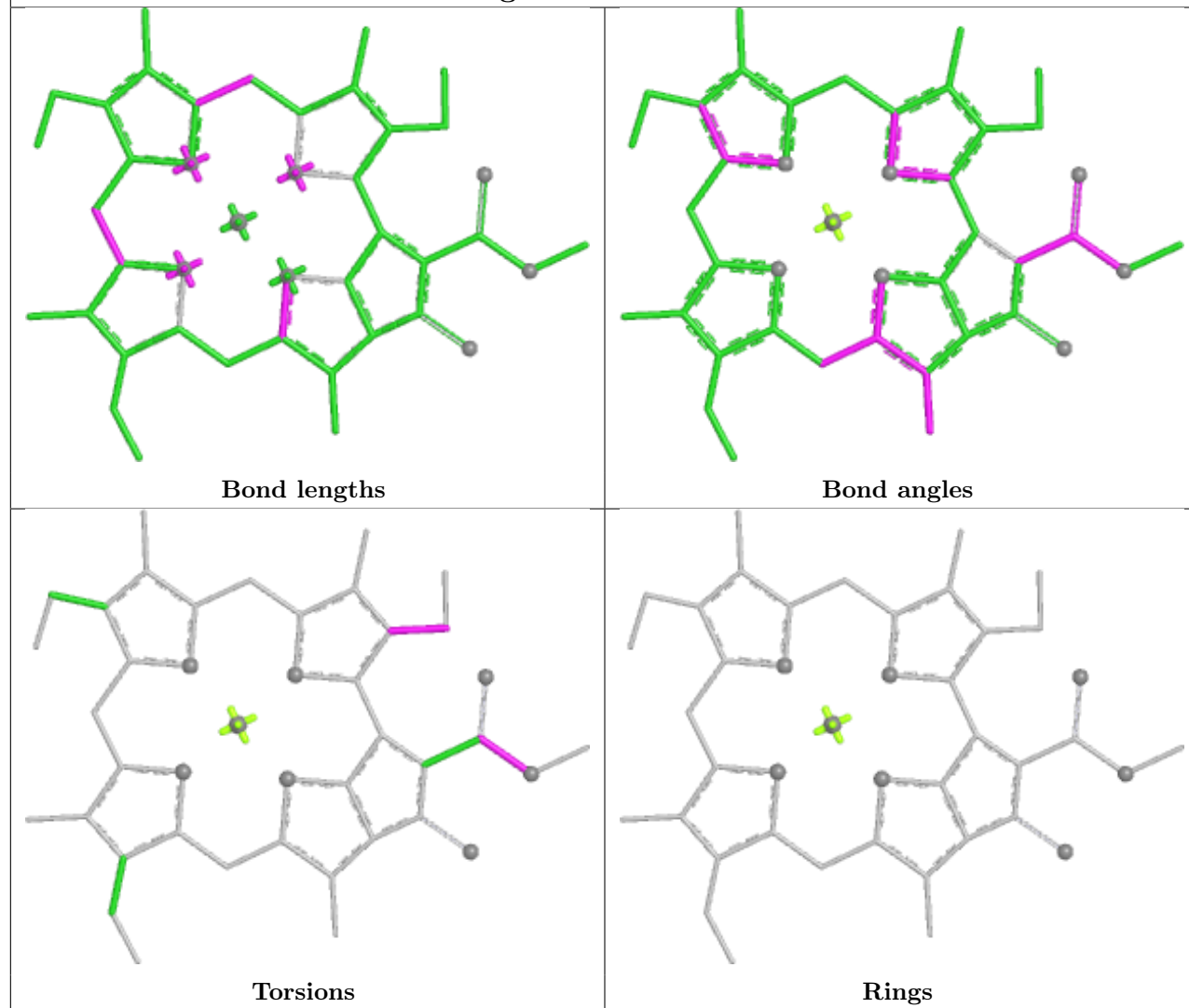




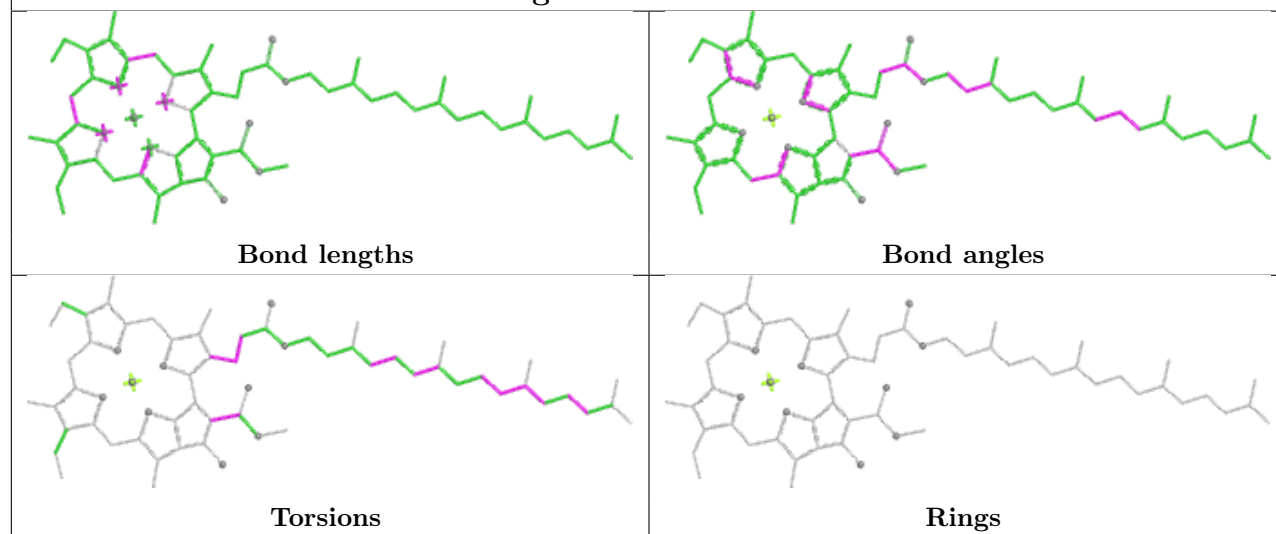


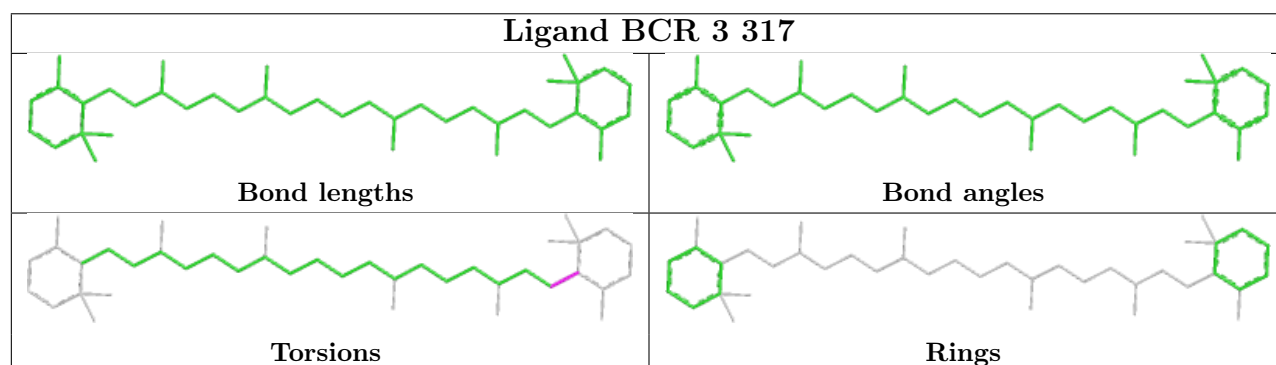
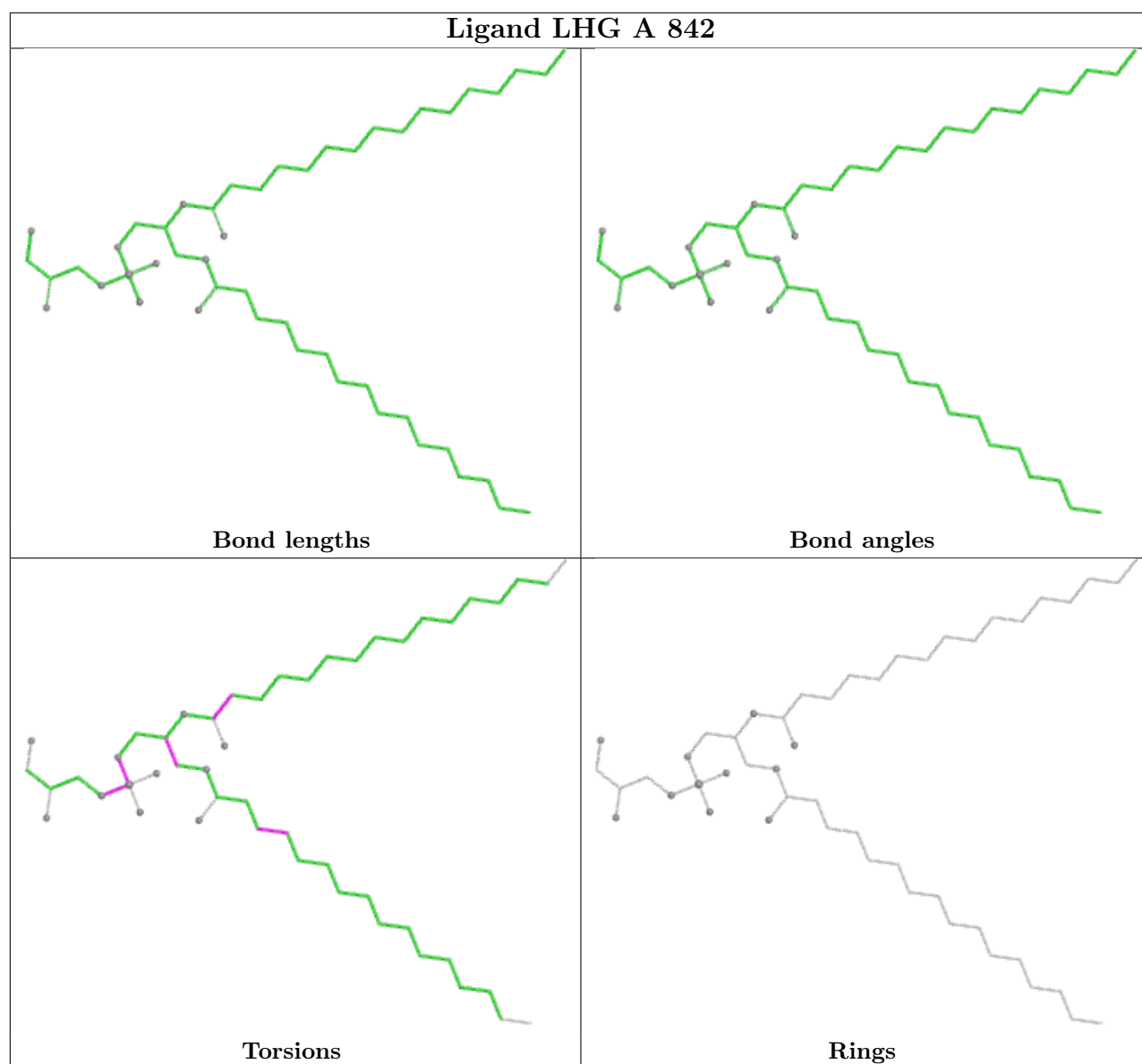


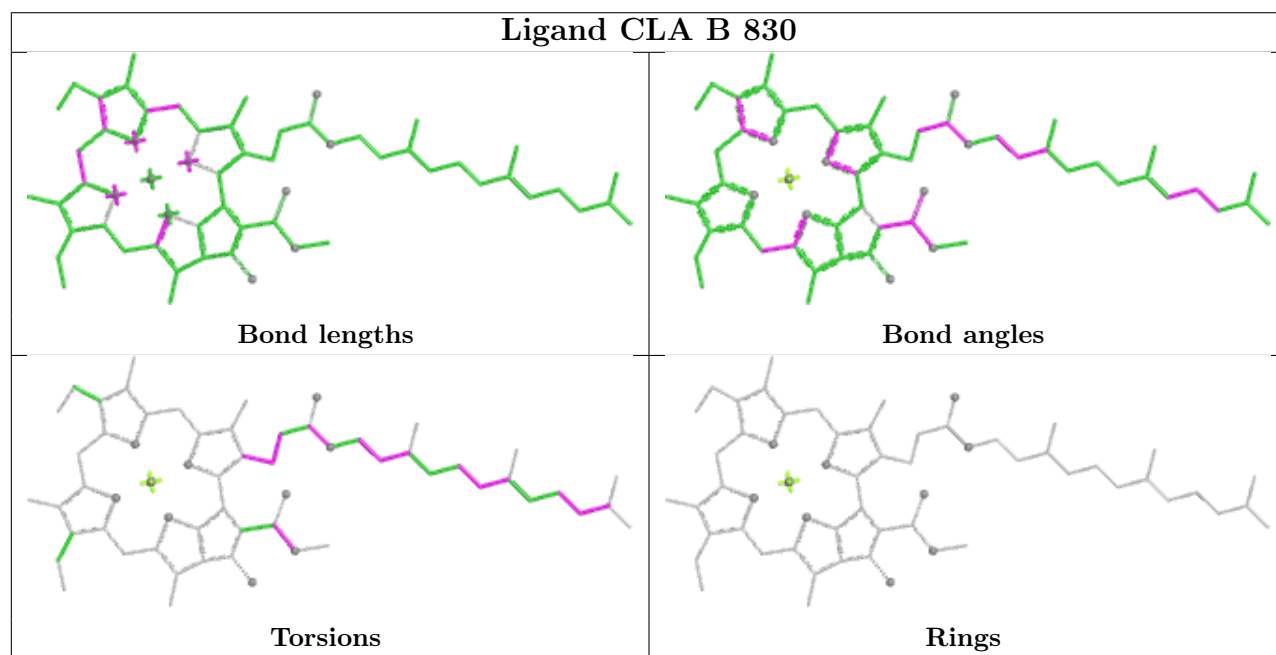
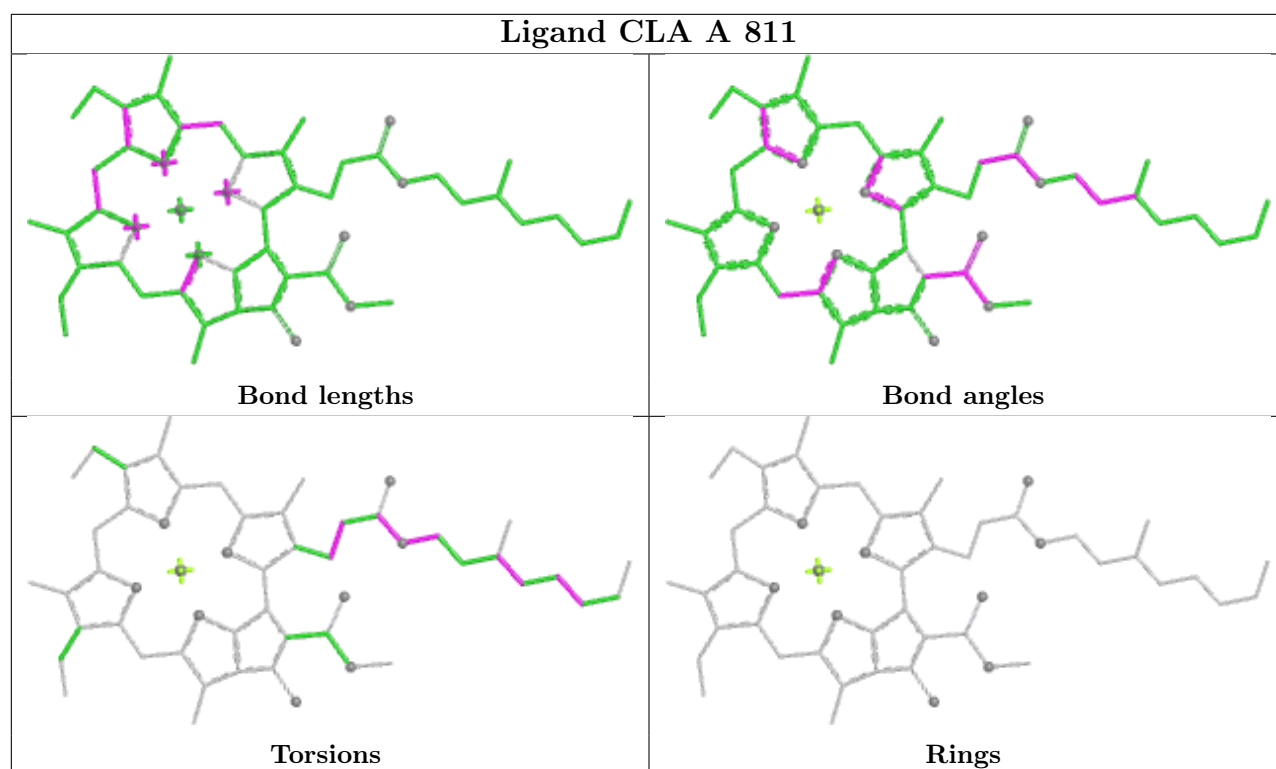
## Ligand CLA 1 305



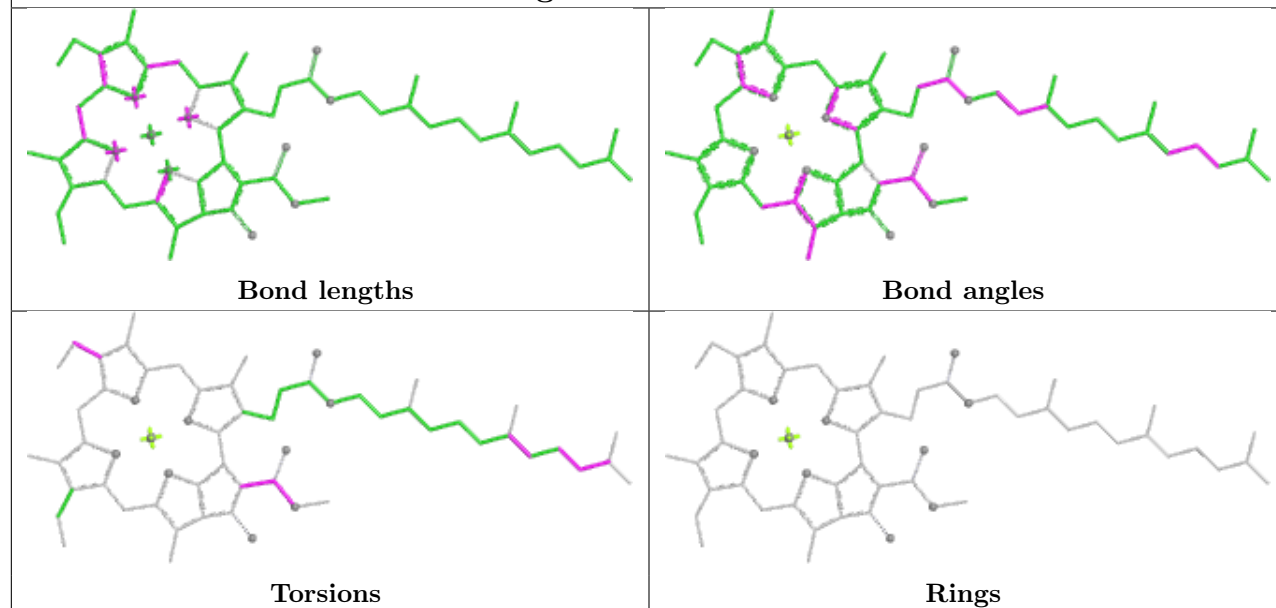
## Ligand CLA B 825



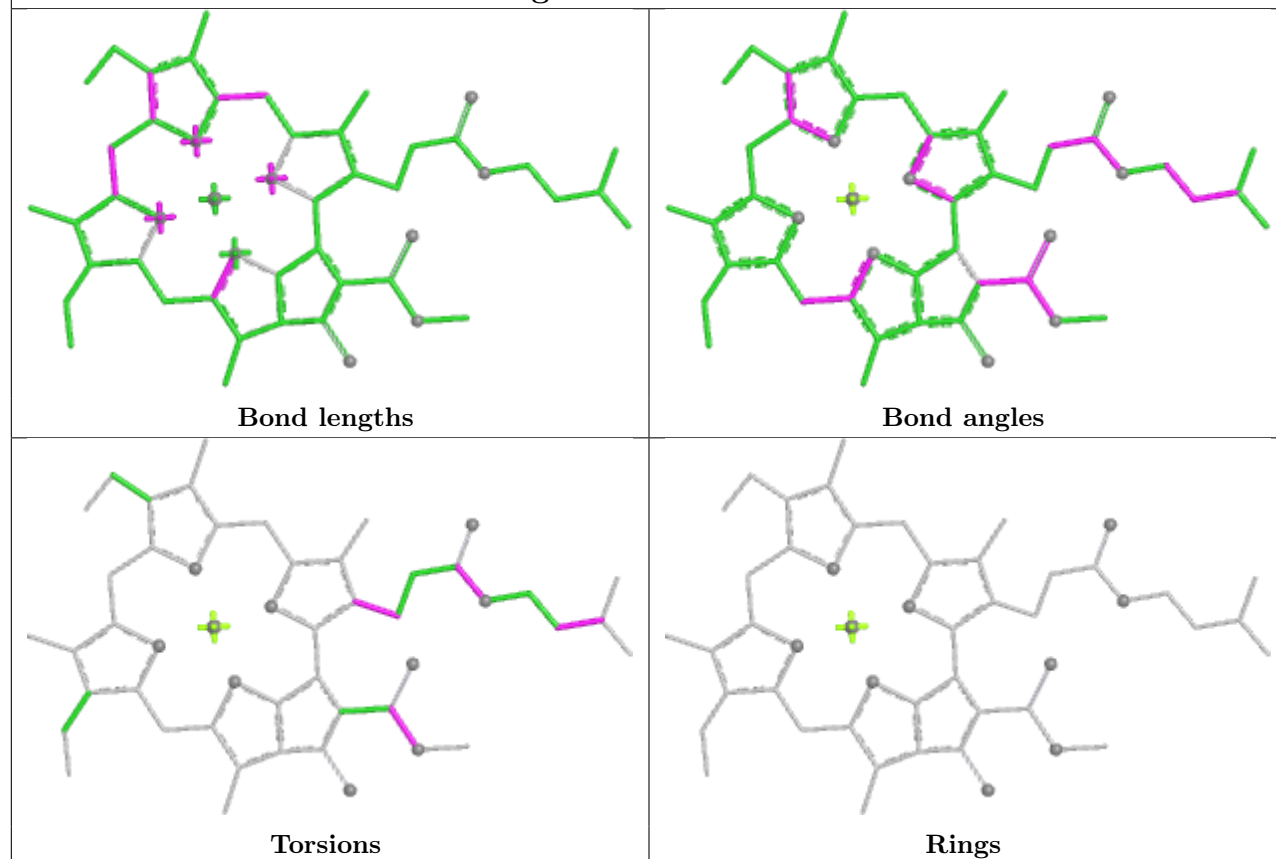


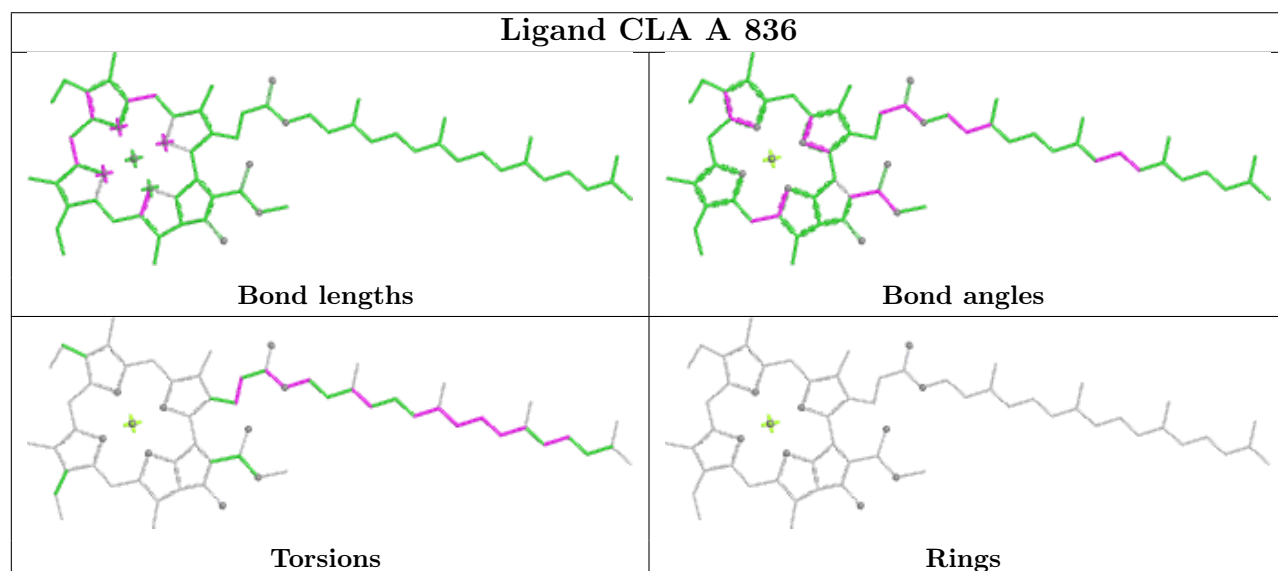
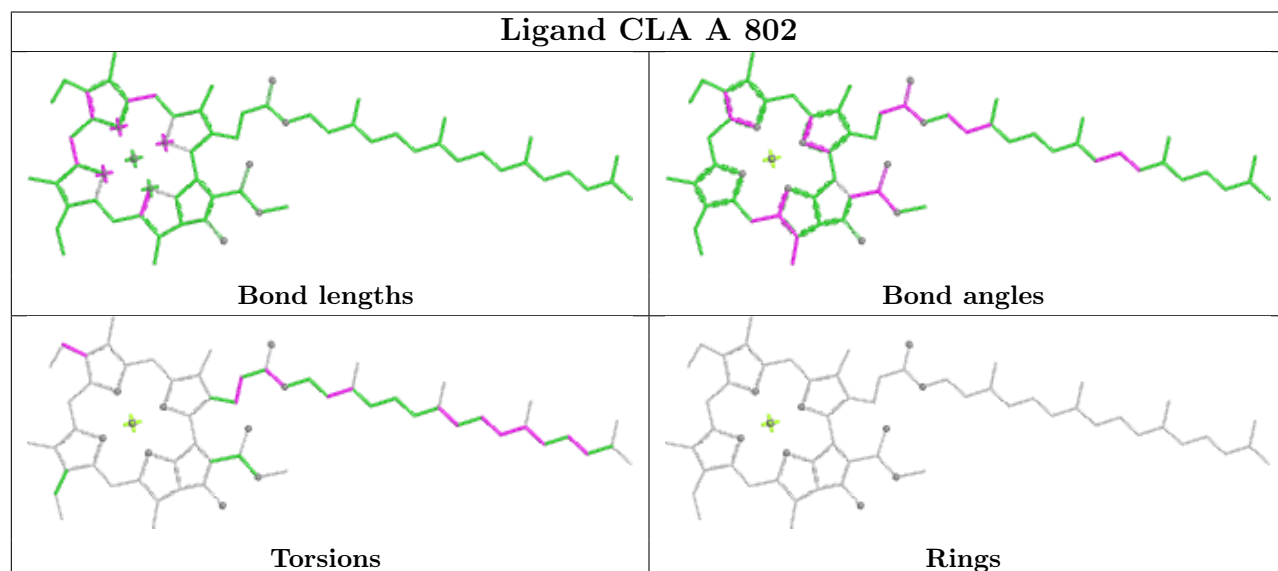
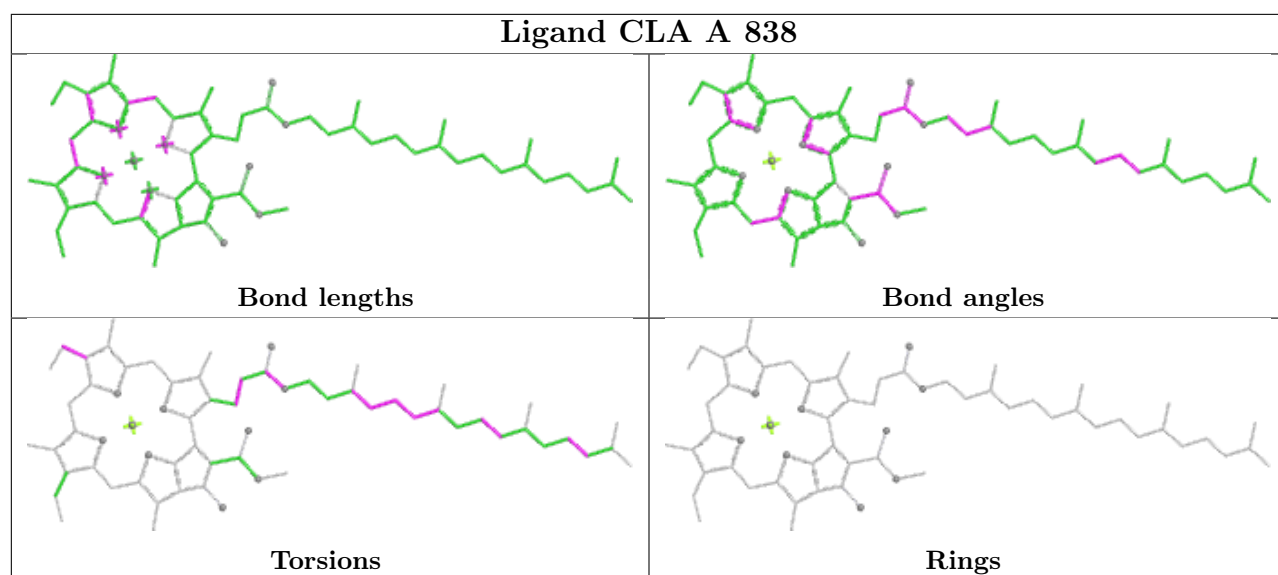


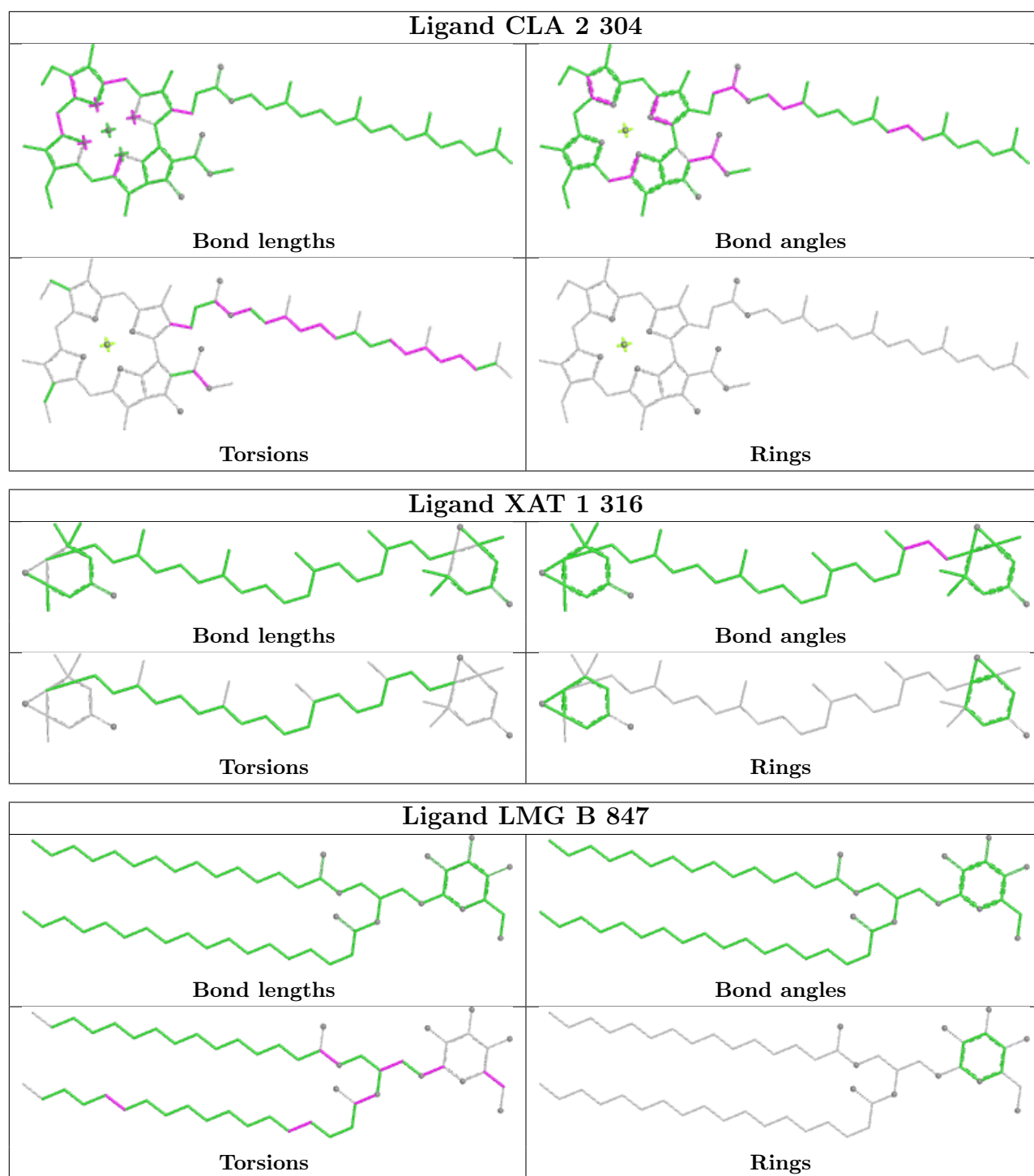
## Ligand CLA 1 302

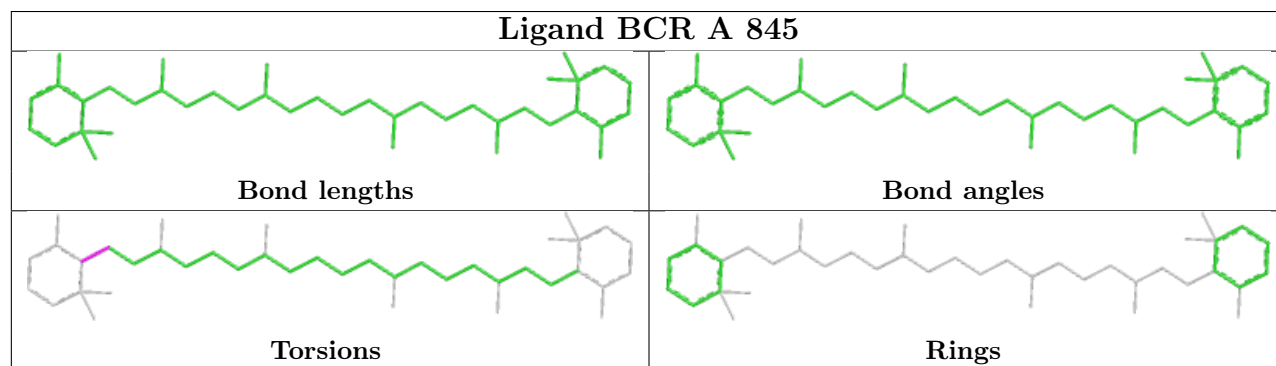
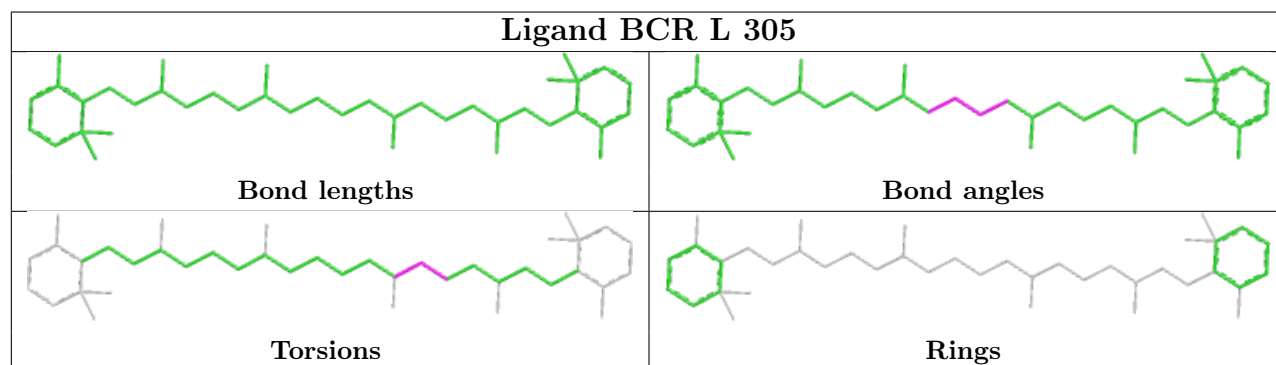
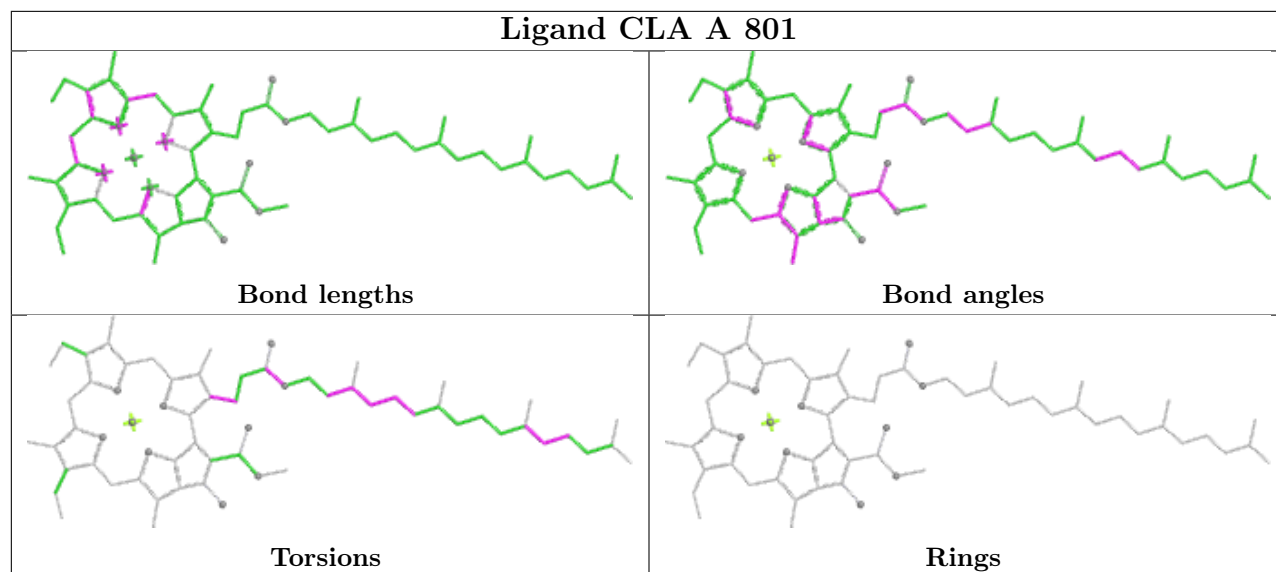


## Ligand CLA A 803



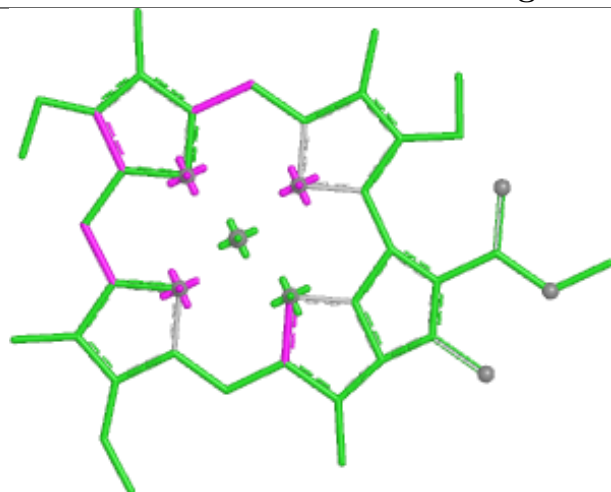




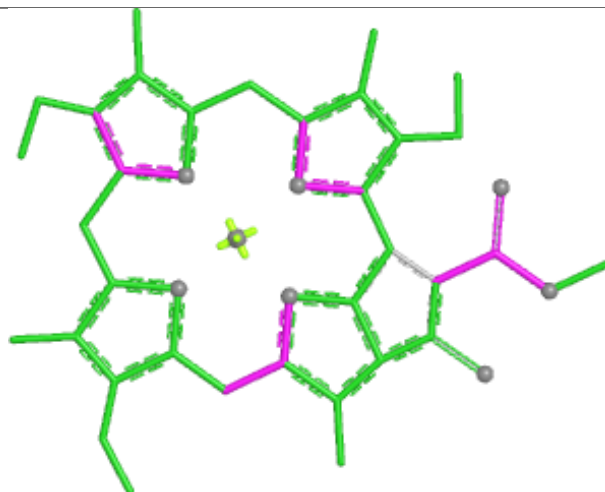




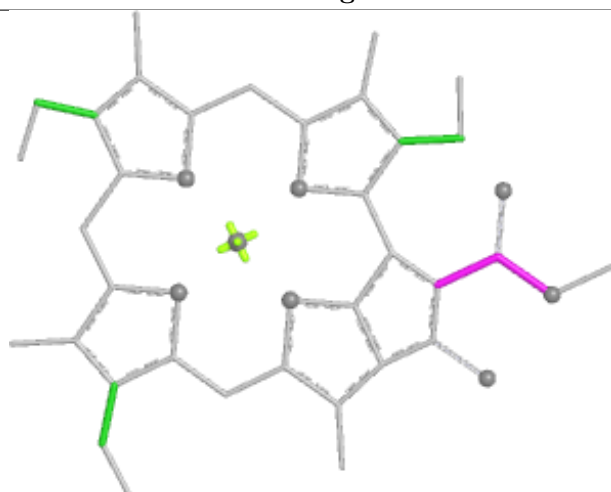
## Ligand CLA J 102



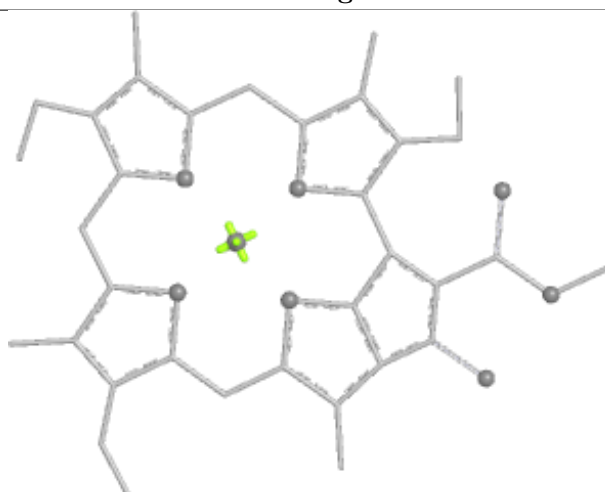
Bond lengths



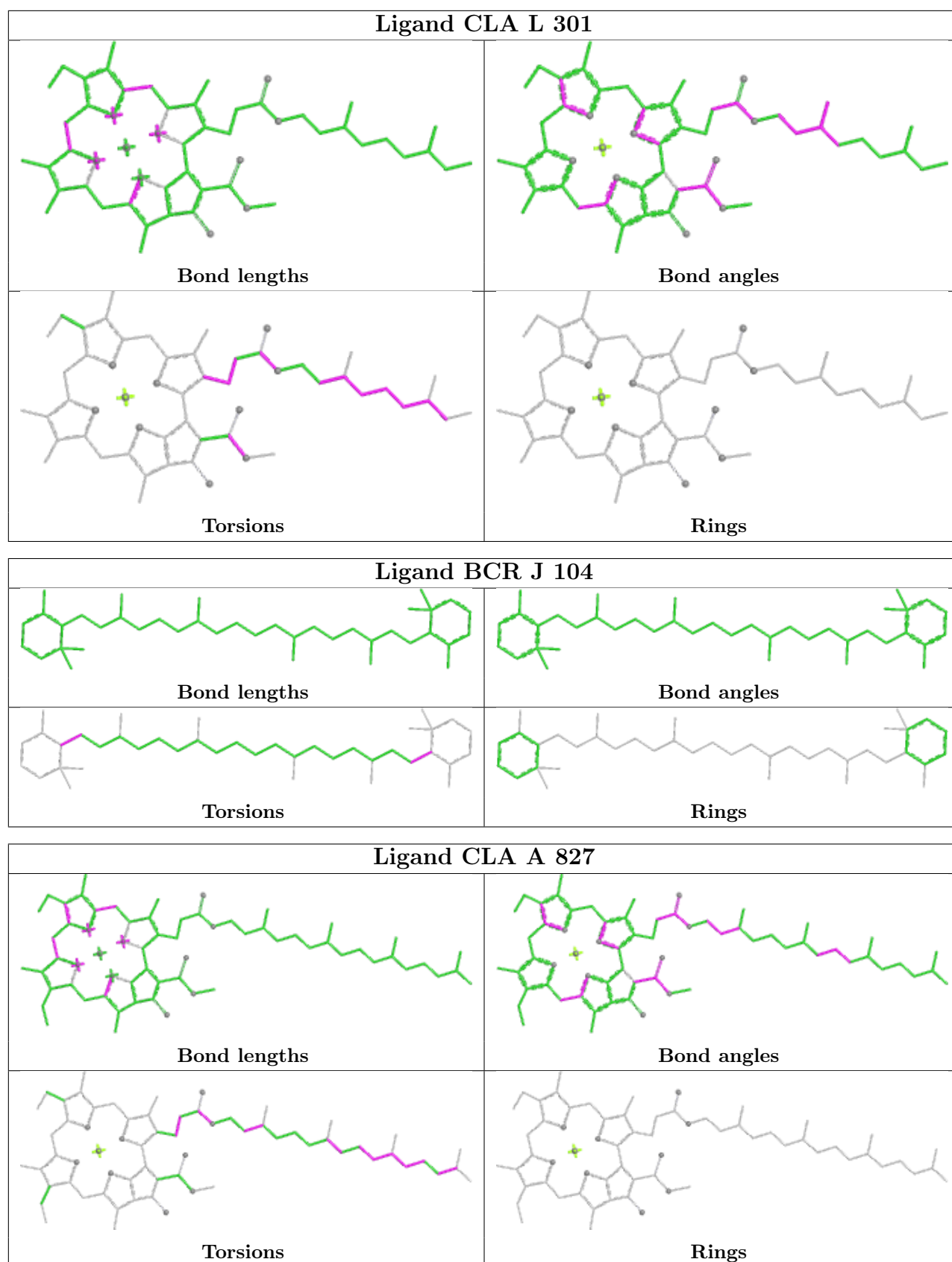
Bond angles

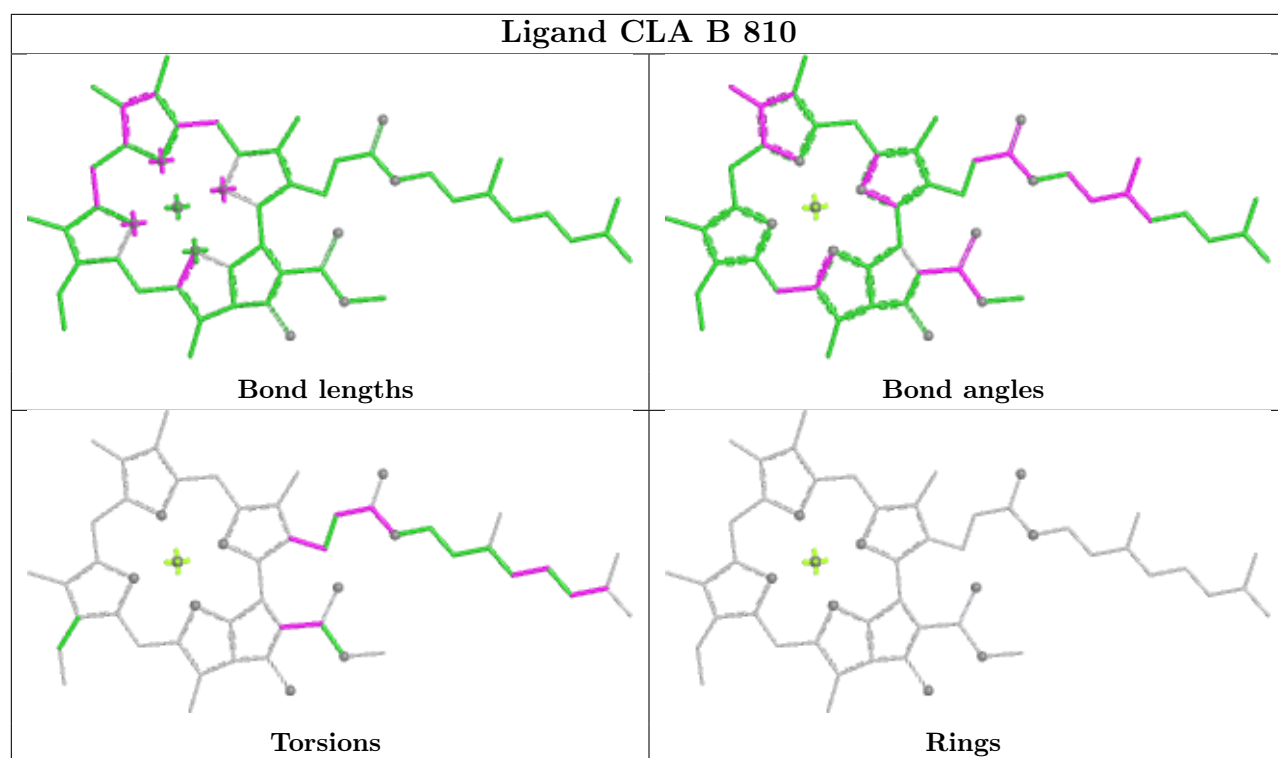


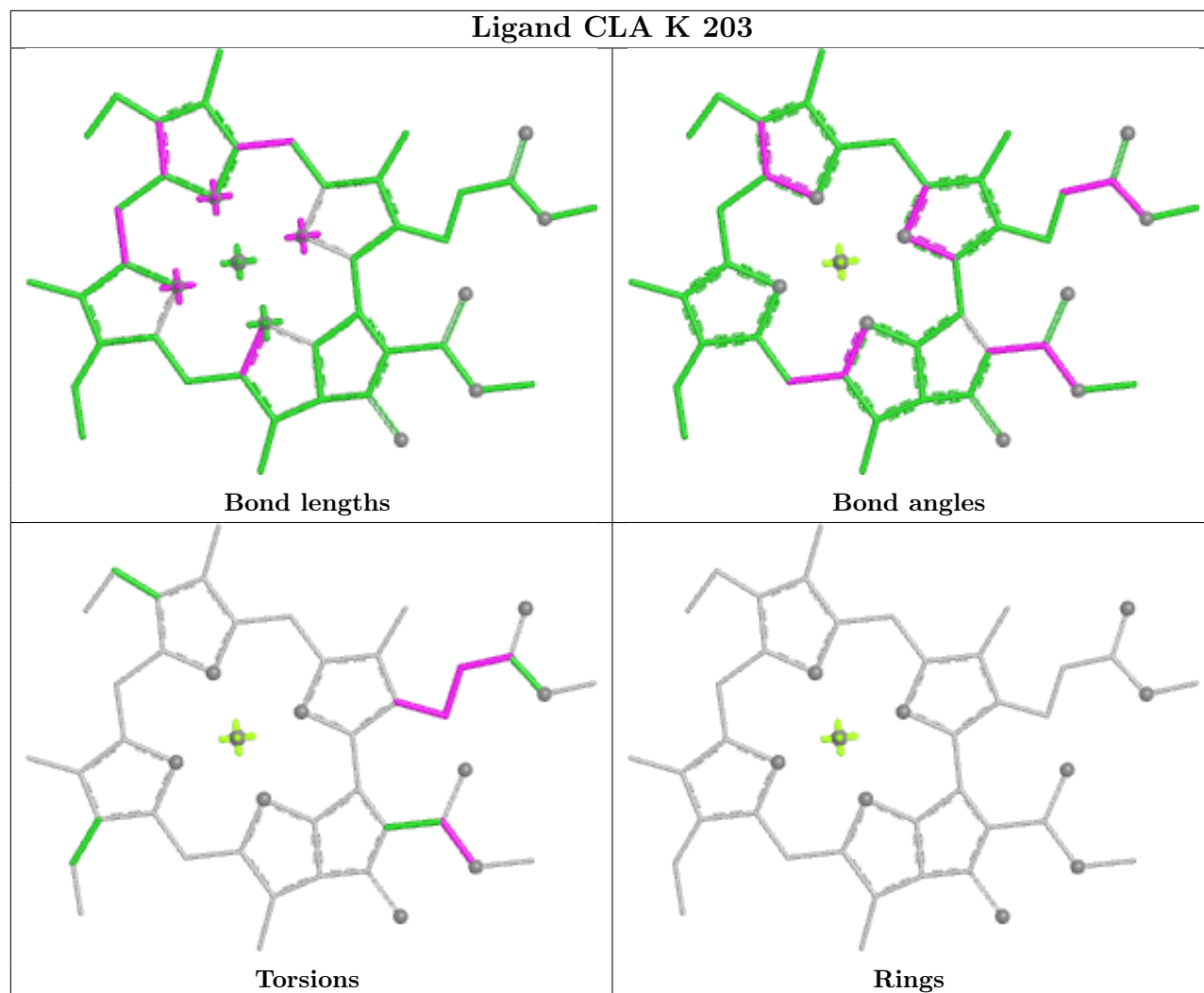
Torsions



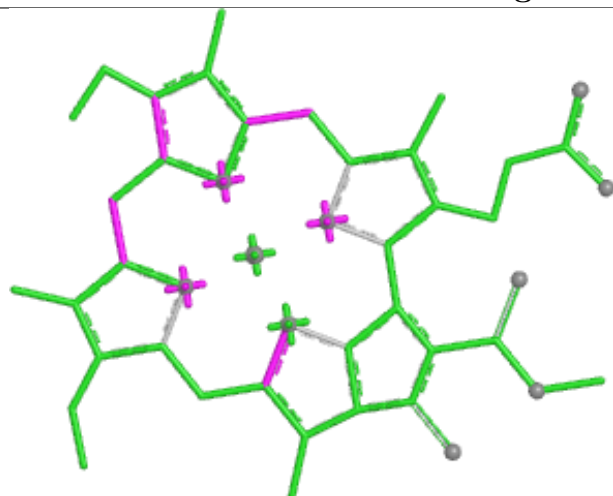
Rings



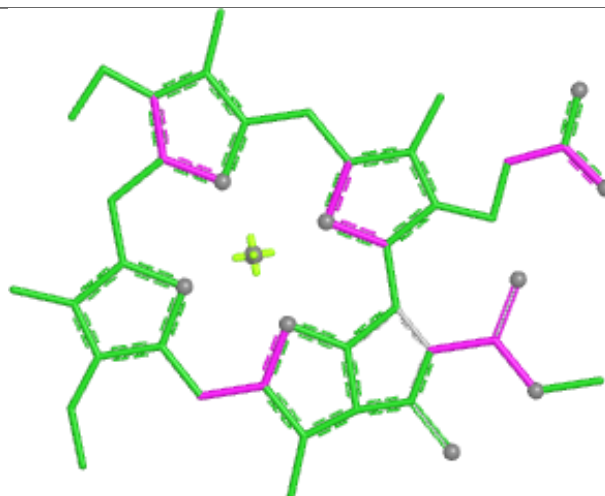




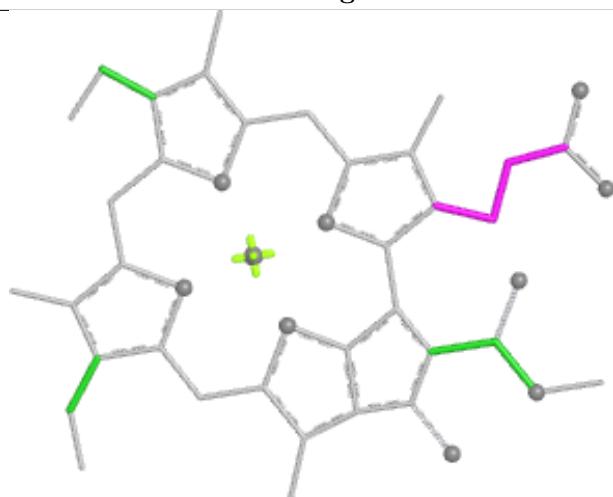
## Ligand CLA B 833



Bond lengths



Bond angles

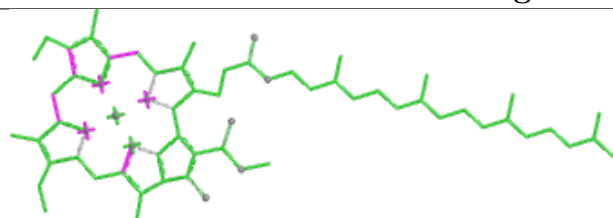


Torsions

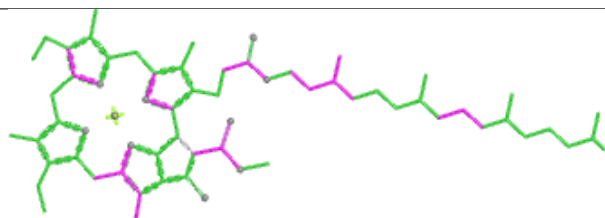


Rings

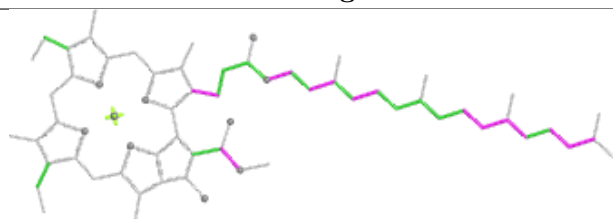
## Ligand CLA A 810



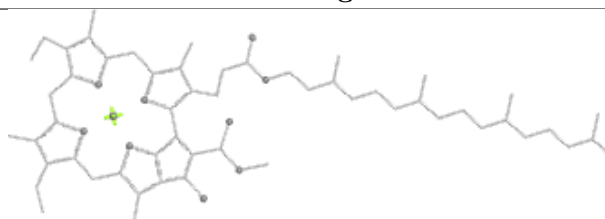
Bond lengths



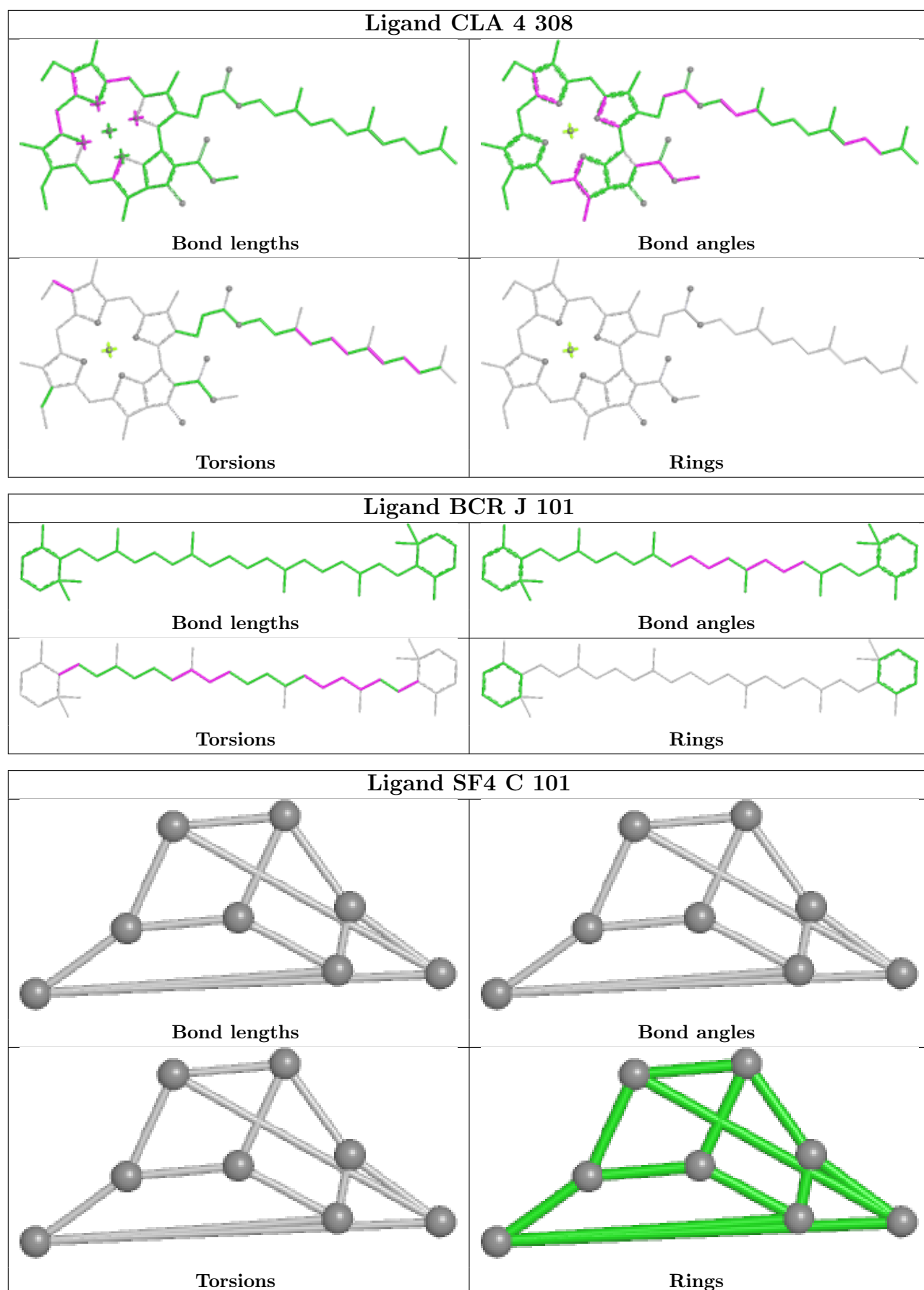
Bond angles

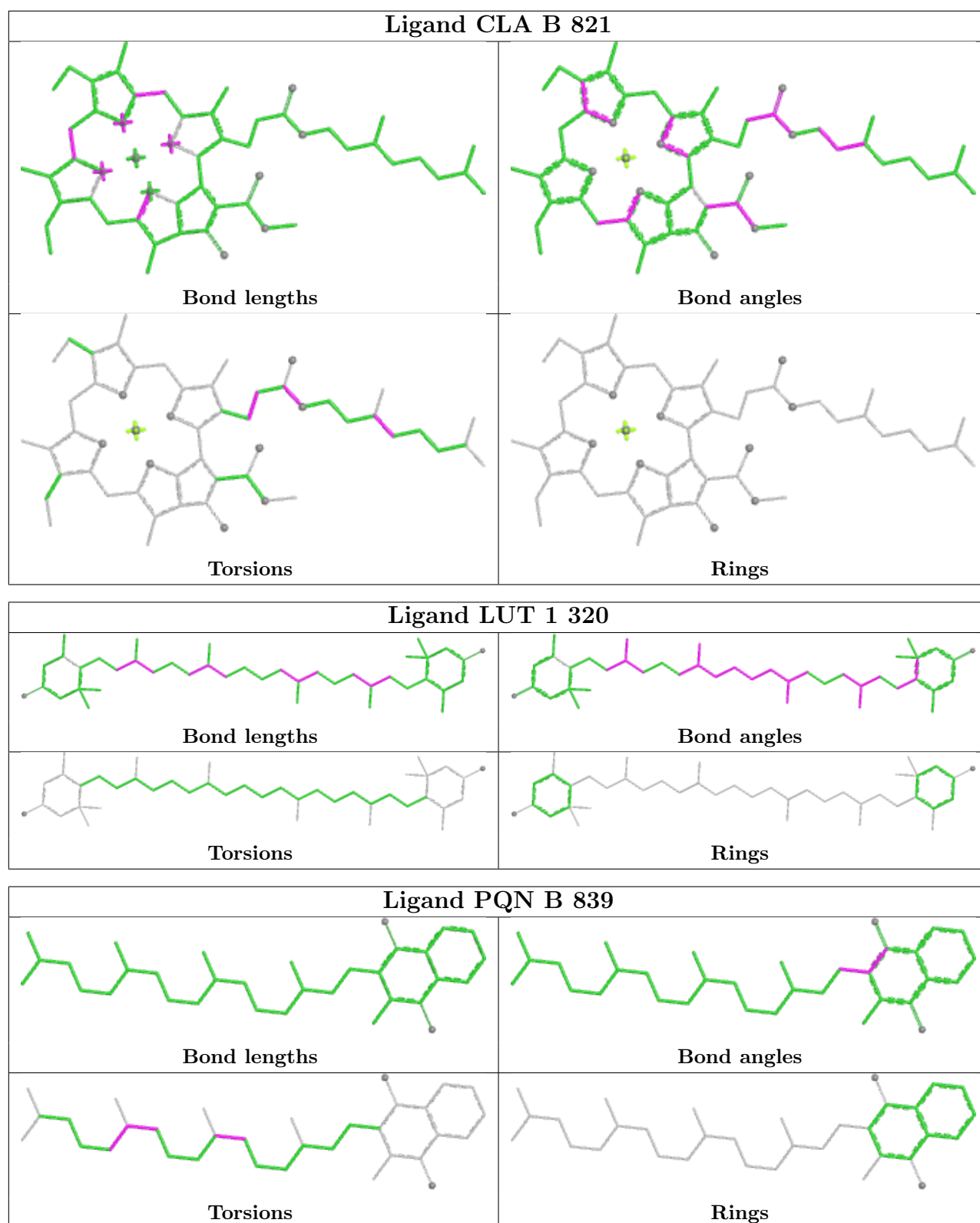


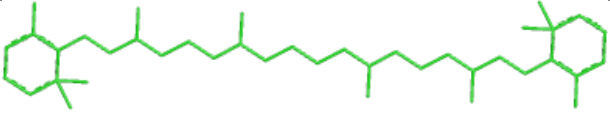
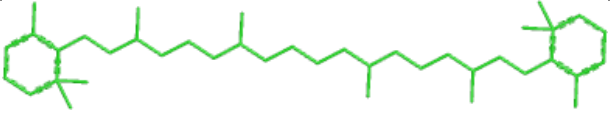
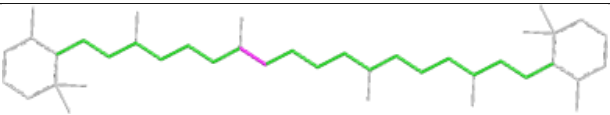
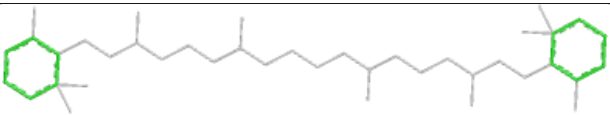


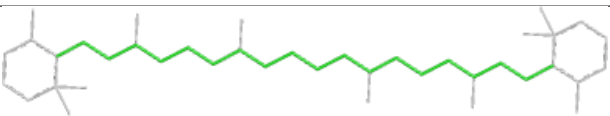
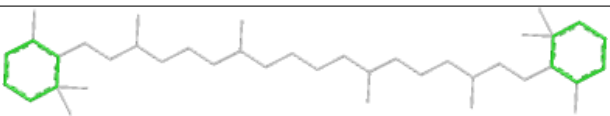
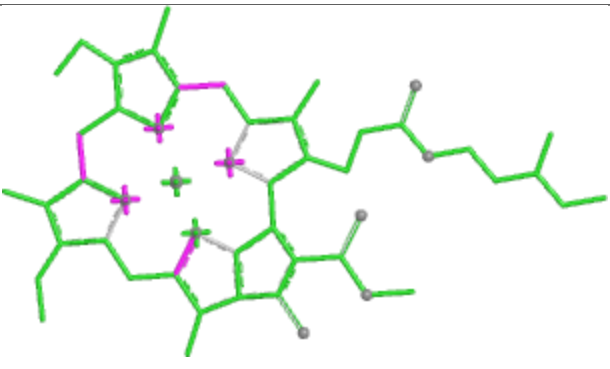
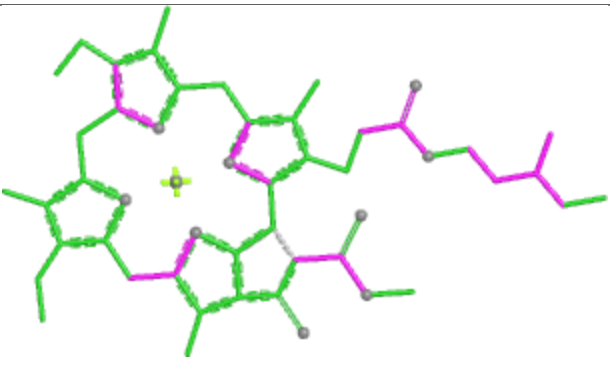
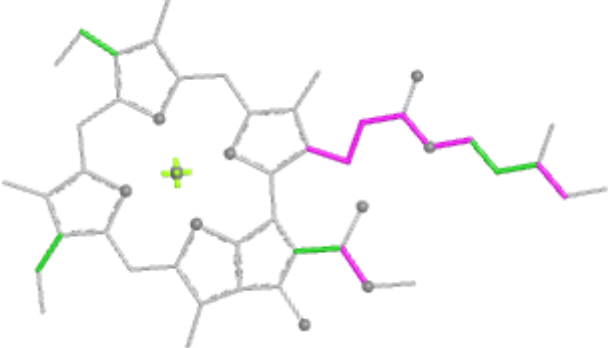
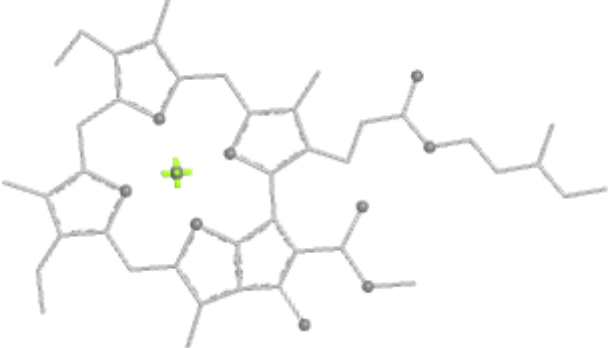
Torsions



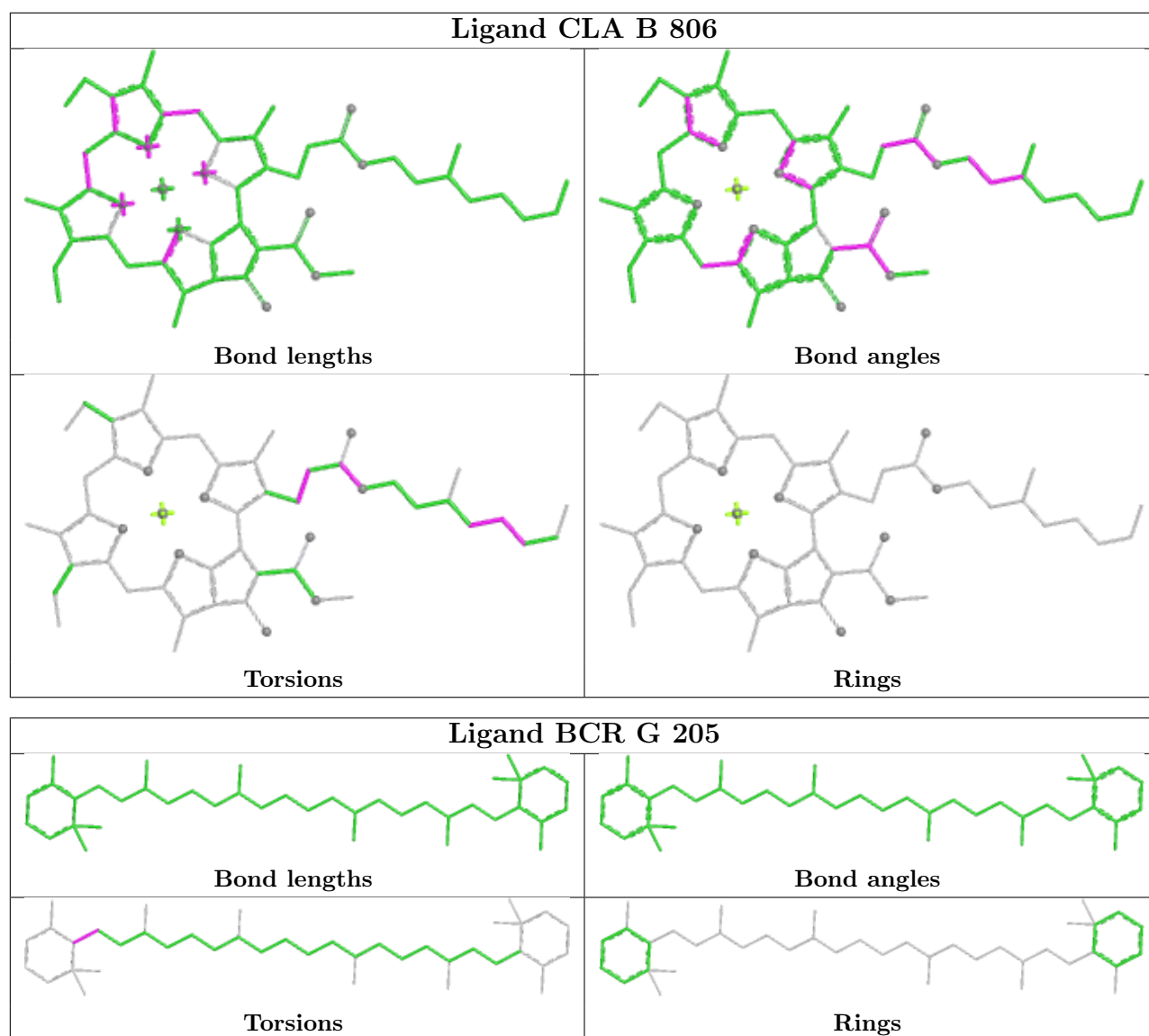
Rings



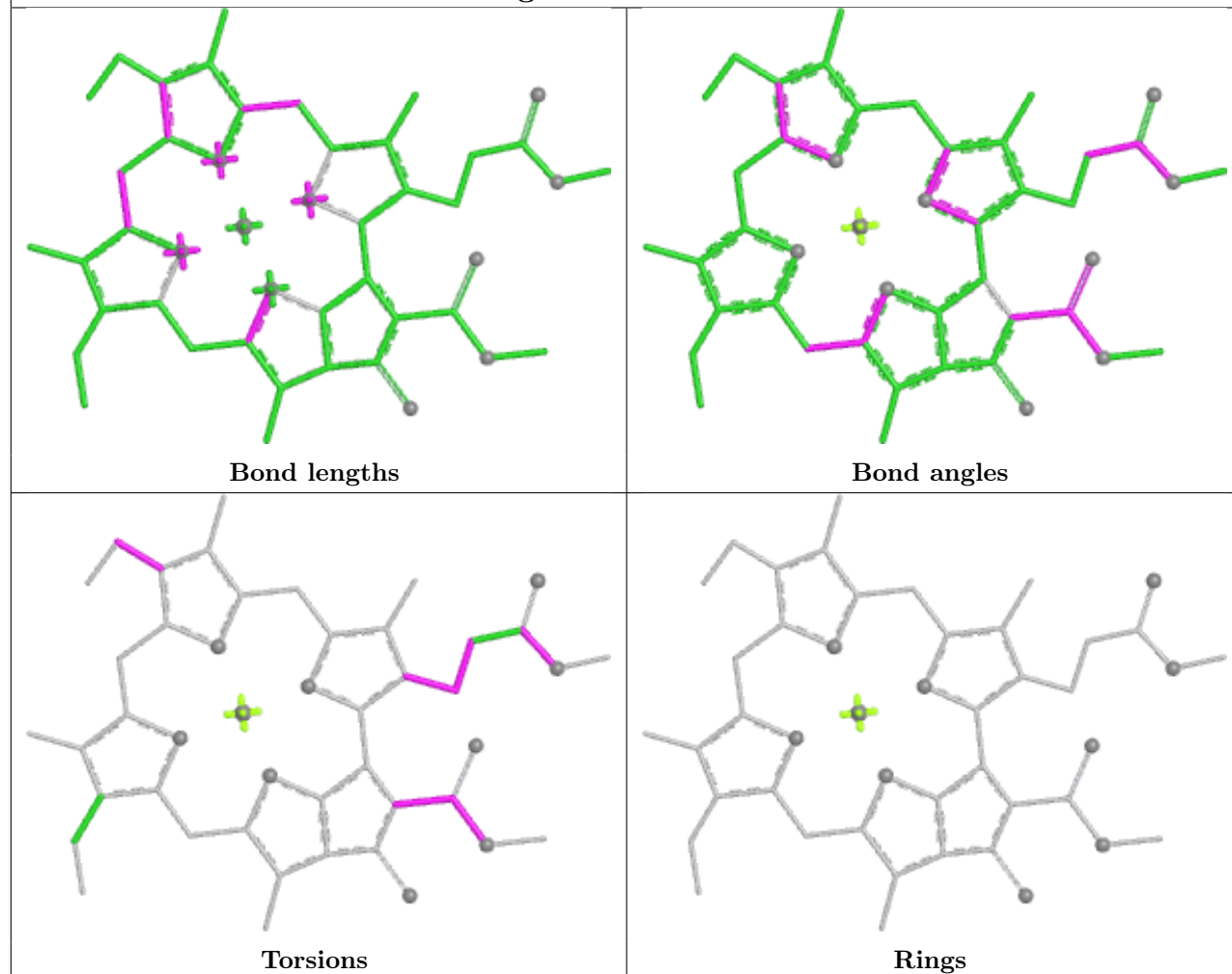


Ligand BCR F 305	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 848	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 822	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

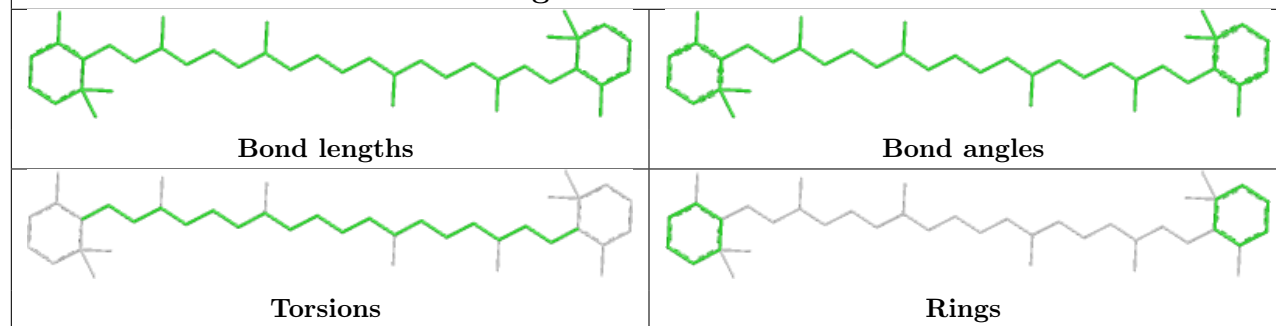




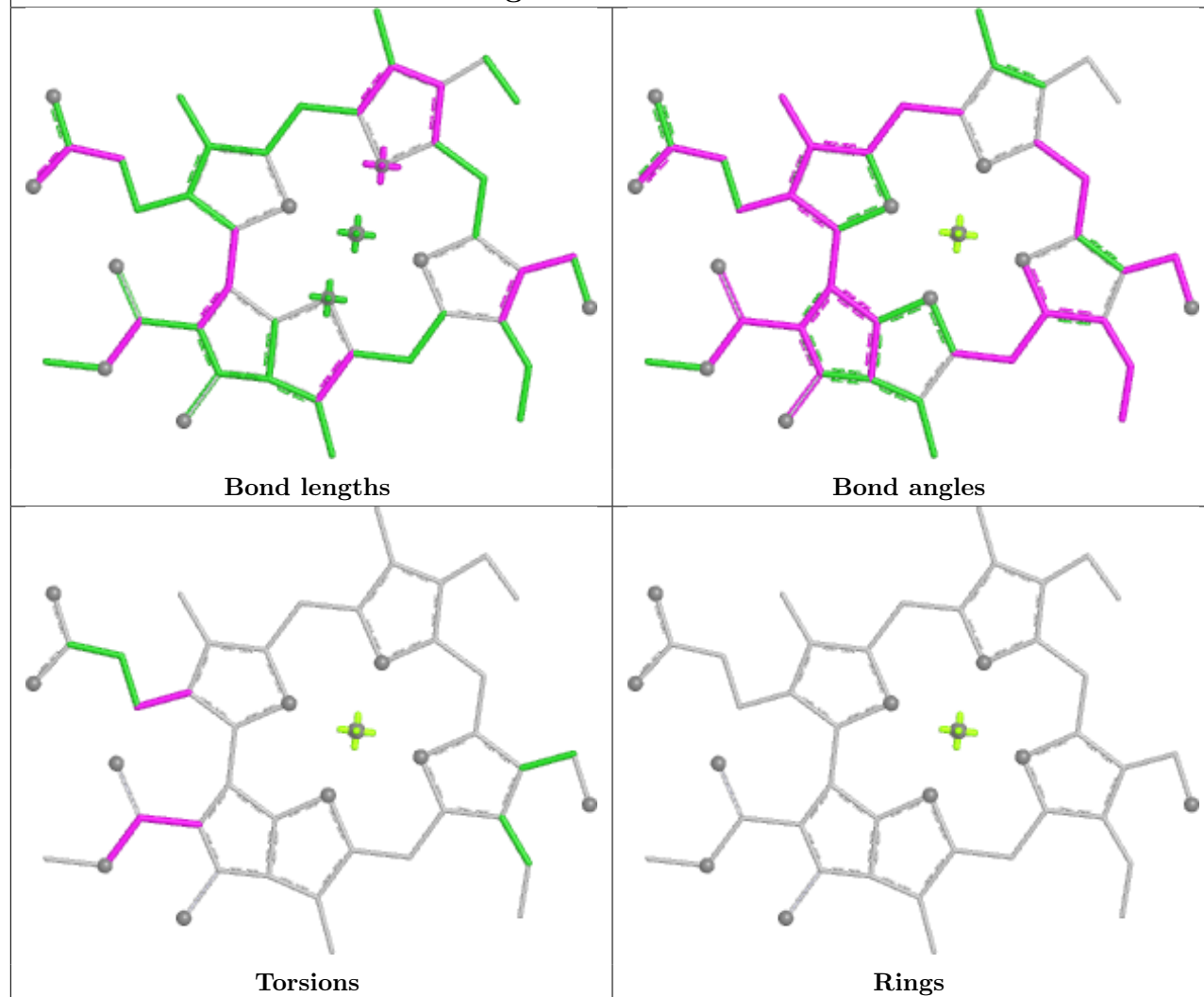
## Ligand CLA 3 314



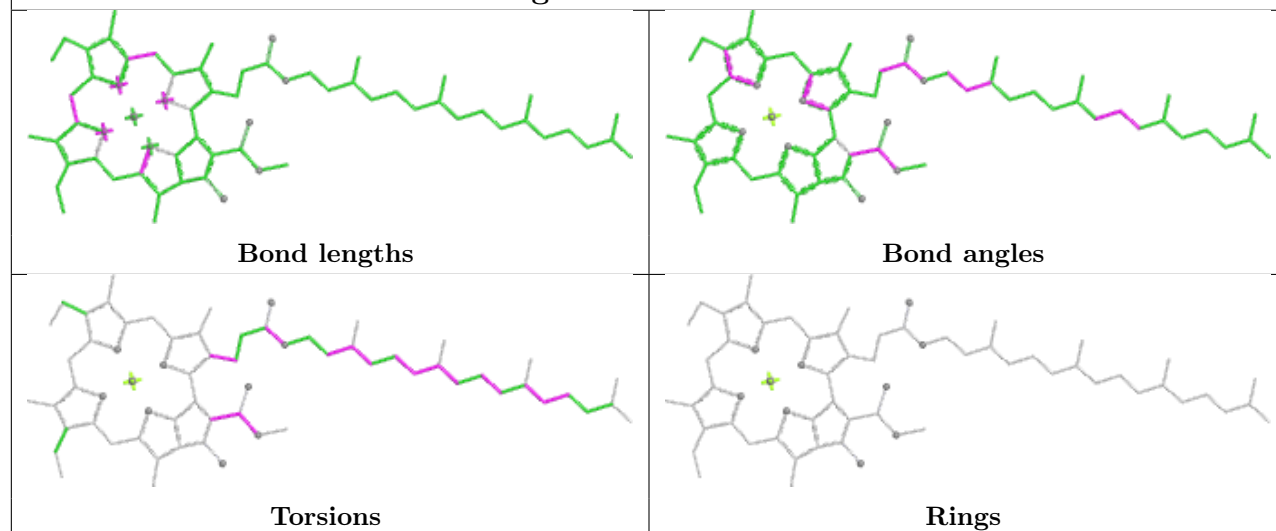
## Ligand BCR F 306

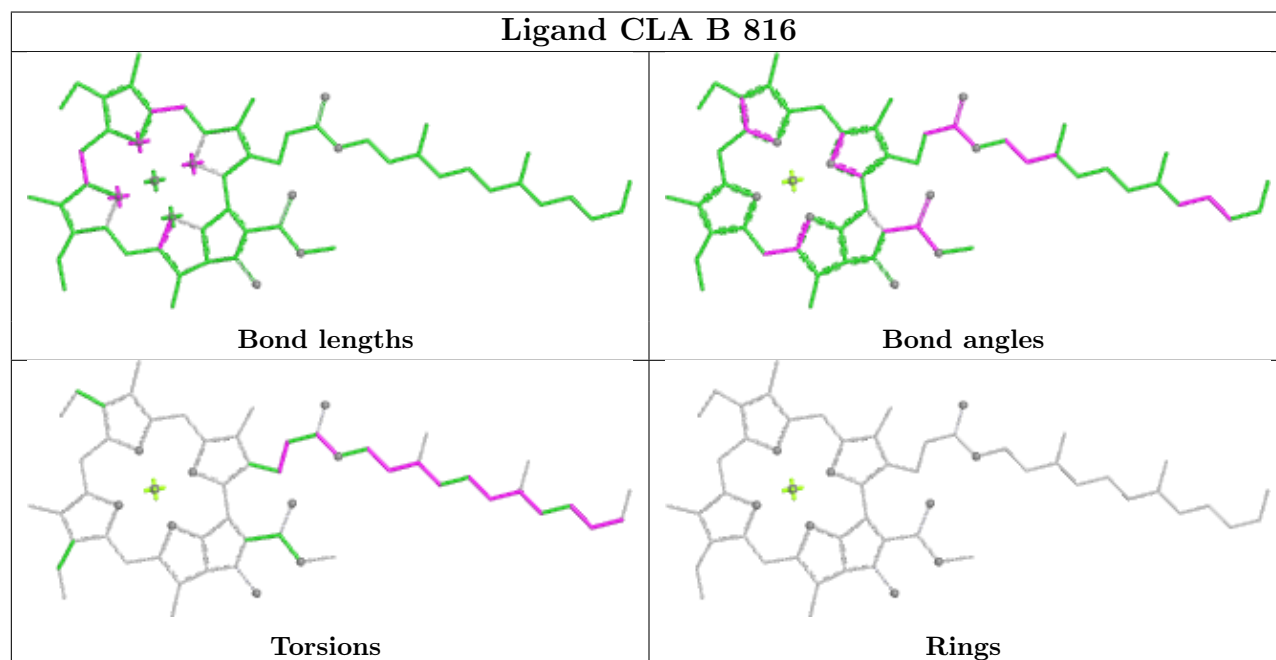
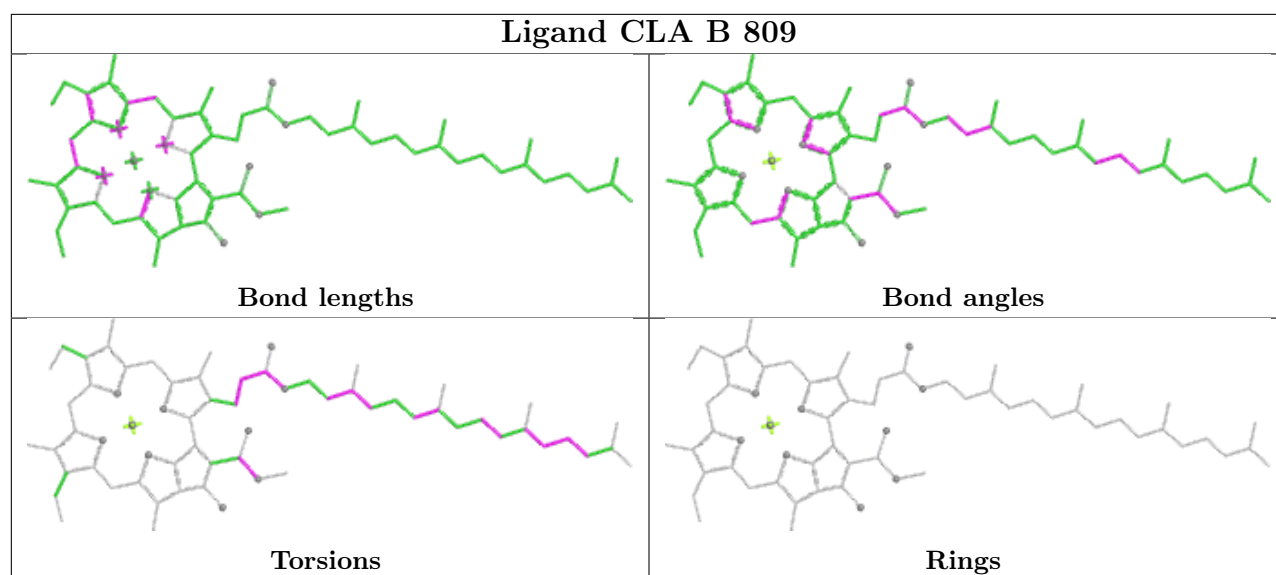


## Ligand CHL 2 307

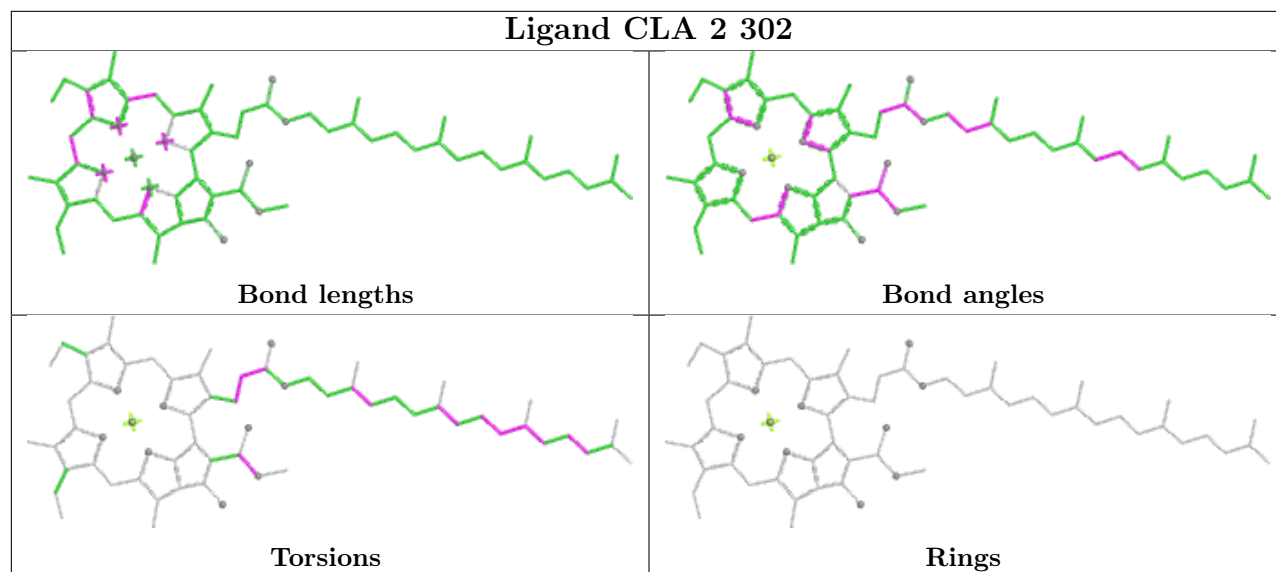


## Ligand CLA A 832

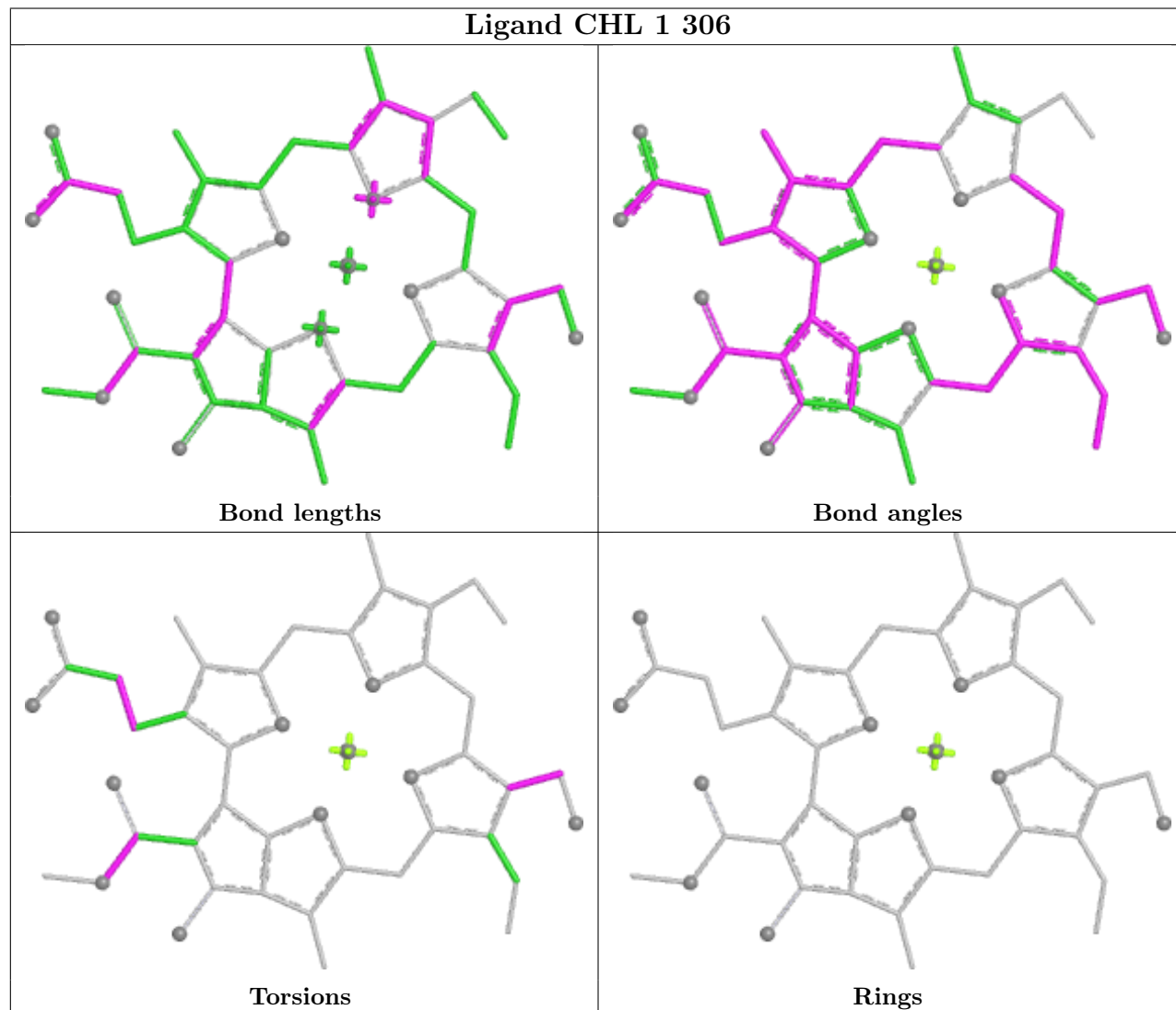


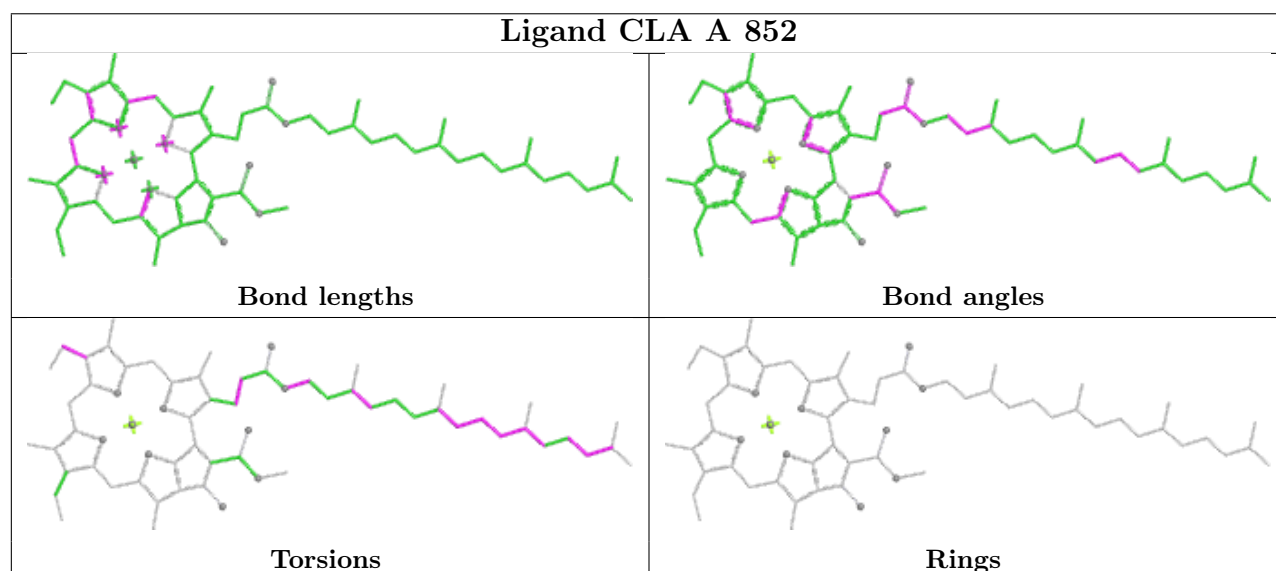
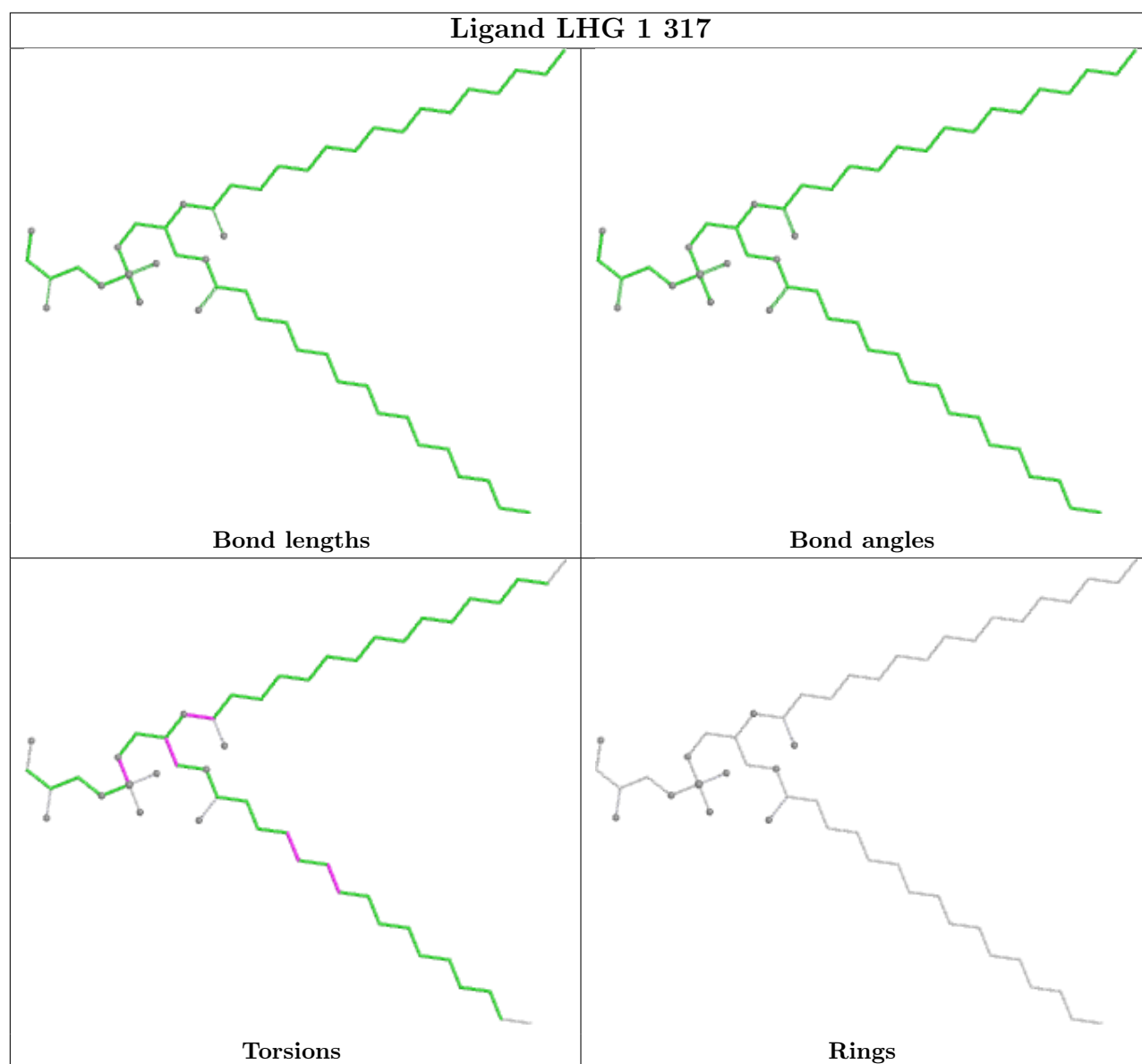


## Ligand CLA 2 302

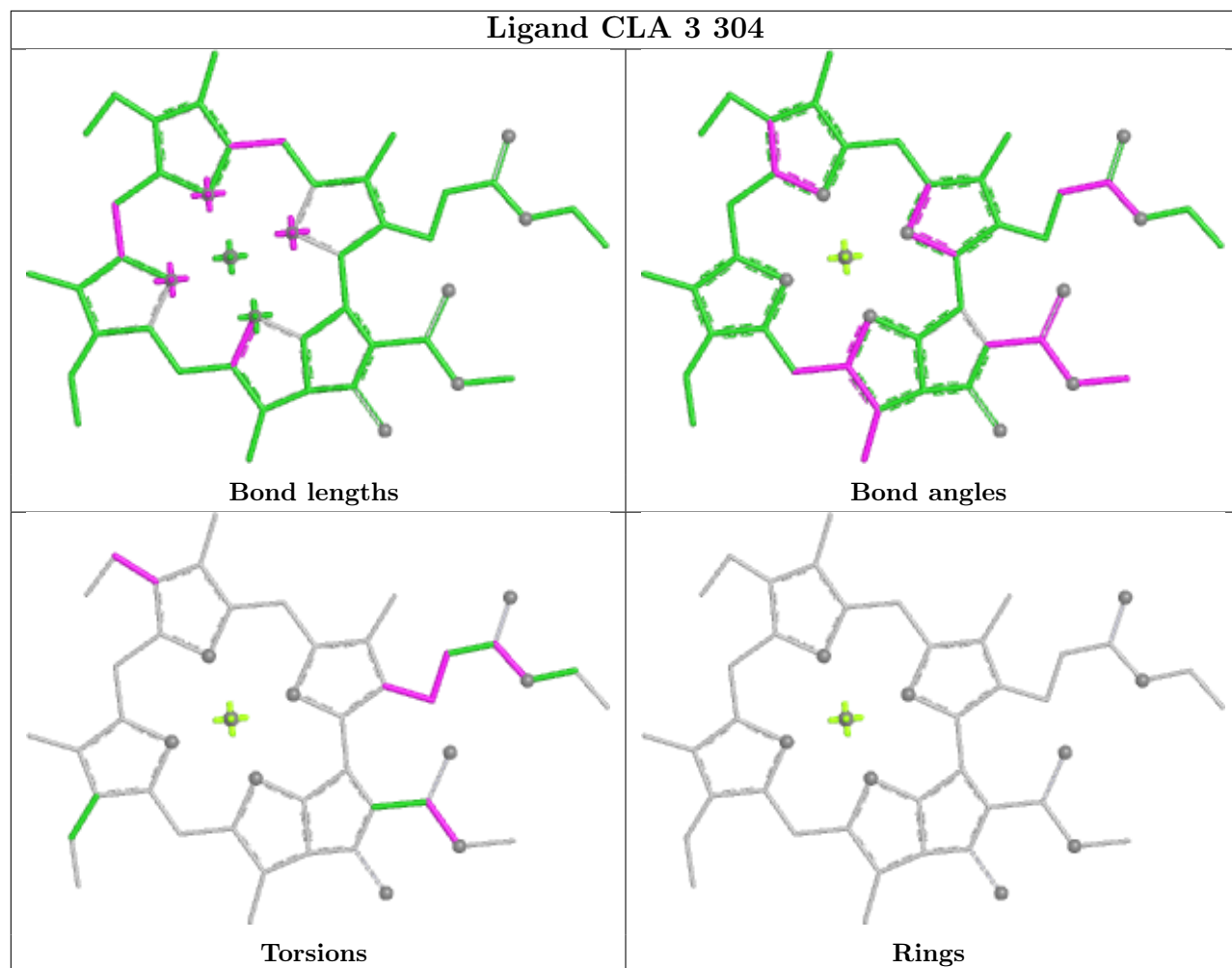


## Ligand CHL 1 306

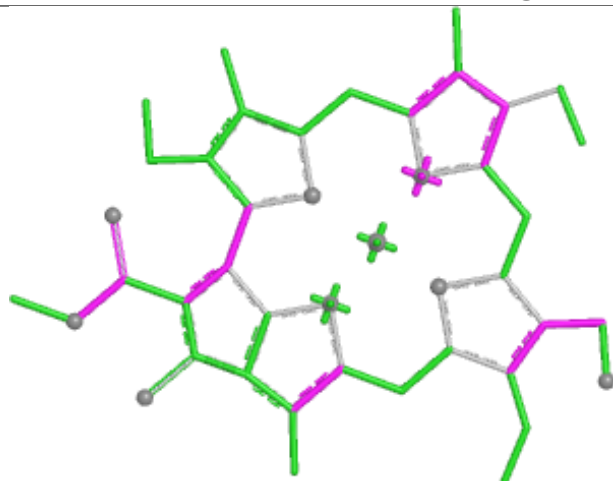




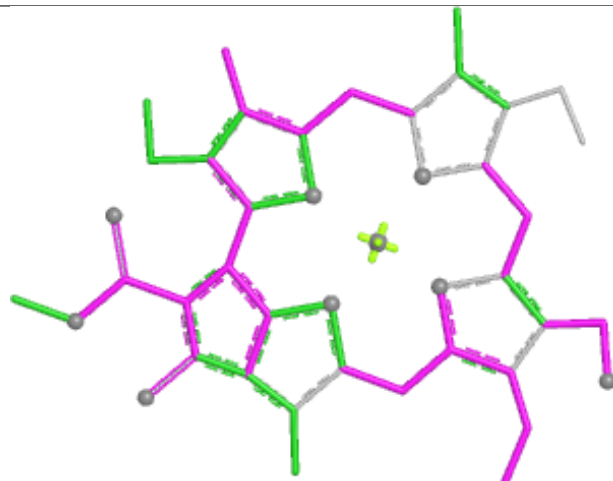
## Ligand CLA 3 304



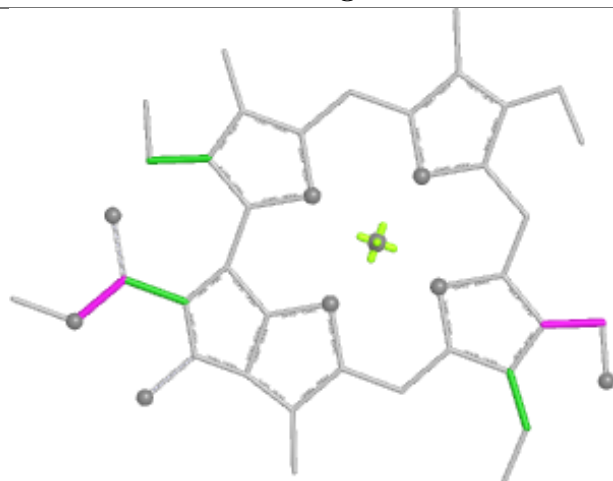
## Ligand CHL 2 305



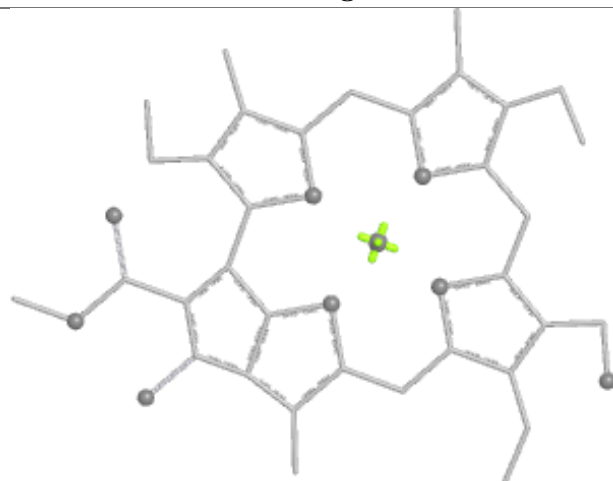
Bond lengths



Bond angles

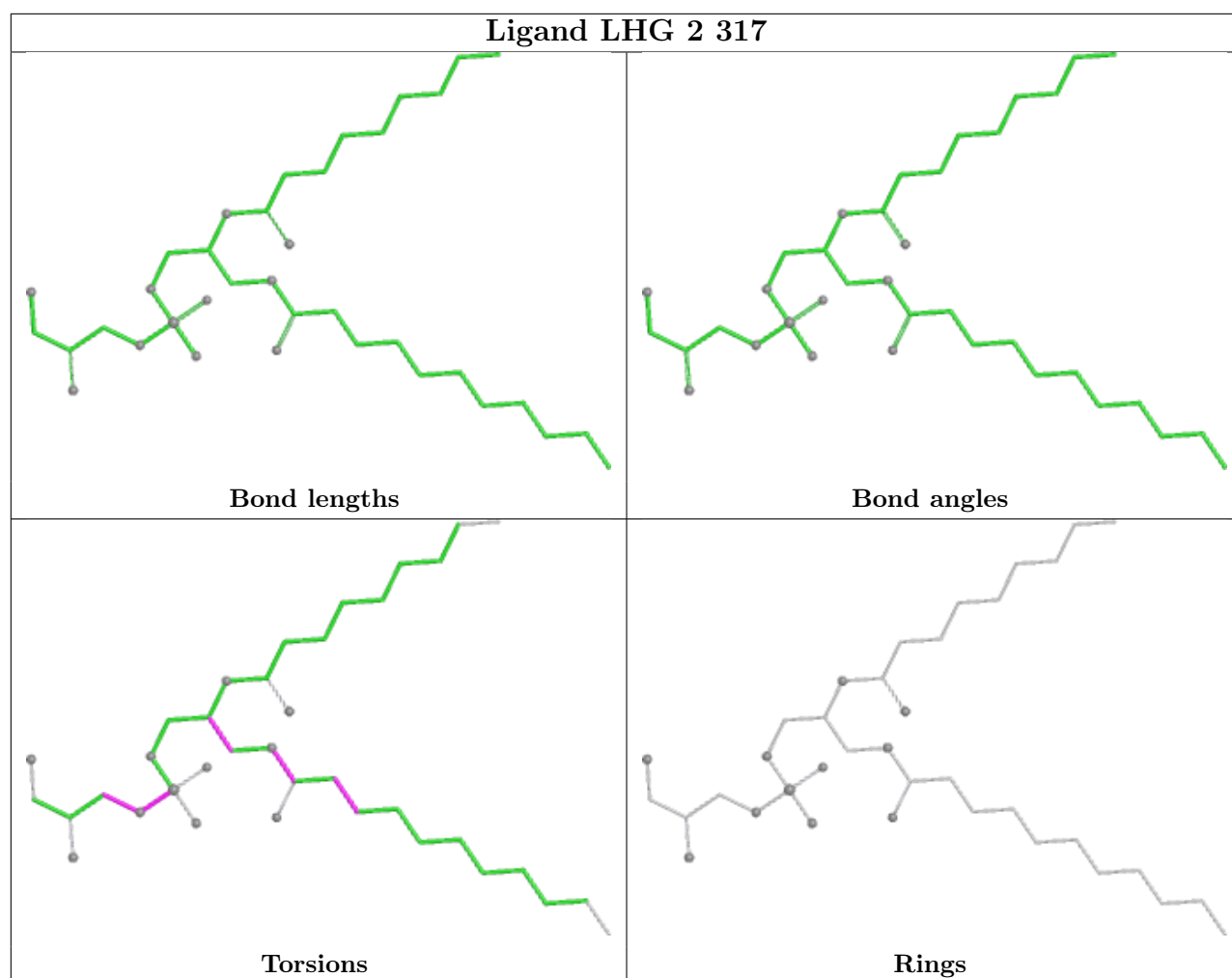


Torsions

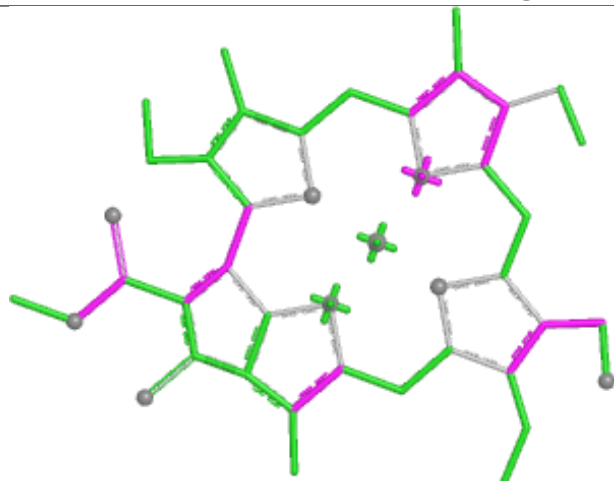


Rings

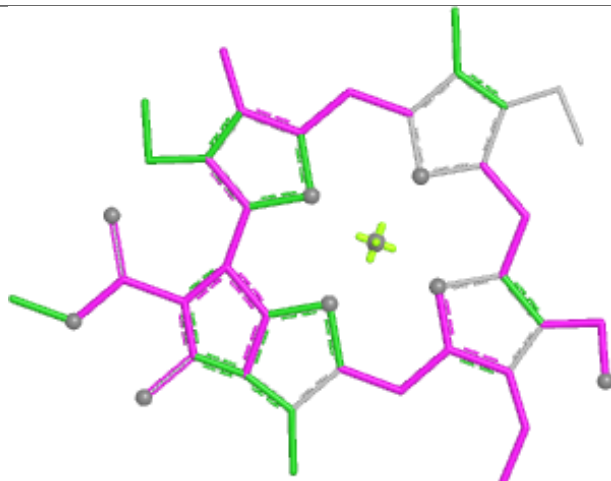




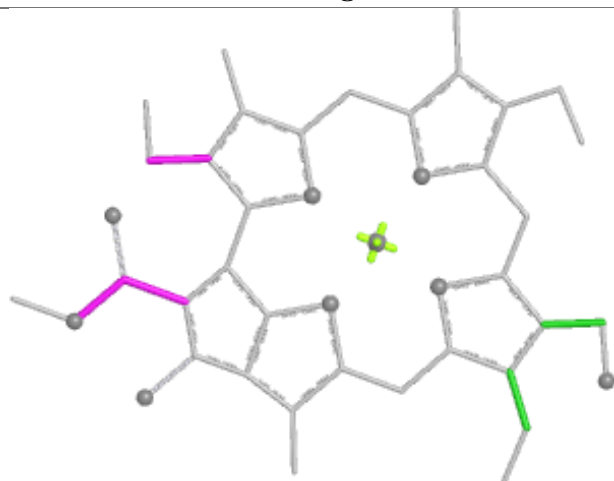
## Ligand CHL 2 314



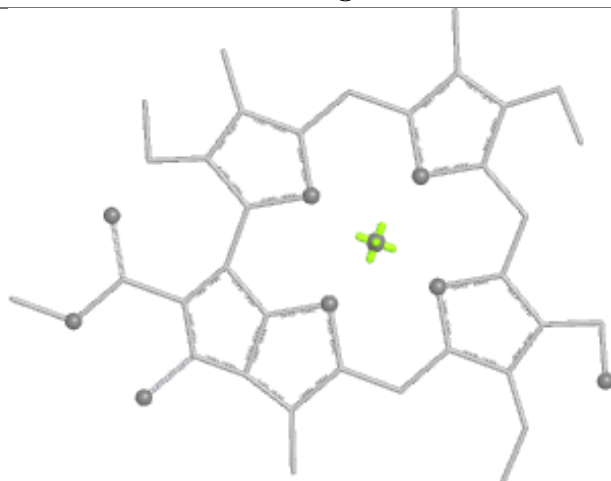
Bond lengths



Bond angles

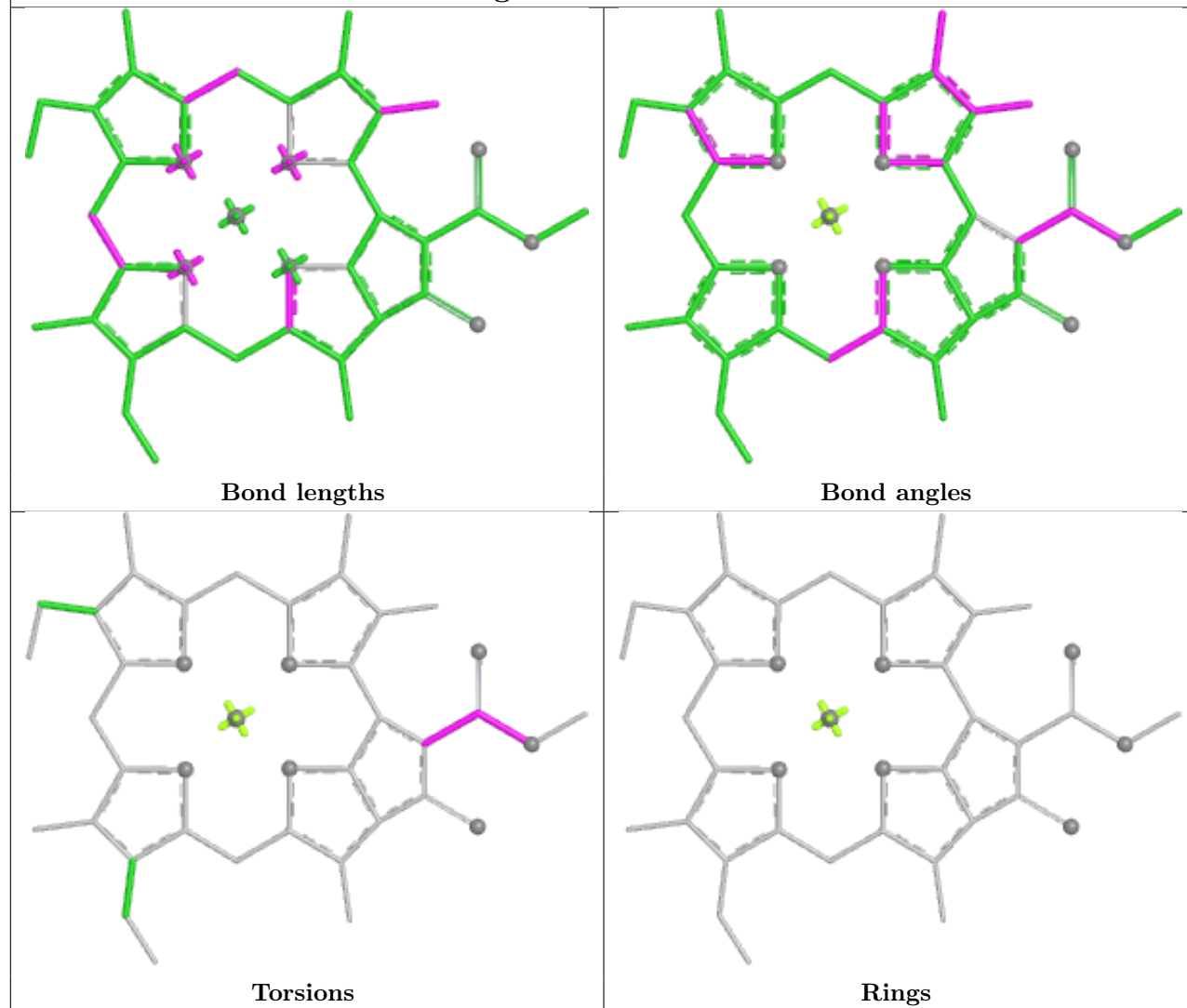


Torsions

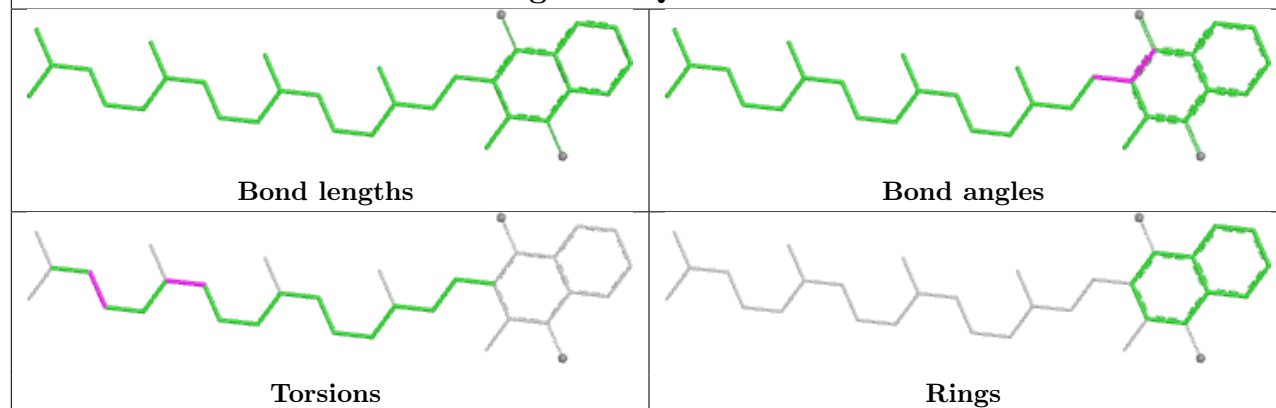


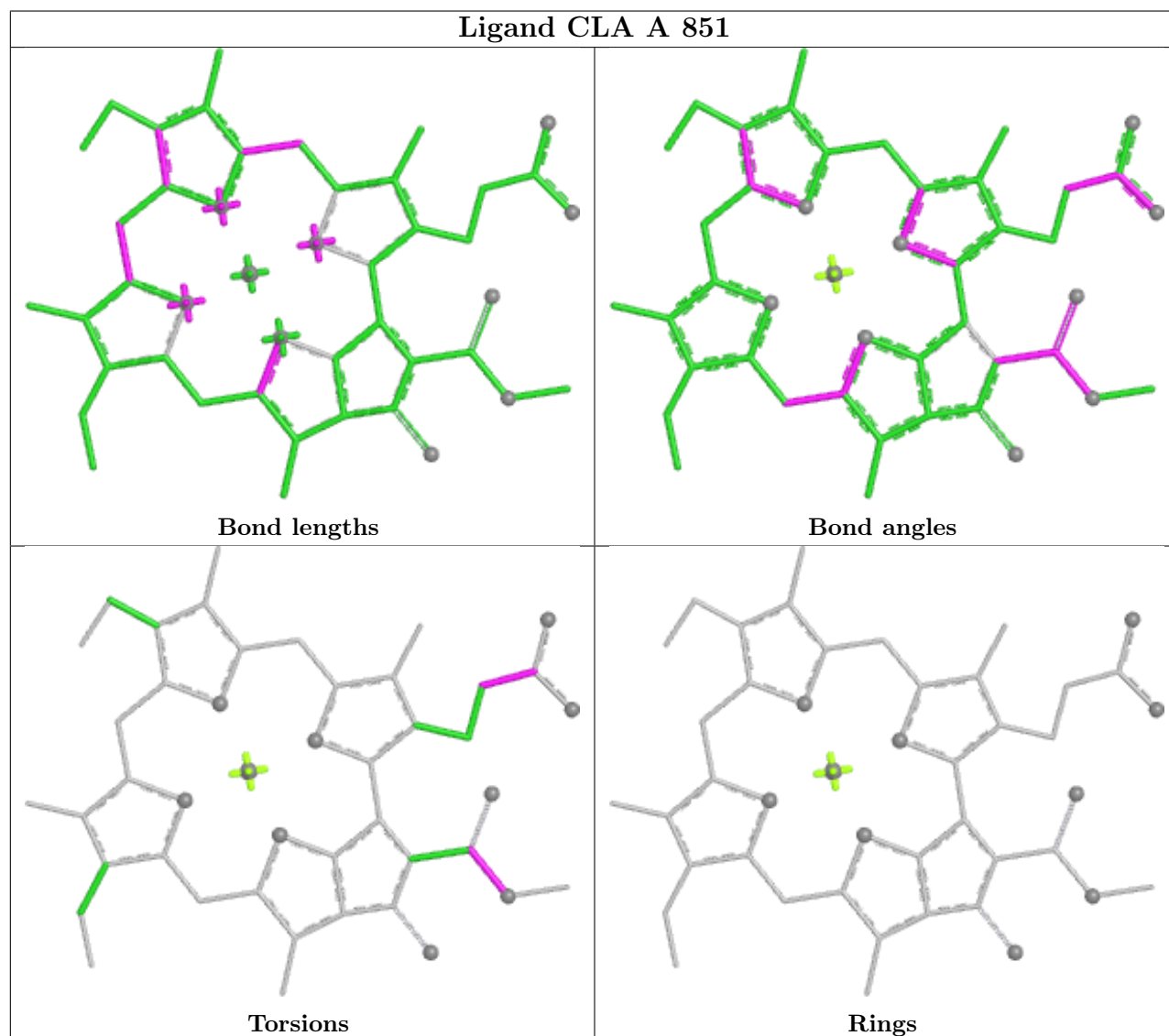
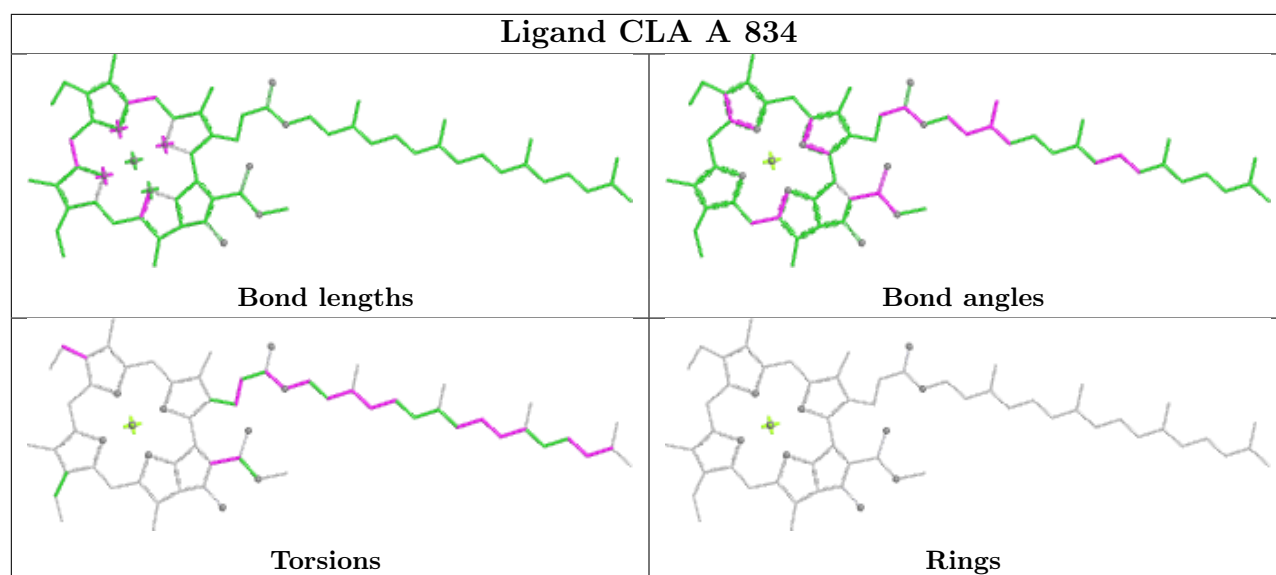
Rings

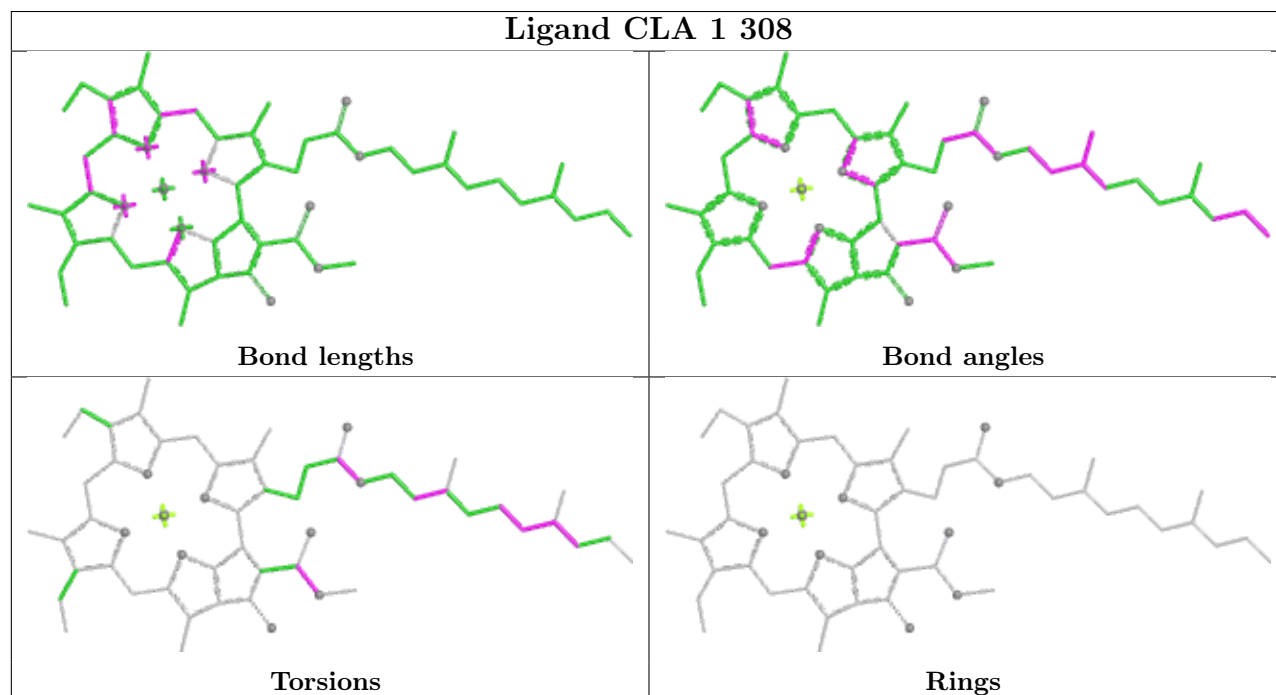
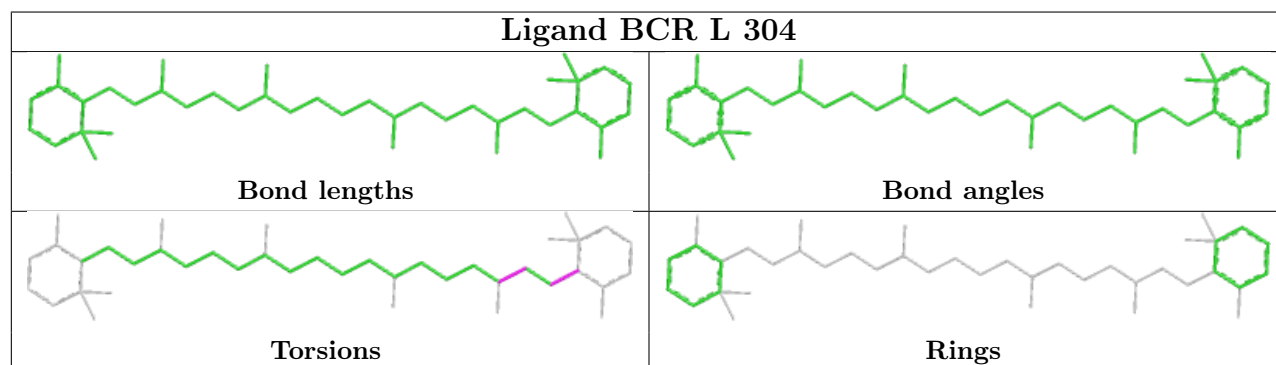
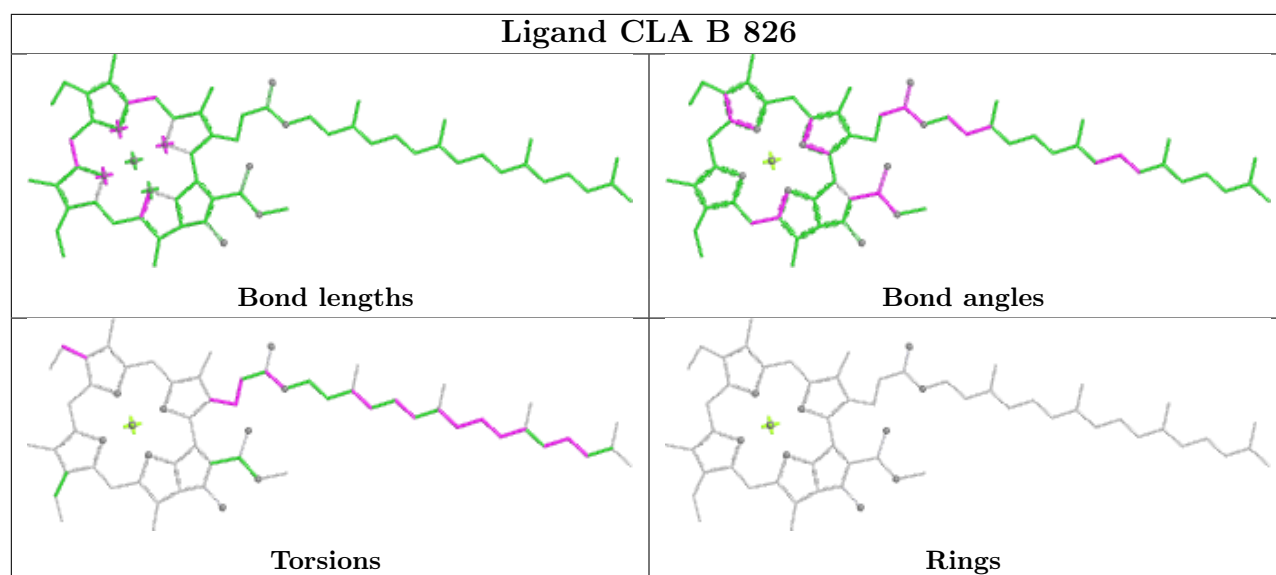
## Ligand CLA G 202

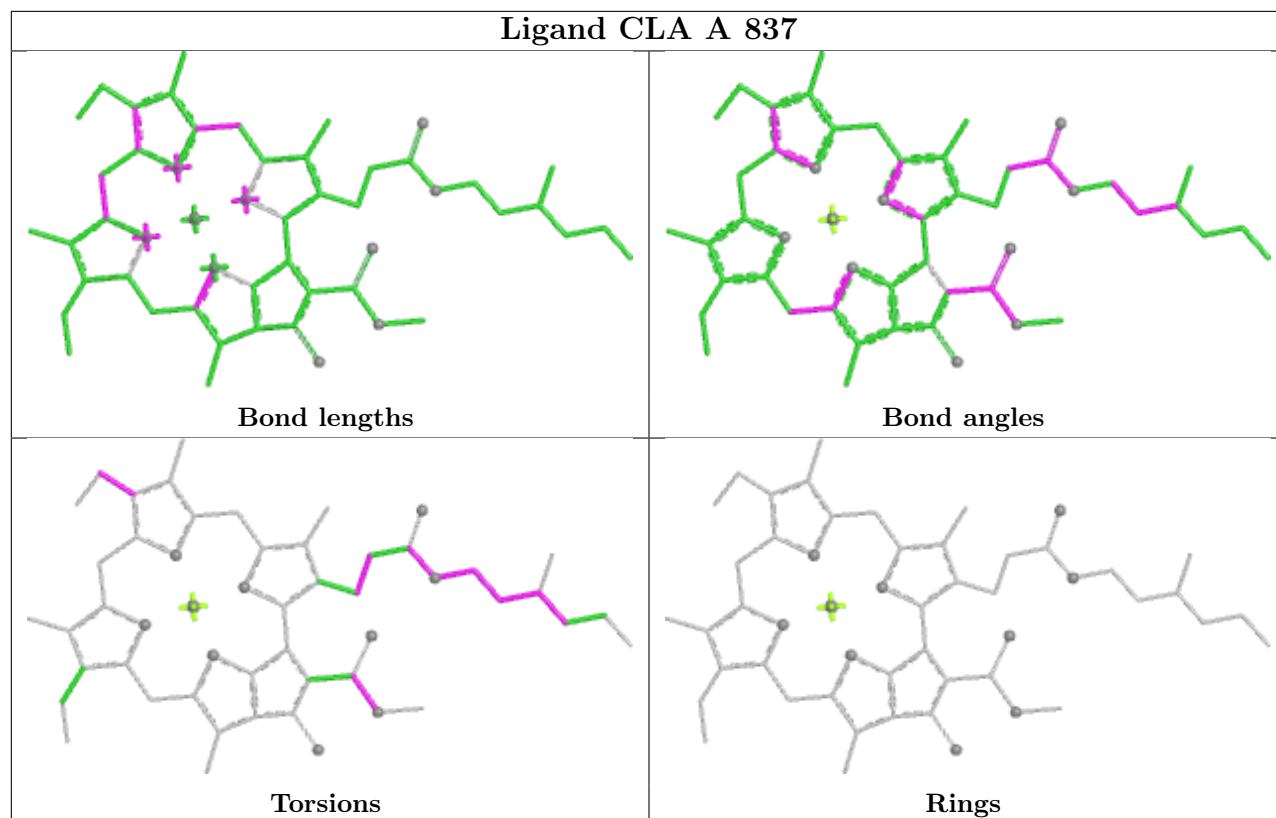


## Ligand PQN A 841

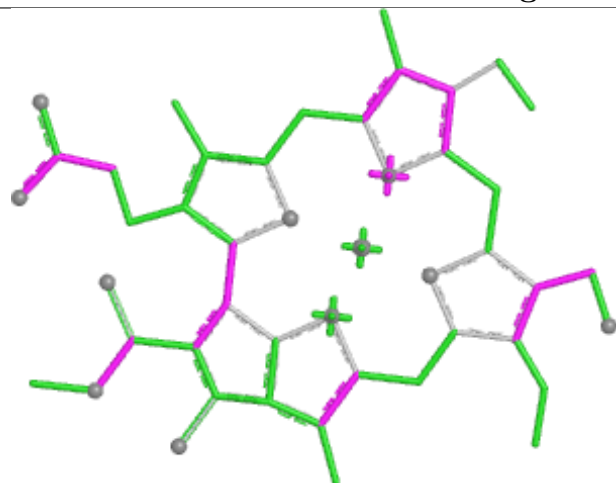




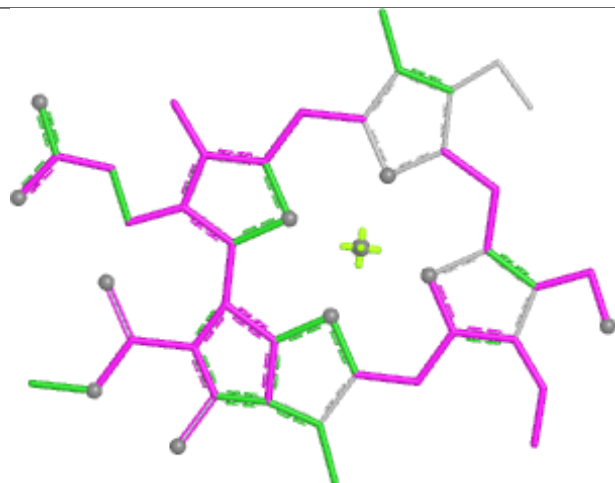




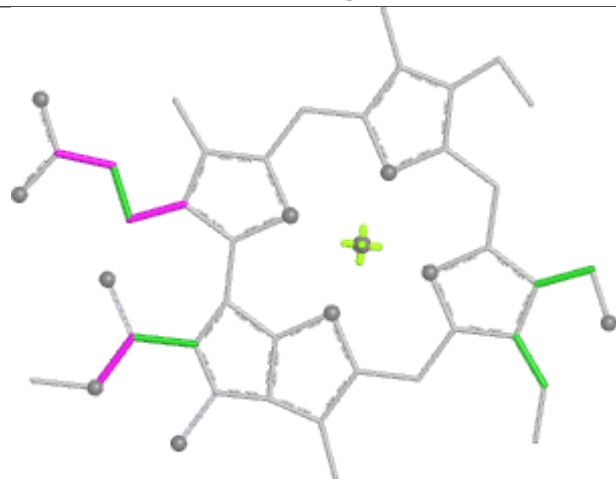
## Ligand CHL 4 305



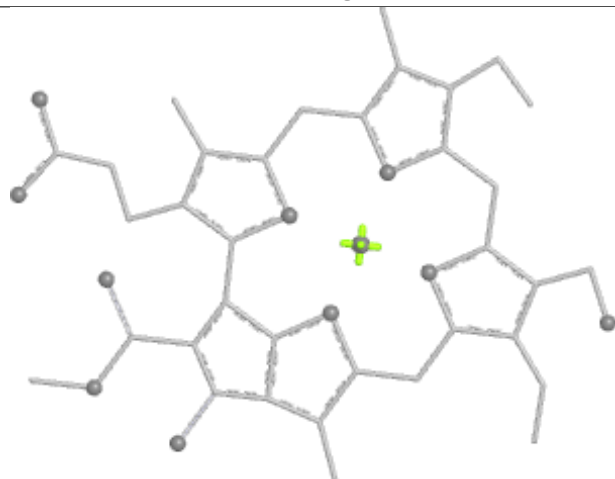
Bond lengths



Bond angles

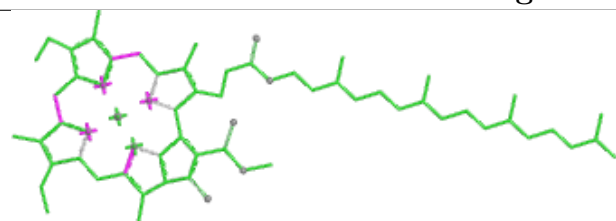


Torsions

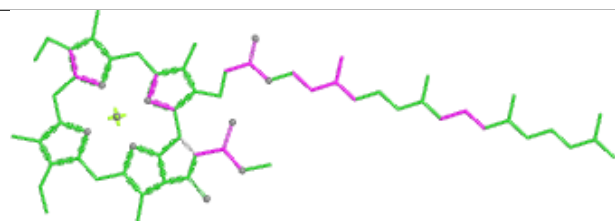


Rings

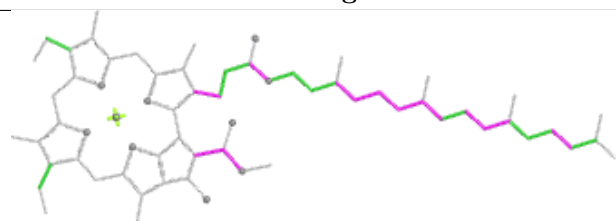
## Ligand CLA A 805



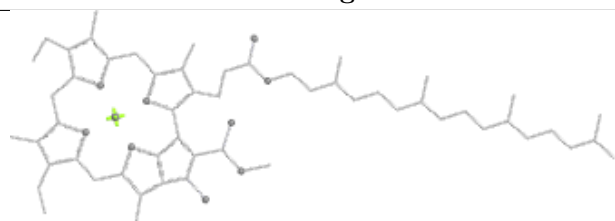
Bond lengths



Bond angles

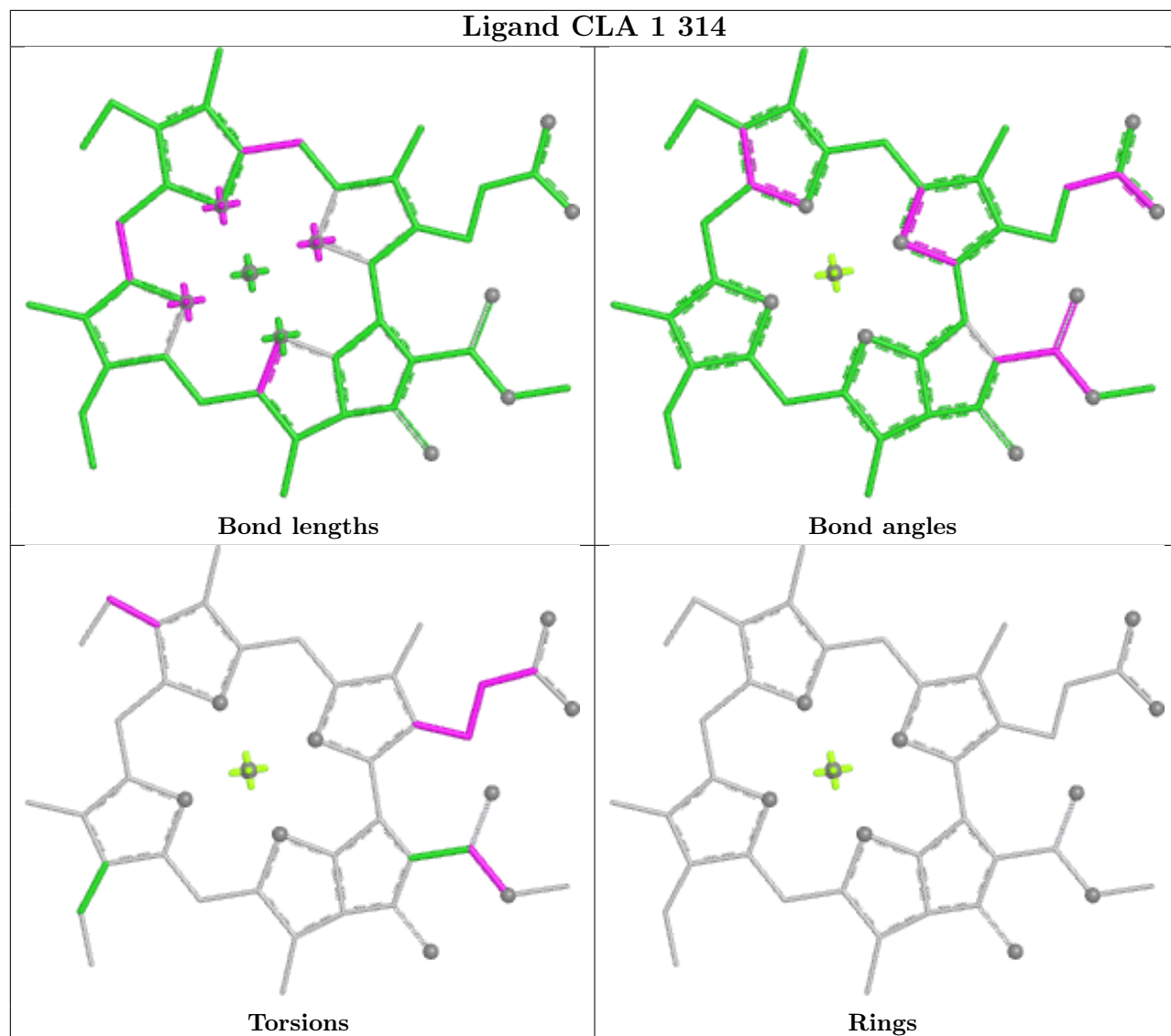


Torsions



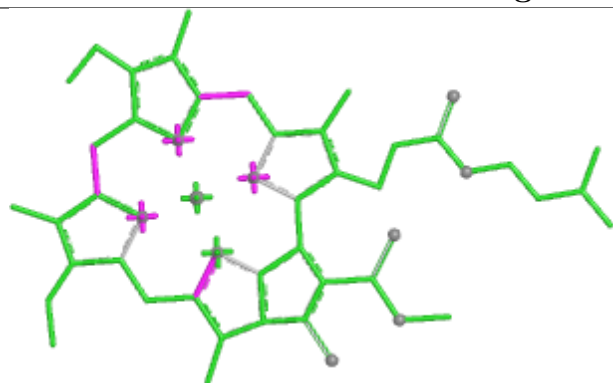
Rings

## Ligand CLA 1 314

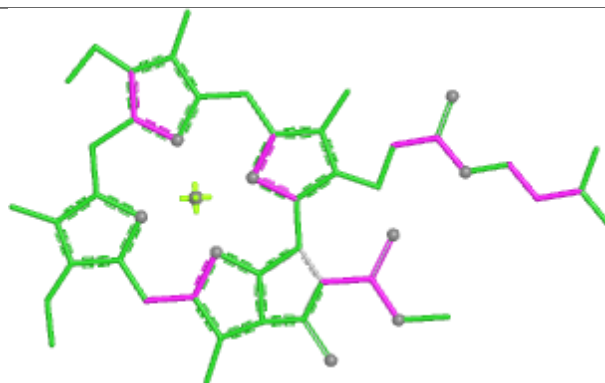




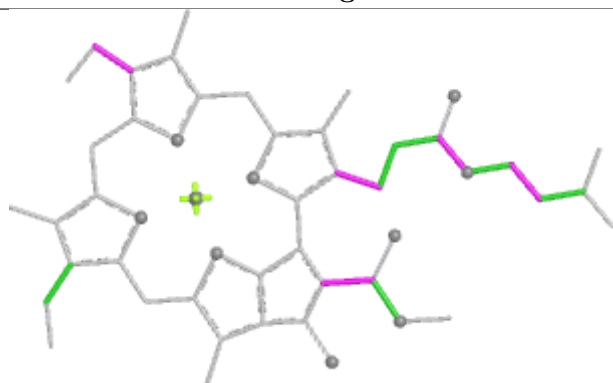
## Ligand CLA B 829



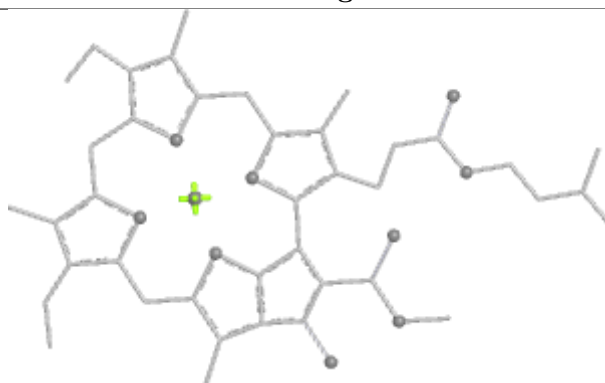
Bond lengths



Bond angles

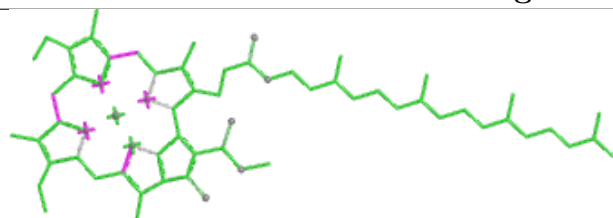


Torsions

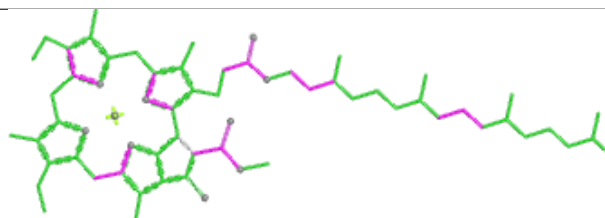


Rings

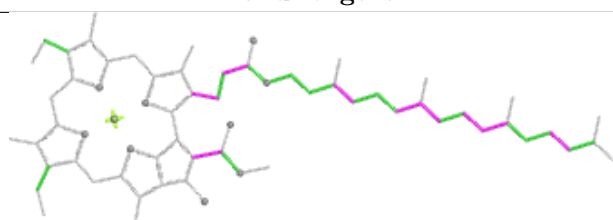
## Ligand CLA B 838



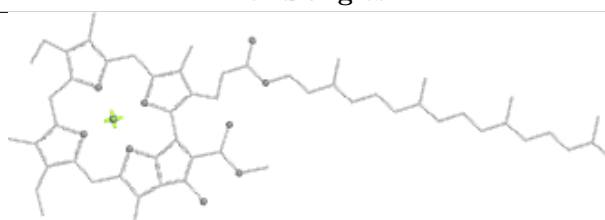
Bond lengths



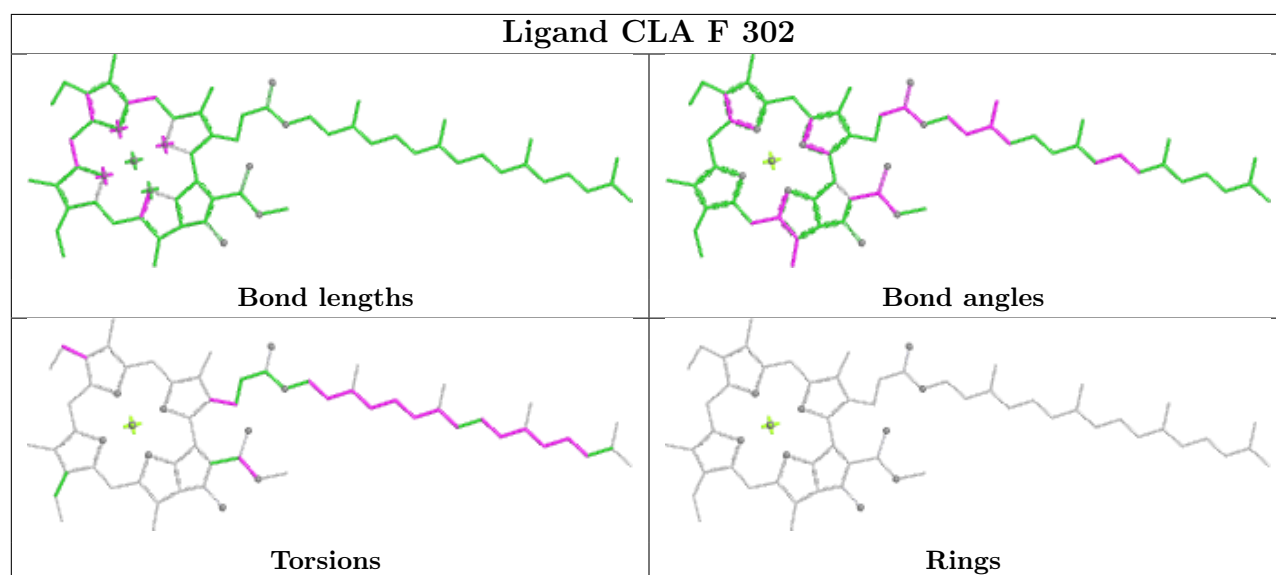
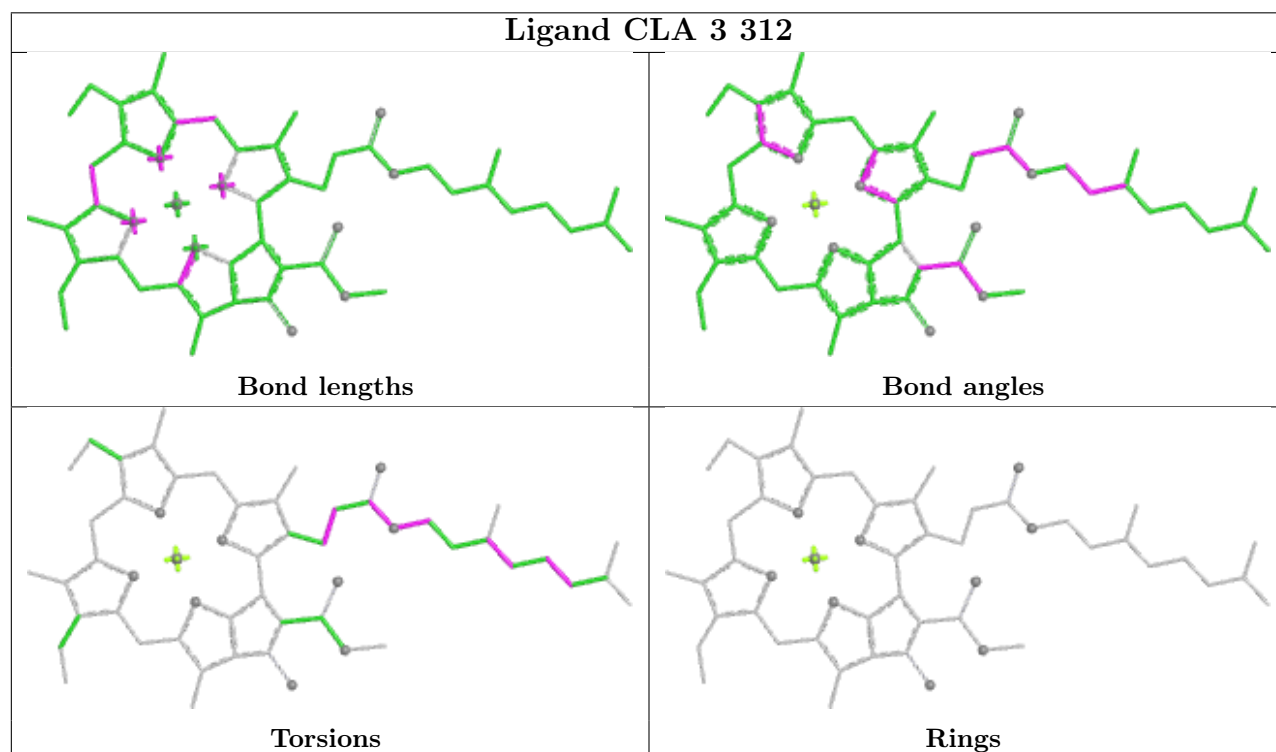
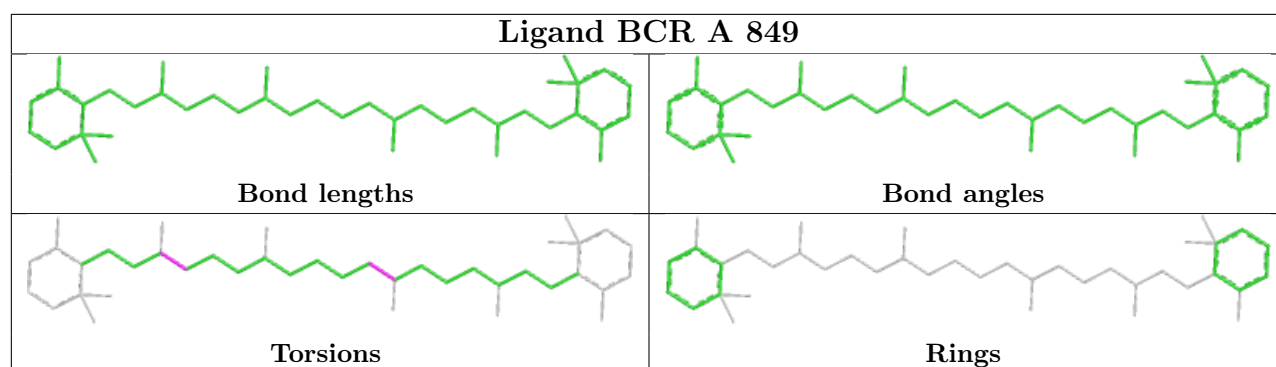
Bond angles

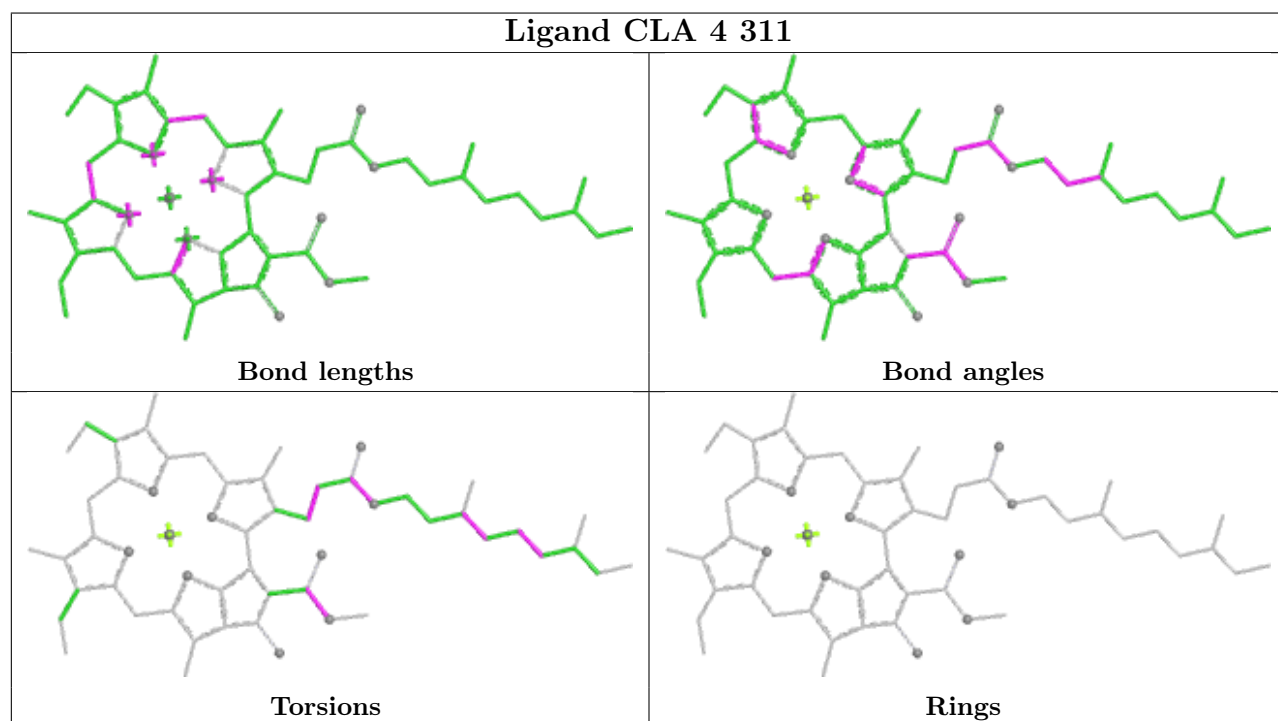
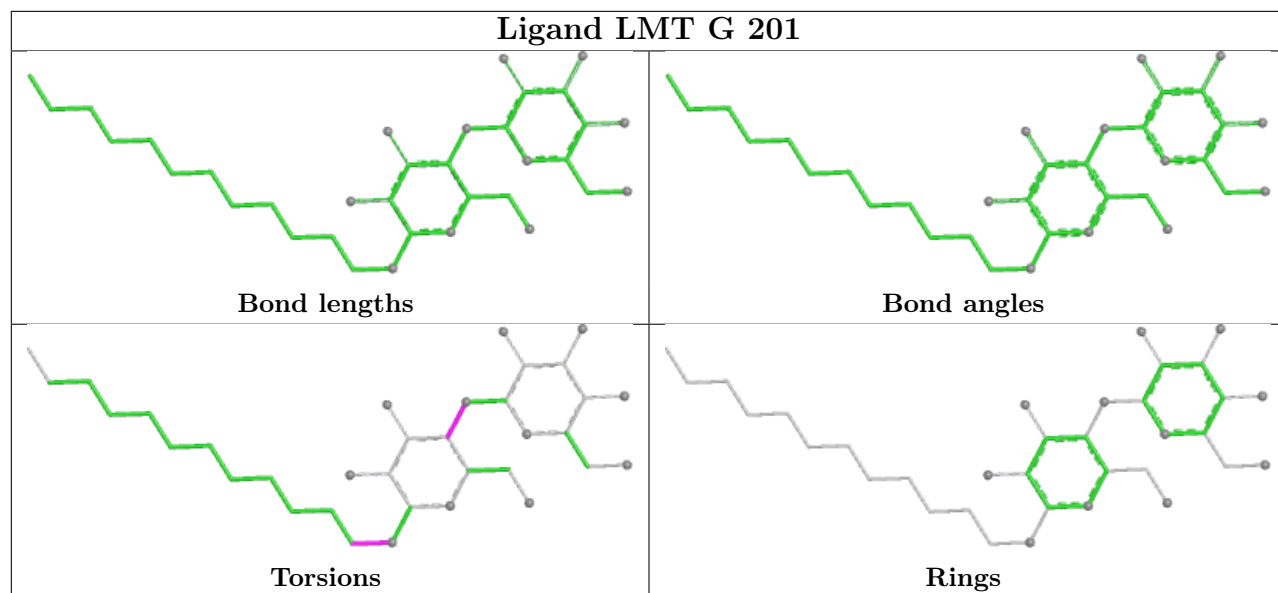


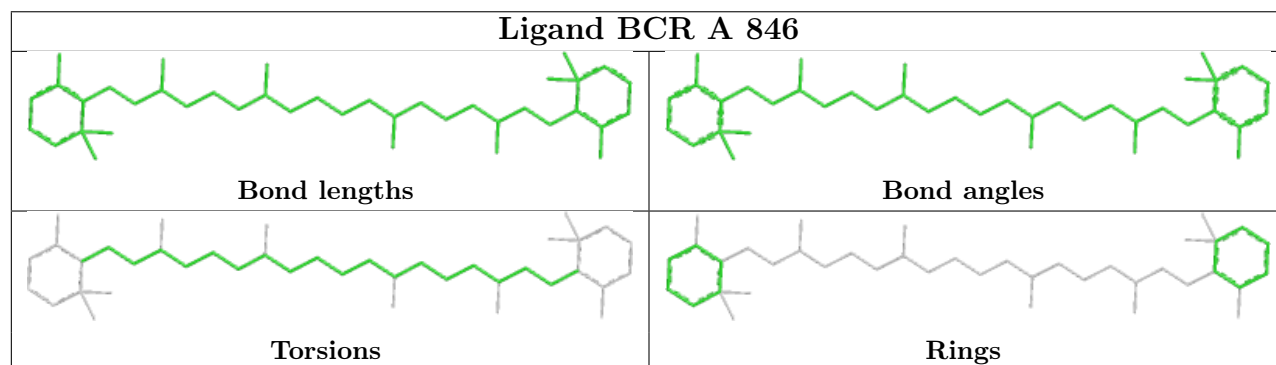
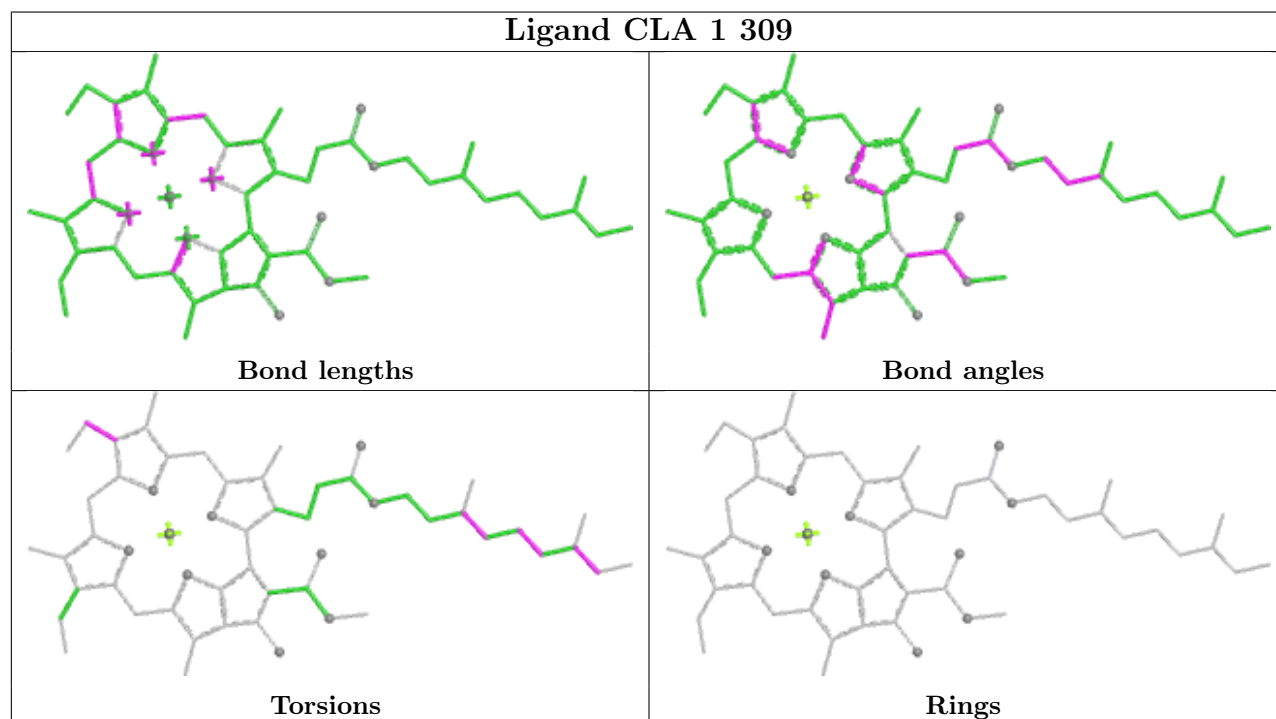
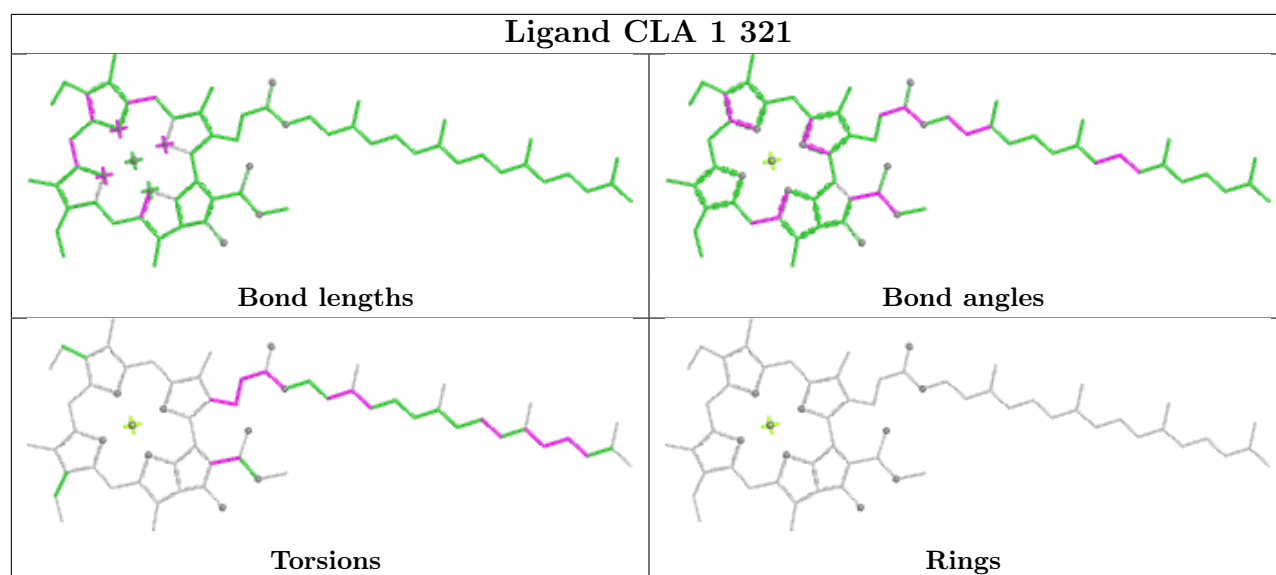
Torsions



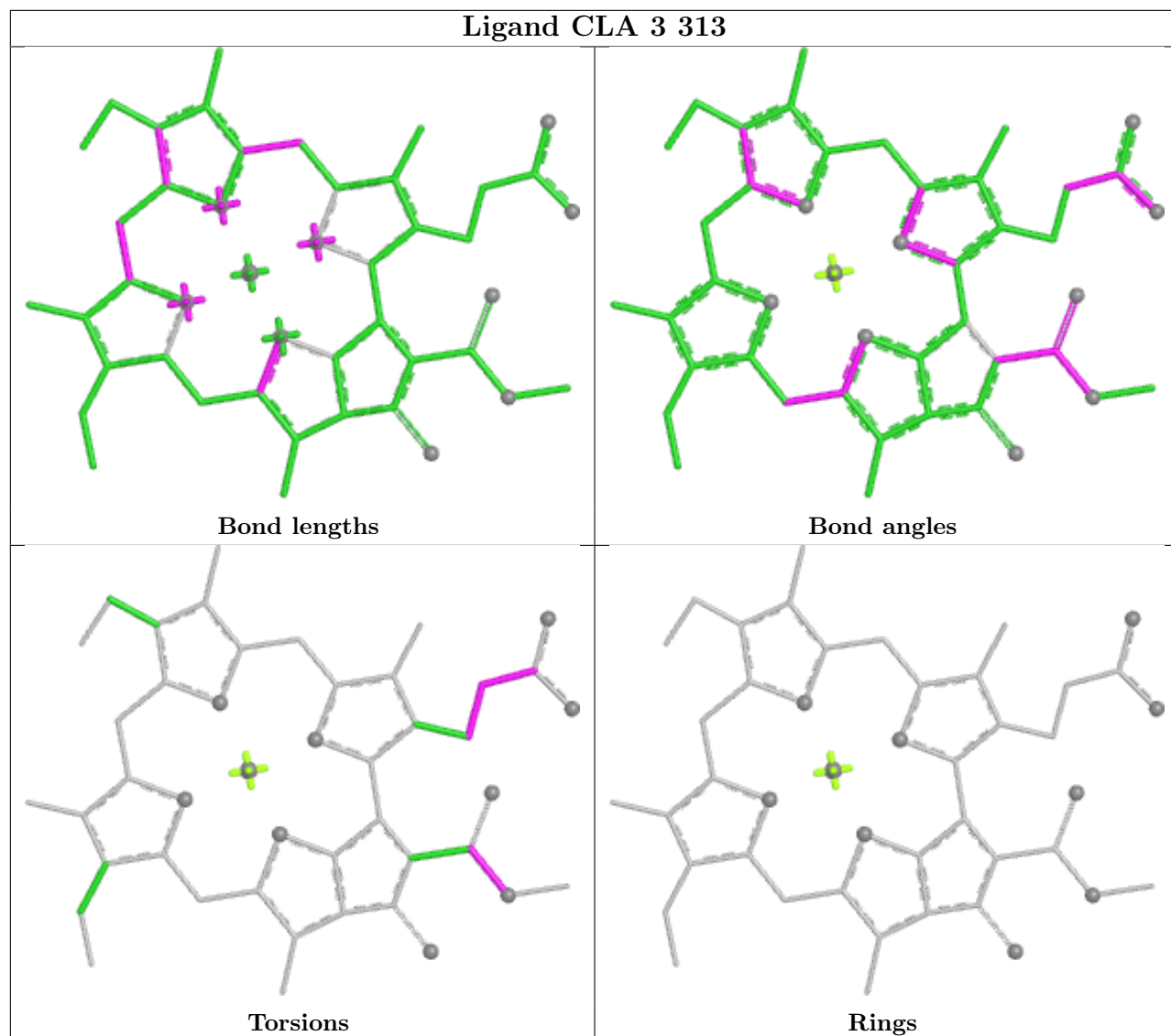
Rings

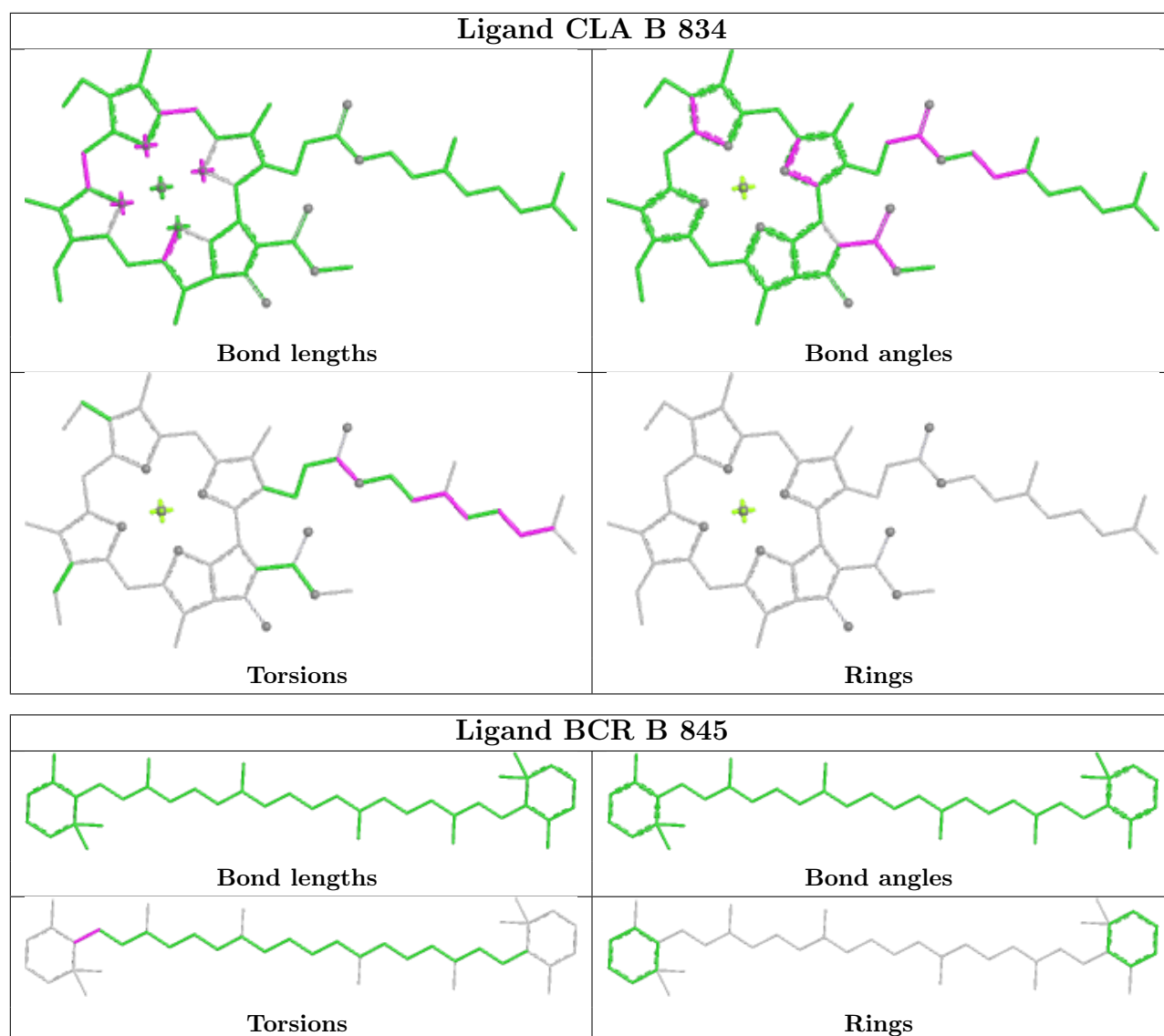




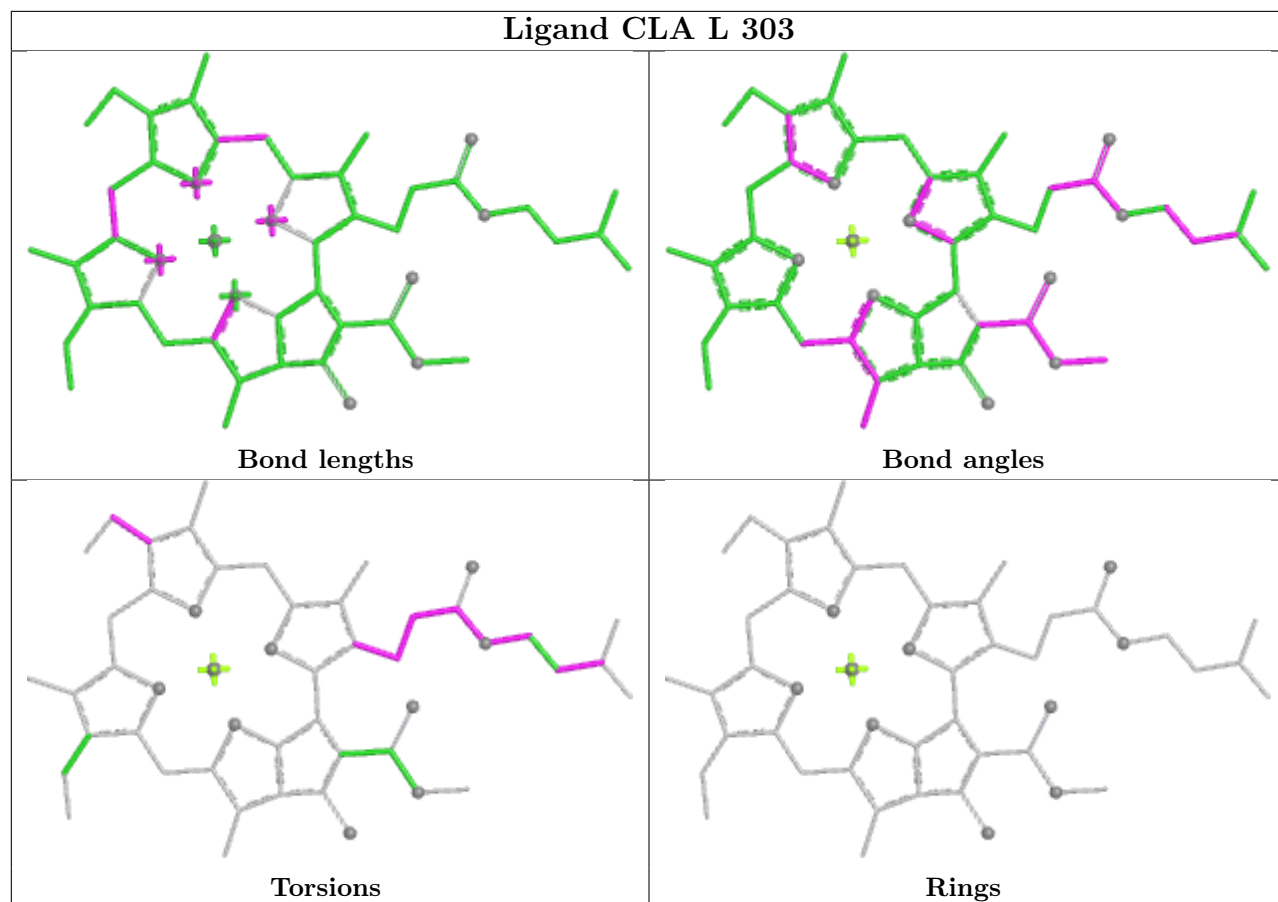


## Ligand CLA 3 313

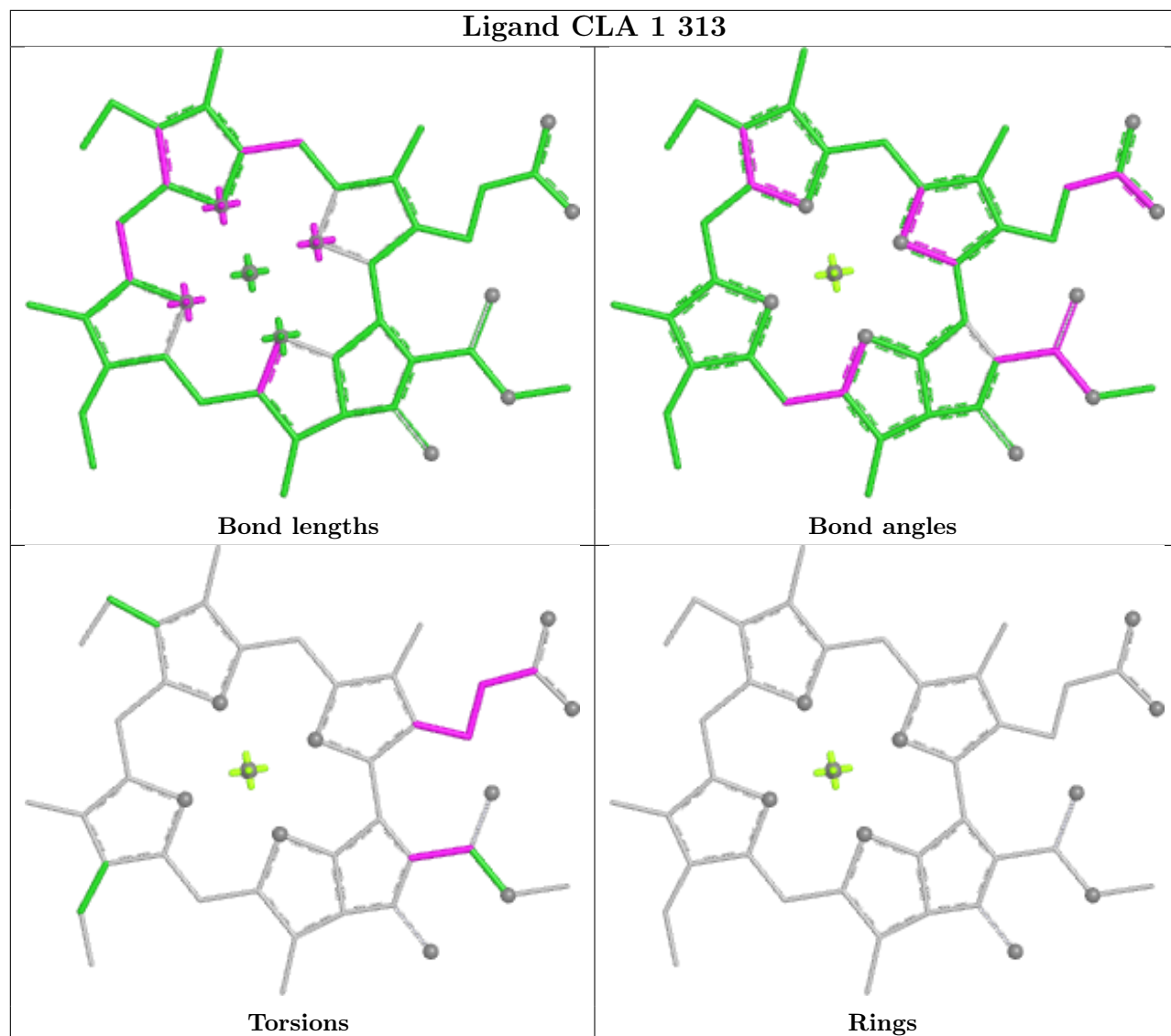




## Ligand CLA L 303

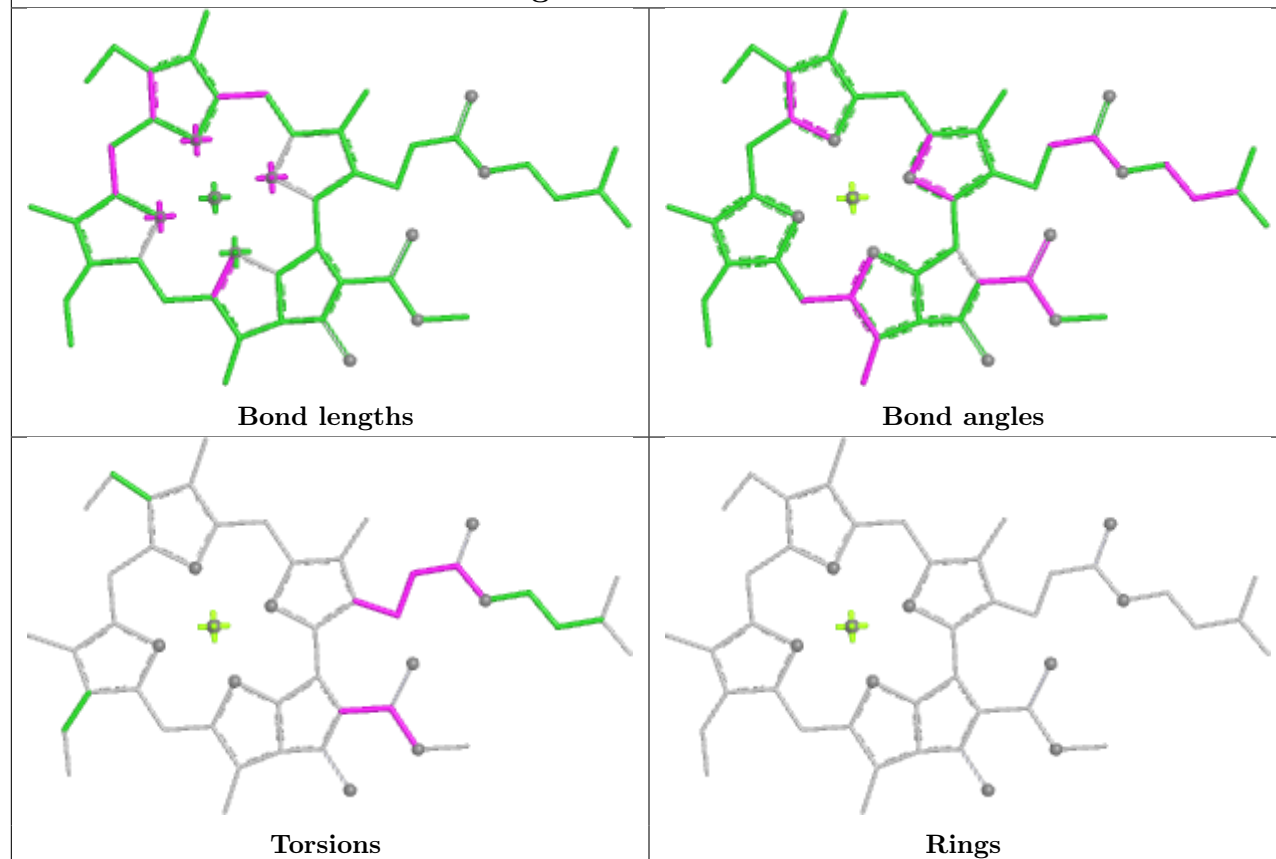


## Ligand CLA 1 313

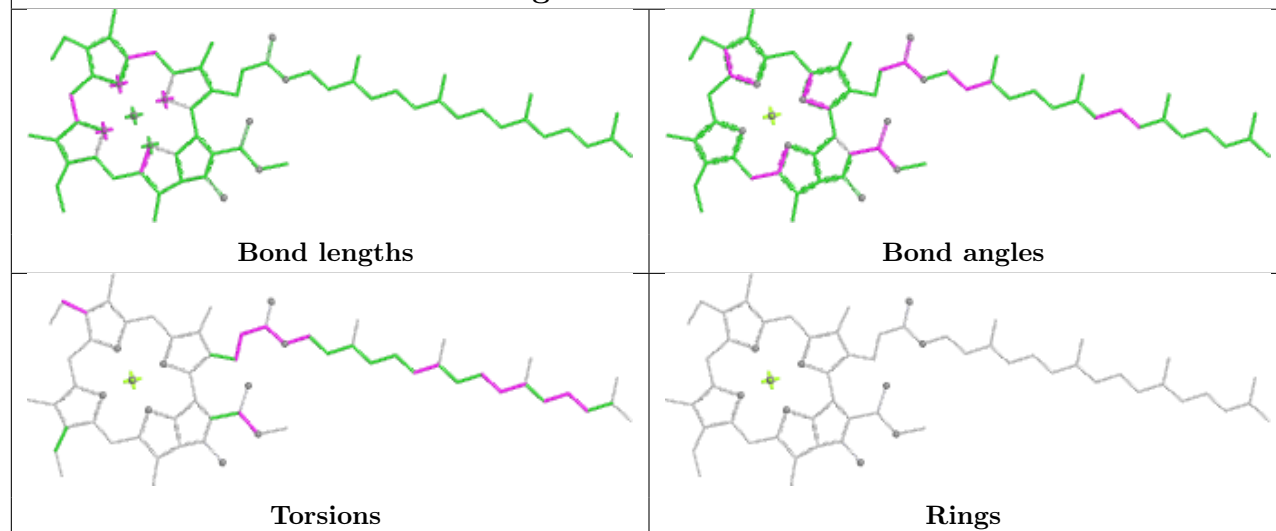




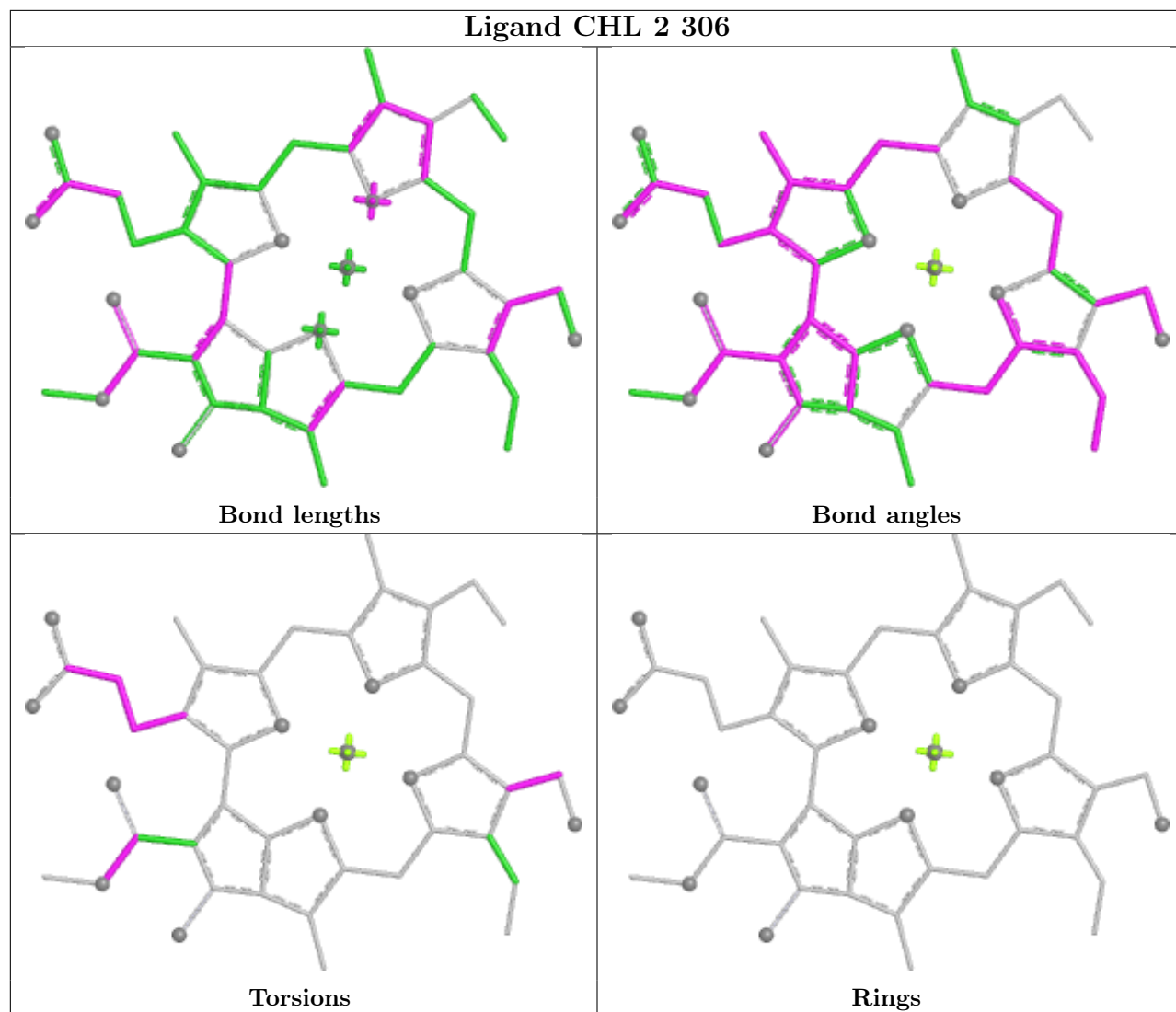
## Ligand CLA A 830



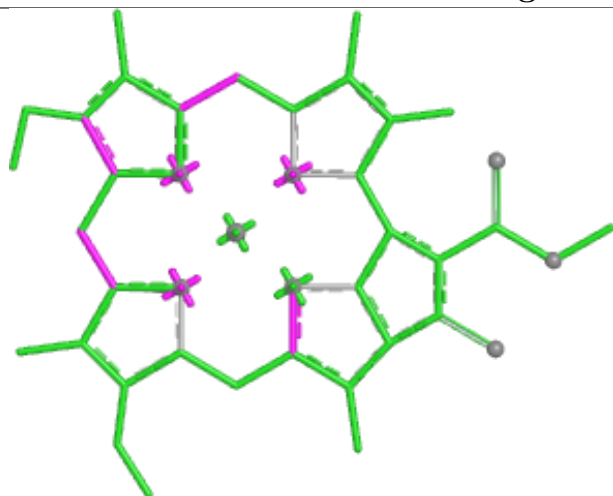
## Ligand CLA B 802



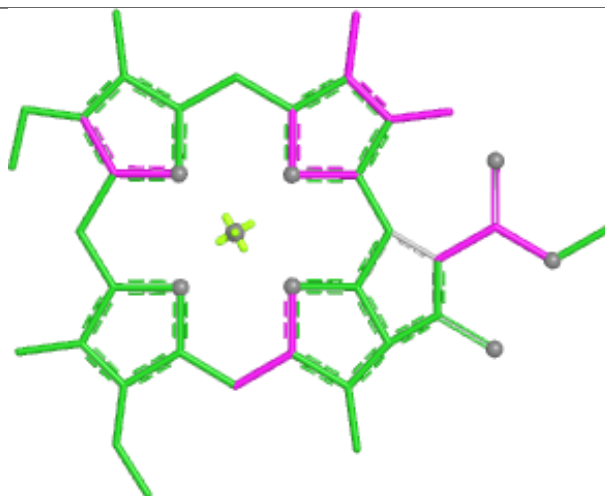
## Ligand CHL 2 306



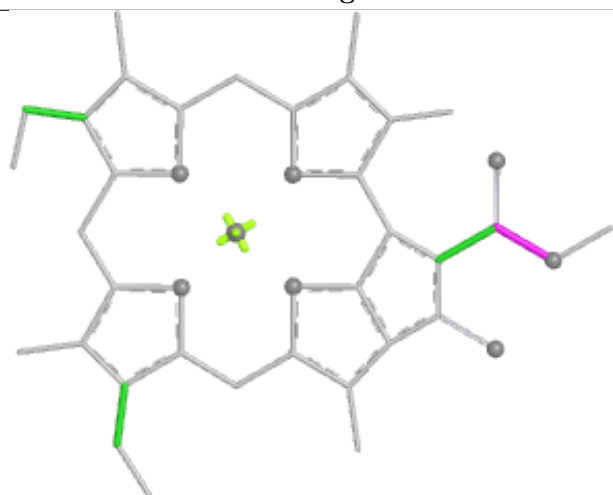
## Ligand CLA 2 310



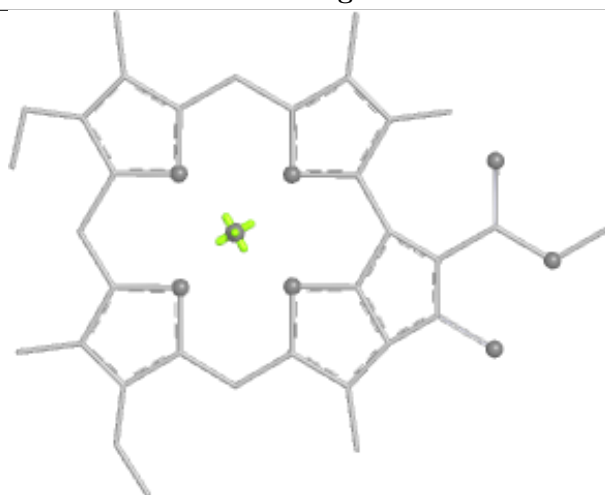
Bond lengths



Bond angles

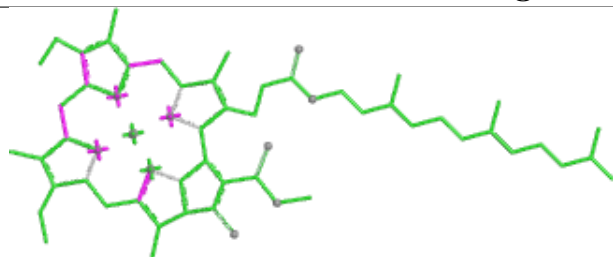


Torsions

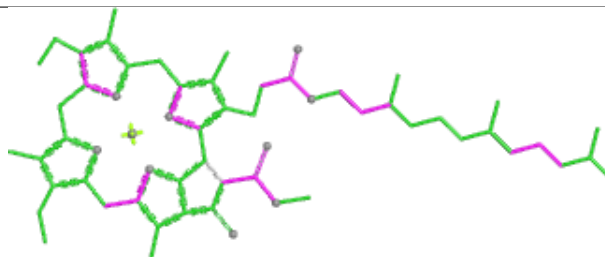


Rings

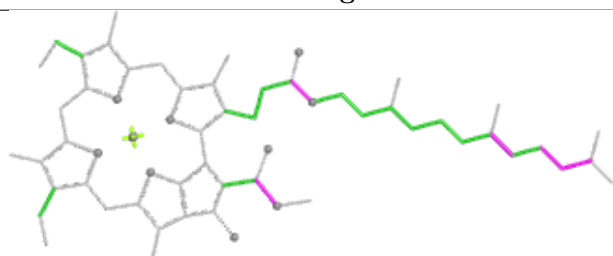
## Ligand CLA B 818



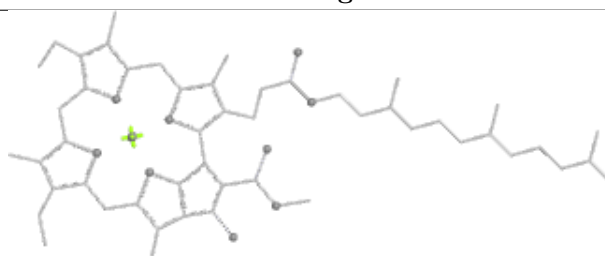
Bond lengths



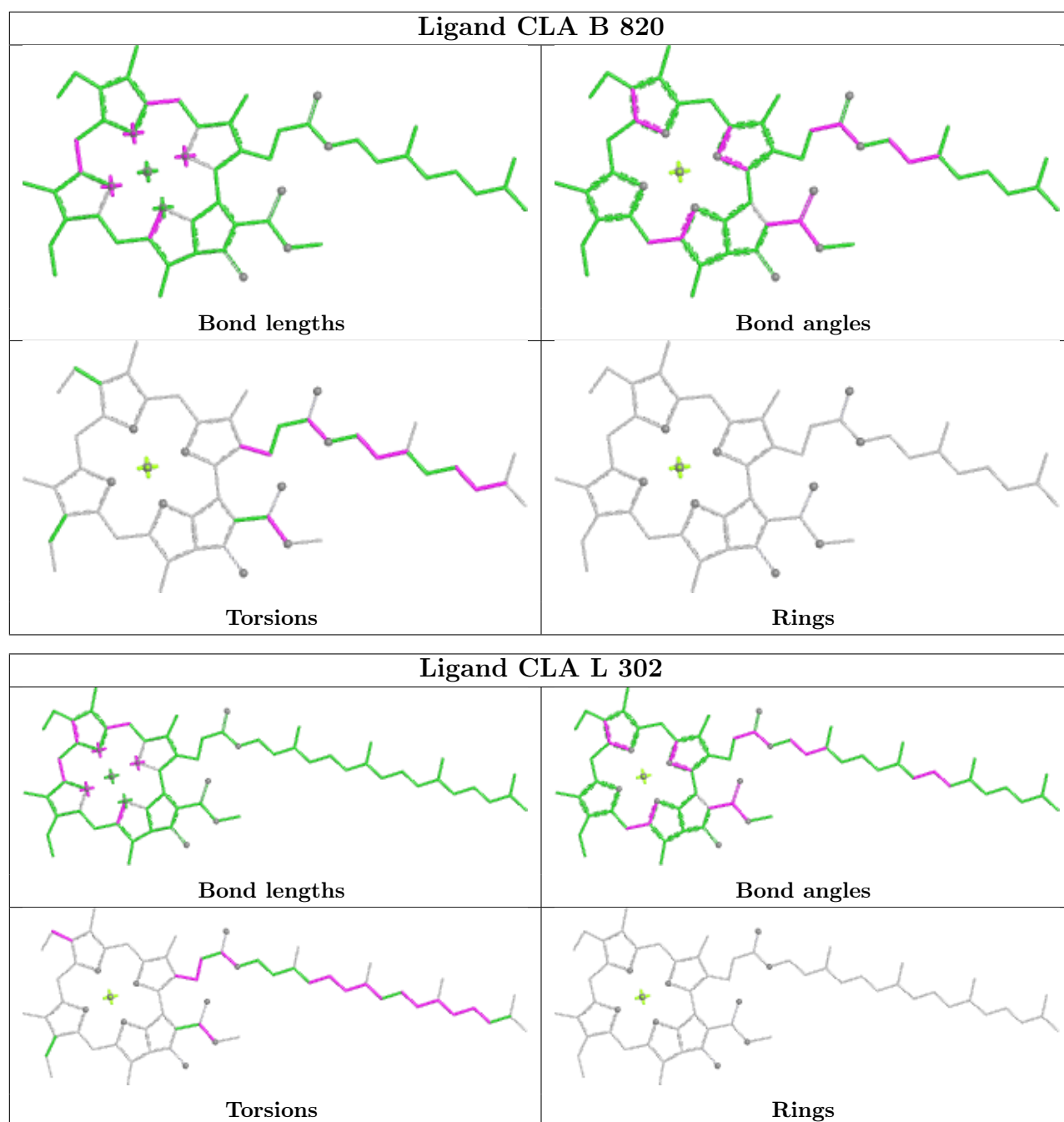
Bond angles



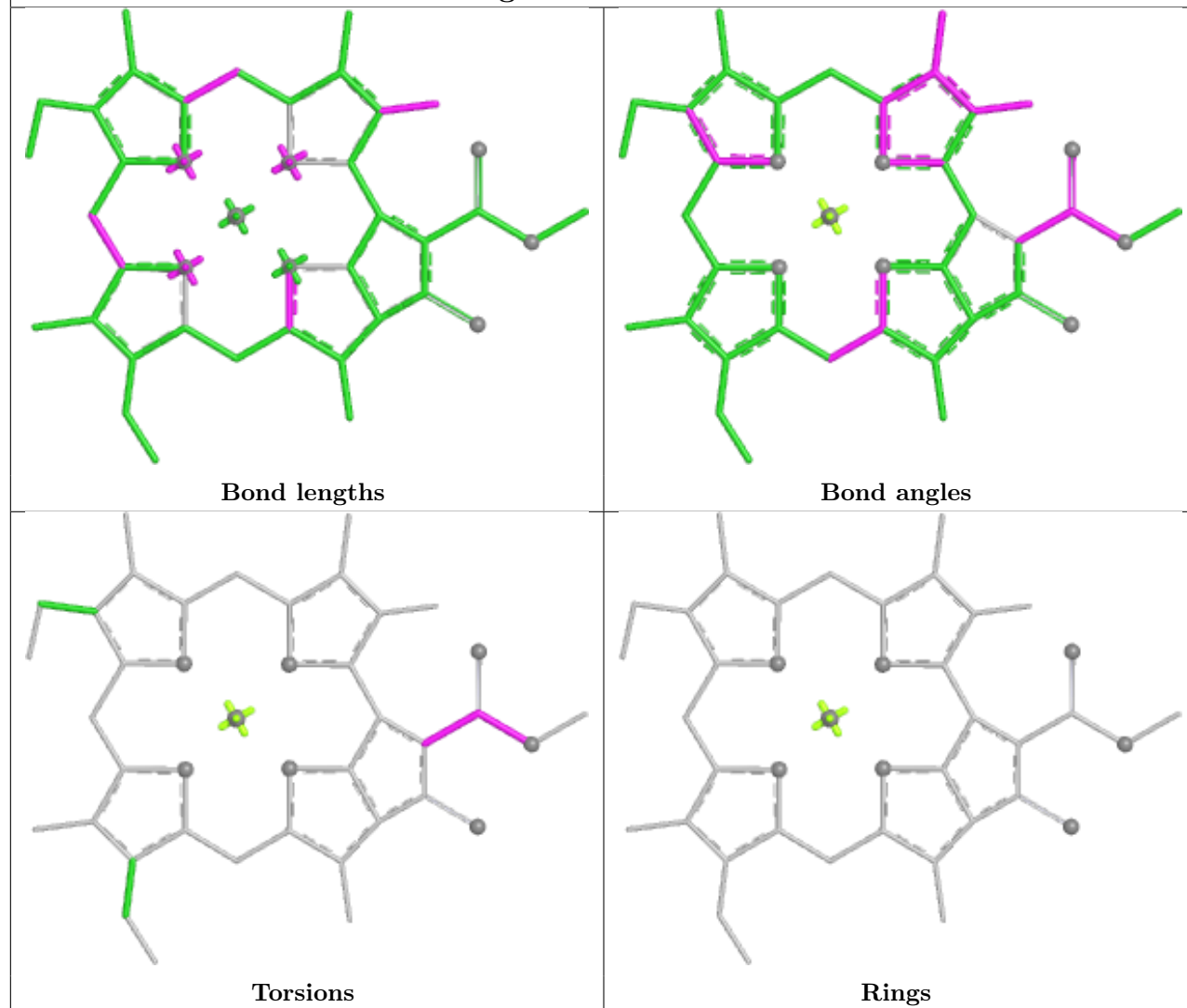
Torsions



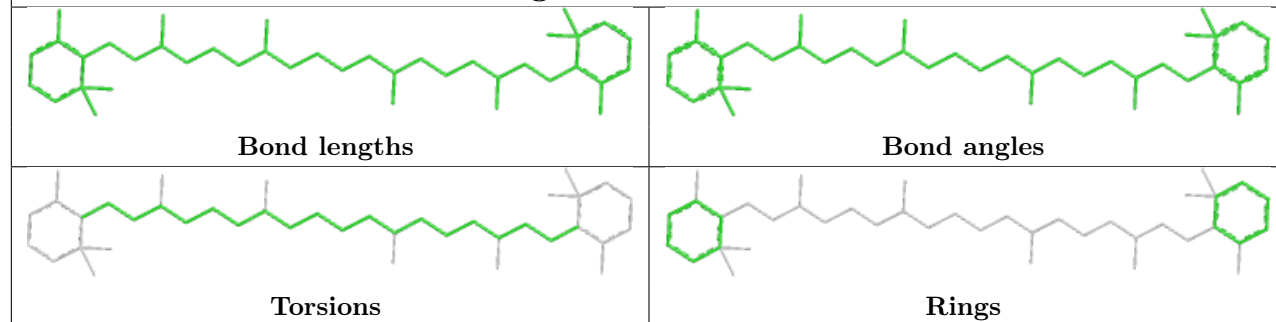
Rings



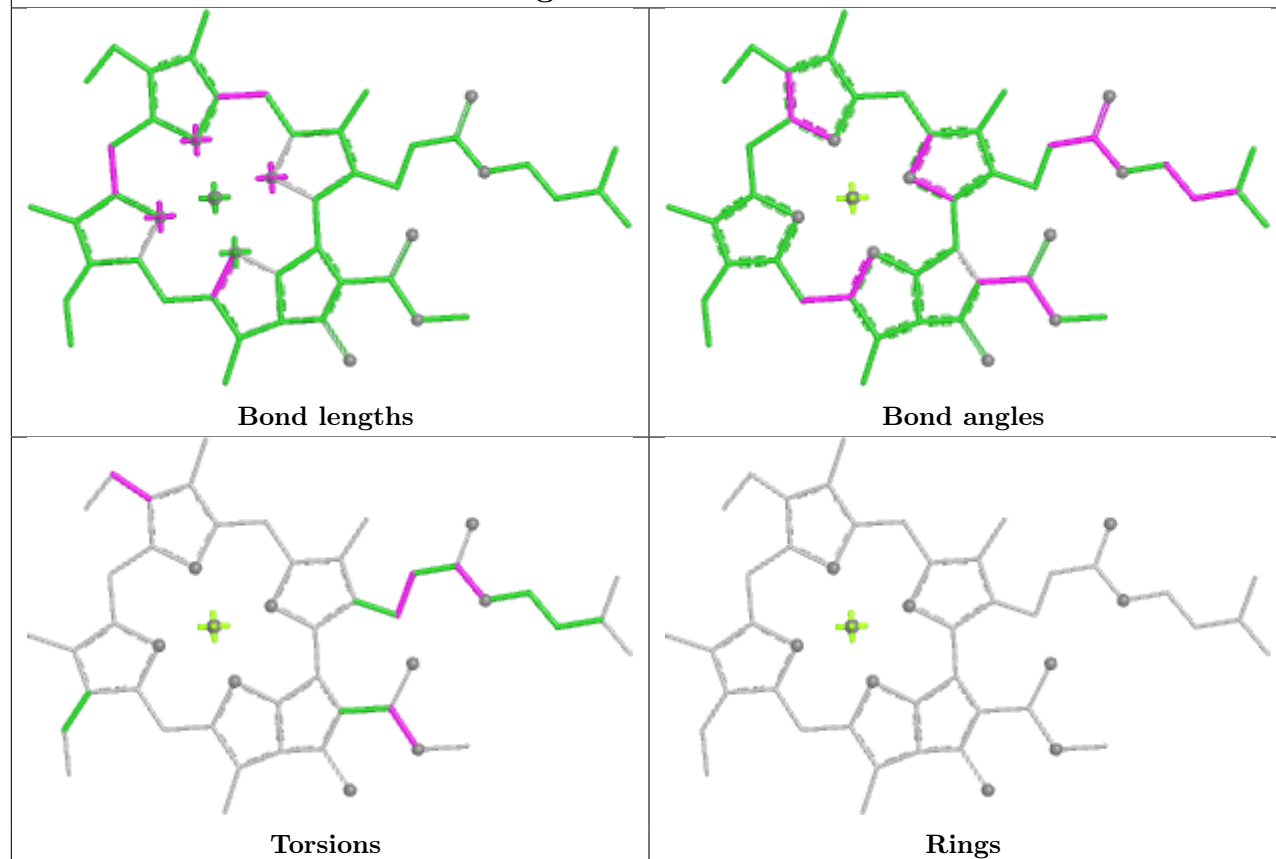
## Ligand CLA 3 310



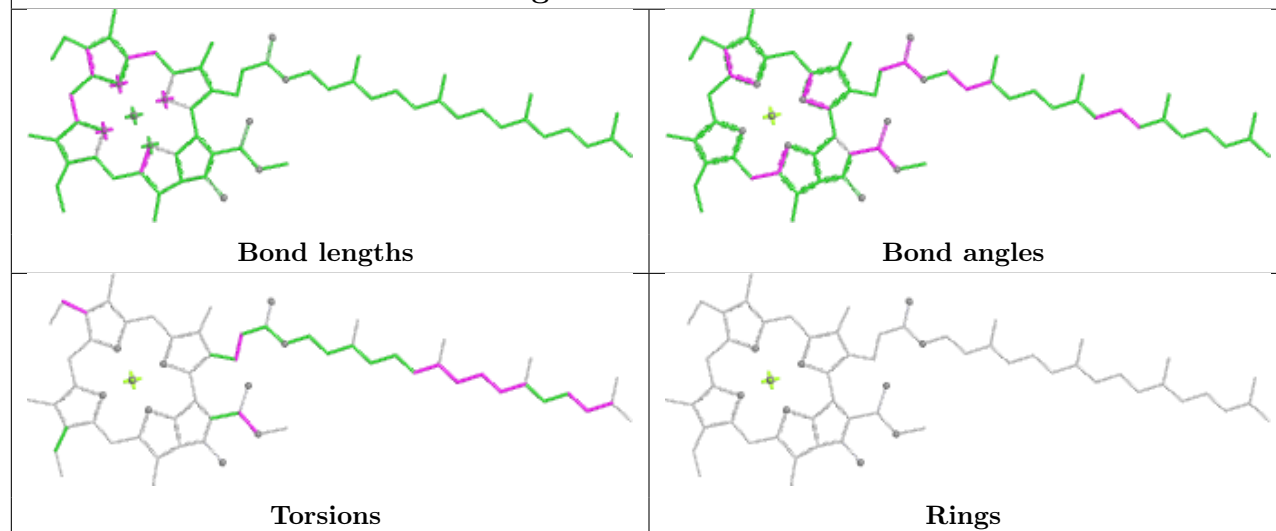
## Ligand BCR B 843

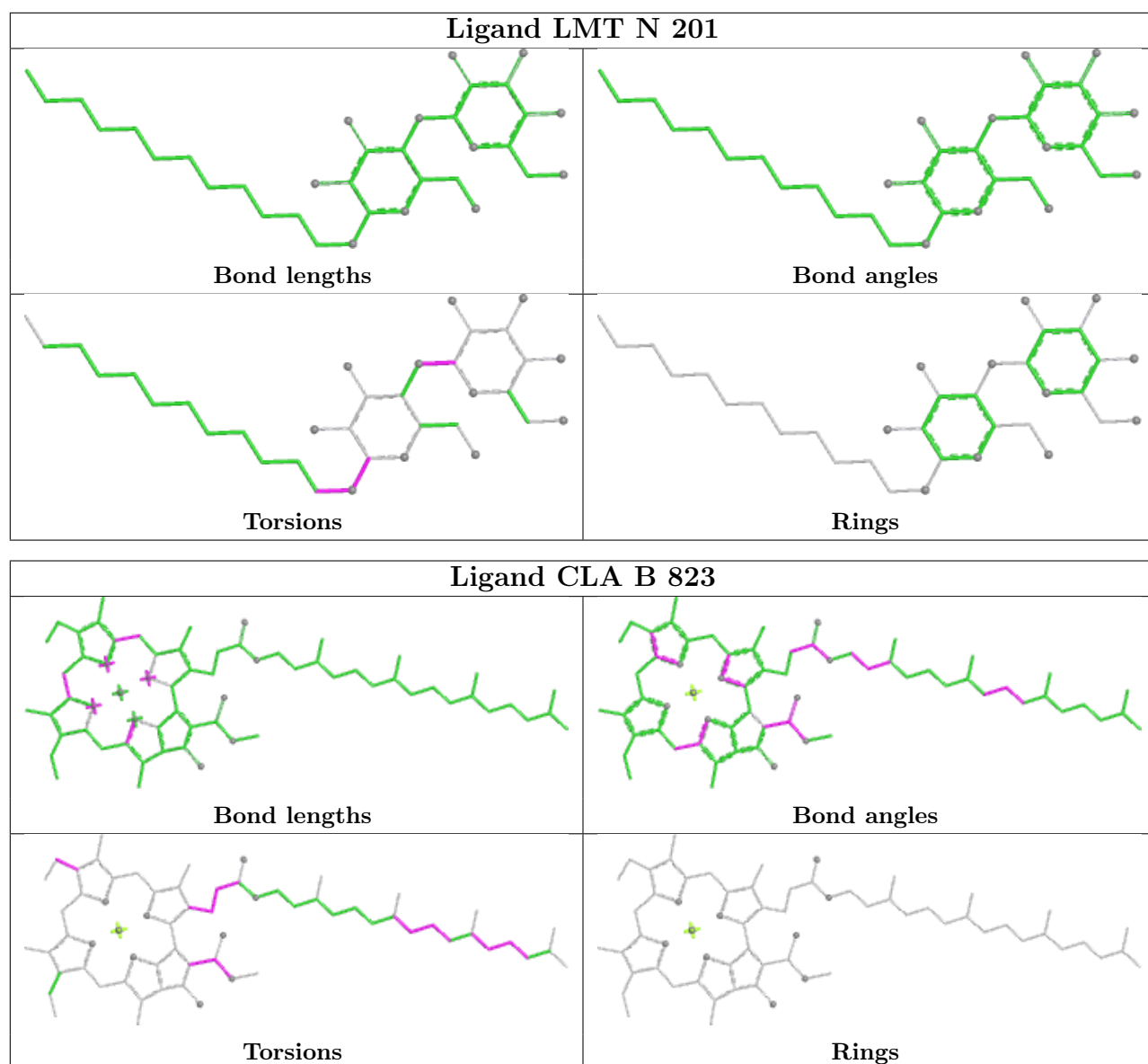


## Ligand CLA 2 303

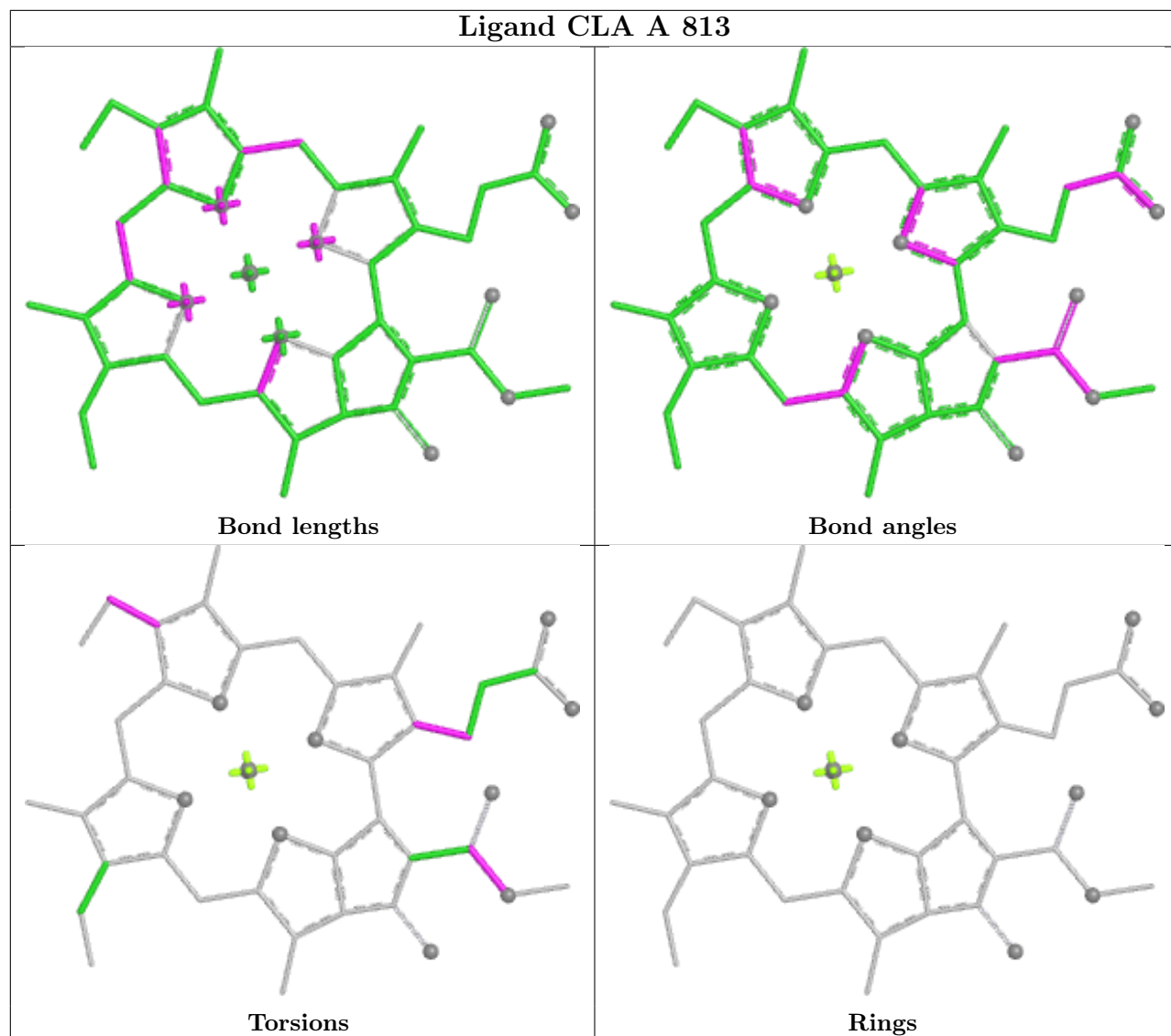


## Ligand CLA A 828



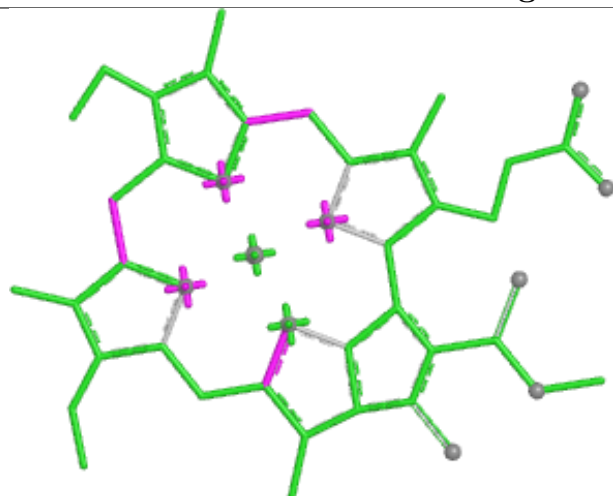


## Ligand CLA A 813

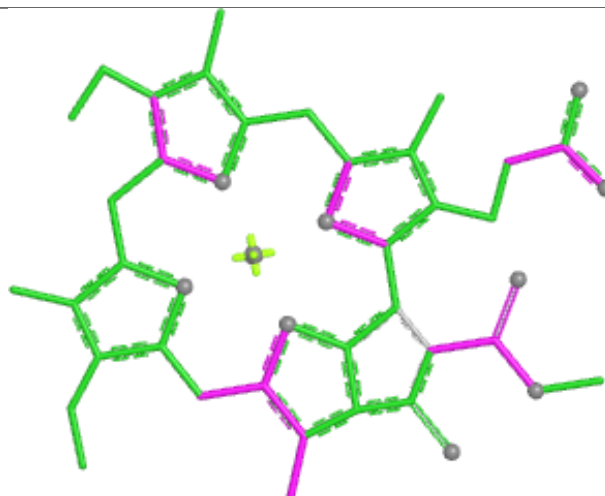




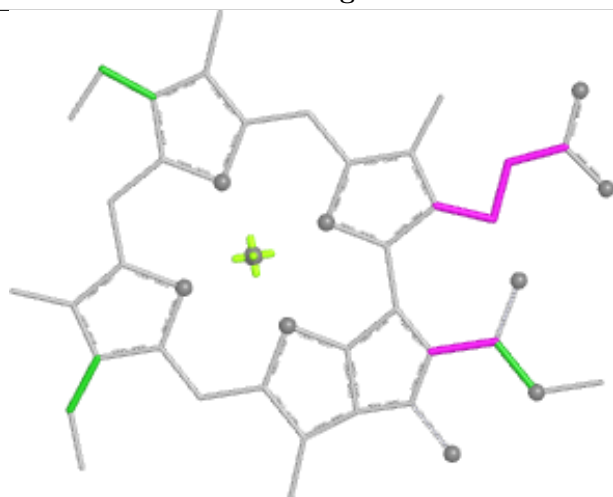
## Ligand CLA 3 303



Bond lengths



Bond angles

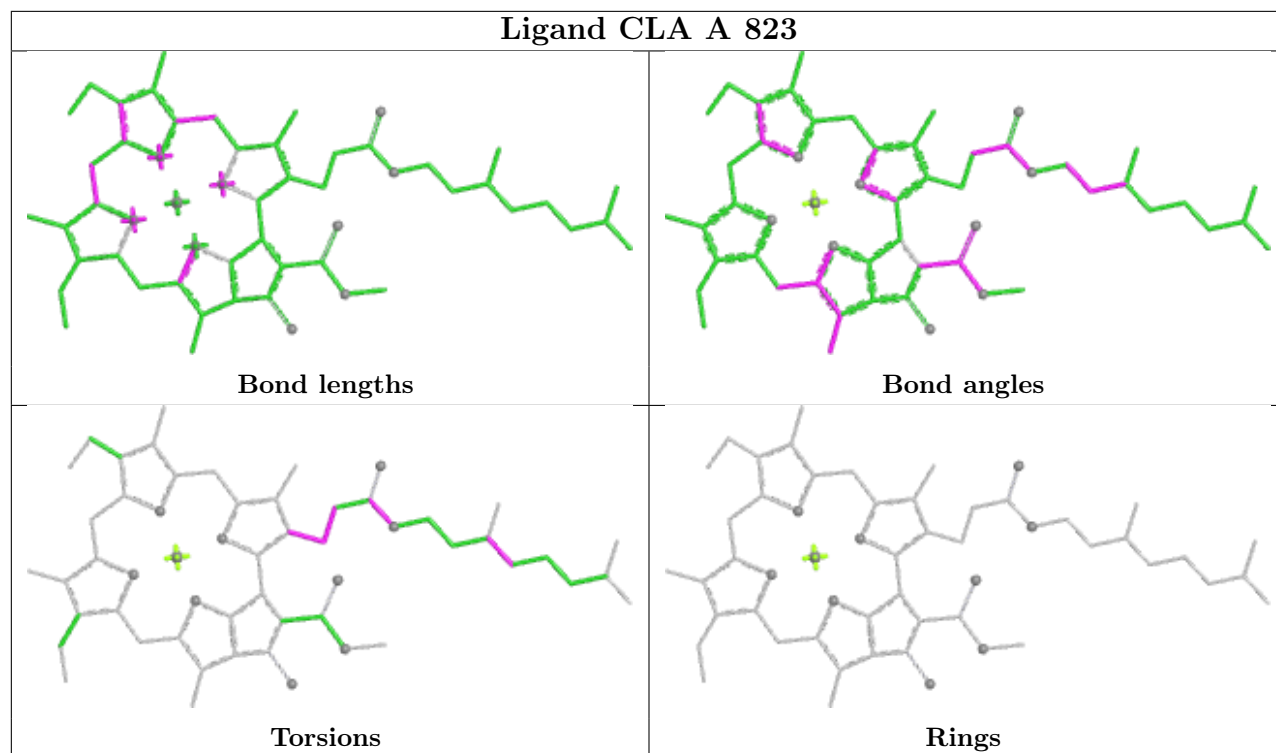


Torsions

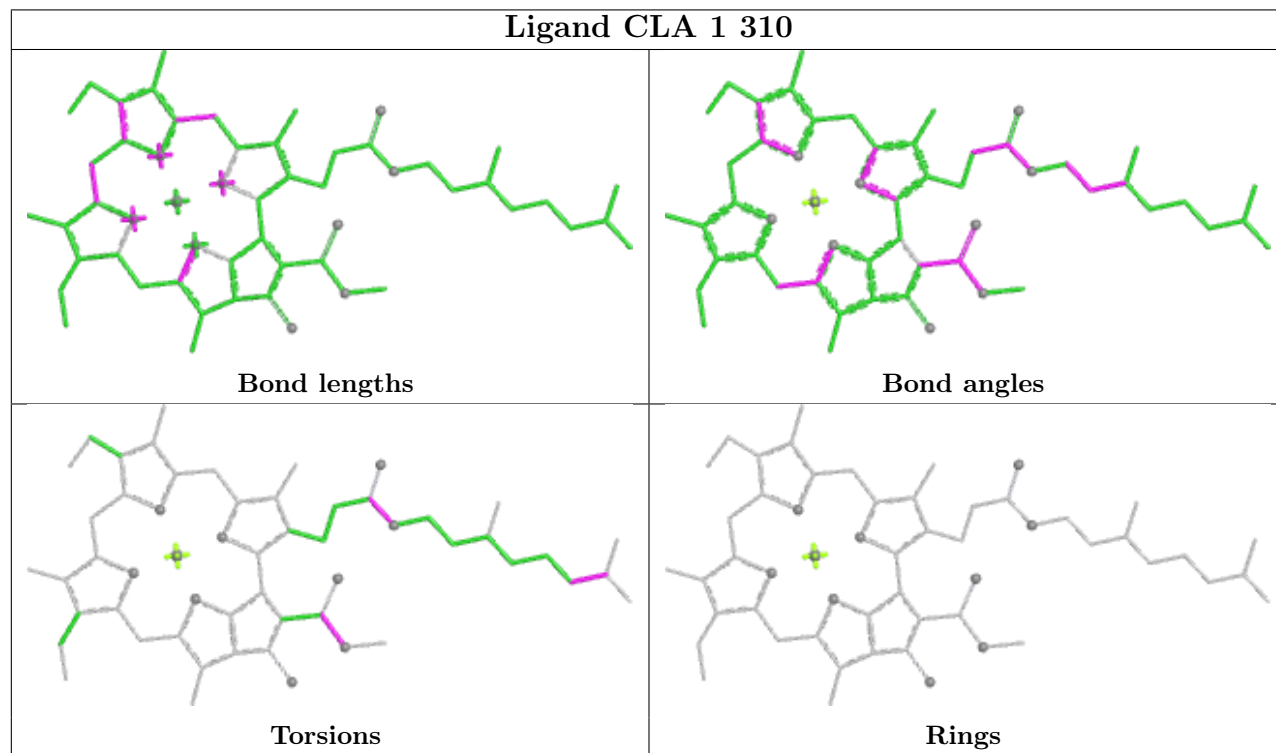


Rings

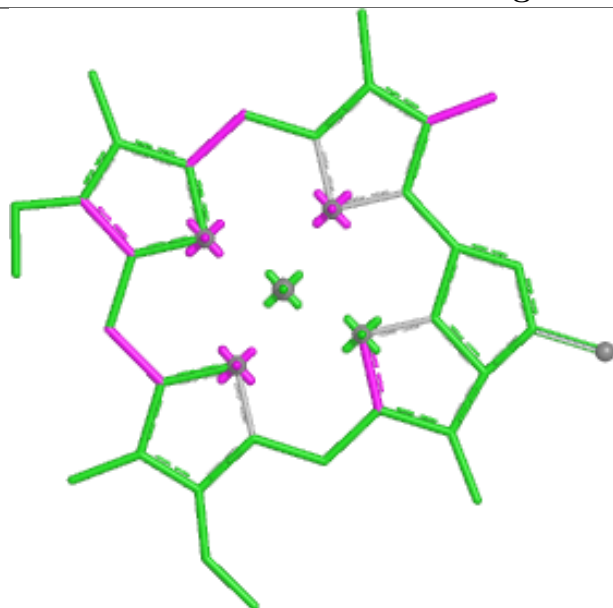
## Ligand CLA A 823



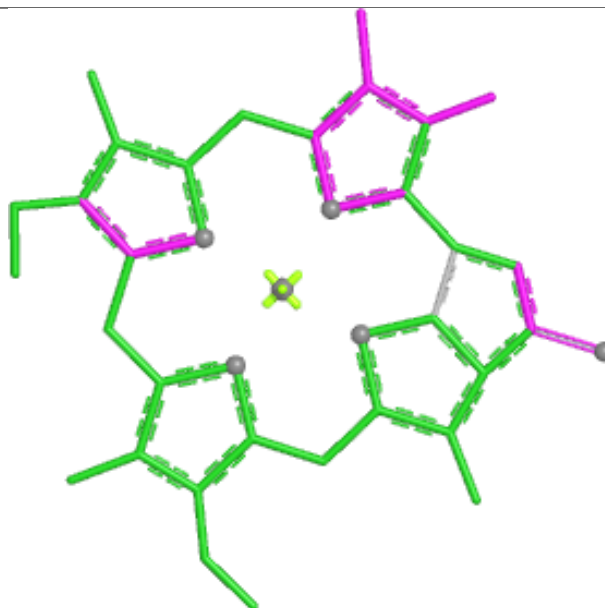
## Ligand CLA 1 310



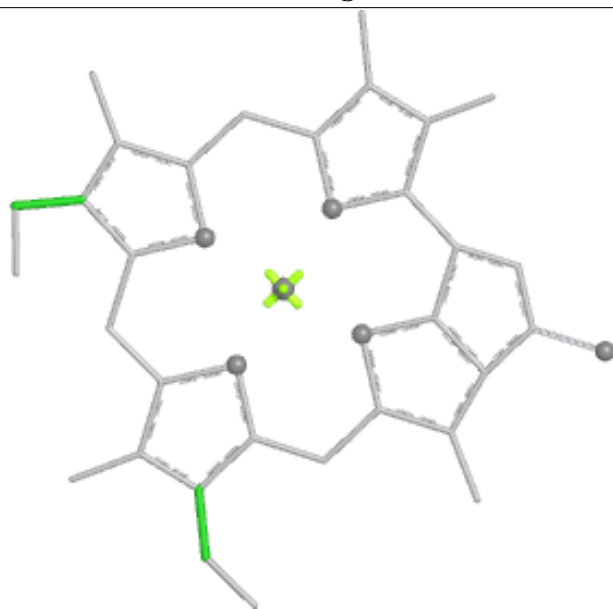
## Ligand CLA K 204



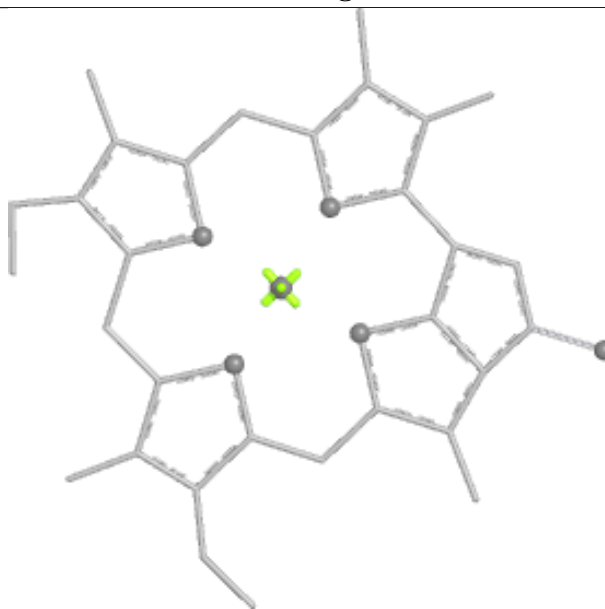
Bond lengths



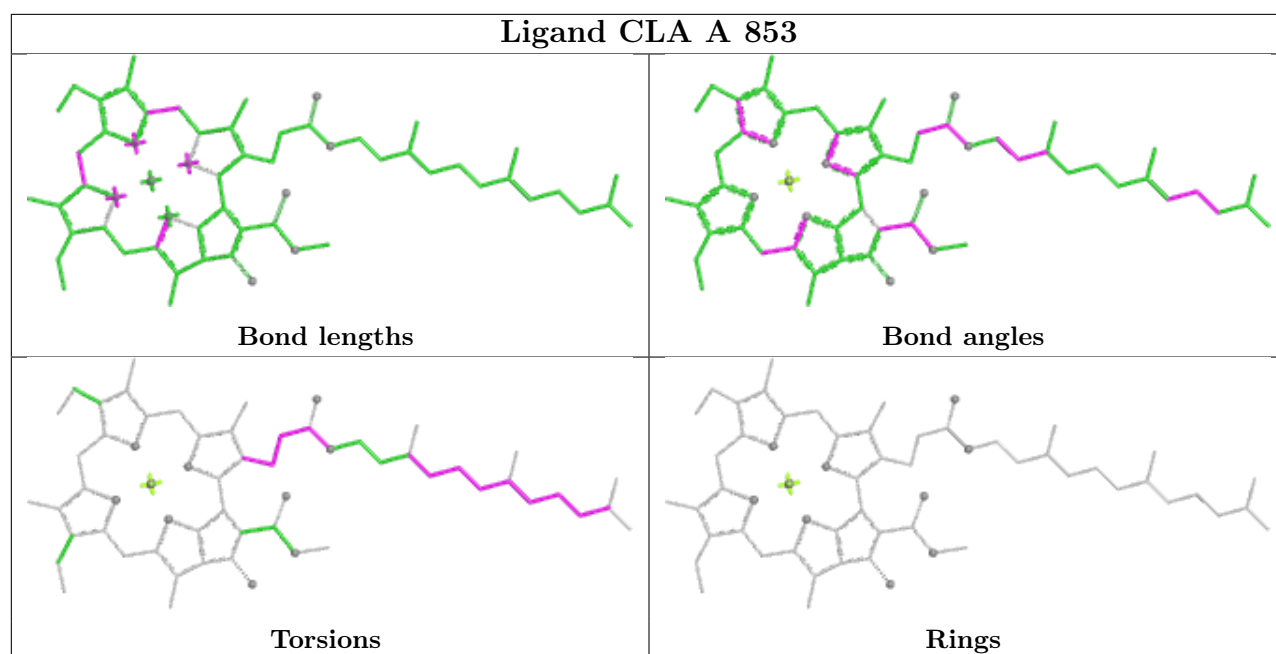
Bond angles



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.

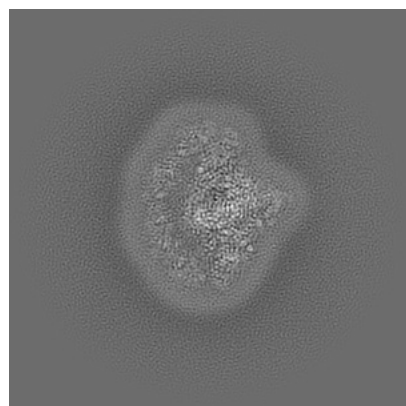
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51219. These allow visual inspection of the internal detail of the map and identification of artifacts.

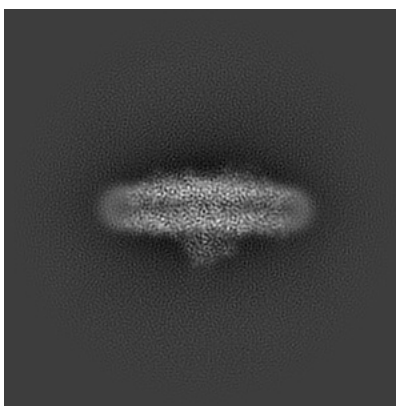
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

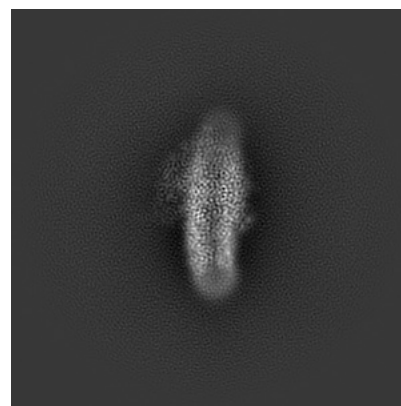
#### 6.1.1 Primary map



X

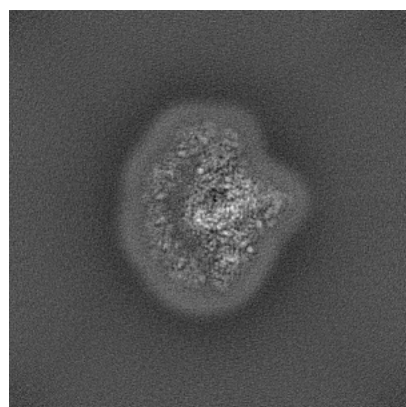


Y

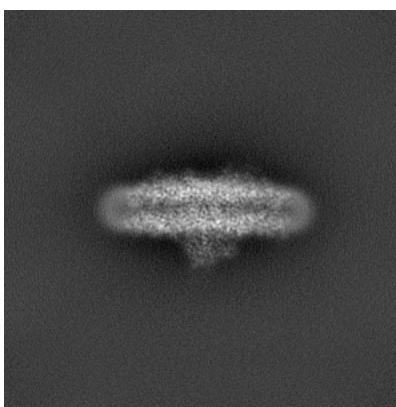


Z

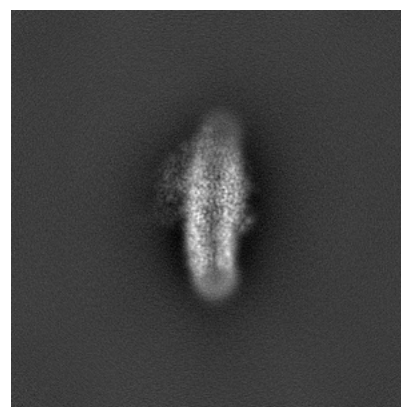
#### 6.1.2 Raw map



X



Y

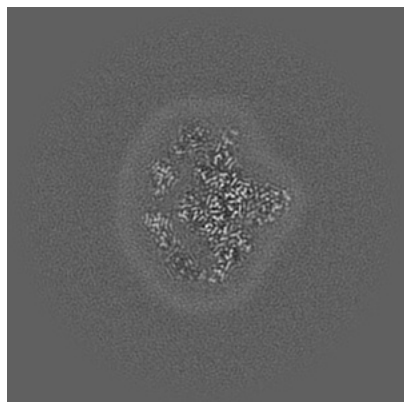


Z

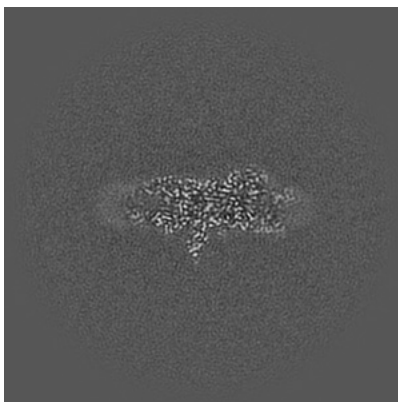
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

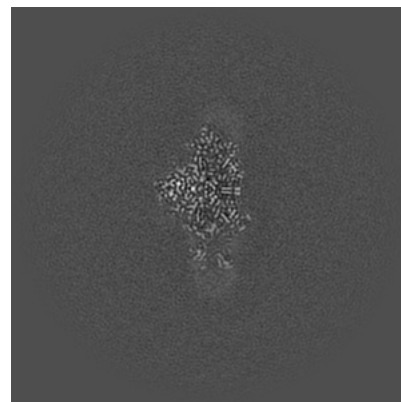
### 6.2.1 Primary map



X Index: 224

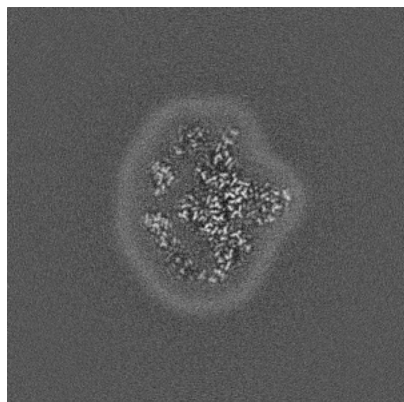


Y Index: 224

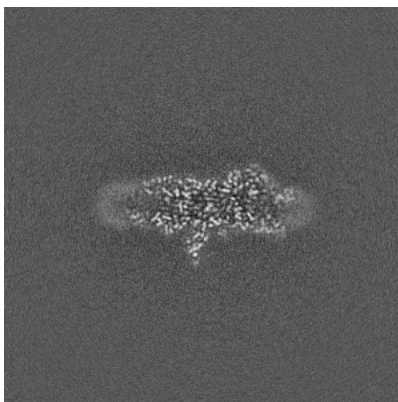


Z Index: 224

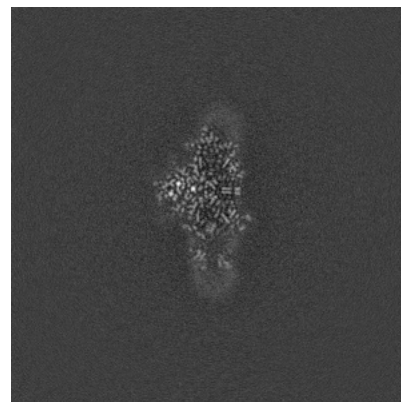
### 6.2.2 Raw map



X Index: 224



Y Index: 224



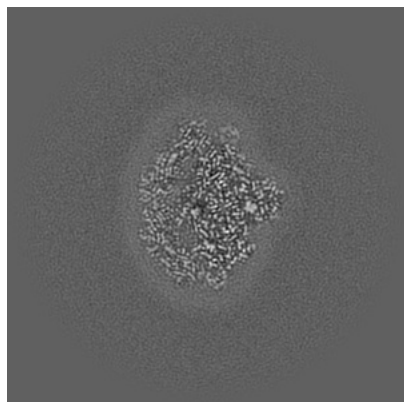
Z Index: 224

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

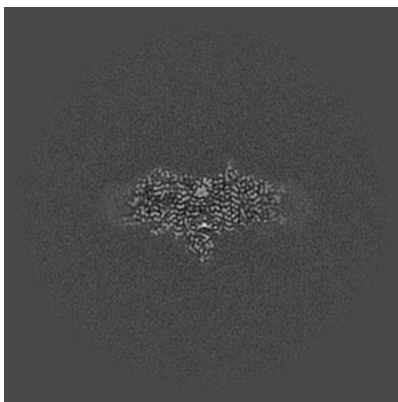


## 6.3 Largest variance slices [i](#)

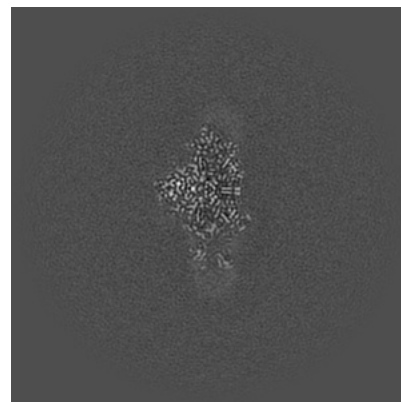
### 6.3.1 Primary map



X Index: 212

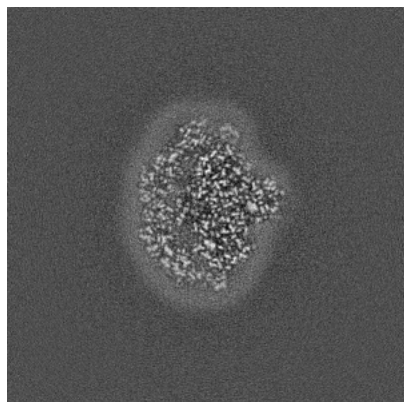


Y Index: 244

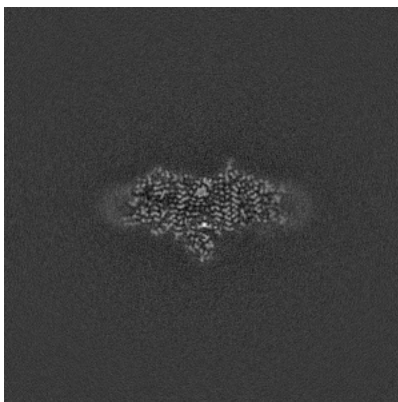


Z Index: 224

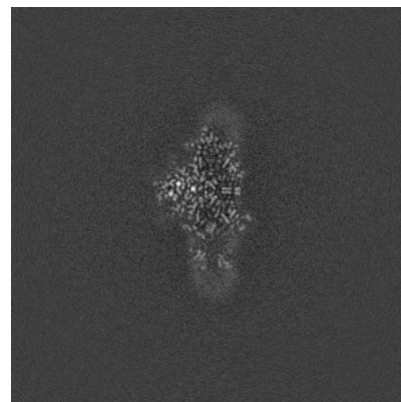
### 6.3.2 Raw map



X Index: 211



Y Index: 244

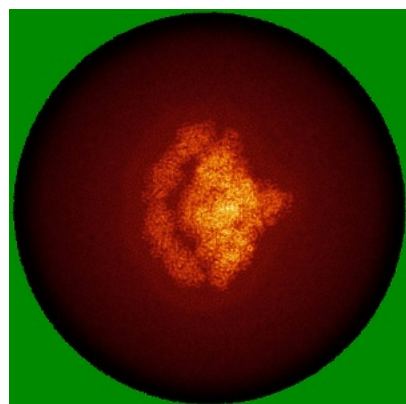


Z Index: 224

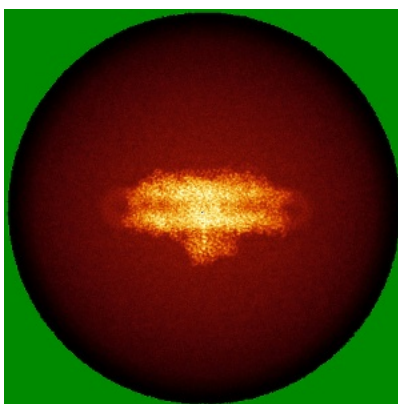
The images above show the largest variance slices of the map in three orthogonal directions.

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

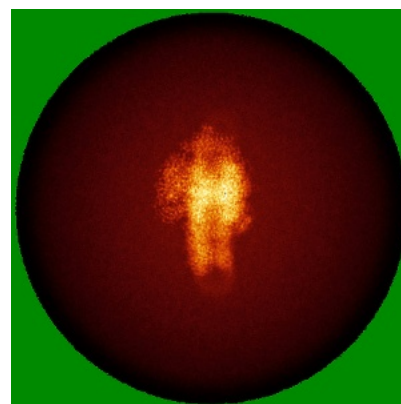
### 6.4.1 Primary map



X

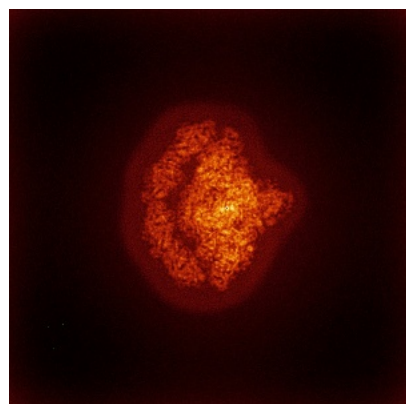


Y

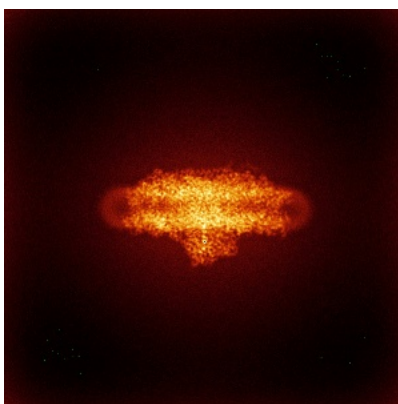


Z

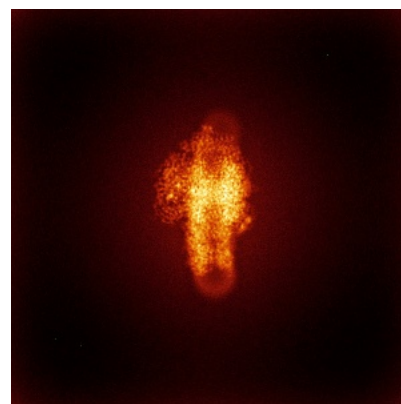
### 6.4.2 Raw map



X



Y



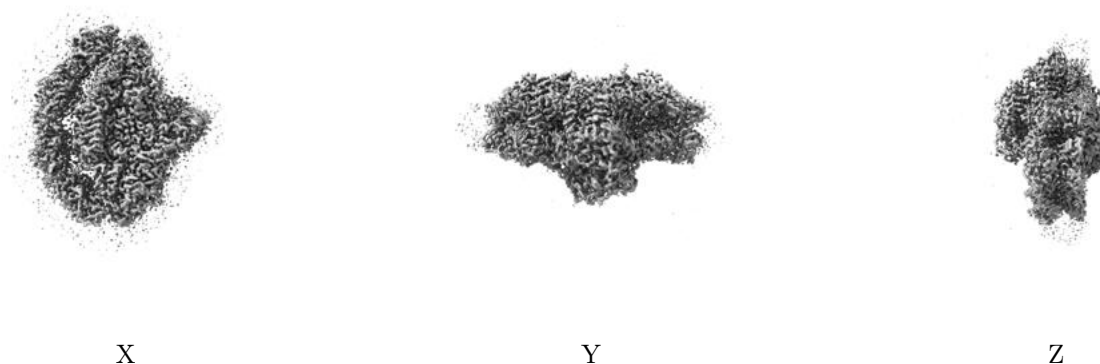
Z

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



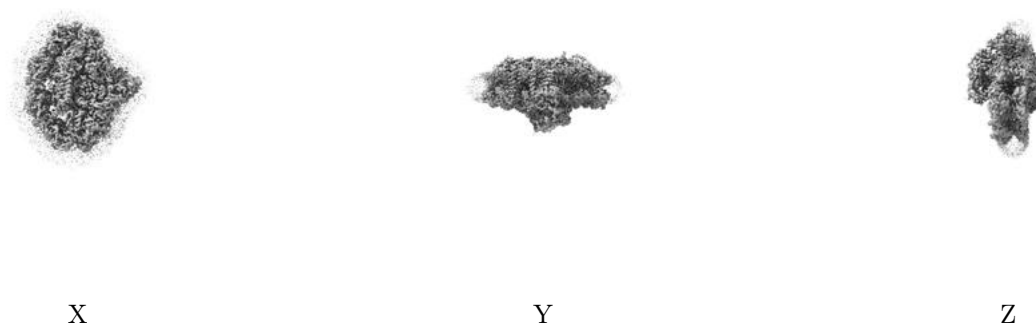
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

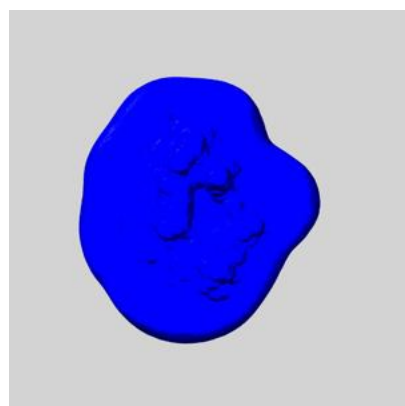
## 6.6 Mask visualisation [i](#)

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

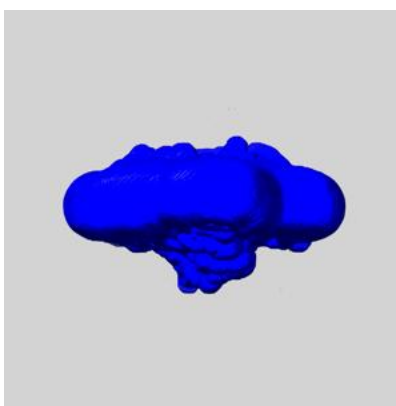
A mask typically either:

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

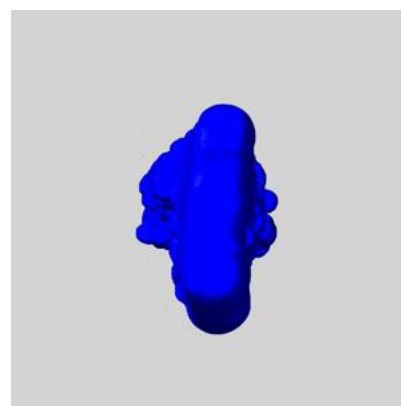
### 6.6.1 emd\_51219\_msk\_1.map [i](#)



X



Y

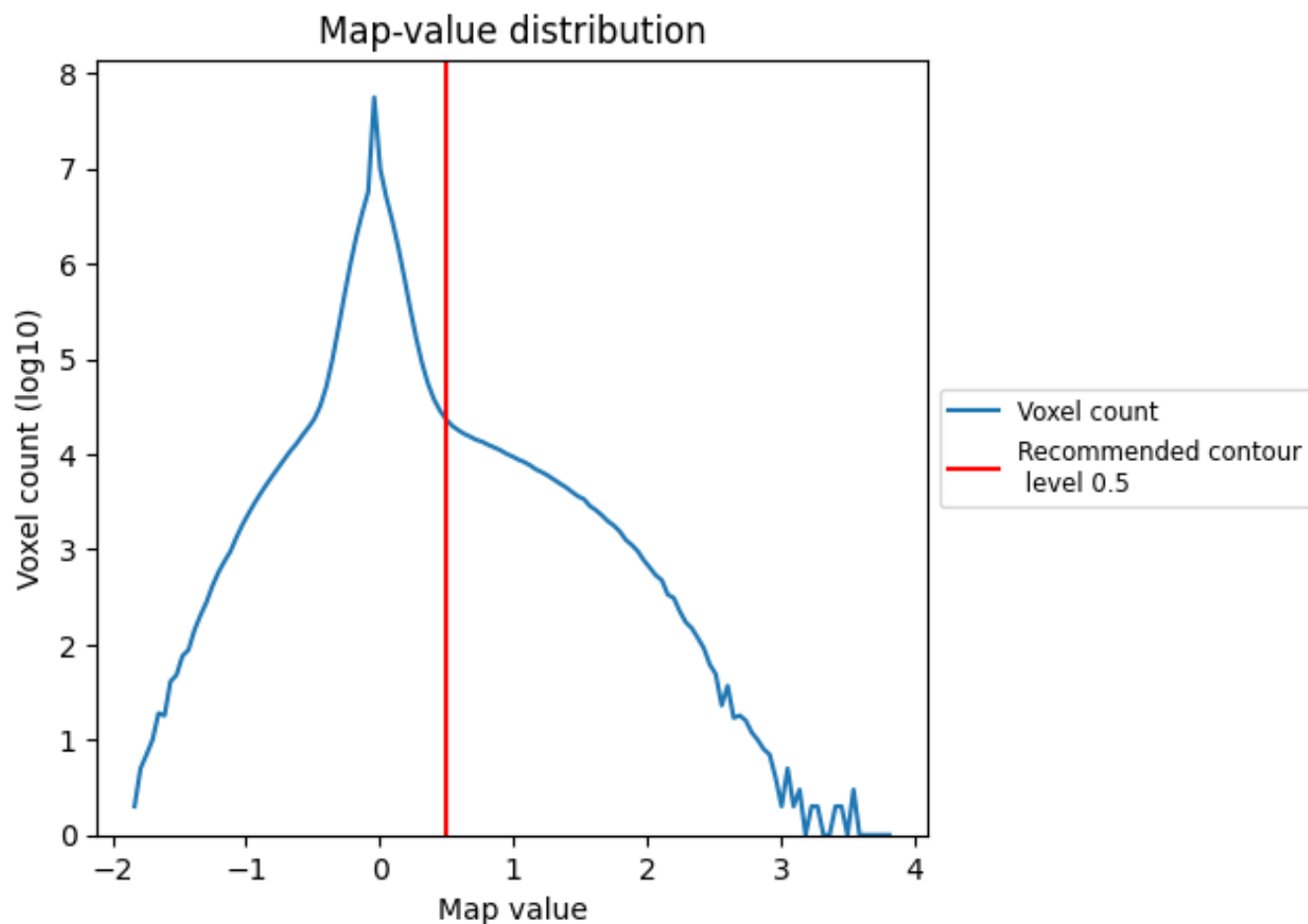


Z

## 7 Map analysis [i](#)

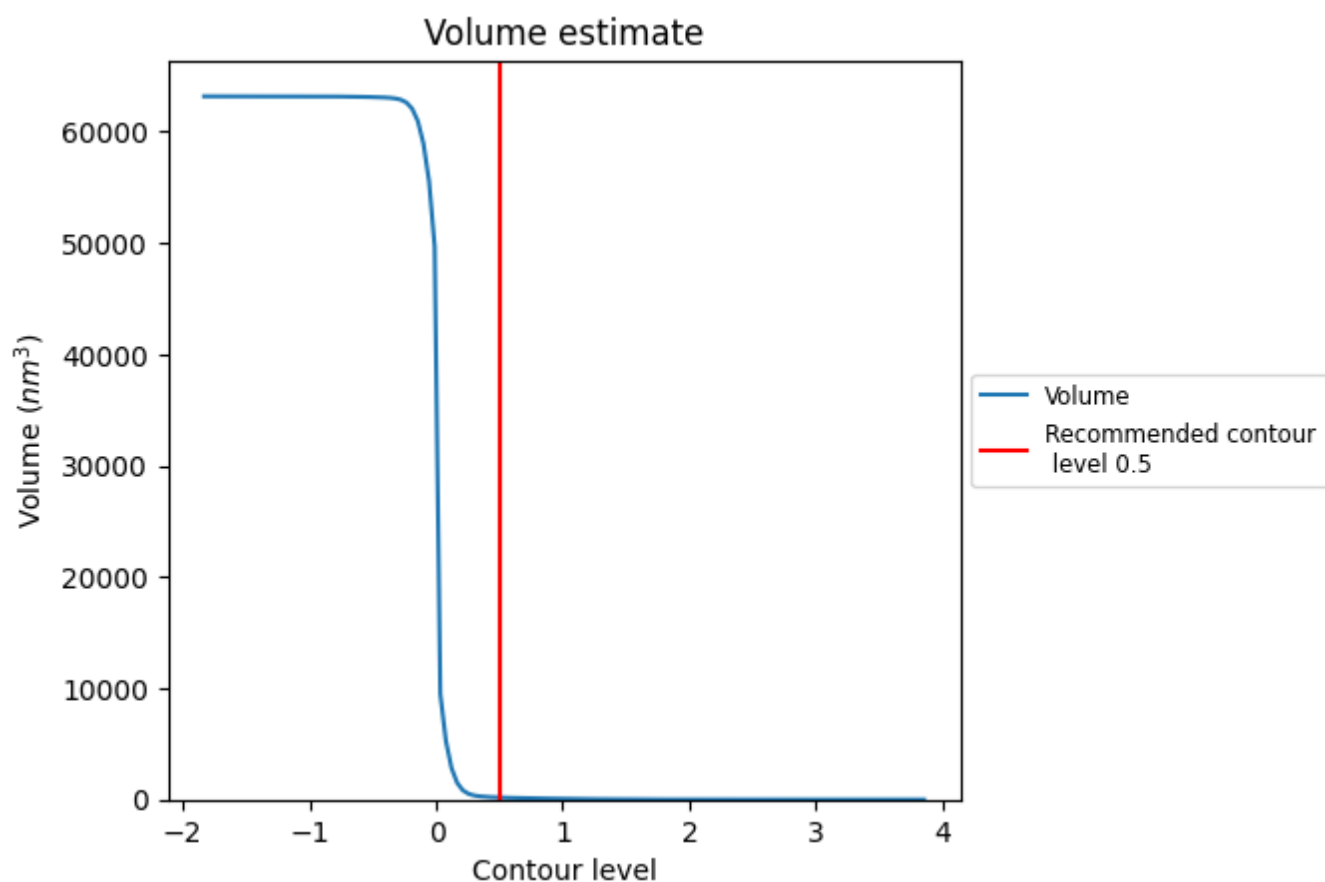
This section contains the results of statistical analysis of the map.

### 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.

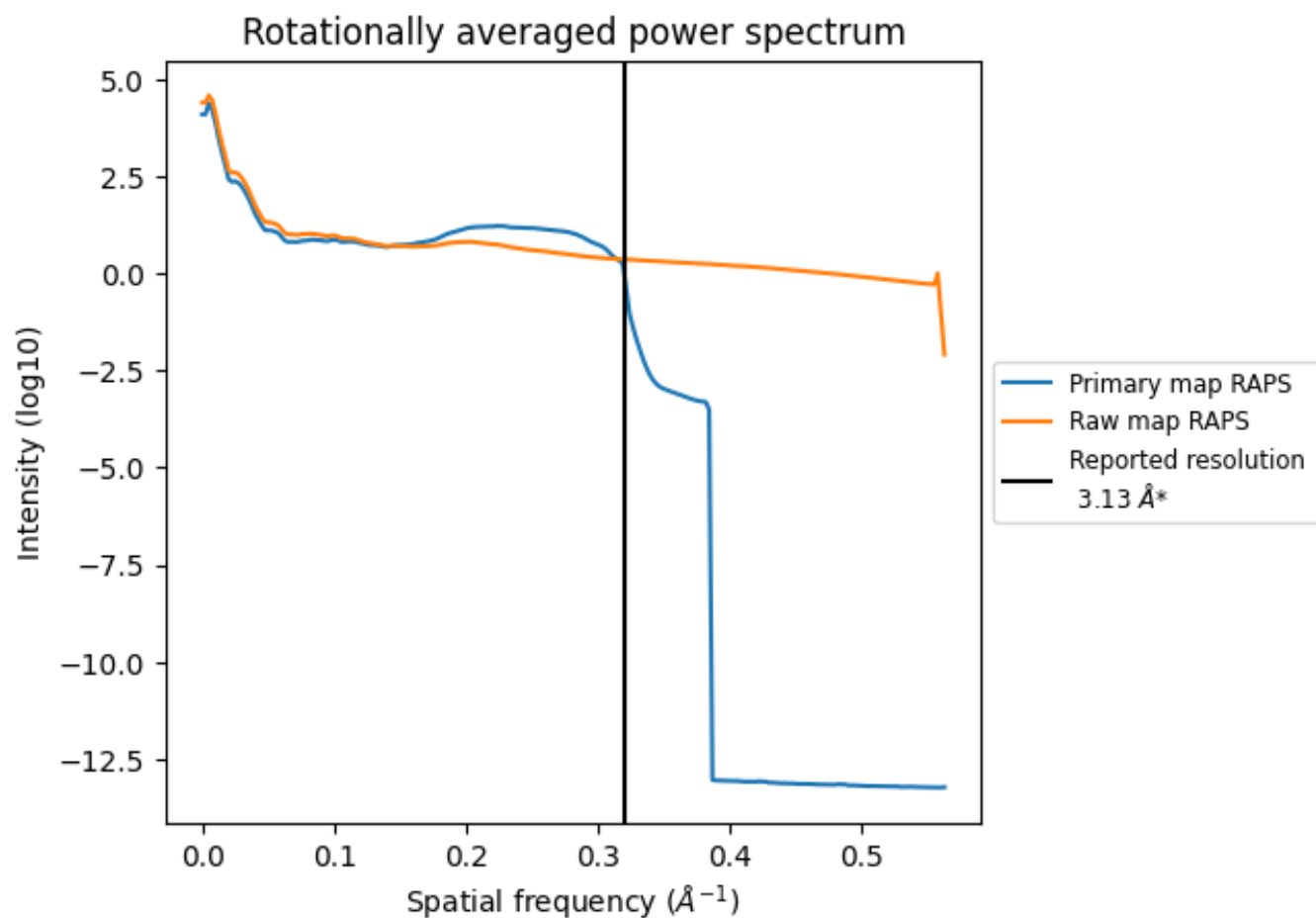
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185  $\text{nm}^3$ ; this corresponds to an approximate mass of 167 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 ⓘ

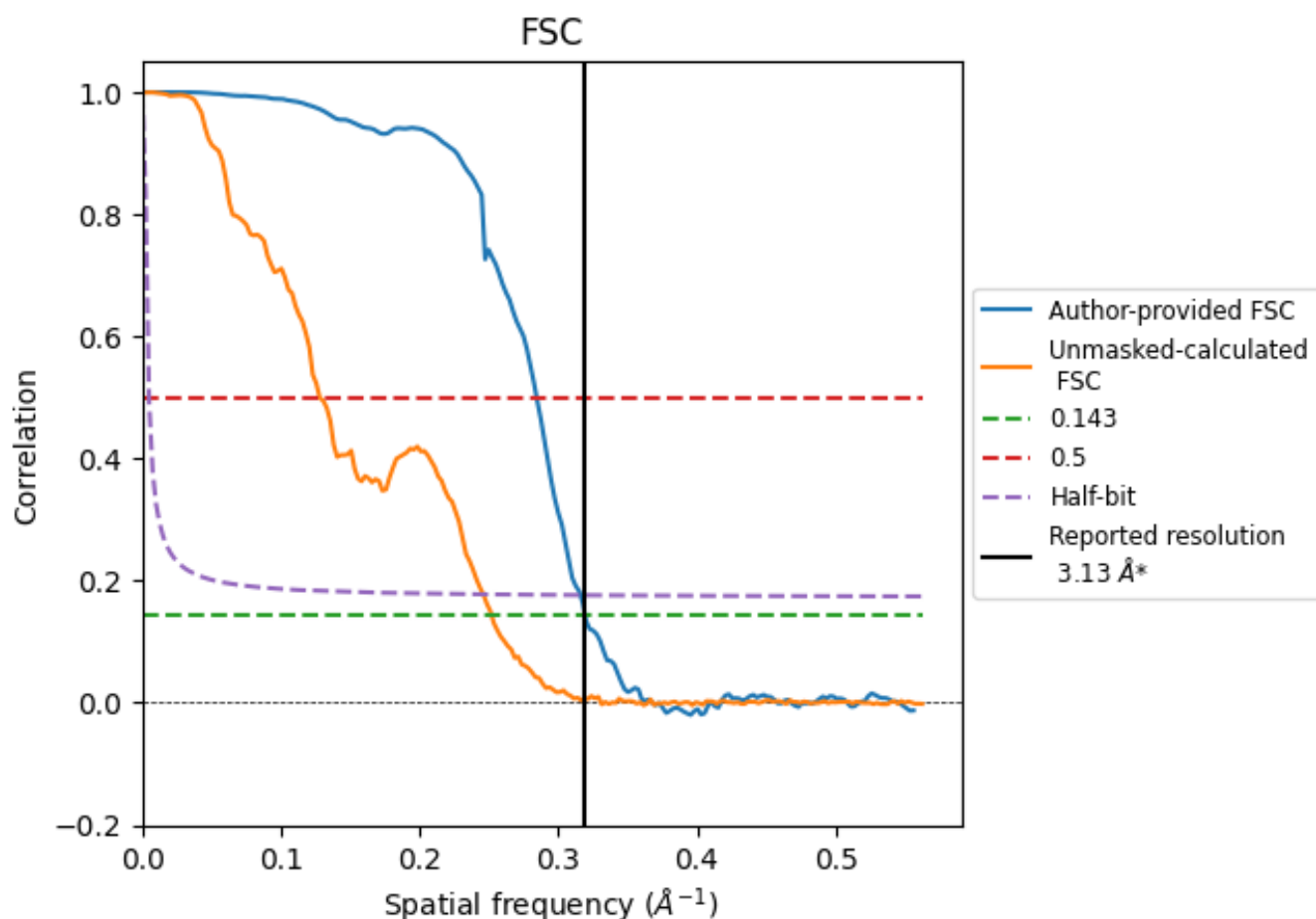


\*Reported resolution corresponds to spatial frequency of 0.319 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.319  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

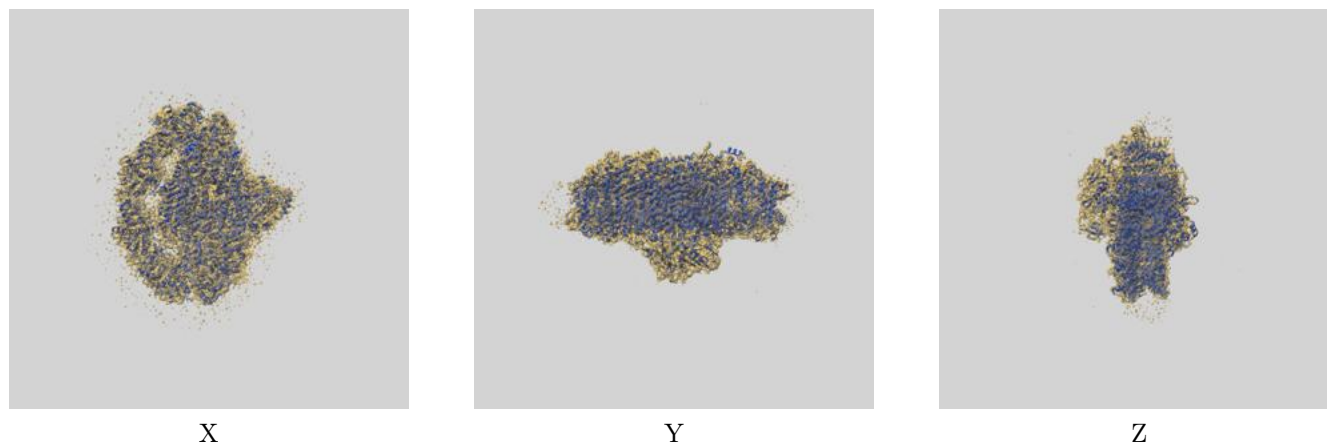
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.52	3.16
Unmasked-calculated*	3.97	7.82	4.07

\*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 3.13 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-51219 and PDB model 9GBI. Per-residue inclusion information can be found in section [3](#) on page [27](#).

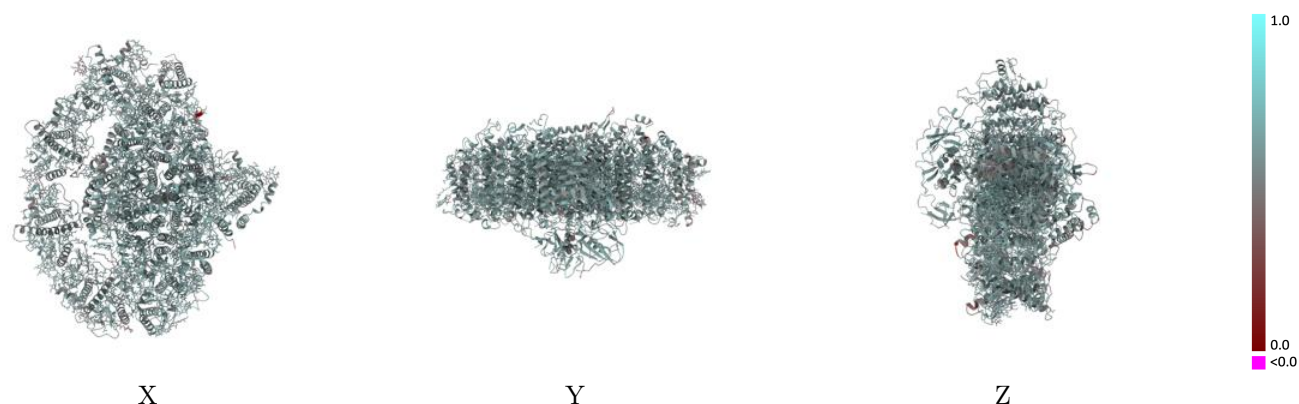
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

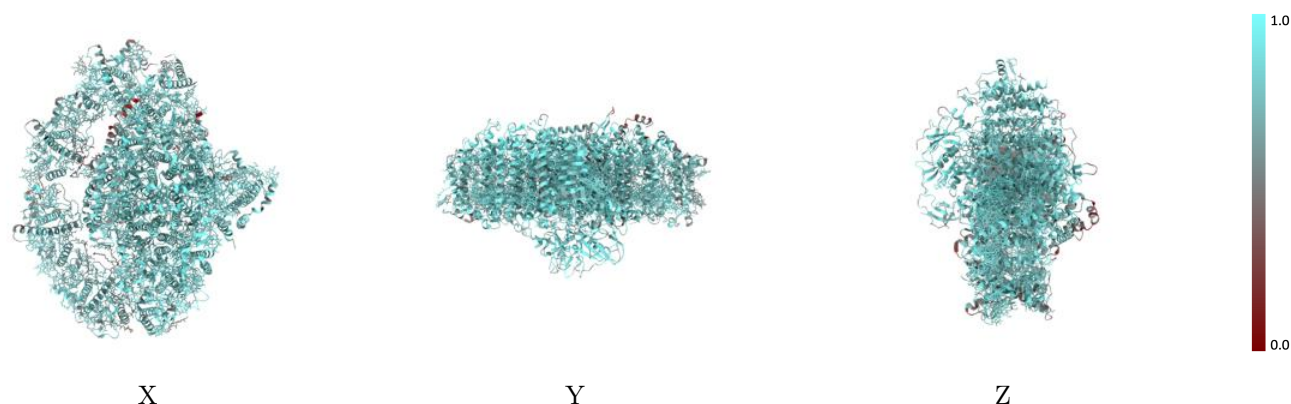


## 9.2 Q-score mapped to coordinate model [i](#)



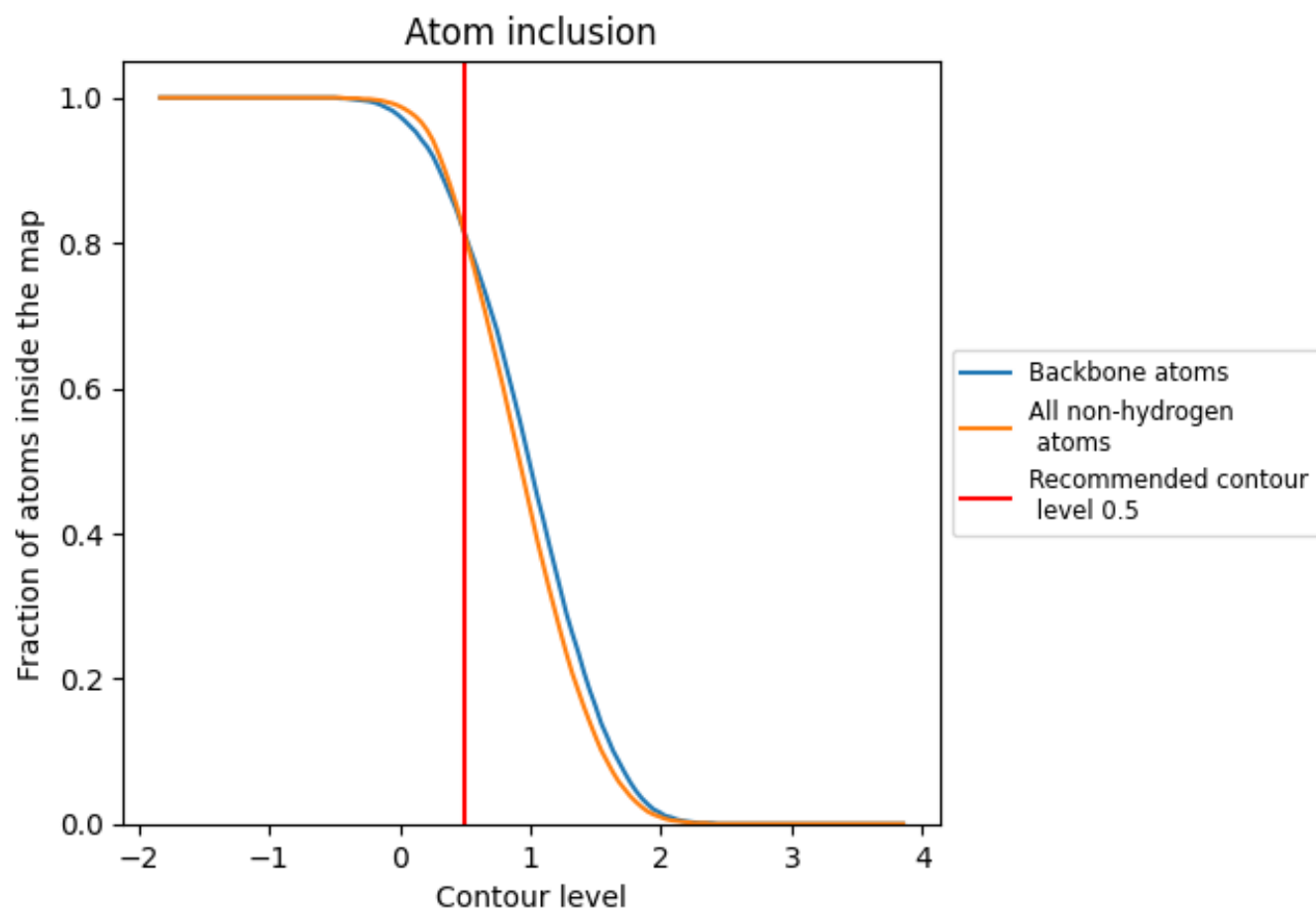
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8100	<div></div> 0.5720
1	<div></div> 0.7480	<div></div> 0.5530
2	<div></div> 0.7420	<div></div> 0.5490
3	<div></div> 0.7740	<div></div> 0.5550
4	<div></div> 0.7570	<div></div> 0.5570
A	<div></div> 0.8570	<div></div> 0.5870
B	<div></div> 0.8660	<div></div> 0.5900
C	<div></div> 0.8880	<div></div> 0.5820
D	<div></div> 0.8120	<div></div> 0.5720
E	<div></div> 0.7580	<div></div> 0.5670
F	<div></div> 0.8020	<div></div> 0.5720
G	<div></div> 0.7750	<div></div> 0.5630
H	<div></div> 0.7410	<div></div> 0.5500
I	<div></div> 0.8190	<div></div> 0.5630
J	<div></div> 0.7680	<div></div> 0.5590
K	<div></div> 0.6570	<div></div> 0.5110
L	<div></div> 0.8080	<div></div> 0.5620
N	<div></div> 0.4300	<div></div> 0.5010

