



Full wwPDB EM Validation Report ⓘ

Sep 17, 2025 – 01:42 pm BST

PDB ID : 9GC2 / pdb_00009gc2
EMDB ID : EMD-51227
Title : Cryo-EM structure of Arabidopsis thaliana PSI-LHCI- a603-NH mutant
Authors : Capaldi, S.; Chaves-Sanjuan, A.; Bonnet, D.M.V.; Bassi, R.
Deposited on : 2024-08-01
Resolution : 3.29 Å(reported)
Based on initial model : 9GBI

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

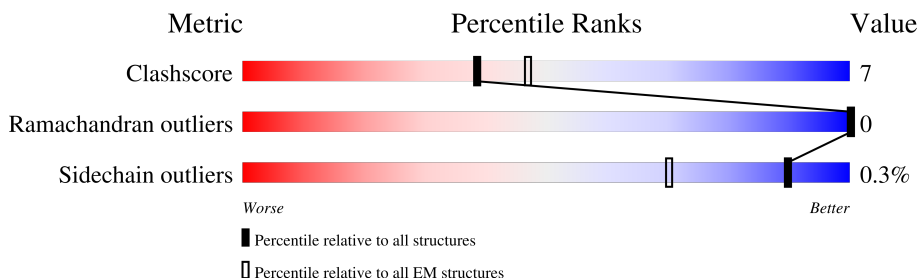
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 Å.

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





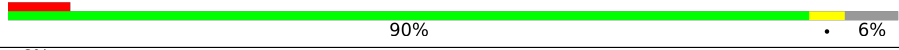



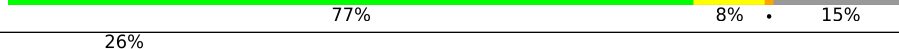
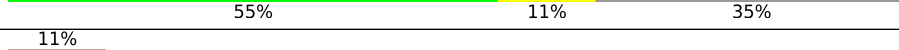
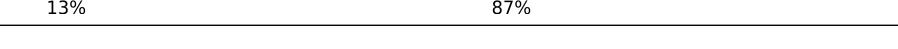
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	206	<div> <div>13%</div> <div>78%</div> <div>17%</div> <div>6%</div> </div>
2	2	214	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
3	3	234	<div> <div>6%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
4	4	199	<div> <div>6%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
5	A	750	<div> <div>.</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
6	B	734	<div> <div>89%</div> <div>11%</div> </div>
7	C	81	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
8	D	160	<div> <div>72%</div> <div>15%</div> <div>.</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
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	305	X	-	-	-
18	CHL	4	306	X	-	-	-
18	CHL	4	307	X	-	-	-
18	CHL	4	314	X	-	-	-
19	CLA	1	302	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	1	318	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	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	304	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	851	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	H	201	X	-	-	-
19	CLA	H	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J	102	X	-	-	-
19	CLA	K	201	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	302	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 35543 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
			1680	1102	270	303	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	103	HIS	ASN	engineered mutation	UNP Q9SY97

- 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
			1564	1024	255	282	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	99	HIS	ASN	engineered mutation	UNP P27521

- 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	94	Total	C	N	O	0	0
			731	472	121	138		

- 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		

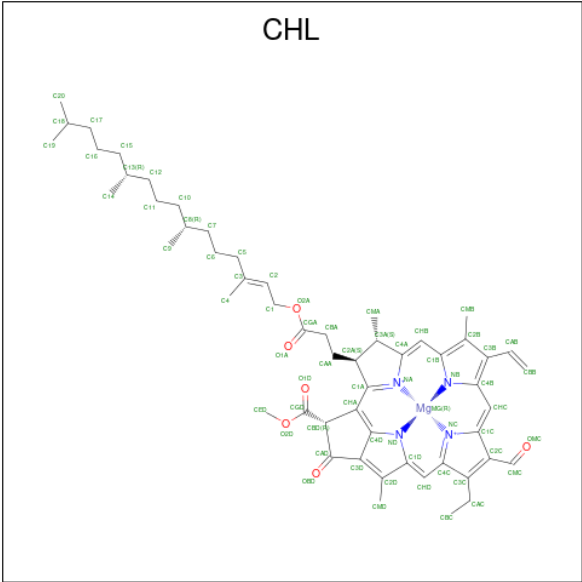
- Molecule 16 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

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.

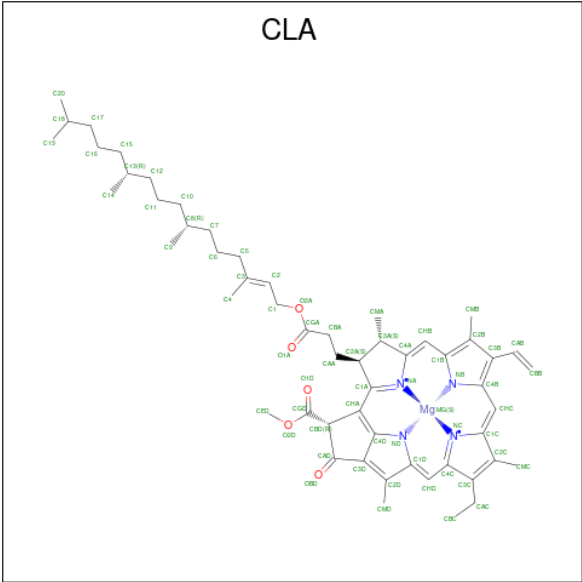
Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	11	Total	C	N	O	0	0
			80	51	15	14		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (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	
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: C₅₅H₇₂MgN₄O₅) (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
			60	50	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
			50	40	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	

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Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			50	40	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
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	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
			43	35	1	4	3	
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	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	4	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 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 63	C 53	Mg 1	N 4	O 5	0
19	A	1	Total 59	C 49	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 54	C 44	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
			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	
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
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	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	
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
			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
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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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
			51	41	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
			52	42	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
			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
			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
			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
			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	

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Mol	Chain	Residues	Atoms					AltConf
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
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	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
			50	40	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
			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
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	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
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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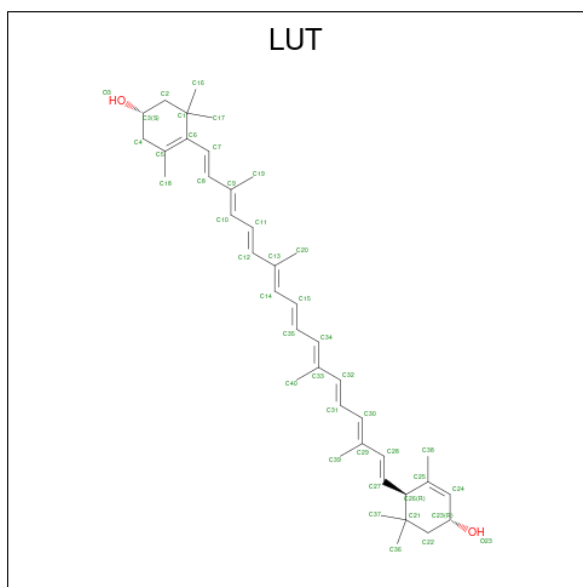
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 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	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
19	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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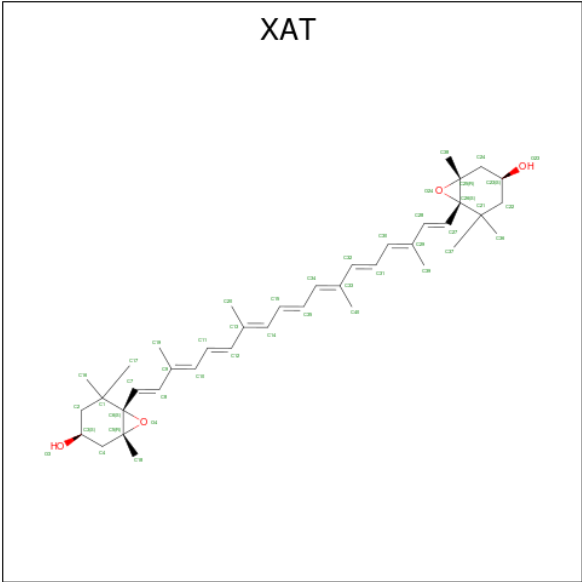
Mol	Chain	Residues	Atoms					AltConf
19	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	

- Molecule 20 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



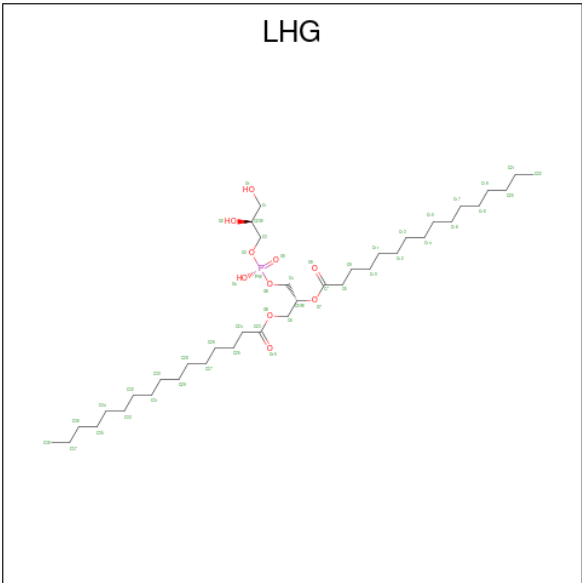
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O		0
			42	40	2		
20	1	1	Total	C	O		0
			42	40	2		
20	2	1	Total	C	O		0
			42	40	2		
20	3	1	Total	C	O		0
			42	40	2		
20	4	1	Total	C	O		0
			42	40	2		

- 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



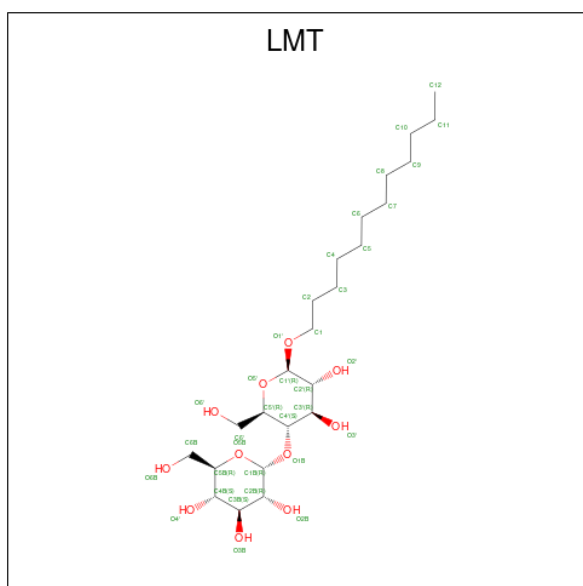
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



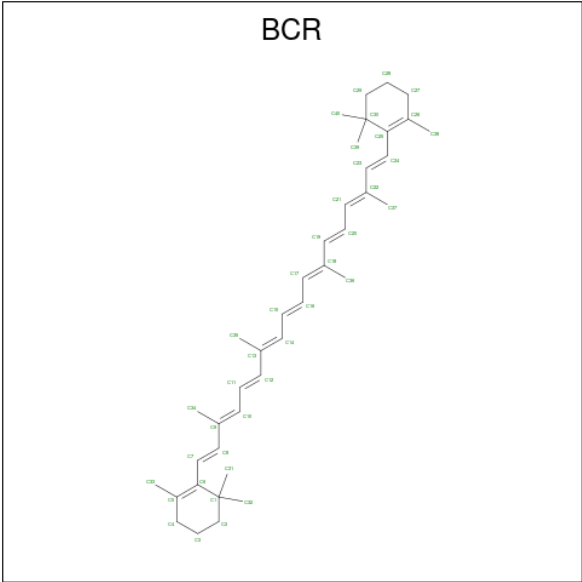
Mol	Chain	Residues	Atoms				AltConf
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	2	1	Total	C	O	P	0
			37	26	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			35	24	11	
23	A	1	Total	C	O	0
			35	24	11	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



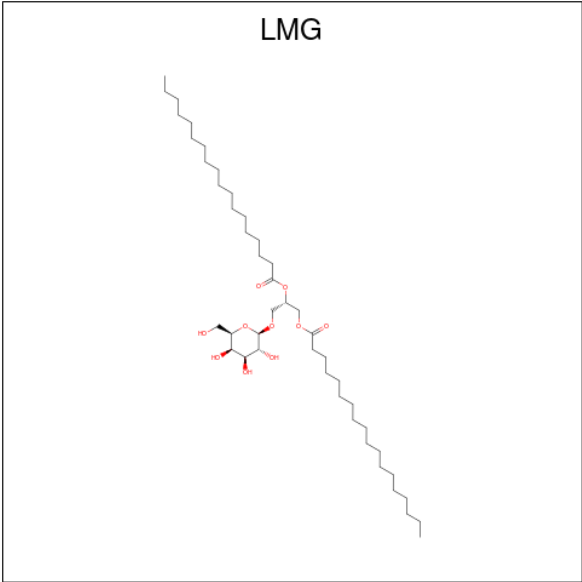
Mol	Chain	Residues	Atoms	AltConf
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0

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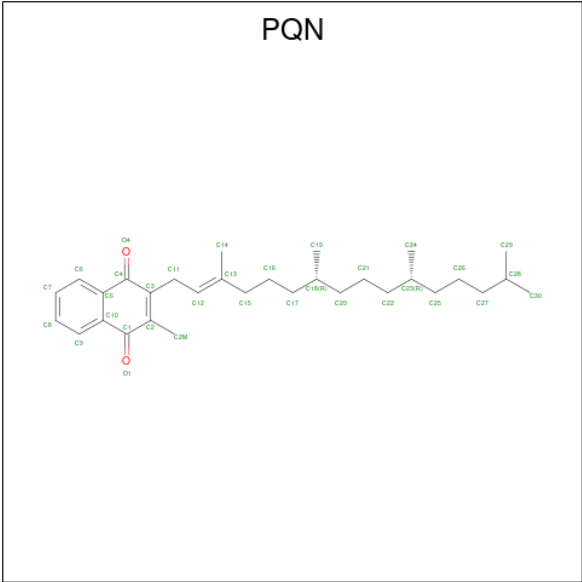
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	L	1	Total C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

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



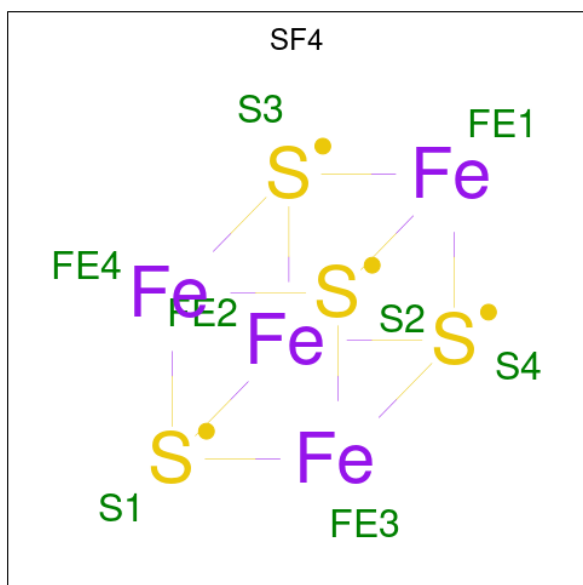
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			36	26	10	
25	B	1	Total	C	O	0
			52	42	10	
25	F	1	Total	C	O	0
			30	20	10	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



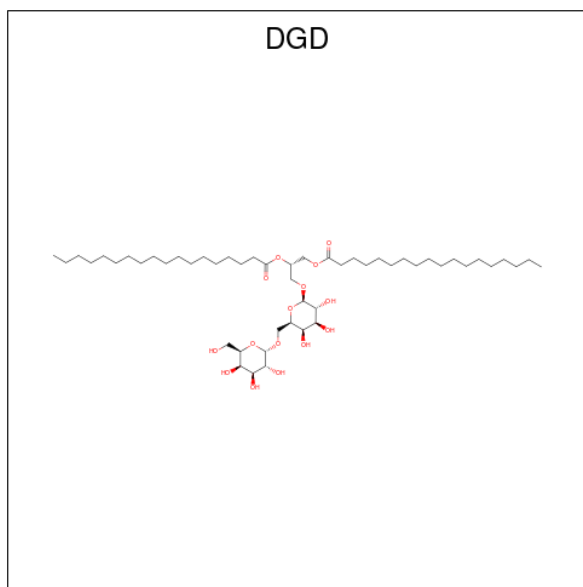
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_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).

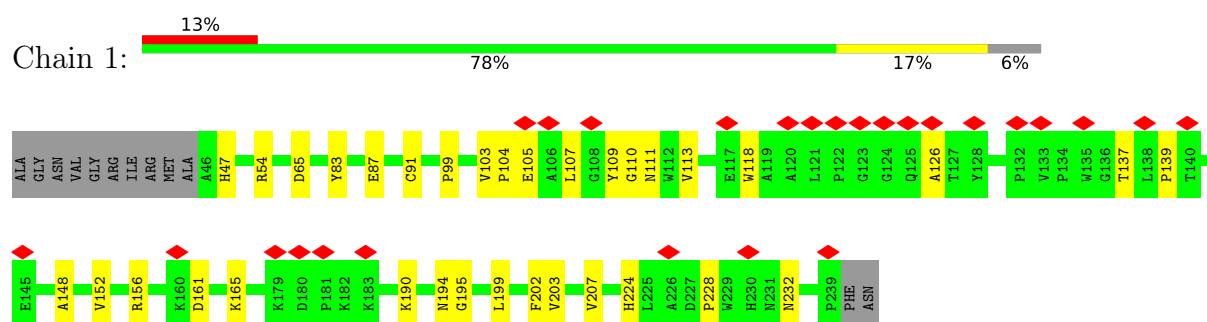


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B	1	66	51	15	0

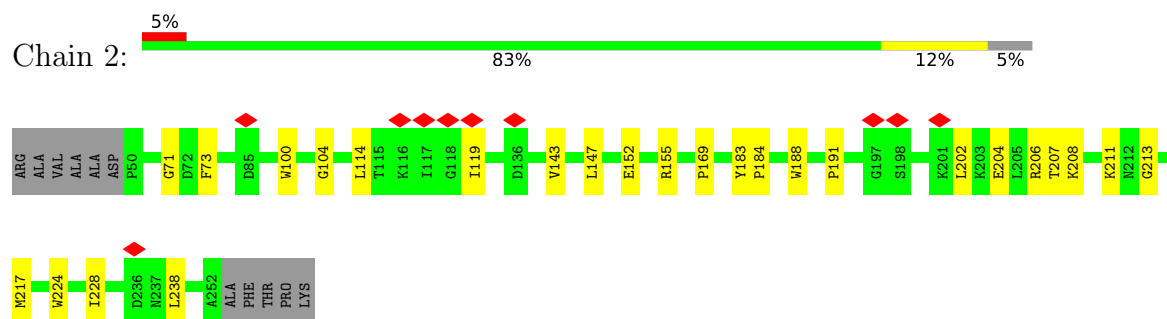
3 Residue-property plots [i](#)

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.

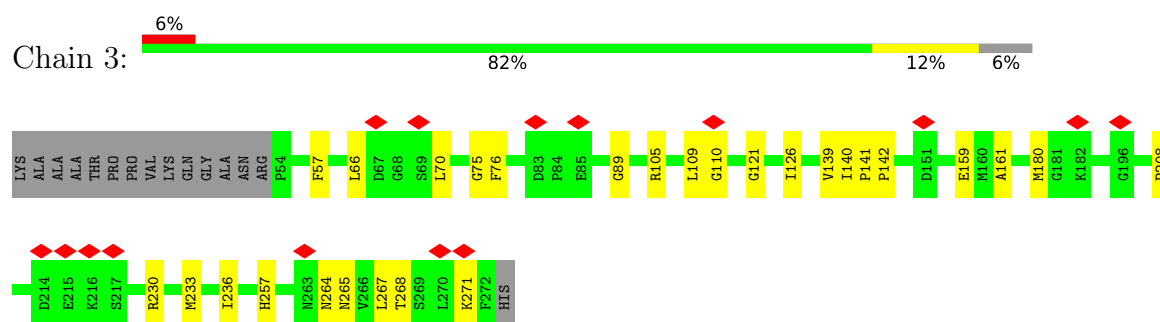
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



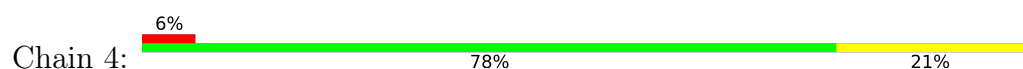
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

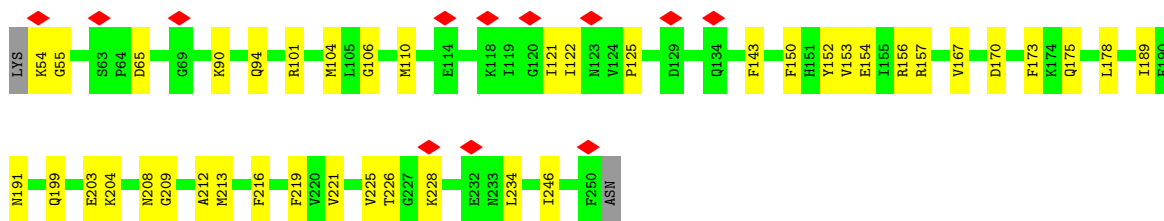


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



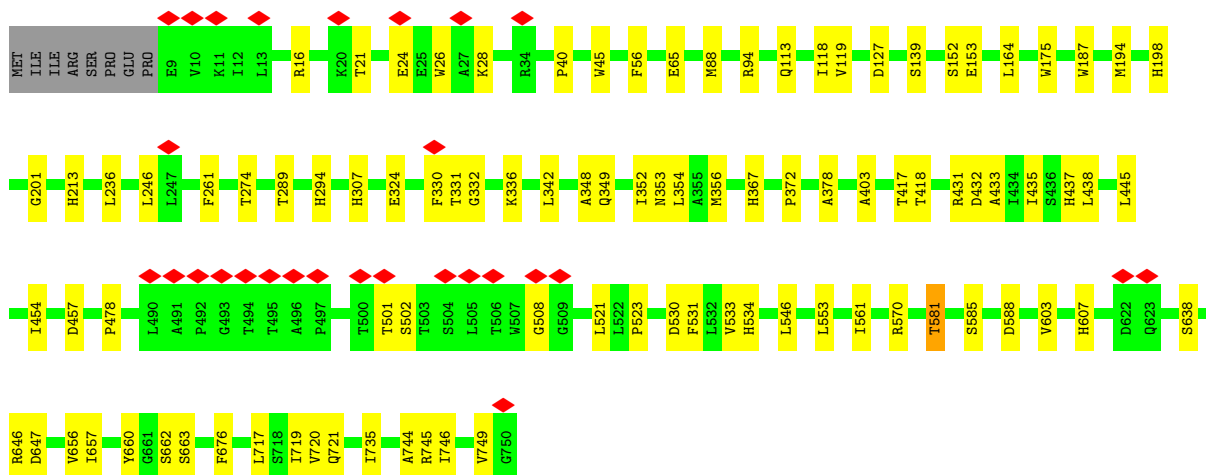
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic





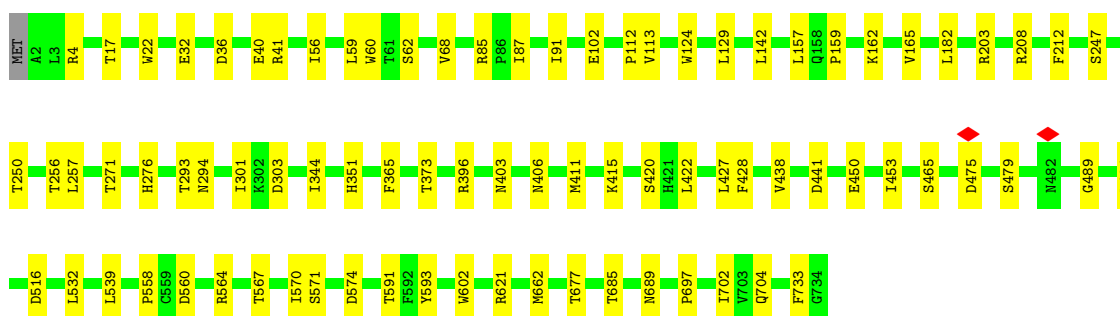
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 86% 13%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 89% 11%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 79% 20%

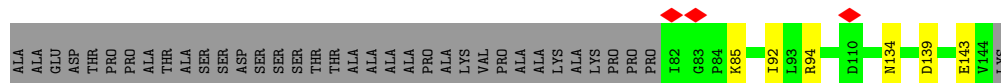


- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

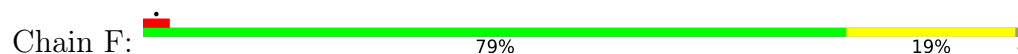
Chain D: 72% 15% 12%



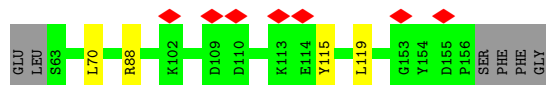
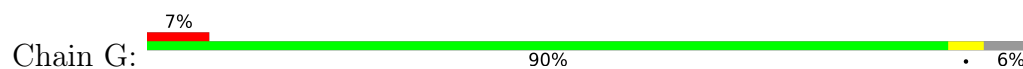
- Molecule 9: Photosystem I reaction center subunit IV B, chloroplastic



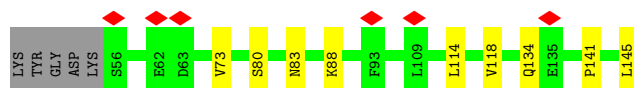
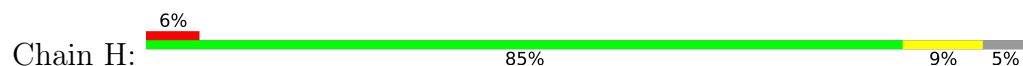
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



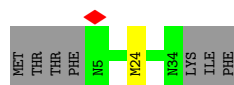
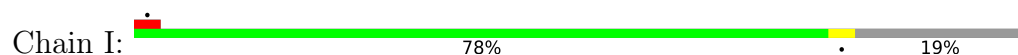
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



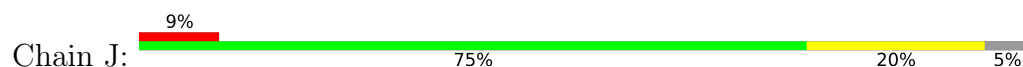
- Molecule 12: Photosystem I reaction center subunit VI-1, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII



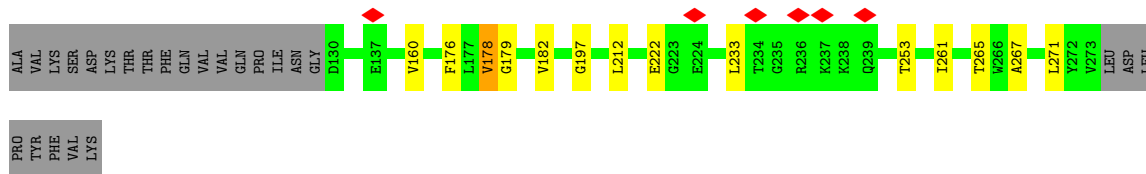
- Molecule 14: Photosystem I reaction center subunit IX





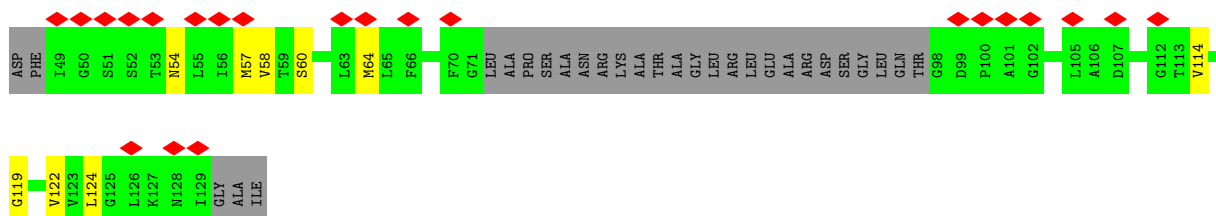
- Molecule 15: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 77% 8% 15%



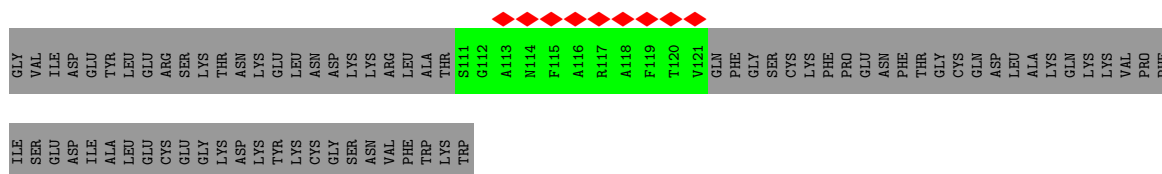
- Molecule 16: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 26% 55% 11% 35%



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

Chain N: 11% 13% 87%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	3.611	Depositor
Minimum map value	-1.558	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	398.272, 398.272, 398.272	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: LMT, DGD, LUT, LHG, BCR, CLA, SF4, LMG, CHL, PQN, XAT

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	0.12	0/1551	0.27	0/2117
2	2	0.12	0/1639	0.26	0/2242
3	3	0.14	0/1733	0.29	0/2356
4	4	0.13	0/1614	0.28	0/2198
5	A	0.14	0/6031	0.27	0/8226
6	B	0.14	0/6063	0.27	0/8281
7	C	0.16	0/628	0.35	0/852
8	D	0.12	0/1140	0.28	0/1542
9	E	0.11	0/519	0.28	0/703
10	F	0.14	0/1238	0.31	0/1670
11	G	0.10	0/749	0.21	0/1016
12	H	0.11	0/712	0.28	0/968
13	I	0.15	0/236	0.37	0/322
14	J	0.12	0/349	0.25	0/476
15	L	0.12	0/1108	0.25	0/1512
16	K	0.10	0/385	0.30	0/520
17	N	0.07	0/81	0.14	0/108
All	All	0.13	0/25776	0.28	0/35109

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	23	0
2	2	1582	0	1533	21	0
3	3	1680	0	1647	23	0
4	4	1564	0	1518	31	0
5	A	5834	0	5683	76	0
6	B	5852	0	5639	58	0
7	C	615	0	592	15	0
8	D	1112	0	1122	19	0
9	E	509	0	518	5	0
10	F	1208	0	1241	21	0
11	G	731	0	712	3	0
12	H	692	0	693	8	0
13	I	230	0	245	0	0
14	J	339	0	357	8	0
15	L	1076	0	1081	11	0
16	K	382	0	399	8	0
17	N	80	0	75	0	0
18	1	102	0	78	3	0
18	2	229	0	157	8	0
18	3	47	0	31	0	0
18	4	195	0	141	4	0
19	1	693	0	616	16	0
19	2	459	0	403	5	0
19	3	646	0	538	14	0
19	4	527	0	458	14	0
19	A	2569	0	2615	74	0
19	B	2434	0	2441	56	0
19	F	90	0	66	1	0
19	G	137	0	101	1	0
19	H	100	0	74	4	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	115	0	111	2	0
20	1	84	0	112	7	0
20	2	42	0	56	4	0
20	3	42	0	56	6	0
20	4	42	0	56	7	0
21	1	44	0	56	3	0
21	2	44	0	56	1	0
21	3	44	0	56	2	0
21	4	44	0	56	1	0
22	1	98	0	148	5	0
22	2	37	0	44	2	0
22	A	49	0	74	0	0
22	B	49	0	74	5	0
23	2	35	0	46	1	0
23	A	35	0	46	1	0
24	2	40	0	56	6	0
24	3	40	0	56	4	0
24	4	40	0	56	0	0
24	A	280	0	392	20	0
24	B	240	0	336	9	0
24	F	80	0	112	4	0
24	G	80	0	112	5	0
24	I	40	0	56	4	0
24	J	120	0	168	10	0
24	L	120	0	168	10	0
25	4	36	0	42	0	0
25	B	52	0	77	1	0
25	F	30	0	30	2	0
26	A	33	0	46	0	0
26	B	33	0	46	2	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	B	66	0	96	2	0
All	All	35543	0	35268	504	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 (504) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:315:LUT:H171	20:3:315:LUT:H8	1.58	0.85
20:4:315:LUT:H171	20:4:315:LUT:H8	1.60	0.84
19:B:851:CLA:HBA1	19:B:851:CLA:HBD	1.64	0.80
20:1:315:LUT:H8	20:1:315:LUT:H171	1.62	0.79
19:A:808:CLA:HBB2	19:A:811:CLA:HMA3	1.67	0.77
20:1:319:LUT:H8	20:1:319:LUT:H181	1.67	0.76
8:D:199:LYS:HD2	8:D:204:LEU:HD21	1.66	0.76
7:C:61:ASP:HB3	9:E:134:ASN:HD21	1.50	0.76
18:2:301:CHL:H2	3:3:161:ALA:HA	1.69	0.75
18:1:306:CHL:HBB1	21:1:316:XAT:H161	1.69	0.75
24:L:304:BCR:H361	24:L:304:BCR:H21C	1.68	0.74
3:3:230:ARG:HA	3:3:233:MET:HE2	1.70	0.74
10:F:148:GLY:HA2	10:F:152:THR:HB	1.69	0.73
24:2:319:BCR:H331	24:2:319:BCR:H343	1.71	0.73
4:4:221:VAL:HG11	19:4:312:CLA:HAC2	1.71	0.73
5:A:745:ARG:HH11	5:A:749:VAL:HG11	1.53	0.73
3:3:236:ILE:HG21	21:3:316:XAT:H12	1.69	0.73
15:L:222:GLU:N	15:L:222:GLU:OE2	2.23	0.71
10:F:126:TYR:HB3	14:J:38:ILE:HD11	1.73	0.71
8:D:127:ARG:NH2	8:D:129:GLU:OE1	2.23	0.71
10:F:75:CYS:SG	10:F:130:CYS:N	2.65	0.69
19:A:806:CLA:HAB	24:J:103:BCR:H352	1.77	0.67
4:4:156:ARG:NH2	4:4:167:VAL:O	2.29	0.66
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.29	0.65
6:B:40:GLU:HG2	6:B:165:VAL:HG23	1.78	0.65
4:4:175:GLN:OE1	4:4:175:GLN:N	2.27	0.65
8:D:107:GLU:O	8:D:137:ARG:NH1	2.30	0.65
10:F:102:GLU:OE1	10:F:102:GLU:N	2.25	0.64
5:A:118:ILE:HG12	5:A:119:VAL:HG23	1.80	0.64
19:A:807:CLA:H122	23:A:851:LMT:H102	1.80	0.64
8:D:166:VAL:HG11	8:D:172:ASN:HD22	1.62	0.63
19:A:833:CLA:H42	24:A:849:BCR:H362	1.81	0.62
5:A:530:ASP:O	5:A:534:HIS:ND1	2.30	0.62
4:4:204:LYS:O	4:4:208:ASN:ND2	2.27	0.61
5:A:353:ASN:ND2	19:A:803:CLA:OBD	2.30	0.61
4:4:225:VAL:HG13	4:4:226:THR:HG23	1.81	0.61
19:B:812:CLA:HAC2	19:B:813:CLA:HAB	1.83	0.61
2:2:184:PRO:HB3	18:2:307:CHL:HBC2	1.82	0.61
2:2:183:TYR:HB3	19:2:309:CLA:HED2	1.83	0.60
5:A:433:ALA:O	5:A:437:HIS:ND1	2.31	0.60
8:D:69:ASP:N	8:D:69:ASP:OD1	2.35	0.60
3:3:105:ARG:HB3	19:3:309:CLA:HBC3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:843:BCR:H10C	24:A:843:BCR:H352	1.84	0.59
24:A:844:BCR:H352	24:A:844:BCR:H10C	1.85	0.59
7:C:32:ASP:OD1	7:C:32:ASP:N	2.35	0.59
1:1:111:ASN:HD21	1:1:113:VAL:HB	1.68	0.59
7:C:61:ASP:HB3	9:E:134:ASN:ND2	2.17	0.59
20:1:319:LUT:H181	20:1:319:LUT:C8	2.32	0.59
5:A:356:MET:HG3	19:A:823:CLA:HMA1	1.85	0.59
24:B:842:BCR:H362	24:G:205:BCR:H312	1.84	0.59
22:B:850:LHG:H272	22:B:850:LHG:H322	1.84	0.59
9:E:143:GLU:N	9:E:143:GLU:OE2	2.35	0.59
24:L:304:BCR:H361	24:L:304:BCR:C21	2.30	0.59
4:4:154:GLU:OE1	4:4:157:ARG:NH2	2.33	0.58
15:L:182:VAL:HG12	15:L:197:GLY:HA3	1.84	0.58
6:B:32:GLU:OE1	6:B:396:ARG:NH1	2.36	0.58
4:4:106:GLY:O	4:4:110:MET:HG2	2.04	0.58
19:A:805:CLA:H2A	19:A:807:CLA:HED1	1.86	0.58
4:4:191:ASN:OD1	20:4:315:LUT:O23	2.20	0.58
18:2:301:CHL:HHC	18:2:301:CHL:HBB1	1.86	0.58
5:A:152:SER:OG	5:A:153:GLU:N	2.35	0.58
5:A:432:ASP:OD2	8:D:81:THR:OG1	2.21	0.58
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.68	0.58
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.85	0.58
19:B:822:CLA:HBC2	19:B:823:CLA:HBA1	1.86	0.58
15:L:265:THR:HG23	24:L:304:BCR:H333	1.85	0.58
5:A:662:SER:OG	5:A:663:SER:N	2.37	0.57
4:4:143:PHE:HB2	18:4:306:CHL:HBC1	1.85	0.57
4:4:101:ARG:NH1	18:4:307:CHL:OBD	2.37	0.57
2:2:152:GLU:OE1	2:2:155:ARG:NH2	2.33	0.57
22:B:850:LHG:H242	22:B:850:LHG:H102	1.87	0.57
8:D:128:LYS:HE3	8:D:160:LEU:HD13	1.87	0.57
2:2:213:GLY:O	2:2:217:MET:HG3	2.05	0.57
24:L:305:BCR:H352	24:L:305:BCR:H10C	1.85	0.56
19:A:833:CLA:H172	24:A:849:BCR:H12C	1.87	0.56
6:B:59:LEU:HD21	19:B:807:CLA:H101	1.86	0.56
6:B:415:LYS:HB3	6:B:539:LEU:HD13	1.87	0.56
22:1:320:LHG:O2	22:1:320:LHG:O9	2.23	0.56
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.87	0.56
5:A:656:VAL:HG22	5:A:744:ALA:HB3	1.88	0.56
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.86	0.56
2:2:104:GLY:HA2	21:2:316:XAT:H181	1.88	0.56
1:1:47:HIS:HD2	1:1:54:ARG:HG3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:147:LEU:HD22	24:2:319:BCR:H23C	1.88	0.55
19:A:840:CLA:H152	24:L:305:BCR:H17C	1.88	0.55
5:A:367:HIS:ND1	19:A:816:CLA:OBD	2.38	0.55
1:1:190:LYS:O	1:1:194:ASN:ND2	2.31	0.55
3:3:66:LEU:HD13	3:3:75:GLY:HA2	1.88	0.55
19:B:818:CLA:HAB	19:B:818:CLA:H8	1.89	0.55
6:B:36:ASP:O	6:B:41:ARG:NH1	2.40	0.55
6:B:203:ARG:O	6:B:247:SER:OG	2.22	0.55
24:G:201:BCR:H23C	24:G:201:BCR:H403	1.89	0.55
18:2:301:CHL:HAC1	24:3:317:BCR:HC31	1.87	0.54
19:4:312:CLA:HAA1	19:4:312:CLA:HBD	1.90	0.54
19:B:813:CLA:H92	19:B:824:CLA:H42	1.88	0.54
19:4:303:CLA:H11	10:F:205:VAL:HG13	1.89	0.54
3:3:121:GLY:HA2	3:3:126:ILE:HG22	1.89	0.54
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.40	0.54
16:K:64:MET:HE2	16:K:114:VAL:HG11	1.90	0.54
2:2:202:LEU:HD22	2:2:206:ARG:HE	1.73	0.53
6:B:276:HIS:HB2	19:B:817:CLA:C1B	2.39	0.53
19:B:806:CLA:H151	19:B:828:CLA:HBB2	1.91	0.53
4:4:104:MET:HE1	19:4:309:CLA:HHC	1.90	0.53
19:B:838:CLA:H193	24:I:101:BCR:H362	1.91	0.53
5:A:570:ARG:HD3	5:A:720:VAL:HG11	1.89	0.53
5:A:403:ALA:HB2	24:A:848:BCR:H323	1.91	0.53
19:A:807:CLA:H151	19:A:809:CLA:H142	1.91	0.53
2:2:238:LEU:HB2	20:2:315:LUT:H22	1.91	0.52
10:F:68:ASP:N	10:F:72:LEU:O	2.42	0.52
3:3:89:GLY:H	5:A:16:ARG:HH11	1.56	0.52
6:B:62:SER:HB2	6:B:142:LEU:HB2	1.90	0.52
8:D:197:THR:OG1	8:D:199:LYS:NZ	2.43	0.52
4:4:199:GLN:NE2	4:4:203:GLU:OE2	2.42	0.52
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.91	0.52
19:A:811:CLA:H92	19:A:811:CLA:H41	1.91	0.52
19:A:838:CLA:H141	25:F:305:LMG:H151	1.92	0.52
6:B:257:LEU:HD13	19:B:817:CLA:HMB3	1.92	0.52
19:B:826:CLA:H13	24:B:846:BCR:H15C	1.92	0.52
1:1:224:HIS:HB2	19:1:312:CLA:HED1	1.92	0.52
5:A:21:THR:HG21	5:A:175:TRP:HE1	1.74	0.52
4:4:125:PRO:HD2	19:4:304:CLA:HED3	1.92	0.52
5:A:194:MET:HE2	19:A:811:CLA:HBC2	1.91	0.51
19:B:827:CLA:HBC3	28:B:848:DGD:HBV2	1.93	0.51
2:2:147:LEU:HD13	24:2:319:BCR:H24C	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:274:THR:OG1	5:A:289:THR:OG1	2.22	0.51
8:D:161:HIS:CG	8:D:162:PRO:HD3	2.46	0.51
4:4:121:ILE:HG22	4:4:122:ILE:HG13	1.93	0.51
4:4:170:ASP:HB3	4:4:173:PHE:O	2.10	0.51
7:C:18:VAL:HG21	7:C:28:MET:HG2	1.93	0.51
7:C:80:ALA:HB2	8:D:127:ARG:HD2	1.92	0.51
3:3:140:ILE:HG22	3:3:142:PRO:HG2	1.92	0.51
19:B:831:CLA:H12	24:F:303:BCR:H353	1.93	0.51
5:A:139:SER:OG	19:A:806:CLA:OBD	2.29	0.51
12:H:80:SER:HB2	15:L:160:VAL:HG22	1.92	0.50
5:A:561:ILE:HD11	5:A:581:THR:HG21	1.93	0.50
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.94	0.50
6:B:428:PHE:CZ	24:J:101:BCR:H292	2.46	0.50
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.76	0.50
6:B:102:GLU:OE2	12:H:134:GLN:N	2.38	0.50
19:A:833:CLA:HBB1	19:A:852:CLA:HMB2	1.94	0.50
6:B:159:PRO:HA	6:B:162:LYS:HE3	1.94	0.50
3:3:89:GLY:H	5:A:16:ARG:NH1	2.10	0.50
6:B:558:PRO:HB3	6:B:702:ILE:HD12	1.92	0.50
14:J:13:VAL:O	14:J:17:LEU:HG	2.11	0.50
19:B:821:CLA:HAA1	19:B:821:CLA:HBD	1.94	0.50
16:K:57:MET:HB2	16:K:119:GLY:HA3	1.93	0.50
1:1:148:ALA:HB1	24:G:201:BCR:H16C	1.94	0.49
2:2:224:TRP:O	2:2:228:ILE:HG22	2.12	0.49
19:A:822:CLA:H42	24:A:848:BCR:H363	1.93	0.49
10:F:106:ALA:O	10:F:110:ASN:ND2	2.45	0.49
19:1:312:CLA:C4B	20:1:315:LUT:H183	2.42	0.49
5:A:119:VAL:HG11	19:B:832:CLA:HMD1	1.93	0.49
19:A:837:CLA:HED2	6:B:420:SER:HB3	1.94	0.49
10:F:103:SER:HB2	10:F:105:PRO:HD2	1.94	0.49
5:A:431:ARG:NH2	8:D:110:THR:O	2.44	0.49
6:B:571:SER:OG	6:B:574:ASP:OD2	2.30	0.49
22:2:317:LHG:HC92	24:3:317:BCR:HC42	1.94	0.49
6:B:293:THR:HG22	6:B:294:ASN:H	1.77	0.49
19:1:302:CLA:HAC2	22:1:317:LHG:H112	1.95	0.49
6:B:256:THR:OG1	6:B:271:THR:OG1	2.27	0.49
10:F:96:LEU:HA	10:F:109:LEU:HD13	1.95	0.49
24:J:101:BCR:H361	24:J:101:BCR:C21	2.42	0.49
19:3:312:CLA:C1B	20:3:315:LUT:H183	2.43	0.49
4:4:216:PHE:CD2	21:4:316:XAT:H14	2.47	0.49
4:4:65:ASP:OD1	4:4:65:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:585:SER:OG	5:A:588:ASP:OD2	2.29	0.48
19:A:827:CLA:H61	24:A:846:BCR:H342	1.96	0.48
1:1:228:PRO:O	1:1:232:ASN:ND2	2.39	0.48
3:3:230:ARG:HB3	19:3:301:CLA:HBC2	1.95	0.48
5:A:501:THR:OG1	5:A:502:SER:N	2.47	0.48
5:A:676:PHE:HB2	19:A:833:CLA:O1A	2.14	0.48
15:L:178:VAL:HG21	15:L:267:ALA:HB3	1.96	0.48
2:2:114:LEU:HD22	2:2:119:ILE:HG21	1.96	0.48
6:B:60:TRP:HA	19:B:807:CLA:HBB2	1.96	0.48
8:D:103:GLU:HG3	8:D:117:ARG:HA	1.95	0.48
9:E:85:LYS:HB2	9:E:85:LYS:NZ	2.28	0.48
19:A:853:CLA:H42	19:L:301:CLA:H102	1.95	0.47
6:B:411:MET:SD	24:B:845:BCR:H292	2.54	0.47
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.96	0.47
20:3:315:LUT:H171	20:3:315:LUT:C8	2.38	0.47
4:4:150:PHE:HA	4:4:153:VAL:HG22	1.96	0.47
4:4:234:LEU:HB2	20:4:315:LUT:O3	2.14	0.47
19:A:811:CLA:H41	19:A:811:CLA:H61	1.66	0.47
19:A:828:CLA:HAA1	19:A:828:CLA:HBD	1.97	0.47
6:B:489:GLY:C	6:B:494:LEU:HD12	2.39	0.47
4:4:90:LYS:O	4:4:94:GLN:HG2	2.14	0.47
1:1:87:GLU:HB2	19:1:302:CLA:C1B	2.45	0.47
2:2:238:LEU:HD22	20:2:315:LUT:H172	1.96	0.47
6:B:4:ARG:HA	6:B:4:ARG:HD2	1.75	0.47
6:B:453:ILE:HD13	24:J:101:BCR:H20C	1.96	0.47
12:H:73:VAL:HA	15:L:233:LEU:HD11	1.95	0.47
19:B:851:CLA:H112	19:B:851:CLA:H152	1.67	0.47
18:1:301:CHL:HBA2	18:1:301:CHL:H3A	1.76	0.47
4:4:209:GLY:O	4:4:213:MET:HG2	2.15	0.47
5:A:113:GLN:NE2	19:A:807:CLA:OBD	2.47	0.47
8:D:116:MET:HB2	8:D:121:ASN:ND2	2.29	0.47
5:A:445:LEU:HD11	19:A:835:CLA:HMB2	1.96	0.47
5:A:478:PRO:HG3	5:A:531:PHE:HB2	1.95	0.47
19:A:823:CLA:H192	19:A:823:CLA:H161	1.71	0.47
10:F:100:ALA:O	10:F:103:SER:OG	2.33	0.47
10:F:140:VAL:HG12	10:F:150:PHE:HB2	1.97	0.47
3:3:265:ASN:H	3:3:268:THR:HG22	1.79	0.47
5:A:65:GLU:OE1	5:A:65:GLU:N	2.48	0.47
6:B:17:THR:HG21	7:C:77:MET:HE3	1.97	0.47
16:K:54:ASN:ND2	19:K:201:CLA:OBD	2.32	0.47
5:A:638:SER:OG	5:A:638:SER:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:87:ILE:HG12	6:B:113:VAL:HG21	1.97	0.46
19:B:813:CLA:H172	24:B:843:BCR:H271	1.96	0.46
19:B:838:CLA:HAA1	19:B:838:CLA:HBD	1.96	0.46
5:A:454:ILE:HG22	19:A:831:CLA:HBC2	1.95	0.46
6:B:124:TRP:HB3	6:B:129:LEU:HD12	1.97	0.46
19:3:306:CLA:H3A	19:3:306:CLA:HBA2	1.50	0.46
6:B:685:THR:O	6:B:689:ASN:ND2	2.48	0.46
19:3:304:CLA:H12	19:3:304:CLA:H2A	1.97	0.46
19:1:302:CLA:CBB	21:1:316:XAT:H32	2.46	0.46
19:1:308:CLA:H92	19:1:308:CLA:H61	1.72	0.46
22:1:317:LHG:HC81	22:1:317:LHG:HC5	1.39	0.46
19:A:828:CLA:H203	19:A:828:CLA:H161	1.83	0.46
2:2:73:PHE:HZ	2:2:211:LYS:HE2	1.80	0.46
19:A:803:CLA:HBA1	19:A:803:CLA:H3A	1.78	0.46
16:K:57:MET:HA	16:K:60:SER:OG	2.16	0.46
2:2:204:GLU:O	2:2:208:LYS:HG3	2.15	0.46
3:3:180:MET:HE3	3:3:180:MET:O	2.16	0.46
8:D:70:PRO:C	8:D:71:ASN:HD22	2.23	0.46
1:1:202:PHE:CE1	21:1:316:XAT:H10	2.51	0.46
18:2:306:CHL:HHC	18:2:306:CHL:HBB1	1.98	0.46
19:A:833:CLA:C4B	19:A:852:CLA:HBB1	2.45	0.46
14:J:33:PHE:HB3	24:J:101:BCR:HC7	1.96	0.46
19:3:303:CLA:HBA2	19:3:304:CLA:HHD	1.98	0.46
4:4:104:MET:HG3	4:4:212:ALA:HB2	1.97	0.46
19:A:853:CLA:H61	19:A:853:CLA:H41	1.58	0.46
19:B:832:CLA:HBA2	24:J:101:BCR:H352	1.97	0.46
5:A:28:LYS:HB2	5:A:28:LYS:HE2	1.77	0.45
5:A:307:HIS:CE1	24:A:844:BCR:H363	2.51	0.45
5:A:324:GLU:HG2	5:A:336:LYS:HD2	1.97	0.45
1:1:83:TYR:OH	22:B:850:LHG:O1	2.30	0.45
1:1:190:LYS:HD3	19:1:311:CLA:HBD	1.96	0.45
19:A:801:CLA:HBA1	19:A:801:CLA:H3A	1.67	0.45
19:A:819:CLA:HMB2	19:A:823:CLA:HMA3	1.96	0.45
19:A:840:CLA:H191	15:L:176:PHE:HE2	1.81	0.45
15:L:212:LEU:HB3	15:L:253:THR:HG22	1.99	0.45
19:4:301:CLA:HBB2	19:4:302:CLA:HBC2	1.98	0.45
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.97	0.45
19:A:807:CLA:H93	19:A:807:CLA:H61	1.69	0.45
14:J:37:LEU:O	24:J:101:BCR:H15C	2.15	0.45
19:K:201:CLA:H3A	19:K:201:CLA:HBA1	1.52	0.45
24:2:319:BCR:H371	24:2:319:BCR:C25	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:94:ARG:HA	5:A:94:ARG:HD3	1.77	0.45
24:A:847:BCR:H20C	24:A:847:BCR:H361	1.86	0.45
22:2:317:LHG:HC62	22:2:317:LHG:H242	1.54	0.45
18:4:306:CHL:H2A	18:4:306:CHL:HED2	1.98	0.45
6:B:182:LEU:HD21	19:B:813:CLA:H2	1.98	0.45
6:B:567:THR:O	6:B:567:THR:OG1	2.29	0.45
24:L:305:BCR:H10C	24:L:305:BCR:C35	2.46	0.45
19:1:308:CLA:HBA1	19:1:308:CLA:H3A	1.81	0.45
19:1:313:CLA:HBA2	19:1:313:CLA:H3A	1.63	0.45
20:2:315:LUT:C8	20:2:315:LUT:H181	2.46	0.45
19:H:202:CLA:H3A	19:H:202:CLA:HBA2	1.53	0.45
6:B:373:THR:HG23	6:B:591:THR:HG21	1.98	0.45
6:B:403:ASN:HB3	6:B:406:ASN:HD21	1.81	0.45
19:1:318:CLA:HBA2	19:1:318:CLA:H3A	1.44	0.45
19:B:829:CLA:HBD	19:B:829:CLA:HAA1	1.99	0.45
19:A:854:CLA:H62	19:A:854:CLA:H101	1.76	0.45
19:B:826:CLA:H152	24:B:846:BCR:H17C	1.98	0.45
4:4:101:ARG:HD3	19:4:309:CLA:C4C	2.47	0.45
19:4:312:CLA:C1B	20:4:315:LUT:H183	2.47	0.45
6:B:203:ARG:HD3	6:B:250:THR:HB	1.99	0.45
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.29	0.45
19:B:806:CLA:H192	19:B:806:CLA:H161	1.74	0.45
22:B:850:LHG:H181	22:B:850:LHG:H141	1.98	0.45
19:A:815:CLA:H61	19:A:815:CLA:H41	1.58	0.44
24:B:844:BCR:H20C	24:B:844:BCR:H361	1.79	0.44
5:A:294:HIS:HB2	19:A:816:CLA:C1B	2.47	0.44
19:A:833:CLA:H52	6:B:438:VAL:HG13	1.99	0.44
7:C:2:SER:N	7:C:71:HIS:O	2.50	0.44
2:2:71:GLY:HA2	2:2:207:THR:HG23	1.98	0.44
19:2:302:CLA:H192	19:2:302:CLA:H162	1.75	0.44
5:A:746:ILE:HD12	5:A:746:ILE:HA	1.83	0.44
3:3:267:LEU:O	3:3:271:LYS:N	2.50	0.44
5:A:533:VAL:HG11	5:A:607:HIS:CG	2.52	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.53	0.44
1:1:103:VAL:HB	1:1:104:PRO:HD3	2.00	0.44
22:1:320:LHG:HC62	22:1:320:LHG:H241	1.45	0.44
5:A:40:PRO:HB3	5:A:45:TRP:CE3	2.53	0.44
19:A:839:CLA:H61	19:A:839:CLA:H41	1.46	0.44
19:B:814:CLA:C1B	24:B:844:BCR:H352	2.47	0.44
2:2:211:LYS:NZ	19:2:310:CLA:O1D	2.37	0.44
19:3:302:CLA:H72	19:A:811:CLA:H201	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:521:LEU:HD12	5:A:521:LEU:HA	1.84	0.44
5:A:531:PHE:CE1	24:A:843:BCR:H313	2.52	0.44
19:A:813:CLA:HBA2	19:A:813:CLA:H3A	1.57	0.44
7:C:23:THR:HG21	7:C:47:ASP:O	2.18	0.44
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.53	0.44
24:2:319:BCR:H371	24:2:319:BCR:H402	1.99	0.44
19:4:303:CLA:H2	10:F:205:VAL:HG22	1.99	0.44
22:B:850:LHG:H261	22:B:850:LHG:H121	2.00	0.44
15:L:271:LEU:HD23	15:L:271:LEU:HA	1.85	0.44
5:A:24:GLU:OE1	5:A:24:GLU:N	2.50	0.44
5:A:201:GLY:HA2	19:A:818:CLA:HBC1	2.00	0.44
5:A:553:LEU:HD23	5:A:553:LEU:HA	1.85	0.44
19:A:853:CLA:H112	19:A:853:CLA:H152	1.89	0.44
19:B:805:CLA:HBA1	19:B:805:CLA:H3A	1.65	0.44
4:4:228:LYS:HE2	4:4:228:LYS:HB2	1.67	0.43
11:G:115:TYR:O	11:G:119:LEU:HG	2.18	0.43
5:A:531:PHE:HE1	24:A:843:BCR:H313	1.84	0.43
6:B:182:LEU:HD13	19:B:813:CLA:HBB	2.00	0.43
2:2:191:PRO:HD2	20:2:315:LUT:H23	2.00	0.43
20:4:315:LUT:H7	20:4:315:LUT:H181	1.78	0.43
19:G:203:CLA:H3A	19:G:203:CLA:HBA2	1.59	0.43
1:1:91:CYS:HB3	1:1:195:GLY:HA3	2.00	0.43
19:3:310:CLA:H2A	19:3:310:CLA:HED2	2.00	0.43
5:A:213:HIS:HB2	19:A:812:CLA:C1C	2.47	0.43
19:A:819:CLA:H92	19:A:819:CLA:H62	1.82	0.43
19:A:824:CLA:H62	19:A:824:CLA:H102	1.63	0.43
19:B:806:CLA:H3A	19:B:829:CLA:HAB	2.00	0.43
10:F:149:GLU:HA	14:J:38:ILE:HG22	1.99	0.43
24:L:305:BCR:H24C	24:L:305:BCR:H371	1.86	0.43
16:K:122:VAL:HG12	19:K:202:CLA:HBB1	1.99	0.43
18:4:305:CHL:H62	18:4:305:CHL:H41	1.77	0.43
5:A:646:ARG:NH1	5:A:647:ASP:OD2	2.51	0.43
6:B:22:TRP:CG	6:B:704:GLN:HE22	2.36	0.43
6:B:475:ASP:OD1	6:B:475:ASP:N	2.50	0.43
19:B:818:CLA:H3A	19:B:818:CLA:HBA2	1.56	0.43
16:K:58:VAL:CG2	19:K:201:CLA:HBD	2.49	0.43
1:1:199:LEU:O	1:1:203:VAL:HG23	2.19	0.43
19:1:302:CLA:HBC1	22:1:317:LHG:H121	2.01	0.43
19:4:302:CLA:H91	19:4:303:CLA:H13	2.01	0.43
10:F:90:LYS:HD2	10:F:90:LYS:HA	1.72	0.43
5:A:198:HIS:ND1	19:A:823:CLA:OBD	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:354:LEU:HD21	19:A:828:CLA:HBB1	2.01	0.43
6:B:208:ARG:O	6:B:212:PHE:HB3	2.19	0.43
19:B:826:CLA:H141	19:B:826:CLA:H161	1.83	0.43
24:F:304:BCR:H24C	24:F:304:BCR:H371	1.85	0.43
24:L:304:BCR:H24C	24:L:304:BCR:H371	1.85	0.43
1:1:156:ARG:NH2	19:1:308:CLA:O1D	2.41	0.43
3:3:70:LEU:HD23	3:3:70:LEU:HA	1.92	0.43
5:A:660:TYR:OH	6:B:441:ASP:OD1	2.15	0.43
6:B:85:ARG:NH2	12:H:145:LEU:O	2.36	0.43
9:E:92:ILE:HG22	9:E:94:ARG:H	1.84	0.43
19:A:853:CLA:H3A	19:A:853:CLA:HBA2	1.48	0.43
24:F:303:BCR:H24C	24:F:303:BCR:H371	1.86	0.43
5:A:330:PHE:CD1	5:A:330:PHE:N	2.87	0.43
24:A:847:BCR:H371	24:A:847:BCR:H24C	1.84	0.43
19:A:828:CLA:H92	19:A:828:CLA:H61	1.73	0.42
6:B:697:PRO:O	7:C:81:TYR:OH	2.36	0.42
25:B:849:LMG:HC8	25:B:849:LMG:H111	1.32	0.42
11:G:70:LEU:HD23	11:G:70:LEU:HA	1.85	0.42
2:2:143:VAL:O	2:2:147:LEU:HG	2.19	0.42
3:3:139:VAL:HG13	3:3:140:ILE:HG13	2.01	0.42
19:A:830:CLA:H62	19:A:830:CLA:H102	1.85	0.42
24:A:844:BCR:H361	24:A:844:BCR:H20C	1.74	0.42
1:1:105:GLU:HG3	1:1:110:GLY:O	2.19	0.42
24:3:317:BCR:H24C	24:3:317:BCR:H371	1.91	0.42
19:B:812:CLA:HBB1	19:B:820:CLA:HBC2	2.00	0.42
24:B:842:BCR:H20C	24:B:842:BCR:H361	1.89	0.42
8:D:108:MET:HE3	8:D:108:MET:HB3	1.85	0.42
19:F:301:CLA:HBA1	19:F:301:CLA:H3A	1.74	0.42
24:I:101:BCR:H24C	24:I:101:BCR:H371	1.86	0.42
14:J:28:GLU:HG3	19:J:102:CLA:C1B	2.49	0.42
5:A:342:LEU:O	5:A:349:GLN:NE2	2.52	0.42
19:B:804:CLA:HBD	19:B:804:CLA:HBA1	2.01	0.42
10:F:186:ILE:HG13	10:F:187:ILE:HG13	2.01	0.42
3:3:57:PHE:HB2	3:3:76:PHE:HD1	1.84	0.42
19:3:312:CLA:HBD	19:3:312:CLA:O1A	2.19	0.42
19:A:804:CLA:H93	19:A:804:CLA:H61	1.71	0.42
1:1:99:PRO:O	1:1:103:VAL:HG23	2.19	0.42
4:4:178:LEU:HD21	4:4:189:ILE:HG22	2.00	0.42
5:A:261:PHE:CZ	24:A:844:BCR:H343	2.54	0.42
19:H:202:CLA:H102	19:H:202:CLA:H62	1.68	0.42
3:3:141:PRO:N	3:3:142:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:312:CLA:H11	19:4:312:CLA:HBA2	1.70	0.42
19:B:836:CLA:H192	19:B:836:CLA:H161	1.80	0.42
3:3:109:LEU:HD23	3:3:109:LEU:HA	1.89	0.42
19:3:302:CLA:H13	19:3:308:CLA:H42	2.01	0.42
5:A:236:LEU:HD11	19:A:814:CLA:HED2	2.00	0.42
5:A:435:ILE:HB	6:B:677:THR:HG21	2.02	0.42
19:A:808:CLA:H2	19:A:811:CLA:H193	2.02	0.42
19:A:823:CLA:H93	19:A:823:CLA:H62	1.73	0.42
6:B:465:SER:O	6:B:479:SER:OG	2.25	0.42
19:B:810:CLA:H62	19:B:810:CLA:H41	1.77	0.42
19:B:812:CLA:HAA1	19:B:812:CLA:HBD	2.02	0.42
19:B:830:CLA:HMC1	19:B:840:CLA:H142	2.02	0.42
15:L:261:ILE:O	15:L:265:THR:HG22	2.20	0.42
1:1:161:ASP:O	1:1:165:LYS:HG3	2.19	0.42
19:2:308:CLA:HBA1	23:2:318:LMT:H11	2.01	0.42
19:A:835:CLA:H91	19:L:301:CLA:H191	2.02	0.42
24:A:844:BCR:H10C	24:A:844:BCR:C35	2.49	0.42
19:B:808:CLA:H192	19:B:808:CLA:H161	1.77	0.42
19:B:834:CLA:HAA1	19:B:834:CLA:HBD	2.02	0.42
3:3:265:ASN:H	3:3:268:THR:CG2	2.33	0.42
5:A:531:PHE:HZ	24:A:843:BCR:H322	1.84	0.42
24:A:845:BCR:H20C	24:A:845:BCR:H361	1.92	0.42
19:B:833:CLA:H61	19:B:833:CLA:H41	1.51	0.42
19:B:839:CLA:H62	19:B:839:CLA:H41	1.69	0.42
26:B:841:PQN:H301	28:B:848:DGD:HAT1	2.02	0.42
7:C:21:CYS:HA	7:C:22:PRO:HD3	1.87	0.42
7:C:61:ASP:OD1	7:C:62:PHE:N	2.49	0.42
7:C:70:TRP:CE3	7:C:70:TRP:HA	2.55	0.42
5:A:26:TRP:NE1	19:A:809:CLA:HBA1	2.35	0.41
5:A:164:LEU:HD23	5:A:164:LEU:HA	1.88	0.41
5:A:603:VAL:HG21	19:A:801:CLA:H202	2.02	0.41
19:A:811:CLA:H92	19:A:811:CLA:H61	1.79	0.41
7:C:15:THR:HG22	7:C:28:MET:HE2	2.02	0.41
1:1:107:LEU:HD12	1:1:109:TYR:HE2	1.84	0.41
5:A:735:ILE:HG23	19:A:826:CLA:HBB1	2.02	0.41
10:F:189:ASP:OD1	10:F:192:LEU:HB3	2.20	0.41
24:F:303:BCR:H20C	24:F:303:BCR:H361	1.89	0.41
25:F:305:LMG:HC72	14:J:5:LYS:HB3	2.02	0.41
1:1:65:ASP:C	1:1:65:ASP:OD2	2.62	0.41
2:2:188:TRP:HZ3	18:2:307:CHL:HAB	1.84	0.41
4:4:219:PHE:HZ	20:4:315:LUT:H173	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:417:THR:OG1	5:A:418:THR:N	2.54	0.41
19:A:816:CLA:H3A	19:A:816:CLA:HBA2	1.69	0.41
19:B:823:CLA:HMA1	19:B:840:CLA:HED3	2.02	0.41
10:F:92:LEU:HD23	10:F:92:LEU:HA	1.89	0.41
10:F:179:LYS:HB2	10:F:179:LYS:HE2	1.79	0.41
24:I:101:BCR:H20C	24:I:101:BCR:H361	1.92	0.41
24:L:304:BCR:H21C	24:L:304:BCR:C36	2.42	0.41
16:K:64:MET:HG2	16:K:114:VAL:HG13	2.01	0.41
2:2:169:PRO:HB2	24:2:319:BCR:H10C	2.01	0.41
19:3:308:CLA:HBA2	19:3:314:CLA:HBB1	2.02	0.41
19:B:812:CLA:HBA2	19:B:812:CLA:H12	1.84	0.41
7:C:77:MET:HE2	7:C:77:MET:HB2	1.95	0.41
24:G:201:BCR:H371	24:G:201:BCR:H24C	1.87	0.41
24:J:104:BCR:H23C	24:J:104:BCR:H403	2.03	0.41
19:1:309:CLA:H62	19:1:309:CLA:H41	1.84	0.41
5:A:348:ALA:O	5:A:352:ILE:HG13	2.20	0.41
19:A:806:CLA:H3A	19:A:806:CLA:HBA2	1.63	0.41
19:A:852:CLA:H3A	19:A:852:CLA:CGA	2.51	0.41
8:D:103:GLU:HA	8:D:116:MET:O	2.20	0.41
11:G:88:ARG:HA	11:G:88:ARG:HD3	1.88	0.41
12:H:83:ASN:CG	19:H:201:CLA:HMA3	2.46	0.41
1:1:152:VAL:HG21	24:G:201:BCR:H362	2.02	0.41
18:2:301:CHL:HMD2	24:3:317:BCR:HC21	2.01	0.41
19:3:308:CLA:H2	19:3:308:CLA:H62	1.83	0.41
19:3:311:CLA:H3A	19:3:311:CLA:HBA1	1.85	0.41
4:4:104:MET:CE	19:4:309:CLA:HHC	2.49	0.41
5:A:330:PHE:N	5:A:330:PHE:HD1	2.19	0.41
24:A:846:BCR:H371	24:A:846:BCR:H24C	1.85	0.41
6:B:301:ILE:HG21	19:B:824:CLA:HAC1	2.02	0.41
19:B:825:CLA:H41	19:B:835:CLA:H8	2.01	0.41
19:B:826:CLA:H72	19:B:826:CLA:H111	1.75	0.41
19:B:832:CLA:H12	24:J:101:BCR:H341	2.02	0.41
8:D:70:PRO:C	8:D:71:ASN:ND2	2.78	0.41
10:F:70:SER:OG	10:F:70:SER:O	2.39	0.41
19:H:201:CLA:H3A	19:H:201:CLA:HBA2	1.48	0.41
15:L:179:GLY:O	15:L:182:VAL:HG22	2.20	0.41
5:A:56:PHE:CD2	19:A:803:CLA:HMC2	2.56	0.41
5:A:431:ARG:H	5:A:431:ARG:HG2	1.69	0.41
6:B:344:ILE:HD12	19:B:818:CLA:H101	2.02	0.41
3:3:126:ILE:HD12	3:3:126:ILE:HA	1.84	0.41
12:H:114:LEU:O	12:H:118:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:309:CLA:H92	19:1:309:CLA:H61	1.81	0.41
20:1:315:LUT:H7	20:1:315:LUT:H181	1.79	0.41
20:1:315:LUT:H11	20:1:315:LUT:H191	1.96	0.41
19:1:318:CLA:HBC3	20:1:319:LUT:H28	2.03	0.41
19:A:815:CLA:CHD	19:A:816:CLA:HBB2	2.51	0.41
19:A:830:CLA:H143	26:B:841:PQN:H191	2.02	0.41
6:B:662:MET:HE1	19:B:803:CLA:HMA3	2.03	0.41
6:B:733:PHE:HD2	12:H:141:PRO:HG2	1.86	0.41
19:B:816:CLA:H61	19:B:816:CLA:H41	1.74	0.41
12:H:88:LYS:HA	12:H:88:LYS:HD3	1.73	0.41
24:J:103:BCR:H20C	24:J:103:BCR:H361	1.90	0.41
19:3:309:CLA:CBB	20:3:315:LUT:H32	2.50	0.41
4:4:54:LYS:HB3	4:4:55:GLY:H	1.64	0.41
5:A:127:ASP:N	5:A:127:ASP:OD1	2.42	0.41
5:A:307:HIS:NE2	24:A:844:BCR:H363	2.36	0.41
5:A:719:ILE:H	5:A:719:ILE:HG13	1.73	0.41
6:B:351:HIS:ND1	19:B:817:CLA:OBD	2.53	0.41
19:B:838:CLA:H51	19:B:839:CLA:H142	2.03	0.41
16:K:124:LEU:HD13	16:K:124:LEU:HA	1.94	0.41
1:1:118:TRP:CZ2	1:1:126:ALA:HB2	2.55	0.40
3:3:208:PRO:HD2	20:3:315:LUT:H23	2.02	0.40
3:3:257:HIS:ND1	3:3:264:ASN:O	2.53	0.40
19:4:312:CLA:H93	19:4:312:CLA:H61	1.82	0.40
24:A:844:BCR:H24C	24:A:844:BCR:H371	1.78	0.40
6:B:157:LEU:HD23	6:B:157:LEU:HA	1.87	0.40
19:B:823:CLA:HBC3	24:B:845:BCR:H372	2.02	0.40
8:D:67:GLN:N	8:D:67:GLN:OE1	2.54	0.40
19:A:822:CLA:HBA2	19:A:822:CLA:H3A	1.48	0.40
19:A:826:CLA:H193	19:A:833:CLA:H122	2.02	0.40
19:A:835:CLA:H41	19:A:835:CLA:H62	1.80	0.40
19:B:806:CLA:H92	19:B:806:CLA:H61	1.81	0.40
19:B:807:CLA:H111	19:B:807:CLA:H72	1.81	0.40
3:3:110:GLY:HA2	21:3:316:XAT:H181	2.03	0.40
20:3:315:LUT:H35	20:3:315:LUT:H401	1.92	0.40
6:B:56:ILE:HD11	19:B:807:CLA:H18	2.04	0.40
1:1:207:VAL:HG11	19:1:312:CLA:HHD	2.03	0.40
4:4:219:PHE:CZ	20:4:315:LUT:H173	2.56	0.40
5:A:88:MET:HE1	19:A:806:CLA:HMA2	2.03	0.40
5:A:331:THR:OG1	5:A:332:GLY:N	2.53	0.40
6:B:567:THR:HB	6:B:570:ILE:HD12	2.03	0.40
19:B:838:CLA:H112	24:I:101:BCR:H382	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:137:THR:HG23	1:1:139:PRO:HD2	2.04	0.40
18:1:301:CHL:H11	4:4:152:TYR:HB2	2.02	0.40
2:2:100:TRP:CE2	18:2:307:CHL:HED3	2.56	0.40
19:2:309:CLA:H62	19:2:309:CLA:H41	1.90	0.40
4:4:246:ILE:HG22	19:4:312:CLA:O1A	2.22	0.40
5:A:187:TRP:CD1	19:A:810:CLA:HED1	2.57	0.40
5:A:372:PRO:HG2	5:A:378:ALA:HB2	2.04	0.40
19:A:825:CLA:H202	19:A:825:CLA:H161	1.75	0.40
19:A:840:CLA:H62	19:A:840:CLA:H41	1.85	0.40
6:B:427:LEU:HD23	6:B:427:LEU:HA	1.95	0.40
24:L:304:BCR:H15C	24:L:304:BCR:H351	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/206 (93%)	187 (97%)	5 (3%)	0	100	100
2	2	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
3	3	217/234 (93%)	213 (98%)	4 (2%)	0	100	100
4	4	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
5	A	740/750 (99%)	727 (98%)	13 (2%)	0	100	100
6	B	731/734 (100%)	718 (98%)	13 (2%)	0	100	100
7	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	D	139/160 (87%)	131 (94%)	8 (6%)	0	100	100
9	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
10	F	150/154 (97%)	147 (98%)	3 (2%)	0	100	100
11	G	92/100 (92%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	88/95 (93%)	87 (99%)	1 (1%)	0	100	100
13	I	28/37 (76%)	27 (96%)	1 (4%)	0	100	100
14	J	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
15	L	142/169 (84%)	140 (99%)	2 (1%)	0	100	100
16	K	51/84 (61%)	49 (96%)	2 (4%)	0	100	100
17	N	9/85 (11%)	9 (100%)	0	0	100	100
All	All	3154/3445 (92%)	3081 (98%)	73 (2%)	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%)	153 (100%)	0	100	100
2	2	164/171 (96%)	164 (100%)	0	100	100
3	3	169/179 (94%)	168 (99%)	1 (1%)	84	90
4	4	164/166 (99%)	164 (100%)	0	100	100
5	A	601/609 (99%)	598 (100%)	3 (0%)	86	91
6	B	597/598 (100%)	596 (100%)	1 (0%)	92	95
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	120/134 (90%)	119 (99%)	1 (1%)	79	87
9	E	56/80 (70%)	55 (98%)	1 (2%)	54	74
10	F	125/127 (98%)	125 (100%)	0	100	100
11	G	79/84 (94%)	79 (100%)	0	100	100
12	H	75/79 (95%)	75 (100%)	0	100	100
13	I	26/33 (79%)	25 (96%)	1 (4%)	28	56
14	J	36/38 (95%)	36 (100%)	0	100	100
15	L	111/134 (83%)	110 (99%)	1 (1%)	75	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	K	41/61 (67%)	41 (100%)	0	100	100
17	N	7/73 (10%)	7 (100%)	0	100	100
All	All	2594/2798 (93%)	2585 (100%)	9 (0%)	90	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	159	GLU
5	A	246	LEU
5	A	457	ASP
5	A	581	THR
6	B	303	ASP
8	D	161	HIS
9	E	139	ASP
13	I	24	MET
15	L	178	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
1	1	209	GLN
2	2	92	GLN
2	2	131	GLN
2	2	166	ASN
3	3	61	GLN
3	3	242	GLN
4	4	75	ASN
4	4	99	HIS
4	4	168	ASN
4	4	222	GLN
4	4	223	HIS
5	A	50	HIS
5	A	113	GLN
5	A	136	GLN
5	A	238	HIS
5	A	366	HIS
5	A	448	HIS
5	A	658	GLN
5	A	713	GLN

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Mol	Chain	Res	Type
6	B	64	ASN
6	B	236	ASN
6	B	248	GLN
6	B	299	HIS
6	B	333	GLN
6	B	403	ASN
6	B	504	ASN
6	B	610	ASN
7	C	16	GLN
8	D	71	ASN
8	D	147	GLN
8	D	161	HIS
9	E	134	ASN
10	F	110	ASN
10	F	122	ASN
11	G	87	GLN
11	G	90	ASN
11	G	99	GLN
11	G	104	HIS
12	H	134	GLN
16	K	128	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](#)

206 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LUT	4	315	-	42,43,43	1.61	8 (19%)	51,60,60	1.59	11 (21%)
24	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.65	2 (3%)
19	CLA	B	840	22	65,73,73	1.35	7 (10%)	76,113,113	1.77	11 (14%)
19	CLA	B	833	-	56,64,73	1.45	7 (12%)	65,102,113	1.89	9 (13%)
19	CLA	B	820	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	6 (11%)
19	CLA	A	826	-	65,73,73	1.33	7 (10%)	76,113,113	1.74	8 (10%)
25	LMG	B	849	-	52,52,55	0.19	0	60,60,63	0.15	0
19	CLA	A	829	-	65,73,73	1.36	7 (10%)	76,113,113	1.74	9 (11%)
18	CHL	4	307	-	51,59,74	1.66	10 (19%)	55,96,114	2.06	12 (21%)
19	CLA	B	806	-	65,73,73	1.34	7 (10%)	76,113,113	1.79	13 (17%)
22	LHG	1	320	-	48,48,48	0.30	0	51,54,54	0.28	0
19	CLA	B	839	-	65,73,73	1.34	7 (10%)	76,113,113	1.67	10 (13%)
19	CLA	B	816	-	55,63,73	1.45	7 (12%)	64,101,113	1.80	10 (15%)
19	CLA	B	811	-	54,62,73	1.42	7 (12%)	67,100,113	1.91	14 (20%)
19	CLA	2	302	2	65,73,73	1.35	7 (10%)	76,113,113	1.67	10 (13%)
19	CLA	3	314	-	46,54,73	1.56	7 (15%)	53,90,113	1.90	8 (15%)
22	LHG	2	317	19	36,36,48	0.34	0	39,42,54	0.31	0
19	CLA	A	807	5	62,70,73	1.37	7 (11%)	72,109,113	1.79	9 (12%)
19	CLA	A	832	-	45,53,73	1.58	7 (15%)	52,89,113	1.92	7 (13%)
19	CLA	A	825	-	65,73,73	1.33	7 (10%)	76,113,113	1.79	11 (14%)
19	CLA	A	827	-	65,73,73	1.35	7 (10%)	76,113,113	1.70	10 (13%)
19	CLA	B	819	-	60,68,73	1.40	7 (11%)	70,107,113	1.74	9 (12%)
19	CLA	3	312	-	55,63,73	1.45	7 (12%)	64,101,113	1.82	7 (10%)
19	CLA	A	814	-	45,53,73	1.57	7 (15%)	52,89,113	1.98	7 (13%)
19	CLA	A	822	-	55,63,73	1.46	7 (12%)	64,101,113	1.75	9 (14%)
24	BCR	J	101	-	41,41,41	0.18	0	56,56,56	0.93	4 (7%)
19	CLA	F	301	-	45,53,73	1.57	7 (15%)	52,89,113	1.95	7 (13%)
22	LHG	1	317	19	48,48,48	0.30	0	51,54,54	0.31	0
24	BCR	B	845	-	41,41,41	0.11	0	56,56,56	0.30	0
19	CLA	G	204	11	46,54,73	1.55	7 (15%)	53,90,113	1.93	8 (15%)
19	CLA	3	313	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	7 (13%)
19	CLA	1	307	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	XAT	4	316	-	39,47,47	0.09	0	54,74,74	0.80	3 (5%)
18	CHL	1	306	1	46,54,74	1.73	11 (23%)	49,90,114	2.11	10 (20%)
19	CLA	A	812	-	45,53,73	1.56	7 (15%)	52,89,113	1.99	9 (17%)
19	CLA	A	808	-	59,67,73	1.41	7 (11%)	68,105,113	1.80	9 (13%)
24	BCR	G	205	-	41,41,41	0.11	0	56,56,56	0.31	0
24	BCR	L	304	-	41,41,41	0.22	0	56,56,56	0.87	2 (3%)
18	CHL	3	307	-	47,55,74	1.67	9 (19%)	50,91,114	2.23	10 (20%)
19	CLA	A	811	-	65,73,73	1.33	7 (10%)	76,113,113	1.79	12 (15%)
19	CLA	A	824	-	65,73,73	1.35	6 (9%)	76,113,113	1.71	11 (14%)
19	CLA	B	818	-	60,68,73	1.40	7 (11%)	70,107,113	1.83	12 (17%)
24	BCR	4	317	-	41,41,41	0.13	0	56,56,56	0.32	0
20	LUT	2	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)
19	CLA	A	840	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	9 (11%)
23	LMT	2	318	-	36,36,36	0.11	0	47,47,47	0.13	0
19	CLA	A	820	-	45,53,73	1.58	7 (15%)	52,89,113	1.92	7 (13%)
19	CLA	A	817	-	65,73,73	1.35	7 (10%)	76,113,113	1.65	11 (14%)
19	CLA	1	314	1	45,53,73	1.56	7 (15%)	52,89,113	1.93	8 (15%)
20	LUT	1	319	-	42,43,43	1.65	8 (19%)	51,60,60	1.63	10 (19%)
19	CLA	A	806	5	65,73,73	1.34	7 (10%)	76,113,113	1.64	12 (15%)
19	CLA	B	807	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	B	815	-	55,63,73	1.46	7 (12%)	64,101,113	1.86	9 (14%)
24	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.30	0
19	CLA	A	839	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	11 (14%)
18	CHL	2	314	2	43,51,74	1.66	9 (20%)	45,86,114	1.94	9 (20%)
19	CLA	4	313	-	45,53,73	1.57	7 (15%)	52,89,113	1.84	8 (15%)
19	CLA	B	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.68	10 (13%)
24	BCR	L	303	-	41,41,41	0.16	0	56,56,56	0.31	0
24	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.29	0
19	CLA	A	838	-	65,73,73	1.34	7 (10%)	76,113,113	1.79	13 (17%)
19	CLA	1	308	1	57,65,73	1.42	7 (12%)	66,103,113	2.01	11 (16%)
18	CHL	2	306	-	46,54,74	1.74	9 (19%)	49,90,114	2.20	11 (22%)
19	CLA	4	301	4	46,54,73	1.54	7 (15%)	53,90,113	1.96	9 (16%)
19	CLA	K	201	-	45,53,73	1.57	7 (15%)	52,89,113	1.90	8 (15%)
19	CLA	B	836	-	65,73,73	1.33	7 (10%)	76,113,113	1.72	9 (11%)
21	XAT	2	316	-	39,47,47	0.14	0	54,74,74	0.75	2 (3%)
19	CLA	1	311	1	50,58,73	1.53	7 (14%)	58,95,113	1.91	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	311	-	45,53,73	1.59	7 (15%)	52,89,113	1.99	8 (15%)
19	CLA	B	809	6	65,73,73	1.36	7 (10%)	76,113,113	1.72	11 (14%)
19	CLA	3	304	-	47,55,73	1.52	7 (14%)	54,91,113	1.95	10 (18%)
19	CLA	1	305	-	42,50,73	1.58	7 (16%)	48,85,113	1.92	7 (14%)
19	CLA	A	837	-	65,73,73	1.32	7 (10%)	76,113,113	1.72	13 (17%)
19	CLA	B	821	-	50,58,73	1.52	7 (14%)	58,95,113	1.88	9 (15%)
20	LUT	1	315	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	11 (21%)
22	LHG	B	850	19	48,48,48	0.30	0	51,54,54	0.28	0
24	BCR	A	848	-	41,41,41	0.13	0	56,56,56	0.20	0
24	BCR	3	317	-	41,41,41	0.11	0	56,56,56	0.28	0
19	CLA	B	802	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	11 (14%)
19	CLA	1	313	-	45,53,73	1.56	7 (15%)	52,89,113	1.88	7 (13%)
19	CLA	1	312	-	60,68,73	1.40	7 (11%)	70,107,113	1.81	12 (17%)
19	CLA	B	831	-	60,68,73	1.40	7 (11%)	70,107,113	1.74	11 (15%)
19	CLA	F	302	-	45,53,73	1.57	7 (15%)	52,89,113	1.97	8 (15%)
19	CLA	B	828	-	65,73,73	1.35	7 (10%)	76,113,113	1.71	11 (14%)
19	CLA	A	818	-	45,53,73	1.55	7 (15%)	52,89,113	1.91	6 (11%)
19	CLA	A	853	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	8 (10%)
19	CLA	2	310	22	41,49,73	1.61	7 (17%)	47,84,113	2.01	9 (19%)
19	CLA	3	308	3	65,73,73	1.35	7 (10%)	76,113,113	1.71	10 (13%)
19	CLA	A	833	-	65,73,73	1.34	7 (10%)	76,113,113	1.61	11 (14%)
19	CLA	2	309	2	60,68,73	1.40	7 (11%)	70,107,113	1.76	10 (14%)
19	CLA	4	302	4	60,68,73	1.41	7 (11%)	70,107,113	1.81	10 (14%)
19	CLA	4	303	-	60,68,73	1.40	7 (11%)	70,107,113	1.84	12 (17%)
19	CLA	K	202	-	46,54,73	1.57	7 (15%)	53,90,113	1.94	7 (13%)
19	CLA	B	827	-	60,68,73	1.39	7 (11%)	70,107,113	1.70	11 (15%)
19	CLA	4	304	-	45,53,73	1.58	7 (15%)	52,89,113	1.95	6 (11%)
19	CLA	3	301	3	60,68,73	1.41	7 (11%)	70,107,113	1.75	13 (18%)
19	CLA	B	810	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	9 (11%)
19	CLA	B	835	-	55,63,73	1.47	7 (12%)	64,101,113	1.84	7 (10%)
20	LUT	3	315	-	42,43,43	1.64	8 (19%)	51,60,60	1.63	12 (23%)
24	BCR	I	101	-	41,41,41	0.13	0	56,56,56	0.22	0
24	BCR	A	843	-	41,41,41	0.14	0	56,56,56	0.43	0
19	CLA	B	803	-	65,73,73	1.34	6 (9%)	76,113,113	1.74	11 (14%)
18	CHL	2	307	-	46,54,74	1.74	10 (21%)	49,90,114	2.17	9 (18%)
19	CLA	A	819	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	805	-	65,73,73	1.35	7 (10%)	76,113,113	1.79	10 (13%)
19	CLA	A	816	-	55,63,73	1.45	7 (12%)	64,101,113	1.82	8 (12%)
19	CLA	B	832	-	58,66,73	1.40	7 (12%)	67,104,113	1.80	7 (10%)
19	CLA	L	302	-	50,58,73	1.53	7 (14%)	58,95,113	1.79	9 (15%)
19	CLA	B	825	-	55,63,73	1.47	7 (12%)	64,101,113	1.84	11 (17%)
19	CLA	2	312	-	65,73,73	1.34	7 (10%)	76,113,113	1.74	8 (10%)
25	LMG	4	318	-	36,36,55	0.20	0	44,44,63	0.19	0
19	CLA	B	851	-	65,73,73	1.33	7 (10%)	76,113,113	1.77	12 (15%)
26	PQN	A	841	-	34,34,34	0.26	0	42,45,45	0.50	1 (2%)
19	CLA	B	822	-	55,63,73	1.45	7 (12%)	64,101,113	1.77	10 (15%)
19	CLA	1	310	22	55,63,73	1.47	7 (12%)	64,101,113	1.91	10 (15%)
19	CLA	2	304	-	45,53,73	1.58	7 (15%)	52,89,113	2.03	10 (19%)
24	BCR	A	846	-	41,41,41	0.11	0	56,56,56	0.19	0
19	CLA	A	821	-	51,59,73	1.50	7 (13%)	59,96,113	1.91	9 (15%)
19	CLA	A	831	-	65,73,73	1.35	7 (10%)	76,113,113	1.64	11 (14%)
19	CLA	B	826	-	65,73,73	1.35	7 (10%)	76,113,113	1.81	11 (14%)
19	CLA	B	823	-	55,63,73	1.46	7 (12%)	64,101,113	1.71	10 (15%)
19	CLA	G	203	-	50,58,73	1.54	7 (14%)	58,95,113	1.93	9 (15%)
19	CLA	A	854	-	65,73,73	1.33	7 (10%)	76,113,113	1.78	13 (17%)
19	CLA	4	310	-	60,68,73	1.40	7 (11%)	70,107,113	1.69	11 (15%)
19	CLA	H	201	12	45,53,73	1.56	7 (15%)	52,89,113	1.84	9 (17%)
19	CLA	3	302	-	60,68,73	1.40	7 (11%)	70,107,113	1.78	10 (14%)
19	CLA	1	304	-	51,59,73	1.51	7 (13%)	59,96,113	1.96	11 (18%)
19	CLA	3	303	-	45,53,73	1.57	7 (15%)	52,89,113	1.91	10 (19%)
19	CLA	L	301	-	65,73,73	1.35	7 (10%)	76,113,113	1.66	10 (13%)
26	PQN	B	841	-	34,34,34	0.26	0	42,45,45	0.51	1 (2%)
24	BCR	F	304	-	41,41,41	0.14	0	56,56,56	0.34	0
23	LMT	A	851	-	36,36,36	0.10	0	47,47,47	0.26	0
19	CLA	B	829	-	65,73,73	1.36	7 (10%)	76,113,113	1.77	11 (14%)
18	CHL	4	314	4	41,50,74	1.69	8 (19%)	42,85,114	2.14	8 (19%)
25	LMG	F	305	-	30,30,55	0.21	0	38,38,63	0.15	0
19	CLA	B	804	-	45,53,73	1.58	7 (15%)	52,89,113	1.93	8 (15%)
19	CLA	A	810	-	54,62,73	1.46	7 (12%)	62,99,113	1.84	10 (16%)
19	CLA	A	835	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	10 (13%)
19	CLA	3	310	-	41,49,73	1.60	7 (17%)	47,84,113	2.03	9 (19%)
24	BCR	G	201	-	41,41,41	0.13	0	56,56,56	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	303	-	58,66,73	1.42	7 (12%)	67,104,113	1.82	11 (16%)
19	CLA	3	309	3	50,58,73	1.52	7 (14%)	58,95,113	1.86	11 (18%)
19	CLA	A	813	-	50,58,73	1.53	7 (14%)	58,95,113	1.87	7 (12%)
24	BCR	F	303	-	41,41,41	0.11	0	56,56,56	0.27	0
21	XAT	1	316	-	39,47,47	0.11	0	54,74,74	0.87	3 (5%)
19	CLA	A	805	-	50,58,73	1.53	7 (14%)	58,95,113	1.89	10 (17%)
18	CHL	4	306	-	46,54,74	1.74	10 (21%)	49,90,114	2.09	11 (22%)
19	CLA	A	834	-	51,59,73	1.51	7 (13%)	59,96,113	1.99	8 (13%)
18	CHL	4	305	-	56,64,74	1.61	9 (16%)	61,102,114	2.00	11 (18%)
18	CHL	2	301	2	51,59,74	1.67	10 (19%)	55,96,114	2.11	13 (23%)
19	CLA	2	308	2	45,53,73	1.57	7 (15%)	52,89,113	1.90	7 (13%)
19	CLA	3	306	3	45,53,73	1.57	7 (15%)	52,89,113	1.88	8 (15%)
19	CLA	B	838	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	11 (14%)
24	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.33	0
24	BCR	L	305	-	41,41,41	0.15	0	56,56,56	0.43	0
19	CLA	A	836	-	52,60,73	1.51	7 (13%)	60,97,113	1.84	8 (13%)
19	CLA	K	203	16	38,45,73	1.69	7 (18%)	43,78,113	2.07	8 (18%)
19	CLA	A	809	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	A	830	-	65,73,73	1.35	7 (10%)	76,113,113	1.74	12 (15%)
19	CLA	2	311	2	45,53,73	1.57	7 (15%)	52,89,113	1.98	8 (15%)
19	CLA	J	102	14	42,50,73	1.58	7 (16%)	48,85,113	1.83	8 (16%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
19	CLA	A	815	-	63,72,73	1.36	7 (11%)	73,112,113	1.63	9 (12%)
19	CLA	B	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.65	9 (11%)
19	CLA	B	817	-	59,67,73	1.40	7 (11%)	68,105,113	1.69	10 (14%)
24	BCR	2	319	-	41,41,41	0.19	0	56,56,56	0.77	3 (5%)
19	CLA	A	804	5	65,73,73	1.33	7 (10%)	76,113,113	1.70	14 (18%)
19	CLA	G	202	-	41,49,73	1.63	7 (17%)	47,84,113	1.93	9 (19%)
19	CLA	A	828	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
24	BCR	A	845	-	41,41,41	0.12	0	56,56,56	0.22	0
19	CLA	A	802	-	50,58,73	1.53	7 (14%)	58,95,113	1.89	8 (13%)
19	CLA	4	311	4	45,53,73	1.58	7 (15%)	52,89,113	1.97	7 (13%)
19	CLA	1	302	1	60,68,73	1.39	7 (11%)	70,107,113	1.77	11 (15%)
19	CLA	3	305	-	42,50,73	1.59	7 (16%)	48,85,113	1.90	7 (14%)
18	CHL	1	301	1	56,64,74	1.59	10 (17%)	61,102,114	2.05	15 (24%)
24	BCR	B	842	-	41,41,41	0.13	0	56,56,56	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	313	-	43,51,73	1.56	7 (16%)	49,86,113	1.96	6 (12%)
19	CLA	A	823	-	65,73,73	1.34	7 (10%)	76,113,113	1.63	11 (14%)
27	SF4	A	850	6,5	0,12,12	-	-	-		
19	CLA	1	318	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	B	813	-	65,73,73	1.33	7 (10%)	76,113,113	1.75	12 (15%)
19	CLA	B	814	-	65,73,73	1.34	7 (10%)	76,113,113	1.74	11 (14%)
21	XAT	3	316	-	39,47,47	0.11	0	54,74,74	0.93	4 (7%)
19	CLA	B	834	-	45,53,73	1.58	7 (15%)	52,89,113	1.95	5 (9%)
19	CLA	B	830	-	50,58,73	1.55	7 (14%)	58,95,113	1.78	9 (15%)
28	DGD	B	848	-	67,67,67	0.16	0	81,81,81	0.15	0
24	BCR	A	844	-	41,41,41	0.24	0	56,56,56	0.76	2 (3%)
18	CHL	2	305	-	43,51,74	1.66	8 (18%)	45,86,114	2.13	10 (22%)
19	CLA	A	803	-	65,73,73	1.34	7 (10%)	76,113,113	1.82	11 (14%)
19	CLA	H	202	15	55,63,73	1.46	7 (12%)	64,101,113	1.73	10 (15%)
19	CLA	4	308	4	50,58,73	1.53	7 (14%)	58,95,113	1.91	7 (12%)
19	CLA	B	837	-	47,55,73	1.53	7 (14%)	54,91,113	1.91	8 (14%)
24	BCR	J	104	-	41,41,41	0.13	0	56,56,56	0.27	0
24	BCR	J	103	-	41,41,41	0.13	0	56,56,56	0.23	0
27	SF4	C	101	7	0,12,12	-	-	-		
24	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.33	0
19	CLA	2	303	-	50,58,73	1.53	7 (14%)	58,95,113	1.85	9 (15%)
19	CLA	1	309	1	60,68,73	1.39	7 (11%)	70,107,113	1.78	11 (15%)
19	CLA	4	312	-	56,64,73	1.45	7 (12%)	65,102,113	1.77	9 (13%)
19	CLA	A	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.74	13 (17%)
22	LHG	A	842	-	48,48,48	0.29	0	51,54,54	0.28	0
19	CLA	B	812	-	55,63,73	1.46	7 (12%)	64,101,113	1.85	9 (14%)
24	BCR	A	847	-	41,41,41	0.13	0	56,56,56	0.56	1 (1%)
19	CLA	4	309	4	60,68,73	1.38	7 (11%)	70,107,113	1.80	12 (17%)
19	CLA	A	852	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	11 (14%)
19	CLA	B	808	-	65,73,73	1.33	7 (10%)	76,113,113	1.72	11 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LUT	4	315	-	-	0/29/67/67	0/2/2/2
24	BCR	B	844	-	-	6/29/63/63	0/2/2/2
19	CLA	B	840	22	1/1/15/20	16/37/115/115	-
19	CLA	B	833	-	1/1/13/20	12/27/105/115	-
19	CLA	B	820	-	1/1/11/20	2/13/91/115	-
19	CLA	A	826	-	1/1/15/20	22/37/115/115	-
25	LMG	B	849	-	-	11/47/67/70	0/1/1/1
19	CLA	A	829	-	1/1/15/20	18/37/115/115	-
18	CHL	4	307	-	3/3/17/26	9/21/119/137	-
19	CLA	B	806	-	1/1/15/20	16/37/115/115	-
22	LHG	1	320	-	-	17/53/53/53	-
19	CLA	B	839	-	1/1/15/20	12/37/115/115	-
19	CLA	B	816	-	1/1/13/20	9/25/103/115	-
19	CLA	B	811	-	1/1/13/20	10/25/101/115	-
19	CLA	2	302	2	1/1/15/20	14/37/115/115	-
19	CLA	3	314	-	1/1/11/20	8/15/93/115	-
22	LHG	2	317	19	-	11/41/41/53	-
19	CLA	A	807	5	1/1/14/20	16/34/112/115	-
19	CLA	A	832	-	1/1/11/20	3/13/91/115	-
19	CLA	A	825	-	1/1/15/20	10/37/115/115	-
19	CLA	A	827	-	1/1/15/20	15/37/115/115	-
19	CLA	B	819	-	1/1/14/20	16/31/109/115	-
19	CLA	3	312	-	1/1/13/20	7/25/103/115	-
19	CLA	A	814	-	1/1/11/20	4/13/91/115	-
19	CLA	A	822	-	1/1/13/20	9/25/103/115	-
24	BCR	J	101	-	-	13/29/63/63	0/2/2/2
19	CLA	F	301	-	1/1/11/20	6/13/91/115	-
22	LHG	1	317	19	-	9/53/53/53	-
24	BCR	B	845	-	-	0/29/63/63	0/2/2/2
19	CLA	G	204	11	1/1/11/20	7/15/93/115	-
19	CLA	3	313	-	1/1/11/20	5/13/91/115	-
19	CLA	1	307	-	1/1/11/20	2/13/91/115	-
21	XAT	4	316	-	-	0/31/93/93	0/4/4/4
18	CHL	1	306	1	2/2/16/26	4/15/113/137	-
19	CLA	A	812	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	808	-	1/1/13/20	14/30/108/115	-
24	BCR	G	205	-	-	1/29/63/63	0/2/2/2
24	BCR	L	304	-	-	1/29/63/63	0/2/2/2
18	CHL	3	307	-	3/3/16/26	4/17/115/137	-
19	CLA	A	811	-	1/1/15/20	23/37/115/115	-
19	CLA	A	824	-	1/1/15/20	8/37/115/115	-
19	CLA	B	818	-	1/1/14/20	16/31/109/115	-
24	BCR	4	317	-	-	2/29/63/63	0/2/2/2
20	LUT	2	315	-	-	1/29/67/67	0/2/2/2
19	CLA	A	840	-	1/1/15/20	17/37/115/115	-
23	LMT	2	318	-	-	4/21/61/61	0/2/2/2
19	CLA	A	820	-	1/1/11/20	6/13/91/115	-
19	CLA	A	817	-	1/1/15/20	11/37/115/115	-
19	CLA	1	314	1	1/1/11/20	8/13/91/115	-
20	LUT	1	319	-	-	2/29/67/67	0/2/2/2
19	CLA	A	806	5	1/1/15/20	18/37/115/115	-
19	CLA	B	807	-	1/1/15/20	14/37/115/115	-
19	CLA	B	815	-	1/1/13/20	10/25/103/115	-
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
19	CLA	A	839	-	1/1/15/20	20/37/115/115	-
18	CHL	2	314	2	2/2/15/26	2/12/110/137	-
19	CLA	4	313	-	1/1/11/20	4/13/91/115	-
19	CLA	B	824	-	1/1/15/20	15/37/115/115	-
24	BCR	L	303	-	-	4/29/63/63	0/2/2/2
24	BCR	B	843	-	-	4/29/63/63	0/2/2/2
19	CLA	A	838	-	1/1/15/20	18/37/115/115	-
19	CLA	1	308	1	1/1/13/20	12/28/106/115	-
18	CHL	2	306	-	3/3/16/26	6/15/113/137	-
19	CLA	4	301	4	1/1/11/20	6/15/93/115	-
19	CLA	K	201	-	1/1/11/20	5/13/91/115	-
19	CLA	B	836	-	1/1/15/20	16/37/115/115	-
21	XAT	2	316	-	-	3/31/93/93	0/4/4/4
19	CLA	1	311	1	1/1/12/20	8/19/97/115	-
19	CLA	3	311	-	1/1/11/20	7/13/91/115	-
19	CLA	B	809	6	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	304	-	1/1/11/20	6/16/94/115	-
19	CLA	1	305	-	1/1/10/20	4/10/88/115	-
19	CLA	A	837	-	1/1/15/20	16/37/115/115	-
19	CLA	B	821	-	1/1/12/20	11/19/97/115	-
20	LUT	1	315	-	-	0/29/67/67	0/2/2/2
22	LHG	B	850	19	-	8/53/53/53	-
24	BCR	A	848	-	-	0/29/63/63	0/2/2/2
24	BCR	3	317	-	-	0/29/63/63	0/2/2/2
19	CLA	B	802	-	1/1/15/20	17/37/115/115	-
19	CLA	1	313	-	1/1/11/20	5/13/91/115	-
19	CLA	1	312	-	1/1/14/20	12/31/109/115	-
19	CLA	B	831	-	1/1/14/20	16/31/109/115	-
19	CLA	F	302	-	1/1/11/20	6/13/91/115	-
19	CLA	B	828	-	1/1/15/20	17/37/115/115	-
19	CLA	A	818	-	1/1/11/20	0/13/91/115	-
19	CLA	A	853	-	1/1/15/20	23/37/115/115	-
19	CLA	2	310	22	1/1/10/20	3/8/86/115	-
19	CLA	3	308	3	1/1/15/20	14/37/115/115	-
19	CLA	A	833	-	1/1/15/20	20/37/115/115	-
19	CLA	2	309	2	1/1/14/20	11/31/109/115	-
19	CLA	4	302	4	1/1/14/20	6/31/109/115	-
19	CLA	4	303	-	1/1/14/20	17/31/109/115	-
19	CLA	K	202	-	1/1/11/20	7/15/93/115	-
19	CLA	B	827	-	1/1/14/20	12/31/109/115	-
19	CLA	4	304	-	1/1/11/20	4/13/91/115	-
19	CLA	3	301	3	1/1/14/20	12/31/109/115	-
19	CLA	B	810	-	1/1/15/20	22/37/115/115	-
19	CLA	B	835	-	1/1/13/20	7/25/103/115	-
20	LUT	3	315	-	-	0/29/67/67	0/2/2/2
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
24	BCR	A	843	-	-	8/29/63/63	0/2/2/2
19	CLA	B	803	-	1/1/15/20	14/37/115/115	-
18	CHL	2	307	-	3/3/16/26	6/15/113/137	-
19	CLA	A	819	-	1/1/15/20	10/37/115/115	-
19	CLA	B	805	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	816	-	1/1/13/20	9/25/103/115	-
19	CLA	B	832	-	1/1/13/20	14/29/107/115	-
19	CLA	L	302	-	1/1/12/20	11/19/97/115	-
19	CLA	B	825	-	1/1/13/20	7/25/103/115	-
19	CLA	2	312	-	1/1/15/20	19/37/115/115	-
25	LMG	4	318	-	-	5/31/51/70	0/1/1/1
19	CLA	B	851	-	1/1/15/20	18/37/115/115	-
26	PQN	A	841	-	-	5/23/43/43	0/2/2/2
19	CLA	B	822	-	1/1/13/20	9/25/103/115	-
19	CLA	1	310	22	1/1/13/20	9/25/103/115	-
19	CLA	2	304	-	1/1/11/20	4/13/91/115	-
24	BCR	A	846	-	-	0/29/63/63	0/2/2/2
19	CLA	A	821	-	1/1/12/20	9/21/99/115	-
19	CLA	A	831	-	1/1/15/20	21/37/115/115	-
19	CLA	B	826	-	1/1/15/20	13/37/115/115	-
19	CLA	B	823	-	1/1/13/20	8/25/103/115	-
19	CLA	G	203	-	1/1/12/20	8/19/97/115	-
19	CLA	A	854	-	1/1/15/20	15/37/115/115	-
19	CLA	4	310	-	1/1/14/20	15/31/109/115	-
19	CLA	H	201	12	1/1/11/20	7/13/91/115	-
19	CLA	3	302	-	1/1/14/20	14/31/109/115	-
19	CLA	1	304	-	1/1/12/20	11/21/99/115	-
19	CLA	3	303	-	1/1/11/20	6/13/91/115	-
19	CLA	L	301	-	1/1/15/20	14/37/115/115	-
26	PQN	B	841	-	-	6/23/43/43	0/2/2/2
24	BCR	F	304	-	-	0/29/63/63	0/2/2/2
23	LMT	A	851	-	-	4/21/61/61	0/2/2/2
19	CLA	B	829	-	1/1/15/20	11/37/115/115	-
18	CHL	4	314	4	3/3/15/26	0/10/108/137	-
25	LMG	F	305	-	-	1/25/45/70	0/1/1/1
19	CLA	B	804	-	1/1/11/20	7/13/91/115	-
19	CLA	A	810	-	1/1/12/20	9/24/102/115	-
19	CLA	A	835	-	1/1/15/20	21/37/115/115	-
19	CLA	3	310	-	1/1/10/20	3/8/86/115	-
24	BCR	G	201	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	303	-	1/1/13/20	9/29/107/115	-
19	CLA	3	309	3	1/1/12/20	6/19/97/115	-
19	CLA	A	813	-	1/1/12/20	8/19/97/115	-
24	BCR	F	303	-	-	2/29/63/63	0/2/2/2
21	XAT	1	316	-	-	0/31/93/93	0/4/4/4
19	CLA	A	805	-	1/1/12/20	3/19/97/115	-
18	CHL	4	306	-	3/3/16/26	6/15/113/137	-
19	CLA	A	834	-	1/1/12/20	10/21/99/115	-
18	CHL	4	305	-	3/3/18/26	11/27/125/137	-
18	CHL	2	301	2	3/3/17/26	9/21/119/137	-
19	CLA	2	308	2	1/1/11/20	3/13/91/115	-
19	CLA	3	306	3	1/1/11/20	5/13/91/115	-
19	CLA	B	838	-	1/1/15/20	18/37/115/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
24	BCR	L	305	-	-	3/29/63/63	0/2/2/2
19	CLA	A	836	-	1/1/12/20	7/22/100/115	-
19	CLA	K	203	16	1/1/8/20	0/2/76/115	-
19	CLA	A	809	-	1/1/15/20	9/37/115/115	-
19	CLA	A	830	-	1/1/15/20	19/37/115/115	-
19	CLA	2	311	2	1/1/11/20	5/13/91/115	-
19	CLA	J	102	14	1/1/10/20	5/10/88/115	-
27	SF4	C	102	7	-	-	0/6/5/5
19	CLA	A	815	-	1/1/15/20	22/35/113/115	-
19	CLA	B	801	-	1/1/15/20	12/37/115/115	-
19	CLA	B	817	-	1/1/13/20	13/30/108/115	-
24	BCR	2	319	-	-	15/29/63/63	0/2/2/2
19	CLA	A	804	5	1/1/15/20	14/37/115/115	-
19	CLA	G	202	-	1/1/10/20	4/8/86/115	-
19	CLA	A	828	-	1/1/15/20	16/37/115/115	-
24	BCR	A	845	-	-	2/29/63/63	0/2/2/2
19	CLA	A	802	-	1/1/12/20	9/19/97/115	-
19	CLA	4	311	4	1/1/11/20	3/13/91/115	-
19	CLA	1	302	1	1/1/14/20	9/31/109/115	-
19	CLA	3	305	-	1/1/10/20	2/10/88/115	-
18	CHL	1	301	1	3/3/18/26	11/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
19	CLA	2	313	-	1/1/10/20	0/11/89/115	-
19	CLA	A	823	-	1/1/15/20	19/37/115/115	-
27	SF4	A	850	6,5	-	-	0/6/5/5
19	CLA	1	318	-	1/1/15/20	19/37/115/115	-
19	CLA	B	813	-	1/1/15/20	20/37/115/115	-
19	CLA	B	814	-	1/1/15/20	20/37/115/115	-
21	XAT	3	316	-	-	1/31/93/93	0/4/4/4
19	CLA	B	834	-	1/1/11/20	9/13/91/115	-
19	CLA	B	830	-	1/1/12/20	7/19/97/115	-
28	DGD	B	848	-	-	12/55/95/95	0/2/2/2
24	BCR	A	844	-	-	1/29/63/63	0/2/2/2
18	CHL	2	305	-	3/3/15/26	5/12/110/137	-
19	CLA	A	803	-	1/1/15/20	14/37/115/115	-
19	CLA	H	202	15	1/1/13/20	11/25/103/115	-
19	CLA	4	308	4	1/1/12/20	8/19/97/115	-
19	CLA	B	837	-	1/1/11/20	2/16/94/115	-
24	BCR	J	104	-	-	4/29/63/63	0/2/2/2
24	BCR	J	103	-	-	2/29/63/63	0/2/2/2
27	SF4	C	101	7	-	-	0/6/5/5
24	BCR	A	849	-	-	4/29/63/63	0/2/2/2
19	CLA	2	303	-	1/1/12/20	7/19/97/115	-
19	CLA	1	309	1	1/1/14/20	9/31/109/115	-
19	CLA	4	312	-	1/1/13/20	8/27/105/115	-
19	CLA	A	801	-	1/1/15/20	18/37/115/115	-
22	LHG	A	842	-	-	5/53/53/53	-
19	CLA	B	812	-	1/1/13/20	11/25/103/115	-
24	BCR	A	847	-	-	4/29/63/63	0/2/2/2
19	CLA	4	309	4	1/1/14/20	6/31/109/115	-
19	CLA	A	852	-	1/1/15/20	11/37/115/115	-
19	CLA	B	808	-	1/1/15/20	12/37/115/115	-

All (1145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	305	CHL	CMC-C2C	5.43	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	305	CHL	CMC-C2C	5.41	1.56	1.45
18	4	306	CHL	CMC-C2C	5.41	1.56	1.45
18	1	306	CHL	CMC-C2C	5.41	1.56	1.45
18	2	301	CHL	CMC-C2C	5.39	1.56	1.45
18	2	314	CHL	CMC-C2C	5.39	1.56	1.45
18	4	314	CHL	CMC-C2C	5.38	1.56	1.45
18	2	306	CHL	CMC-C2C	5.36	1.56	1.45
18	2	307	CHL	CMC-C2C	5.34	1.56	1.45
18	3	307	CHL	CMC-C2C	5.34	1.56	1.45
18	1	301	CHL	CMC-C2C	5.29	1.56	1.45
18	4	307	CHL	CMC-C2C	5.29	1.56	1.45
19	A	832	CLA	MG-NA	5.07	2.18	2.06
19	K	202	CLA	MG-NA	5.05	2.18	2.06
19	3	311	CLA	MG-NA	5.03	2.18	2.06
19	4	311	CLA	MG-NA	5.02	2.18	2.06
19	F	302	CLA	MG-NA	5.02	2.18	2.06
19	F	301	CLA	MG-NA	5.02	2.18	2.06
19	A	820	CLA	MG-NA	5.02	2.18	2.06
19	1	304	CLA	MG-NA	5.02	2.18	2.06
19	G	202	CLA	MG-NA	5.01	2.18	2.06
19	A	821	CLA	MG-NA	5.01	2.18	2.06
19	2	304	CLA	MG-NA	5.01	2.18	2.06
19	H	201	CLA	MG-NA	5.01	2.18	2.06
19	B	840	CLA	MG-NA	5.00	2.18	2.06
19	B	835	CLA	MG-NA	5.00	2.18	2.06
19	B	829	CLA	MG-NA	4.99	2.18	2.06
19	3	312	CLA	MG-NA	4.99	2.18	2.06
19	3	305	CLA	MG-NA	4.99	2.18	2.06
19	B	830	CLA	MG-NA	4.98	2.18	2.06
19	B	809	CLA	MG-NA	4.98	2.18	2.06
19	4	312	CLA	MG-NA	4.98	2.18	2.06
19	4	304	CLA	MG-NA	4.98	2.18	2.06
19	A	834	CLA	MG-NA	4.98	2.18	2.06
19	A	830	CLA	MG-NA	4.98	2.18	2.06
19	G	203	CLA	MG-NA	4.97	2.18	2.06
19	2	310	CLA	MG-NA	4.97	2.18	2.06
19	B	807	CLA	MG-NA	4.97	2.18	2.06
19	B	851	CLA	MG-NA	4.97	2.18	2.06
19	1	312	CLA	MG-NA	4.96	2.18	2.06
19	A	836	CLA	MG-NA	4.96	2.18	2.06
19	A	828	CLA	MG-NA	4.96	2.18	2.06
19	1	303	CLA	MG-NA	4.96	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	833	CLA	MG-NA	4.96	2.18	2.06
19	K	201	CLA	MG-NA	4.96	2.18	2.06
19	A	814	CLA	MG-NA	4.96	2.18	2.06
19	H	202	CLA	MG-NA	4.96	2.18	2.06
19	A	853	CLA	MG-NA	4.96	2.18	2.06
19	B	811	CLA	MG-NA	4.96	2.18	2.06
19	A	823	CLA	MG-NA	4.96	2.18	2.06
19	4	308	CLA	MG-NA	4.96	2.18	2.06
19	A	840	CLA	MG-NA	4.96	2.18	2.06
19	1	310	CLA	MG-NA	4.96	2.18	2.06
19	2	303	CLA	MG-NA	4.95	2.18	2.06
19	B	805	CLA	MG-NA	4.95	2.18	2.06
19	4	313	CLA	MG-NA	4.95	2.18	2.06
19	1	307	CLA	MG-NA	4.95	2.18	2.06
19	B	806	CLA	MG-NA	4.95	2.18	2.06
19	B	834	CLA	MG-NA	4.95	2.18	2.06
19	3	301	CLA	MG-NA	4.95	2.18	2.06
19	A	827	CLA	MG-NA	4.95	2.18	2.06
19	B	813	CLA	MG-NA	4.95	2.18	2.06
19	B	810	CLA	MG-NA	4.95	2.18	2.06
19	A	838	CLA	MG-NA	4.95	2.18	2.06
19	3	302	CLA	MG-NA	4.94	2.18	2.06
19	1	314	CLA	MG-NA	4.94	2.18	2.06
19	4	310	CLA	MG-NA	4.94	2.18	2.06
19	B	803	CLA	MG-NA	4.94	2.18	2.06
19	B	804	CLA	MG-NA	4.94	2.18	2.06
19	B	821	CLA	MG-NA	4.94	2.18	2.06
19	4	303	CLA	MG-NA	4.94	2.18	2.06
19	3	303	CLA	MG-NA	4.94	2.18	2.06
19	B	812	CLA	MG-NA	4.94	2.18	2.06
19	G	204	CLA	MG-NA	4.94	2.18	2.06
19	2	312	CLA	MG-NA	4.94	2.18	2.06
19	A	829	CLA	MG-NA	4.94	2.18	2.06
19	3	304	CLA	MG-NA	4.94	2.18	2.06
19	2	311	CLA	MG-NA	4.93	2.18	2.06
19	B	838	CLA	MG-NA	4.93	2.18	2.06
19	A	816	CLA	MG-NA	4.93	2.18	2.06
19	1	311	CLA	MG-NA	4.93	2.18	2.06
19	B	826	CLA	MG-NA	4.93	2.18	2.06
19	A	813	CLA	MG-NA	4.93	2.18	2.06
19	1	318	CLA	MG-NA	4.93	2.18	2.06
19	B	815	CLA	MG-NA	4.93	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	831	CLA	MG-NA	4.93	2.18	2.06
19	3	313	CLA	MG-NA	4.92	2.18	2.06
19	1	302	CLA	MG-NA	4.92	2.18	2.06
19	A	809	CLA	MG-NA	4.92	2.17	2.06
19	A	811	CLA	MG-NA	4.92	2.17	2.06
19	4	301	CLA	MG-NA	4.91	2.17	2.06
19	A	819	CLA	MG-NA	4.91	2.17	2.06
19	A	812	CLA	MG-NA	4.91	2.17	2.06
19	4	302	CLA	MG-NA	4.91	2.17	2.06
19	A	804	CLA	MG-NA	4.91	2.17	2.06
19	B	837	CLA	MG-NA	4.91	2.17	2.06
19	A	805	CLA	MG-NA	4.91	2.17	2.06
19	B	814	CLA	MG-NA	4.91	2.17	2.06
19	A	835	CLA	MG-NA	4.90	2.17	2.06
19	A	817	CLA	MG-NA	4.90	2.17	2.06
19	L	302	CLA	MG-NA	4.90	2.17	2.06
19	2	313	CLA	MG-NA	4.90	2.17	2.06
19	3	306	CLA	MG-NA	4.90	2.17	2.06
19	J	102	CLA	MG-NA	4.90	2.17	2.06
19	2	302	CLA	MG-NA	4.90	2.17	2.06
19	3	314	CLA	MG-NA	4.90	2.17	2.06
19	A	839	CLA	MG-NA	4.90	2.17	2.06
19	B	816	CLA	MG-NA	4.90	2.17	2.06
19	A	815	CLA	MG-NA	4.90	2.17	2.06
19	A	825	CLA	MG-NA	4.90	2.17	2.06
19	B	822	CLA	MG-NA	4.90	2.17	2.06
19	A	822	CLA	MG-NA	4.90	2.17	2.06
19	A	808	CLA	MG-NA	4.89	2.17	2.06
19	3	308	CLA	MG-NA	4.89	2.17	2.06
19	B	808	CLA	MG-NA	4.89	2.17	2.06
19	1	305	CLA	MG-NA	4.89	2.17	2.06
19	A	854	CLA	MG-NA	4.89	2.17	2.06
19	B	824	CLA	MG-NA	4.89	2.17	2.06
19	1	313	CLA	MG-NA	4.89	2.17	2.06
19	2	309	CLA	MG-NA	4.88	2.17	2.06
19	B	825	CLA	MG-NA	4.88	2.17	2.06
19	3	310	CLA	MG-NA	4.88	2.17	2.06
19	A	803	CLA	MG-NA	4.88	2.17	2.06
19	B	828	CLA	MG-NA	4.88	2.17	2.06
19	A	810	CLA	MG-NA	4.88	2.17	2.06
19	2	308	CLA	MG-NA	4.87	2.17	2.06
19	B	819	CLA	MG-NA	4.87	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	802	CLA	MG-NA	4.87	2.17	2.06
19	A	801	CLA	MG-NA	4.87	2.17	2.06
19	B	827	CLA	MG-NA	4.87	2.17	2.06
19	A	833	CLA	MG-NA	4.86	2.17	2.06
19	B	818	CLA	MG-NA	4.86	2.17	2.06
19	B	823	CLA	MG-NA	4.86	2.17	2.06
19	A	807	CLA	MG-NA	4.86	2.17	2.06
19	B	820	CLA	MG-NA	4.86	2.17	2.06
19	3	309	CLA	MG-NA	4.85	2.17	2.06
19	B	839	CLA	MG-NA	4.85	2.17	2.06
19	B	831	CLA	MG-NA	4.85	2.17	2.06
19	B	836	CLA	MG-NA	4.85	2.17	2.06
19	L	301	CLA	MG-NA	4.84	2.17	2.06
19	A	818	CLA	MG-NA	4.84	2.17	2.06
19	A	837	CLA	MG-NA	4.84	2.17	2.06
19	A	802	CLA	MG-NA	4.84	2.17	2.06
19	B	817	CLA	MG-NA	4.82	2.17	2.06
19	1	309	CLA	MG-NA	4.82	2.17	2.06
19	B	832	CLA	MG-NA	4.82	2.17	2.06
19	K	203	CLA	MG-NA	4.81	2.17	2.06
19	A	806	CLA	MG-NA	4.81	2.17	2.06
19	4	309	CLA	MG-NA	4.79	2.17	2.06
19	A	852	CLA	MG-NA	4.79	2.17	2.06
19	A	824	CLA	MG-NA	4.79	2.17	2.06
19	B	801	CLA	MG-NA	4.79	2.17	2.06
19	1	308	CLA	MG-NA	4.79	2.17	2.06
19	A	826	CLA	MG-NA	4.77	2.17	2.06
19	3	311	CLA	C4B-NB	4.27	1.39	1.35
19	K	202	CLA	C4B-NB	4.23	1.39	1.35
19	1	304	CLA	C4B-NB	4.21	1.39	1.35
19	3	306	CLA	C4B-NB	4.21	1.39	1.35
19	G	202	CLA	C4B-NB	4.20	1.39	1.35
19	L	302	CLA	C4B-NB	4.19	1.39	1.35
19	3	305	CLA	C4B-NB	4.19	1.38	1.35
19	G	203	CLA	C4B-NB	4.19	1.38	1.35
19	B	834	CLA	C4B-NB	4.17	1.38	1.35
19	3	313	CLA	C4B-NB	4.16	1.38	1.35
19	A	809	CLA	C4B-NB	4.16	1.38	1.35
19	4	304	CLA	C4B-NB	4.16	1.38	1.35
19	1	303	CLA	C4B-NB	4.15	1.38	1.35
19	K	201	CLA	C4B-NB	4.14	1.38	1.35
19	B	809	CLA	C4B-NB	4.14	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	305	CLA	C4B-NB	4.12	1.38	1.35
19	4	311	CLA	C4B-NB	4.12	1.38	1.35
19	J	102	CLA	C4B-NB	4.12	1.38	1.35
19	1	307	CLA	C4B-NB	4.12	1.38	1.35
19	B	840	CLA	C4B-NB	4.11	1.38	1.35
19	2	311	CLA	C4B-NB	4.11	1.38	1.35
19	1	312	CLA	C4B-NB	4.10	1.38	1.35
19	A	820	CLA	C4B-NB	4.10	1.38	1.35
19	A	830	CLA	C4B-NB	4.09	1.38	1.35
19	G	204	CLA	C4B-NB	4.09	1.38	1.35
19	A	833	CLA	C4B-NB	4.09	1.38	1.35
19	1	311	CLA	C4B-NB	4.08	1.38	1.35
19	A	832	CLA	C4B-NB	4.08	1.38	1.35
19	4	313	CLA	C4B-NB	4.08	1.38	1.35
19	1	314	CLA	C4B-NB	4.08	1.38	1.35
19	A	821	CLA	C4B-NB	4.08	1.38	1.35
19	2	310	CLA	C4B-NB	4.07	1.38	1.35
19	4	312	CLA	C4B-NB	4.07	1.38	1.35
19	4	302	CLA	C4B-NB	4.07	1.38	1.35
19	A	836	CLA	C4B-NB	4.07	1.38	1.35
19	B	826	CLA	C4B-NB	4.07	1.38	1.35
19	A	817	CLA	C4B-NB	4.06	1.38	1.35
19	A	814	CLA	C4B-NB	4.06	1.38	1.35
19	A	823	CLA	C4B-NB	4.06	1.38	1.35
19	2	302	CLA	C4B-NB	4.05	1.38	1.35
19	1	313	CLA	C4B-NB	4.05	1.38	1.35
20	1	319	LUT	C34-C33	4.05	1.41	1.35
19	3	302	CLA	C4B-NB	4.05	1.38	1.35
19	1	309	CLA	C4B-NB	4.05	1.38	1.35
19	2	304	CLA	C4B-NB	4.05	1.38	1.35
19	A	829	CLA	C4B-NB	4.05	1.38	1.35
19	2	303	CLA	C4B-NB	4.05	1.38	1.35
19	F	302	CLA	C4B-NB	4.04	1.38	1.35
19	4	308	CLA	C4B-NB	4.04	1.38	1.35
19	B	804	CLA	C4B-NB	4.04	1.38	1.35
19	1	310	CLA	C4B-NB	4.04	1.38	1.35
19	F	301	CLA	C4B-NB	4.04	1.38	1.35
20	1	319	LUT	C14-C13	4.04	1.41	1.35
19	2	313	CLA	C4B-NB	4.03	1.38	1.35
19	A	801	CLA	C4B-NB	4.03	1.38	1.35
19	B	818	CLA	C4B-NB	4.03	1.38	1.35
19	2	308	CLA	C4B-NB	4.03	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	304	CLA	C4B-NB	4.03	1.38	1.35
19	3	310	CLA	C4B-NB	4.03	1.38	1.35
19	A	819	CLA	C4B-NB	4.03	1.38	1.35
19	4	310	CLA	C4B-NB	4.03	1.38	1.35
19	B	820	CLA	C4B-NB	4.03	1.38	1.35
19	3	314	CLA	C4B-NB	4.03	1.38	1.35
19	3	303	CLA	C4B-NB	4.02	1.38	1.35
19	H	202	CLA	C4B-NB	4.02	1.38	1.35
19	2	309	CLA	C4B-NB	4.02	1.38	1.35
19	A	813	CLA	C4B-NB	4.01	1.38	1.35
19	H	201	CLA	C4B-NB	4.01	1.38	1.35
19	B	835	CLA	C4B-NB	4.01	1.38	1.35
20	3	315	LUT	C34-C33	4.01	1.41	1.35
19	3	301	CLA	C4B-NB	4.01	1.38	1.35
19	B	822	CLA	C4B-NB	4.00	1.38	1.35
19	B	837	CLA	C4B-NB	4.00	1.38	1.35
19	3	312	CLA	C4B-NB	4.00	1.38	1.35
19	A	834	CLA	C4B-NB	4.00	1.38	1.35
19	B	829	CLA	C4B-NB	3.99	1.38	1.35
19	B	830	CLA	C4B-NB	3.99	1.38	1.35
19	A	826	CLA	C4B-NB	3.99	1.38	1.35
19	K	203	CLA	C4B-NB	3.99	1.38	1.35
19	A	831	CLA	C4B-NB	3.99	1.38	1.35
19	A	840	CLA	C4B-NB	3.99	1.38	1.35
19	A	822	CLA	C4B-NB	3.99	1.38	1.35
19	B	825	CLA	C4B-NB	3.99	1.38	1.35
20	1	319	LUT	C10-C9	3.98	1.41	1.35
20	1	319	LUT	C30-C29	3.98	1.41	1.35
19	A	802	CLA	C4B-NB	3.98	1.38	1.35
19	B	831	CLA	C4B-NB	3.98	1.38	1.35
19	L	301	CLA	C4B-NB	3.98	1.38	1.35
19	A	835	CLA	C4B-NB	3.97	1.38	1.35
19	A	818	CLA	C4B-NB	3.97	1.38	1.35
19	1	302	CLA	C4B-NB	3.97	1.38	1.35
19	1	318	CLA	C4B-NB	3.97	1.38	1.35
19	2	312	CLA	C4B-NB	3.97	1.38	1.35
19	B	801	CLA	C4B-NB	3.97	1.38	1.35
19	B	851	CLA	C4B-NB	3.97	1.38	1.35
20	2	315	LUT	C34-C33	3.97	1.41	1.35
19	4	303	CLA	C4B-NB	3.97	1.38	1.35
19	B	824	CLA	C4B-NB	3.97	1.38	1.35
20	3	315	LUT	C14-C13	3.96	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	315	LUT	C30-C29	3.96	1.41	1.35
19	B	814	CLA	C4B-NB	3.96	1.38	1.35
19	A	838	CLA	C4B-NB	3.96	1.38	1.35
19	B	815	CLA	C4B-NB	3.96	1.38	1.35
19	B	807	CLA	C4B-NB	3.96	1.38	1.35
19	A	839	CLA	C4B-NB	3.95	1.38	1.35
19	A	824	CLA	C4B-NB	3.95	1.38	1.35
19	A	854	CLA	C4B-NB	3.95	1.38	1.35
19	1	308	CLA	C4B-NB	3.95	1.38	1.35
20	1	315	LUT	C34-C33	3.95	1.41	1.35
19	B	806	CLA	C4B-NB	3.94	1.38	1.35
19	A	812	CLA	C4B-NB	3.94	1.38	1.35
19	B	811	CLA	C4B-NB	3.94	1.38	1.35
19	B	823	CLA	C4B-NB	3.94	1.38	1.35
19	3	308	CLA	C4B-NB	3.93	1.38	1.35
20	2	315	LUT	C14-C13	3.93	1.41	1.35
19	A	827	CLA	C4B-NB	3.93	1.38	1.35
19	B	828	CLA	C4B-NB	3.93	1.38	1.35
19	B	836	CLA	C4B-NB	3.93	1.38	1.35
20	2	315	LUT	C10-C9	3.93	1.41	1.35
19	B	817	CLA	C4B-NB	3.92	1.38	1.35
19	A	816	CLA	C4B-NB	3.92	1.38	1.35
19	B	816	CLA	C4B-NB	3.92	1.38	1.35
20	3	315	LUT	C10-C9	3.92	1.41	1.35
19	B	827	CLA	C4B-NB	3.92	1.38	1.35
19	B	802	CLA	C4B-NB	3.91	1.38	1.35
19	B	810	CLA	C4B-NB	3.91	1.38	1.35
20	2	315	LUT	C30-C29	3.91	1.41	1.35
19	A	852	CLA	C4B-NB	3.91	1.38	1.35
19	A	804	CLA	C4B-NB	3.91	1.38	1.35
19	B	821	CLA	C4B-NB	3.90	1.38	1.35
19	B	819	CLA	C4B-NB	3.90	1.38	1.35
19	A	853	CLA	C4B-NB	3.90	1.38	1.35
20	1	315	LUT	C10-C9	3.90	1.40	1.35
19	A	815	CLA	C4B-NB	3.90	1.38	1.35
19	A	810	CLA	C4B-NB	3.89	1.38	1.35
19	4	301	CLA	C4B-NB	3.88	1.38	1.35
19	B	812	CLA	C4B-NB	3.88	1.38	1.35
19	B	808	CLA	C4B-NB	3.87	1.38	1.35
19	A	828	CLA	C4B-NB	3.87	1.38	1.35
20	1	315	LUT	C14-C13	3.87	1.40	1.35
20	3	315	LUT	C30-C29	3.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	806	CLA	C4B-NB	3.87	1.38	1.35
19	B	838	CLA	C4B-NB	3.87	1.38	1.35
19	B	805	CLA	C4B-NB	3.87	1.38	1.35
19	B	839	CLA	C4B-NB	3.86	1.38	1.35
19	A	805	CLA	C4B-NB	3.86	1.38	1.35
20	4	315	LUT	C30-C29	3.86	1.40	1.35
18	2	306	CHL	C4B-NB	3.85	1.38	1.35
19	A	808	CLA	C4B-NB	3.84	1.38	1.35
19	B	833	CLA	C4B-NB	3.83	1.38	1.35
19	A	811	CLA	C4B-NB	3.83	1.38	1.35
19	B	832	CLA	C4B-NB	3.83	1.38	1.35
19	4	309	CLA	C4B-NB	3.81	1.38	1.35
19	3	309	CLA	C4B-NB	3.80	1.38	1.35
19	A	807	CLA	C4B-NB	3.80	1.38	1.35
19	A	803	CLA	C4B-NB	3.79	1.38	1.35
20	4	315	LUT	C14-C13	3.78	1.40	1.35
20	4	315	LUT	C34-C33	3.77	1.40	1.35
18	4	306	CHL	C4B-NB	3.76	1.38	1.35
19	A	837	CLA	C4B-NB	3.75	1.38	1.35
18	4	305	CHL	C4B-NB	3.75	1.38	1.35
18	4	314	CHL	C4B-NB	3.73	1.38	1.35
19	A	825	CLA	C4B-NB	3.73	1.38	1.35
18	2	307	CHL	C4B-NB	3.72	1.38	1.35
19	B	813	CLA	C4B-NB	3.71	1.38	1.35
18	2	301	CHL	C4B-NB	3.71	1.38	1.35
18	3	307	CHL	C4B-NB	3.68	1.38	1.35
18	4	307	CHL	C4B-NB	3.68	1.38	1.35
19	B	803	CLA	C4B-NB	3.65	1.38	1.35
18	2	305	CHL	C4B-NB	3.61	1.38	1.35
18	2	307	CHL	C3B-C2B	-3.60	1.35	1.40
18	2	314	CHL	C4B-NB	3.59	1.38	1.35
18	1	306	CHL	C4B-NB	3.59	1.38	1.35
20	4	315	LUT	C10-C9	3.56	1.40	1.35
18	1	301	CHL	C4B-NB	3.56	1.38	1.35
18	4	314	CHL	C3B-C2B	-3.53	1.35	1.40
18	2	306	CHL	O2D-CGD	3.50	1.41	1.33
18	2	314	CHL	O2D-CGD	3.49	1.41	1.33
18	2	305	CHL	O2D-CGD	3.47	1.41	1.33
18	2	301	CHL	C3B-C2B	-3.47	1.35	1.40
18	4	306	CHL	C3B-C2B	-3.46	1.35	1.40
18	4	307	CHL	C3B-C2B	-3.46	1.35	1.40
18	4	305	CHL	O2D-CGD	3.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	307	CHL	C3B-C2B	-3.45	1.35	1.40
18	1	306	CHL	O2D-CGD	3.43	1.41	1.33
18	4	306	CHL	O2D-CGD	3.42	1.41	1.33
18	4	305	CHL	C3B-C2B	-3.42	1.35	1.40
18	2	307	CHL	O2D-CGD	3.42	1.41	1.33
18	4	314	CHL	O2D-CGD	3.39	1.41	1.30
18	2	306	CHL	C3B-C2B	-3.38	1.35	1.40
18	3	307	CHL	O2D-CGD	3.37	1.41	1.33
18	2	301	CHL	O2D-CGD	3.37	1.41	1.33
18	4	306	CHL	O2A-CGA	3.37	1.42	1.30
18	1	301	CHL	C3B-C2B	-3.37	1.35	1.40
18	2	306	CHL	O2A-CGA	3.36	1.42	1.30
18	2	307	CHL	O2A-CGA	3.36	1.42	1.30
18	1	306	CHL	O2A-CGA	3.36	1.42	1.30
19	B	833	CLA	CHC-C1C	3.36	1.43	1.35
18	4	307	CHL	O2D-CGD	3.36	1.41	1.33
18	2	305	CHL	C3B-C2B	-3.35	1.35	1.40
18	1	301	CHL	O2D-CGD	3.35	1.41	1.33
18	1	306	CHL	C3B-C2B	-3.35	1.35	1.40
19	A	824	CLA	CHC-C1C	3.35	1.43	1.35
19	B	832	CLA	CHC-C1C	3.35	1.43	1.35
19	K	203	CLA	CHC-C1C	3.34	1.43	1.35
19	3	301	CLA	CHC-C1C	3.34	1.43	1.35
19	B	825	CLA	CHC-C1C	3.34	1.43	1.35
19	B	801	CLA	CHC-C1C	3.33	1.43	1.35
19	A	831	CLA	C3B-C2B	-3.33	1.35	1.40
19	B	803	CLA	CHC-C1C	3.32	1.43	1.35
19	A	852	CLA	CHC-C1C	3.32	1.43	1.35
19	A	802	CLA	CHC-C1C	3.31	1.43	1.35
19	A	837	CLA	CHC-C1C	3.31	1.43	1.35
19	A	826	CLA	CHC-C1C	3.31	1.43	1.35
19	B	814	CLA	C3B-C2B	-3.30	1.35	1.40
19	B	818	CLA	CHC-C1C	3.30	1.43	1.35
19	B	829	CLA	C3B-C2B	-3.30	1.35	1.40
19	3	314	CLA	CHC-C1C	3.30	1.43	1.35
19	1	309	CLA	CHC-C1C	3.29	1.43	1.35
19	3	309	CLA	CHC-C1C	3.29	1.43	1.35
19	A	822	CLA	CHC-C1C	3.29	1.43	1.35
19	A	832	CLA	CHC-C1C	3.29	1.43	1.35
19	A	807	CLA	CHC-C1C	3.29	1.43	1.35
19	A	812	CLA	CHC-C1C	3.29	1.43	1.35
19	A	836	CLA	CHC-C1C	3.29	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	828	CLA	C3B-C2B	-3.29	1.35	1.40
19	B	823	CLA	CHC-C1C	3.29	1.43	1.35
19	A	817	CLA	CHC-C1C	3.28	1.43	1.35
19	G	203	CLA	CHC-C1C	3.28	1.43	1.35
19	B	809	CLA	C3B-C2B	-3.28	1.35	1.40
19	B	818	CLA	C3B-C2B	-3.28	1.35	1.40
19	4	303	CLA	CHC-C1C	3.28	1.43	1.35
19	B	812	CLA	CHC-C1C	3.28	1.43	1.35
19	B	851	CLA	CHC-C1C	3.28	1.43	1.35
19	2	302	CLA	CHC-C1C	3.28	1.43	1.35
19	B	813	CLA	C3B-C2B	-3.28	1.35	1.40
19	B	840	CLA	CHC-C1C	3.28	1.43	1.35
19	B	804	CLA	C3B-C2B	-3.28	1.35	1.40
19	L	301	CLA	CHC-C1C	3.28	1.43	1.35
19	B	830	CLA	CHC-C1C	3.28	1.43	1.35
19	B	829	CLA	CHC-C1C	3.27	1.43	1.35
19	A	829	CLA	CHC-C1C	3.27	1.43	1.35
19	A	828	CLA	CHC-C1C	3.27	1.43	1.35
19	A	806	CLA	CHC-C1C	3.27	1.43	1.35
19	1	314	CLA	CHC-C1C	3.27	1.43	1.35
19	B	816	CLA	CHC-C1C	3.27	1.43	1.35
19	4	301	CLA	CHC-C1C	3.27	1.43	1.35
19	B	820	CLA	CHC-C1C	3.26	1.43	1.35
19	A	824	CLA	C3B-C2B	-3.26	1.35	1.40
19	B	825	CLA	C3B-C2B	-3.26	1.35	1.40
19	3	310	CLA	CHC-C1C	3.26	1.43	1.35
19	A	802	CLA	C3B-C2B	-3.26	1.35	1.40
19	3	302	CLA	CHC-C1C	3.26	1.43	1.35
19	B	821	CLA	CHC-C1C	3.26	1.43	1.35
19	A	803	CLA	CHC-C1C	3.26	1.43	1.35
19	B	815	CLA	CHC-C1C	3.26	1.43	1.35
19	B	828	CLA	C3B-C2B	-3.26	1.35	1.40
19	A	808	CLA	CHC-C1C	3.26	1.43	1.35
19	A	804	CLA	CHC-C1C	3.26	1.43	1.35
19	2	308	CLA	CHC-C1C	3.26	1.43	1.35
18	2	314	CHL	C3B-C2B	-3.26	1.35	1.40
19	B	805	CLA	C3B-C2B	-3.26	1.35	1.40
19	1	303	CLA	CHC-C1C	3.25	1.43	1.35
19	B	814	CLA	CHC-C1C	3.25	1.43	1.35
19	1	310	CLA	CHC-C1C	3.25	1.43	1.35
19	A	829	CLA	C3B-C2B	-3.25	1.35	1.40
19	B	808	CLA	C3B-C2B	-3.25	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	839	CLA	CHC-C1C	3.25	1.43	1.35
19	B	806	CLA	CHC-C1C	3.25	1.43	1.35
19	B	809	CLA	CHC-C1C	3.25	1.43	1.35
19	H	202	CLA	CHC-C1C	3.25	1.43	1.35
19	B	807	CLA	CHC-C1C	3.25	1.43	1.35
19	A	817	CLA	C3B-C2B	-3.25	1.35	1.40
19	3	306	CLA	CHC-C1C	3.25	1.43	1.35
19	2	311	CLA	CHC-C1C	3.25	1.43	1.35
19	A	805	CLA	CHC-C1C	3.25	1.43	1.35
19	A	811	CLA	CHC-C1C	3.25	1.43	1.35
19	2	303	CLA	CHC-C1C	3.24	1.43	1.35
19	A	833	CLA	CHC-C1C	3.24	1.43	1.35
19	A	806	CLA	C3B-C2B	-3.24	1.35	1.40
19	2	309	CLA	CHC-C1C	3.24	1.43	1.35
19	2	302	CLA	C3B-C2B	-3.24	1.35	1.40
19	3	304	CLA	CHC-C1C	3.24	1.43	1.35
19	3	313	CLA	CHC-C1C	3.24	1.43	1.35
19	A	853	CLA	CHC-C1C	3.24	1.43	1.35
19	K	201	CLA	CHC-C1C	3.24	1.43	1.35
19	4	302	CLA	CHC-C1C	3.24	1.43	1.35
19	3	308	CLA	CHC-C1C	3.24	1.43	1.35
19	1	307	CLA	CHC-C1C	3.24	1.43	1.35
19	B	835	CLA	C3B-C2B	-3.24	1.35	1.40
19	B	836	CLA	CHC-C1C	3.24	1.43	1.35
19	G	202	CLA	CHC-C1C	3.24	1.43	1.35
19	F	302	CLA	CHC-C1C	3.23	1.43	1.35
19	B	804	CLA	CHC-C1C	3.23	1.43	1.35
19	J	102	CLA	CHC-C1C	3.23	1.43	1.35
19	A	810	CLA	CHC-C1C	3.23	1.43	1.35
19	A	834	CLA	CHC-C1C	3.23	1.43	1.35
19	B	826	CLA	CHC-C1C	3.23	1.43	1.35
19	A	827	CLA	CHC-C1C	3.23	1.43	1.35
19	B	834	CLA	CHC-C1C	3.23	1.43	1.35
19	B	837	CLA	CHC-C1C	3.23	1.43	1.35
19	2	312	CLA	C3B-C2B	-3.23	1.35	1.40
19	3	305	CLA	CHC-C1C	3.23	1.43	1.35
19	1	318	CLA	CHC-C1C	3.23	1.43	1.35
19	A	836	CLA	C3B-C2B	-3.23	1.35	1.40
19	A	820	CLA	CHC-C1C	3.23	1.43	1.35
19	A	804	CLA	C3B-C2B	-3.23	1.35	1.40
19	A	853	CLA	C3B-C2B	-3.23	1.35	1.40
19	3	311	CLA	CHC-C1C	3.23	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	809	CLA	CHC-C1C	3.23	1.43	1.35
19	A	819	CLA	CHC-C1C	3.22	1.43	1.35
19	A	854	CLA	CHC-C1C	3.22	1.43	1.35
19	B	831	CLA	CHC-C1C	3.22	1.43	1.35
19	4	311	CLA	CHC-C1C	3.22	1.43	1.35
19	A	813	CLA	CHC-C1C	3.22	1.43	1.35
19	1	302	CLA	CHC-C1C	3.22	1.43	1.35
19	B	835	CLA	CHC-C1C	3.22	1.43	1.35
19	4	310	CLA	CHC-C1C	3.22	1.43	1.35
19	H	201	CLA	CHC-C1C	3.22	1.43	1.35
19	2	304	CLA	CHC-C1C	3.22	1.43	1.35
19	B	817	CLA	CHC-C1C	3.22	1.43	1.35
19	2	310	CLA	CHC-C1C	3.22	1.43	1.35
19	4	308	CLA	C3B-C2B	-3.22	1.35	1.40
19	1	308	CLA	CHC-C1C	3.22	1.43	1.35
19	1	311	CLA	CHC-C1C	3.22	1.43	1.35
19	A	827	CLA	C3B-C2B	-3.22	1.35	1.40
19	A	840	CLA	C3B-C2B	-3.22	1.35	1.40
19	A	834	CLA	C3B-C2B	-3.21	1.35	1.40
19	B	806	CLA	C3B-C2B	-3.21	1.35	1.40
19	K	202	CLA	CHC-C1C	3.21	1.43	1.35
19	B	819	CLA	CHC-C1C	3.21	1.43	1.35
19	A	830	CLA	C3B-C2B	-3.21	1.35	1.40
19	B	807	CLA	C3B-C2B	-3.21	1.35	1.40
19	B	827	CLA	C3B-C2B	-3.21	1.35	1.40
19	1	313	CLA	CHC-C1C	3.21	1.43	1.35
19	4	304	CLA	CHC-C1C	3.21	1.43	1.35
19	G	204	CLA	CHC-C1C	3.20	1.43	1.35
19	A	819	CLA	C3B-C2B	-3.20	1.35	1.40
19	A	815	CLA	CHC-C1C	3.20	1.43	1.35
19	L	302	CLA	CHC-C1C	3.20	1.43	1.35
19	3	303	CLA	CHC-C1C	3.20	1.43	1.35
19	A	839	CLA	CHC-C1C	3.20	1.43	1.35
19	A	818	CLA	CHC-C1C	3.20	1.43	1.35
19	F	301	CLA	CHC-C1C	3.20	1.43	1.35
19	B	828	CLA	CHC-C1C	3.20	1.43	1.35
19	B	810	CLA	CHC-C1C	3.20	1.43	1.35
19	B	839	CLA	C3B-C2B	-3.20	1.35	1.40
19	B	824	CLA	CHC-C1C	3.20	1.43	1.35
19	4	312	CLA	CHC-C1C	3.19	1.43	1.35
19	B	815	CLA	C3B-C2B	-3.19	1.35	1.40
19	A	825	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	304	CLA	CHC-C1C	3.19	1.43	1.35
19	4	308	CLA	CHC-C1C	3.19	1.43	1.35
19	A	814	CLA	CHC-C1C	3.19	1.43	1.35
19	A	835	CLA	CHC-C1C	3.19	1.43	1.35
19	A	823	CLA	CHC-C1C	3.18	1.43	1.35
19	B	823	CLA	C3B-C2B	-3.18	1.35	1.40
19	A	830	CLA	CHC-C1C	3.18	1.43	1.35
19	B	811	CLA	CHC-C1C	3.18	1.43	1.35
19	1	312	CLA	CHC-C1C	3.18	1.43	1.35
19	L	302	CLA	C3B-C2B	-3.18	1.36	1.40
19	A	816	CLA	CHC-C1C	3.18	1.43	1.35
19	A	801	CLA	CHC-C1C	3.18	1.43	1.35
19	A	840	CLA	CHC-C1C	3.18	1.43	1.35
19	3	308	CLA	C3B-C2B	-3.18	1.36	1.40
19	B	805	CLA	CHC-C1C	3.18	1.43	1.35
19	B	822	CLA	CHC-C1C	3.18	1.43	1.35
19	L	301	CLA	C3B-C2B	-3.18	1.36	1.40
19	4	313	CLA	CHC-C1C	3.18	1.43	1.35
19	A	821	CLA	CHC-C1C	3.17	1.43	1.35
19	B	802	CLA	CHC-C1C	3.17	1.43	1.35
19	4	309	CLA	CHC-C1C	3.17	1.43	1.35
19	B	819	CLA	C3B-C2B	-3.17	1.36	1.40
19	1	312	CLA	C3B-C2B	-3.17	1.36	1.40
19	B	838	CLA	CHC-C1C	3.17	1.43	1.35
19	4	302	CLA	C3B-C2B	-3.17	1.36	1.40
19	3	303	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	826	CLA	C3B-C2B	-3.16	1.36	1.40
19	4	304	CLA	C3B-C2B	-3.16	1.36	1.40
19	2	312	CLA	CHC-C1C	3.16	1.43	1.35
19	B	827	CLA	CHC-C1C	3.16	1.43	1.35
19	2	313	CLA	CHC-C1C	3.16	1.43	1.35
19	1	305	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	813	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	822	CLA	C3B-C2B	-3.16	1.36	1.40
19	A	838	CLA	CHC-C1C	3.16	1.43	1.35
19	A	810	CLA	C3B-C2B	-3.16	1.36	1.40
19	B	813	CLA	CHC-C1C	3.16	1.43	1.35
19	A	805	CLA	C3B-C2B	-3.16	1.36	1.40
19	B	808	CLA	CHC-C1C	3.15	1.43	1.35
19	1	311	CLA	C3B-C2B	-3.15	1.36	1.40
19	A	831	CLA	CHC-C1C	3.15	1.43	1.35
19	1	305	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	834	CLA	C3B-C2B	-3.15	1.36	1.40
19	A	854	CLA	C3B-C2B	-3.14	1.36	1.40
19	2	311	CLA	C3B-C2B	-3.14	1.36	1.40
19	B	822	CLA	C3B-C2B	-3.14	1.36	1.40
19	B	816	CLA	C3B-C2B	-3.14	1.36	1.40
19	4	310	CLA	C3B-C2B	-3.14	1.36	1.40
19	B	836	CLA	C3B-C2B	-3.14	1.36	1.40
19	3	301	CLA	C3B-C2B	-3.13	1.36	1.40
19	A	816	CLA	C3B-C2B	-3.13	1.36	1.40
19	3	312	CLA	CHC-C1C	3.13	1.43	1.35
19	B	821	CLA	C3B-C2B	-3.13	1.36	1.40
19	A	814	CLA	C3B-C2B	-3.13	1.36	1.40
19	B	826	CLA	C3B-C2B	-3.13	1.36	1.40
19	3	305	CLA	C3B-C2B	-3.12	1.36	1.40
19	B	838	CLA	C3B-C2B	-3.12	1.36	1.40
19	A	808	CLA	C3B-C2B	-3.12	1.36	1.40
19	1	303	CLA	C3B-C2B	-3.12	1.36	1.40
19	A	835	CLA	C3B-C2B	-3.12	1.36	1.40
19	B	817	CLA	C3B-C2B	-3.12	1.36	1.40
19	B	812	CLA	C3B-C2B	-3.12	1.36	1.40
19	3	309	CLA	C3B-C2B	-3.11	1.36	1.40
19	1	318	CLA	C3B-C2B	-3.11	1.36	1.40
18	4	306	CHL	MG-NA	3.11	2.13	2.06
19	B	840	CLA	C3B-C2B	-3.10	1.36	1.40
19	4	313	CLA	C3B-C2B	-3.10	1.36	1.40
19	B	824	CLA	C3B-C2B	-3.10	1.36	1.40
19	A	815	CLA	C3B-C2B	-3.10	1.36	1.40
19	B	802	CLA	C3B-C2B	-3.10	1.36	1.40
19	A	818	CLA	C3B-C2B	-3.10	1.36	1.40
19	A	837	CLA	C3B-C2B	-3.09	1.36	1.40
19	3	314	CLA	C3B-C2B	-3.09	1.36	1.40
19	A	838	CLA	C3B-C2B	-3.09	1.36	1.40
19	4	312	CLA	C3B-C2B	-3.09	1.36	1.40
19	H	202	CLA	C3B-C2B	-3.09	1.36	1.40
19	3	302	CLA	C3B-C2B	-3.09	1.36	1.40
19	B	820	CLA	C3B-C2B	-3.09	1.36	1.40
19	B	837	CLA	C3B-C2B	-3.08	1.36	1.40
18	2	307	CHL	MG-NA	3.08	2.13	2.06
19	G	203	CLA	C3B-C2B	-3.08	1.36	1.40
19	A	809	CLA	C3B-C2B	-3.08	1.36	1.40
19	2	303	CLA	C3B-C2B	-3.08	1.36	1.40
19	1	308	CLA	C3B-C2B	-3.08	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	309	CLA	C3B-C2B	-3.08	1.36	1.40
19	1	307	CLA	C3B-C2B	-3.07	1.36	1.40
19	A	823	CLA	C3B-C2B	-3.07	1.36	1.40
19	A	832	CLA	C3B-C2B	-3.07	1.36	1.40
19	2	308	CLA	C3B-C2B	-3.07	1.36	1.40
19	K	201	CLA	C3B-C2B	-3.07	1.36	1.40
19	A	801	CLA	C3B-C2B	-3.07	1.36	1.40
19	3	312	CLA	C3B-C2B	-3.07	1.36	1.40
19	A	803	CLA	C3B-C2B	-3.07	1.36	1.40
19	B	831	CLA	C3B-C2B	-3.06	1.36	1.40
19	1	304	CLA	C3B-C2B	-3.06	1.36	1.40
19	3	311	CLA	C3B-C2B	-3.06	1.36	1.40
19	B	830	CLA	C3B-C2B	-3.06	1.36	1.40
19	A	812	CLA	C3B-C2B	-3.06	1.36	1.40
19	B	810	CLA	C3B-C2B	-3.06	1.36	1.40
19	G	204	CLA	C3B-C2B	-3.05	1.36	1.40
19	1	310	CLA	C3B-C2B	-3.05	1.36	1.40
19	2	313	CLA	C3B-C2B	-3.05	1.36	1.40
19	A	839	CLA	C3B-C2B	-3.05	1.36	1.40
19	J	102	CLA	C3B-C2B	-3.05	1.36	1.40
19	2	304	CLA	C3B-C2B	-3.04	1.36	1.40
19	G	202	CLA	C3B-C2B	-3.04	1.36	1.40
18	4	314	CHL	MG-NA	3.04	2.13	2.06
19	B	803	CLA	C3B-C2B	-3.04	1.36	1.40
19	K	202	CLA	C3B-C2B	-3.04	1.36	1.40
19	2	310	CLA	C3B-C2B	-3.04	1.36	1.40
19	4	311	CLA	C3B-C2B	-3.04	1.36	1.40
19	3	306	CLA	C3B-C2B	-3.03	1.36	1.40
19	1	313	CLA	C3B-C2B	-3.03	1.36	1.40
19	1	302	CLA	C3B-C2B	-3.03	1.36	1.40
19	3	313	CLA	C3B-C2B	-3.02	1.36	1.40
19	4	303	CLA	C3B-C2B	-3.02	1.36	1.40
19	F	301	CLA	C3B-C2B	-3.02	1.36	1.40
18	4	307	CHL	MG-NA	3.01	2.13	2.06
18	1	306	CHL	MG-NA	3.01	2.13	2.06
18	4	307	CHL	O2A-CGA	3.00	1.42	1.33
19	A	807	CLA	C3B-C2B	-3.00	1.36	1.40
19	4	301	CLA	C3B-C2B	-3.00	1.36	1.40
19	A	821	CLA	C3B-C2B	-3.00	1.36	1.40
19	A	833	CLA	C3B-C2B	-3.00	1.36	1.40
19	B	833	CLA	C3B-C2B	-2.99	1.36	1.40
18	2	306	CHL	MG-NA	2.99	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	201	CLA	C3B-C2B	-2.99	1.36	1.40
19	A	825	CLA	C3B-C2B	-2.98	1.36	1.40
19	B	801	CLA	C3B-C2B	-2.98	1.36	1.40
19	A	811	CLA	C3B-C2B	-2.98	1.36	1.40
18	2	305	CHL	MG-NA	2.97	2.13	2.06
18	4	305	CHL	O2A-CGA	2.97	1.42	1.33
19	A	820	CLA	C3B-C2B	-2.97	1.36	1.40
18	3	307	CHL	MG-NA	2.97	2.13	2.06
19	F	302	CLA	C3B-C2B	-2.97	1.36	1.40
18	2	301	CHL	MG-NA	2.96	2.13	2.06
19	B	832	CLA	C3B-C2B	-2.96	1.36	1.40
19	4	309	CLA	C3B-C2B	-2.95	1.36	1.40
20	4	315	LUT	C8-C9	-2.95	1.39	1.45
19	3	304	CLA	C3B-C2B	-2.95	1.36	1.40
19	A	852	CLA	C3B-C2B	-2.95	1.36	1.40
18	2	314	CHL	MG-NA	2.94	2.13	2.06
19	1	314	CLA	C3B-C2B	-2.94	1.36	1.40
18	1	301	CHL	O2A-CGA	2.93	1.41	1.33
18	4	305	CHL	MG-NA	2.92	2.13	2.06
18	2	301	CHL	O2A-CGA	2.91	1.41	1.33
19	1	309	CLA	C3B-C2B	-2.91	1.36	1.40
19	A	803	CLA	C1D-ND	-2.90	1.34	1.37
18	1	301	CHL	MG-NA	2.90	2.13	2.06
19	3	310	CLA	C3B-C2B	-2.89	1.36	1.40
20	1	315	LUT	C8-C9	-2.85	1.39	1.45
19	K	203	CLA	C3B-C2B	-2.83	1.36	1.40
19	A	824	CLA	C1D-ND	-2.83	1.34	1.37
19	A	825	CLA	C1D-ND	-2.82	1.34	1.37
19	B	829	CLA	C1D-ND	-2.81	1.34	1.37
19	A	807	CLA	C1D-ND	-2.80	1.34	1.37
19	A	852	CLA	C1D-ND	-2.80	1.34	1.37
18	3	307	CHL	O2A-CGA	2.80	1.41	1.33
19	A	833	CLA	C1D-ND	-2.79	1.34	1.37
19	B	801	CLA	C1D-ND	-2.79	1.34	1.37
20	2	315	LUT	C8-C9	-2.78	1.40	1.45
20	3	315	LUT	C8-C9	-2.78	1.40	1.45
19	3	308	CLA	C1D-ND	-2.78	1.34	1.37
19	B	803	CLA	C1D-ND	-2.77	1.34	1.37
19	L	301	CLA	C1D-ND	-2.77	1.34	1.37
19	A	828	CLA	C1D-ND	-2.76	1.34	1.37
19	B	828	CLA	C1D-ND	-2.76	1.34	1.37
19	1	310	CLA	C1D-ND	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	825	CLA	C1D-ND	-2.76	1.34	1.37
19	B	833	CLA	C1D-ND	-2.76	1.34	1.37
19	B	832	CLA	C1D-ND	-2.75	1.34	1.37
19	A	806	CLA	C1D-ND	-2.75	1.34	1.37
19	A	808	CLA	C1D-ND	-2.75	1.34	1.37
19	B	802	CLA	C1D-ND	-2.75	1.34	1.37
19	B	812	CLA	C1D-ND	-2.75	1.34	1.37
19	B	805	CLA	C1D-ND	-2.74	1.34	1.37
19	B	810	CLA	C1D-ND	-2.74	1.34	1.37
20	1	319	LUT	C8-C9	-2.74	1.40	1.45
19	B	809	CLA	C1D-ND	-2.74	1.34	1.37
19	A	819	CLA	C1D-ND	-2.74	1.34	1.37
19	B	823	CLA	C1D-ND	-2.73	1.34	1.37
19	A	826	CLA	C1D-ND	-2.72	1.34	1.37
19	B	839	CLA	C1D-ND	-2.72	1.34	1.37
19	2	304	CLA	C1D-ND	-2.72	1.34	1.37
19	4	302	CLA	C1D-ND	-2.72	1.34	1.37
19	A	805	CLA	C1D-ND	-2.72	1.34	1.37
19	A	839	CLA	C1D-ND	-2.72	1.34	1.37
19	B	837	CLA	C1D-ND	-2.72	1.34	1.37
19	B	851	CLA	C3B-C2B	-2.72	1.36	1.40
19	4	301	CLA	C1D-ND	-2.72	1.34	1.37
19	B	819	CLA	C1D-ND	-2.72	1.34	1.37
19	1	308	CLA	C1D-ND	-2.72	1.34	1.37
19	A	816	CLA	C1D-ND	-2.72	1.34	1.37
19	A	829	CLA	C1D-ND	-2.71	1.34	1.37
19	A	809	CLA	C1D-ND	-2.71	1.34	1.37
19	B	808	CLA	C1D-ND	-2.71	1.34	1.37
19	3	314	CLA	C1D-ND	-2.70	1.34	1.37
19	B	814	CLA	C1D-ND	-2.70	1.34	1.37
19	B	831	CLA	C1D-ND	-2.70	1.34	1.37
19	2	308	CLA	C1D-ND	-2.70	1.34	1.37
19	4	309	CLA	C1D-ND	-2.70	1.34	1.37
19	B	811	CLA	C1D-ND	-2.70	1.34	1.37
19	3	301	CLA	C1D-ND	-2.70	1.34	1.37
19	1	312	CLA	C1D-ND	-2.69	1.34	1.37
19	A	836	CLA	C1D-ND	-2.69	1.34	1.37
19	B	830	CLA	C1D-ND	-2.69	1.34	1.37
19	B	840	CLA	C1D-ND	-2.69	1.34	1.37
19	A	827	CLA	C1D-ND	-2.69	1.34	1.37
19	B	817	CLA	C1D-ND	-2.69	1.34	1.37
19	B	821	CLA	C1D-ND	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	C1D-ND	-2.69	1.34	1.37
19	H	202	CLA	C1D-ND	-2.69	1.34	1.37
19	A	840	CLA	C1D-ND	-2.68	1.34	1.37
19	4	308	CLA	C1D-ND	-2.68	1.34	1.37
19	B	835	CLA	C1D-ND	-2.68	1.34	1.37
19	A	835	CLA	C1D-ND	-2.68	1.34	1.37
19	A	837	CLA	C1D-ND	-2.68	1.34	1.37
19	A	802	CLA	C1D-ND	-2.68	1.34	1.37
19	B	836	CLA	C1D-ND	-2.68	1.34	1.37
19	B	826	CLA	C1D-ND	-2.67	1.34	1.37
19	2	309	CLA	C1D-ND	-2.67	1.34	1.37
19	A	817	CLA	C1D-ND	-2.67	1.34	1.37
19	B	838	CLA	C1D-ND	-2.67	1.34	1.37
19	B	813	CLA	C1D-ND	-2.67	1.34	1.37
19	B	824	CLA	C1D-ND	-2.67	1.34	1.37
19	A	853	CLA	C1D-ND	-2.66	1.34	1.37
19	A	815	CLA	C1D-ND	-2.66	1.34	1.37
19	2	302	CLA	C1D-ND	-2.66	1.34	1.37
19	1	318	CLA	C1D-ND	-2.66	1.34	1.37
19	4	303	CLA	C1D-ND	-2.66	1.34	1.37
19	A	804	CLA	C1D-ND	-2.66	1.34	1.37
19	A	830	CLA	C1D-ND	-2.66	1.34	1.37
19	A	810	CLA	C1D-ND	-2.65	1.34	1.37
19	A	822	CLA	C1D-ND	-2.65	1.34	1.37
19	4	310	CLA	C1D-ND	-2.65	1.34	1.37
19	A	811	CLA	C1D-ND	-2.65	1.34	1.37
19	4	304	CLA	C1D-ND	-2.65	1.34	1.37
19	1	309	CLA	C1D-ND	-2.64	1.34	1.37
19	B	818	CLA	C1D-ND	-2.64	1.34	1.37
19	A	820	CLA	C1D-ND	-2.64	1.34	1.37
19	A	813	CLA	C1D-ND	-2.63	1.34	1.37
19	A	831	CLA	C1D-ND	-2.63	1.34	1.37
19	3	303	CLA	C1D-ND	-2.63	1.34	1.37
19	B	806	CLA	C1D-ND	-2.63	1.34	1.37
19	B	827	CLA	C1D-ND	-2.63	1.34	1.37
19	F	301	CLA	C1D-ND	-2.63	1.34	1.37
19	A	838	CLA	C1D-ND	-2.63	1.34	1.37
19	B	816	CLA	C1D-ND	-2.62	1.34	1.37
19	A	812	CLA	C1D-ND	-2.62	1.34	1.37
19	B	851	CLA	C1D-ND	-2.62	1.34	1.37
19	1	307	CLA	C1D-ND	-2.62	1.34	1.37
19	2	311	CLA	C1D-ND	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	312	CLA	C1D-ND	-2.62	1.34	1.37
19	B	820	CLA	C1D-ND	-2.62	1.34	1.37
19	B	822	CLA	C1D-ND	-2.61	1.34	1.37
19	2	310	CLA	C1D-ND	-2.61	1.34	1.37
19	A	823	CLA	C1D-ND	-2.61	1.34	1.37
19	A	854	CLA	C1D-ND	-2.61	1.34	1.37
19	3	302	CLA	C1D-ND	-2.61	1.34	1.37
19	2	312	CLA	C1D-ND	-2.61	1.34	1.37
19	3	305	CLA	C1D-ND	-2.61	1.34	1.37
19	3	309	CLA	C1D-ND	-2.60	1.34	1.37
19	4	311	CLA	C1D-ND	-2.60	1.34	1.37
19	3	306	CLA	C1D-ND	-2.60	1.34	1.37
19	H	201	CLA	C1D-ND	-2.60	1.34	1.37
19	3	310	CLA	C1D-ND	-2.60	1.34	1.37
19	G	203	CLA	C1D-ND	-2.60	1.34	1.37
19	4	312	CLA	C1D-ND	-2.60	1.34	1.37
19	2	313	CLA	C1D-ND	-2.59	1.34	1.37
19	3	311	CLA	C1D-ND	-2.59	1.34	1.37
19	A	832	CLA	C1D-ND	-2.59	1.34	1.37
19	L	302	CLA	C1D-ND	-2.59	1.34	1.37
19	1	313	CLA	C1D-ND	-2.59	1.34	1.37
19	A	801	CLA	C1D-ND	-2.59	1.34	1.37
19	B	815	CLA	C1D-ND	-2.59	1.34	1.37
19	B	804	CLA	C1D-ND	-2.58	1.34	1.37
19	J	102	CLA	C1D-ND	-2.58	1.34	1.37
19	1	302	CLA	C1D-ND	-2.58	1.34	1.37
19	1	303	CLA	C1D-ND	-2.58	1.34	1.37
19	2	303	CLA	C1D-ND	-2.57	1.34	1.37
19	A	814	CLA	C1D-ND	-2.56	1.34	1.37
19	4	313	CLA	C1D-ND	-2.56	1.34	1.37
19	B	807	CLA	C1D-ND	-2.56	1.34	1.37
19	K	202	CLA	C1D-ND	-2.56	1.34	1.37
19	F	302	CLA	C1D-ND	-2.55	1.34	1.37
19	B	834	CLA	C1D-ND	-2.55	1.34	1.37
19	G	202	CLA	C1D-ND	-2.55	1.34	1.37
19	1	304	CLA	C1D-ND	-2.55	1.34	1.37
19	G	204	CLA	C1D-ND	-2.54	1.34	1.37
19	K	203	CLA	C1D-ND	-2.54	1.34	1.37
19	1	314	CLA	C1D-ND	-2.53	1.34	1.37
19	1	305	CLA	C1D-ND	-2.53	1.34	1.37
18	2	314	CHL	CHC-C1C	2.52	1.41	1.35
20	4	315	LUT	C12-C13	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	304	CLA	C1D-ND	-2.52	1.34	1.37
19	K	201	CLA	C1D-ND	-2.51	1.34	1.37
19	1	311	CLA	C1D-ND	-2.50	1.34	1.37
19	A	818	CLA	C1D-ND	-2.50	1.34	1.37
19	B	830	CLA	C1B-CHB	-2.50	1.34	1.41
19	A	830	CLA	C1B-CHB	-2.49	1.34	1.41
19	A	840	CLA	C1B-CHB	-2.48	1.34	1.41
18	4	305	CHL	C2-C3	2.48	1.38	1.33
19	A	821	CLA	C1D-ND	-2.48	1.34	1.37
18	1	301	CHL	C2-C3	2.47	1.38	1.33
19	B	803	CLA	C1B-CHB	-2.47	1.34	1.41
19	A	811	CLA	C1B-CHB	-2.47	1.34	1.41
18	2	306	CHL	CHC-C1C	2.46	1.41	1.35
19	3	313	CLA	C1D-ND	-2.46	1.34	1.37
19	B	806	CLA	C1B-CHB	-2.46	1.34	1.41
19	A	854	CLA	C1B-CHB	-2.46	1.34	1.41
19	A	833	CLA	C1B-CHB	-2.46	1.34	1.41
19	A	827	CLA	C1B-CHB	-2.46	1.34	1.41
19	B	838	CLA	C1B-CHB	-2.46	1.34	1.41
19	B	835	CLA	C1B-CHB	-2.45	1.34	1.41
19	A	802	CLA	C1B-CHB	-2.45	1.34	1.41
19	B	824	CLA	C1B-CHB	-2.45	1.34	1.41
19	B	829	CLA	C1B-CHB	-2.45	1.34	1.41
18	4	306	CHL	CBA-CGA	2.45	1.56	1.50
19	A	805	CLA	C1B-CHB	-2.45	1.34	1.41
19	A	834	CLA	C1B-CHB	-2.44	1.34	1.41
18	4	305	CHL	CHC-C1C	2.44	1.41	1.35
18	2	307	CHL	CBA-CGA	2.44	1.56	1.50
19	4	312	CLA	C1B-CHB	-2.44	1.34	1.41
18	1	306	CHL	CBA-CGA	2.44	1.56	1.50
19	B	804	CLA	C1B-CHB	-2.44	1.34	1.41
19	B	822	CLA	C1B-CHB	-2.44	1.34	1.41
19	A	814	CLA	C1B-CHB	-2.44	1.34	1.41
19	A	836	CLA	C1B-CHB	-2.44	1.34	1.41
19	B	809	CLA	C1B-CHB	-2.44	1.34	1.41
19	3	303	CLA	C1B-CHB	-2.44	1.34	1.41
19	H	202	CLA	C1B-CHB	-2.44	1.34	1.41
19	A	816	CLA	C1B-CHB	-2.43	1.34	1.41
19	2	311	CLA	C1B-CHB	-2.43	1.34	1.41
19	4	311	CLA	C1B-CHB	-2.43	1.34	1.41
19	A	810	CLA	C1B-CHB	-2.43	1.34	1.41
19	B	816	CLA	C1B-CHB	-2.43	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	825	CLA	C1B-CHB	-2.43	1.34	1.41
19	2	304	CLA	C1B-CHB	-2.43	1.34	1.41
19	3	309	CLA	C1B-CHB	-2.43	1.34	1.41
19	B	851	CLA	C1B-CHB	-2.43	1.34	1.41
19	A	823	CLA	C1B-CHB	-2.43	1.34	1.41
19	B	813	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	812	CLA	C1B-CHB	-2.42	1.34	1.41
19	3	305	CLA	C1B-CHB	-2.42	1.34	1.41
19	4	304	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	819	CLA	C1B-CHB	-2.42	1.34	1.41
19	B	805	CLA	C1B-CHB	-2.42	1.34	1.41
19	3	312	CLA	C1B-CHB	-2.42	1.34	1.41
18	2	305	CHL	CHC-C1C	2.42	1.41	1.35
18	4	314	CHL	CHC-C1C	2.42	1.41	1.35
19	1	311	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	804	CLA	C1B-CHB	-2.42	1.34	1.41
19	1	302	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	818	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	831	CLA	C1B-CHB	-2.42	1.34	1.41
19	A	838	CLA	C1B-CHB	-2.42	1.34	1.41
19	B	815	CLA	C1B-CHB	-2.42	1.34	1.41
19	4	310	CLA	C1B-CHB	-2.42	1.34	1.41
19	B	818	CLA	C1B-CHB	-2.42	1.34	1.41
19	4	313	CLA	C1B-CHB	-2.42	1.34	1.41
19	K	202	CLA	C1B-CHB	-2.41	1.34	1.41
19	2	302	CLA	C1B-CHB	-2.41	1.34	1.41
19	3	301	CLA	C1B-CHB	-2.41	1.34	1.41
19	B	812	CLA	C1B-CHB	-2.41	1.34	1.41
19	B	811	CLA	C1B-CHB	-2.41	1.34	1.41
18	2	306	CHL	CBA-CGA	2.41	1.56	1.50
19	3	314	CLA	C1B-CHB	-2.41	1.34	1.41
19	A	820	CLA	C1B-CHB	-2.41	1.34	1.41
19	F	302	CLA	C1B-CHB	-2.41	1.34	1.41
19	1	307	CLA	C1B-CHB	-2.41	1.34	1.41
19	3	313	CLA	C1B-CHB	-2.41	1.34	1.41
19	A	817	CLA	C1B-CHB	-2.41	1.34	1.41
19	G	203	CLA	C1B-CHB	-2.41	1.34	1.41
19	3	308	CLA	C1B-CHB	-2.41	1.34	1.41
19	B	836	CLA	C1B-CHB	-2.41	1.34	1.41
19	A	824	CLA	C1B-CHB	-2.40	1.34	1.41
19	F	301	CLA	C1B-CHB	-2.40	1.34	1.41
18	2	301	CHL	CHC-C1C	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	302	CLA	C1B-CHB	-2.40	1.34	1.41
19	A	853	CLA	C1B-CHB	-2.40	1.34	1.41
19	1	309	CLA	C1B-CHB	-2.40	1.34	1.41
19	1	305	CLA	C1B-CHB	-2.40	1.34	1.41
19	3	306	CLA	C1B-CHB	-2.40	1.34	1.41
19	A	837	CLA	C1B-CHB	-2.40	1.34	1.41
19	H	201	CLA	C1B-CHB	-2.40	1.34	1.41
19	A	815	CLA	C1B-CHB	-2.40	1.34	1.41
19	A	828	CLA	C1B-CHB	-2.40	1.34	1.41
19	B	828	CLA	C1B-CHB	-2.40	1.34	1.41
19	A	829	CLA	C1B-CHB	-2.40	1.34	1.41
19	B	807	CLA	C1B-CHB	-2.40	1.34	1.41
19	B	827	CLA	C1B-CHB	-2.40	1.34	1.41
19	L	301	CLA	C1B-CHB	-2.40	1.34	1.41
18	4	306	CHL	CHC-C1C	2.40	1.41	1.35
19	B	840	CLA	C1B-CHB	-2.40	1.34	1.41
19	1	318	CLA	C1B-CHB	-2.40	1.34	1.41
19	1	304	CLA	C1B-CHB	-2.40	1.34	1.41
19	2	309	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	819	CLA	C1B-CHB	-2.39	1.34	1.41
19	L	302	CLA	C1B-CHB	-2.39	1.34	1.41
19	1	314	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	801	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	810	CLA	C1B-CHB	-2.39	1.34	1.41
20	4	315	LUT	C32-C33	-2.39	1.40	1.45
19	A	839	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	839	CLA	C1B-CHB	-2.39	1.34	1.41
19	A	813	CLA	C1B-CHB	-2.39	1.34	1.41
19	A	806	CLA	C1B-CHB	-2.39	1.34	1.41
19	G	202	CLA	C1B-CHB	-2.39	1.34	1.41
19	A	852	CLA	C1B-CHB	-2.39	1.34	1.41
19	3	311	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	834	CLA	C1B-CHB	-2.39	1.34	1.41
18	1	301	CHL	CHC-C1C	2.39	1.41	1.35
19	4	303	CLA	C1B-CHB	-2.39	1.34	1.41
19	4	308	CLA	C1B-CHB	-2.39	1.34	1.41
19	B	826	CLA	C1B-CHB	-2.39	1.34	1.41
19	4	302	CLA	C1B-CHB	-2.38	1.34	1.41
18	3	307	CHL	CHC-C1C	2.38	1.41	1.35
19	1	312	CLA	C1B-CHB	-2.38	1.34	1.41
19	A	821	CLA	C1B-CHB	-2.38	1.34	1.41
18	1	306	CHL	CHC-C1C	2.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	822	CLA	C1B-CHB	-2.38	1.34	1.41
19	A	807	CLA	C1B-CHB	-2.38	1.34	1.41
19	2	313	CLA	C1B-CHB	-2.38	1.34	1.41
19	A	808	CLA	C1B-CHB	-2.38	1.34	1.41
19	2	308	CLA	C1B-CHB	-2.38	1.34	1.41
20	2	315	LUT	C32-C33	-2.38	1.40	1.45
19	B	823	CLA	C1B-CHB	-2.38	1.34	1.41
19	1	310	CLA	C1B-CHB	-2.38	1.34	1.41
19	1	303	CLA	C1B-CHB	-2.38	1.34	1.41
19	B	802	CLA	C1B-CHB	-2.37	1.34	1.41
19	3	304	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	820	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	814	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	831	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	837	CLA	C1B-CHB	-2.37	1.34	1.41
19	K	201	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	808	CLA	C1B-CHB	-2.37	1.34	1.41
19	1	313	CLA	C1B-CHB	-2.37	1.34	1.41
19	B	821	CLA	C1B-CHB	-2.37	1.34	1.41
19	A	825	CLA	C1B-CHB	-2.37	1.34	1.41
19	4	309	CLA	C1B-CHB	-2.37	1.34	1.41
19	3	310	CLA	C1B-CHB	-2.37	1.34	1.41
19	A	832	CLA	C1B-CHB	-2.37	1.34	1.41
20	3	315	LUT	C12-C13	-2.37	1.40	1.45
19	G	204	CLA	C1B-CHB	-2.36	1.34	1.41
19	2	310	CLA	C1B-CHB	-2.36	1.34	1.41
19	A	809	CLA	C1B-CHB	-2.36	1.34	1.41
19	A	826	CLA	C1B-CHB	-2.36	1.34	1.41
19	B	833	CLA	C1B-CHB	-2.36	1.34	1.41
20	1	315	LUT	C12-C13	-2.36	1.40	1.45
19	4	301	CLA	C1B-CHB	-2.36	1.34	1.41
18	2	307	CHL	CHC-C1C	2.35	1.41	1.35
20	3	315	LUT	C32-C33	-2.35	1.40	1.45
19	J	102	CLA	C1B-CHB	-2.35	1.34	1.41
19	B	817	CLA	C1B-CHB	-2.35	1.34	1.41
19	2	303	CLA	C1B-CHB	-2.35	1.34	1.41
19	A	835	CLA	C1B-CHB	-2.35	1.34	1.41
19	A	803	CLA	C1B-CHB	-2.35	1.34	1.41
20	2	315	LUT	C28-C29	-2.35	1.40	1.45
20	1	315	LUT	C28-C29	-2.35	1.40	1.45
19	2	312	CLA	C1B-CHB	-2.34	1.34	1.41
18	4	307	CHL	CHC-C1C	2.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	315	LUT	C32-C33	-2.34	1.40	1.45
18	2	301	CHL	C2-C3	2.34	1.39	1.32
20	3	315	LUT	C28-C29	-2.33	1.40	1.45
20	4	315	LUT	C28-C29	-2.33	1.40	1.45
19	1	308	CLA	C1B-CHB	-2.33	1.34	1.41
20	2	315	LUT	C12-C13	-2.33	1.40	1.45
18	4	307	CHL	C2-C3	2.33	1.39	1.32
19	A	801	CLA	C1B-CHB	-2.32	1.34	1.41
19	K	203	CLA	C1B-CHB	-2.30	1.34	1.41
19	B	832	CLA	C1B-CHB	-2.29	1.34	1.41
20	1	319	LUT	C32-C33	-2.28	1.41	1.45
20	1	319	LUT	C12-C13	-2.26	1.41	1.45
19	K	202	CLA	MG-NC	2.25	2.11	2.06
19	B	830	CLA	MG-NC	2.25	2.11	2.06
20	1	319	LUT	C28-C29	-2.24	1.41	1.45
18	4	306	CHL	MG-NC	2.24	2.11	2.06
18	4	314	CHL	MG-NC	2.24	2.11	2.06
19	4	312	CLA	MG-NC	2.23	2.11	2.06
19	3	311	CLA	MG-NC	2.23	2.11	2.06
19	A	821	CLA	MG-NC	2.23	2.11	2.06
19	4	311	CLA	MG-NC	2.22	2.11	2.06
19	G	202	CLA	MG-NC	2.21	2.11	2.06
19	F	302	CLA	MG-NC	2.21	2.11	2.06
19	A	834	CLA	MG-NC	2.21	2.11	2.06
19	1	304	CLA	MG-NC	2.21	2.11	2.06
19	A	830	CLA	MG-NC	2.21	2.11	2.06
18	1	306	CHL	MG-NC	2.20	2.11	2.06
19	B	835	CLA	MG-NC	2.20	2.11	2.06
19	A	820	CLA	MG-NC	2.20	2.11	2.06
19	A	836	CLA	MG-NC	2.19	2.11	2.06
19	A	838	CLA	MG-NC	2.19	2.11	2.06
19	F	301	CLA	MG-NC	2.19	2.11	2.06
19	H	201	CLA	MG-NC	2.19	2.11	2.06
19	1	312	CLA	MG-NC	2.18	2.11	2.06
19	A	823	CLA	MG-NC	2.18	2.11	2.06
18	1	301	CHL	C3B-CAB	-2.18	1.43	1.47
19	3	313	CLA	MG-NC	2.18	2.11	2.06
19	B	834	CLA	MG-NC	2.18	2.11	2.06
19	3	305	CLA	MG-NC	2.18	2.11	2.06
19	4	313	CLA	MG-NC	2.17	2.11	2.06
19	A	814	CLA	MG-NC	2.17	2.11	2.06
19	B	840	CLA	MG-NC	2.17	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	CLA	MG-NC	2.17	2.11	2.06
19	4	308	CLA	MG-NC	2.17	2.11	2.06
19	A	827	CLA	MG-NC	2.17	2.11	2.06
19	B	806	CLA	MG-NC	2.17	2.11	2.06
19	3	312	CLA	MG-NC	2.17	2.11	2.06
19	2	302	CLA	MG-NC	2.17	2.11	2.06
18	1	301	CHL	MG-NC	2.17	2.11	2.06
19	A	832	CLA	MG-NC	2.17	2.11	2.06
19	B	851	CLA	MG-NC	2.17	2.11	2.06
18	2	307	CHL	MG-NC	2.16	2.11	2.06
19	B	804	CLA	MG-NC	2.16	2.11	2.06
19	1	311	CLA	MG-NC	2.16	2.11	2.06
18	2	301	CHL	MG-NC	2.16	2.11	2.06
19	3	301	CLA	MG-NC	2.16	2.11	2.06
19	4	304	CLA	MG-NC	2.16	2.11	2.06
19	A	829	CLA	MG-NC	2.16	2.11	2.06
19	A	816	CLA	MG-NC	2.16	2.11	2.06
19	2	312	CLA	MG-NC	2.15	2.11	2.06
19	2	303	CLA	MG-NC	2.15	2.11	2.06
19	2	311	CLA	MG-NC	2.15	2.11	2.06
19	G	204	CLA	MG-NC	2.15	2.11	2.06
19	B	822	CLA	MG-NC	2.15	2.11	2.06
19	1	305	CLA	MG-NC	2.15	2.11	2.06
19	1	310	CLA	MG-NC	2.15	2.11	2.06
19	4	310	CLA	MG-NC	2.15	2.11	2.06
19	G	203	CLA	MG-NC	2.15	2.11	2.06
18	4	307	CHL	MG-NC	2.14	2.11	2.06
19	A	813	CLA	MG-NC	2.14	2.11	2.06
19	4	303	CLA	MG-NC	2.14	2.11	2.06
19	J	102	CLA	MG-NC	2.14	2.11	2.06
19	B	824	CLA	MG-NC	2.14	2.11	2.06
19	A	840	CLA	MG-NC	2.14	2.11	2.06
19	3	304	CLA	MG-NC	2.14	2.11	2.06
19	2	313	CLA	MG-NC	2.14	2.11	2.06
19	K	201	CLA	MG-NC	2.14	2.11	2.06
19	1	302	CLA	MG-NC	2.14	2.11	2.06
19	A	825	CLA	MG-NC	2.13	2.11	2.06
19	1	307	CLA	MG-NC	2.13	2.11	2.06
18	4	305	CHL	MG-NC	2.13	2.11	2.06
19	1	303	CLA	MG-NC	2.13	2.11	2.06
19	B	838	CLA	MG-NC	2.13	2.11	2.06
19	3	303	CLA	MG-NC	2.13	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	305	CHL	MG-NC	2.13	2.11	2.06
19	3	314	CLA	MG-NC	2.13	2.11	2.06
19	A	833	CLA	MG-NC	2.13	2.11	2.06
19	B	813	CLA	MG-NC	2.13	2.11	2.06
19	L	302	CLA	MG-NC	2.13	2.11	2.06
19	B	810	CLA	MG-NC	2.13	2.11	2.06
19	H	202	CLA	MG-NC	2.13	2.11	2.06
19	B	826	CLA	MG-NC	2.12	2.11	2.06
19	B	827	CLA	MG-NC	2.12	2.11	2.06
19	1	318	CLA	MG-NC	2.12	2.11	2.06
19	1	313	CLA	MG-NC	2.12	2.11	2.06
19	B	808	CLA	MG-NC	2.12	2.11	2.06
19	2	304	CLA	MG-NC	2.12	2.11	2.06
19	2	310	CLA	MG-NC	2.12	2.11	2.06
19	A	815	CLA	MG-NC	2.12	2.11	2.06
19	B	815	CLA	MG-NC	2.12	2.11	2.06
19	A	812	CLA	MG-NC	2.12	2.11	2.06
18	2	307	CHL	C3B-CAB	-2.12	1.43	1.47
19	B	807	CLA	MG-NC	2.12	2.11	2.06
18	3	307	CHL	MG-NC	2.12	2.11	2.06
19	3	309	CLA	MG-NC	2.12	2.11	2.06
19	B	809	CLA	MG-NC	2.11	2.11	2.06
19	B	837	CLA	MG-NC	2.11	2.11	2.06
19	3	310	CLA	MG-NC	2.11	2.11	2.06
19	A	831	CLA	MG-NC	2.11	2.11	2.06
19	B	829	CLA	MG-NC	2.11	2.11	2.06
19	3	306	CLA	MG-NC	2.11	2.11	2.06
19	3	308	CLA	MG-NC	2.11	2.11	2.06
19	A	853	CLA	MG-NC	2.11	2.11	2.06
19	A	818	CLA	MG-NC	2.10	2.11	2.06
19	A	839	CLA	MG-NC	2.10	2.11	2.06
18	2	306	CHL	MG-NC	2.10	2.11	2.06
19	B	816	CLA	MG-NC	2.10	2.11	2.06
19	B	828	CLA	MG-NC	2.10	2.11	2.06
18	1	306	CHL	C3B-CAB	-2.10	1.43	1.47
19	B	831	CLA	MG-NC	2.10	2.11	2.06
19	B	811	CLA	CAA-C2A	2.10	1.58	1.54
19	B	821	CLA	MG-NC	2.10	2.11	2.06
19	4	302	CLA	MG-NC	2.10	2.11	2.06
19	B	819	CLA	MG-NC	2.10	2.11	2.06
19	B	823	CLA	MG-NC	2.10	2.11	2.06
19	A	819	CLA	MG-NC	2.10	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	309	CLA	MG-NC	2.10	2.11	2.06
19	A	835	CLA	MG-NC	2.10	2.11	2.06
19	A	828	CLA	MG-NC	2.10	2.11	2.06
19	L	301	CLA	MG-NC	2.10	2.11	2.06
18	2	314	CHL	MG-NC	2.09	2.11	2.06
19	A	837	CLA	MG-NC	2.09	2.11	2.06
19	4	301	CLA	MG-NC	2.09	2.11	2.06
19	A	804	CLA	MG-NC	2.09	2.11	2.06
19	B	820	CLA	MG-NC	2.09	2.11	2.06
19	A	817	CLA	MG-NC	2.08	2.11	2.06
19	A	822	CLA	MG-NC	2.08	2.11	2.06
19	B	811	CLA	MG-NC	2.08	2.11	2.06
19	B	825	CLA	MG-NC	2.08	2.11	2.06
18	4	307	CHL	C3B-CAB	-2.08	1.43	1.47
19	2	308	CLA	MG-NC	2.07	2.11	2.06
19	K	203	CLA	MG-NC	2.07	2.11	2.06
19	A	802	CLA	MG-NC	2.07	2.11	2.06
19	A	854	CLA	MG-NC	2.07	2.11	2.06
19	B	805	CLA	MG-NC	2.07	2.11	2.06
19	A	809	CLA	MG-NC	2.07	2.11	2.06
19	A	801	CLA	MG-NC	2.07	2.11	2.06
19	A	811	CLA	MG-NC	2.07	2.11	2.06
19	A	806	CLA	MG-NC	2.07	2.11	2.06
19	B	812	CLA	MG-NC	2.07	2.11	2.06
19	B	833	CLA	MG-NC	2.07	2.11	2.06
19	B	802	CLA	MG-NC	2.06	2.11	2.06
19	A	805	CLA	MG-NC	2.06	2.11	2.06
19	3	302	CLA	MG-NC	2.06	2.11	2.06
19	B	817	CLA	MG-NC	2.06	2.11	2.06
19	A	810	CLA	MG-NC	2.06	2.11	2.06
18	3	307	CHL	C3B-CAB	-2.05	1.43	1.47
19	A	807	CLA	MG-NC	2.05	2.11	2.06
19	A	808	CLA	MG-NC	2.05	2.11	2.06
19	B	814	CLA	MG-NC	2.05	2.11	2.06
18	4	314	CHL	C3B-CAB	-2.05	1.43	1.47
19	A	826	CLA	MG-NC	2.05	2.11	2.06
19	4	309	CLA	MG-NC	2.05	2.11	2.06
19	B	836	CLA	MG-NC	2.05	2.11	2.06
19	B	832	CLA	MG-NC	2.05	2.11	2.06
19	B	818	CLA	MG-NC	2.04	2.11	2.06
19	A	803	CLA	MG-NC	2.04	2.11	2.06
19	B	801	CLA	MG-NC	2.04	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	309	CLA	MG-NC	2.04	2.11	2.06
19	B	839	CLA	MG-NC	2.03	2.11	2.06
18	2	314	CHL	C3B-CAB	-2.02	1.43	1.47
18	2	301	CHL	C3B-CAB	-2.01	1.43	1.47
19	A	852	CLA	MG-NC	2.01	2.11	2.06
18	2	314	CHL	O1D-CGD	2.01	1.26	1.21
19	1	308	CLA	MG-NC	2.01	2.11	2.06
18	1	306	CHL	O1D-CGD	2.01	1.26	1.21
18	4	306	CHL	C3B-CAB	-2.01	1.43	1.47
18	2	305	CHL	C3B-CAB	-2.00	1.43	1.47

All (1570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	308	CLA	C4A-NA-C1A	11.53	111.89	106.71
19	A	803	CLA	C4A-NA-C1A	11.17	111.73	106.71
18	3	307	CHL	C4A-NA-C1A	10.94	111.62	106.71
19	B	826	CLA	C4A-NA-C1A	10.81	111.57	106.71
18	1	301	CHL	C4A-NA-C1A	10.76	111.54	106.71
19	B	805	CLA	C4A-NA-C1A	10.76	111.54	106.71
19	A	825	CLA	C4A-NA-C1A	10.74	111.53	106.71
18	2	306	CHL	C4A-NA-C1A	10.66	111.50	106.71
19	B	806	CLA	C4A-NA-C1A	10.65	111.50	106.71
19	3	311	CLA	C4A-NA-C1A	10.65	111.49	106.71
19	K	203	CLA	C4A-NA-C1A	10.65	111.49	106.71
19	B	840	CLA	C4A-NA-C1A	10.58	111.46	106.71
19	A	838	CLA	C4A-NA-C1A	10.57	111.46	106.71
19	B	833	CLA	C4A-NA-C1A	10.56	111.45	106.71
18	2	307	CHL	C4A-NA-C1A	10.51	111.43	106.71
19	1	310	CLA	C4A-NA-C1A	10.50	111.42	106.71
19	A	811	CLA	C4A-NA-C1A	10.48	111.42	106.71
19	A	814	CLA	C4A-NA-C1A	10.48	111.42	106.71
19	4	311	CLA	C4A-NA-C1A	10.46	111.41	106.71
19	2	311	CLA	C4A-NA-C1A	10.43	111.40	106.71
19	2	312	CLA	C4A-NA-C1A	10.43	111.39	106.71
19	1	311	CLA	C4A-NA-C1A	10.42	111.39	106.71
19	A	834	CLA	C4A-NA-C1A	10.41	111.39	106.71
19	A	854	CLA	C4A-NA-C1A	10.38	111.37	106.71
19	K	202	CLA	C4A-NA-C1A	10.36	111.36	106.71
19	B	813	CLA	C4A-NA-C1A	10.36	111.36	106.71
19	4	303	CLA	C4A-NA-C1A	10.35	111.36	106.71
19	B	815	CLA	C4A-NA-C1A	10.35	111.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	829	CLA	C4A-NA-C1A	10.33	111.35	106.71
19	2	304	CLA	C4A-NA-C1A	10.32	111.35	106.71
19	G	203	CLA	C4A-NA-C1A	10.32	111.35	106.71
19	2	313	CLA	C4A-NA-C1A	10.30	111.34	106.71
19	4	301	CLA	C4A-NA-C1A	10.27	111.33	106.71
19	G	204	CLA	C4A-NA-C1A	10.26	111.32	106.71
19	F	302	CLA	C4A-NA-C1A	10.25	111.31	106.71
19	B	818	CLA	C4A-NA-C1A	10.23	111.31	106.71
19	A	830	CLA	C4A-NA-C1A	10.23	111.30	106.71
19	B	803	CLA	C4A-NA-C1A	10.23	111.30	106.71
19	B	814	CLA	C4A-NA-C1A	10.20	111.29	106.71
18	2	301	CHL	C4A-NA-C1A	10.19	111.29	106.71
19	1	304	CLA	C4A-NA-C1A	10.18	111.28	106.71
19	1	312	CLA	C4A-NA-C1A	10.17	111.28	106.71
19	A	812	CLA	C4A-NA-C1A	10.16	111.27	106.71
19	4	302	CLA	C4A-NA-C1A	10.15	111.27	106.71
19	A	821	CLA	C4A-NA-C1A	10.15	111.27	106.71
19	4	309	CLA	C4A-NA-C1A	10.13	111.26	106.71
19	A	807	CLA	C4A-NA-C1A	10.13	111.26	106.71
19	4	308	CLA	C4A-NA-C1A	10.12	111.25	106.71
19	B	834	CLA	C4A-NA-C1A	10.11	111.25	106.71
19	3	312	CLA	C4A-NA-C1A	10.10	111.25	106.71
18	4	305	CHL	C4A-NA-C1A	10.10	111.25	106.71
18	4	314	CHL	C4A-NA-C1A	10.09	111.24	106.71
19	A	853	CLA	C4A-NA-C1A	10.08	111.24	106.71
19	4	304	CLA	C4A-NA-C1A	10.08	111.24	106.71
19	1	303	CLA	C4A-NA-C1A	10.07	111.23	106.71
19	B	835	CLA	C4A-NA-C1A	10.07	111.23	106.71
19	A	828	CLA	C4A-NA-C1A	10.06	111.23	106.71
19	3	310	CLA	C4A-NA-C1A	10.04	111.22	106.71
19	A	840	CLA	C4A-NA-C1A	10.03	111.22	106.71
18	1	306	CHL	C4A-NA-C1A	10.03	111.21	106.71
19	F	301	CLA	C4A-NA-C1A	10.02	111.21	106.71
19	B	812	CLA	C4A-NA-C1A	10.02	111.21	106.71
19	3	304	CLA	C4A-NA-C1A	9.99	111.20	106.71
19	A	820	CLA	C4A-NA-C1A	9.97	111.19	106.71
19	A	837	CLA	C4A-NA-C1A	9.96	111.19	106.71
19	A	826	CLA	C4A-NA-C1A	9.96	111.19	106.71
19	B	807	CLA	C4A-NA-C1A	9.94	111.17	106.71
19	A	829	CLA	C4A-NA-C1A	9.90	111.16	106.71
19	3	314	CLA	C4A-NA-C1A	9.88	111.15	106.71
19	B	808	CLA	C4A-NA-C1A	9.88	111.15	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	809	CLA	C4A-NA-C1A	9.87	111.14	106.71
19	A	818	CLA	C4A-NA-C1A	9.87	111.14	106.71
19	1	318	CLA	C4A-NA-C1A	9.87	111.14	106.71
19	B	804	CLA	C4A-NA-C1A	9.86	111.14	106.71
19	1	314	CLA	C4A-NA-C1A	9.84	111.13	106.71
18	4	307	CHL	C4A-NA-C1A	9.84	111.13	106.71
19	B	821	CLA	C4A-NA-C1A	9.83	111.13	106.71
19	B	837	CLA	C4A-NA-C1A	9.83	111.13	106.71
19	A	819	CLA	C4A-NA-C1A	9.83	111.12	106.71
19	A	802	CLA	C4A-NA-C1A	9.81	111.12	106.71
19	A	816	CLA	C4A-NA-C1A	9.81	111.11	106.71
19	B	810	CLA	C4A-NA-C1A	9.80	111.11	106.71
19	3	313	CLA	C4A-NA-C1A	9.80	111.11	106.71
19	A	808	CLA	C4A-NA-C1A	9.79	111.11	106.71
19	2	309	CLA	C4A-NA-C1A	9.78	111.10	106.71
19	3	309	CLA	C4A-NA-C1A	9.78	111.10	106.71
18	4	306	CHL	C4A-NA-C1A	9.77	111.10	106.71
19	B	828	CLA	C4A-NA-C1A	9.76	111.09	106.71
19	A	813	CLA	C4A-NA-C1A	9.74	111.09	106.71
19	A	805	CLA	C4A-NA-C1A	9.74	111.08	106.71
19	B	851	CLA	C4A-NA-C1A	9.74	111.08	106.71
19	B	809	CLA	C4A-NA-C1A	9.73	111.08	106.71
19	3	308	CLA	C4A-NA-C1A	9.73	111.08	106.71
19	4	312	CLA	C4A-NA-C1A	9.72	111.08	106.71
19	3	303	CLA	C4A-NA-C1A	9.70	111.07	106.71
19	1	302	CLA	C4A-NA-C1A	9.69	111.06	106.71
19	1	305	CLA	C4A-NA-C1A	9.68	111.06	106.71
19	2	310	CLA	C4A-NA-C1A	9.68	111.06	106.71
19	A	824	CLA	C4A-NA-C1A	9.67	111.06	106.71
19	B	825	CLA	C4A-NA-C1A	9.64	111.04	106.71
19	A	804	CLA	C4A-NA-C1A	9.64	111.04	106.71
19	A	832	CLA	C4A-NA-C1A	9.63	111.04	106.71
19	K	201	CLA	C4A-NA-C1A	9.63	111.04	106.71
19	A	839	CLA	C4A-NA-C1A	9.63	111.03	106.71
19	3	302	CLA	C4A-NA-C1A	9.62	111.03	106.71
19	A	815	CLA	C4A-NA-C1A	9.62	111.03	106.71
19	A	827	CLA	C4A-NA-C1A	9.60	111.02	106.71
19	2	303	CLA	C4A-NA-C1A	9.60	111.02	106.71
19	1	307	CLA	C4A-NA-C1A	9.60	111.02	106.71
19	B	836	CLA	C4A-NA-C1A	9.59	111.02	106.71
19	2	302	CLA	C4A-NA-C1A	9.58	111.01	106.71
19	1	313	CLA	C4A-NA-C1A	9.57	111.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	309	CLA	C4A-NA-C1A	9.56	111.00	106.71
19	A	801	CLA	C4A-NA-C1A	9.56	111.00	106.71
19	A	835	CLA	C4A-NA-C1A	9.56	111.00	106.71
19	B	819	CLA	C4A-NA-C1A	9.55	111.00	106.71
19	3	301	CLA	C4A-NA-C1A	9.53	110.99	106.71
19	B	831	CLA	C4A-NA-C1A	9.52	110.99	106.71
19	2	308	CLA	C4A-NA-C1A	9.51	110.98	106.71
19	B	832	CLA	C4A-NA-C1A	9.49	110.97	106.71
19	B	820	CLA	C4A-NA-C1A	9.47	110.96	106.71
19	B	816	CLA	C4A-NA-C1A	9.42	110.94	106.71
18	2	305	CHL	C4A-NA-C1A	9.42	110.94	106.71
19	B	802	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	A	810	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	B	822	CLA	C4A-NA-C1A	9.38	110.92	106.71
19	A	836	CLA	C4A-NA-C1A	9.36	110.92	106.71
19	3	306	CLA	C4A-NA-C1A	9.35	110.91	106.71
19	G	202	CLA	C4A-NA-C1A	9.35	110.91	106.71
19	B	838	CLA	C4A-NA-C1A	9.35	110.91	106.71
19	4	313	CLA	C4A-NA-C1A	9.34	110.91	106.71
19	B	839	CLA	C4A-NA-C1A	9.29	110.88	106.71
19	B	824	CLA	C4A-NA-C1A	9.29	110.88	106.71
19	A	852	CLA	C4A-NA-C1A	9.28	110.88	106.71
19	L	301	CLA	C4A-NA-C1A	9.25	110.86	106.71
19	B	830	CLA	C4A-NA-C1A	9.25	110.86	106.71
19	A	831	CLA	C4A-NA-C1A	9.24	110.86	106.71
19	3	305	CLA	C4A-NA-C1A	9.18	110.83	106.71
19	H	201	CLA	C4A-NA-C1A	9.12	110.80	106.71
19	L	302	CLA	C4A-NA-C1A	9.04	110.77	106.71
19	A	823	CLA	C4A-NA-C1A	8.94	110.73	106.71
19	A	817	CLA	C4A-NA-C1A	8.92	110.72	106.71
19	4	310	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	H	202	CLA	C4A-NA-C1A	8.88	110.70	106.71
19	A	822	CLA	C4A-NA-C1A	8.87	110.70	106.71
19	B	827	CLA	C4A-NA-C1A	8.87	110.69	106.71
19	A	806	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	B	811	CLA	C4A-NA-C1A	8.74	110.64	106.71
19	B	823	CLA	C4A-NA-C1A	8.72	110.62	106.71
19	J	102	CLA	C4A-NA-C1A	8.61	110.58	106.71
19	B	801	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	B	817	CLA	C4A-NA-C1A	8.11	110.35	106.71
19	A	833	CLA	C4A-NA-C1A	7.92	110.27	106.71
18	2	314	CHL	C4A-NA-C1A	7.16	109.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	811	CLA	CAB-C3B-C4B	5.73	137.27	128.46
19	B	836	CLA	O2D-CGD-CBD	4.58	119.41	111.27
19	B	829	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	B	810	CLA	O2D-CGD-CBD	4.49	119.25	111.27
19	A	801	CLA	O2D-CGD-CBD	4.41	119.11	111.27
19	A	854	CLA	O2D-CGD-CBD	4.35	118.99	111.27
19	B	811	CLA	CAB-C3B-C2B	-4.33	116.21	124.69
19	A	810	CLA	O2D-CGD-CBD	4.29	118.90	111.27
19	A	820	CLA	O2D-CGD-CBD	4.25	118.82	111.27
19	A	853	CLA	O2D-CGD-CBD	4.23	118.78	111.27
19	B	818	CLA	O2D-CGD-CBD	4.22	118.76	111.27
20	1	319	LUT	C35-C15-C14	4.21	132.09	123.47
19	A	802	CLA	O2D-CGD-CBD	4.20	118.73	111.27
20	1	319	LUT	C19-C9-C10	-4.20	117.04	122.92
18	4	314	CHL	CAA-C2A-C3A	-4.18	103.81	114.26
18	1	306	CHL	O2D-CGD-CBD	4.18	118.70	111.27
19	4	304	CLA	O2D-CGD-CBD	4.17	118.69	111.27
19	B	839	CLA	O2D-CGD-CBD	4.14	118.63	111.27
18	2	314	CHL	CAA-C2A-C3A	-4.14	103.92	114.26
18	2	305	CHL	CAA-C2A-C3A	-4.14	103.92	114.26
19	A	834	CLA	C4-C3-C5	-4.11	111.29	115.98
19	B	838	CLA	O2D-CGD-CBD	4.10	118.55	111.27
19	B	832	CLA	O2D-CGD-CBD	4.09	118.54	111.27
19	A	816	CLA	O2D-CGD-CBD	4.09	118.53	111.27
19	B	816	CLA	O2D-CGD-CBD	4.08	118.53	111.27
19	B	807	CLA	O2D-CGD-CBD	4.08	118.52	111.27
19	A	825	CLA	O2D-CGD-CBD	4.08	118.52	111.27
19	4	311	CLA	O2D-CGD-CBD	4.07	118.50	111.27
19	B	809	CLA	O2D-CGD-CBD	4.06	118.49	111.27
19	3	308	CLA	O2D-CGD-CBD	4.06	118.49	111.27
19	A	840	CLA	O2D-CGD-CBD	4.06	118.48	111.27
19	A	809	CLA	O2D-CGD-CBD	4.05	118.46	111.27
19	A	829	CLA	O2D-CGD-CBD	4.05	118.46	111.27
19	3	303	CLA	O2D-CGD-CBD	4.04	118.45	111.27
19	B	828	CLA	O2D-CGD-CBD	4.04	118.45	111.27
19	B	805	CLA	O2D-CGD-CBD	4.04	118.45	111.27
19	A	835	CLA	O2D-CGD-CBD	4.03	118.44	111.27
19	2	312	CLA	O2D-CGD-CBD	4.03	118.43	111.27
19	A	826	CLA	O2D-CGD-CBD	4.03	118.42	111.27
19	2	310	CLA	O2D-CGD-CBD	4.02	118.42	111.27
19	A	832	CLA	O2D-CGD-CBD	4.02	118.41	111.27
19	A	827	CLA	O2D-CGD-CBD	4.02	118.41	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	836	CLA	O2D-CGD-CBD	4.02	118.41	111.27
19	B	817	CLA	O2D-CGD-CBD	4.02	118.41	111.27
19	B	820	CLA	O2D-CGD-CBD	4.02	118.40	111.27
19	A	807	CLA	O2D-CGD-CBD	4.01	118.40	111.27
19	4	308	CLA	O2D-CGD-CBD	4.00	118.38	111.27
19	B	834	CLA	O2D-CGD-CBD	4.00	118.37	111.27
19	G	203	CLA	O2D-CGD-CBD	3.99	118.36	111.27
19	J	102	CLA	O2D-CGD-CBD	3.99	118.36	111.27
19	A	852	CLA	O2D-CGD-CBD	3.99	118.36	111.27
19	3	312	CLA	O2D-CGD-CBD	3.99	118.36	111.27
19	A	808	CLA	O2D-CGD-CBD	3.99	118.35	111.27
19	B	837	CLA	O2D-CGD-CBD	3.98	118.34	111.27
19	A	805	CLA	O2D-CGD-CBD	3.96	118.31	111.27
19	A	817	CLA	O2D-CGD-CBD	3.96	118.31	111.27
19	4	309	CLA	O2D-CGD-CBD	3.96	118.31	111.27
19	B	814	CLA	O2D-CGD-CBD	3.95	118.30	111.27
19	A	818	CLA	O2D-CGD-CBD	3.95	118.29	111.27
19	A	811	CLA	O2D-CGD-CBD	3.95	118.29	111.27
19	2	304	CLA	O2D-CGD-CBD	3.95	118.28	111.27
19	1	312	CLA	O2D-CGD-CBD	3.94	118.28	111.27
19	2	309	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	3	316	XAT	C7-C8-C9	3.94	131.65	125.53
18	4	305	CHL	O2D-CGD-CBD	3.94	118.27	111.27
19	A	803	CLA	O2D-CGD-CBD	3.92	118.23	111.27
19	B	824	CLA	O2D-CGD-CBD	3.92	118.23	111.27
19	2	308	CLA	O2D-CGD-CBD	3.91	118.22	111.27
18	3	307	CHL	O2D-CGD-CBD	3.91	118.22	111.27
19	1	303	CLA	O2D-CGD-CBD	3.91	118.22	111.27
19	B	804	CLA	O2D-CGD-CBD	3.91	118.21	111.27
19	B	801	CLA	O2D-CGD-CBD	3.90	118.20	111.27
19	B	803	CLA	O2D-CGD-CBD	3.90	118.20	111.27
19	A	834	CLA	O2D-CGD-CBD	3.90	118.19	111.27
19	1	314	CLA	O2D-CGD-CBD	3.89	118.19	111.27
20	1	319	LUT	C39-C29-C30	-3.89	117.47	122.92
19	B	808	CLA	O2D-CGD-CBD	3.89	118.18	111.27
19	1	309	CLA	O2D-CGD-CBD	3.89	118.17	111.27
19	B	819	CLA	O2D-CGD-CBD	3.88	118.17	111.27
19	A	839	CLA	O2D-CGD-CBD	3.88	118.16	111.27
19	F	302	CLA	O2D-CGD-CBD	3.88	118.16	111.27
20	2	315	LUT	C19-C9-C10	-3.88	117.49	122.92
19	B	851	CLA	O2D-CGD-CBD	3.88	118.16	111.27
19	A	813	CLA	O2D-CGD-CBD	3.87	118.15	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	840	CLA	O2D-CGD-CBD	3.87	118.14	111.27
19	B	835	CLA	O2D-CGD-CBD	3.87	118.14	111.27
19	3	302	CLA	O2D-CGD-CBD	3.87	118.14	111.27
20	1	315	LUT	C15-C35-C34	3.87	131.39	123.47
18	2	314	CHL	O2D-CGD-CBD	3.86	118.13	111.27
19	A	824	CLA	O2D-CGD-CBD	3.85	118.11	111.27
19	B	826	CLA	O2D-CGD-CBD	3.85	118.10	111.27
19	4	313	CLA	O2D-CGD-CBD	3.84	118.10	111.27
19	B	851	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	4	301	CLA	O2D-CGD-CBD	3.84	118.10	111.27
19	3	310	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	B	831	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	1	313	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	3	306	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	1	307	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	A	833	CLA	O2D-CGD-CBD	3.83	118.07	111.27
20	4	315	LUT	C39-C29-C30	-3.83	117.56	122.92
19	F	301	CLA	O2D-CGD-CBD	3.83	118.07	111.27
19	A	806	CLA	O2D-CGD-CBD	3.81	118.05	111.27
19	2	313	CLA	O2D-CGD-CBD	3.81	118.04	111.27
19	3	309	CLA	O2D-CGD-CBD	3.81	118.03	111.27
19	G	202	CLA	O2D-CGD-CBD	3.81	118.03	111.27
18	4	306	CHL	O2D-CGD-CBD	3.80	118.03	111.27
20	3	315	LUT	C39-C29-C30	-3.80	117.60	122.92
19	B	813	CLA	O2D-CGD-CBD	3.80	118.02	111.27
19	K	202	CLA	O2D-CGD-CBD	3.80	118.02	111.27
19	B	822	CLA	O2D-CGD-CBD	3.80	118.02	111.27
19	A	823	CLA	O2D-CGD-CBD	3.80	118.02	111.27
19	A	838	CLA	O2D-CGD-CBD	3.79	118.01	111.27
19	1	305	CLA	O2D-CGD-CBD	3.79	118.01	111.27
19	3	314	CLA	O2D-CGD-CBD	3.79	118.01	111.27
19	A	828	CLA	O2D-CGD-CBD	3.79	118.01	111.27
20	1	315	LUT	C19-C9-C10	-3.78	117.63	122.92
19	L	302	CLA	O2D-CGD-CBD	3.77	117.98	111.27
19	1	318	CLA	O2D-CGD-CBD	3.77	117.97	111.27
19	A	812	CLA	O2D-CGD-CBD	3.77	117.96	111.27
20	1	315	LUT	C39-C29-C30	-3.76	117.65	122.92
20	3	315	LUT	C19-C9-C10	-3.76	117.66	122.92
19	3	305	CLA	O2D-CGD-CBD	3.76	117.95	111.27
19	A	821	CLA	O2D-CGD-CBD	3.76	117.94	111.27
19	H	202	CLA	O2D-CGD-CBD	3.76	117.94	111.27
19	B	833	CLA	O2D-CGD-CBD	3.76	117.94	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	302	CLA	O2D-CGD-CBD	3.75	117.94	111.27
19	A	819	CLA	O2D-CGD-CBD	3.75	117.94	111.27
19	2	311	CLA	O2D-CGD-CBD	3.75	117.94	111.27
20	2	315	LUT	C15-C35-C34	3.75	131.16	123.47
19	A	814	CLA	O2D-CGD-CBD	3.75	117.93	111.27
19	1	311	CLA	O2D-CGD-CBD	3.75	117.93	111.27
19	1	308	CLA	CHD-C1D-ND	-3.75	121.01	124.45
19	G	204	CLA	O2D-CGD-CBD	3.74	117.92	111.27
19	B	827	CLA	O2D-CGD-CBD	3.74	117.91	111.27
20	2	315	LUT	C39-C29-C30	-3.73	117.70	122.92
18	4	307	CHL	O2D-CGD-CBD	3.71	117.87	111.27
19	B	812	CLA	O2D-CGD-CBD	3.71	117.86	111.27
18	2	307	CHL	O2D-CGD-CBD	3.71	117.86	111.27
19	3	313	CLA	O2D-CGD-CBD	3.69	117.83	111.27
19	1	308	CLA	O2D-CGD-CBD	3.69	117.82	111.27
19	1	304	CLA	O2D-CGD-CBD	3.68	117.81	111.27
18	2	306	CHL	O2D-CGD-CBD	3.67	117.80	111.27
19	1	302	CLA	O2D-CGD-CBD	3.67	117.78	111.27
19	2	302	CLA	O2D-CGD-CBD	3.67	117.78	111.27
19	2	303	CLA	O2D-CGD-CBD	3.66	117.78	111.27
19	B	811	CLA	O2D-CGD-CBD	3.65	117.75	111.27
19	H	201	CLA	O2D-CGD-CBD	3.62	117.70	111.27
19	B	802	CLA	O2D-CGD-CBD	3.61	117.69	111.27
20	4	315	LUT	C19-C9-C10	-3.61	117.86	122.92
19	4	312	CLA	O2D-CGD-CBD	3.61	117.69	111.27
20	3	315	LUT	C15-C35-C34	3.61	130.87	123.47
18	1	301	CHL	C1-C2-C3	3.61	132.28	126.04
19	L	301	CLA	O2D-CGD-CBD	3.61	117.68	111.27
19	B	821	CLA	O2D-CGD-CBD	3.61	117.67	111.27
19	4	310	CLA	O2D-CGD-CBD	3.56	117.60	111.27
19	K	201	CLA	O2D-CGD-CBD	3.56	117.59	111.27
19	A	804	CLA	O2D-CGD-CBD	3.55	117.58	111.27
19	B	806	CLA	O2D-CGD-CBD	3.53	117.54	111.27
19	A	822	CLA	O2D-CGD-CBD	3.52	117.53	111.27
19	B	815	CLA	O2D-CGD-CBD	3.52	117.52	111.27
19	A	830	CLA	O2D-CGD-CBD	3.52	117.52	111.27
19	3	304	CLA	O2D-CGD-CBD	3.51	117.51	111.27
19	1	309	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
18	2	301	CHL	C1-C2-C3	3.49	132.41	126.75
19	B	825	CLA	O2D-CGD-CBD	3.49	117.47	111.27
24	J	101	BCR	C16-C15-C14	3.47	130.59	123.47
19	B	801	CLA	CMB-C2B-C1B	-3.47	123.13	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	301	CLA	O2D-CGD-CBD	3.47	117.44	111.27
19	A	837	CLA	O2D-CGD-CBD	3.44	117.38	111.27
18	4	305	CHL	CAA-C2A-C3A	-3.44	103.37	112.78
20	1	319	LUT	C20-C13-C14	-3.43	118.11	122.92
18	4	306	CHL	CAA-C2A-C3A	-3.43	103.40	112.78
19	1	304	CLA	C4-C3-C5	-3.41	112.08	115.98
18	2	301	CHL	O2D-CGD-CBD	3.41	117.33	111.27
19	1	310	CLA	O2D-CGD-CBD	3.41	117.32	111.27
21	1	316	XAT	C7-C8-C9	3.40	130.81	125.53
19	B	817	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
18	1	301	CHL	CAA-C2A-C3A	-3.37	103.54	112.78
18	2	301	CHL	CAA-C2A-C3A	-3.35	103.61	112.78
19	A	826	CLA	CHD-C1D-ND	-3.34	121.38	124.45
18	2	306	CHL	CHD-C1D-ND	-3.34	121.38	124.45
19	B	825	CLA	CHD-C1D-ND	-3.34	121.38	124.45
19	F	302	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
19	1	310	CLA	CHD-C1D-ND	-3.33	121.39	124.45
19	A	811	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
20	4	315	LUT	C19-C9-C8	3.33	123.32	118.08
19	A	833	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
19	A	801	CLA	CHD-C1D-ND	-3.32	121.40	124.45
19	A	831	CLA	O2D-CGD-CBD	3.32	117.16	111.27
19	3	311	CLA	O2D-CGD-CBD	3.31	117.15	111.27
18	3	307	CHL	CAA-C2A-C3A	-3.31	103.71	112.78
19	1	302	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
18	2	305	CHL	O2D-CGD-CBD	3.31	117.14	111.27
19	A	832	CLA	CHD-C1D-ND	-3.30	121.42	124.45
21	3	316	XAT	O24-C25-C24	-3.29	110.91	113.38
19	4	303	CLA	O2D-CGD-CBD	3.28	117.11	111.27
19	B	838	CLA	O2A-CGA-CBA	3.28	122.21	111.91
19	A	823	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
19	B	801	CLA	O2A-CGA-CBA	3.28	122.20	111.91
19	2	304	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	A	852	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	2	304	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	B	801	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	1	301	CHL	O2D-CGD-CBD	3.26	117.06	111.27
19	1	314	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
19	B	809	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
18	2	307	CHL	CAA-C2A-C3A	-3.25	103.88	112.78
19	1	310	CLA	O2A-CGA-CBA	3.25	122.10	111.91
19	B	823	CLA	O2D-CGD-CBD	3.25	117.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	CHD-C1D-ND	-3.24	121.47	124.45
24	L	304	BCR	C16-C15-C14	3.24	130.12	123.47
19	A	840	CLA	O2A-CGA-CBA	3.24	122.07	111.91
19	2	308	CLA	CHD-C1D-ND	-3.23	121.48	124.45
19	B	830	CLA	O2D-CGD-CBD	3.23	117.01	111.27
18	2	306	CHL	CAA-C2A-C3A	-3.22	103.96	112.78
19	A	807	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
19	B	822	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
18	2	314	CHL	CHD-C1D-ND	-3.21	121.50	124.45
20	1	315	LUT	C40-C33-C34	-3.21	118.43	122.92
19	A	812	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
19	B	832	CLA	O2A-CGA-CBA	3.20	121.95	111.91
19	L	301	CLA	O2A-CGA-CBA	3.20	121.95	111.91
19	A	825	CLA	O2A-CGA-CBA	3.20	121.95	111.91
19	A	805	CLA	O2A-CGA-CBA	3.19	121.93	111.91
21	4	316	XAT	C7-C8-C9	3.19	130.47	125.53
19	3	304	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
20	3	315	LUT	C35-C15-C14	3.18	129.99	123.47
19	A	834	CLA	O2A-CGA-CBA	3.18	121.88	111.91
19	B	824	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
19	B	828	CLA	O2A-CGA-CBA	3.17	121.85	111.91
19	B	811	CLA	CHD-C1D-ND	-3.17	121.54	124.45
19	A	839	CLA	O2A-CGA-CBA	3.17	121.85	111.91
19	A	802	CLA	O2A-CGA-CBA	3.17	121.85	111.91
19	A	838	CLA	O2A-CGA-CBA	3.17	121.84	111.91
19	A	819	CLA	O2A-CGA-CBA	3.16	121.84	111.91
19	3	302	CLA	O2A-CGA-CBA	3.16	121.83	111.91
19	B	826	CLA	O2A-CGA-CBA	3.16	121.83	111.91
18	2	305	CHL	CHD-C1D-ND	-3.16	121.55	124.45
19	A	830	CLA	O2A-CGA-CBA	3.16	121.81	111.91
19	A	819	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
19	A	826	CLA	O2A-CGA-CBA	3.16	121.81	111.91
18	4	305	CHL	CHD-C1D-ND	-3.15	121.56	124.45
19	B	808	CLA	O2A-CGA-CBA	3.15	121.81	111.91
19	A	807	CLA	O2A-CGA-CBA	3.15	121.79	111.91
19	A	811	CLA	O2A-CGA-CBA	3.15	121.79	111.91
19	B	821	CLA	O2A-CGA-CBA	3.15	121.78	111.91
18	4	307	CHL	CAA-C2A-C3A	-3.14	104.17	112.78
20	1	319	LUT	C12-C13-C14	3.14	123.76	118.94
19	A	806	CLA	O2A-CGA-CBA	3.14	121.77	111.91
19	A	819	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	K	203	CLA	CMB-C2B-C1B	-3.14	123.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	833	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	A	813	CLA	O2A-CGA-CBA	3.14	121.75	111.91
19	A	831	CLA	O2A-CGA-CBA	3.13	121.73	111.91
19	A	816	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	4	309	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	A	833	CLA	O2A-CGA-CBA	3.12	121.70	111.91
19	3	312	CLA	O2A-CGA-CBA	3.11	121.68	111.91
19	A	835	CLA	O2A-CGA-CBA	3.11	121.68	111.91
19	4	303	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
19	3	303	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
19	F	301	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
19	2	310	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	A	830	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
19	A	811	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	4	309	CLA	O2A-CGA-CBA	3.11	121.66	111.91
19	A	809	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	B	805	CLA	O2A-CGA-CBA	3.11	121.66	111.91
20	1	319	LUT	C40-C33-C34	-3.10	118.57	122.92
19	B	851	CLA	CHD-C1D-ND	-3.10	121.60	124.45
19	3	306	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
19	1	318	CLA	CHD-C1D-ND	-3.10	121.60	124.45
19	B	835	CLA	O2A-CGA-CBA	3.10	121.64	111.91
18	1	306	CHL	CAA-C2A-C3A	-3.10	104.29	112.78
19	A	817	CLA	O2A-CGA-CBA	3.10	121.63	111.91
19	B	817	CLA	C12-C11-C10	-3.10	102.67	113.62
19	1	312	CLA	O2A-CGA-CBA	3.09	121.61	111.91
19	4	308	CLA	O2A-CGA-CBA	3.09	121.61	111.91
19	2	302	CLA	O2A-CGA-CBA	3.09	121.61	111.91
20	2	315	LUT	C40-C33-C34	-3.09	118.59	122.92
19	A	854	CLA	O2A-CGA-CBA	3.09	121.61	111.91
20	4	315	LUT	C15-C35-C34	3.09	129.80	123.47
19	A	829	CLA	CHD-C1D-ND	-3.09	121.62	124.45
24	J	101	BCR	C21-C20-C19	3.09	132.84	123.22
19	B	802	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	B	836	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
20	3	315	LUT	C40-C33-C34	-3.08	118.61	122.92
19	1	308	CLA	C1-C2-C3	3.08	131.37	126.04
19	H	201	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	4	302	CLA	CHD-C1D-ND	-3.08	121.63	124.45
19	A	821	CLA	O2A-CGA-CBA	3.08	121.56	111.91
19	2	312	CLA	O2A-CGA-CBA	3.08	121.56	111.91
19	B	818	CLA	O2A-CGA-CBA	3.08	121.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	308	CLA	O2A-CGA-CBA	3.07	121.55	111.91
19	2	309	CLA	O2A-CGA-CBA	3.07	121.55	111.91
19	B	836	CLA	O2A-CGA-CBA	3.07	121.55	111.91
19	J	102	CLA	CHD-C1D-ND	-3.07	121.63	124.45
19	B	813	CLA	O2A-CGA-CBA	3.07	121.54	111.91
19	3	302	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	1	313	CLA	CHD-C1D-ND	-3.07	121.63	124.45
19	1	304	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	G	203	CLA	O2A-CGA-CBA	3.06	121.53	111.91
19	3	310	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	G	204	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	A	838	CLA	CHD-C1D-ND	-3.06	121.64	124.45
19	1	309	CLA	CHD-C1D-ND	-3.06	121.64	124.45
19	A	810	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	3	304	CLA	O2A-CGA-CBA	3.06	121.51	111.91
19	B	817	CLA	O2A-CGA-CBA	3.06	121.51	111.91
19	4	311	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
20	1	319	LUT	C15-C35-C34	3.06	129.74	123.47
19	4	302	CLA	O2A-CGA-CBA	3.06	121.50	111.91
19	3	305	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
19	B	807	CLA	O2A-CGA-CBA	3.06	121.50	111.91
19	3	302	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	A	837	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
19	1	311	CLA	O2A-CGA-CBA	3.05	121.49	111.91
19	2	309	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	A	822	CLA	O2A-CGA-CBA	3.05	121.48	111.91
19	B	836	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	H	202	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
19	4	301	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
19	A	828	CLA	O2A-CGA-CBA	3.05	121.47	111.91
19	A	805	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
19	A	839	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
24	L	304	BCR	C15-C16-C17	3.04	129.71	123.47
19	2	310	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	B	831	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	4	304	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	A	813	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	A	825	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	B	803	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
20	4	315	LUT	C35-C15-C14	3.04	129.70	123.47
19	2	309	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
18	4	305	CHL	C1-C2-C3	3.04	131.29	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	303	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	B	812	CLA	O2A-CGA-CBA	3.04	121.44	111.91
19	B	819	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
20	3	315	LUT	C20-C13-C14	-3.04	118.67	122.92
19	B	833	CLA	O2A-CGA-CBA	3.03	121.43	111.91
19	J	102	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
19	A	833	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	837	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
19	3	309	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
19	B	809	CLA	O2A-CGA-CBA	3.03	121.42	111.91
19	1	304	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	809	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	834	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	827	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
19	B	839	CLA	O2A-CGA-CBA	3.03	121.40	111.91
19	3	308	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	812	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	816	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
19	B	840	CLA	O2A-CGA-CBA	3.02	121.40	111.91
19	B	829	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	A	802	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	A	815	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	1	310	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	B	830	CLA	O2A-CGA-CBA	3.02	121.38	111.91
19	4	304	CLA	CHD-C1D-ND	-3.02	121.68	124.45
19	B	819	CLA	O2A-CGA-CBA	3.02	121.38	111.91
19	1	307	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	G	203	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	G	202	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	4	312	CLA	O2A-CGA-CBA	3.01	121.36	111.91
19	4	309	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	4	308	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	3	312	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	B	832	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	1	309	CLA	O2A-CGA-CBA	3.01	121.34	111.91
19	B	830	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	4	301	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	B	811	CLA	O2A-CGA-CBA	3.00	121.34	111.91
19	B	808	CLA	CHD-C1D-ND	-3.00	121.69	124.45
19	A	809	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	3	308	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	B	839	CLA	CMB-C2B-C1B	-3.00	123.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	854	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	B	823	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	4	308	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	A	808	CLA	C12-C11-C10	-3.00	103.01	113.62
19	B	837	CLA	O2A-CGA-CBA	3.00	121.31	111.91
19	A	835	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
19	4	313	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	B	820	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	B	813	CLA	CHD-C1D-ND	-2.99	121.70	124.45
19	B	815	CLA	CHD-C1D-ND	-2.99	121.70	124.45
19	G	203	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	4	307	CHL	C1-C2-C3	2.99	131.59	126.75
19	4	310	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	837	CLA	O2A-CGA-CBA	2.99	121.29	111.91
18	4	307	CHL	O2A-CGA-CBA	2.99	121.29	111.91
19	B	814	CLA	CHD-C1D-ND	-2.99	121.71	124.45
19	1	318	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	801	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
20	1	315	LUT	C20-C13-C14	-2.99	118.73	122.92
19	A	817	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	802	CLA	CHD-C1D-ND	-2.99	121.71	124.45
19	B	825	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	821	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	3	314	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	832	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	818	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	B	815	CLA	O2A-CGA-CBA	2.99	121.28	111.91
19	3	301	CLA	O2A-CGA-CBA	2.99	121.28	111.91
19	2	311	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
19	B	833	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
18	2	301	CHL	CHD-C1D-ND	-2.98	121.71	124.45
19	L	301	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	1	303	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	K	202	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	B	802	CLA	CHD-C1D-ND	-2.98	121.71	124.45
19	B	840	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	4	312	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	K	201	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	A	810	CLA	O2A-CGA-CBA	2.98	121.26	111.91
19	4	302	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
19	A	829	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
19	1	312	CLA	CMB-C2B-C1B	-2.98	123.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	A	806	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	B	813	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
19	A	825	CLA	CHD-C1D-ND	-2.98	121.72	124.45
24	2	319	BCR	C7-C8-C9	2.97	130.73	126.23
19	1	318	CLA	O2A-CGA-CBA	2.97	121.24	111.91
19	B	806	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
19	B	825	CLA	O2A-CGA-CBA	2.97	121.24	111.91
19	A	834	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
19	2	313	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
26	B	841	PQN	C11-C3-C4	-2.97	115.32	118.50
19	2	308	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
19	A	822	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
19	1	311	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
19	A	829	CLA	O2A-CGA-CBA	2.97	121.22	111.91
19	B	827	CLA	O2A-CGA-CBA	2.97	121.22	111.91
19	A	822	CLA	CHD-C1D-ND	-2.97	121.73	124.45
19	3	301	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
19	3	313	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
19	B	831	CLA	O2A-CGA-CBA	2.97	121.21	111.91
20	4	315	LUT	C40-C33-C34	-2.97	118.77	122.92
19	B	812	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	A	828	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	A	853	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	A	836	CLA	O2A-CGA-CBA	2.96	121.19	111.91
19	B	835	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
19	1	313	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
19	A	835	CLA	CHD-C1D-ND	-2.96	121.74	124.45
19	B	810	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
19	A	852	CLA	CHD-C1D-ND	-2.95	121.74	124.45
19	1	304	CLA	O2A-CGA-CBA	2.95	121.18	111.91
19	B	814	CLA	O2A-CGA-CBA	2.95	121.17	111.91
19	B	838	CLA	CHD-C1D-ND	-2.95	121.74	124.45
19	A	804	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	B	818	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	A	824	CLA	O2A-CGA-CBA	2.95	121.17	111.91
19	A	840	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	A	827	CLA	O2A-CGA-CBA	2.95	121.16	111.91
19	A	836	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	H	202	CLA	O2A-CGA-CBA	2.95	121.16	111.91
19	4	310	CLA	CHD-C1D-ND	-2.95	121.75	124.45
19	B	807	CLA	CMB-C2B-C1B	-2.94	123.94	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	302	CLA	O2A-CGA-CBA	2.94	121.15	111.91
19	A	808	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	A	838	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	A	820	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	B	826	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
20	2	315	LUT	C20-C13-C14	-2.94	118.81	122.92
19	B	827	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
19	3	309	CLA	O2A-CGA-CBA	2.94	121.12	111.91
19	B	838	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
19	1	312	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	A	814	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
19	B	821	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	B	829	CLA	O2A-CGA-CBA	2.93	121.10	111.91
19	A	854	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	B	811	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	3	309	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	B	807	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	A	803	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	A	813	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	3	311	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
19	B	815	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
19	B	804	CLA	CHD-C1D-ND	-2.93	121.77	124.45
19	B	826	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	836	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	B	828	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
19	B	806	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	B	824	CLA	O2A-CGA-CBA	2.92	121.07	111.91
18	4	305	CHL	O2A-CGA-CBA	2.92	121.07	111.91
19	2	302	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
19	4	303	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	A	808	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	A	806	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
19	B	834	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
19	B	820	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	A	803	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
19	2	303	CLA	O2A-CGA-CBA	2.91	121.03	111.91
18	4	314	CHL	CHD-C1D-ND	-2.90	121.79	124.45
18	3	307	CHL	CHD-C1D-ND	-2.90	121.79	124.45
19	B	808	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
19	B	851	CLA	O2A-CGA-CBA	2.90	121.01	111.91
19	1	308	CLA	O2A-CGA-CBA	2.90	121.00	111.91
19	B	827	CLA	CHD-C1D-ND	-2.90	121.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	804	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
19	B	806	CLA	O2A-CGA-CBA	2.90	121.00	111.91
19	A	807	CLA	CHD-C1D-ND	-2.90	121.79	124.45
19	B	832	CLA	CHD-C1D-ND	-2.89	121.79	124.45
19	A	823	CLA	CHD-C1D-ND	-2.89	121.80	124.45
19	A	828	CLA	CHD-C1D-ND	-2.89	121.80	124.45
19	2	302	CLA	CHD-C1D-ND	-2.88	121.80	124.45
19	1	305	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
19	A	853	CLA	O2A-CGA-CBA	2.88	120.95	111.91
19	B	816	CLA	O2A-CGA-CBA	2.88	120.95	111.91
19	A	826	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
19	A	831	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
19	L	302	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
19	3	311	CLA	CHD-C1D-ND	-2.88	121.81	124.45
19	4	303	CLA	O2A-CGA-CBA	2.88	120.94	111.91
20	2	315	LUT	C35-C15-C14	2.88	129.37	123.47
19	F	301	CLA	CHD-C1D-ND	-2.88	121.81	124.45
19	A	823	CLA	O2A-CGA-CBA	2.88	120.93	111.91
19	B	825	CLA	O1D-CGD-CBD	-2.87	118.60	124.48
19	A	805	CLA	CHD-C1D-ND	-2.87	121.81	124.45
19	B	816	CLA	CHD-C1D-ND	-2.87	121.81	124.45
19	A	821	CLA	C4-C3-C5	-2.87	112.70	115.98
19	4	310	CLA	O2A-CGA-CBA	2.87	120.90	111.91
19	2	312	CLA	CHD-C1D-ND	-2.86	121.82	124.45
19	3	303	CLA	CHD-C1D-ND	-2.86	121.82	124.45
19	B	829	CLA	C1-C2-C3	2.86	130.99	126.04
19	A	809	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	B	823	CLA	O2A-CGA-CBA	2.86	120.88	111.91
19	A	837	CLA	CHD-C1D-ND	-2.86	121.83	124.45
19	3	304	CLA	CHD-C1D-ND	-2.85	121.83	124.45
26	A	841	PQN	C11-C3-C4	-2.85	115.45	118.50
19	A	840	CLA	CHD-C1D-ND	-2.85	121.83	124.45
21	1	316	XAT	O24-C25-C24	-2.85	111.24	113.38
19	2	303	CLA	CHD-C1D-ND	-2.85	121.83	124.45
19	2	311	CLA	CHD-C1D-ND	-2.85	121.83	124.45
19	A	816	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	4	307	CHL	CHD-C1D-ND	-2.85	121.84	124.45
19	B	829	CLA	CHD-C1D-ND	-2.85	121.84	124.45
19	A	824	CLA	C1-C2-C3	2.85	130.96	126.04
24	J	101	BCR	C15-C16-C17	-2.85	117.65	123.47
19	B	810	CLA	O2A-CGA-CBA	2.84	120.83	111.91
19	1	303	CLA	CHD-C1D-ND	-2.84	121.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	307	CLA	CHD-C1D-ND	-2.84	121.84	124.45
19	H	201	CLA	CHD-C1D-ND	-2.84	121.84	124.45
21	2	316	XAT	O4-C5-C4	-2.84	111.25	113.38
19	3	301	CLA	CHD-C1D-ND	-2.84	121.84	124.45
19	B	823	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	L	302	CLA	O2A-CGA-CBA	2.84	120.81	111.91
18	2	301	CHL	O2A-CGA-CBA	2.84	120.81	111.91
19	1	318	CLA	C1-C2-C3	2.84	130.95	126.04
19	3	306	CLA	CHD-C1D-ND	-2.83	121.85	124.45
19	A	839	CLA	CHD-C1D-ND	-2.83	121.85	124.45
19	4	303	CLA	C1-C2-C3	2.82	130.93	126.04
19	A	831	CLA	CHD-C1D-ND	-2.82	121.86	124.45
21	4	316	XAT	O24-C25-C24	-2.82	111.26	113.38
19	B	812	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	B	803	CLA	O2A-CGA-CBA	2.82	120.76	111.91
19	A	824	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
19	A	807	CLA	C1-C2-C3	2.82	130.92	126.04
19	B	817	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	B	822	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	B	805	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
21	1	316	XAT	O4-C5-C4	-2.81	111.27	113.38
19	A	809	CLA	C1-C2-C3	2.81	130.91	126.04
18	3	307	CHL	CMB-C2B-C1B	-2.81	124.14	128.46
19	A	810	CLA	CHD-C1D-ND	-2.81	121.87	124.45
19	B	805	CLA	CHD-C1D-ND	-2.81	121.88	124.45
19	L	302	CLA	CHD-C1D-ND	-2.80	121.88	124.45
19	A	822	CLA	C1-C2-C3	2.80	130.89	126.04
19	A	808	CLA	O2A-CGA-CBA	2.80	120.69	111.91
19	B	814	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
18	4	306	CHL	CHD-C1D-ND	-2.79	121.89	124.45
19	B	835	CLA	CHD-C1D-ND	-2.79	121.89	124.45
18	1	306	CHL	CHD-C1D-ND	-2.79	121.89	124.45
19	A	827	CLA	CHD-C1D-ND	-2.79	121.89	124.45
19	A	852	CLA	O2A-CGA-CBA	2.79	120.66	111.91
20	4	315	LUT	C20-C13-C14	-2.79	119.02	122.92
19	A	816	CLA	O2A-CGA-CBA	2.79	120.66	111.91
19	1	308	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
19	A	801	CLA	O2A-CGA-CBA	2.79	120.65	111.91
19	A	815	CLA	CHD-C1D-ND	-2.79	121.89	124.45
19	B	819	CLA	CHD-C1D-ND	-2.78	121.90	124.45
19	A	829	CLA	C1-C2-C3	2.77	130.84	126.04
18	1	301	CHL	CHD-C1D-ND	-2.77	121.91	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	O2A-CGA-CBA	2.77	120.60	111.91
19	A	804	CLA	O2A-CGA-CBA	2.77	120.59	111.91
19	A	810	CLA	C1-C2-C3	2.77	130.83	126.04
24	B	844	BCR	C16-C15-C14	2.77	129.14	123.47
19	B	828	CLA	CHD-C1D-ND	-2.77	121.91	124.45
19	B	821	CLA	CHD-C1D-ND	-2.76	121.91	124.45
19	B	837	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	G	202	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	B	810	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	1	305	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	F	302	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	1	302	CLA	C1-C2-C3	2.75	130.81	126.04
19	A	817	CLA	CHD-C1D-ND	-2.75	121.92	124.45
19	B	814	CLA	C1-C2-C3	2.75	130.80	126.04
19	2	310	CLA	CMA-C3A-C2A	-2.74	109.69	116.10
19	1	302	CLA	CHD-C1D-ND	-2.74	121.93	124.45
19	A	803	CLA	O2A-CGA-CBA	2.74	120.51	111.91
19	2	312	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
18	3	307	CHL	C2C-C3C-C4C	2.74	108.44	106.49
19	3	312	CLA	CHD-C1D-ND	-2.74	121.94	124.45
19	B	851	CLA	CMB-C2B-C3B	2.74	129.80	124.68
19	A	830	CLA	C1-C2-C3	2.74	130.78	126.04
19	G	204	CLA	CHD-C1D-ND	-2.73	121.94	124.45
19	4	302	CLA	C1-C2-C3	2.73	130.77	126.04
18	2	307	CHL	CHD-C1D-ND	-2.73	121.94	124.45
19	3	310	CLA	CHD-C1D-ND	-2.73	121.94	124.45
19	3	314	CLA	CHD-C1D-ND	-2.73	121.94	124.45
20	1	315	LUT	C35-C15-C14	2.73	129.07	123.47
19	B	838	CLA	C1-C2-C3	2.73	130.77	126.04
19	A	830	CLA	CHD-C1D-ND	-2.73	121.95	124.45
19	K	202	CLA	CHD-C1D-ND	-2.72	121.95	124.45
20	3	315	LUT	C19-C9-C8	2.72	122.37	118.08
19	H	202	CLA	CHD-C1D-ND	-2.72	121.95	124.45
19	B	832	CLA	C1-C2-C3	2.72	130.75	126.04
19	A	818	CLA	CHD-C1D-ND	-2.72	121.95	124.45
19	G	202	CLA	CMA-C3A-C2A	-2.72	109.75	116.10
19	B	839	CLA	CHD-C1D-ND	-2.72	121.96	124.45
19	B	816	CLA	C1-C2-C3	2.72	130.74	126.04
19	K	201	CLA	CHD-C1D-ND	-2.71	121.96	124.45
19	B	802	CLA	O2A-CGA-CBA	2.71	120.42	111.91
19	L	301	CLA	CHD-C1D-ND	-2.71	121.96	124.45
19	A	804	CLA	CHD-C1D-ND	-2.71	121.97	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	202	CLA	C1-C2-C3	2.70	130.71	126.04
19	A	853	CLA	CHD-C1D-ND	-2.70	121.98	124.45
18	2	307	CHL	CMB-C2B-C1B	-2.69	124.33	128.46
20	2	315	LUT	C39-C29-C28	2.69	122.31	118.08
19	1	303	CLA	O2A-CGA-CBA	2.69	120.34	111.91
19	4	312	CLA	CHD-C1D-ND	-2.68	121.99	124.45
19	4	313	CLA	CHD-C1D-ND	-2.68	121.99	124.45
24	A	844	BCR	C15-C16-C17	2.68	128.96	123.47
19	B	803	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	1	314	CLA	CHD-C1D-ND	-2.67	122.00	124.45
18	2	305	CHL	CMB-C2B-C1B	-2.67	124.36	128.46
19	3	305	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	4	308	CLA	C1-C2-C3	2.66	131.06	126.75
19	B	805	CLA	C1-C2-C3	2.66	130.65	126.04
19	K	203	CLA	CMA-C3A-C2A	-2.66	109.89	116.10
19	B	819	CLA	C1-C2-C3	2.65	130.63	126.04
19	A	823	CLA	C1-C2-C3	2.65	130.63	126.04
19	B	831	CLA	C1-C2-C3	2.65	130.63	126.04
20	1	315	LUT	C32-C33-C34	2.65	123.00	118.94
19	B	822	CLA	C1-C2-C3	2.65	130.62	126.04
19	B	840	CLA	CHD-C1D-ND	-2.64	122.02	124.45
19	B	825	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	1	301	CHL	O2A-CGA-CBA	2.64	120.20	111.91
19	A	831	CLA	C1-C2-C3	2.64	130.61	126.04
19	B	821	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
19	A	839	CLA	C1-C2-C3	2.64	130.61	126.04
19	4	303	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
18	2	301	CHL	CMB-C2B-C1B	-2.64	124.41	128.46
19	4	311	CLA	CHD-C1D-ND	-2.63	122.03	124.45
19	1	311	CLA	CHD-C1D-ND	-2.63	122.03	124.45
19	B	830	CLA	CHD-C1D-ND	-2.63	122.04	124.45
19	1	310	CLA	C1-C2-C3	2.62	130.58	126.04
19	3	302	CLA	C1-C2-C3	2.62	130.58	126.04
18	4	305	CHL	CMB-C2B-C1B	-2.62	124.44	128.46
18	4	307	CHL	CMB-C2B-C1B	-2.62	124.44	128.46
19	3	312	CLA	C1-C2-C3	2.62	130.57	126.04
19	L	301	CLA	C1-C2-C3	2.61	130.56	126.04
19	3	313	CLA	CHD-C1D-ND	-2.61	122.05	124.45
19	2	313	CLA	CHD-C1D-ND	-2.61	122.05	124.45
19	4	309	CLA	C1-C2-C3	2.61	130.56	126.04
20	1	319	LUT	C8-C9-C10	2.61	122.94	118.94
19	B	822	CLA	O2A-CGA-CBA	2.60	120.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	C1-C2-C3	2.60	130.55	126.04
19	B	831	CLA	CHD-C1D-ND	-2.60	122.06	124.45
19	B	812	CLA	C1-C2-C3	2.60	130.54	126.04
19	A	854	CLA	C1-C2-C3	2.60	130.53	126.04
19	A	806	CLA	C4-C3-C5	-2.59	110.91	115.27
19	A	838	CLA	C1-C2-C3	2.59	130.53	126.04
19	1	310	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
19	B	825	CLA	C1-C2-C3	2.59	130.52	126.04
19	3	308	CLA	C1-C2-C3	2.59	130.51	126.04
19	B	810	CLA	C1-C2-C3	2.58	130.51	126.04
19	A	816	CLA	C1-C2-C3	2.58	130.50	126.04
19	A	833	CLA	C4-C3-C5	-2.58	110.94	115.27
19	A	820	CLA	CHD-C1D-ND	-2.57	122.09	124.45
19	B	851	CLA	C4-C3-C5	-2.57	110.94	115.27
19	K	203	CLA	CHD-C1D-ND	-2.57	122.09	124.45
19	B	824	CLA	CHD-C1D-ND	-2.57	122.09	124.45
19	B	811	CLA	C1-C2-C3	2.57	130.49	126.04
19	B	824	CLA	C1-C2-C3	2.57	130.48	126.04
19	B	817	CLA	C1-C2-C3	2.56	130.48	126.04
20	1	319	LUT	C32-C33-C34	2.56	122.87	118.94
19	A	821	CLA	CHD-C1D-ND	-2.56	122.10	124.45
19	A	821	CLA	C1-C2-C3	2.56	130.47	126.04
19	A	834	CLA	CHD-C1D-ND	-2.56	122.10	124.45
19	A	801	CLA	C1-C2-C3	2.56	130.46	126.04
18	2	306	CHL	CMB-C2B-C1B	-2.55	124.54	128.46
19	B	813	CLA	C12-C11-C10	-2.55	101.52	113.24
19	3	310	CLA	CMA-C3A-C2A	-2.55	110.15	116.10
18	4	306	CHL	CMB-C2B-C1B	-2.55	124.55	128.46
19	B	827	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
19	B	806	CLA	C4-C3-C5	-2.54	110.99	115.27
18	1	301	CHL	CMB-C2B-C1B	-2.54	124.56	128.46
20	3	315	LUT	C32-C33-C34	2.54	122.83	118.94
24	A	847	BCR	C10-C11-C12	2.53	131.11	123.22
19	B	801	CLA	C1-C2-C3	2.53	130.42	126.04
19	K	203	CLA	OBD-CAD-CBD	-2.53	120.81	125.97
18	4	314	CHL	CMB-C2B-C1B	-2.53	124.58	128.46
18	2	306	CHL	O1D-CGD-CBD	-2.52	119.32	124.48
19	1	312	CLA	C1-C2-C3	2.52	130.40	126.04
20	2	315	LUT	C32-C33-C34	2.52	122.81	118.94
24	B	844	BCR	C15-C16-C17	2.52	128.63	123.47
19	A	836	CLA	C1-C2-C3	2.51	130.39	126.04
18	2	307	CHL	C2A-C3A-C4A	2.51	105.92	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	C1-C2-C3	2.51	130.38	126.04
18	2	307	CHL	C2C-C3C-C4C	2.50	108.27	106.49
18	1	301	CHL	C2A-C1A-CHA	2.50	128.22	123.86
19	B	838	CLA	C4-C3-C5	-2.49	111.08	115.27
19	A	806	CLA	C1-C2-C3	2.49	130.35	126.04
19	A	813	CLA	C1-C2-C3	2.48	130.77	126.75
19	B	835	CLA	C1-C2-C3	2.48	130.34	126.04
18	2	314	CHL	CMB-C2B-C1B	-2.48	124.66	128.46
19	1	304	CLA	C1-C2-C3	2.47	130.32	126.04
19	4	310	CLA	C12-C11-C10	-2.47	101.87	113.24
19	B	826	CLA	C1-C2-C3	2.47	130.32	126.04
19	A	817	CLA	C1-C2-C3	2.47	130.32	126.04
18	2	314	CHL	C2C-C3C-C4C	2.47	108.25	106.49
19	B	809	CLA	C1-C2-C3	2.47	130.31	126.04
19	A	814	CLA	CHD-C1D-ND	-2.47	122.19	124.45
19	A	835	CLA	C1-C2-C3	2.47	130.31	126.04
19	4	310	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
19	A	814	CLA	O2A-CGA-CBA	2.46	121.95	114.03
19	A	811	CLA	C1-C2-C3	2.46	130.30	126.04
19	A	825	CLA	C1-C2-C3	2.46	130.30	126.04
19	B	823	CLA	C1-C2-C3	2.46	130.29	126.04
18	1	306	CHL	CMB-C2B-C1B	-2.46	124.69	128.46
19	A	826	CLA	C4-C3-C5	-2.46	111.14	115.27
20	3	315	LUT	C39-C29-C28	2.45	121.93	118.08
18	3	307	CHL	C2A-C3A-C4A	2.44	105.81	101.87
20	1	315	LUT	C39-C29-C28	2.44	121.92	118.08
19	A	804	CLA	C12-C11-C10	-2.44	102.04	113.24
19	1	302	CLA	C12-C11-C10	-2.44	102.04	113.24
19	B	808	CLA	C1-C2-C3	2.44	130.26	126.04
19	A	840	CLA	C12-C11-C10	-2.44	102.05	113.24
19	A	805	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
19	B	823	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
19	4	310	CLA	C1-C2-C3	2.43	130.25	126.04
19	L	301	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
18	4	306	CHL	C2C-C3C-C4C	2.43	108.22	106.49
21	3	316	XAT	O4-C5-C4	-2.43	111.56	113.38
21	4	316	XAT	O4-C5-C4	-2.43	111.56	113.38
19	A	817	CLA	C12-C11-C10	-2.43	102.08	113.24
18	1	306	CHL	C4D-CHA-C1A	2.43	124.20	121.25
19	B	836	CLA	C1-C2-C3	2.43	130.24	126.04
19	1	309	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	1	309	CLA	C1-C2-C3	2.42	130.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	301	CHL	O1D-CGD-CBD	-2.42	119.53	124.48
19	A	810	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
18	1	301	CHL	C2A-C3A-C4A	2.42	105.78	101.87
19	B	821	CLA	C1-C2-C3	2.42	130.67	126.75
19	4	301	CLA	O2A-CGA-CBA	2.42	121.79	112.23
19	2	312	CLA	C1-C2-C3	2.42	130.22	126.04
20	3	315	LUT	C12-C13-C14	2.41	122.65	118.94
19	B	818	CLA	C12-C11-C10	-2.41	102.14	113.24
18	2	301	CHL	C2A-C3A-C4A	2.41	105.76	101.87
18	4	307	CHL	C2C-C3C-C4C	2.41	108.21	106.49
19	H	201	CLA	O2A-CGA-CBA	2.41	121.75	112.23
19	B	803	CLA	C1-C2-C3	2.40	130.20	126.04
19	3	308	CLA	C12-C11-C10	-2.40	102.19	113.24
19	B	851	CLA	C12-C11-C10	-2.40	102.20	113.24
19	B	840	CLA	C1-C2-C3	2.40	130.20	126.04
19	A	840	CLA	C1-C2-C3	2.40	130.20	126.04
19	A	812	CLA	O2A-CGA-CBA	2.40	121.75	114.03
20	1	315	LUT	C19-C9-C8	2.40	121.86	118.08
19	A	839	CLA	C12-C11-C10	-2.40	102.21	113.24
19	B	820	CLA	O2A-CGA-CBA	2.40	121.74	114.03
19	A	834	CLA	C1-C2-C3	2.40	130.19	126.04
18	2	301	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
19	B	819	CLA	C12-C11-C10	-2.39	102.26	113.24
19	A	830	CLA	C12-C11-C10	-2.39	102.26	113.24
21	3	316	XAT	C27-C28-C29	2.39	129.23	125.53
19	A	819	CLA	C12-C11-C10	-2.39	102.28	113.24
19	A	823	CLA	C12-C11-C10	-2.39	102.28	113.24
19	B	801	CLA	CMB-C2B-C3B	2.38	129.14	124.68
19	2	302	CLA	C1-C2-C3	2.38	130.16	126.04
19	B	808	CLA	C12-C11-C10	-2.38	102.29	113.24
19	2	309	CLA	C12-C11-C10	-2.38	102.29	113.24
19	B	810	CLA	C12-C11-C10	-2.38	102.31	113.24
19	2	311	CLA	O2A-CGA-CBA	2.38	121.67	114.03
19	B	827	CLA	C12-C11-C10	-2.38	102.31	113.24
19	1	312	CLA	C12-C11-C10	-2.38	102.31	113.24
19	K	201	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
24	2	319	BCR	C24-C23-C22	2.38	129.83	126.23
19	B	839	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
19	B	826	CLA	C12-C11-C10	-2.37	102.33	113.24
19	B	804	CLA	O2A-CGA-CBA	2.37	121.66	114.03
19	A	826	CLA	C12-C11-C10	-2.37	102.33	113.24
19	4	312	CLA	C1-C2-C3	2.37	130.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	803	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	1	304	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
19	2	312	CLA	C12-C11-C10	-2.36	102.37	113.24
18	2	301	CHL	C4D-CHA-C1A	2.36	124.12	121.25
19	K	202	CLA	O2A-CGA-CBA	2.36	121.56	112.23
19	3	311	CLA	O2A-CGA-CBA	2.36	121.61	114.03
19	A	809	CLA	C12-C11-C10	-2.36	102.40	113.24
19	3	301	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
19	A	819	CLA	C1-C2-C3	2.36	130.12	126.04
19	K	201	CLA	O2A-CGA-CBA	2.36	121.61	114.03
19	3	314	CLA	O2A-CGA-CBA	2.36	121.55	112.23
21	2	316	XAT	O24-C25-C24	-2.35	111.61	113.38
19	1	318	CLA	C12-C11-C10	-2.35	102.43	113.24
19	A	853	CLA	C12-C11-C10	-2.35	102.43	113.24
18	2	305	CHL	C2A-C3A-C4A	2.35	105.67	101.87
18	4	307	CHL	C2A-C3A-C4A	2.35	105.67	101.87
19	B	840	CLA	C12-C11-C10	-2.35	102.44	113.24
19	B	806	CLA	C12-C11-C10	-2.35	102.44	113.24
19	4	311	CLA	O2A-CGA-CBA	2.35	121.58	114.03
19	A	838	CLA	C12-C11-C10	-2.35	102.45	113.24
19	B	838	CLA	C12-C11-C10	-2.34	102.47	113.24
20	1	319	LUT	C39-C29-C28	2.34	121.77	118.08
19	G	204	CLA	O2A-CGA-CBA	2.34	121.49	112.23
19	B	821	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
19	B	824	CLA	C12-C11-C10	-2.34	102.48	113.24
19	A	824	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
19	A	852	CLA	C12-C11-C10	-2.34	102.48	113.24
19	A	819	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
19	B	839	CLA	C1-C2-C3	2.34	130.09	126.04
19	A	804	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
19	B	805	CLA	C12-C11-C10	-2.34	102.50	113.24
19	1	312	CLA	C4-C3-C5	-2.34	111.34	115.27
19	A	818	CLA	O2A-CGA-CBA	2.33	121.53	114.03
19	A	854	CLA	C12-C11-C10	-2.33	102.52	113.24
19	A	801	CLA	C4D-C3D-CAD	-2.33	105.35	108.10
19	A	811	CLA	CMB-C2B-C3B	2.33	129.04	124.68
19	A	801	CLA	C12-C11-C10	-2.33	102.53	113.24
19	A	806	CLA	C12-C11-C10	-2.33	102.53	113.24
19	A	835	CLA	C12-C11-C10	-2.33	102.53	113.24
19	3	314	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
19	4	302	CLA	C12-C11-C10	-2.33	102.54	113.24
19	B	801	CLA	C12-C11-C10	-2.33	102.54	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	820	CLA	O2A-CGA-CBA	2.33	121.51	114.03
19	K	203	CLA	C3C-C4C-NC	-2.32	107.96	110.57
19	A	815	CLA	C12-C11-C10	-2.32	102.56	113.24
19	A	811	CLA	C4-C3-C5	-2.32	111.36	115.27
19	A	837	CLA	C12-C11-C10	-2.32	102.57	113.24
19	1	312	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
19	A	837	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
19	2	304	CLA	O2A-CGA-CBA	2.32	121.48	114.03
19	A	827	CLA	C12-C11-C10	-2.32	102.59	113.24
19	B	802	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
19	1	309	CLA	C12-C11-C10	-2.32	102.60	113.24
18	1	301	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
19	A	817	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	4	303	CLA	C12-C11-C10	-2.31	102.61	113.24
19	3	304	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	B	806	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	B	803	CLA	C12-C11-C10	-2.31	102.62	113.24
19	B	817	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	B	829	CLA	C12-C11-C10	-2.31	102.62	113.24
19	2	308	CLA	O2A-CGA-CBA	2.31	121.45	114.03
19	3	301	CLA	C12-C11-C10	-2.31	102.62	113.24
19	B	839	CLA	C12-C11-C10	-2.31	102.62	113.24
19	B	831	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
19	B	828	CLA	C12-C11-C10	-2.31	102.63	113.24
20	1	315	LUT	C12-C13-C14	2.31	122.48	118.94
19	A	803	CLA	C12-C11-C10	-2.31	102.63	113.24
19	K	202	CLA	C2D-C1D-ND	2.31	111.80	110.10
19	A	804	CLA	C3C-C4C-NC	-2.31	107.98	110.57
19	A	827	CLA	C1-C2-C3	2.31	130.03	126.04
18	4	307	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
19	A	828	CLA	C12-C11-C10	-2.30	102.65	113.24
18	2	314	CHL	C2A-C3A-C4A	2.30	105.59	101.87
19	A	829	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
19	A	803	CLA	C4-C3-C5	-2.30	111.40	115.27
19	1	314	CLA	O2A-CGA-CBA	2.30	121.42	114.03
19	B	802	CLA	C1-C2-C3	2.30	130.02	126.04
19	A	828	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
19	A	833	CLA	CMB-C2B-C3B	2.30	128.98	124.68
19	L	301	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
19	B	817	CLA	C3C-C4C-NC	-2.30	108.00	110.57
19	B	812	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
19	B	831	CLA	C12-C11-C10	-2.30	102.69	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	306	CHL	C2A-C3A-C4A	2.29	105.58	101.87
19	A	808	CLA	C1-C2-C3	2.29	130.01	126.04
19	2	302	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
19	B	830	CLA	C1-C2-C3	2.29	130.46	126.75
19	K	201	CLA	C3C-C4C-NC	-2.29	108.00	110.57
19	B	809	CLA	C12-C11-C10	-2.29	102.72	113.24
19	B	814	CLA	C12-C11-C10	-2.29	102.72	113.24
19	4	309	CLA	C12-C11-C10	-2.29	102.73	113.24
19	1	302	CLA	CMB-C2B-C3B	2.29	128.96	124.68
19	A	807	CLA	C12-C11-C10	-2.28	102.74	113.24
19	1	302	CLA	C3C-C4C-NC	-2.28	108.01	110.57
19	A	833	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
19	A	810	CLA	C3C-C4C-NC	-2.28	108.01	110.57
19	A	810	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
19	B	834	CLA	O2A-CGA-CBA	2.28	121.36	114.03
19	1	318	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
19	A	822	CLA	C3C-C4C-NC	-2.28	108.02	110.57
19	2	309	CLA	C1-C2-C3	2.28	129.98	126.04
18	3	307	CHL	C4D-CHA-C1A	2.28	124.02	121.25
19	2	302	CLA	C12-C11-C10	-2.28	102.78	113.24
19	A	833	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
19	L	302	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
19	L	302	CLA	C1-C2-C3	2.27	130.43	126.75
20	4	315	LUT	C39-C29-C28	2.27	121.66	118.08
19	F	302	CLA	O2A-CGA-CBA	2.27	121.33	114.03
19	1	310	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
19	H	202	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
19	2	313	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
19	A	829	CLA	C12-C11-C10	-2.27	102.81	113.24
19	A	824	CLA	C12-C11-C10	-2.27	102.81	113.24
19	B	833	CLA	C1-C2-C3	2.27	129.96	126.04
19	A	811	CLA	C12-C11-C10	-2.27	102.83	113.24
19	A	833	CLA	C12-C11-C10	-2.27	102.83	113.24
19	3	306	CLA	O2A-CGA-CBA	2.26	121.30	114.03
19	A	852	CLA	C3C-C4C-NC	-2.26	108.03	110.57
19	A	853	CLA	C1-C2-C3	2.26	129.96	126.04
19	A	832	CLA	O2A-CGA-CBA	2.26	121.30	114.03
19	3	311	CLA	C2D-C1D-ND	2.26	111.77	110.10
19	A	814	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
18	4	305	CHL	C2A-C3A-C4A	2.26	105.52	101.87
19	3	313	CLA	O2A-CGA-CBA	2.26	121.29	114.03
19	A	852	CLA	CMB-C2B-C3B	2.26	128.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	315	LUT	C1-C6-C7	2.26	122.16	115.78
24	A	844	BCR	C16-C15-C14	2.26	128.09	123.47
19	3	305	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
19	1	308	CLA	C3C-C4C-NC	-2.25	108.04	110.57
19	3	306	CLA	C3C-C4C-NC	-2.25	108.04	110.57
19	4	304	CLA	O2A-CGA-CBA	2.25	121.27	114.03
20	4	315	LUT	C11-C10-C9	2.25	130.53	127.31
19	B	815	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
19	A	837	CLA	C1-C2-C3	2.25	129.94	126.04
19	1	311	CLA	C1-C2-C3	2.25	130.39	126.75
20	2	315	LUT	C19-C9-C8	2.25	121.62	118.08
19	B	802	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
19	A	831	CLA	C12-C11-C10	-2.25	102.90	113.24
19	B	816	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	2	301	CHL	C2C-C3C-C4C	2.25	108.09	106.49
19	F	302	CLA	CMB-C2B-C3B	2.25	128.88	124.68
19	B	826	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
19	A	801	CLA	C3C-C4C-NC	-2.24	108.06	110.57
19	B	805	CLA	C3C-C4C-NC	-2.24	108.06	110.57
19	A	805	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	G	202	CLA	CAA-C2A-C3A	-2.24	110.87	116.10
19	3	304	CLA	CMD-C2D-C1D	2.24	128.66	124.71
19	L	301	CLA	C12-C11-C10	-2.24	102.94	113.24
19	B	836	CLA	C12-C11-C10	-2.24	102.95	113.24
19	2	303	CLA	C1-C2-C3	2.24	130.37	126.75
19	F	301	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
19	1	307	CLA	O2A-CGA-CBA	2.23	121.21	114.03
19	4	301	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
19	A	823	CLA	CMB-C2B-C3B	2.23	128.85	124.68
19	B	824	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
19	1	305	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
19	1	302	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
18	1	301	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
18	2	301	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
19	A	838	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
19	B	828	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
19	B	818	CLA	C3C-C4C-NC	-2.23	108.08	110.57
19	B	815	CLA	C1-C2-C3	2.22	129.89	126.04
19	K	201	CLA	CMD-C2D-C1D	2.22	128.63	124.71
20	4	315	LUT	C32-C33-C34	2.22	122.35	118.94
19	A	808	CLA	C3C-C4C-NC	-2.22	108.08	110.57
24	J	101	BCR	C20-C19-C18	2.22	132.66	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	825	CLA	C12-C11-C10	-2.22	103.03	113.24
19	2	304	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
18	3	307	CHL	O2A-CGA-CBA	2.22	121.00	112.23
19	B	808	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
19	B	826	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
19	A	835	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
19	B	813	CLA	C4-C3-C5	-2.21	111.55	115.27
19	1	314	CLA	CMB-C2B-C3B	2.21	128.82	124.68
19	1	308	CLA	C12-C11-C10	-2.21	102.60	113.29
19	B	851	CLA	C1-C2-C3	2.21	129.87	126.04
19	A	833	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
19	A	801	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
19	A	804	CLA	C1-C2-C3	2.21	129.87	126.04
19	B	802	CLA	C12-C11-C10	-2.21	103.09	113.24
19	1	303	CLA	C1-C2-C3	2.21	129.86	126.04
19	A	812	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	3	306	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
19	B	803	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	3	310	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
19	B	823	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	4	314	CHL	C2C-C3C-C4C	2.21	108.06	106.49
19	4	313	CLA	O2A-CGA-CBA	2.21	121.12	114.03
19	A	838	CLA	C4-C3-C5	-2.21	111.56	115.27
19	A	805	CLA	C1-C2-C3	2.20	130.32	126.75
19	1	309	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
19	B	840	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
19	3	310	CLA	C3C-C4C-NC	-2.20	108.10	110.57
20	4	315	LUT	C1-C6-C7	2.20	122.00	115.78
19	A	802	CLA	C3C-C4C-NC	-2.20	108.11	110.57
19	1	307	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
19	3	311	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
19	1	312	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
19	B	839	CLA	C3C-C4C-NC	-2.20	108.11	110.57
19	H	202	CLA	C4-C3-C5	-2.19	111.58	115.27
19	2	304	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	B	833	CLA	C3C-C4C-NC	-2.19	108.11	110.57
19	B	837	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
19	B	813	CLA	C1-C2-C3	2.19	129.84	126.04
19	4	311	CLA	C2D-C1D-ND	2.19	111.72	110.10
18	4	305	CHL	C2C-C3C-C4C	2.19	108.05	106.49
19	H	201	CLA	C3C-C4C-NC	-2.19	108.18	110.57
19	F	302	CLA	O1D-CGD-CBD	-2.19	120.00	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	203	CLA	C1-C2-C3	2.19	130.30	126.75
19	A	805	CLA	C3C-C4C-NC	-2.19	108.11	110.57
19	A	803	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	2	319	BCR	C8-C7-C6	2.19	133.35	127.20
19	A	808	CLA	C4-C3-C5	-2.19	111.59	115.27
19	A	822	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
18	1	306	CHL	O2A-CGA-CBA	2.18	121.05	114.03
19	F	301	CLA	O2A-CGA-CBA	2.18	121.05	114.03
19	A	806	CLA	C3C-C4C-NC	-2.18	108.12	110.57
18	4	307	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
19	A	807	CLA	CMB-C2B-C3B	2.18	128.76	124.68
19	2	308	CLA	C3C-C4C-NC	-2.18	108.12	110.57
19	3	302	CLA	C12-C11-C10	-2.18	103.22	113.24
19	B	837	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
19	A	839	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
19	B	817	CLA	CMB-C2B-C3B	2.18	128.75	124.68
18	4	305	CHL	C4D-CHA-C1A	2.17	123.89	121.25
19	B	820	CLA	C3C-C4C-NC	-2.17	108.13	110.57
19	B	828	CLA	C1-C2-C3	2.17	129.80	126.04
20	1	315	LUT	C1-C6-C7	2.17	121.92	115.78
19	2	310	CLA	CAA-C2A-C3A	-2.17	111.03	116.10
19	3	304	CLA	C3C-C4C-NC	-2.17	108.14	110.57
19	B	832	CLA	C3C-C4C-NC	-2.17	108.14	110.57
19	1	312	CLA	C2D-C1D-ND	2.17	111.70	110.10
19	B	833	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	2	306	CHL	C2A-C3A-C4A	2.17	105.38	101.87
19	A	818	CLA	C3C-C4C-NC	-2.17	108.14	110.57
19	A	854	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
19	B	808	CLA	C4-C3-C5	-2.17	111.62	115.27
20	2	315	LUT	C12-C13-C14	2.17	122.27	118.94
19	B	803	CLA	C3C-C4C-NC	-2.17	108.14	110.57
19	B	816	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
19	B	826	CLA	C4-C3-C5	-2.17	111.62	115.27
19	A	807	CLA	C3C-C4C-NC	-2.17	108.14	110.57
19	A	821	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
19	B	851	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
19	4	303	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
19	B	807	CLA	C12-C11-C10	-2.16	103.31	113.24
19	3	308	CLA	C3C-C4C-NC	-2.16	108.15	110.57
19	A	837	CLA	C3C-C4C-NC	-2.16	108.15	110.57
19	A	803	CLA	C1-C2-C3	2.16	129.78	126.04
19	B	812	CLA	C3C-C4C-NC	-2.16	108.15	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	305	CHL	C4D-CHA-C1A	2.16	123.88	121.25
18	4	306	CHL	C4D-CHA-C1A	2.16	123.88	121.25
19	B	827	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
19	B	821	CLA	C3C-C4C-NC	-2.16	108.15	110.57
19	A	824	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
19	A	812	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
19	1	308	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
19	A	853	CLA	C3C-C4C-NC	-2.16	108.15	110.57
19	A	824	CLA	C3C-C4C-NC	-2.16	108.15	110.57
19	B	827	CLA	C1-C2-C3	2.16	129.77	126.04
18	2	305	CHL	C2C-C3C-C4C	2.15	108.03	106.49
19	B	836	CLA	C3C-C4C-NC	-2.15	108.16	110.57
19	L	302	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
19	2	303	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
19	B	838	CLA	C3C-C4C-NC	-2.15	108.16	110.57
19	H	202	CLA	C3C-C4C-NC	-2.15	108.22	110.57
19	1	303	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	B	811	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	B	828	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	2	305	CHL	O1D-CGD-CBD	-2.15	120.09	124.48
19	3	309	CLA	C1-C2-C3	2.15	130.23	126.75
19	3	302	CLA	CMD-C2D-C1D	2.15	128.50	124.71
19	B	837	CLA	C3C-C4C-NC	-2.15	108.16	110.57
19	A	830	CLA	C2D-C1D-ND	2.15	111.69	110.10
19	3	301	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
19	B	806	CLA	C2D-C1D-ND	2.14	111.68	110.10
19	B	805	CLA	C4-C3-C5	-2.14	111.67	115.27
19	1	309	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
19	B	814	CLA	C2D-C1D-ND	2.14	111.68	110.10
19	B	824	CLA	CMB-C2B-C3B	2.14	128.68	124.68
18	4	307	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
19	A	816	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	B	851	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
19	A	815	CLA	C3C-C4C-NC	-2.14	108.17	110.57
19	A	837	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	K	203	CLA	CAA-C2A-C3A	-2.14	111.11	116.10
19	3	302	CLA	C3C-C4C-NC	-2.14	108.18	110.57
19	A	817	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
19	A	852	CLA	C4-C3-C5	-2.13	111.68	115.27
19	3	301	CLA	C2D-C1D-ND	2.13	111.68	110.10
19	B	833	CLA	C4D-CHA-C1A	2.13	123.84	121.25
19	1	309	CLA	C3C-C4C-NC	-2.13	108.18	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	811	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
19	K	202	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
19	4	309	CLA	C3C-C4C-NC	-2.13	108.18	110.57
19	3	304	CLA	CMB-C2B-C3B	2.13	128.66	124.68
19	3	309	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	B	828	CLA	C5-C3-C2	2.13	125.43	121.12
19	B	824	CLA	C3C-C4C-NC	-2.13	108.18	110.57
19	4	301	CLA	C3C-C4C-NC	-2.13	108.19	110.57
19	B	829	CLA	CMD-C2D-C1D	2.13	128.46	124.71
19	B	822	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
18	4	314	CHL	C4D-CHA-C1A	2.12	123.83	121.25
19	1	303	CLA	C4-C3-C5	-2.12	111.70	115.27
19	4	308	CLA	C2D-C1D-ND	2.12	111.67	110.10
19	1	318	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	A	809	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	A	812	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	B	831	CLA	C4-C3-C5	-2.12	111.70	115.27
19	B	818	CLA	C1-C2-C3	2.12	129.71	126.04
19	F	301	CLA	CMB-C2B-C3B	2.12	128.65	124.68
18	2	307	CHL	O2A-CGA-CBA	2.12	120.85	114.03
19	3	301	CLA	C4-C3-C5	-2.12	111.70	115.27
19	2	312	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	2	313	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	3	308	CLA	C4-C3-C5	-2.12	111.71	115.27
19	2	311	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
19	B	830	CLA	C3C-C4C-NC	-2.12	108.19	110.57
19	B	830	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
19	A	802	CLA	C1-C2-C3	2.12	130.18	126.75
19	1	313	CLA	O2A-CGA-CBA	2.12	120.83	114.03
19	B	822	CLA	C3C-C4C-NC	-2.12	108.20	110.57
19	B	818	CLA	C4-C3-C5	-2.12	111.71	115.27
19	B	802	CLA	C3C-C4C-NC	-2.12	108.20	110.57
19	A	827	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
19	B	831	CLA	C3C-C4C-NC	-2.12	108.20	110.57
19	G	204	CLA	C3C-C4C-NC	-2.12	108.20	110.57
19	B	839	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
19	2	311	CLA	C2D-C1D-ND	2.11	111.66	110.10
19	A	804	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
19	1	311	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
19	A	830	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	2	306	CHL	C2C-C3C-C4C	2.11	108.00	106.49
19	H	201	CLA	O1D-CGD-CBD	-2.11	120.16	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	852	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	1	308	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
19	B	825	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	A	852	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
19	A	828	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
19	4	309	CLA	CMB-C2B-C3B	2.11	128.62	124.68
19	A	832	CLA	C3C-C4C-NC	-2.11	108.21	110.57
19	L	301	CLA	C3C-C4C-NC	-2.11	108.21	110.57
19	2	302	CLA	C3C-C4C-NC	-2.11	108.21	110.57
19	1	311	CLA	C2D-C1D-ND	2.10	111.66	110.10
19	4	310	CLA	C2D-C1D-ND	2.10	111.66	110.10
19	A	854	CLA	CMD-C2D-C1D	2.10	128.42	124.71
19	1	303	CLA	C3C-C4C-NC	-2.10	108.21	110.57
19	A	836	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
19	1	311	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
19	A	839	CLA	C3C-C4C-NC	-2.10	108.21	110.57
19	B	825	CLA	C3C-C4C-NC	-2.10	108.21	110.57
19	4	312	CLA	C2D-C1D-ND	2.10	111.65	110.10
19	B	818	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	1	314	CLA	C3C-C4C-NC	-2.10	108.22	110.57
18	4	306	CHL	O2A-CGA-CBA	2.10	120.78	114.03
19	A	835	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
19	3	310	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
19	A	817	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	3	303	CLA	O2A-CGA-CBA	2.10	120.77	114.03
19	B	838	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	4	304	CLA	C2D-C1D-ND	2.10	111.65	110.10
19	A	822	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
19	B	811	CLA	C3C-C4C-NC	-2.10	108.22	110.57
19	J	102	CLA	C3C-C4C-NC	-2.10	108.22	110.57
19	A	837	CLA	CED-O2D-CGD	2.10	120.68	115.94
19	1	314	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
19	A	831	CLA	C3C-C4C-NC	-2.10	108.22	110.57
19	B	804	CLA	C3C-C4C-NC	-2.10	108.22	110.57
18	4	314	CHL	C2A-C3A-C4A	2.10	105.25	101.87
19	A	804	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	A	840	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
19	3	303	CLA	C3C-C4C-NC	-2.09	108.22	110.57
18	2	307	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
19	A	829	CLA	C3C-C4C-NC	-2.09	108.22	110.57
19	A	835	CLA	C3C-C4C-NC	-2.09	108.22	110.57
19	B	809	CLA	C3C-C4C-NC	-2.09	108.22	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	822	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	4	303	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
19	B	813	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
19	3	303	CLA	CMD-C2D-C1D	2.09	128.40	124.71
19	B	829	CLA	C3C-C4C-NC	-2.09	108.22	110.57
19	B	818	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
18	4	314	CHL	C2A-C1A-CHA	2.09	127.52	123.86
19	H	201	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	A	838	CLA	C3C-C4C-NC	-2.09	108.22	110.57
19	B	813	CLA	CMD-C2D-C1D	2.09	128.40	124.71
18	2	306	CHL	C2A-C1A-CHA	2.09	127.52	123.86
19	A	837	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	B	840	CLA	C2D-C1D-ND	2.09	111.64	110.10
19	B	823	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	A	803	CLA	C3C-C4C-NC	-2.09	108.23	110.57
19	L	302	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	1	306	CHL	C2C-C3C-C4C	2.09	107.98	106.49
19	B	814	CLA	C3C-C4C-NC	-2.09	108.23	110.57
19	A	854	CLA	C2D-C1D-ND	2.09	111.64	110.10
19	4	310	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
19	3	313	CLA	C3C-C4C-NC	-2.09	108.23	110.57
19	B	809	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
19	A	820	CLA	C2D-C1D-ND	2.08	111.64	110.10
19	B	807	CLA	C3C-C4C-NC	-2.08	108.23	110.57
19	B	815	CLA	C3C-C4C-NC	-2.08	108.23	110.57
19	3	301	CLA	C1-C2-C3	2.08	129.65	126.04
19	2	304	CLA	C3C-C4C-NC	-2.08	108.23	110.57
19	1	303	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
18	4	305	CHL	OMC-CMC-C2C	-2.08	120.98	125.69
18	1	301	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
19	B	806	CLA	C3C-C4C-NC	-2.08	108.24	110.57
18	3	307	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
19	A	825	CLA	CMB-C2B-C3B	2.08	128.57	124.68
19	A	811	CLA	CMD-C2D-C1D	2.08	128.38	124.71
19	A	819	CLA	C4-C3-C5	-2.08	111.78	115.27
19	B	814	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
19	G	202	CLA	CMD-C2D-C1D	2.08	128.37	124.71
19	1	305	CLA	C3C-C4C-NC	-2.08	108.24	110.57
19	1	310	CLA	C3C-C4C-NC	-2.08	108.24	110.57
19	B	828	CLA	C3C-C4C-NC	-2.08	108.24	110.57
19	3	301	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	1	303	CLA	C2D-C1D-ND	2.07	111.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	839	CLA	CMB-C2B-C3B	2.07	128.56	124.68
19	B	809	CLA	C4-C3-C5	-2.07	111.78	115.27
19	4	312	CLA	CMD-C2D-C1D	2.07	128.37	124.71
19	B	835	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
19	B	806	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
19	A	817	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	A	811	CLA	C2D-C1D-ND	2.07	111.63	110.10
19	H	201	CLA	CMD-C2D-C1D	2.07	128.36	124.71
19	2	303	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	3	305	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	B	813	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	J	102	CLA	CMD-C2D-C1D	2.07	128.36	124.71
19	A	834	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
19	G	203	CLA	CMD-C2D-C1D	2.07	128.36	124.71
19	K	203	CLA	CMB-C2B-C3B	2.07	128.55	124.68
19	B	829	CLA	C4-C3-C5	-2.07	111.79	115.27
19	2	309	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	1	313	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	B	851	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	3	305	CLA	CMD-C2D-C1D	2.07	128.35	124.71
19	4	309	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
19	A	828	CLA	C2D-C1D-ND	2.07	111.63	110.10
19	B	810	CLA	C3C-C4C-NC	-2.07	108.25	110.57
19	A	811	CLA	C3C-C4C-NC	-2.06	108.26	110.57
19	3	303	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
19	A	830	CLA	CMB-C2B-C3B	2.06	128.54	124.68
18	1	301	CHL	C2C-C3C-C4C	2.06	107.96	106.49
19	A	854	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
19	4	303	CLA	CMB-C2B-C3B	2.06	128.54	124.68
19	A	815	CLA	CMB-C2B-C3B	2.06	128.54	124.68
19	4	303	CLA	C3C-C4C-NC	-2.06	108.26	110.57
19	A	825	CLA	C4-C3-C5	-2.06	111.80	115.27
19	B	836	CLA	CMB-C2B-C3B	2.06	128.54	124.68
18	4	306	CHL	O2A-CGA-O1A	-2.06	118.16	123.30
19	4	302	CLA	C3C-C4C-NC	-2.06	108.26	110.57
19	B	819	CLA	C3C-C4C-NC	-2.06	108.26	110.57
19	B	806	CLA	CMD-C2D-C1D	2.06	128.35	124.71
18	2	306	CHL	O2A-CGA-CBA	2.06	120.65	114.03
19	G	203	CLA	C2D-C1D-ND	2.06	111.62	110.10
18	4	306	CHL	C2A-C3A-C4A	2.06	105.19	101.87
19	B	807	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
19	1	313	CLA	CMD-C2D-C1D	2.06	128.34	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	836	CLA	C3C-C4C-NC	-2.06	108.26	110.57
19	A	824	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
19	A	832	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
19	3	309	CLA	CED-O2D-CGD	2.06	120.59	115.94
19	B	827	CLA	C3C-C4C-NC	-2.06	108.27	110.57
19	A	815	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
19	A	823	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
19	A	838	CLA	CMD-C2D-C1D	2.06	128.34	124.71
19	4	313	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
19	A	806	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
19	B	830	CLA	CED-O2D-CGD	2.05	120.58	115.94
19	4	302	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
19	3	313	CLA	CMD-C2D-C1D	2.05	128.33	124.71
19	2	310	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
19	A	813	CLA	C3C-C4C-NC	-2.05	108.27	110.57
19	H	202	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	3	312	CLA	C3C-C4C-NC	-2.05	108.27	110.57
19	B	811	CLA	CMD-C2D-C1D	2.05	128.32	124.71
19	3	309	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	3	306	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	A	819	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	B	804	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
19	2	308	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
19	2	304	CLA	CED-O2D-CGD	2.05	120.56	115.94
19	A	814	CLA	C3C-C4C-NC	-2.05	108.28	110.57
19	G	202	CLA	C2D-C1D-ND	2.04	111.61	110.10
19	B	819	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
19	A	854	CLA	C3C-C4C-NC	-2.04	108.28	110.57
19	A	804	CLA	C2A-C1A-CHA	2.04	127.43	123.86
19	J	102	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
19	A	805	CLA	CMB-C2B-C3B	2.04	128.50	124.68
19	B	827	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
19	B	829	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
19	J	102	CLA	CMB-C2B-C3B	2.04	128.50	124.68
19	A	831	CLA	C4-C3-C5	-2.04	111.84	115.27
19	G	203	CLA	C3C-C4C-NC	-2.04	108.28	110.57
19	A	816	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
19	B	838	CLA	CMB-C2B-C3B	2.04	128.50	124.68
19	1	304	CLA	CMB-C2B-C3B	2.04	128.50	124.68
19	2	309	CLA	C2D-C1D-ND	2.04	111.61	110.10
19	B	823	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
19	A	801	CLA	C2D-C1D-ND	2.04	111.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	802	CLA	CMB-C2B-C3B	2.04	128.49	124.68
19	4	301	CLA	CMB-C2B-C3B	2.04	128.49	124.68
19	A	806	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	3	311	CLA	CED-O2D-CGD	2.04	120.55	115.94
19	B	816	CLA	CMD-C2D-C1D	2.04	128.30	124.71
19	B	809	CLA	CMB-C2B-C3B	2.04	128.49	124.68
19	4	311	CLA	CMB-C2B-C3B	2.04	128.49	124.68
18	1	301	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
19	B	801	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
19	B	816	CLA	CMB-C2B-C3B	2.04	128.49	124.68
19	G	204	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
19	A	823	CLA	C2D-C1D-ND	2.04	111.60	110.10
19	B	813	CLA	CMB-C2B-C3B	2.04	128.49	124.68
18	4	306	CHL	CBC-CAC-C3C	-2.04	106.82	112.43
19	A	830	CLA	CMD-C2D-C1D	2.04	128.30	124.71
19	4	309	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
19	1	307	CLA	C3C-C4C-NC	-2.03	108.29	110.57
19	B	826	CLA	C3C-C4C-NC	-2.03	108.29	110.57
19	B	811	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
20	2	315	LUT	C31-C30-C29	2.03	130.21	127.31
19	2	309	CLA	CMB-C2B-C3B	2.03	128.48	124.68
19	B	840	CLA	C3C-C4C-NC	-2.03	108.29	110.57
19	A	804	CLA	C4-C3-C5	-2.03	111.85	115.27
19	A	809	CLA	C2D-C1D-ND	2.03	111.60	110.10
19	A	838	CLA	C2D-C1D-ND	2.03	111.60	110.10
19	G	204	CLA	CMD-C2D-C1D	2.03	128.29	124.71
19	B	806	CLA	C1-C2-C3	2.03	129.55	126.04
19	4	313	CLA	C3C-C4C-NC	-2.03	108.30	110.57
19	A	823	CLA	C3C-C4C-NC	-2.03	108.30	110.57
19	3	309	CLA	CMD-C2D-C1D	2.03	128.29	124.71
19	2	310	CLA	CMB-C2B-C3B	2.03	128.47	124.68
19	1	310	CLA	CMB-C2B-C3B	2.03	128.47	124.68
19	A	837	CLA	C4D-CHA-C1A	2.03	123.72	121.25
19	A	825	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	A	830	CLA	CED-O2D-CGD	2.03	120.52	115.94
18	2	314	CHL	C2A-C1A-CHA	2.03	127.40	123.86
19	1	312	CLA	CMD-C2D-C1D	2.03	128.28	124.71
19	A	801	CLA	C4-C3-C5	-2.02	111.86	115.27
19	1	304	CLA	C2D-C1D-ND	2.02	111.60	110.10
19	A	803	CLA	C2D-C1D-ND	2.02	111.60	110.10
18	2	305	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
19	2	311	CLA	C3C-C4C-NC	-2.02	108.30	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	302	CLA	C3C-C4C-NC	-2.02	108.30	110.57
19	A	810	CLA	CMB-C2B-C3B	2.02	128.46	124.68
19	4	310	CLA	CMB-C2B-C3B	2.02	128.46	124.68
19	A	801	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
19	G	202	CLA	C3C-C4C-NC	-2.02	108.30	110.57
19	A	809	CLA	CMD-C2D-C1D	2.02	128.28	124.71
19	3	309	CLA	C2D-C1D-ND	2.02	111.59	110.10
19	A	831	CLA	C2D-C1D-ND	2.02	111.59	110.10
19	A	825	CLA	C3C-C4C-NC	-2.02	108.30	110.57
19	A	854	CLA	CMB-C2B-C3B	2.02	128.46	124.68
19	1	308	CLA	CMD-C2D-C1D	2.02	128.28	124.71
19	B	808	CLA	C2D-C1D-ND	2.02	111.59	110.10
19	B	811	CLA	C2D-C1D-ND	2.02	111.59	110.10
19	1	304	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	B	822	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	A	827	CLA	C3C-C4C-NC	-2.02	108.31	110.57
19	B	810	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	4	301	CLA	CMD-C2D-C1D	2.02	128.27	124.71
19	B	807	CLA	CMD-C2D-C1D	2.02	128.27	124.71
19	B	840	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	B	805	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
19	A	839	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
19	2	302	CLA	C4-C3-C5	-2.02	111.88	115.27
19	3	314	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
19	B	807	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	3	310	CLA	CMB-C2B-C3B	2.01	128.45	124.68
19	1	311	CLA	C3C-C4C-NC	-2.01	108.31	110.57
19	A	821	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	4	309	CLA	CMD-C2D-C1D	2.01	128.26	124.71
18	2	314	CHL	C3C-C4C-NC	-2.01	108.31	110.57
19	B	804	CLA	CMD-C2D-C1D	2.01	128.26	124.71
19	A	802	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	B	812	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	1	301	CHL	C4D-CHA-C1A	2.01	123.70	121.25
19	1	307	CLA	CMD-C2D-C1D	2.01	128.26	124.71
19	A	820	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	1	302	CLA	CMD-C2D-C1D	2.01	128.26	124.71
19	3	308	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	B	825	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	B	814	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	A	840	CLA	C3C-C4C-NC	-2.01	108.32	110.57
19	A	806	CLA	O2D-CGD-O1D	-2.01	119.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	306	CHL	O2A-CGA-O1A	-2.01	118.29	123.30
19	2	310	CLA	C3C-C4C-NC	-2.01	108.32	110.57
19	4	312	CLA	CMB-C2B-C3B	2.01	128.43	124.68
19	B	815	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
19	3	301	CLA	CMB-C2B-C3B	2.01	128.43	124.68
19	3	303	CLA	CMB-C2B-C3B	2.01	128.43	124.68
19	A	838	CLA	CMB-C2B-C3B	2.01	128.43	124.68
19	A	831	CLA	CED-O2D-CGD	2.01	120.47	115.94
19	B	808	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
20	3	315	LUT	C7-C8-C9	2.01	129.27	126.23
19	A	819	CLA	C2D-C1D-ND	2.01	111.58	110.10
19	A	826	CLA	C2D-C1D-ND	2.01	111.58	110.10
19	4	313	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
19	B	818	CLA	CMD-C2D-C1D	2.00	128.25	124.71
19	2	303	CLA	CMD-C2D-C1D	2.00	128.24	124.71
19	3	304	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
19	3	302	CLA	CMB-C2B-C3B	2.00	128.43	124.68
19	1	305	CLA	CMD-C2D-C1D	2.00	128.24	124.71
19	2	304	CLA	CMD-C2D-C1D	2.00	128.24	124.71
19	3	314	CLA	C3C-C4C-NC	-2.00	108.33	110.57
19	1	318	CLA	CMB-C2B-C3B	2.00	128.42	124.68
19	B	803	CLA	C2C-C1C-NC	-2.00	108.10	109.97
19	B	831	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
19	3	303	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
19	4	302	CLA	C4-C3-C5	-2.00	111.91	115.27
19	A	804	CLA	CMD-C2D-C1D	2.00	128.24	124.71
19	A	827	CLA	CMB-C2B-C3B	2.00	128.42	124.68
18	1	306	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
19	A	812	CLA	CMD-C2D-C1D	2.00	128.24	124.71
19	A	819	CLA	C3C-C4C-NC	-2.00	108.33	110.57

All (176) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
18	2	305	CHL	ND
18	2	305	CHL	NA
18	2	305	CHL	NC
18	2	306	CHL	ND
18	2	306	CHL	NA
18	2	306	CHL	NC
18	2	307	CHL	ND
18	2	307	CHL	NA
18	2	307	CHL	NC
18	2	314	CHL	ND
18	2	314	CHL	NC
18	3	307	CHL	ND
18	3	307	CHL	NA
18	3	307	CHL	NC
18	4	305	CHL	ND
18	4	305	CHL	NA
18	4	305	CHL	NC
18	4	306	CHL	ND
18	4	306	CHL	NA
18	4	306	CHL	NC
18	4	307	CHL	ND
18	4	307	CHL	NA
18	4	307	CHL	NC
18	4	314	CHL	ND
18	4	314	CHL	NA
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	318	CLA	ND
19	2	302	CLA	ND
19	2	303	CLA	ND
19	2	304	CLA	ND

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Mol	Chain	Res	Type	Atom
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
19	2	313	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	304	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

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Mol	Chain	Res	Type	Atom
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	817	CLA	ND
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	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

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Mol	Chain	Res	Type	Atom
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
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	B	839	CLA	ND
19	B	840	CLA	ND
19	B	851	CLA	ND
19	F	301	CLA	ND
19	F	302	CLA	ND
19	G	202	CLA	ND
19	G	203	CLA	ND
19	G	204	CLA	ND
19	H	201	CLA	ND
19	H	202	CLA	ND
19	J	102	CLA	ND
19	L	301	CLA	ND
19	L	302	CLA	ND
19	K	201	CLA	ND
19	K	202	CLA	ND
19	K	203	CLA	ND

All (1799) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	301	CHL	CBD-CGD-O2D-CED
18	1	301	CHL	C1-C2-C3-C5
18	1	306	CHL	C3C-C2C-CMC-OMC
18	1	306	CHL	CHA-CBD-CGD-O2D
18	2	301	CHL	O2A-C1-C2-C3
18	2	301	CHL	C1-C2-C3-C4
18	2	301	CHL	C1-C2-C3-C5
18	2	305	CHL	C3C-C2C-CMC-OMC
18	2	306	CHL	CBD-CGD-O2D-CED
18	2	307	CHL	CHA-CBD-CGD-O1D
18	4	305	CHL	C1C-C2C-CMC-OMC
18	4	306	CHL	CHA-CBD-CGD-O1D
18	4	306	CHL	CHA-CBD-CGD-O2D
18	4	306	CHL	CBD-CGD-O2D-CED
18	4	307	CHL	C1A-C2A-CAA-CBA
18	4	307	CHL	C3A-C2A-CAA-CBA
18	4	307	CHL	C3C-C2C-CMC-OMC
19	1	302	CLA	CHA-CBD-CGD-O1D
19	1	304	CLA	C1A-C2A-CAA-CBA
19	1	304	CLA	C3A-C2A-CAA-CBA
19	1	304	CLA	CHA-CBD-CGD-O1D
19	1	304	CLA	C1-C2-C3-C4
19	1	304	CLA	C1-C2-C3-C5
19	1	304	CLA	C4-C3-C5-C6
19	1	305	CLA	C1A-C2A-CAA-CBA
19	1	305	CLA	C3A-C2A-CAA-CBA
19	1	308	CLA	C1A-C2A-CAA-CBA
19	1	308	CLA	C1-C2-C3-C4
19	1	308	CLA	C1-C2-C3-C5
19	1	310	CLA	CBD-CGD-O2D-CED
19	1	311	CLA	C1-C2-C3-C5
19	1	312	CLA	C1-C2-C3-C4
19	1	312	CLA	C1-C2-C3-C5
19	1	313	CLA	C1A-C2A-CAA-CBA
19	1	313	CLA	C3A-C2A-CAA-CBA
19	1	314	CLA	C1A-C2A-CAA-CBA
19	1	314	CLA	CHA-CBD-CGD-O1D
19	1	318	CLA	C1A-C2A-CAA-CBA
19	1	318	CLA	C3A-C2A-CAA-CBA
19	1	318	CLA	O1A-CGA-O2A-C1
19	1	318	CLA	CHA-CBD-CGD-O2D
19	2	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	2	303	CLA	C1-C2-C3-C5
19	2	304	CLA	C1A-C2A-CAA-CBA
19	2	304	CLA	CBD-CGD-O2D-CED
19	2	304	CLA	O1D-CGD-O2D-CED
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	CHA-CBD-CGD-O1D
19	2	312	CLA	CHA-CBD-CGD-O2D
19	2	312	CLA	CBD-CGD-O2D-CED
19	3	301	CLA	CBD-CGD-O2D-CED
19	3	303	CLA	C1A-C2A-CAA-CBA
19	3	304	CLA	C1A-C2A-CAA-CBA
19	3	304	CLA	CBD-CGD-O2D-CED
19	3	305	CLA	C3A-C2A-CAA-CBA
19	3	305	CLA	CHA-CBD-CGD-O1D
19	3	306	CLA	C3A-C2A-CAA-CBA
19	3	308	CLA	C3A-C2A-CAA-CBA
19	3	314	CLA	C1A-C2A-CAA-CBA
19	3	314	CLA	CBA-CGA-O2A-C1
19	4	301	CLA	CHA-CBD-CGD-O1D
19	4	301	CLA	CAD-CBD-CGD-O1D
19	4	303	CLA	CBD-CGD-O2D-CED
19	4	304	CLA	CHA-CBD-CGD-O1D
19	4	304	CLA	CHA-CBD-CGD-O2D
19	4	308	CLA	C1A-C2A-CAA-CBA
19	4	308	CLA	C3A-C2A-CAA-CBA
19	4	310	CLA	C1A-C2A-CAA-CBA
19	4	310	CLA	C3A-C2A-CAA-CBA
19	4	310	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	C2A-CAA-CBA-CGA
19	4	312	CLA	CBA-CGA-O2A-C1
19	4	312	CLA	O1A-CGA-O2A-C1
19	4	313	CLA	C1A-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	802	CLA	C1A-C2A-CAA-CBA
19	A	803	CLA	C3A-C2A-CAA-CBA
19	A	803	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	CAD-CBD-CGD-O1D
19	A	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C1-C2-C3-C5
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C1-C2-C3-C5
19	A	811	CLA	CHA-CBD-CGD-O1D
19	A	811	CLA	CHA-CBD-CGD-O2D
19	A	811	CLA	CAD-CBD-CGD-O1D
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C1-C2-C3-C5
19	A	811	CLA	C2-C3-C5-C6
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C2A-CAA-CBA-CGA
19	A	815	CLA	O1A-CGA-O2A-C1
19	A	815	CLA	CHA-CBD-CGD-O2D
19	A	815	CLA	C2-C3-C5-C6
19	A	815	CLA	C4-C3-C5-C6
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	817	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	C14-C13-C15-C16
19	A	826	CLA	O2A-C1-C2-C3
19	A	826	CLA	C1-C2-C3-C4
19	A	827	CLA	CHA-CBD-CGD-O1D
19	A	827	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	C4-C3-C5-C6
19	A	829	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	CAD-CBD-CGD-O2D
19	A	831	CLA	C1A-C2A-CAA-CBA
19	A	831	CLA	C3A-C2A-CAA-CBA
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CAD-CBD-CGD-O2D
19	A	834	CLA	C1-C2-C3-C5
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D
19	A	837	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
19	A	838	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C10-C8-C9
19	A	840	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	C4-C3-C5-C6
19	A	853	CLA	C1A-C2A-CAA-CBA
19	A	853	CLA	C3A-C2A-CAA-CBA
19	A	853	CLA	C4-C3-C5-C6
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	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	C1-C2-C3-C4
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	805	CLA	C3A-C2A-CAA-CBA
19	B	805	CLA	C14-C13-C15-C16
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	C1A-C2A-CAA-CBA
19	B	809	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	C1-C2-C3-C4
19	B	810	CLA	C1-C2-C3-C5
19	B	811	CLA	CHA-CBD-CGD-O1D
19	B	811	CLA	C1-C2-C3-C4
19	B	811	CLA	C1-C2-C3-C5
19	B	811	CLA	C4-C3-C5-C6
19	B	812	CLA	CBA-CGA-O2A-C1
19	B	812	CLA	O1A-CGA-O2A-C1
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C1-C2-C3-C5
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	C11-C10-C8-C9
19	B	816	CLA	CHA-CBD-CGD-O1D
19	B	816	CLA	C2-C3-C5-C6
19	B	817	CLA	C2A-CAA-CBA-CGA
19	B	818	CLA	C3A-C2A-CAA-CBA
19	B	818	CLA	C1-C2-C3-C5
19	B	819	CLA	CHA-CBD-CGD-O1D
19	B	820	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C3A-C2A-CAA-CBA
19	B	821	CLA	C1-C2-C3-C5
19	B	822	CLA	CHA-CBD-CGD-O2D
19	B	822	CLA	C4-C3-C5-C6
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	C1A-C2A-CAA-CBA
19	B	826	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	C1-C2-C3-C5
19	B	830	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C3A-C2A-CAA-CBA
19	B	831	CLA	C1-C2-C3-C4
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	C2-C3-C5-C6
19	B	833	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C3A-C2A-CAA-CBA
19	B	834	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	CHA-CBD-CGD-O1D
19	B	836	CLA	CAD-CBD-CGD-O1D
19	B	836	CLA	CAD-CBD-CGD-O2D
19	B	836	CLA	C4-C3-C5-C6
19	B	838	CLA	C1-C2-C3-C4
19	B	838	CLA	C1-C2-C3-C5
19	B	838	CLA	C11-C10-C8-C9
19	B	839	CLA	C2-C3-C5-C6
19	B	840	CLA	C14-C13-C15-C16
19	B	851	CLA	O2A-C1-C2-C3
19	B	851	CLA	C1-C2-C3-C5
19	F	301	CLA	CBD-CGD-O2D-CED
19	F	302	CLA	CHA-CBD-CGD-O1D
19	F	302	CLA	CHA-CBD-CGD-O2D
19	G	202	CLA	CHA-CBD-CGD-O1D
19	G	203	CLA	C1A-C2A-CAA-CBA
19	G	203	CLA	C3A-C2A-CAA-CBA
19	G	203	CLA	CBD-CGD-O2D-CED
19	H	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	H	201	CLA	C3A-C2A-CAA-CBA
19	H	202	CLA	C3A-C2A-CAA-CBA
19	H	202	CLA	O1A-CGA-O2A-C1
19	H	202	CLA	C1-C2-C3-C4
19	H	202	CLA	C1-C2-C3-C5
19	J	102	CLA	C1A-C2A-CAA-CBA
19	J	102	CLA	C3A-C2A-CAA-CBA
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	302	CLA	C1A-C2A-CAA-CBA
19	L	302	CLA	C3A-C2A-CAA-CBA
19	L	302	CLA	C1-C2-C3-C5
19	K	201	CLA	C3A-C2A-CAA-CBA
19	K	202	CLA	C1A-C2A-CAA-CBA
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	320	LHG	C3-O3-P-O4
22	1	320	LHG	C3-O3-P-O5
22	1	320	LHG	C3-O3-P-O6
22	1	320	LHG	C4-O6-P-O4
22	1	320	LHG	O10-C23-O8-C6
22	1	320	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	C4-O6-P-O3
22	2	317	LHG	O10-C23-O8-C6
22	2	317	LHG	C24-C23-O8-C6
22	A	842	LHG	C3-O3-P-O5
22	A	842	LHG	C3-O3-P-O6
22	B	850	LHG	C4-O6-P-O3
22	B	850	LHG	C4-O6-P-O4
22	B	850	LHG	C4-O6-P-O5
23	2	318	LMT	O5'-C1'-O1'-C1
24	2	319	BCR	C1-C6-C7-C8
24	2	319	BCR	C5-C6-C7-C8
24	2	319	BCR	C6-C7-C8-C9
24	2	319	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	2	319	BCR	C7-C8-C9-C34
24	2	319	BCR	C9-C10-C11-C12
24	2	319	BCR	C15-C16-C17-C18
24	2	319	BCR	C36-C18-C19-C20
24	A	843	BCR	C11-C12-C13-C14
24	A	843	BCR	C11-C12-C13-C35
24	A	843	BCR	C21-C22-C23-C24
24	A	843	BCR	C37-C22-C23-C24
24	G	201	BCR	C5-C6-C7-C8
24	G	201	BCR	C11-C12-C13-C14
24	G	201	BCR	C11-C12-C13-C35
24	G	201	BCR	C23-C24-C25-C26
24	G	201	BCR	C23-C24-C25-C30
24	J	101	BCR	C1-C6-C7-C8
24	J	101	BCR	C5-C6-C7-C8
24	J	101	BCR	C11-C12-C13-C14
24	J	101	BCR	C13-C14-C15-C16
24	J	101	BCR	C19-C20-C21-C22
24	J	101	BCR	C21-C22-C23-C24
24	J	104	BCR	C23-C24-C25-C26
24	J	104	BCR	C23-C24-C25-C30
24	L	303	BCR	C21-C22-C23-C24
24	L	303	BCR	C23-C24-C25-C26
24	L	303	BCR	C23-C24-C25-C30
25	B	849	LMG	C2-C1-O1-C7
25	B	849	LMG	O9-C10-O7-C8
25	B	849	LMG	C11-C10-O7-C8
25	B	849	LMG	O10-C28-O8-C9
25	B	849	LMG	C29-C28-O8-C9
28	B	848	DGD	C2D-C1D-O3G-C3G
28	B	848	DGD	O6D-C1D-O3G-C3G
18	1	301	CHL	O1D-CGD-O2D-CED
18	2	306	CHL	O1D-CGD-O2D-CED
19	1	308	CLA	O1D-CGD-O2D-CED
19	4	303	CLA	O1D-CGD-O2D-CED
19	K	201	CLA	O1D-CGD-O2D-CED
19	2	303	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	O1D-CGD-O2D-CED
19	G	203	CLA	O1D-CGD-O2D-CED
18	2	305	CHL	CBD-CGD-O2D-CED
19	1	304	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	2	302	CLA	CBD-CGD-O2D-CED
19	2	310	CLA	CBD-CGD-O2D-CED
19	2	311	CLA	CBD-CGD-O2D-CED
19	3	306	CLA	CBD-CGD-O2D-CED
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	311	CLA	CBD-CGD-O2D-CED
19	3	314	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	CBD-CGD-O2D-CED
19	B	803	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	B	821	CLA	CBD-CGD-O2D-CED
19	B	833	CLA	CBD-CGD-O2D-CED
19	B	851	CLA	CBD-CGD-O2D-CED
19	G	204	CLA	CBD-CGD-O2D-CED
19	K	201	CLA	CBD-CGD-O2D-CED
19	1	312	CLA	O1A-CGA-O2A-C1
19	3	314	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	O1A-CGA-O2A-C1
18	4	306	CHL	O1D-CGD-O2D-CED
19	2	312	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	O1D-CGD-O2D-CED
19	B	815	CLA	O1D-CGD-O2D-CED
18	3	307	CHL	CBA-CGA-O2A-C1
18	2	305	CHL	O1D-CGD-O2D-CED
19	2	311	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	1	312	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	H	202	CLA	CBA-CGA-O2A-C1
18	2	301	CHL	CBD-CGD-O2D-CED
19	1	311	CLA	CBD-CGD-O2D-CED
19	1	314	CLA	CBD-CGD-O2D-CED
19	1	318	CLA	CBD-CGD-O2D-CED
19	3	310	CLA	CBD-CGD-O2D-CED
19	A	834	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	B	810	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	825	CLA	CBD-CGD-O2D-CED
19	B	830	CLA	CBD-CGD-O2D-CED
19	K	202	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	O1A-CGA-O2A-C1
19	A	813	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1
19	3	311	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	CBD-CGD-O2D-CED
19	G	202	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C3-C5-C6-C7
19	A	815	CLA	C3-C5-C6-C7
19	A	829	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	B	813	CLA	C3-C5-C6-C7
19	B	823	CLA	C3-C5-C6-C7
19	1	308	CLA	CBA-CGA-O2A-C1
19	A	813	CLA	CBA-CGA-O2A-C1
19	1	314	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	1	305	CLA	CBD-CGD-O2D-CED
19	4	313	CLA	CBD-CGD-O2D-CED
19	K	202	CLA	O1A-CGA-O2A-C1
19	G	204	CLA	CBA-CGA-O2A-C1
19	K	202	CLA	CBA-CGA-O2A-C1
19	1	309	CLA	C4-C3-C5-C6
19	A	835	CLA	C4-C3-C5-C6
19	B	810	CLA	C4-C3-C5-C6
19	A	807	CLA	C2-C3-C5-C6
19	A	828	CLA	C2-C3-C5-C6
19	A	840	CLA	C2-C3-C5-C6
19	A	853	CLA	C2-C3-C5-C6
18	4	305	CHL	CBD-CGD-O2D-CED
19	A	802	CLA	CBD-CGD-O2D-CED
19	A	828	CLA	CBD-CGD-O2D-CED
19	H	201	CLA	CBD-CGD-O2D-CED
19	1	314	CLA	C2A-CAA-CBA-CGA
19	3	313	CLA	C2A-CAA-CBA-CGA
19	A	801	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	810	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
19	A	853	CLA	C2A-CAA-CBA-CGA
19	A	854	CLA	C2A-CAA-CBA-CGA
19	B	801	CLA	C2A-CAA-CBA-CGA
19	B	810	CLA	C2A-CAA-CBA-CGA
19	B	812	CLA	C2A-CAA-CBA-CGA
19	B	824	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C2A-CAA-CBA-CGA
19	B	833	CLA	C2A-CAA-CBA-CGA
19	B	835	CLA	C2A-CAA-CBA-CGA
19	L	302	CLA	C2A-CAA-CBA-CGA
19	A	817	CLA	O1A-CGA-O2A-C1
19	3	308	CLA	C3-C5-C6-C7
19	1	318	CLA	CBA-CGA-O2A-C1
19	3	312	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	CBA-CGA-O2A-C1
19	A	826	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
19	A	835	CLA	CBA-CGA-O2A-C1
19	B	811	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
19	G	203	CLA	CBA-CGA-O2A-C1
19	A	826	CLA	C1-C2-C3-C5
19	A	833	CLA	C1-C2-C3-C5
19	B	802	CLA	C1-C2-C3-C5
19	B	805	CLA	C1-C2-C3-C5
19	B	816	CLA	C1-C2-C3-C5
19	B	831	CLA	C1-C2-C3-C5
19	A	826	CLA	CBD-CGD-O2D-CED
19	1	305	CLA	O1D-CGD-O2D-CED
19	3	304	CLA	O1D-CGD-O2D-CED
19	H	201	CLA	O1D-CGD-O2D-CED
19	3	304	CLA	O1A-CGA-O2A-C1
19	A	803	CLA	O1A-CGA-O2A-C1
19	A	835	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	O1A-CGA-O2A-C1
19	B	805	CLA	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	O1A-CGA-O2A-C1
19	B	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	816	CLA	O1A-CGA-O2A-C1
19	B	822	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	O1A-CGA-O2A-C1
19	L	302	CLA	O1A-CGA-O2A-C1
24	A	843	BCR	C19-C20-C21-C22
24	A	847	BCR	C9-C10-C11-C12
19	1	303	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	CBD-CGD-O2D-CED
19	L	301	CLA	CBD-CGD-O2D-CED
19	L	302	CLA	CBD-CGD-O2D-CED
19	1	303	CLA	C3-C5-C6-C7
19	A	839	CLA	C3-C5-C6-C7
19	A	834	CLA	CBA-CGA-O2A-C1
19	B	805	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
19	L	302	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
19	1	312	CLA	CBD-CGD-O2D-CED
19	A	819	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	B	801	CLA	CBD-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	B	831	CLA	CBD-CGD-O2D-CED
18	4	307	CHL	O1A-CGA-O2A-C1
19	A	827	CLA	CBD-CGD-O2D-CED
19	L	301	CLA	C3-C5-C6-C7
19	3	312	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	O1A-CGA-O2A-C1
19	A	838	CLA	O1A-CGA-O2A-C1
19	A	833	CLA	C4-C3-C5-C6
19	A	839	CLA	C4-C3-C5-C6
19	B	833	CLA	C4-C3-C5-C6
19	A	839	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	B	833	CLA	C2-C3-C5-C6
19	3	306	CLA	C2A-CAA-CBA-CGA
19	3	314	CLA	C2A-CAA-CBA-CGA
19	A	806	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	826	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	O1A-CGA-O2A-C1
25	B	849	LMG	O6-C1-O1-C7
19	A	803	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	CBA-CGA-O2A-C1
19	B	802	CLA	CBA-CGA-O2A-C1
19	B	809	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	CBA-CGA-O2A-C1
19	G	202	CLA	O1D-CGD-O2D-CED
19	B	830	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	C1-C2-C3-C5
19	A	830	CLA	C1-C2-C3-C5
19	A	831	CLA	C1-C2-C3-C5
19	B	833	CLA	C1-C2-C3-C5
19	1	310	CLA	O1D-CGD-O2D-CED
19	4	312	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	O1D-CGD-O2D-CED
19	F	301	CLA	O1D-CGD-O2D-CED
19	1	313	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	O1D-CGD-O2D-CED
19	4	303	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
18	4	305	CHL	CBA-CGA-O2A-C1
18	4	307	CHL	CBA-CGA-O2A-C1
19	3	304	CLA	CBA-CGA-O2A-C1
19	A	801	CLA	CBA-CGA-O2A-C1
19	A	811	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CBA-CGA-O2A-C1
19	A	853	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	CBA-CGA-O2A-C1
19	B	822	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBD-CGD-O2D-CED
19	G	204	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	C5-C6-C7-C8
19	3	308	CLA	C13-C15-C16-C17
19	A	815	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B	802	CLA	C15-C16-C17-C18
19	B	838	CLA	C5-C6-C7-C8
18	2	301	CHL	O1A-CGA-O2A-C1
23	A	851	LMT	O5B-C1B-O1B-C4'
19	1	318	CLA	C5-C6-C7-C8
19	1	318	CLA	C10-C11-C12-C13
19	A	817	CLA	C15-C16-C17-C18
19	A	854	CLA	C10-C11-C12-C13
19	B	803	CLA	C15-C16-C17-C18
19	B	805	CLA	C15-C16-C17-C18
19	B	808	CLA	C10-C11-C12-C13
19	B	818	CLA	C10-C11-C12-C13
19	B	824	CLA	C13-C15-C16-C17
23	2	318	LMT	C2'-C1'-O1'-C1
23	A	851	LMT	C2'-C1'-O1'-C1
25	B	849	LMG	O1-C7-C8-O7
18	4	305	CHL	O1A-CGA-O2A-C1
19	A	830	CLA	O1A-CGA-O2A-C1
19	A	833	CLA	C2-C3-C5-C6
19	A	852	CLA	C2-C3-C5-C6
19	1	309	CLA	C11-C10-C8-C9
19	2	302	CLA	C11-C12-C13-C14
19	3	302	CLA	C11-C10-C8-C9
19	4	310	CLA	C6-C7-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	A	806	CLA	C6-C7-C8-C9
19	A	807	CLA	C6-C7-C8-C9
19	A	809	CLA	C14-C13-C15-C16
19	A	823	CLA	C6-C7-C8-C9
19	A	826	CLA	C14-C13-C15-C16
19	A	829	CLA	C11-C12-C13-C14
19	A	831	CLA	C11-C10-C8-C9
19	A	831	CLA	C11-C12-C13-C14
19	A	835	CLA	C11-C10-C8-C9
19	A	835	CLA	C14-C13-C15-C16
19	A	839	CLA	C14-C13-C15-C16
19	A	852	CLA	C14-C13-C15-C16
19	B	801	CLA	C11-C12-C13-C14
19	B	803	CLA	C11-C12-C13-C14
19	B	807	CLA	C14-C13-C15-C16
19	B	808	CLA	C11-C12-C13-C14
19	B	810	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B	813	CLA	C11-C10-C8-C9
19	B	813	CLA	C14-C13-C15-C16
19	B	814	CLA	C14-C13-C15-C16
19	B	817	CLA	C11-C10-C8-C9
19	B	826	CLA	C14-C13-C15-C16
19	B	828	CLA	C14-C13-C15-C16
19	B	829	CLA	C11-C12-C13-C14
19	B	831	CLA	C11-C10-C8-C9
19	L	301	CLA	C11-C10-C8-C9
19	A	811	CLA	C2A-CAA-CBA-CGA
19	A	835	CLA	C2A-CAA-CBA-CGA
24	A	847	BCR	C11-C12-C13-C35
24	L	303	BCR	C37-C22-C23-C24
24	2	319	BCR	C17-C18-C19-C20
19	G	203	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C5-C6-C7-C8
19	B	807	CLA	C5-C6-C7-C8
19	B	826	CLA	C10-C11-C12-C13
19	A	828	CLA	CBA-CGA-O2A-C1
19	4	310	CLA	C10-C11-C12-C13
19	A	804	CLA	C10-C11-C12-C13
19	A	808	CLA	C5-C6-C7-C8
19	A	811	CLA	C10-C11-C12-C13
19	A	823	CLA	C15-C16-C17-C18
19	A	825	CLA	C8-C10-C11-C12
19	A	827	CLA	C15-C16-C17-C18
19	A	835	CLA	C10-C11-C12-C13
19	A	837	CLA	C5-C6-C7-C8
19	A	837	CLA	C15-C16-C17-C18
19	A	838	CLA	C5-C6-C7-C8
19	A	853	CLA	C15-C16-C17-C18
19	B	810	CLA	C10-C11-C12-C13
19	B	810	CLA	C15-C16-C17-C18
19	B	838	CLA	C10-C11-C12-C13
19	B	851	CLA	C15-C16-C17-C18
19	A	829	CLA	O1A-CGA-O2A-C1
19	3	308	CLA	C15-C16-C17-C18
19	4	303	CLA	C5-C6-C7-C8
19	4	303	CLA	C10-C11-C12-C13
19	4	309	CLA	C10-C11-C12-C13
19	A	803	CLA	C15-C16-C17-C18
19	A	807	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A	809	CLA	C10-C11-C12-C13
19	A	809	CLA	C15-C16-C17-C18
19	A	817	CLA	C10-C11-C12-C13
19	A	824	CLA	C10-C11-C12-C13
19	A	833	CLA	C15-C16-C17-C18
19	A	835	CLA	C13-C15-C16-C17
19	A	854	CLA	C15-C16-C17-C18
19	B	806	CLA	C5-C6-C7-C8
19	B	809	CLA	C10-C11-C12-C13
19	B	824	CLA	C15-C16-C17-C18
19	A	801	CLA	C1-C2-C3-C5
19	B	840	CLA	C1-C2-C3-C5
19	2	312	CLA	C10-C11-C12-C13
19	A	824	CLA	C15-C16-C17-C18
19	A	825	CLA	C15-C16-C17-C18
19	A	839	CLA	C10-C11-C12-C13
19	A	854	CLA	C5-C6-C7-C8
19	B	813	CLA	C15-C16-C17-C18
19	B	818	CLA	C8-C10-C11-C12
19	B	840	CLA	C10-C11-C12-C13
19	B	810	CLA	O1D-CGD-O2D-CED
19	1	318	CLA	C2-C1-O2A-CGA
19	1	302	CLA	C10-C11-C12-C13
19	2	309	CLA	C10-C11-C12-C13
19	B	801	CLA	C10-C11-C12-C13
19	B	823	CLA	C5-C6-C7-C8
19	B	836	CLA	C15-C16-C17-C18
19	1	313	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	C13-C15-C16-C17
19	B	805	CLA	C10-C11-C12-C13
19	3	309	CLA	O1D-CGD-O2D-CED
19	A	806	CLA	C11-C12-C13-C15
19	A	835	CLA	C11-C12-C13-C15
19	A	840	CLA	C12-C13-C15-C16
19	A	852	CLA	C11-C12-C13-C15
19	A	853	CLA	C11-C12-C13-C15
19	A	854	CLA	C11-C12-C13-C15
19	B	802	CLA	C12-C13-C15-C16
19	B	806	CLA	C12-C13-C15-C16
19	B	809	CLA	C11-C10-C8-C7
19	B	817	CLA	C6-C7-C8-C10
19	B	851	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	811	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	C2A-CAA-CBA-CGA
19	1	318	CLA	C2A-CAA-CBA-CGA
19	4	303	CLA	C2A-CAA-CBA-CGA
19	A	827	CLA	C2A-CAA-CBA-CGA
19	B	811	CLA	C2A-CAA-CBA-CGA
19	B	816	CLA	C2A-CAA-CBA-CGA
19	1	307	CLA	O1D-CGD-O2D-CED
19	2	310	CLA	O1D-CGD-O2D-CED
19	2	302	CLA	C15-C16-C17-C18
19	3	308	CLA	C10-C11-C12-C13
19	A	828	CLA	C10-C11-C12-C13
19	A	840	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
19	B	814	CLA	C15-C16-C17-C18
23	A	851	LMT	C2B-C1B-O1B-C4'
19	A	833	CLA	O1A-CGA-O2A-C1
19	B	803	CLA	O1A-CGA-O2A-C1
19	B	836	CLA	O1A-CGA-O2A-C1
19	A	838	CLA	C10-C11-C12-C13
19	B	806	CLA	C15-C16-C17-C18
19	3	302	CLA	C3-C5-C6-C7
19	1	309	CLA	C10-C11-C12-C13
19	1	312	CLA	C10-C11-C12-C13
19	A	807	CLA	C10-C11-C12-C13
19	A	829	CLA	C15-C16-C17-C18
19	A	830	CLA	C10-C11-C12-C13
19	A	852	CLA	C8-C10-C11-C12
19	A	805	CLA	O1A-CGA-O2A-C1
19	4	302	CLA	C10-C11-C12-C13
19	A	816	CLA	C5-C6-C7-C8
19	A	826	CLA	C10-C11-C12-C13
19	A	829	CLA	C10-C11-C12-C13
19	B	827	CLA	C10-C11-C12-C13
19	A	823	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	2	302	CLA	C10-C11-C12-C13
19	3	312	CLA	C5-C6-C7-C8
19	A	827	CLA	C10-C11-C12-C13
19	A	828	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	824	CLA	C8-C10-C11-C12
19	B	832	CLA	C5-C6-C7-C8
22	2	317	LHG	C3-O3-P-O6
19	A	823	CLA	C3-C5-C6-C7
19	B	833	CLA	C3-C5-C6-C7
19	B	828	CLA	CBA-CGA-O2A-C1
19	A	837	CLA	C8-C10-C11-C12
19	A	840	CLA	C5-C6-C7-C8
19	B	833	CLA	O1D-CGD-O2D-CED
18	4	305	CHL	C4-C3-C5-C6
19	B	839	CLA	C4-C3-C5-C6
19	A	801	CLA	C13-C15-C16-C17
18	3	307	CHL	C2A-CAA-CBA-CGA
19	1	311	CLA	C2A-CAA-CBA-CGA
19	3	312	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	F	302	CLA	C2A-CAA-CBA-CGA
18	4	305	CHL	C6-C7-C8-C9
19	A	833	CLA	C3-C5-C6-C7
18	2	301	CHL	CBA-CGA-O2A-C1
19	4	303	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	CBA-CGA-O2A-C1
22	1	320	LHG	C28-C29-C30-C31
19	3	301	CLA	O1D-CGD-O2D-CED
18	2	307	CHL	O1D-CGD-O2D-CED
19	B	822	CLA	O1D-CGD-O2D-CED
19	4	302	CLA	C11-C12-C13-C15
19	A	827	CLA	C16-C17-C18-C20
19	B	835	CLA	C6-C7-C8-C9
19	B	836	CLA	CBA-CGA-O2A-C1
22	B	850	LHG	C29-C30-C31-C32
25	B	849	LMG	C21-C22-C23-C24
19	B	836	CLA	C5-C6-C7-C8
18	4	307	CHL	C1-C2-C3-C5
19	A	802	CLA	C1-C2-C3-C5
19	A	813	CLA	C1-C2-C3-C5
19	B	821	CLA	C1-C2-C3-C4
19	L	302	CLA	C1-C2-C3-C4
18	3	307	CHL	O1A-CGA-O2A-C1
19	A	823	CLA	C5-C6-C7-C8
19	B	817	CLA	C10-C11-C12-C13
24	J	101	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	C5-C6-C7-C8
19	B	817	CLA	C5-C6-C7-C8
19	A	816	CLA	C6-C7-C8-C10
19	2	302	CLA	O1D-CGD-O2D-CED
19	A	825	CLA	C4-C3-C5-C6
19	B	817	CLA	C4-C3-C5-C6
19	1	303	CLA	C2-C3-C5-C6
19	A	836	CLA	C2-C3-C5-C6
19	B	817	CLA	C2-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
19	H	202	CLA	C2-C3-C5-C6
19	A	807	CLA	C11-C12-C13-C14
19	A	817	CLA	C11-C12-C13-C14
19	A	826	CLA	C6-C7-C8-C9
19	A	826	CLA	C11-C10-C8-C9
19	A	827	CLA	C11-C10-C8-C9
19	B	829	CLA	C6-C7-C8-C9
19	A	815	CLA	C5-C6-C7-C8
19	B	805	CLA	C5-C6-C7-C8
19	B	839	CLA	C8-C10-C11-C12
19	2	309	CLA	C2A-CAA-CBA-CGA
19	3	303	CLA	C2A-CAA-CBA-CGA
19	A	822	CLA	C2A-CAA-CBA-CGA
19	B	822	CLA	C2A-CAA-CBA-CGA
19	K	202	CLA	C2A-CAA-CBA-CGA
19	B	833	CLA	O1A-CGA-O2A-C1
19	1	304	CLA	O1D-CGD-O2D-CED
18	4	305	CHL	C6-C7-C8-C10
19	1	312	CLA	C11-C12-C13-C15
19	2	309	CLA	C11-C12-C13-C14
19	4	302	CLA	C11-C12-C13-C14
19	A	827	CLA	C16-C17-C18-C19
19	B	835	CLA	C6-C7-C8-C10
19	B	819	CLA	C10-C11-C12-C13
19	A	836	CLA	O1D-CGD-O2D-CED
19	2	309	CLA	C8-C10-C11-C12
19	A	828	CLA	C13-C15-C16-C17
19	A	805	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	1	311	CLA	C3A-C2A-CAA-CBA
19	2	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	3	302	CLA	C3A-C2A-CAA-CBA
19	3	314	CLA	C3A-C2A-CAA-CBA
19	4	303	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	830	CLA	C3A-C2A-CAA-CBA
19	A	834	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	833	CLA	C3A-C2A-CAA-CBA
19	B	839	CLA	C3A-C2A-CAA-CBA
19	B	808	CLA	C15-C16-C17-C18
19	1	309	CLA	C11-C12-C13-C15
19	B	819	CLA	C11-C12-C13-C15
19	A	824	CLA	O2A-C1-C2-C3
19	B	851	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	C3-C5-C6-C7
19	1	318	CLA	C15-C16-C17-C18
19	3	302	CLA	C10-C11-C12-C13
19	B	813	CLA	C10-C11-C12-C13
19	B	838	CLA	C15-C16-C17-C18
19	3	301	CLA	C4-C3-C5-C6
19	A	836	CLA	C4-C3-C5-C6
19	B	818	CLA	C4-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	A	827	CLA	C2-C3-C5-C6
19	B	807	CLA	C2-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	A	810	CLA	C1-C2-C3-C5
19	B	834	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	O1D-CGD-O2D-CED
19	1	309	CLA	C5-C6-C7-C8
19	B	808	CLA	C3-C5-C6-C7
22	1	320	LHG	C24-C25-C26-C27
19	1	308	CLA	C5-C6-C7-C8
19	2	312	CLA	C5-C6-C7-C8
19	B	813	CLA	C13-C15-C16-C17
19	A	808	CLA	O1A-CGA-O2A-C1
22	2	317	LHG	C23-C24-C25-C26
19	A	830	CLA	C3-C5-C6-C7
20	1	319	LUT	C1-C6-C7-C8
20	1	319	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	845	BCR	C1-C6-C7-C8
24	A	845	BCR	C5-C6-C7-C8
24	B	843	BCR	C1-C6-C7-C8
24	B	843	BCR	C5-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C26
24	B	846	BCR	C23-C24-C25-C30
24	G	201	BCR	C1-C6-C7-C8
24	J	101	BCR	C23-C24-C25-C26
24	J	101	BCR	C23-C24-C25-C30
24	J	104	BCR	C1-C6-C7-C8
24	J	104	BCR	C5-C6-C7-C8
19	B	802	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	CBA-CGA-O2A-C1
19	3	301	CLA	C10-C11-C12-C13
19	A	819	CLA	C15-C16-C17-C18
19	B	824	CLA	C10-C11-C12-C13
19	B	826	CLA	C13-C15-C16-C17
19	L	301	CLA	C15-C16-C17-C18
19	4	308	CLA	CBD-CGD-O2D-CED
19	1	302	CLA	C4-C3-C5-C6
19	2	312	CLA	C4-C3-C5-C6
19	A	804	CLA	C4-C3-C5-C6
19	A	830	CLA	C4-C3-C5-C6
19	B	815	CLA	C4-C3-C5-C6
19	3	308	CLA	O1D-CGD-O2D-CED
19	2	312	CLA	C2-C3-C5-C6
19	2	312	CLA	C12-C13-C15-C16
19	3	301	CLA	C11-C10-C8-C7
19	A	804	CLA	C6-C7-C8-C10
19	A	807	CLA	C6-C7-C8-C10
19	A	811	CLA	C11-C12-C13-C15
19	A	815	CLA	C11-C10-C8-C7
19	A	817	CLA	C6-C7-C8-C10
19	A	817	CLA	C11-C12-C13-C15
19	A	823	CLA	C6-C7-C8-C10
19	A	826	CLA	C6-C7-C8-C10
19	A	826	CLA	C11-C10-C8-C7
19	A	827	CLA	C6-C7-C8-C10
19	A	829	CLA	C2-C3-C5-C6
19	A	830	CLA	C2-C3-C5-C6
19	A	835	CLA	C12-C13-C15-C16
19	A	838	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C11-C10-C8-C7
19	B	805	CLA	C11-C12-C13-C15
19	B	838	CLA	C11-C10-C8-C7
19	B	839	CLA	C11-C12-C13-C15
19	B	836	CLA	C10-C11-C12-C13
19	B	840	CLA	C8-C10-C11-C12
19	4	303	CLA	C11-C12-C13-C15
19	4	309	CLA	C11-C12-C13-C14
19	F	302	CLA	O1D-CGD-O2D-CED
25	F	305	LMG	C10-C11-C12-C13
19	A	809	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	C2A-CAA-CBA-CGA
19	B	813	CLA	C2A-CAA-CBA-CGA
19	H	201	CLA	C2A-CAA-CBA-CGA
19	A	823	CLA	C10-C11-C12-C13
19	3	308	CLA	C5-C6-C7-C8
19	B	840	CLA	C13-C15-C16-C17
19	3	302	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBA-CGA-O2A-C1
19	3	301	CLA	C5-C6-C7-C8
19	B	824	CLA	O1D-CGD-O2D-CED
22	A	842	LHG	C24-C25-C26-C27
19	A	826	CLA	C13-C15-C16-C17
19	A	803	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	CBD-CGD-O2D-CED
25	4	318	LMG	O6-C5-C6-O5
25	B	849	LMG	O6-C5-C6-O5
19	A	831	CLA	CBD-CGD-O2D-CED
23	2	318	LMT	O5B-C5B-C6B-O6B
19	B	805	CLA	C13-C15-C16-C17
19	A	831	CLA	C4-C3-C5-C6
19	1	309	CLA	C2-C3-C5-C6
19	A	837	CLA	C2-C3-C5-C6
19	L	301	CLA	C2-C3-C5-C6
19	3	301	CLA	C11-C10-C8-C9
19	A	801	CLA	C11-C12-C13-C14
19	A	817	CLA	C6-C7-C8-C9
19	A	827	CLA	C6-C7-C8-C9
19	A	837	CLA	C11-C12-C13-C14
19	A	854	CLA	C14-C13-C15-C16
19	B	801	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	805	CLA	C11-C12-C13-C14
19	B	806	CLA	C14-C13-C15-C16
19	B	809	CLA	C11-C10-C8-C9
19	B	814	CLA	C6-C7-C8-C9
19	B	818	CLA	C6-C7-C8-C9
19	B	828	CLA	C11-C10-C8-C9
19	B	839	CLA	C11-C12-C13-C14
19	3	308	CLA	CBD-CGD-O2D-CED
19	A	814	CLA	O1D-CGD-O2D-CED
19	2	311	CLA	C2A-CAA-CBA-CGA
19	A	833	CLA	C2A-CAA-CBA-CGA
19	A	840	CLA	C2A-CAA-CBA-CGA
19	B	806	CLA	C2A-CAA-CBA-CGA
19	G	204	CLA	C2A-CAA-CBA-CGA
23	2	318	LMT	O5'-C5'-C6'-O6'
25	4	318	LMG	C11-C12-C13-C14
18	2	301	CHL	C1A-C2A-CAA-CBA
18	2	306	CHL	C1A-C2A-CAA-CBA
19	1	311	CLA	C1A-C2A-CAA-CBA
19	3	302	CLA	C1A-C2A-CAA-CBA
19	3	306	CLA	C1A-C2A-CAA-CBA
19	3	308	CLA	C1A-C2A-CAA-CBA
19	4	303	CLA	C1A-C2A-CAA-CBA
19	A	803	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	C1A-C2A-CAA-CBA
19	A	819	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	830	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C1A-C2A-CAA-CBA
19	B	819	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	840	CLA	C1A-C2A-CAA-CBA
19	H	202	CLA	C1A-C2A-CAA-CBA
19	K	201	CLA	C1A-C2A-CAA-CBA
19	2	309	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	815	CLA	C15-C16-C17-C18
19	B	831	CLA	C10-C11-C12-C13
19	B	839	CLA	C5-C6-C7-C8
22	B	850	LHG	C3-O3-P-O6
19	B	807	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	C5-C6-C7-C8
19	B	829	CLA	C10-C11-C12-C13
19	A	839	CLA	C16-C17-C18-C19
19	3	306	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	C15-C16-C17-C18
19	A	833	CLA	CBA-CGA-O2A-C1
19	A	853	CLA	O1A-CGA-O2A-C1
19	B	851	CLA	C2-C3-C5-C6
28	B	848	DGD	CAA-CBA-CCA-CDA
19	4	308	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	C13-C15-C16-C17
18	2	307	CHL	C2A-CAA-CBA-CGA
18	4	307	CHL	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	1	310	CLA	C6-C7-C8-C10
19	A	819	CLA	C16-C17-C18-C19
19	A	827	CLA	C8-C10-C11-C12
19	1	303	CLA	C10-C11-C12-C13
19	3	309	CLA	C2C-C3C-CAC-CBC
28	B	848	DGD	C5B-C6B-C7B-C8B
19	3	308	CLA	C8-C10-C11-C12
19	3	304	CLA	CAA-CBA-CGA-O2A
19	4	310	CLA	CAA-CBA-CGA-O2A
19	B	840	CLA	CAA-CBA-CGA-O2A
19	B	832	CLA	C10-C11-C12-C13
19	1	318	CLA	C4-C3-C5-C6
19	A	829	CLA	C4-C3-C5-C6
19	B	831	CLA	C4-C3-C5-C6
19	A	804	CLA	C2-C3-C5-C6
19	1	310	CLA	C6-C7-C8-C9
19	A	819	CLA	C16-C17-C18-C20
19	B	833	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	C5-C6-C7-C8
19	B	840	CLA	C2A-CAA-CBA-CGA
19	1	304	CLA	O1A-CGA-O2A-C1
19	2	303	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	4	308	CLA	C1-C2-C3-C5
19	3	314	CLA	O1D-CGD-O2D-CED
19	A	839	CLA	C16-C17-C18-C20
22	1	320	LHG	C12-C13-C14-C15
19	A	828	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	C10-C11-C12-C13
24	G	201	BCR	C16-C17-C18-C19
24	J	101	BCR	C11-C10-C9-C8
22	A	842	LHG	O7-C5-C6-O8
18	4	305	CHL	C1-C2-C3-C5
19	A	815	CLA	C1-C2-C3-C5
22	1	320	LHG	C15-C16-C17-C18
19	B	828	CLA	C13-C15-C16-C17
19	B	836	CLA	C13-C15-C16-C17
19	B	827	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	C6-C7-C8-C10
18	1	301	CHL	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	1	309	CLA	C11-C10-C8-C7
19	3	301	CLA	C2-C3-C5-C6
19	3	302	CLA	C11-C10-C8-C7
19	A	801	CLA	C11-C12-C13-C15
19	A	801	CLA	C12-C13-C15-C16
19	A	808	CLA	C11-C10-C8-C7
19	A	811	CLA	C12-C13-C15-C16
19	A	815	CLA	C12-C13-C15-C16
19	A	826	CLA	C12-C13-C15-C16
19	A	830	CLA	C11-C12-C13-C15
19	A	831	CLA	C6-C7-C8-C10
19	A	835	CLA	C11-C10-C8-C7
19	A	837	CLA	C11-C12-C13-C15
19	A	838	CLA	C6-C7-C8-C10
19	A	839	CLA	C6-C7-C8-C10
19	A	854	CLA	C12-C13-C15-C16
19	B	801	CLA	C11-C10-C8-C7
19	B	807	CLA	C12-C13-C15-C16
19	B	814	CLA	C6-C7-C8-C10
19	B	814	CLA	C12-C13-C15-C16
19	B	818	CLA	C6-C7-C8-C10
19	B	824	CLA	C12-C13-C15-C16
19	B	825	CLA	C2-C3-C5-C6
19	B	826	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	827	CLA	C6-C7-C8-C10
19	B	827	CLA	C11-C10-C8-C7
19	B	828	CLA	C11-C10-C8-C7
19	1	303	CLA	C6-C7-C8-C9
19	1	318	CLA	C11-C12-C13-C14
19	2	312	CLA	C14-C13-C15-C16
19	A	803	CLA	C11-C12-C13-C14
19	A	811	CLA	C14-C13-C15-C16
19	A	815	CLA	C11-C10-C8-C9
19	A	815	CLA	C14-C13-C15-C16
19	A	827	CLA	C11-C12-C13-C14
19	A	833	CLA	C11-C12-C13-C14
19	A	837	CLA	C6-C7-C8-C9
19	A	838	CLA	C6-C7-C8-C9
19	A	838	CLA	C14-C13-C15-C16
19	A	839	CLA	C6-C7-C8-C9
19	B	826	CLA	C6-C7-C8-C9
19	B	826	CLA	C11-C12-C13-C14
19	B	827	CLA	C6-C7-C8-C9
19	B	827	CLA	C11-C10-C8-C9
19	B	840	CLA	C11-C10-C8-C9
19	B	851	CLA	C14-C13-C15-C16
19	2	302	CLA	CBA-CGA-O2A-C1
19	A	802	CLA	O1D-CGD-O2D-CED
19	A	839	CLA	C2A-CAA-CBA-CGA
19	A	806	CLA	C15-C16-C17-C18
19	4	309	CLA	C11-C12-C13-C15
19	B	825	CLA	C6-C7-C8-C9
19	B	812	CLA	O1D-CGD-O2D-CED
24	2	319	BCR	C11-C12-C13-C14
19	1	303	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	C13-C15-C16-C17
24	2	319	BCR	C22-C23-C24-C25
19	B	823	CLA	CBD-CGD-O2D-CED
19	A	806	CLA	C8-C10-C11-C12
19	2	309	CLA	C4-C3-C5-C6
19	B	827	CLA	C4-C3-C5-C6
19	H	202	CLA	C4-C3-C5-C6
19	1	302	CLA	C2-C3-C5-C6
19	A	811	CLA	C16-C17-C18-C19
19	1	310	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	2	317	LHG	C2-C3-O3-P
19	3	303	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C3A-C2A-CAA-CBA
19	1	314	CLA	C3A-C2A-CAA-CBA
19	A	802	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	819	CLA	C3A-C2A-CAA-CBA
19	B	812	CLA	C3A-C2A-CAA-CBA
19	B	835	CLA	C3A-C2A-CAA-CBA
19	F	301	CLA	C3A-C2A-CAA-CBA
19	K	202	CLA	C3A-C2A-CAA-CBA
19	A	819	CLA	C8-C10-C11-C12
19	B	826	CLA	C15-C16-C17-C18
19	A	811	CLA	C16-C17-C18-C20
19	A	837	CLA	CBA-CGA-O2A-C1
25	B	849	LMG	O1-C7-C8-C9
19	A	813	CLA	O2A-C1-C2-C3
19	B	830	CLA	O2A-C1-C2-C3
19	2	312	CLA	C3-C5-C6-C7
19	B	832	CLA	C4-C3-C5-C6
19	4	303	CLA	C11-C12-C13-C14
19	A	825	CLA	C2-C3-C5-C6
18	4	305	CHL	C3C-C2C-CMC-OMC
22	1	320	LHG	C4-O6-P-O3
19	A	836	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	C2A-CAA-CBA-CGA
19	B	838	CLA	C2A-CAA-CBA-CGA
19	2	312	CLA	C15-C16-C17-C18
19	2	312	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	C6-C7-C8-C9
19	B	814	CLA	C16-C17-C18-C19
19	1	318	CLA	C3-C5-C6-C7
19	A	807	CLA	C3-C5-C6-C7
24	2	319	BCR	C13-C14-C15-C16
19	4	310	CLA	C11-C12-C13-C15
19	B	818	CLA	C11-C12-C13-C15
23	A	851	LMT	O5'-C1'-O1'-C1
19	B	803	CLA	C13-C15-C16-C17
19	A	801	CLA	C2-C1-O2A-CGA
19	A	825	CLA	C2-C1-O2A-CGA
19	1	308	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C11-C10-C8-C9
19	A	853	CLA	C11-C10-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	B	808	CLA	C14-C13-C15-C16
19	B	810	CLA	C11-C12-C13-C14
19	B	818	CLA	C11-C10-C8-C9
19	B	838	CLA	C6-C7-C8-C9
19	L	301	CLA	C6-C7-C8-C9
19	A	801	CLA	C8-C10-C11-C12
19	A	820	CLA	C2A-CAA-CBA-CGA
19	1	312	CLA	C11-C12-C13-C14
19	B	814	CLA	C16-C17-C18-C20
24	4	317	BCR	C23-C24-C25-C26
24	4	317	BCR	C23-C24-C25-C30
24	A	843	BCR	C5-C6-C7-C8
24	J	101	BCR	C7-C8-C9-C10
19	B	825	CLA	C5-C6-C7-C8
19	1	309	CLA	C11-C12-C13-C14
19	B	808	CLA	C16-C17-C18-C19
19	B	819	CLA	C11-C12-C13-C14
19	1	302	CLA	C11-C10-C8-C7
19	1	303	CLA	C6-C7-C8-C10
19	4	310	CLA	C11-C10-C8-C7
19	A	804	CLA	C11-C12-C13-C15
19	A	806	CLA	C6-C7-C8-C10
19	A	806	CLA	C11-C10-C8-C7
19	A	815	CLA	C6-C7-C8-C10
19	A	827	CLA	C11-C12-C13-C15
19	A	828	CLA	C12-C13-C15-C16
19	A	837	CLA	C6-C7-C8-C10
19	A	838	CLA	C12-C13-C15-C16
19	A	852	CLA	C12-C13-C15-C16
19	A	853	CLA	C6-C7-C8-C10
19	B	803	CLA	C6-C7-C8-C10
19	B	803	CLA	C11-C12-C13-C15
19	B	805	CLA	C12-C13-C15-C16
19	B	806	CLA	C11-C12-C13-C15
19	B	813	CLA	C11-C12-C13-C15
19	B	813	CLA	C12-C13-C15-C16
19	B	814	CLA	C11-C10-C8-C7
19	B	824	CLA	C11-C10-C8-C7
19	B	826	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B	832	CLA	C6-C7-C8-C10
19	B	838	CLA	C6-C7-C8-C10
19	B	840	CLA	C11-C12-C13-C15
19	B	840	CLA	C12-C13-C15-C16
19	B	851	CLA	C12-C13-C15-C16
19	L	301	CLA	C6-C7-C8-C10
19	L	301	CLA	C11-C10-C8-C7
26	B	841	PQN	C16-C17-C18-C20
19	A	806	CLA	C1-C2-C3-C4
19	A	811	CLA	C1-C2-C3-C4
19	A	834	CLA	C1-C2-C3-C4
19	3	302	CLA	C11-C12-C13-C14
19	A	815	CLA	C13-C15-C16-C17
19	B	851	CLA	C10-C11-C12-C13
19	1	307	CLA	C2A-CAA-CBA-CGA
19	G	203	CLA	C2A-CAA-CBA-CGA
19	3	302	CLA	C5-C6-C7-C8
19	B	831	CLA	C3-C5-C6-C7
19	3	301	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	C5-C6-C7-C8
19	B	818	CLA	O1A-CGA-O2A-C1
18	2	301	CHL	CAD-CBD-CGD-O2D
18	3	307	CHL	CAD-CBD-CGD-O2D
19	2	309	CLA	CAD-CBD-CGD-O2D
19	3	302	CLA	CAD-CBD-CGD-O2D
19	4	312	CLA	CAD-CBD-CGD-O2D
19	4	313	CLA	CAD-CBD-CGD-O2D
19	A	801	CLA	CAD-CBD-CGD-O2D
19	A	802	CLA	CAD-CBD-CGD-O2D
19	A	811	CLA	CAD-CBD-CGD-O2D
19	A	813	CLA	CAD-CBD-CGD-O2D
19	A	822	CLA	CAD-CBD-CGD-O2D
19	A	835	CLA	CAD-CBD-CGD-O2D
19	A	839	CLA	CAD-CBD-CGD-O2D
19	B	812	CLA	CAD-CBD-CGD-O2D
19	B	835	CLA	CAD-CBD-CGD-O2D
19	L	302	CLA	CAD-CBD-CGD-O2D
19	A	819	CLA	C5-C6-C7-C8
19	A	824	CLA	C8-C10-C11-C12
19	A	839	CLA	C15-C16-C17-C18
19	B	813	CLA	C5-C6-C7-C8
19	B	806	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	O1A-CGA-O2A-C1
19	B	832	CLA	O1A-CGA-O2A-C1
19	A	828	CLA	C15-C16-C17-C18
19	B	827	CLA	C5-C6-C7-C8
19	B	828	CLA	C10-C11-C12-C13
19	K	201	CLA	C2A-CAA-CBA-CGA
19	4	301	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	C16-C17-C18-C19
19	B	831	CLA	C11-C12-C13-C14
19	3	309	CLA	C4C-C3C-CAC-CBC
18	1	306	CHL	CHA-CBD-CGD-O1D
18	2	307	CHL	CHA-CBD-CGD-O2D
19	1	302	CLA	CHA-CBD-CGD-O2D
19	1	303	CLA	CHA-CBD-CGD-O1D
19	1	312	CLA	CHA-CBD-CGD-O2D
19	2	302	CLA	CHA-CBD-CGD-O1D
19	3	301	CLA	CHA-CBD-CGD-O1D
19	3	303	CLA	CHA-CBD-CGD-O2D
19	3	310	CLA	CHA-CBD-CGD-O1D
19	4	301	CLA	CHA-CBD-CGD-O2D
19	4	302	CLA	CHA-CBD-CGD-O2D
19	4	303	CLA	CHA-CBD-CGD-O2D
19	4	312	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	CHA-CBD-CGD-O2D
19	A	820	CLA	CHA-CBD-CGD-O1D
19	A	820	CLA	CHA-CBD-CGD-O2D
19	A	825	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	829	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	837	CLA	CHA-CBD-CGD-O2D
19	A	854	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	829	CLA	CHA-CBD-CGD-O2D
19	B	832	CLA	CHA-CBD-CGD-O2D
19	G	202	CLA	CHA-CBD-CGD-O2D
19	H	201	CLA	CHA-CBD-CGD-O2D
19	B	819	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	802	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	O1A-CGA-O2A-C1
19	B	801	CLA	O1A-CGA-O2A-C1
19	B	828	CLA	O1A-CGA-O2A-C1
24	J	101	BCR	C20-C21-C22-C23
19	A	853	CLA	C13-C15-C16-C17
19	1	310	CLA	O1A-CGA-O2A-C1
19	L	301	CLA	O1A-CGA-O2A-C1
19	A	803	CLA	C4-C3-C5-C6
19	B	825	CLA	C4-C3-C5-C6
19	A	839	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C11-C12-C13-C14
19	A	853	CLA	C6-C7-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	B	829	CLA	C14-C13-C15-C16
19	B	851	CLA	C11-C10-C8-C9
19	B	818	CLA	O1D-CGD-O2D-CED
19	2	312	CLA	C2A-CAA-CBA-CGA
19	1	311	CLA	O1D-CGD-O2D-CED
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	B	839	CLA	C1A-C2A-CAA-CBA
19	2	302	CLA	C16-C17-C18-C19
19	A	838	CLA	C16-C17-C18-C19
19	B	812	CLA	C6-C7-C8-C10
19	B	824	CLA	C16-C17-C18-C19
19	B	829	CLA	C16-C17-C18-C19
19	1	310	CLA	C5-C6-C7-C8
19	A	823	CLA	CBD-CGD-O2D-CED
19	4	308	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	C5-C6-C7-C8
19	A	810	CLA	C4-C3-C5-C6
19	1	312	CLA	C8-C10-C11-C12
19	L	301	CLA	C8-C10-C11-C12
22	1	320	LHG	C4-O6-P-O5
22	2	317	LHG	C4-O6-P-O4
19	A	835	CLA	C16-C17-C18-C19
19	A	854	CLA	C16-C17-C18-C19
19	B	814	CLA	CBA-CGA-O2A-C1
19	B	819	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	C2A-CAA-CBA-CGA
18	2	305	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	2	302	CLA	CAD-CBD-CGD-O1D
19	3	301	CLA	CAD-CBD-CGD-O1D
19	A	802	CLA	CAD-CBD-CGD-O1D
19	A	805	CLA	CAD-CBD-CGD-O1D
19	A	810	CLA	CAD-CBD-CGD-O1D
19	A	814	CLA	CAD-CBD-CGD-O1D
19	A	821	CLA	C2-C3-C5-C6
19	A	825	CLA	CAD-CBD-CGD-O1D
19	A	833	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CAD-CBD-CGD-O1D
19	B	813	CLA	CAD-CBD-CGD-O1D
19	B	821	CLA	CAD-CBD-CGD-O1D
19	B	824	CLA	CAD-CBD-CGD-O1D
19	B	839	CLA	CAD-CBD-CGD-O1D
19	4	310	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	C16-C17-C18-C19
19	A	852	CLA	C16-C17-C18-C19
19	L	301	CLA	C16-C17-C18-C19
19	A	811	CLA	C4-C3-C5-C6
19	A	837	CLA	C4-C3-C5-C6
19	4	310	CLA	C6-C7-C8-C10
19	A	823	CLA	C11-C12-C13-C15
19	A	829	CLA	C11-C12-C13-C15
19	A	837	CLA	C11-C10-C8-C7
19	A	853	CLA	C12-C13-C15-C16
19	B	810	CLA	C6-C7-C8-C10
19	B	826	CLA	C12-C13-C15-C16
19	B	836	CLA	C12-C13-C15-C16
19	B	838	CLA	C12-C13-C15-C16
26	B	841	PQN	C22-C23-C25-C26
22	B	850	LHG	C14-C15-C16-C17
19	B	806	CLA	C8-C10-C11-C12
19	B	828	CLA	C15-C16-C17-C18
19	A	840	CLA	C16-C17-C18-C20
19	B	809	CLA	C16-C17-C18-C20
18	1	306	CHL	C1C-C2C-CMC-OMC
18	4	307	CHL	C1C-C2C-CMC-OMC
22	1	317	LHG	C4-C5-C6-O8
25	4	318	LMG	C29-C30-C31-C32
19	1	311	CLA	O1A-CGA-O2A-C1
19	1	318	CLA	C13-C15-C16-C17
19	B	851	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	3	302	CLA	O2A-C1-C2-C3
19	B	839	CLA	CAA-CBA-CGA-O2A
19	A	835	CLA	C16-C17-C18-C20
19	A	854	CLA	C16-C17-C18-C20
19	B	819	CLA	C5-C6-C7-C8
19	A	816	CLA	C3-C5-C6-C7
19	B	807	CLA	O1A-CGA-O2A-C1
19	A	835	CLA	C15-C16-C17-C18
19	1	302	CLA	C11-C10-C8-C9
19	2	312	CLA	C6-C7-C8-C9
19	4	310	CLA	C11-C10-C8-C9
19	A	806	CLA	C11-C12-C13-C14
19	A	807	CLA	C11-C10-C8-C9
19	A	808	CLA	C11-C10-C8-C9
19	A	815	CLA	C6-C7-C8-C9
19	A	830	CLA	C14-C13-C15-C16
19	A	831	CLA	C6-C7-C8-C9
19	A	835	CLA	C11-C12-C13-C14
19	A	840	CLA	C11-C12-C13-C14
19	A	852	CLA	C11-C12-C13-C14
19	A	853	CLA	C11-C12-C13-C14
19	B	806	CLA	C11-C12-C13-C14
19	B	814	CLA	C11-C12-C13-C14
19	B	824	CLA	C11-C10-C8-C9
19	B	832	CLA	C6-C7-C8-C9
26	B	841	PQN	C16-C17-C18-C19
19	A	826	CLA	O1D-CGD-O2D-CED
18	1	301	CHL	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
24	2	319	BCR	C18-C19-C20-C21
24	A	843	BCR	C10-C11-C12-C13
24	A	844	BCR	C10-C11-C12-C13
24	A	847	BCR	C10-C11-C12-C13
24	G	201	BCR	C10-C11-C12-C13
24	J	101	BCR	C18-C19-C20-C21
24	L	304	BCR	C18-C19-C20-C21
24	L	305	BCR	C10-C11-C12-C13
19	K	202	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	C3-C5-C6-C7
19	3	302	CLA	O1A-CGA-O2A-C1
19	A	825	CLA	C16-C17-C18-C20
24	A	847	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	809	CLA	C15-C16-C17-C18
19	B	829	CLA	C4-C3-C5-C6
19	A	833	CLA	C8-C10-C11-C12
19	A	837	CLA	C3-C5-C6-C7
19	1	313	CLA	C2A-CAA-CBA-CGA
18	4	305	CHL	C2-C1-O2A-CGA
19	1	310	CLA	C2-C1-O2A-CGA
19	4	310	CLA	C2-C1-O2A-CGA
19	A	835	CLA	C2-C1-O2A-CGA
19	B	803	CLA	C2-C1-O2A-CGA
19	B	813	CLA	C2-C1-O2A-CGA
19	B	817	CLA	C2-C1-O2A-CGA
19	2	312	CLA	CBA-CGA-O2A-C1
19	4	309	CLA	C4-C3-C5-C6
20	2	315	LUT	C1-C6-C7-C8
24	A	843	BCR	C1-C6-C7-C8
24	B	844	BCR	C23-C24-C25-C30
24	L	305	BCR	C1-C6-C7-C8
24	L	305	BCR	C5-C6-C7-C8
19	B	819	CLA	C2-C3-C5-C6
19	1	309	CLA	O1A-CGA-O2A-C1
19	B	808	CLA	C16-C17-C18-C20
19	2	312	CLA	C13-C15-C16-C17
19	A	806	CLA	C10-C11-C12-C13
19	A	839	CLA	C1-C2-C3-C5
22	2	317	LHG	C26-C27-C28-C29
19	2	312	CLA	C6-C7-C8-C10
19	A	809	CLA	C12-C13-C15-C16
19	B	801	CLA	C11-C12-C13-C15
19	B	808	CLA	C11-C12-C13-C15
26	B	841	PQN	C21-C22-C23-C25
19	1	308	CLA	C6-C7-C8-C9
19	A	828	CLA	C14-C13-C15-C16
19	A	837	CLA	C11-C10-C8-C9
19	B	817	CLA	C6-C7-C8-C9
19	B	838	CLA	C11-C12-C13-C14
19	B	840	CLA	C11-C12-C13-C14
18	1	301	CHL	C6-C7-C8-C10
19	A	840	CLA	C16-C17-C18-C19
19	A	826	CLA	C5-C6-C7-C8
22	1	320	LHG	C2-C3-O3-P
19	4	310	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A	823	CLA	C8-C10-C11-C12
19	B	815	CLA	C2-C3-C5-C6
19	1	318	CLA	C16-C17-C18-C20
19	3	308	CLA	C16-C17-C18-C19
19	B	812	CLA	C6-C7-C8-C9
19	B	818	CLA	C11-C12-C13-C14
19	A	808	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CAA-CBA-CGA-O2A
19	B	839	CLA	C15-C16-C17-C18
19	A	839	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
25	B	849	LMG	C12-C13-C14-C15
26	A	841	PQN	C26-C27-C28-C30
19	B	814	CLA	C2-C3-C5-C6
19	4	308	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	C10-C11-C12-C13
19	F	301	CLA	CAA-CBA-CGA-O1A
19	4	303	CLA	C2-C1-O2A-CGA
19	A	821	CLA	C2-C1-O2A-CGA
19	A	826	CLA	C2-C1-O2A-CGA
19	A	852	CLA	C2-C1-O2A-CGA
19	B	814	CLA	C2-C1-O2A-CGA
19	A	853	CLA	C8-C10-C11-C12
19	4	310	CLA	C11-C12-C13-C14
19	A	815	CLA	C16-C17-C18-C19
19	A	810	CLA	C5-C6-C7-C8
19	3	311	CLA	C2A-CAA-CBA-CGA
19	A	837	CLA	C2A-CAA-CBA-CGA
19	B	809	CLA	C2A-CAA-CBA-CGA
22	1	317	LHG	O7-C5-C6-O8
28	B	848	DGD	O1G-C1G-C2G-O2G
19	3	303	CLA	C3A-C2A-CAA-CBA
19	4	304	CLA	C3A-C2A-CAA-CBA
19	A	826	CLA	C3A-C2A-CAA-CBA
19	B	836	CLA	C16-C17-C18-C19
22	2	317	LHG	C24-C25-C26-C27
28	B	848	DGD	C7A-C8A-C9A-CAA
19	2	309	CLA	C11-C10-C8-C9
19	2	312	CLA	C11-C12-C13-C14
19	A	829	CLA	C6-C7-C8-C9
19	A	840	CLA	C14-C13-C15-C16
19	A	854	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	804	CLA	CAA-CBA-CGA-O2A
19	B	834	CLA	CAA-CBA-CGA-O1A
19	A	811	CLA	C8-C10-C11-C12
19	B	817	CLA	O1D-CGD-O2D-CED
21	2	316	XAT	C20-C13-C14-C15
24	2	319	BCR	C20-C21-C22-C37
24	A	849	BCR	C11-C10-C9-C34
24	A	849	BCR	C16-C17-C18-C36
24	B	843	BCR	C11-C10-C9-C34
24	B	844	BCR	C11-C10-C9-C34
24	B	844	BCR	C20-C21-C22-C37
24	F	303	BCR	C35-C13-C14-C15
28	B	848	DGD	O1G-C1G-C2G-C3G
19	B	802	CLA	C2A-CAA-CBA-CGA
19	B	836	CLA	C2A-CAA-CBA-CGA
19	B	851	CLA	C2A-CAA-CBA-CGA
19	1	318	CLA	C16-C17-C18-C19
19	3	308	CLA	C16-C17-C18-C20
19	B	809	CLA	C16-C17-C18-C19
26	A	841	PQN	C26-C27-C28-C29
19	1	310	CLA	O2A-C1-C2-C3
19	4	308	CLA	O2A-C1-C2-C3
19	A	821	CLA	O2A-C1-C2-C3
19	A	828	CLA	O2A-C1-C2-C3
19	A	830	CLA	O2A-C1-C2-C3
19	A	839	CLA	O2A-C1-C2-C3
19	B	802	CLA	O2A-C1-C2-C3
19	B	817	CLA	O2A-C1-C2-C3
19	B	823	CLA	O2A-C1-C2-C3
19	B	801	CLA	CBA-CGA-O2A-C1
28	B	848	DGD	O6E-C1E-O5D-C6D
19	B	810	CLA	C5-C6-C7-C8
18	1	301	CHL	C1A-C2A-CAA-CBA
19	4	304	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	B	812	CLA	C1A-C2A-CAA-CBA
19	B	851	CLA	C1A-C2A-CAA-CBA
19	F	301	CLA	C1A-C2A-CAA-CBA
19	A	831	CLA	C16-C17-C18-C19
19	4	303	CLA	C11-C10-C8-C7
19	A	803	CLA	C11-C12-C13-C15
19	A	830	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	A	831	CLA	C11-C12-C13-C15
19	B	810	CLA	C11-C12-C13-C15
19	B	810	CLA	C12-C13-C15-C16
19	B	826	CLA	C11-C10-C8-C7
19	B	828	CLA	C12-C13-C15-C16
19	L	301	CLA	C11-C12-C13-C15
19	A	808	CLA	C11-C12-C13-C14
19	B	838	CLA	C13-C15-C16-C17
19	3	313	CLA	CAA-CBA-CGA-O2A
19	F	301	CLA	CAA-CBA-CGA-O2A
19	A	840	CLA	C13-C15-C16-C17
19	B	805	CLA	CAA-CBA-CGA-O2A
19	A	832	CLA	CAA-CBA-CGA-O1A
19	A	852	CLA	C15-C16-C17-C18
19	A	852	CLA	C5-C6-C7-C8
18	2	307	CHL	CAA-CBA-CGA-O1A
19	B	801	CLA	C16-C17-C18-C19
19	B	807	CLA	C16-C17-C18-C19
19	B	828	CLA	C2-C3-C5-C6
18	2	306	CHL	CAA-CBA-CGA-O1A
21	2	316	XAT	C12-C13-C14-C15
24	2	319	BCR	C20-C21-C22-C23
24	A	849	BCR	C11-C10-C9-C8
24	A	849	BCR	C16-C17-C18-C19
24	B	843	BCR	C11-C10-C9-C8
24	B	844	BCR	C11-C10-C9-C8
24	B	844	BCR	C20-C21-C22-C23
24	F	303	BCR	C12-C13-C14-C15
19	2	311	CLA	CAA-CBA-CGA-O2A
19	H	202	CLA	C2A-CAA-CBA-CGA
19	B	834	CLA	CAA-CBA-CGA-O2A
19	B	851	CLA	C4-C3-C5-C6
19	A	823	CLA	C2-C1-O2A-CGA
19	A	833	CLA	C2-C1-O2A-CGA
19	B	835	CLA	C2-C1-O2A-CGA
19	A	816	CLA	CAA-CBA-CGA-O2A
19	A	839	CLA	C11-C12-C13-C14
19	B	851	CLA	C11-C12-C13-C14
19	2	302	CLA	O1A-CGA-O2A-C1
19	B	838	CLA	O1A-CGA-O2A-C1
19	3	311	CLA	CAA-CBA-CGA-O1A
19	3	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	821	CLA	C4-C3-C5-C6
19	2	303	CLA	O1A-CGA-O2A-C1
19	2	308	CLA	C2A-CAA-CBA-CGA
19	A	821	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	A	825	CLA	C16-C17-C18-C19
24	B	844	BCR	C23-C24-C25-C26
24	B	847	BCR	C1-C6-C7-C8
24	G	205	BCR	C1-C6-C7-C8
24	J	103	BCR	C23-C24-C25-C26
24	J	103	BCR	C23-C24-C25-C30
22	A	842	LHG	C4-C5-C6-O8
19	B	825	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	C4-C3-C5-C6
19	B	818	CLA	C5-C6-C7-C8
19	B	802	CLA	C8-C10-C11-C12
18	2	307	CHL	CAA-CBA-CGA-O2A
19	A	804	CLA	C16-C17-C18-C19
19	A	815	CLA	C16-C17-C18-C20
19	B	801	CLA	C16-C17-C18-C20
19	B	822	CLA	C6-C7-C8-C10
18	2	306	CHL	C2A-CAA-CBA-CGA
19	A	809	CLA	C16-C17-C18-C19
19	A	831	CLA	C16-C17-C18-C20
19	3	301	CLA	C1-C2-C3-C5
18	1	301	CHL	C2-C3-C5-C6
19	A	831	CLA	C11-C10-C8-C7
19	A	833	CLA	C11-C10-C8-C7
19	A	833	CLA	C12-C13-C15-C16
19	A	835	CLA	C6-C7-C8-C10
19	B	832	CLA	C11-C10-C8-C7
19	B	836	CLA	C2-C3-C5-C6
19	A	810	CLA	C1-C2-C3-C4
19	A	822	CLA	C1-C2-C3-C4
19	A	830	CLA	C1-C2-C3-C4
19	B	801	CLA	C1-C2-C3-C4
19	B	803	CLA	C1-C2-C3-C4
19	B	813	CLA	C1-C2-C3-C4
19	B	818	CLA	C1-C2-C3-C4
19	B	840	CLA	C1-C2-C3-C4
19	B	851	CLA	C1-C2-C3-C4
19	A	803	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	B	838	CLA	C16-C17-C18-C19
28	B	848	DGD	C7B-C8B-C9B-CAB
18	2	306	CHL	CAA-CBA-CGA-O2A
25	4	318	LMG	O7-C10-C11-C12
19	A	829	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	C4-C3-C5-C6
19	A	808	CLA	C4-C3-C5-C6
19	3	302	CLA	C11-C12-C13-C15
19	A	823	CLA	C16-C17-C18-C20
19	B	806	CLA	C16-C17-C18-C20
19	B	807	CLA	C16-C17-C18-C20
19	B	840	CLA	C16-C17-C18-C19
19	A	834	CLA	CAA-CBA-CGA-O2A
19	4	303	CLA	C11-C10-C8-C9
19	A	801	CLA	C11-C10-C8-C9
19	A	823	CLA	C11-C12-C13-C14
19	A	835	CLA	C6-C7-C8-C9
19	A	853	CLA	C14-C13-C15-C16
19	B	838	CLA	C14-C13-C15-C16
26	B	841	PQN	C24-C23-C25-C26
18	4	306	CHL	CAA-CBA-CGA-O2A
18	1	301	CHL	C3A-C2A-CAA-CBA
19	3	311	CLA	C3A-C2A-CAA-CBA
19	A	823	CLA	C3A-C2A-CAA-CBA
22	B	850	LHG	C27-C28-C29-C30
26	B	841	PQN	C23-C25-C26-C27
18	2	314	CHL	CAD-CBD-CGD-O2D
19	3	309	CLA	CAD-CBD-CGD-O2D
19	3	312	CLA	CAD-CBD-CGD-O2D
19	3	314	CLA	CAD-CBD-CGD-O2D
19	A	809	CLA	CAD-CBD-CGD-O2D
19	A	810	CLA	CAD-CBD-CGD-O2D
19	A	812	CLA	CAD-CBD-CGD-O2D
19	A	814	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	A	830	CLA	CAD-CBD-CGD-O2D
19	A	831	CLA	CAD-CBD-CGD-O2D
19	A	838	CLA	CAD-CBD-CGD-O2D
19	B	810	CLA	CAD-CBD-CGD-O2D
19	B	815	CLA	CAD-CBD-CGD-O2D
19	B	819	CLA	CAD-CBD-CGD-O2D
19	B	821	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	830	CLA	CAD-CBD-CGD-O2D
19	B	831	CLA	CAD-CBD-CGD-O2D
19	B	837	CLA	CAD-CBD-CGD-O2D
19	B	840	CLA	CAD-CBD-CGD-O2D
19	B	851	CLA	CAD-CBD-CGD-O2D
19	3	309	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C5-C6-C7-C8
19	B	809	CLA	C8-C10-C11-C12
19	B	831	CLA	C2-C3-C5-C6
19	B	803	CLA	CAA-CBA-CGA-O2A
28	B	848	DGD	C6A-C7A-C8A-C9A
21	2	316	XAT	O4-C6-C7-C8
21	3	316	XAT	O4-C6-C7-C8
19	2	311	CLA	CAA-CBA-CGA-O1A
19	4	311	CLA	CAA-CBA-CGA-O1A
19	A	833	CLA	CBD-CGD-O2D-CED
19	A	853	CLA	C3-C5-C6-C7
19	A	801	CLA	CAA-CBA-CGA-O2A
19	A	838	CLA	CAA-CBA-CGA-O2A
19	A	803	CLA	CAA-CBA-CGA-O1A
19	A	832	CLA	CAA-CBA-CGA-O2A
18	4	307	CHL	O2A-C1-C2-C3
19	2	303	CLA	O2A-C1-C2-C3
19	4	303	CLA	O2A-C1-C2-C3
19	B	805	CLA	O2A-C1-C2-C3
19	B	810	CLA	O2A-C1-C2-C3
19	B	821	CLA	O2A-C1-C2-C3
19	B	831	CLA	O2A-C1-C2-C3
19	B	832	CLA	O2A-C1-C2-C3
19	B	833	CLA	O2A-C1-C2-C3
19	L	302	CLA	O2A-C1-C2-C3
19	A	802	CLA	CBA-CGA-O2A-C1
19	A	854	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	C3-C5-C6-C7
19	B	804	CLA	CAA-CBA-CGA-O1A
19	B	806	CLA	O1D-CGD-O2D-CED
18	1	301	CHL	CHA-CBD-CGD-O2D
18	2	301	CHL	CHA-CBD-CGD-O2D
18	2	305	CHL	CHA-CBD-CGD-O1D
19	1	303	CLA	CHA-CBD-CGD-O2D
19	1	304	CLA	CHA-CBD-CGD-O2D
19	1	314	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	1	318	CLA	CHA-CBD-CGD-O1D
19	2	310	CLA	CHA-CBD-CGD-O2D
19	4	302	CLA	CHA-CBD-CGD-O1D
19	A	808	CLA	CHA-CBD-CGD-O1D
19	A	808	CLA	CHA-CBD-CGD-O2D
19	A	813	CLA	CHA-CBD-CGD-O1D
19	A	825	CLA	CHA-CBD-CGD-O2D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	835	CLA	CHA-CBD-CGD-O1D
19	A	853	CLA	CHA-CBD-CGD-O1D
19	A	853	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	816	CLA	CHA-CBD-CGD-O2D
19	B	819	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	CHA-CBD-CGD-O1D
19	B	822	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D
19	B	829	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	B	836	CLA	CHA-CBD-CGD-O2D
19	H	202	CLA	CHA-CBD-CGD-O2D
19	J	102	CLA	CHA-CBD-CGD-O2D
19	A	853	CLA	C10-C11-C12-C13
19	3	303	CLA	CAA-CBA-CGA-O1A
22	1	320	LHG	O7-C7-C8-C9
19	3	313	CLA	CAA-CBA-CGA-O1A
19	B	839	CLA	CAA-CBA-CGA-O1A
19	A	840	CLA	C15-C16-C17-C18
19	B	807	CLA	C15-C16-C17-C18
19	A	840	CLA	C8-C10-C11-C12
19	3	308	CLA	CAA-CBA-CGA-O2A
19	A	853	CLA	CAA-CBA-CGA-O2A
22	1	320	LHG	O8-C23-C24-C25
19	3	302	CLA	C2A-CAA-CBA-CGA
19	B	816	CLA	C4-C3-C5-C6
19	A	807	CLA	C12-C13-C15-C16
19	A	828	CLA	C11-C10-C8-C7
19	B	808	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B	813	CLA	C11-C10-C8-C7
19	B	838	CLA	C11-C12-C13-C15
26	A	841	PQN	C17-C18-C20-C21
19	3	312	CLA	C6-C7-C8-C9
19	A	804	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	CAA-CBA-CGA-O1A
19	A	820	CLA	CAA-CBA-CGA-O2A
19	A	830	CLA	C11-C12-C13-C14
19	A	833	CLA	C11-C10-C8-C9
19	B	813	CLA	C11-C12-C13-C14
19	B	819	CLA	C11-C10-C8-C9
19	B	836	CLA	C14-C13-C15-C16
22	1	317	LHG	C25-C26-C27-C28
18	1	301	CHL	C6-C7-C8-C9
19	3	312	CLA	C6-C7-C8-C10
19	4	312	CLA	C3-C5-C6-C7
19	A	807	CLA	CAA-CBA-CGA-O1A
19	A	826	CLA	CAA-CBA-CGA-O2A
19	A	831	CLA	C13-C15-C16-C17
19	A	829	CLA	CAA-CBA-CGA-O1A
19	B	813	CLA	CAA-CBA-CGA-O1A
19	G	204	CLA	CAA-CBA-CGA-O1A
19	A	838	CLA	C15-C16-C17-C18
19	3	311	CLA	C1A-C2A-CAA-CBA
19	3	313	CLA	C1A-C2A-CAA-CBA
19	4	301	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C1A-C2A-CAA-CBA
19	B	802	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C16-C17-C18-C19
19	A	806	CLA	CAA-CBA-CGA-O1A
19	A	853	CLA	C2-C1-O2A-CGA
19	B	838	CLA	C2-C1-O2A-CGA
19	2	309	CLA	CAA-CBA-CGA-O1A
19	B	823	CLA	CAA-CBA-CGA-O1A
19	L	302	CLA	CAA-CBA-CGA-O1A
25	4	318	LMG	O9-C10-C11-C12
19	4	303	CLA	CAA-CBA-CGA-O2A
19	2	302	CLA	C2A-CAA-CBA-CGA
19	2	303	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	C2A-CAA-CBA-CGA
19	B	804	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	B	818	CLA	C2A-CAA-CBA-CGA
19	A	815	CLA	CAA-CBA-CGA-O2A
19	G	204	CLA	CAA-CBA-CGA-O2A
19	B	828	CLA	CAA-CBA-CGA-O1A
19	A	835	CLA	C2-C3-C5-C6
18	4	306	CHL	CAA-CBA-CGA-O1A
19	1	314	CLA	CAA-CBA-CGA-O1A
28	B	848	DGD	C2E-C1E-O5D-C6D
22	B	850	LHG	C3-O3-P-O5
22	1	320	LHG	O9-C7-C8-C9
24	B	847	BCR	C5-C6-C7-C8
19	B	824	CLA	CAA-CBA-CGA-O1A
19	B	840	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	CAA-CBA-CGA-O2A
19	F	302	CLA	CAA-CBA-CGA-O1A
19	B	832	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	C2A-CAA-CBA-CGA
19	A	826	CLA	CAA-CBA-CGA-O1A
19	2	302	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	C2-C3-C5-C6
19	F	302	CLA	CAA-CBA-CGA-O2A
18	2	314	CHL	CAD-CBD-CGD-O1D
19	1	304	CLA	C2-C3-C5-C6
19	1	312	CLA	CAD-CBD-CGD-O1D
19	3	313	CLA	CAD-CBD-CGD-O1D
19	A	808	CLA	CAD-CBD-CGD-O1D
19	A	831	CLA	CAD-CBD-CGD-O1D
19	A	839	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O1D
19	H	201	CLA	CAD-CBD-CGD-O1D
19	2	302	CLA	CAA-CBA-CGA-O1A
19	B	831	CLA	CAA-CBA-CGA-O1A
19	A	806	CLA	CAA-CBA-CGA-O2A
19	A	801	CLA	C14-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C9
19	A	828	CLA	C11-C10-C8-C9
19	A	852	CLA	C11-C10-C8-C9
19	B	802	CLA	C14-C13-C15-C16
26	A	841	PQN	C19-C18-C20-C21
22	1	317	LHG	C27-C28-C29-C30
19	2	302	CLA	C13-C15-C16-C17
19	A	809	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	CAA-CBA-CGA-O2A
18	4	305	CHL	O1D-CGD-O2D-CED
22	1	320	LHG	O10-C23-C24-C25
19	A	801	CLA	C15-C16-C17-C18
19	A	819	CLA	C13-C15-C16-C17
19	A	830	CLA	C15-C16-C17-C18
19	B	814	CLA	C10-C11-C12-C13
19	3	308	CLA	C12-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C10
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	C11-C12-C13-C15
19	A	840	CLA	C11-C12-C13-C15
19	B	817	CLA	C11-C10-C8-C7
19	B	819	CLA	C11-C10-C8-C7
19	B	831	CLA	C11-C10-C8-C7
19	A	838	CLA	CAA-CBA-CGA-O1A
28	B	848	DGD	O6D-C5D-C6D-O5D
19	H	202	CLA	CAA-CBA-CGA-O2A
19	A	834	CLA	CAA-CBA-CGA-O1A
19	G	203	CLA	CAA-CBA-CGA-O1A
19	A	831	CLA	C8-C10-C11-C12
19	B	810	CLA	CAA-CBA-CGA-O1A
19	B	819	CLA	CAA-CBA-CGA-O1A
26	A	841	PQN	C25-C26-C27-C28
19	1	308	CLA	CAA-CBA-CGA-O2A
19	1	311	CLA	CAA-CBA-CGA-O2A
19	4	301	CLA	CAA-CBA-CGA-O2A
19	B	806	CLA	CAA-CBA-CGA-O1A
19	A	814	CLA	C2A-CAA-CBA-CGA
19	A	832	CLA	C2A-CAA-CBA-CGA
19	1	318	CLA	CAA-CBA-CGA-O1A
19	4	302	CLA	CAA-CBA-CGA-O1A
19	A	801	CLA	C4-C3-C5-C6
19	2	309	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

156 monomers are involved in 293 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	315	LUT	7	0
24	B	844	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	840	CLA	2	0
19	B	833	CLA	1	0
19	B	820	CLA	1	0
19	A	826	CLA	2	0
25	B	849	LMG	1	0
18	4	307	CHL	1	0
19	B	806	CLA	4	0
22	1	320	LHG	2	0
19	B	839	CLA	2	0
19	B	816	CLA	1	0
19	2	302	CLA	1	0
19	3	314	CLA	1	0
22	2	317	LHG	2	0
19	A	807	CLA	5	0
19	A	825	CLA	1	0
19	A	827	CLA	1	0
19	3	312	CLA	2	0
19	A	814	CLA	1	0
19	A	822	CLA	2	0
24	J	101	BCR	7	0
19	F	301	CLA	1	0
22	1	317	LHG	3	0
24	B	845	BCR	2	0
21	4	316	XAT	1	0
18	1	306	CHL	1	0
19	A	812	CLA	1	0
19	A	808	CLA	2	0
24	G	205	BCR	1	0
24	L	304	BCR	6	0
19	A	811	CLA	7	0
19	A	824	CLA	1	0
19	B	818	CLA	3	0
20	2	315	LUT	4	0
19	A	840	CLA	3	0
23	2	318	LMT	1	0
20	1	319	LUT	3	0
19	A	806	CLA	4	0
19	B	807	CLA	4	0
19	A	839	CLA	1	0
19	B	824	CLA	2	0
24	B	843	BCR	1	0
19	A	838	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	308	CLA	3	0
18	2	306	CHL	1	0
19	4	301	CLA	1	0
19	K	201	CLA	3	0
19	B	836	CLA	1	0
21	2	316	XAT	1	0
19	1	311	CLA	1	0
19	3	311	CLA	1	0
19	3	304	CLA	2	0
19	A	837	CLA	1	0
19	B	821	CLA	1	0
20	1	315	LUT	4	0
22	B	850	LHG	5	0
24	A	848	BCR	2	0
24	3	317	BCR	4	0
19	1	313	CLA	1	0
19	1	312	CLA	3	0
19	B	831	CLA	1	0
19	B	828	CLA	1	0
19	A	818	CLA	1	0
19	A	853	CLA	4	0
19	2	310	CLA	1	0
19	3	308	CLA	3	0
19	A	833	CLA	7	0
19	2	309	CLA	2	0
19	4	302	CLA	2	0
19	4	303	CLA	3	0
19	K	202	CLA	1	0
19	B	827	CLA	1	0
19	4	304	CLA	1	0
19	3	301	CLA	1	0
19	B	810	CLA	1	0
19	B	835	CLA	1	0
20	3	315	LUT	6	0
24	I	101	BCR	4	0
24	A	843	BCR	4	0
19	B	803	CLA	1	0
18	2	307	CHL	3	0
19	A	819	CLA	2	0
19	B	805	CLA	1	0
19	A	816	CLA	4	0
19	B	832	CLA	3	0

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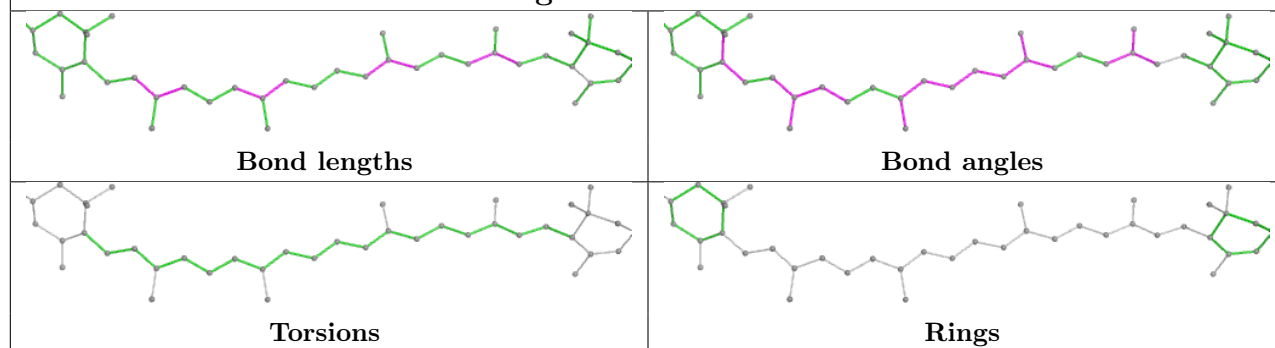
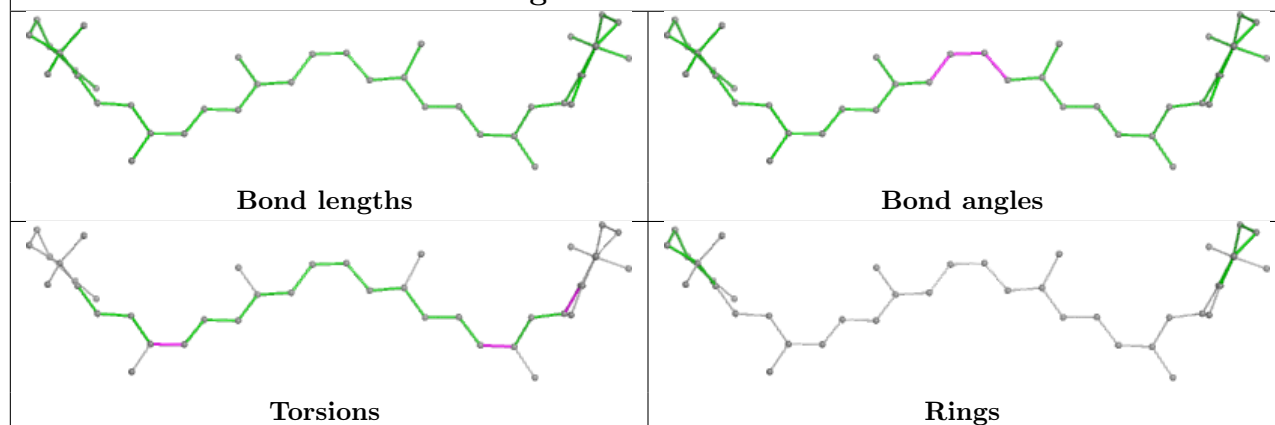
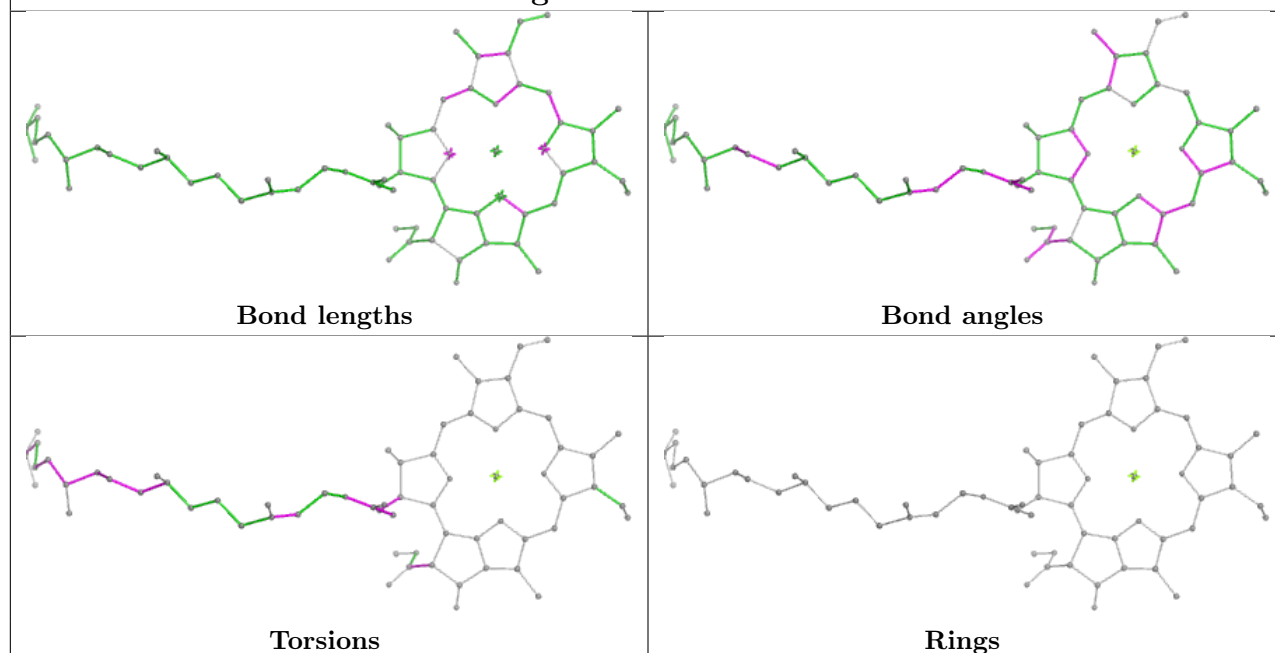
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	825	CLA	1	0
19	B	851	CLA	2	0
19	B	822	CLA	1	0
24	A	846	BCR	2	0
19	A	831	CLA	1	0
19	B	826	CLA	4	0
19	B	823	CLA	3	0
19	G	203	CLA	1	0
19	A	854	CLA	1	0
19	H	201	CLA	2	0
19	3	302	CLA	2	0
19	3	303	CLA	1	0
19	L	301	CLA	2	0
26	B	841	PQN	2	0
24	F	304	BCR	1	0
23	A	851	LMT	1	0
19	B	829	CLA	2	0
25	F	305	LMG	2	0
19	B	804	CLA	1	0
19	A	810	CLA	1	0
19	A	835	CLA	3	0
19	3	310	CLA	1	0
24	G	201	BCR	4	0
19	3	309	CLA	2	0
19	A	813	CLA	1	0
24	F	303	BCR	3	0
21	1	316	XAT	3	0
19	A	805	CLA	1	0
18	4	306	CHL	2	0
18	4	305	CHL	1	0
18	2	301	CHL	4	0
19	2	308	CLA	1	0
19	3	306	CLA	1	0
19	B	838	CLA	4	0
24	B	846	BCR	2	0
24	L	305	BCR	4	0
19	A	809	CLA	2	0
19	A	830	CLA	2	0
19	J	102	CLA	1	0
19	A	815	CLA	2	0
19	B	817	CLA	3	0
24	2	319	BCR	6	0

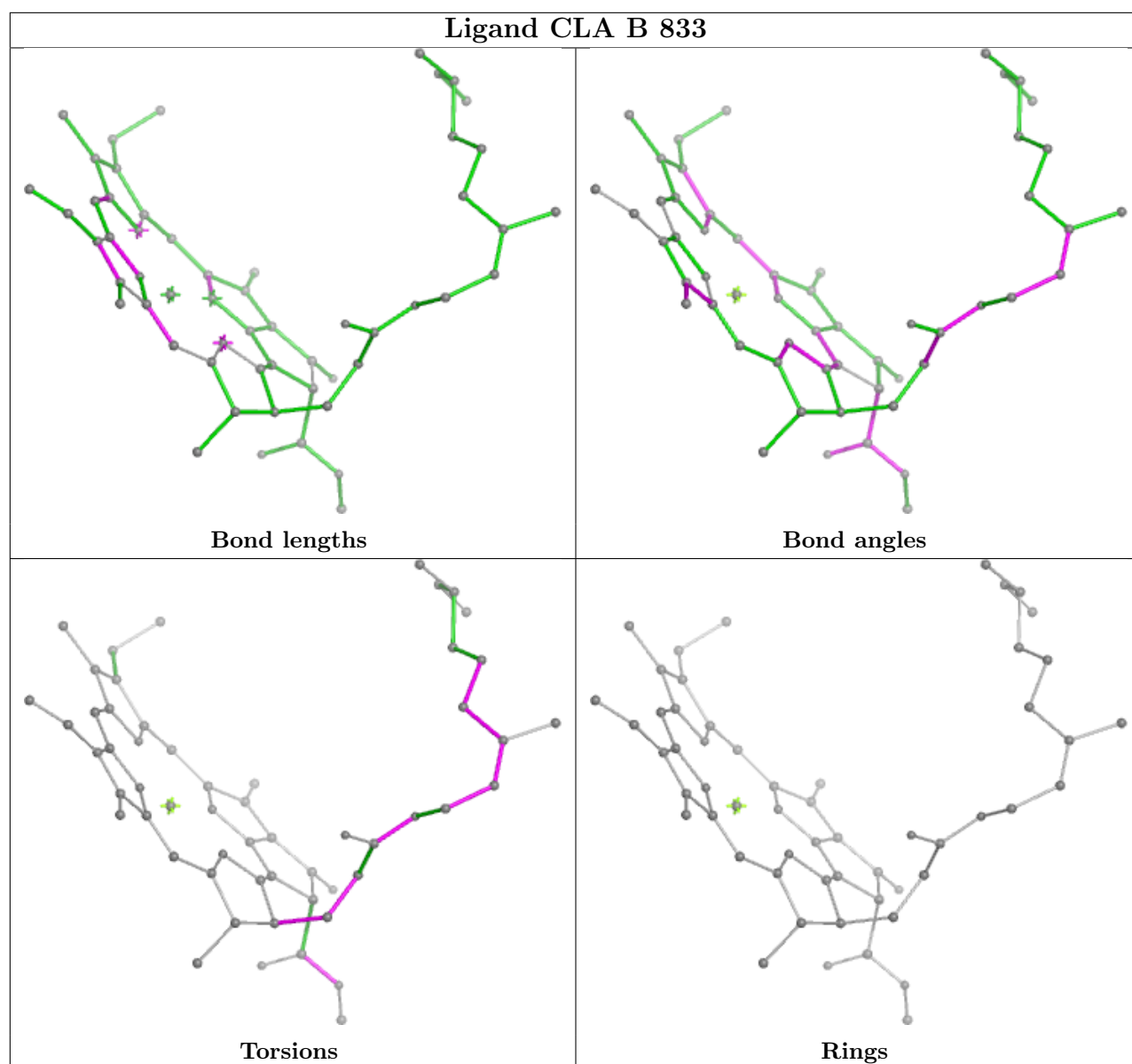
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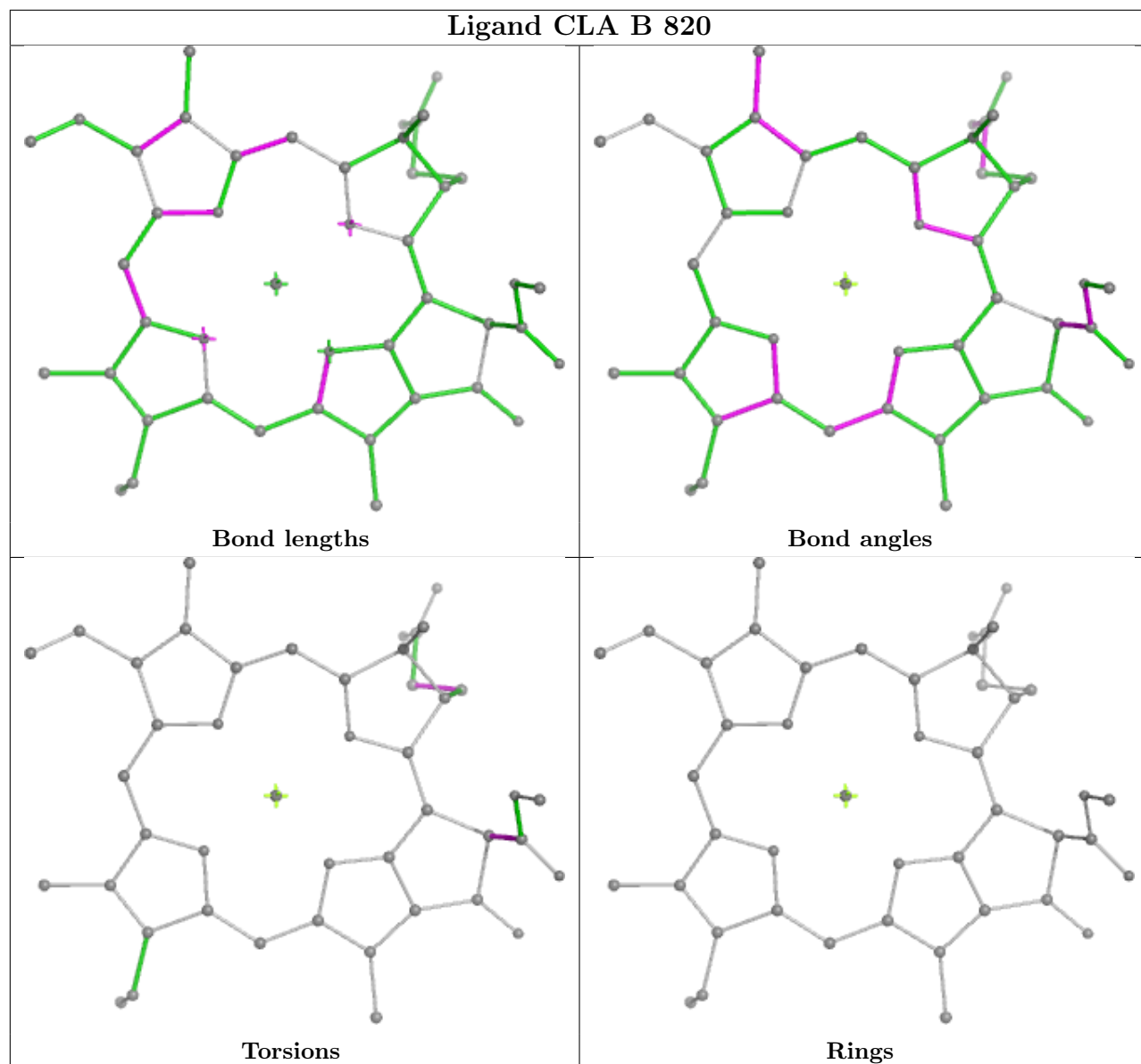
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	804	CLA	1	0
19	A	828	CLA	4	0
24	A	845	BCR	1	0
19	1	302	CLA	4	0
18	1	301	CHL	2	0
24	B	842	BCR	2	0
19	A	823	CLA	5	0
19	1	318	CLA	2	0
19	B	813	CLA	5	0
19	B	814	CLA	1	0
21	3	316	XAT	2	0
19	B	834	CLA	1	0
19	B	830	CLA	1	0
28	B	848	DGD	2	0
24	A	844	BCR	7	0
19	A	803	CLA	3	0
19	H	202	CLA	2	0
24	J	104	BCR	1	0
24	J	103	BCR	2	0
24	A	849	BCR	2	0
19	1	309	CLA	2	0
19	4	312	CLA	6	0
19	A	801	CLA	2	0
19	B	812	CLA	4	0
24	A	847	BCR	2	0
19	4	309	CLA	3	0
19	A	852	CLA	3	0
19	B	808	CLA	1	0

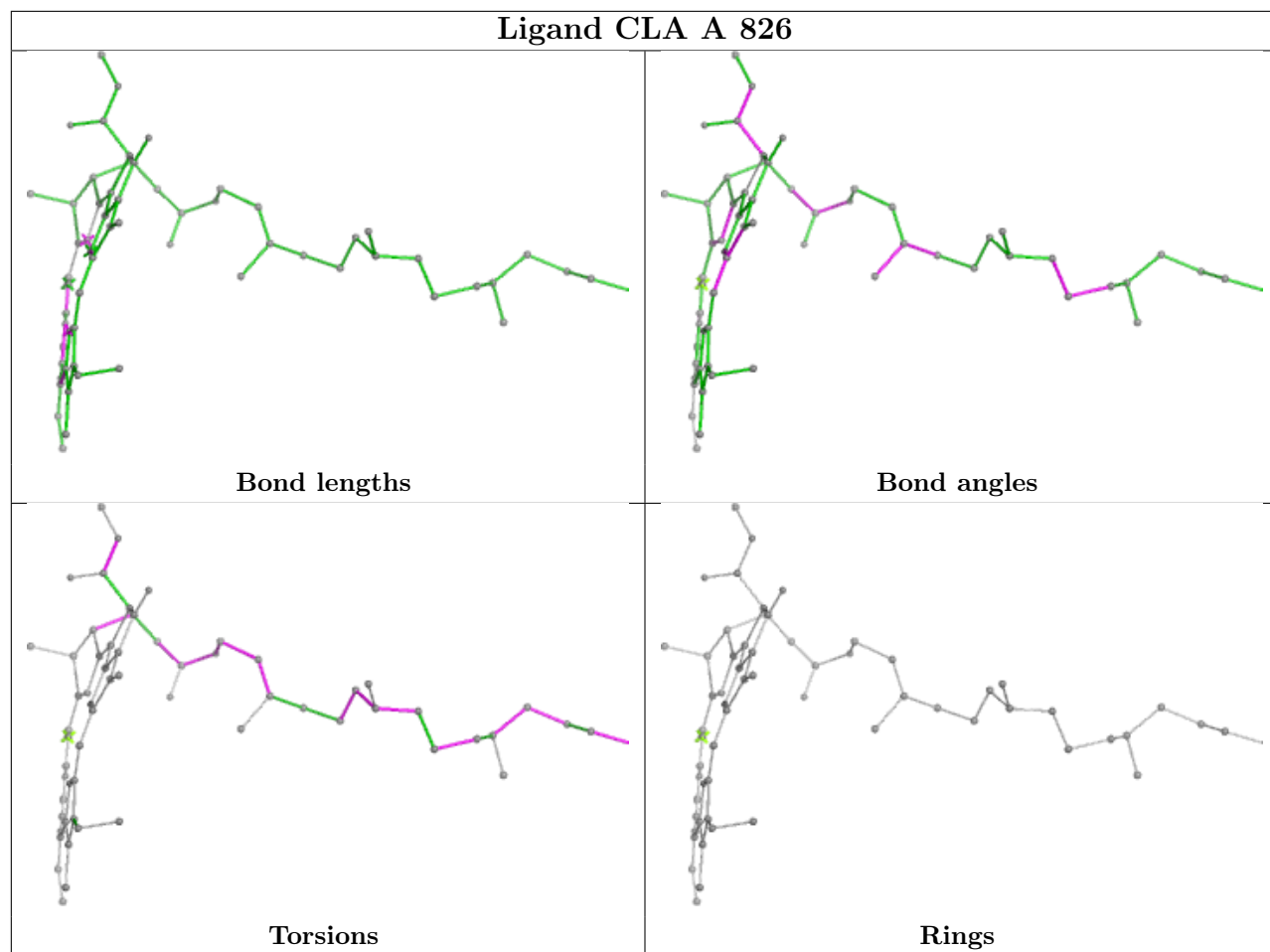
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

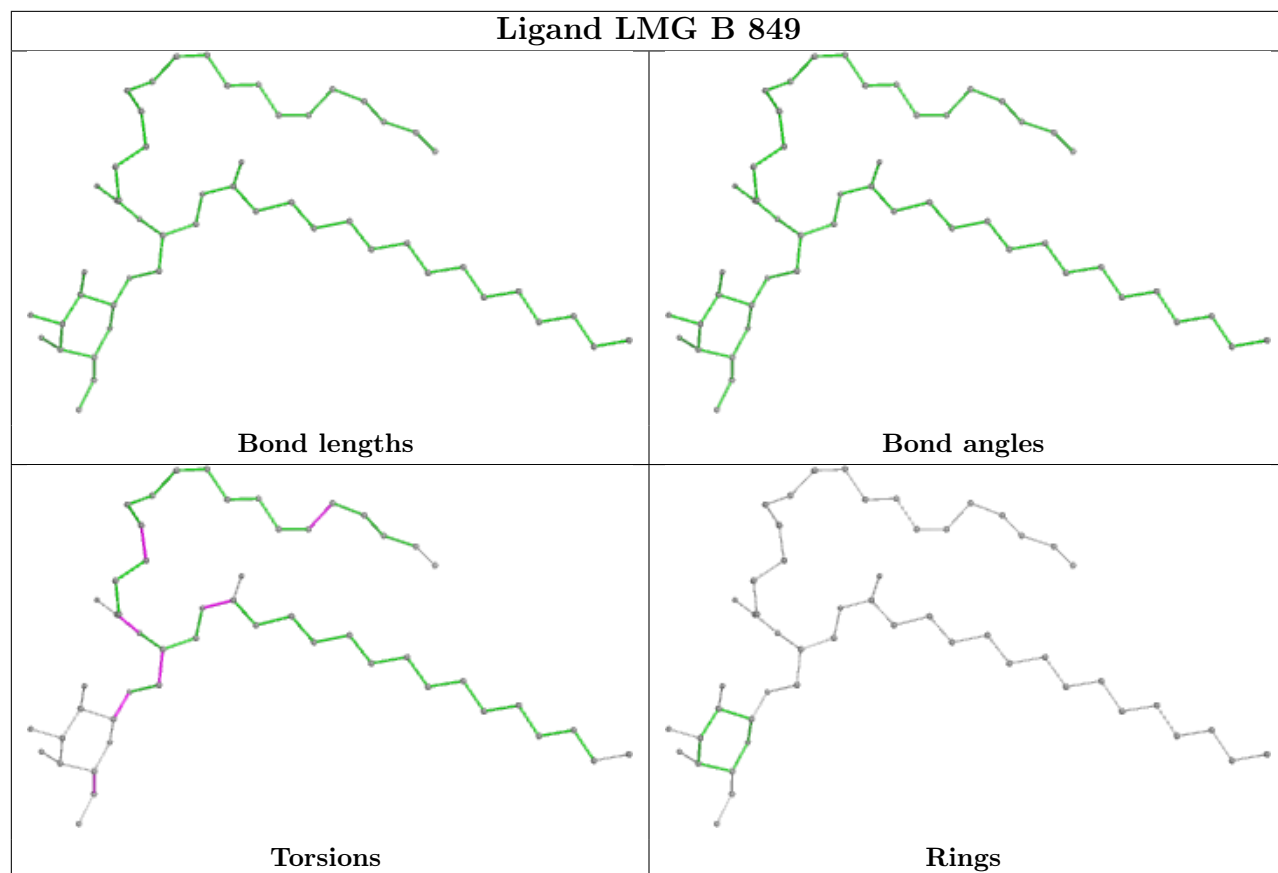
Ligand LUT 4 315**Ligand BCR B 844****Ligand CLA B 840**

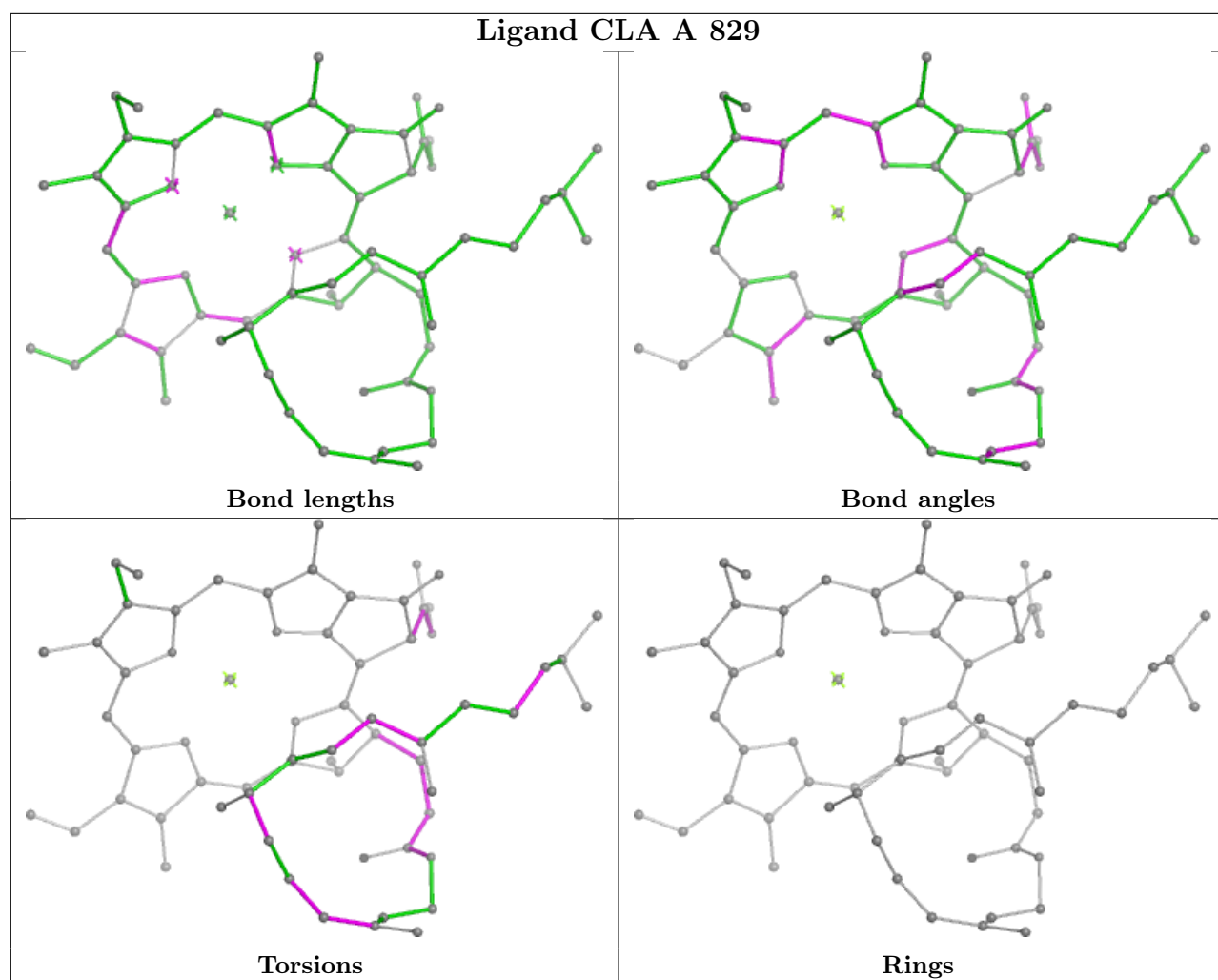


Ligand CLA B 820

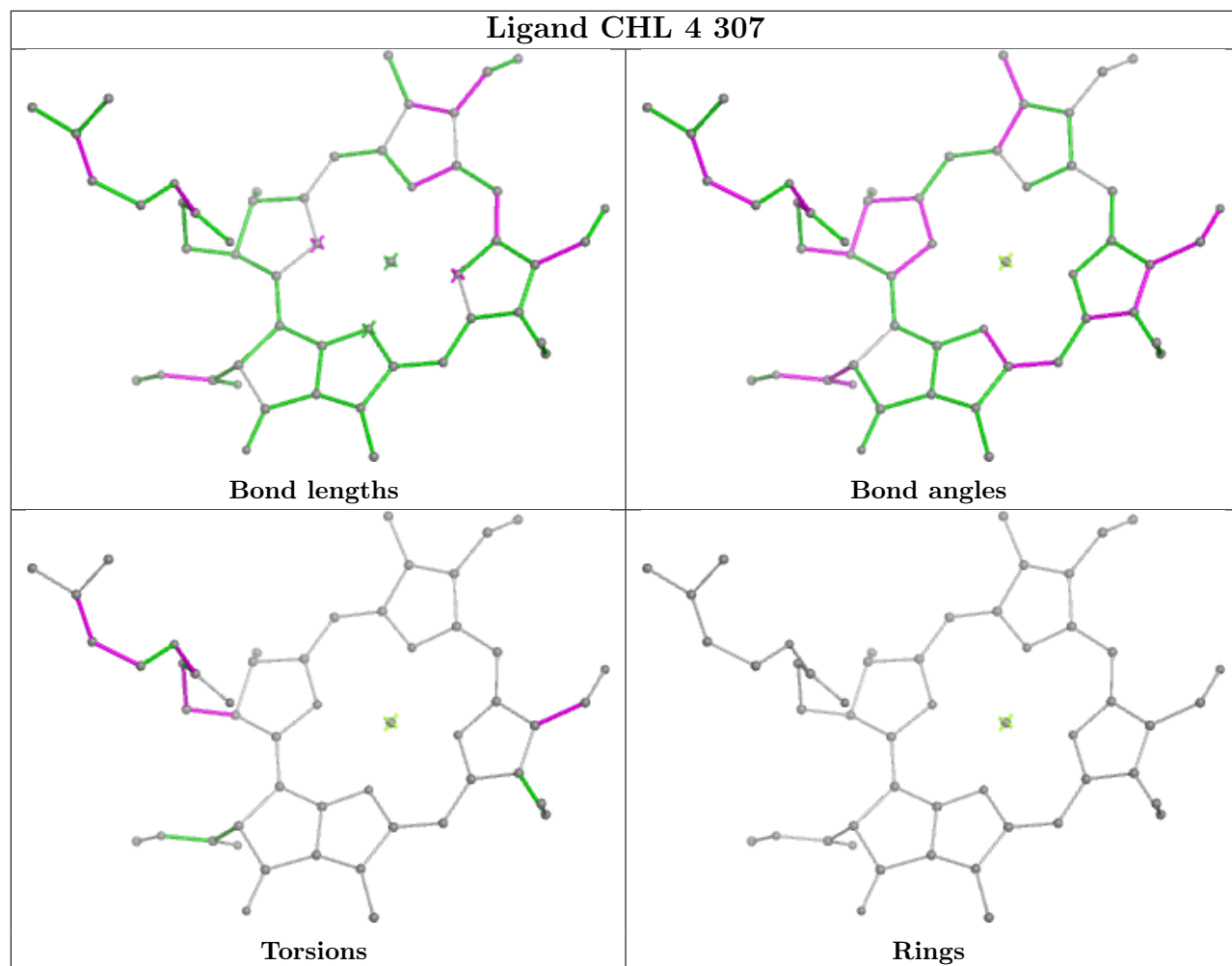




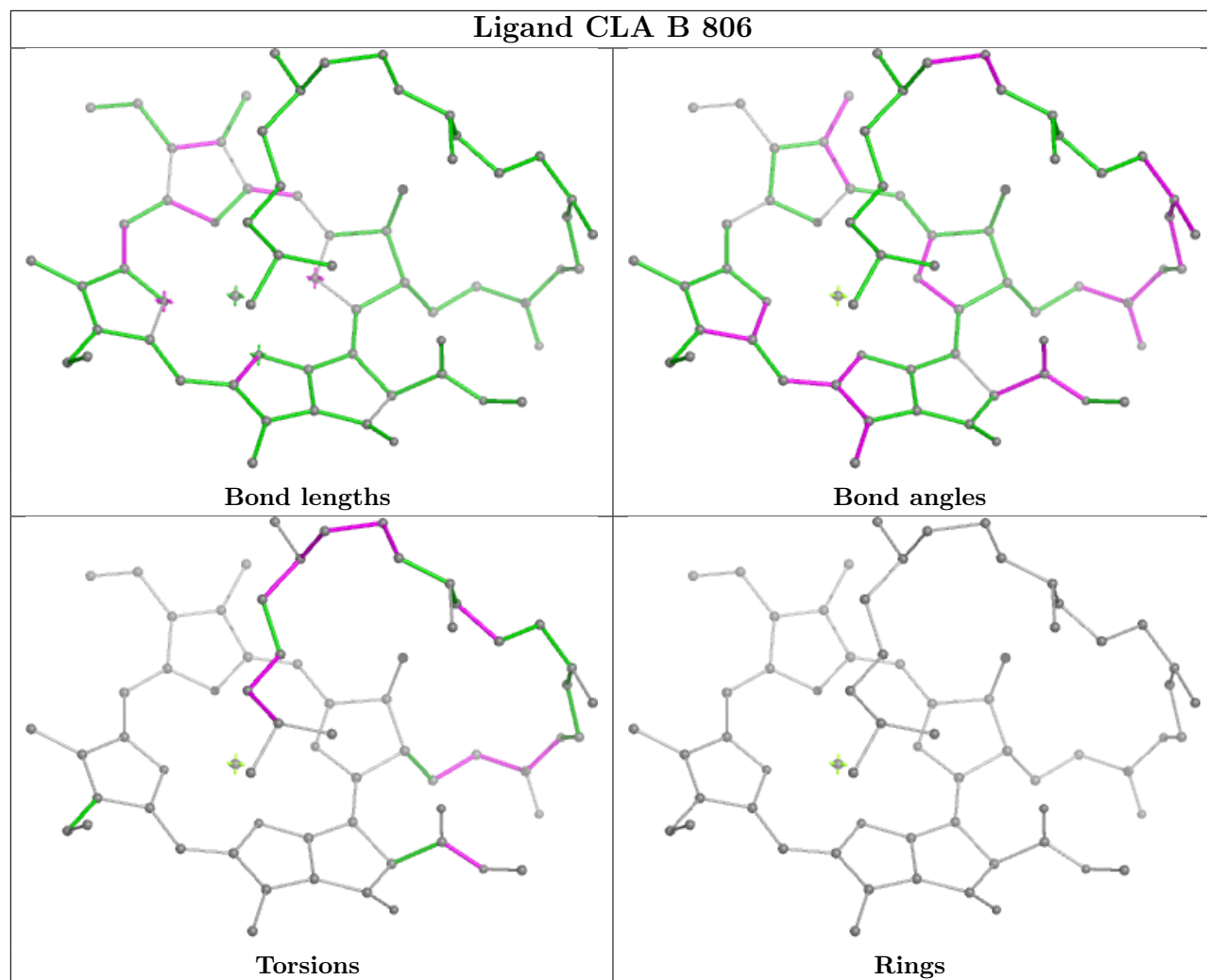


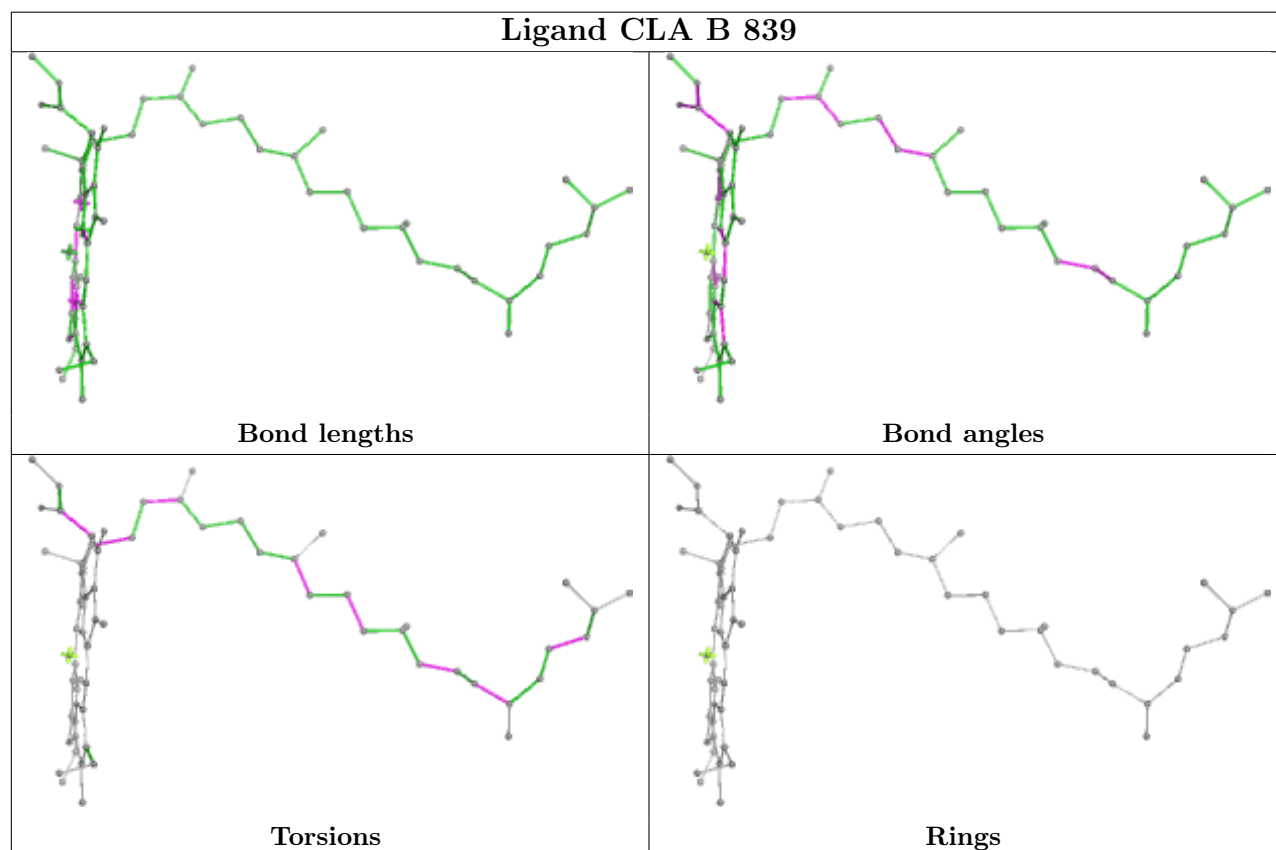
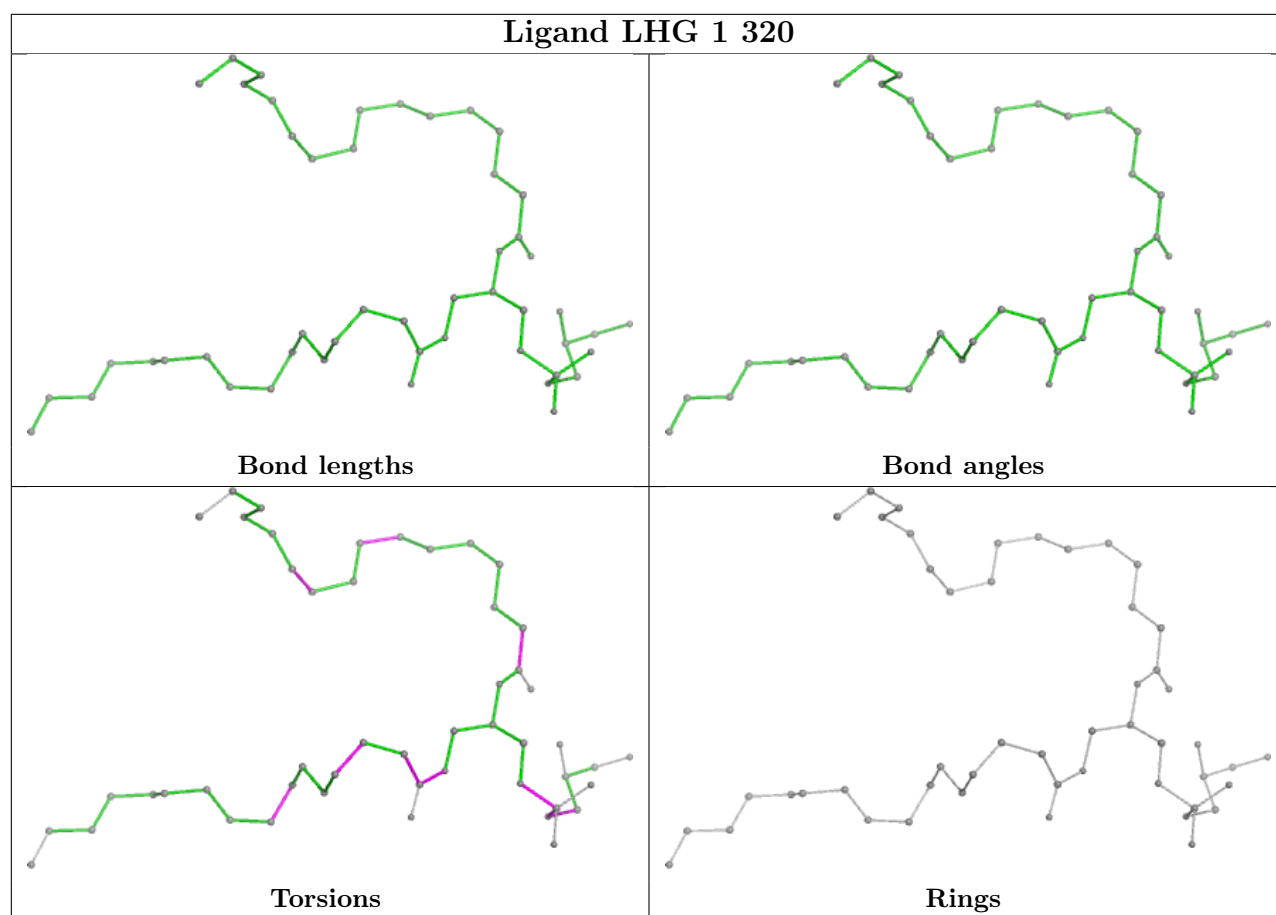


Ligand CHL 4 307

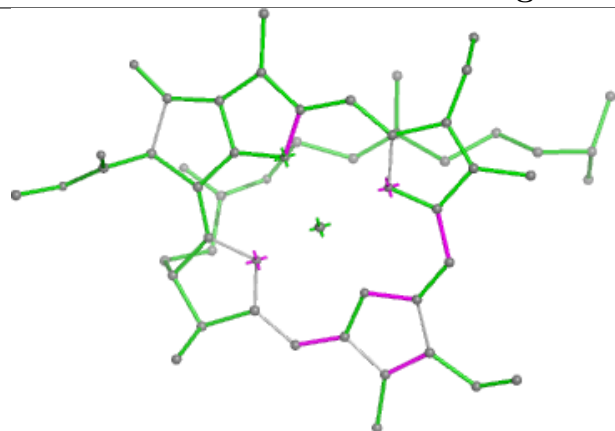


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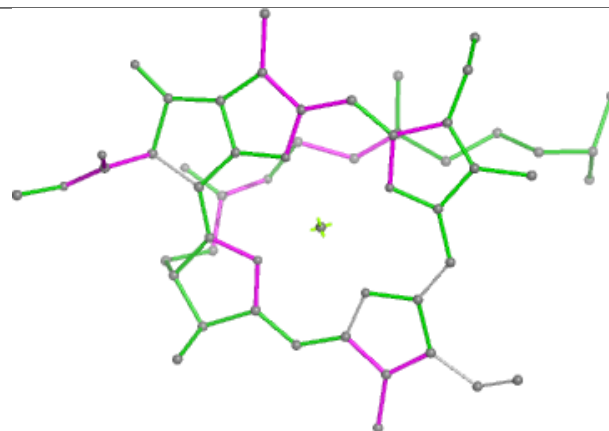




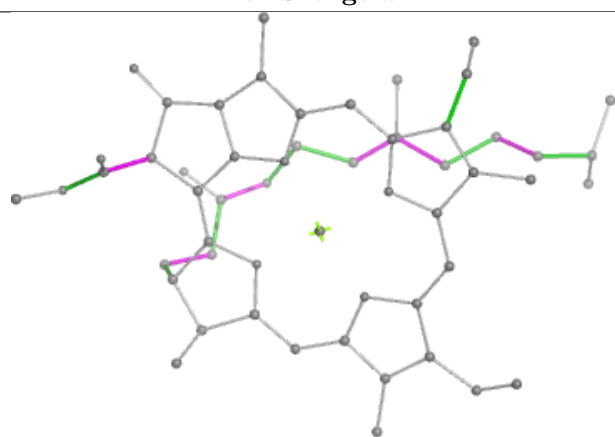
Ligand CLA B 816



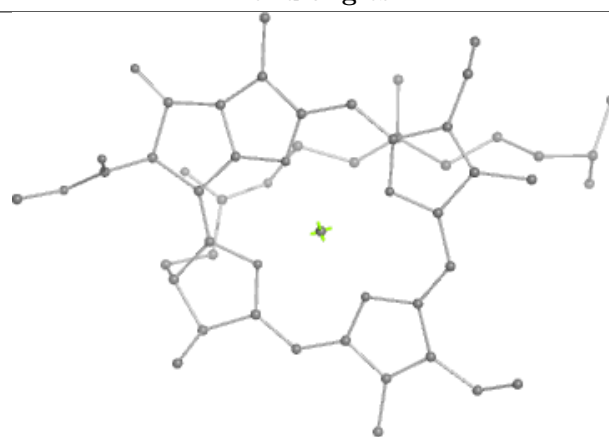
Bond lengths



Bond angles

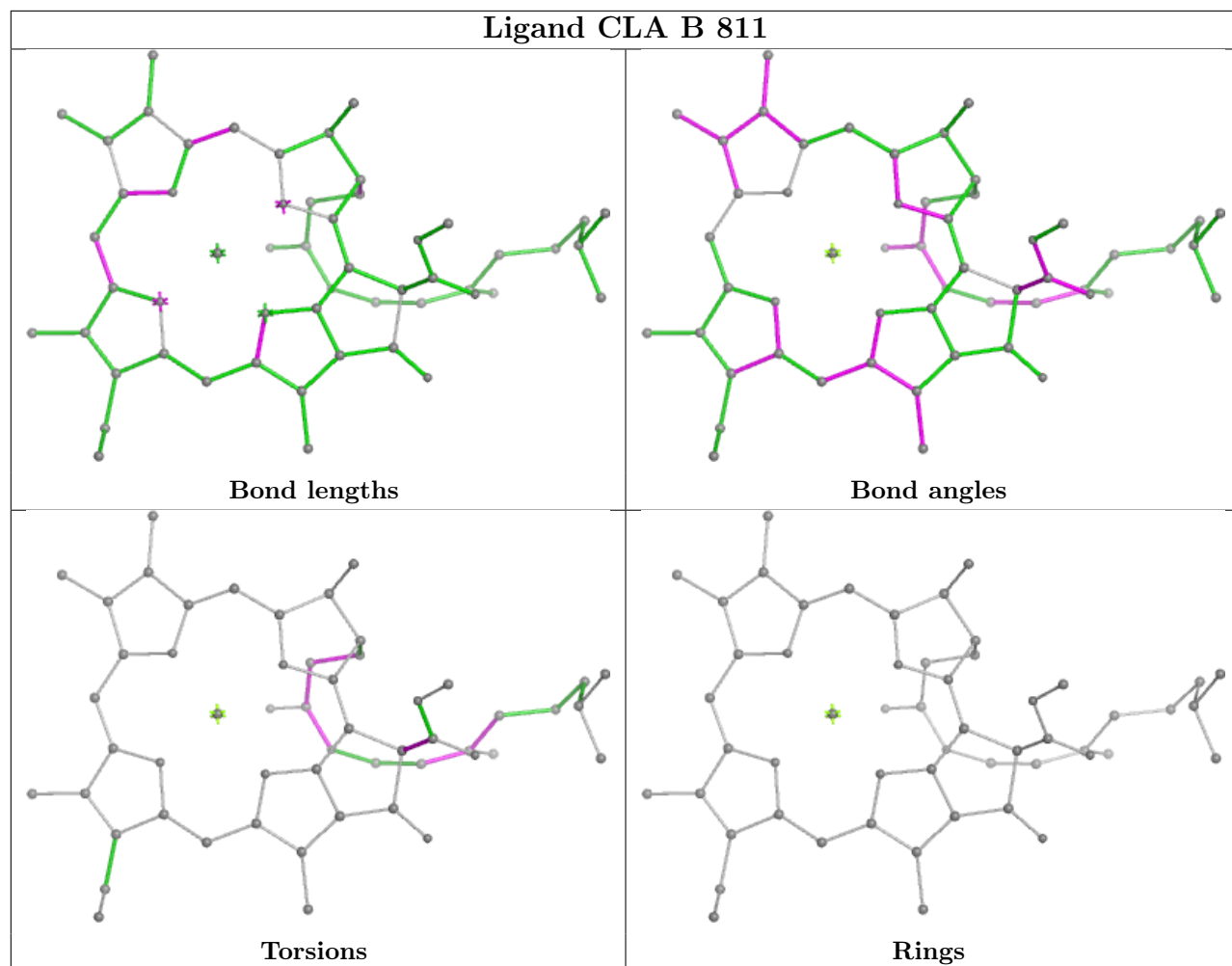


Torsions

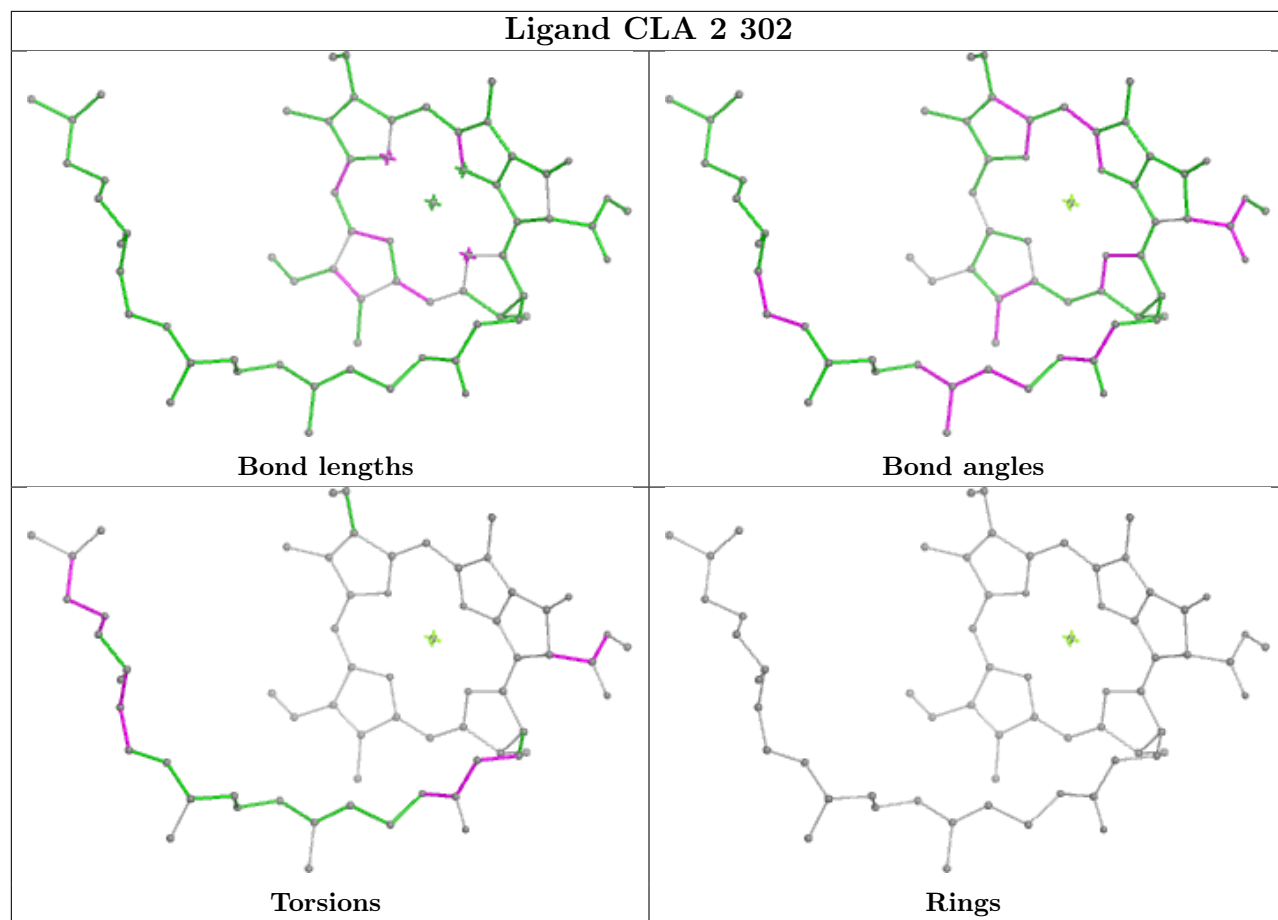


Rings

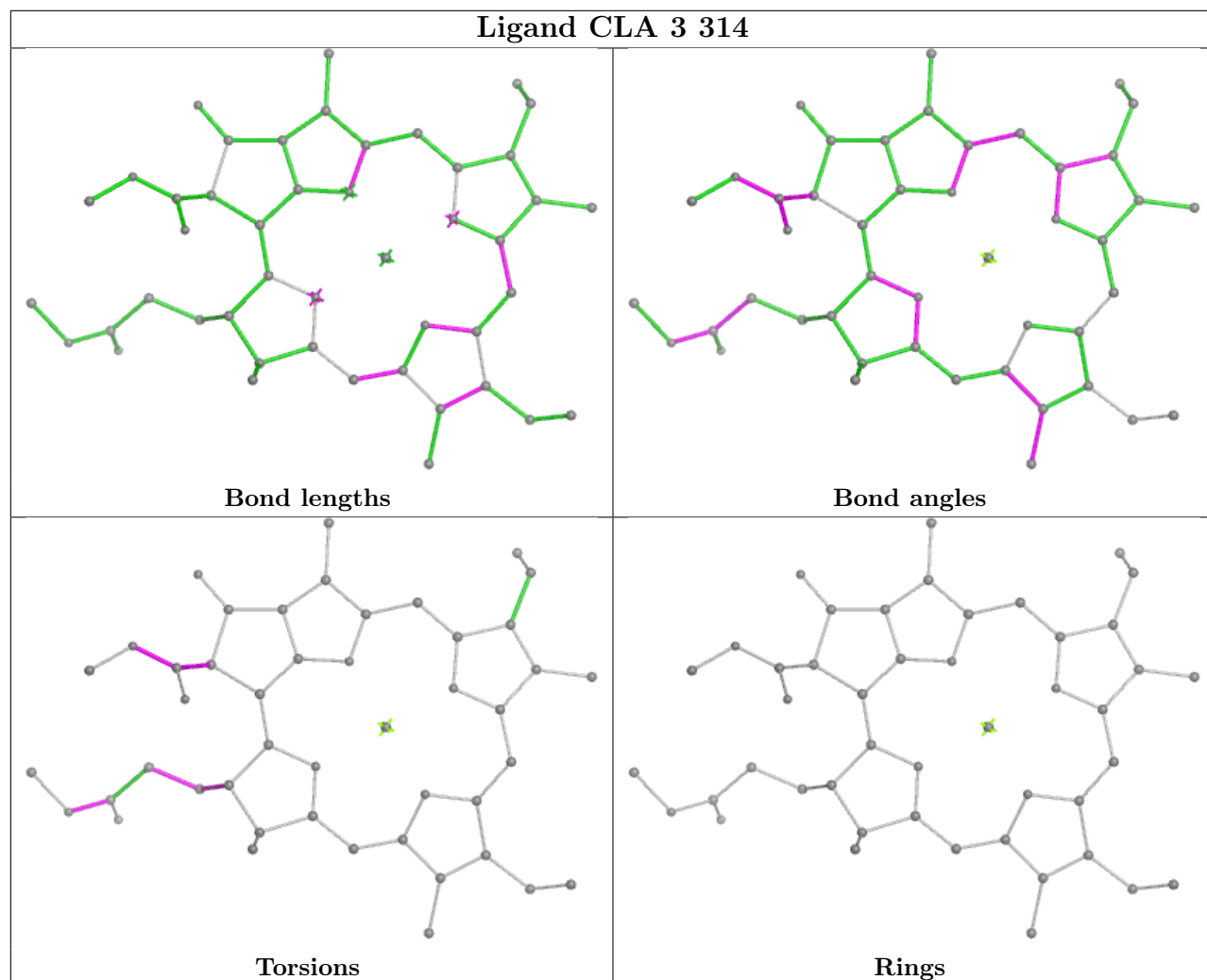
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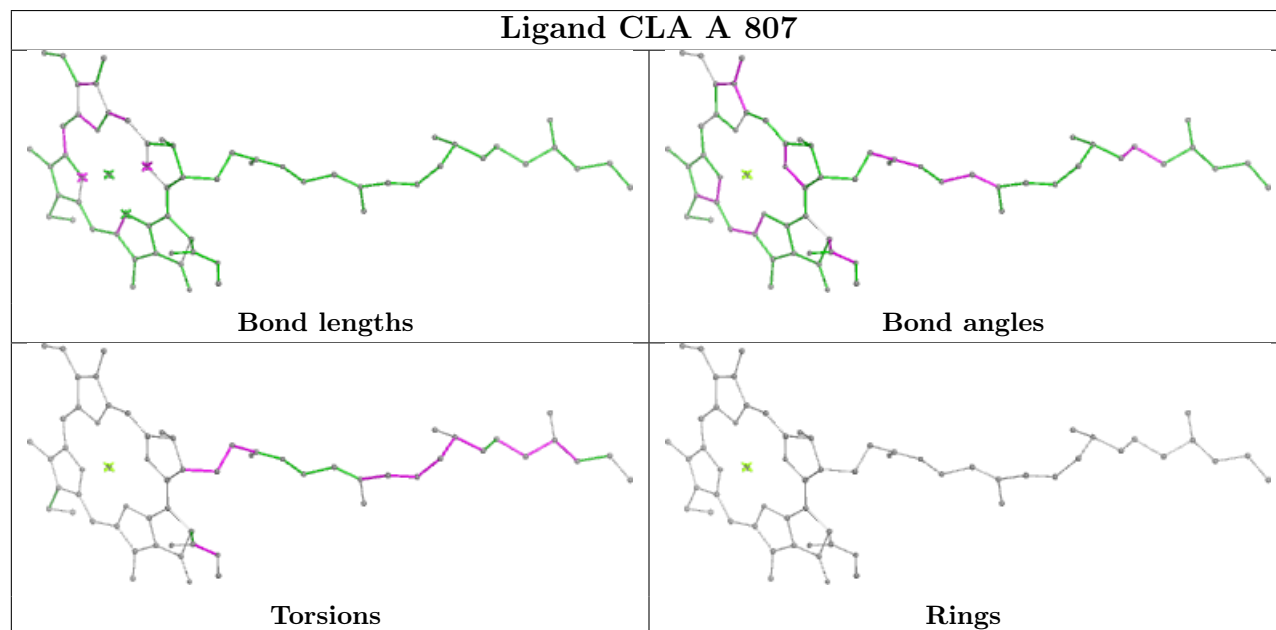
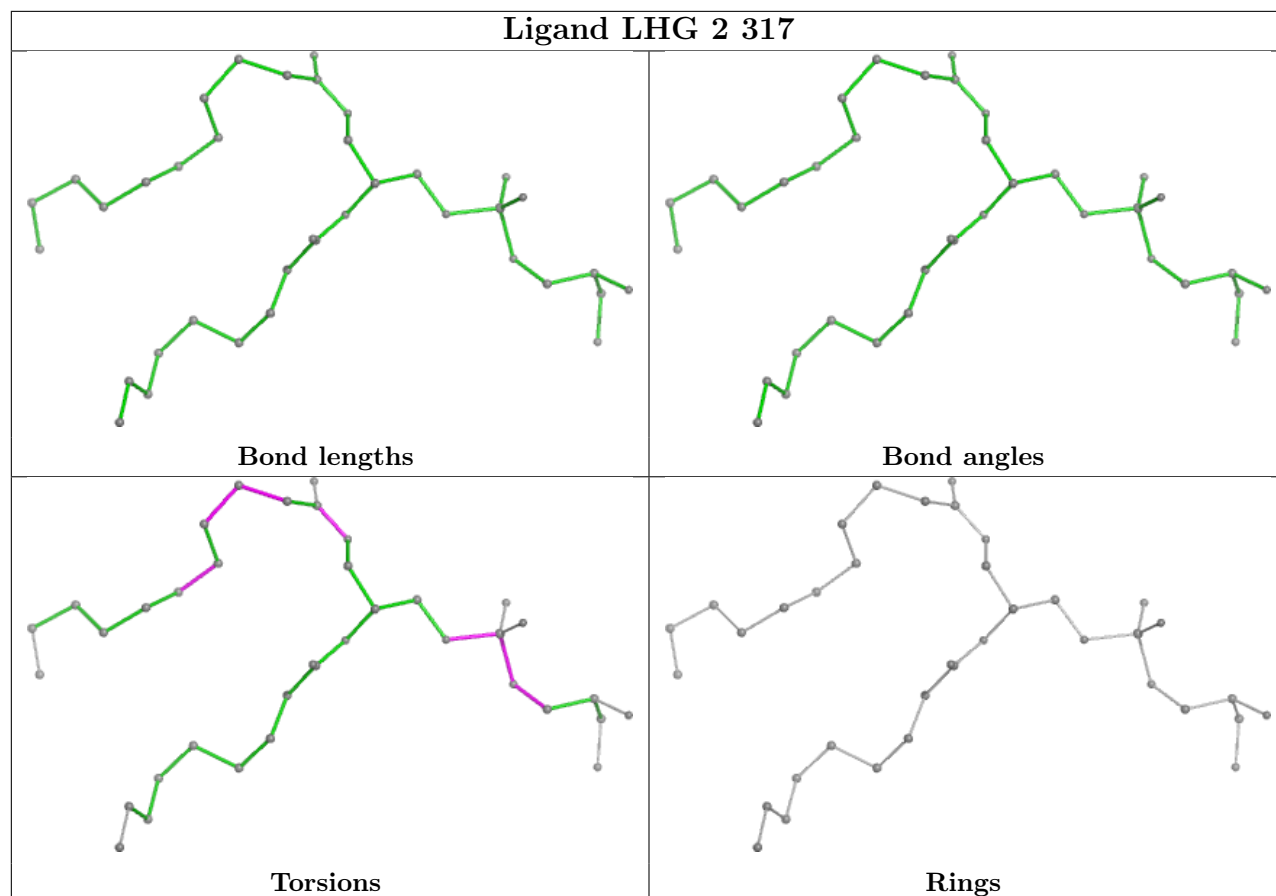


Ligand CLA 2 302

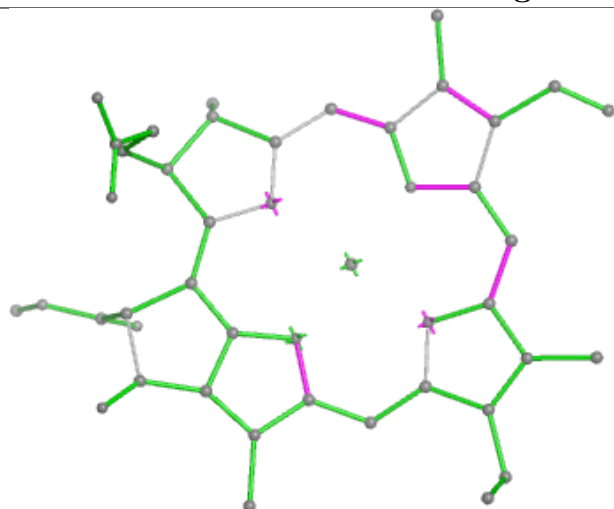


Ligand CLA 3 314

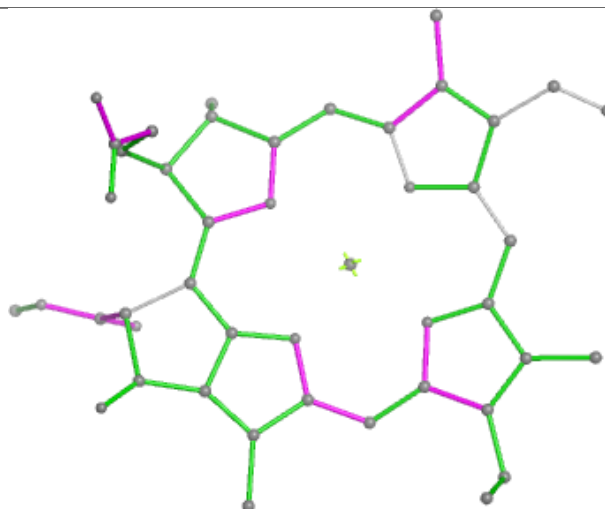




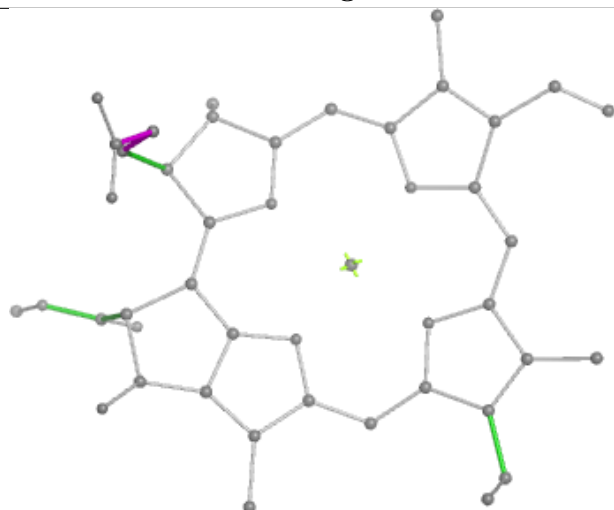
Ligand CLA A 832



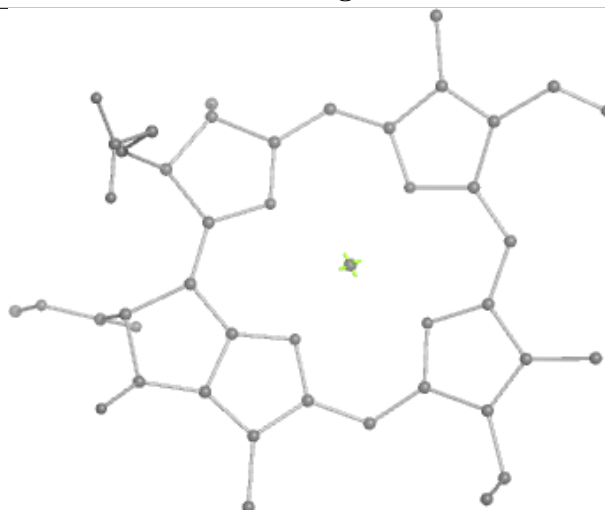
Bond lengths



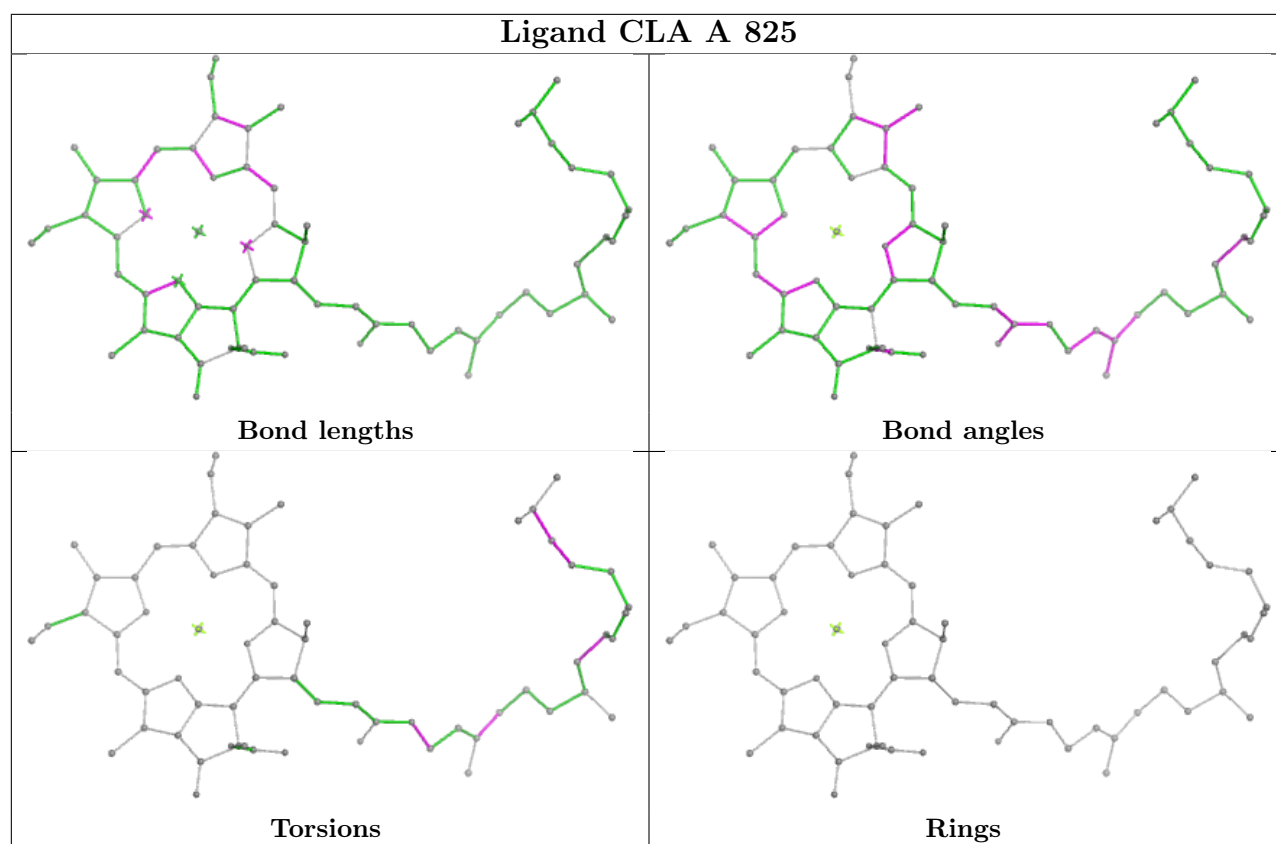
Bond angles



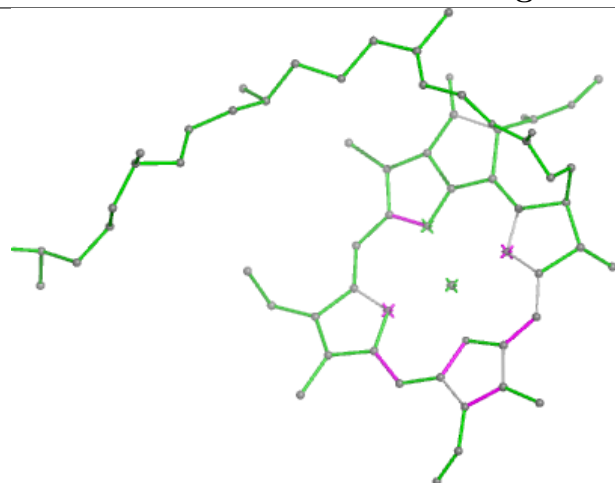
Torsions



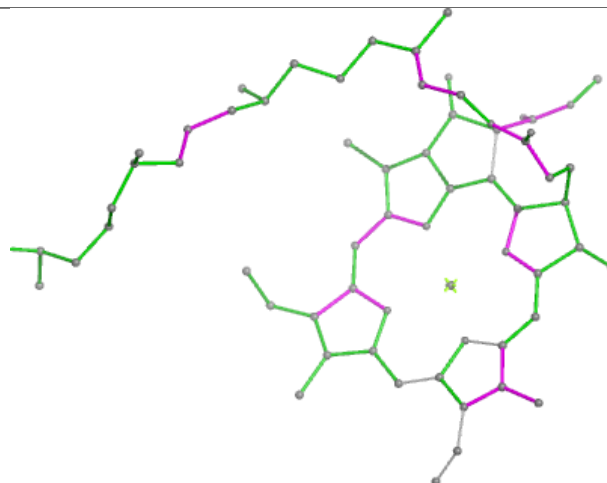
Rings



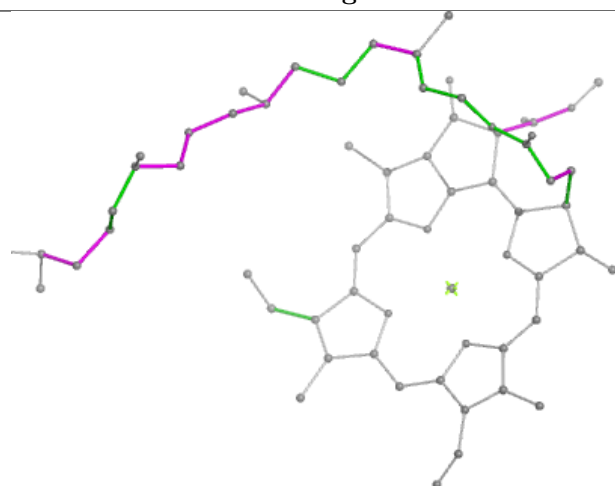
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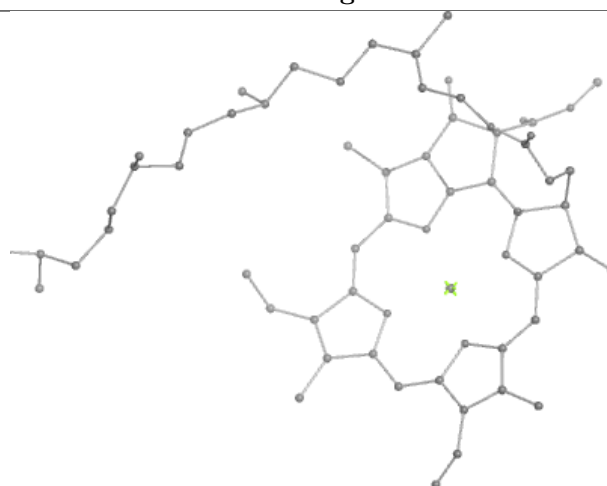
Bond lengths



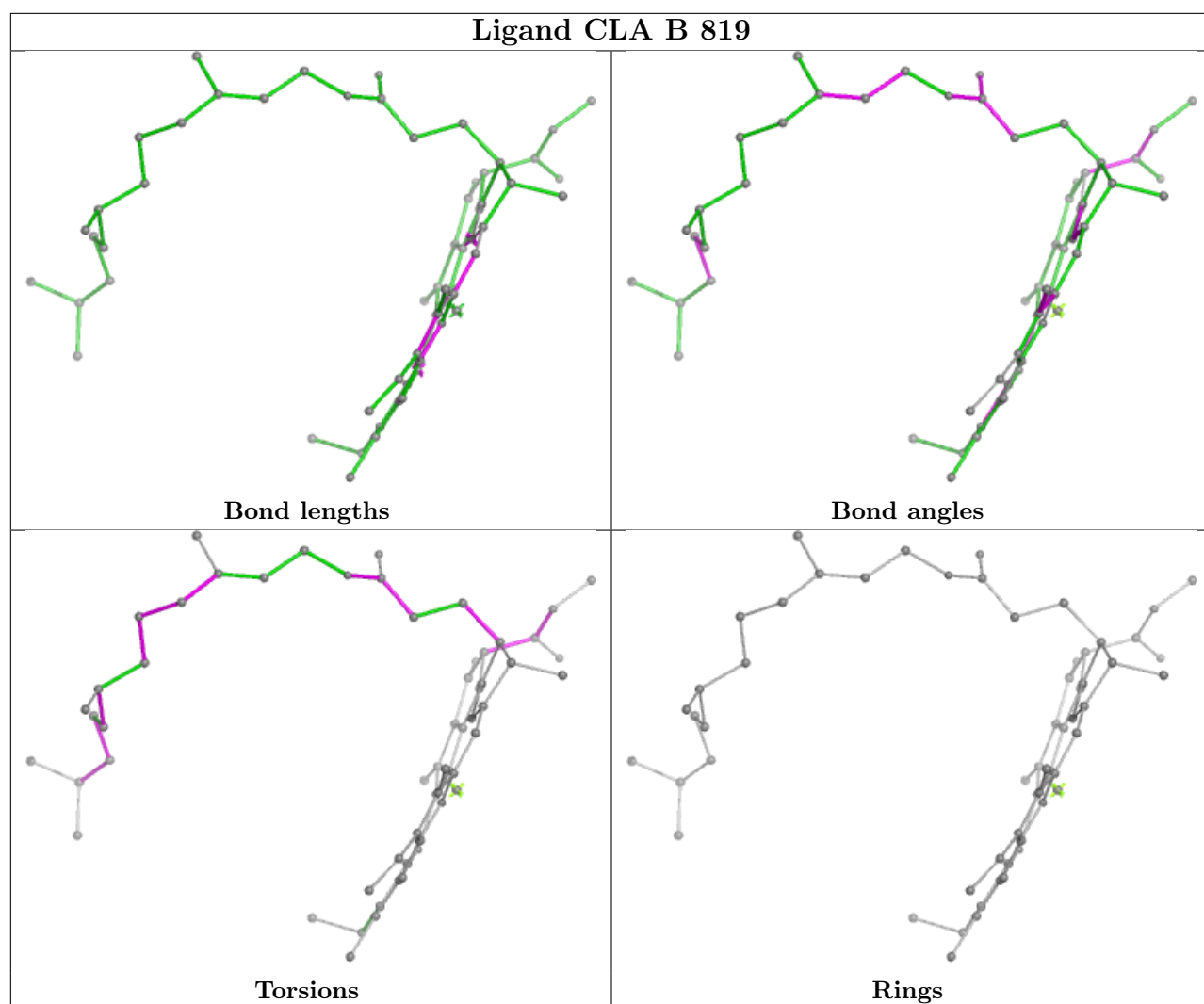
Bond angles



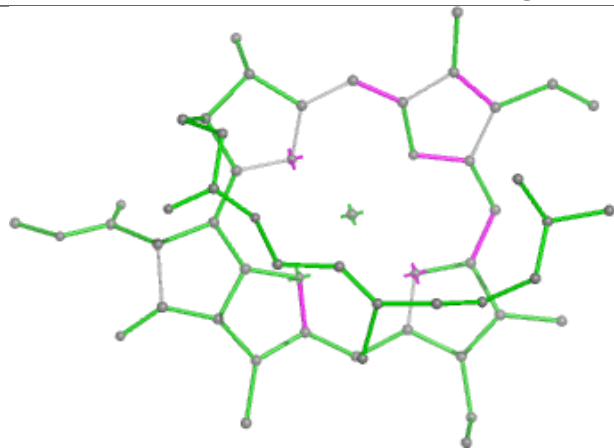
Torsions



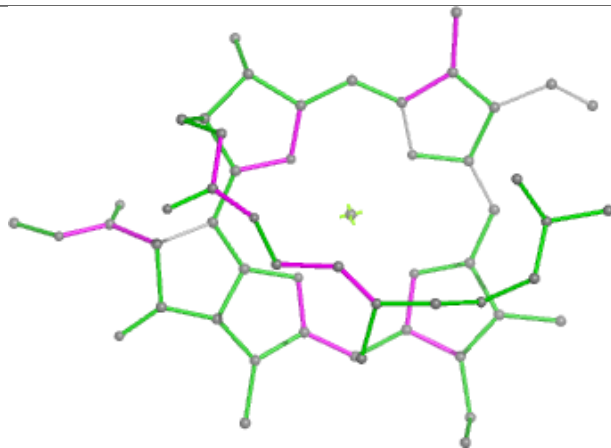
Rings



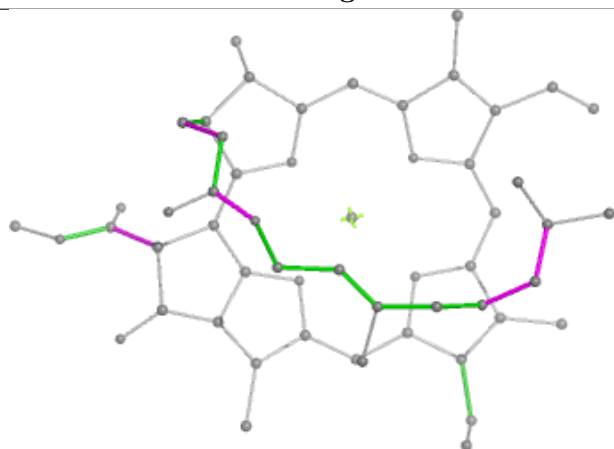
Ligand CLA 3 312



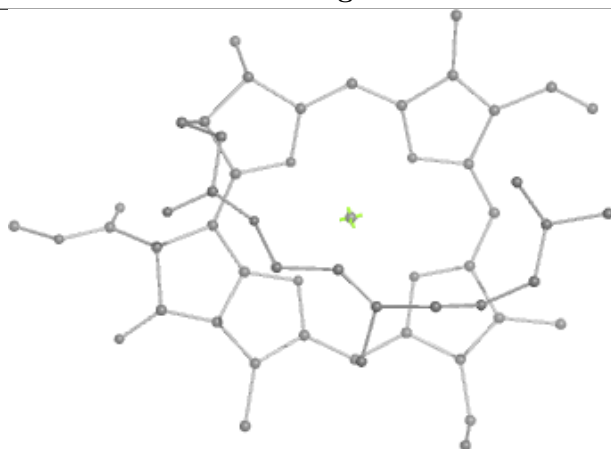
Bond lengths



Bond angles

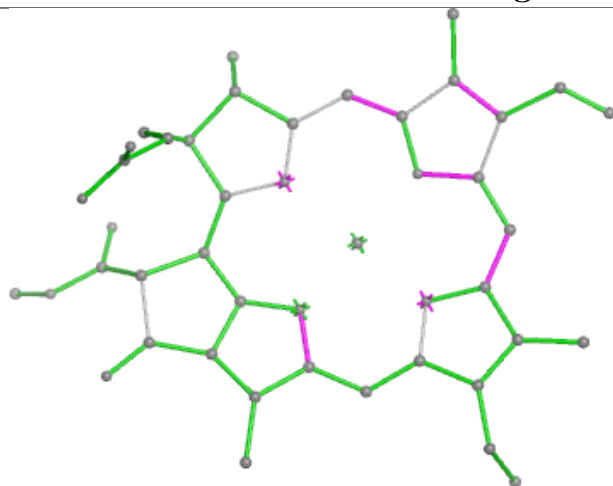


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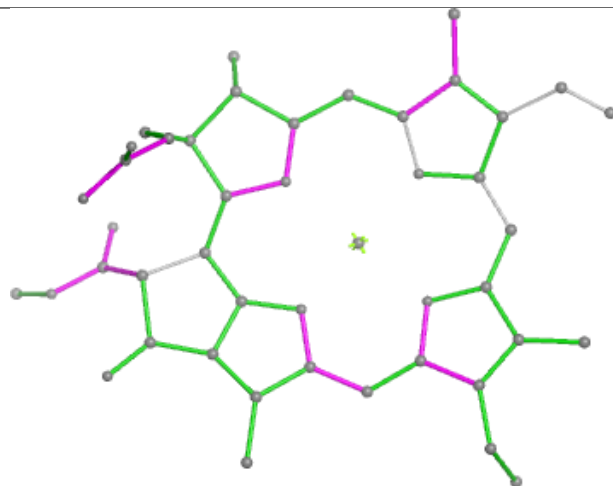


Rings

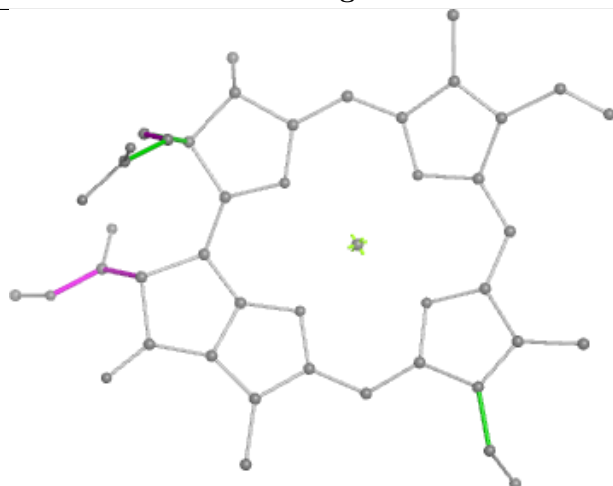
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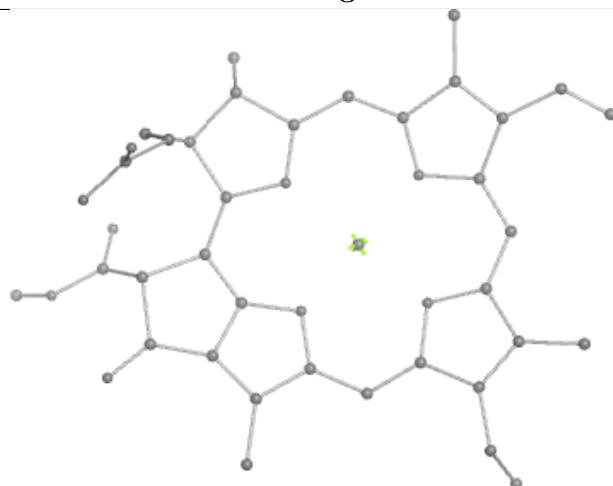
Bond lengths



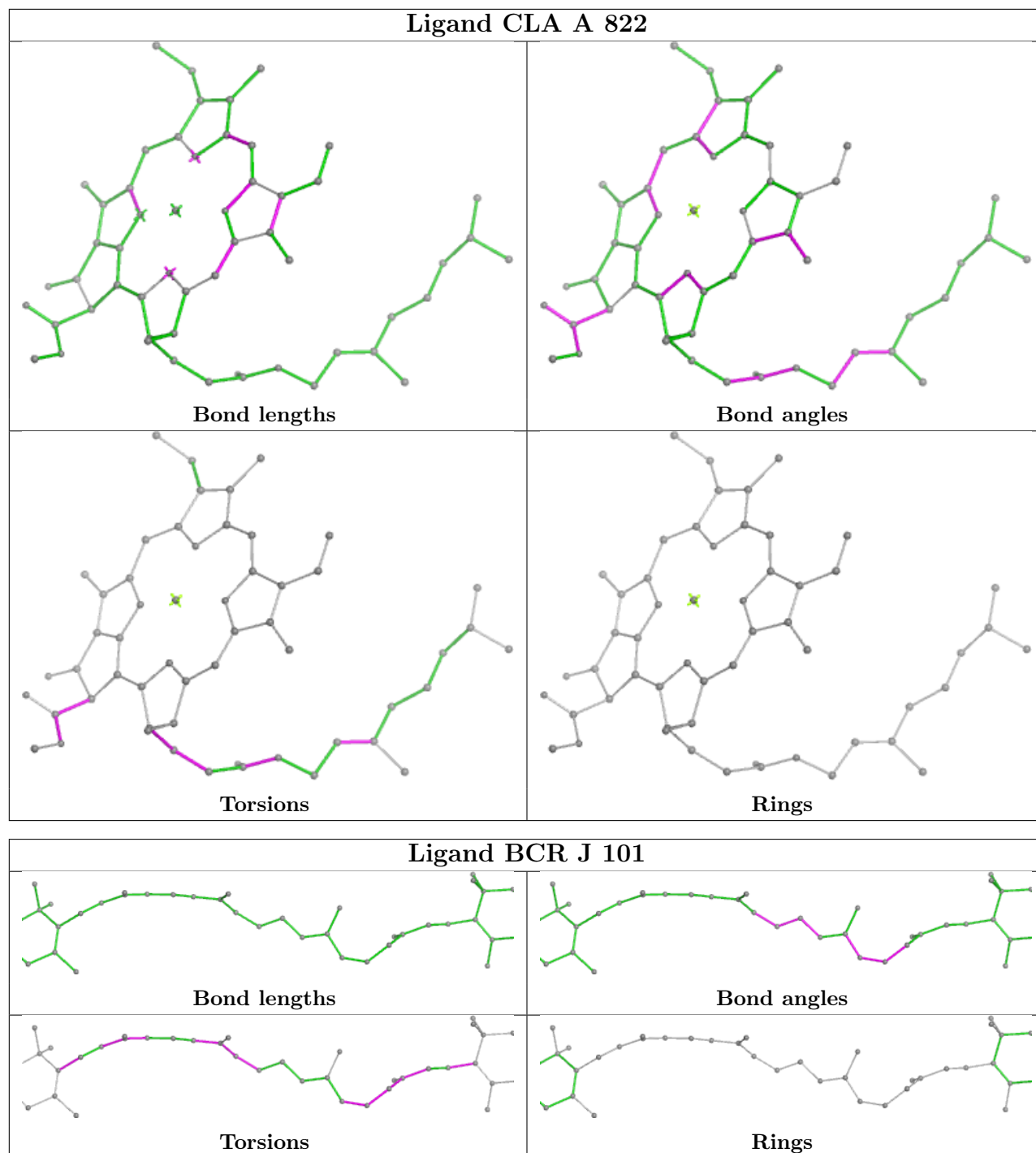
Bond angles



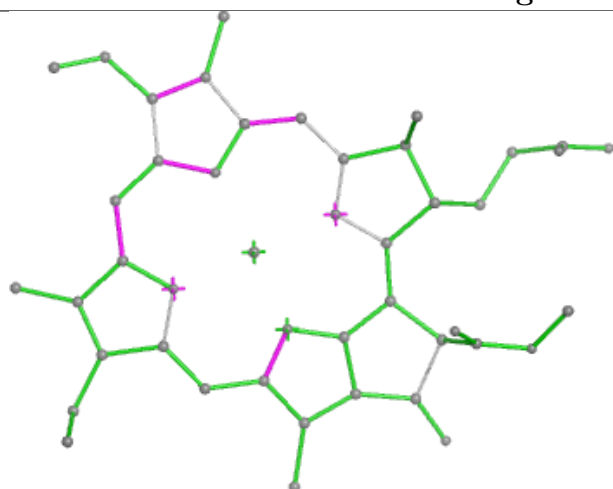
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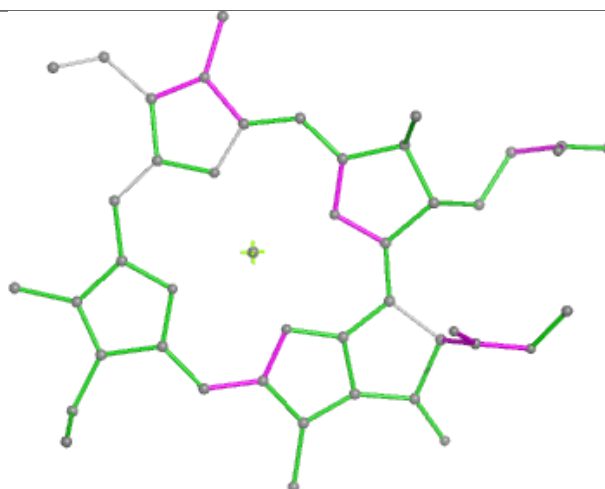
Rings



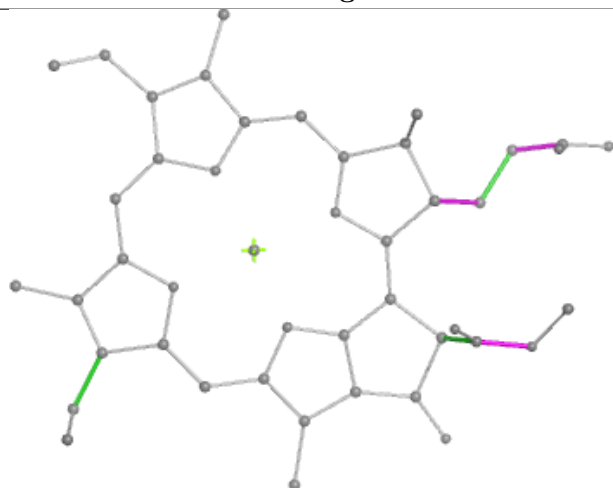
Ligand CLA F 301



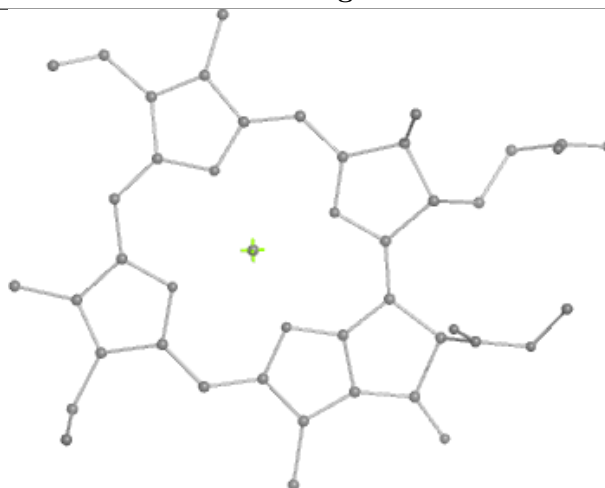
Bond lengths



Bond angles

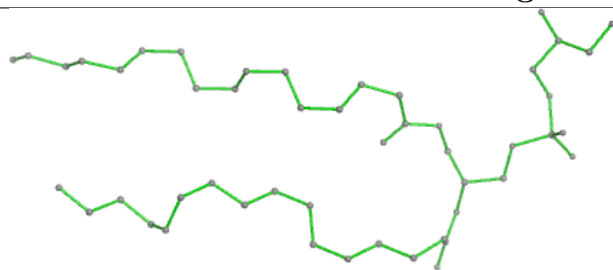


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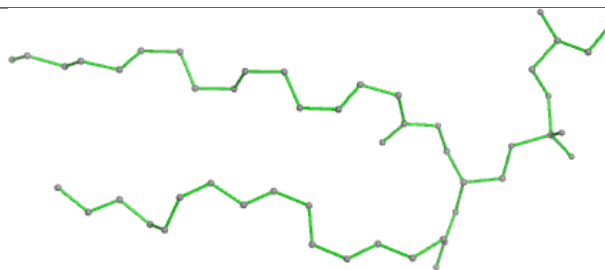


Rings

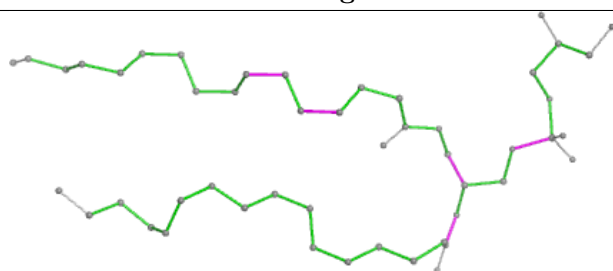
Ligand LHG 1 317



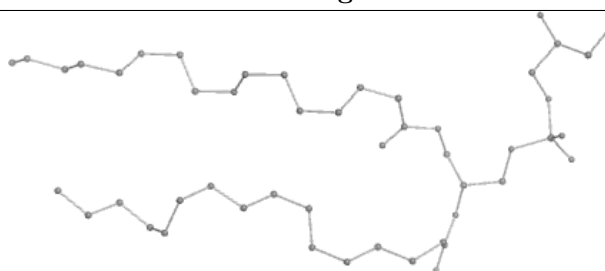
Bond lengths



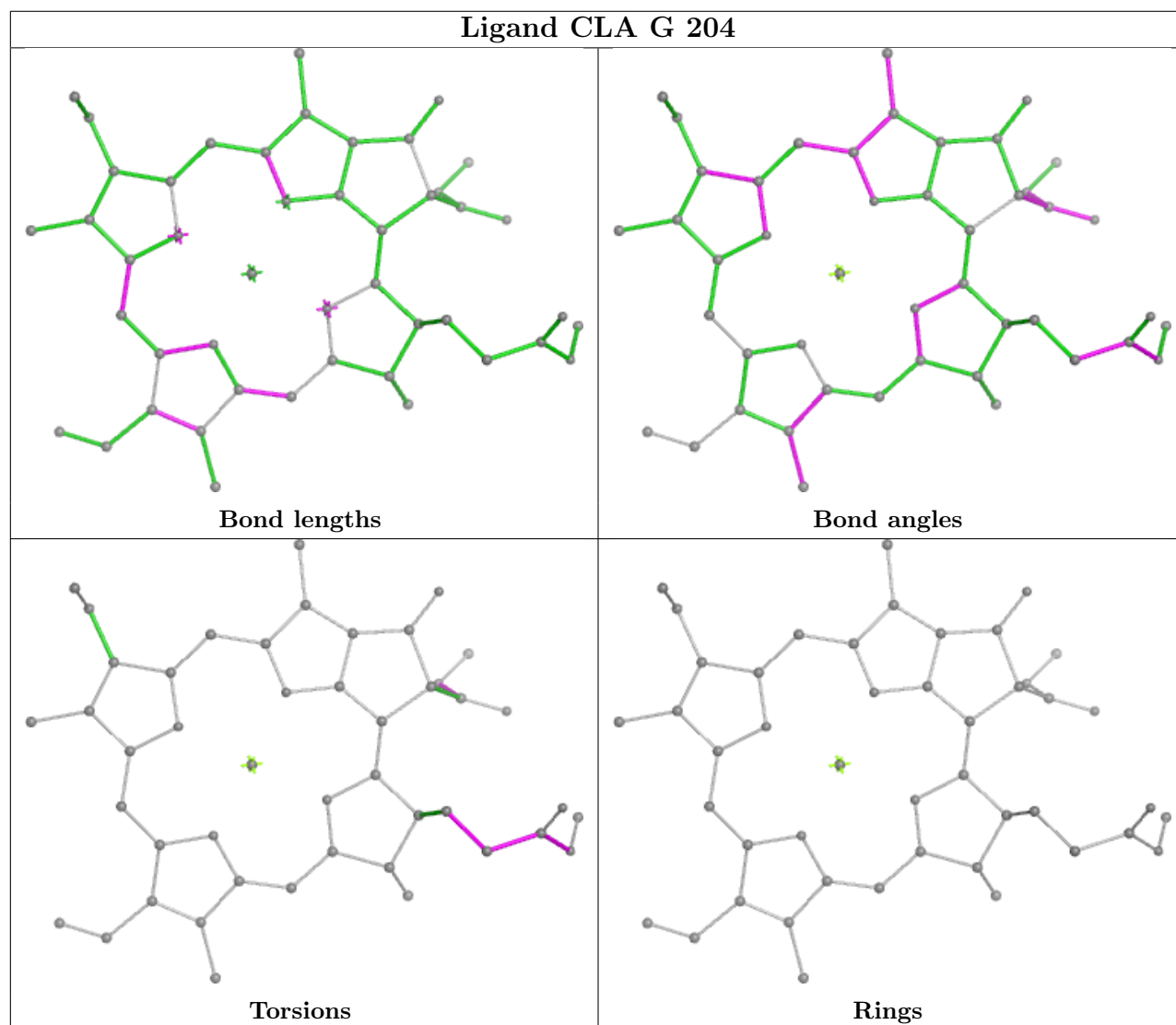
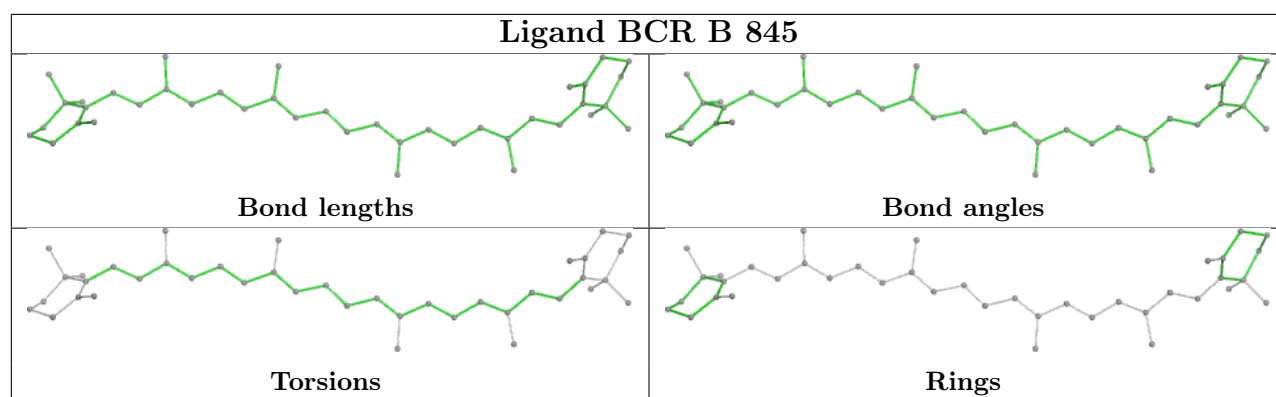
Bond angles



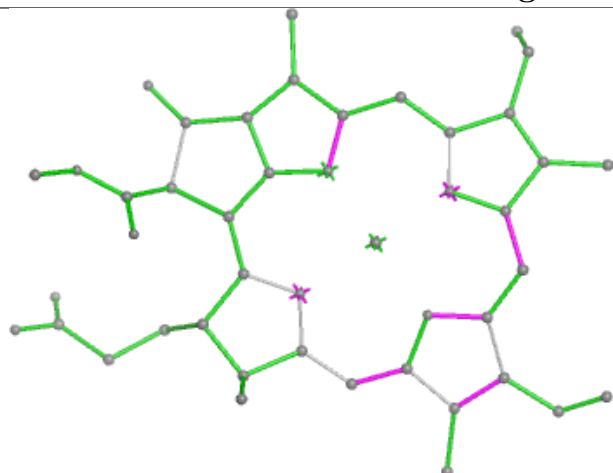
Torsions



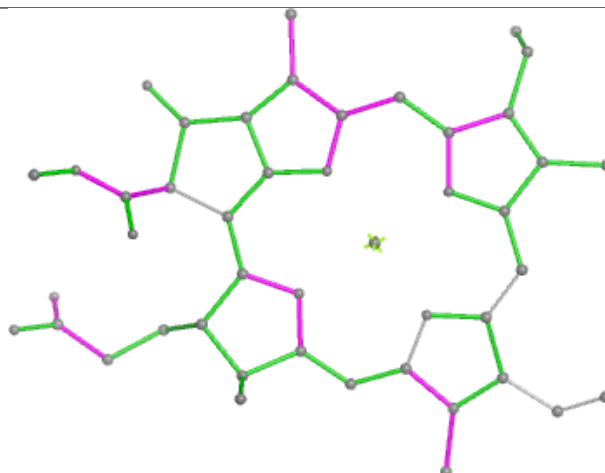
Rings



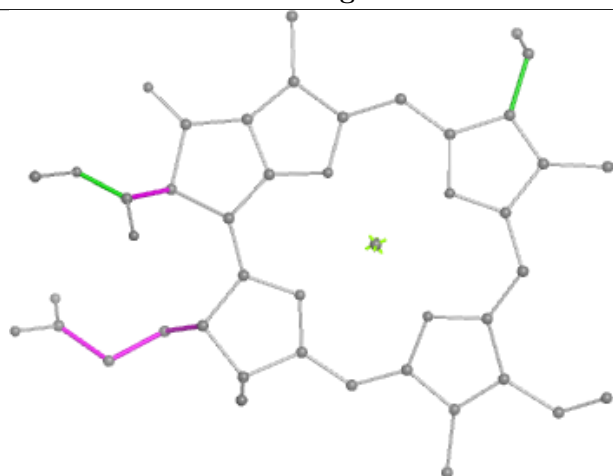
Ligand CLA 3 313



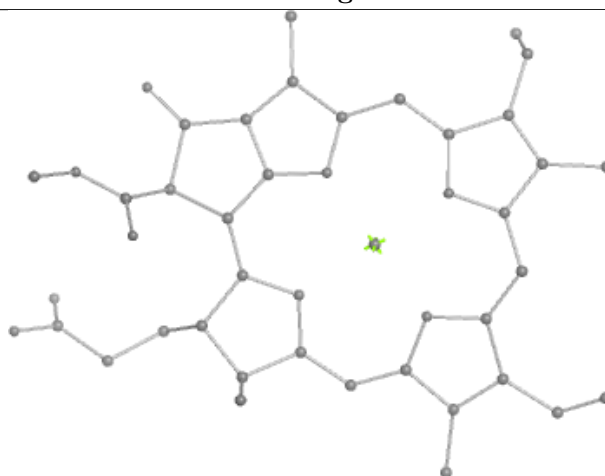
Bond lengths



Bond angles

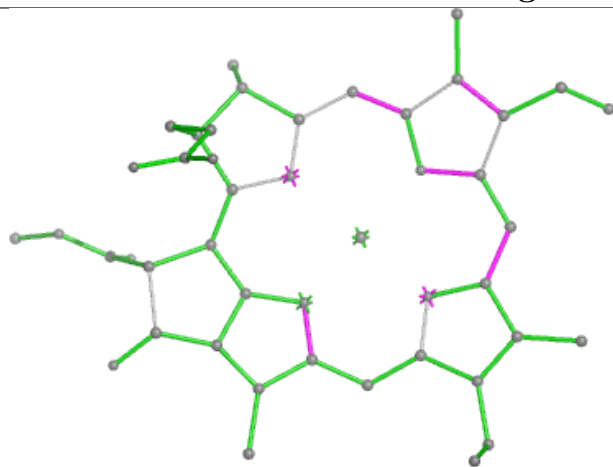


Torsions

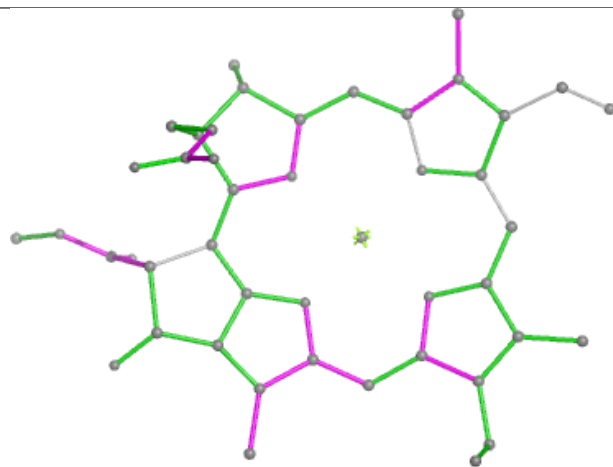


Rings

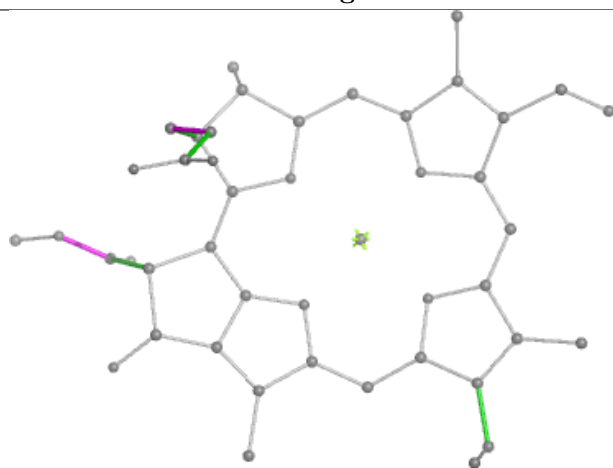
Ligand CLA 1 307



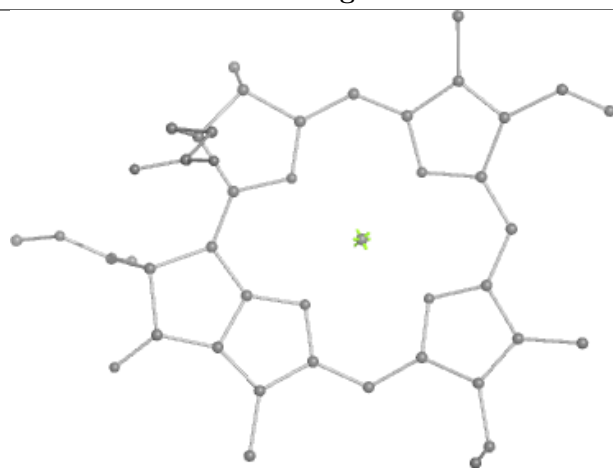
Bond lengths



Bond angles

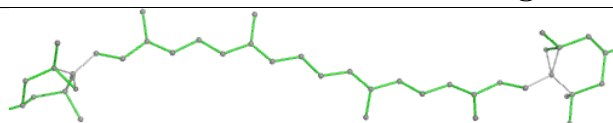


Torsions

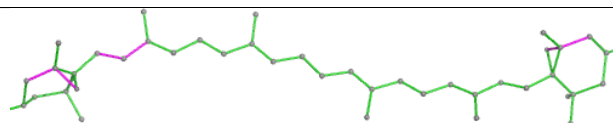


Rings

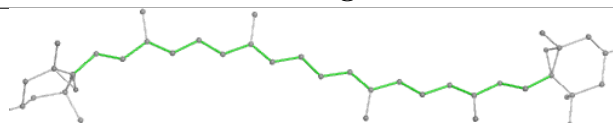
Ligand XAT 4 316



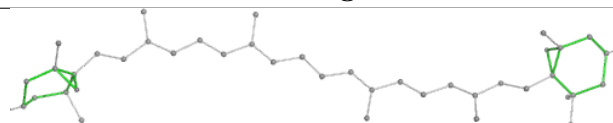
Bond lengths



Bond angles

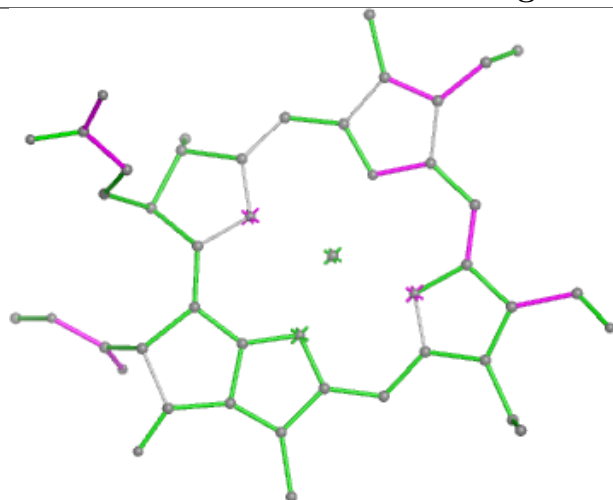


Torsions

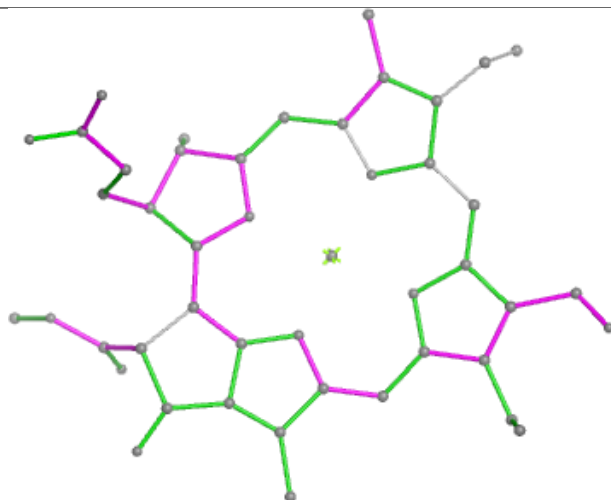


Rings

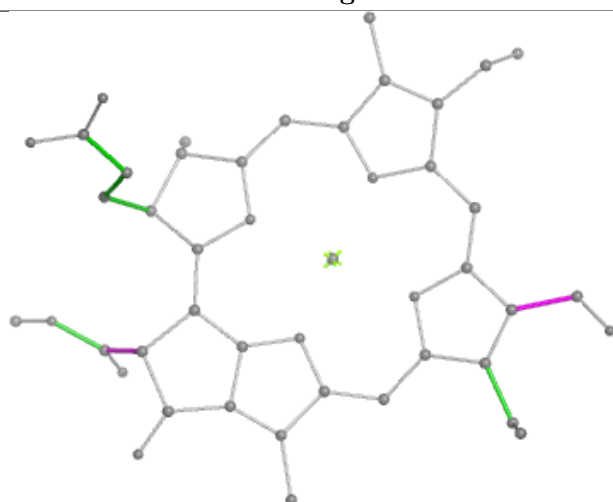
Ligand CHL 1 306



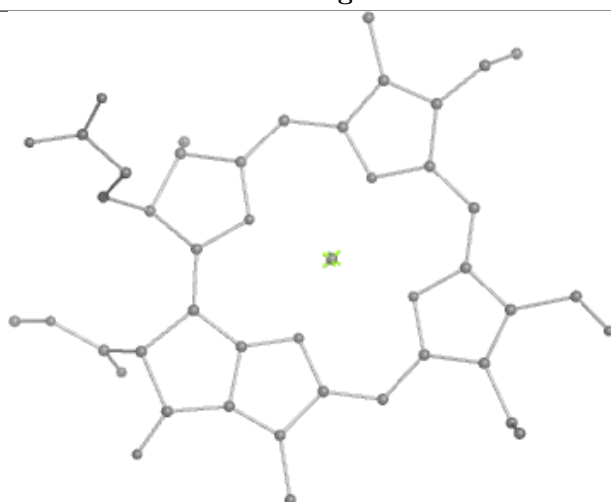
Bond lengths



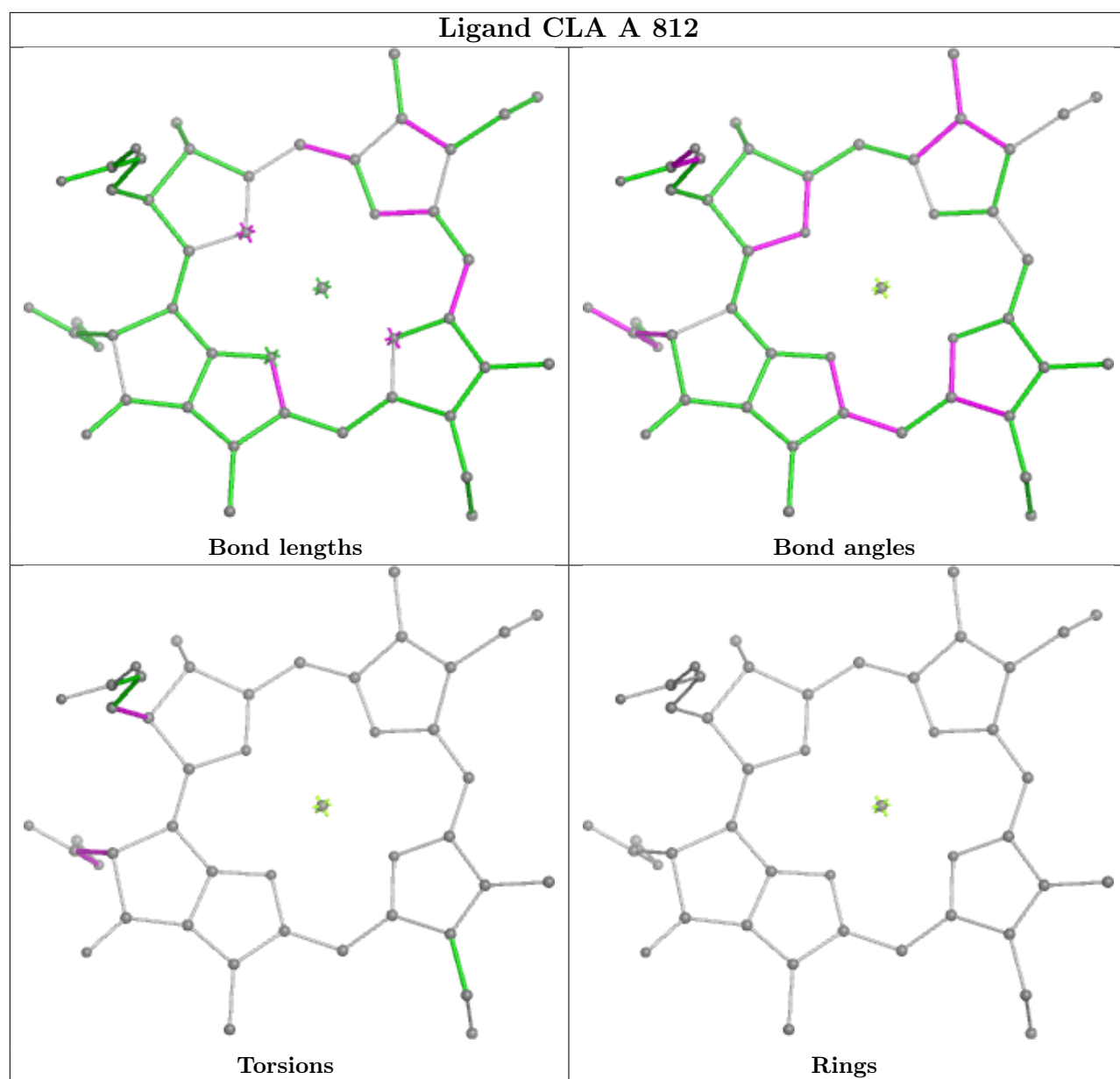
Bond angles

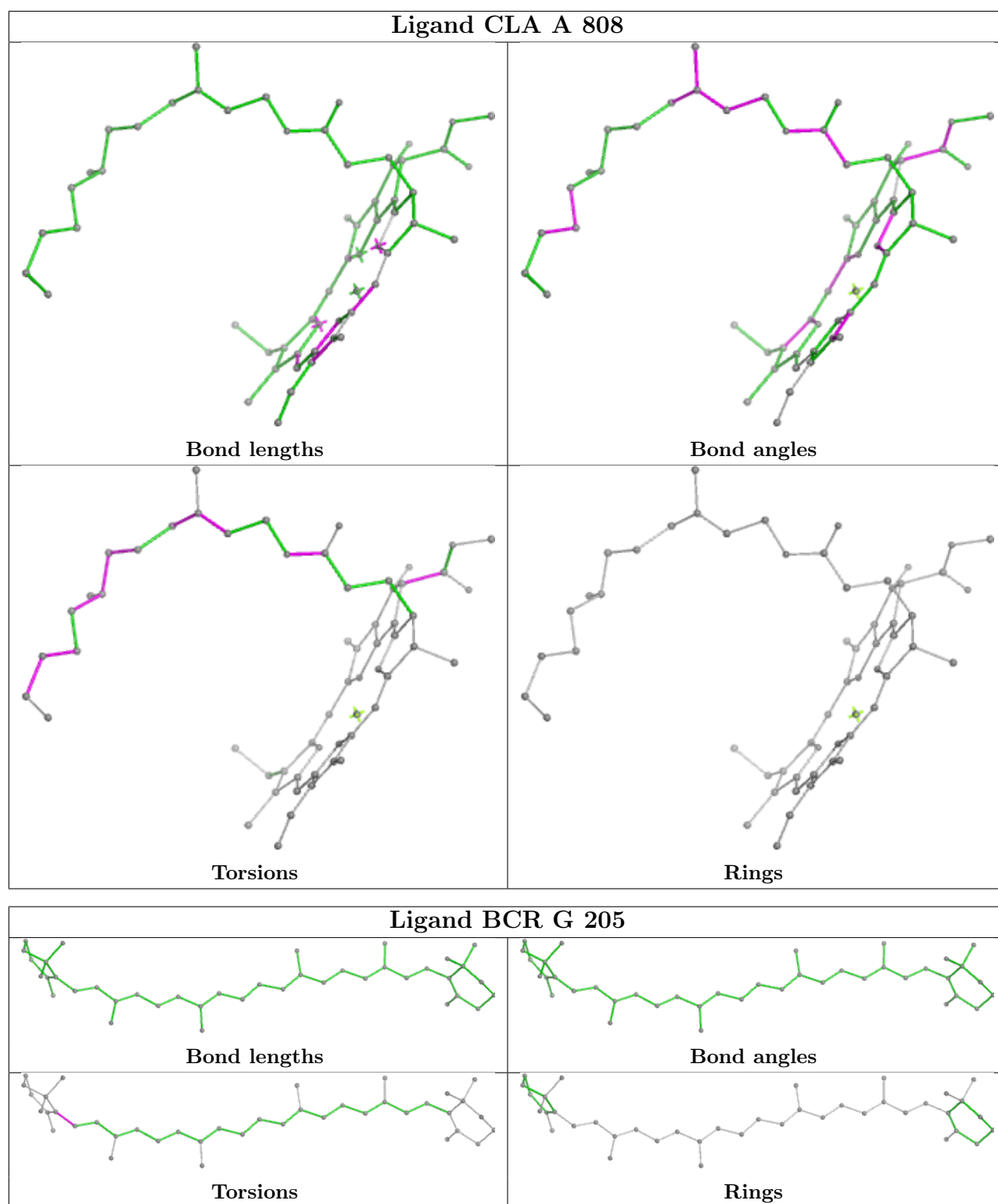


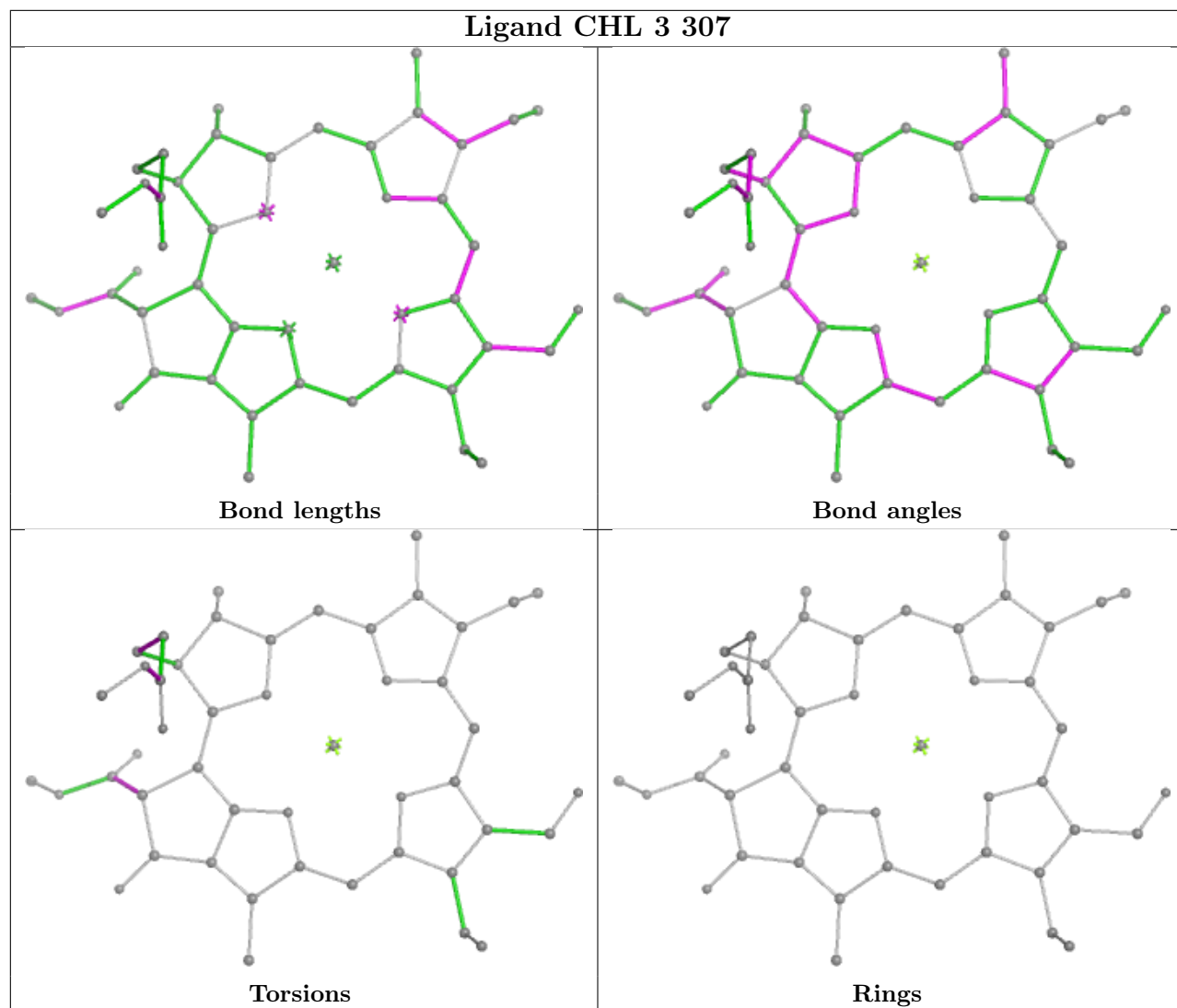
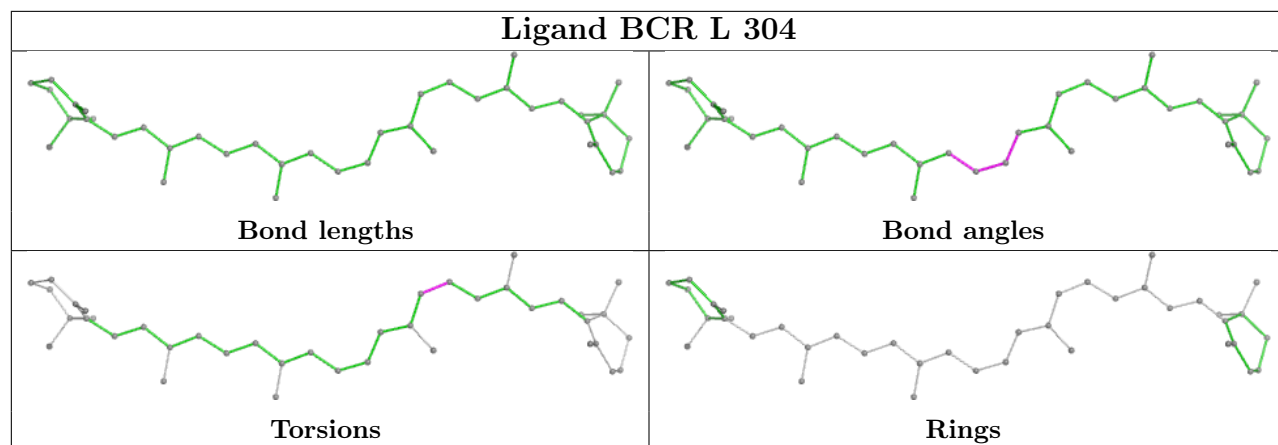
Torsions



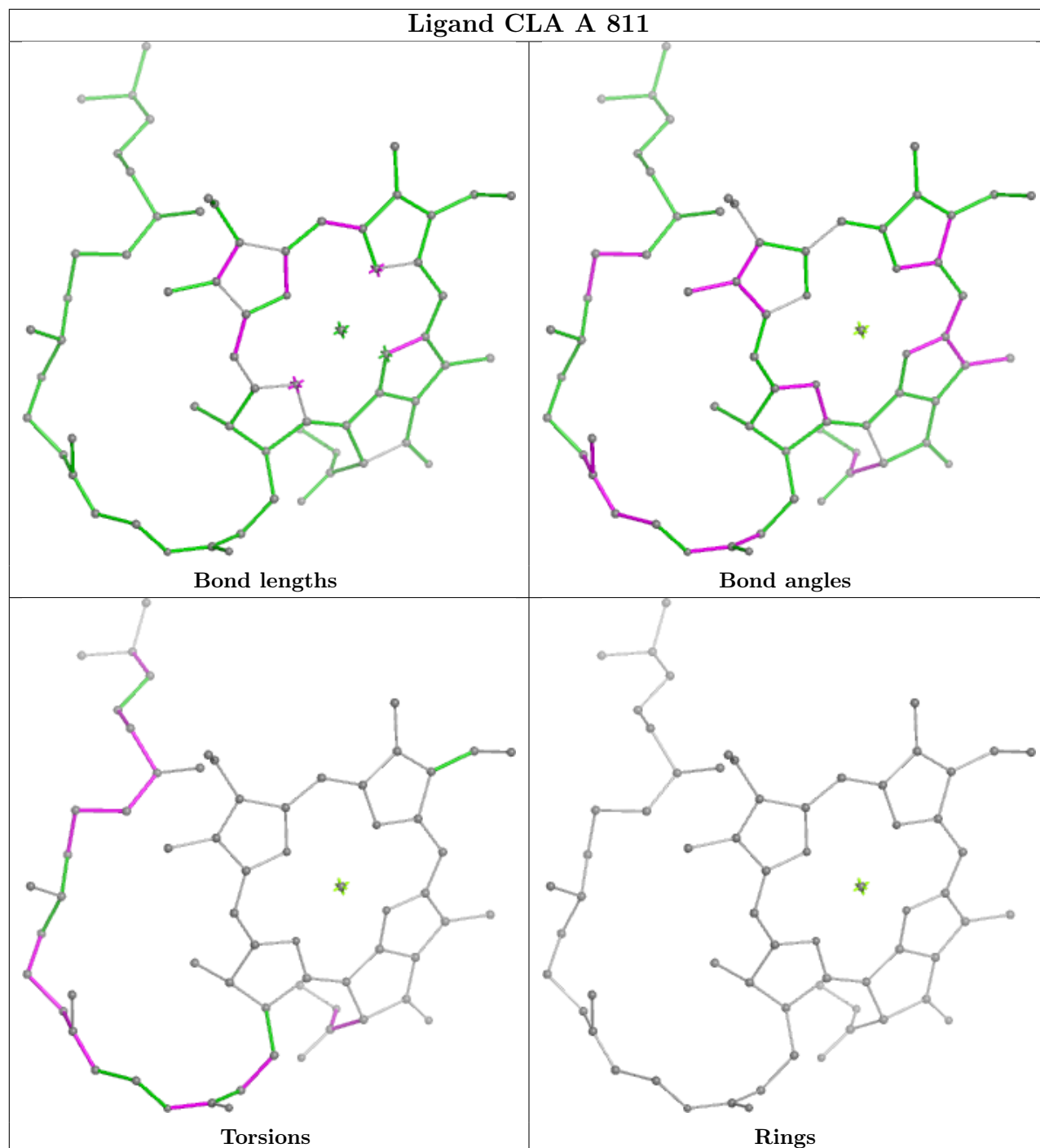
Rings

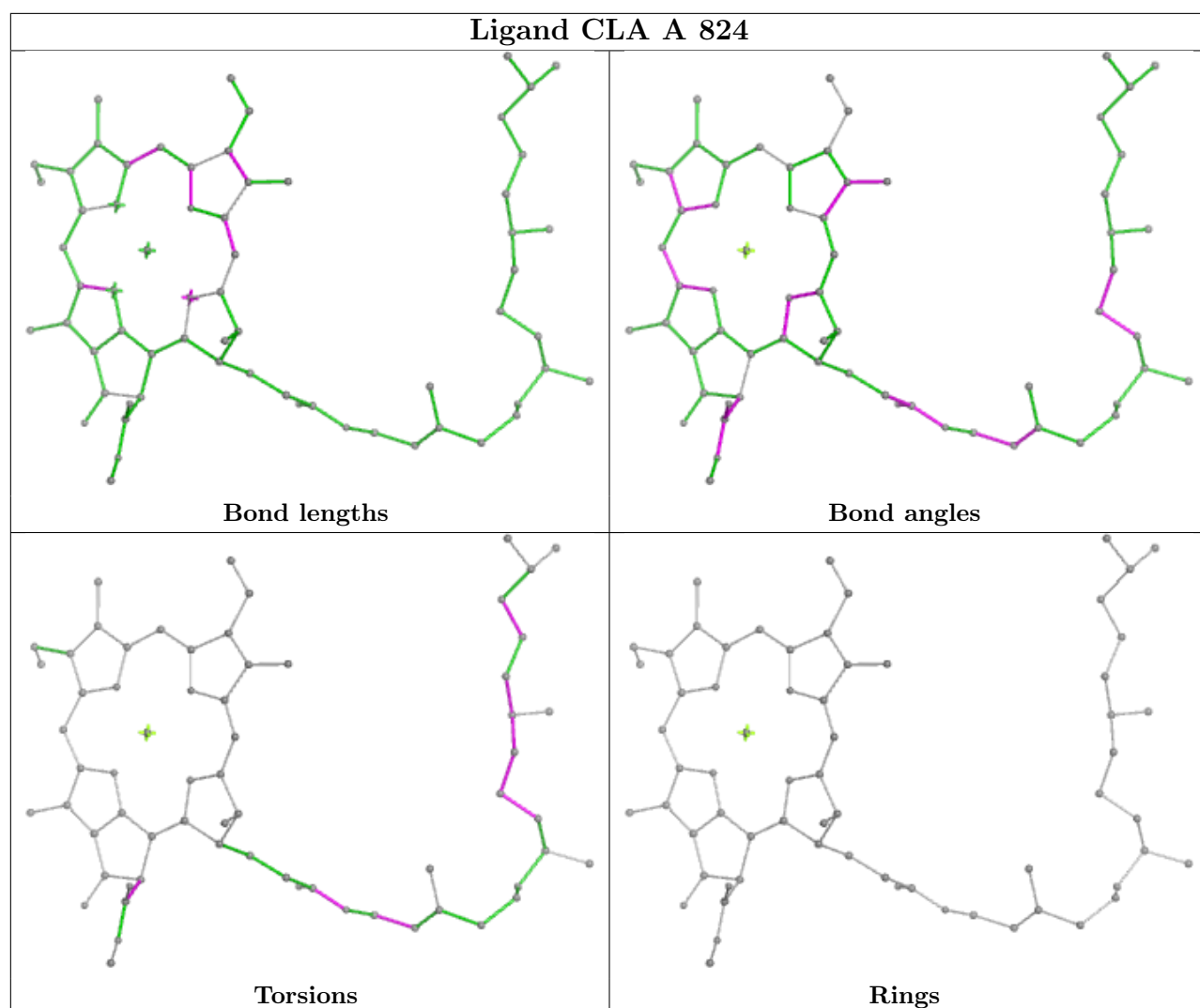


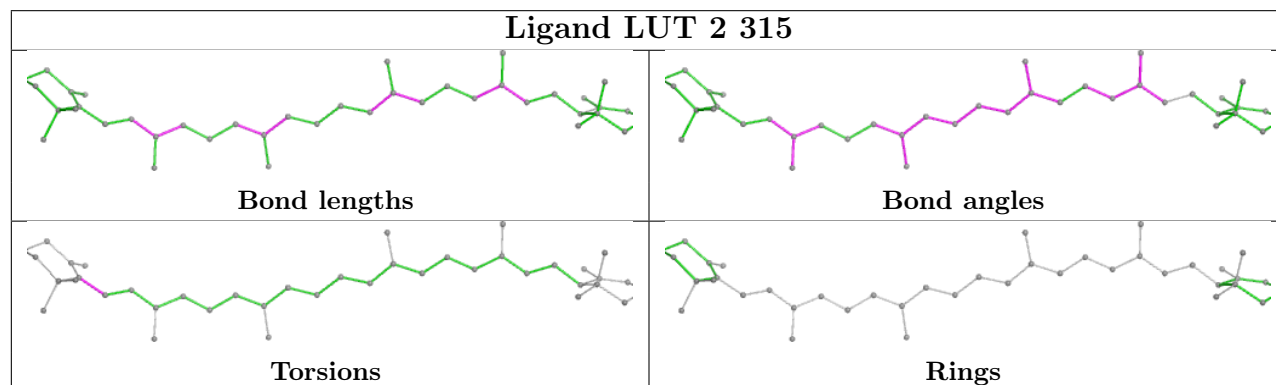
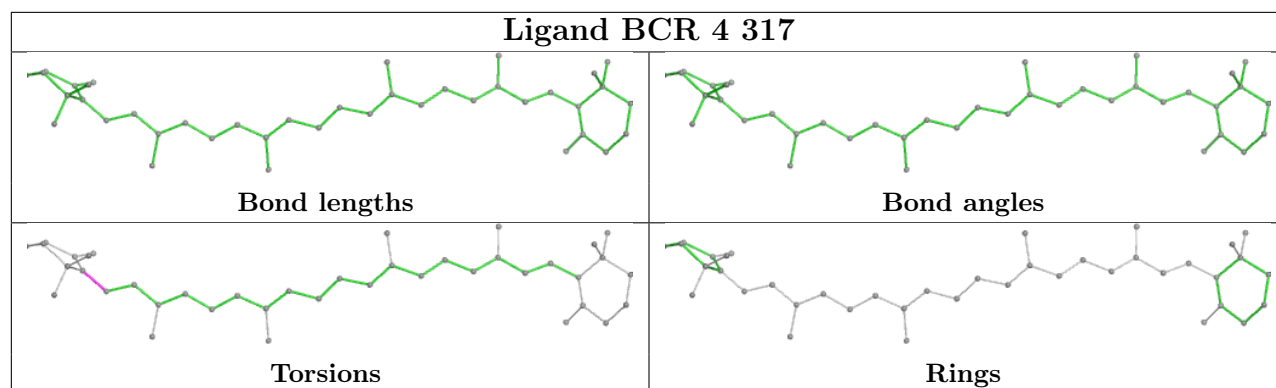
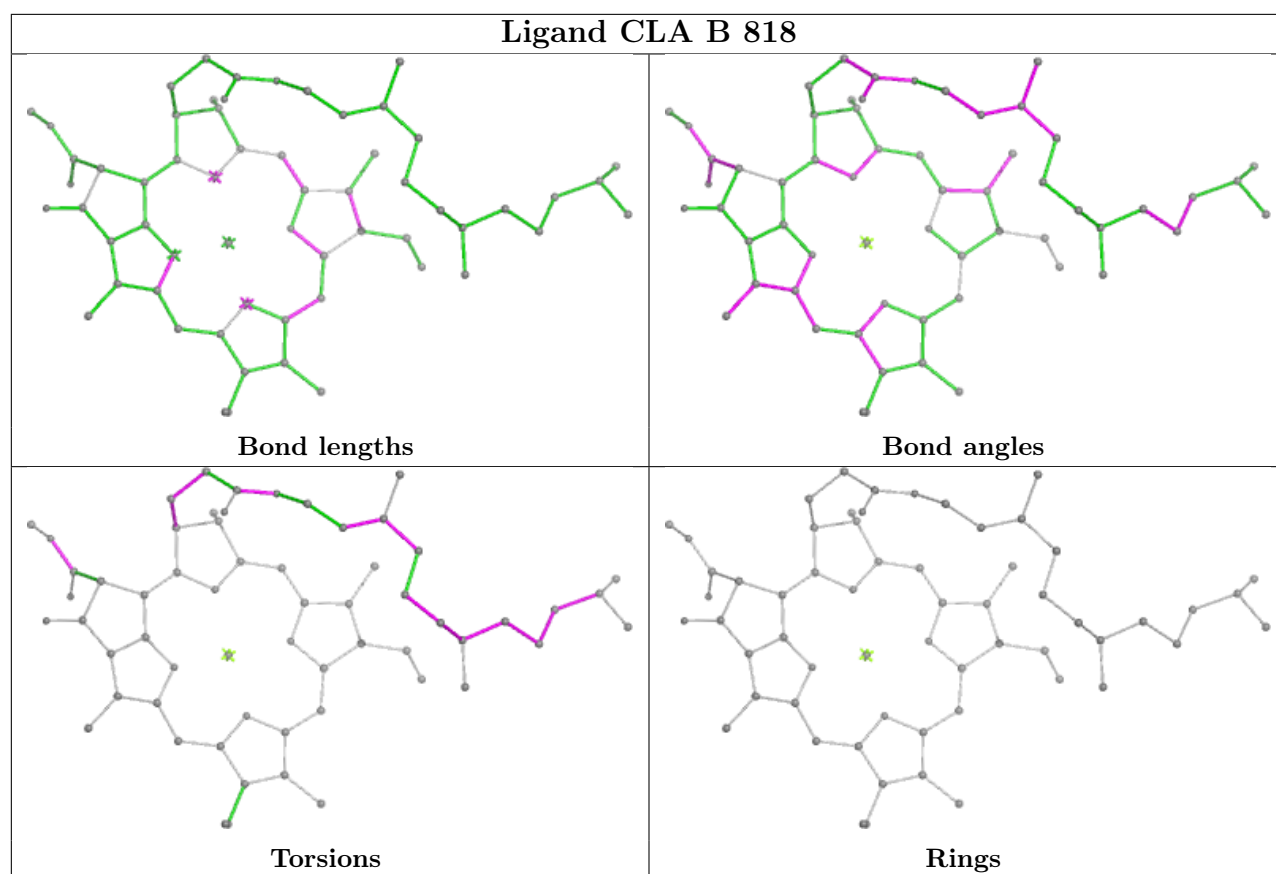


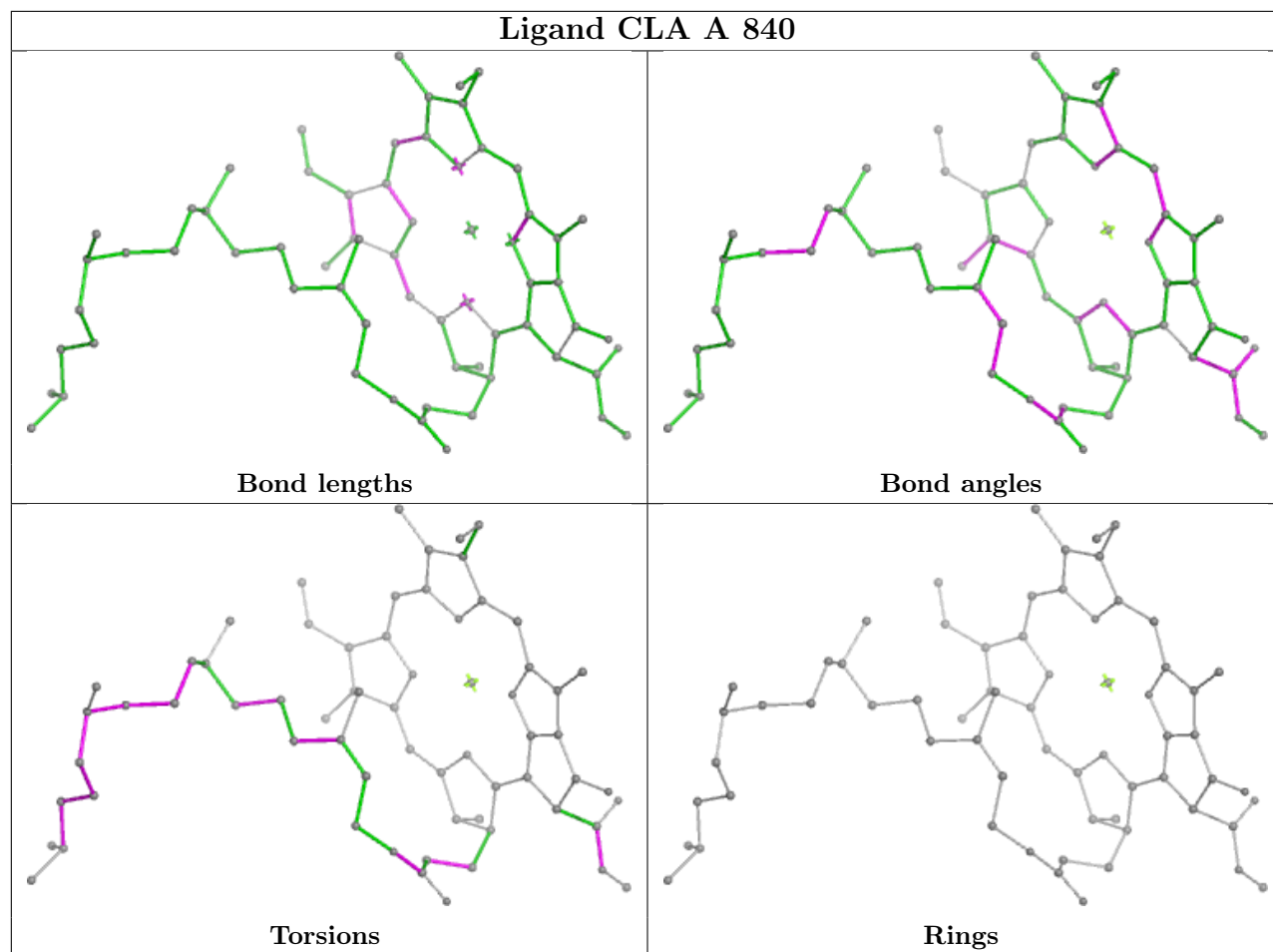


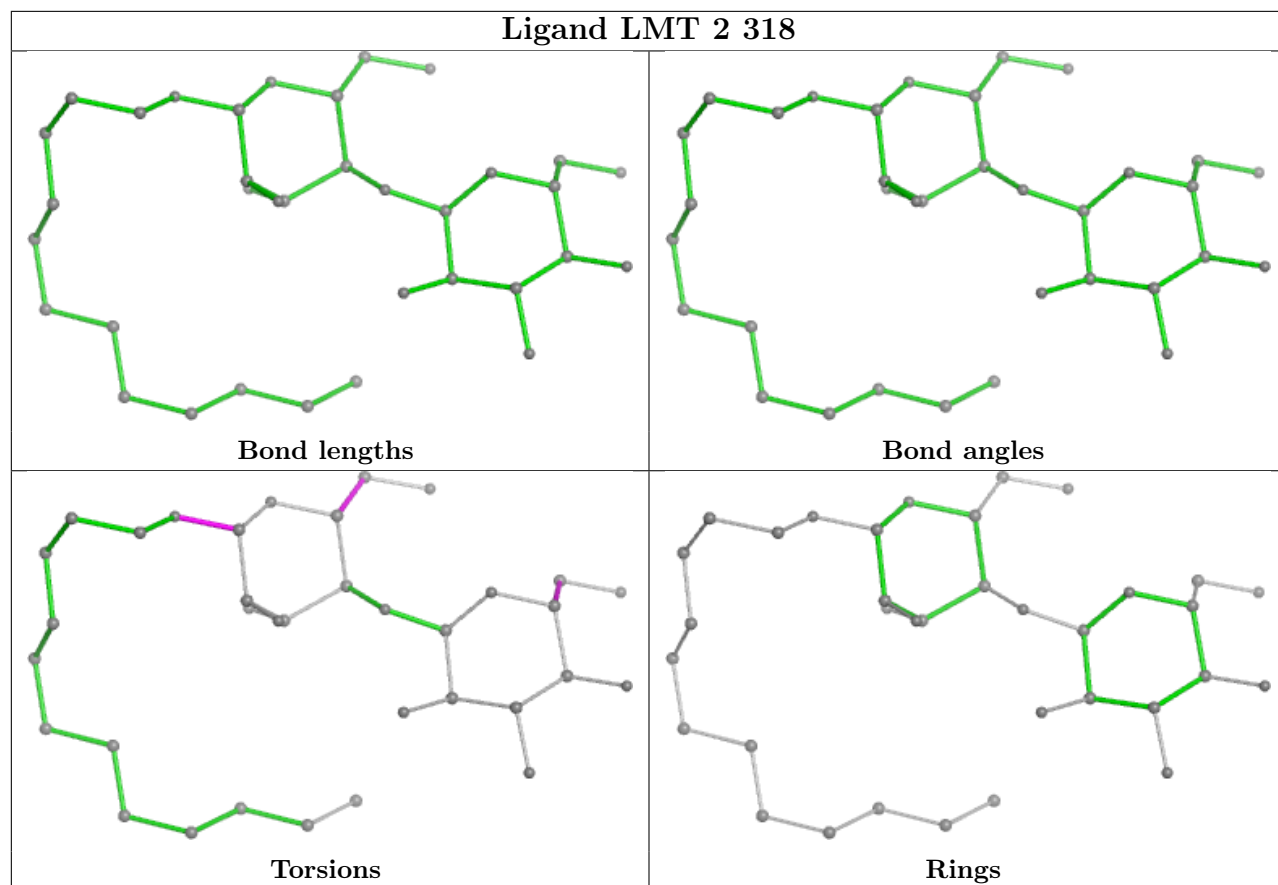
Ligand CLA A 811



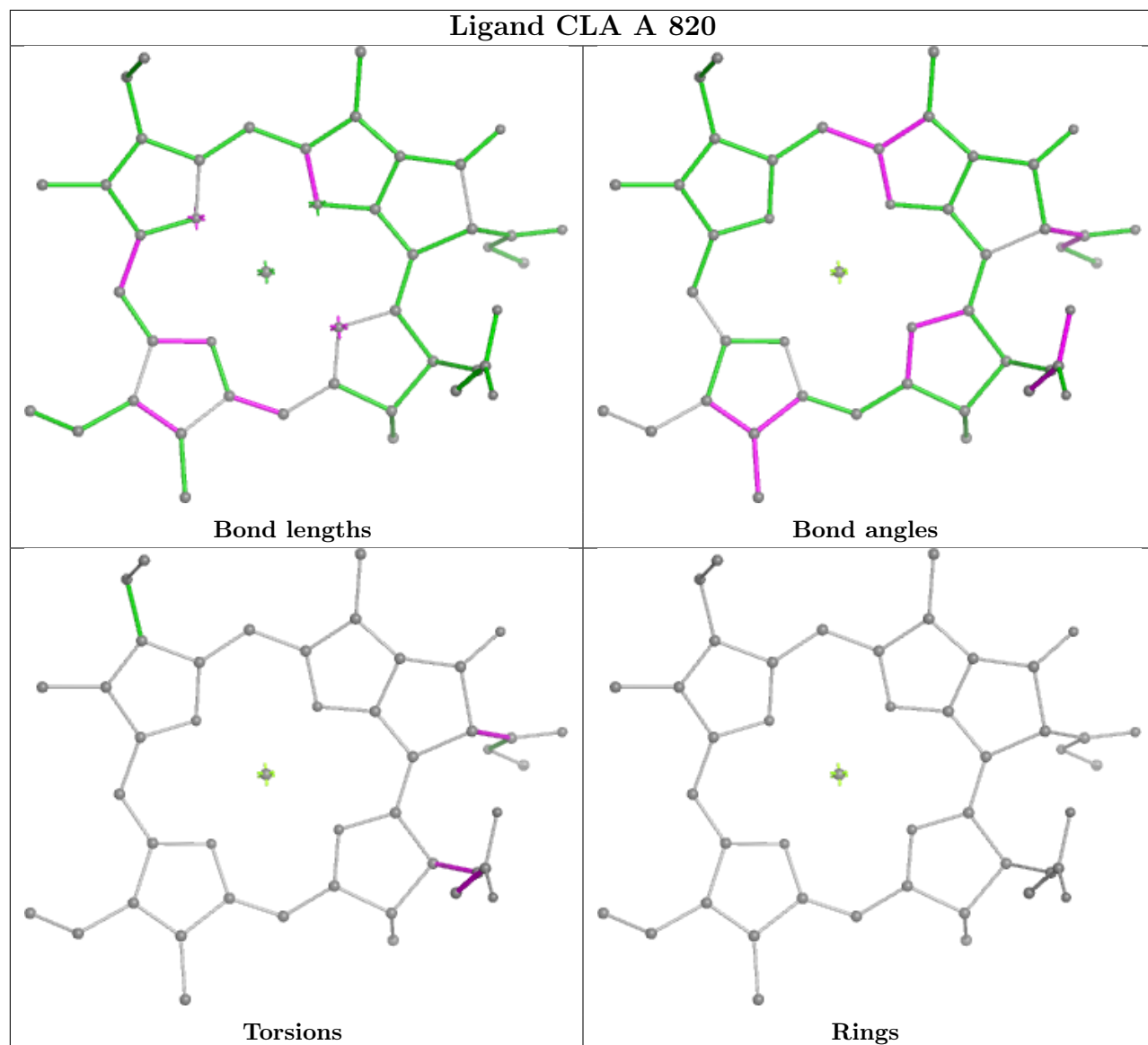


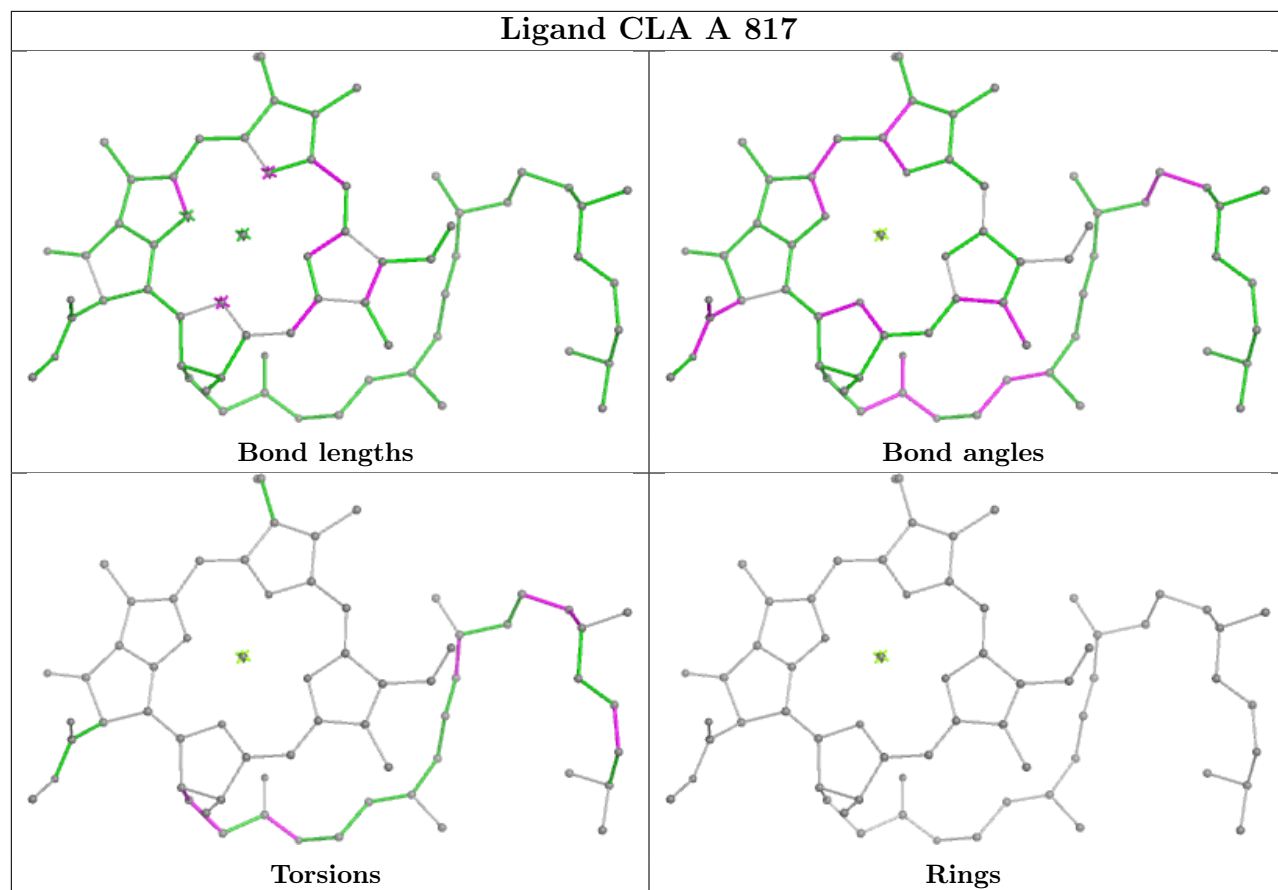




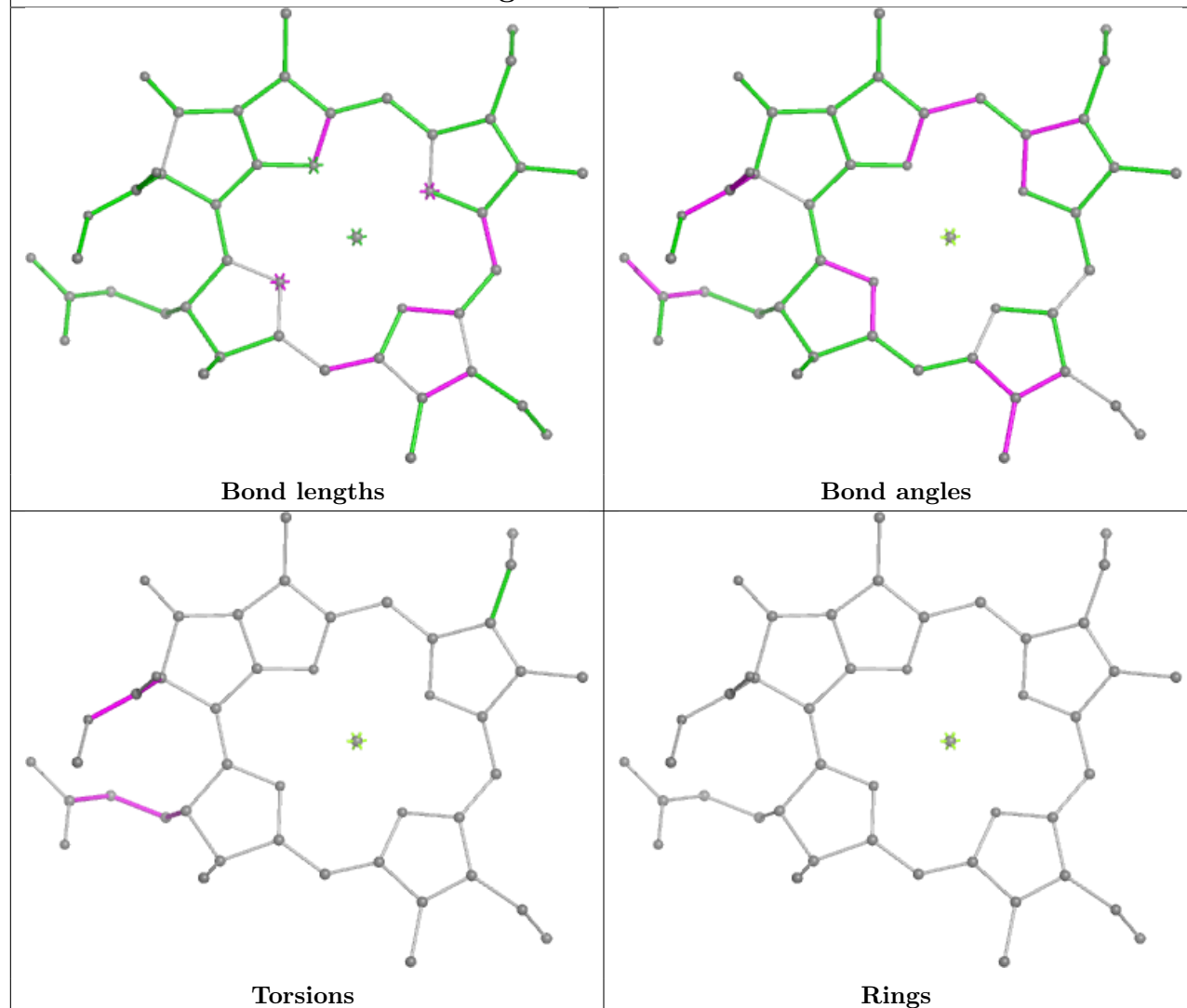


Ligand CLA A 820

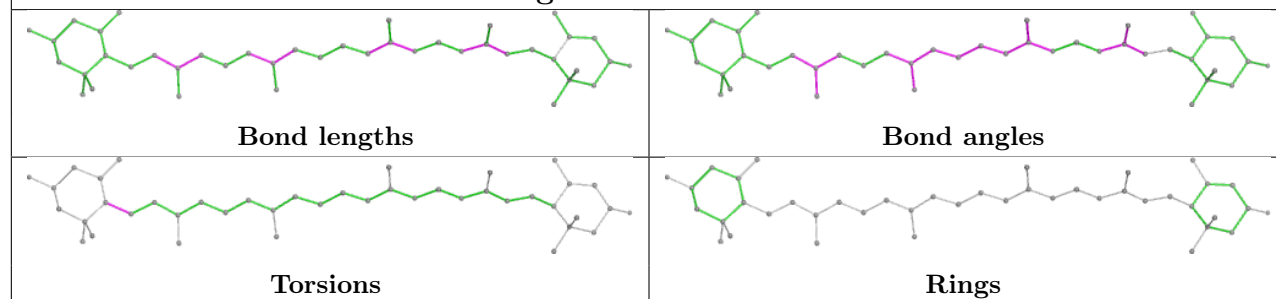


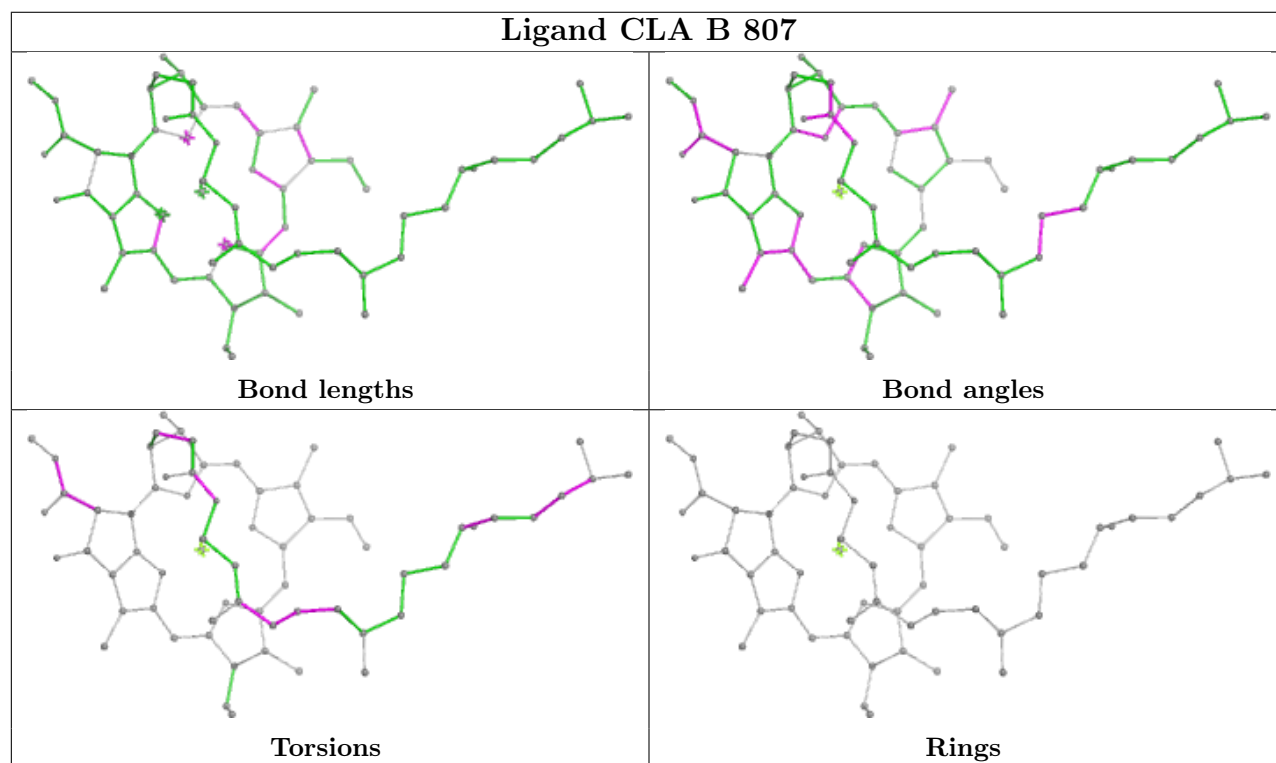
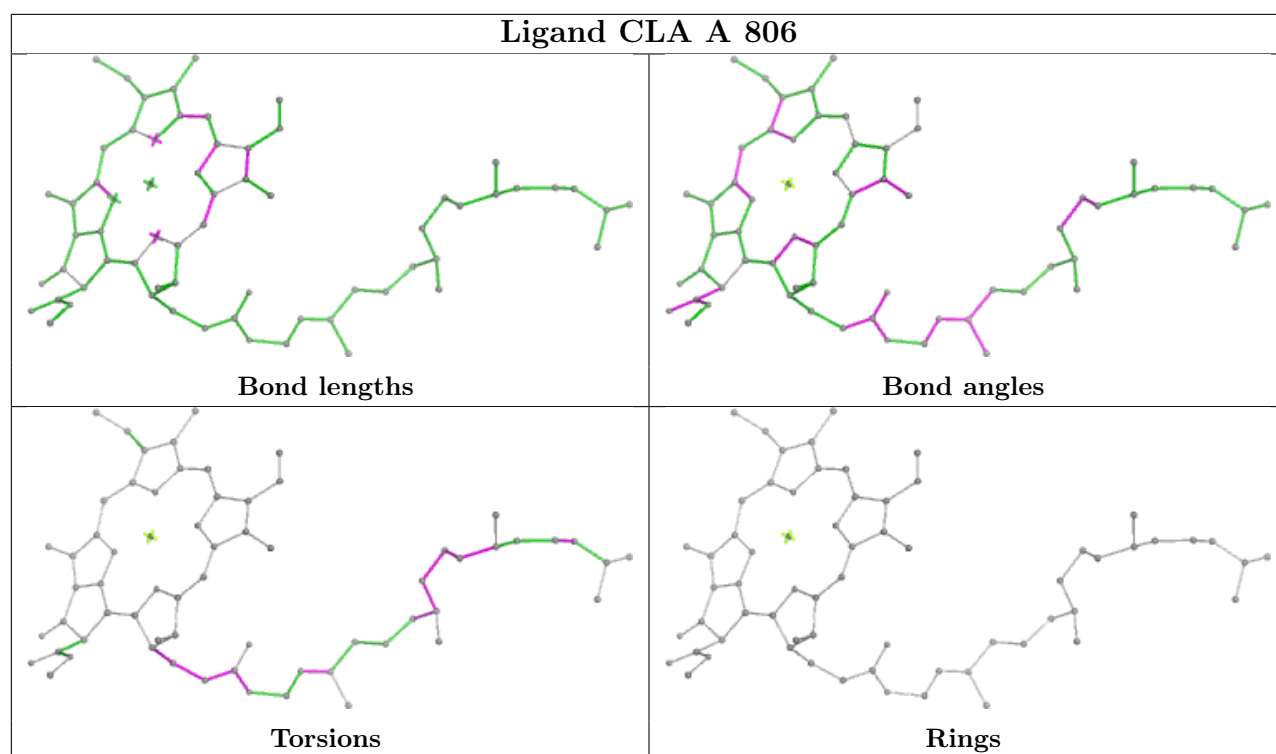


Ligand CLA 1 314

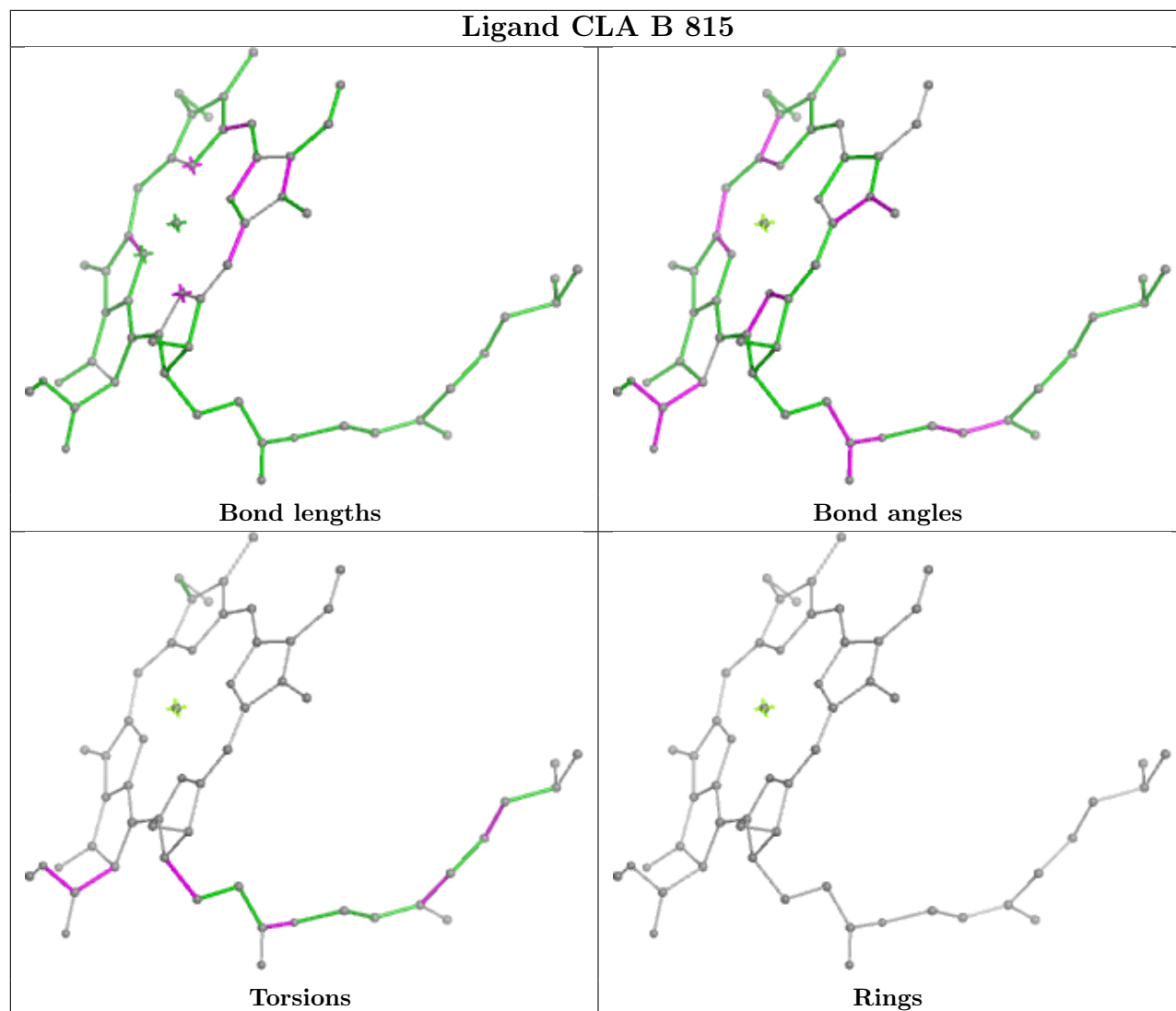


Ligand LUT 1 319

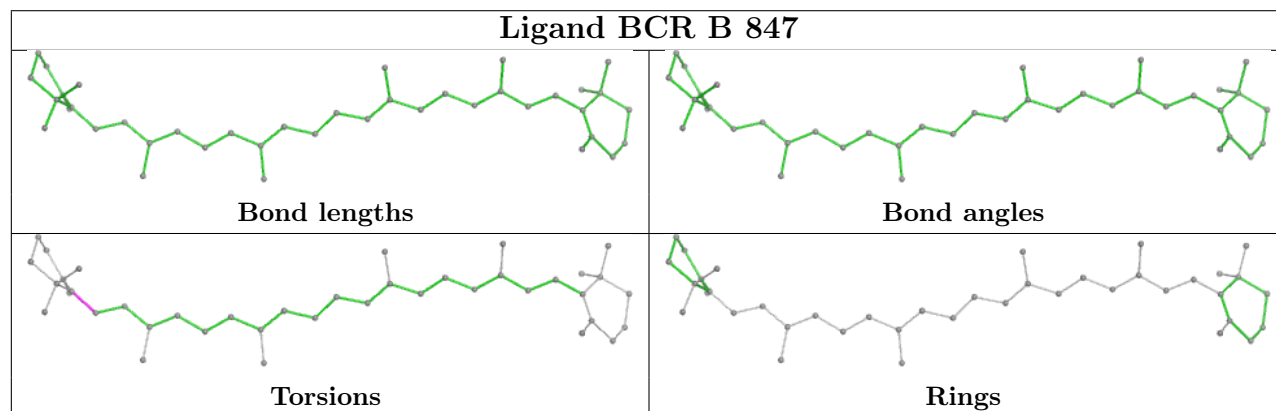


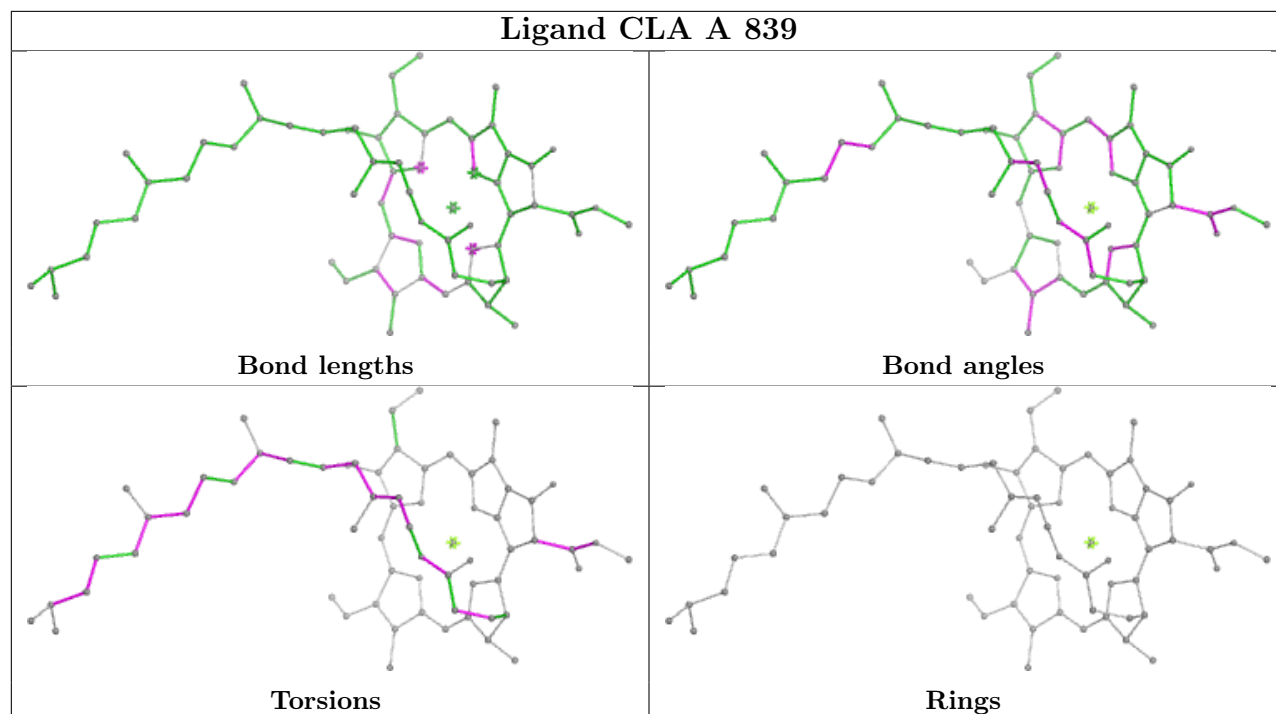


Ligand CLA B 815

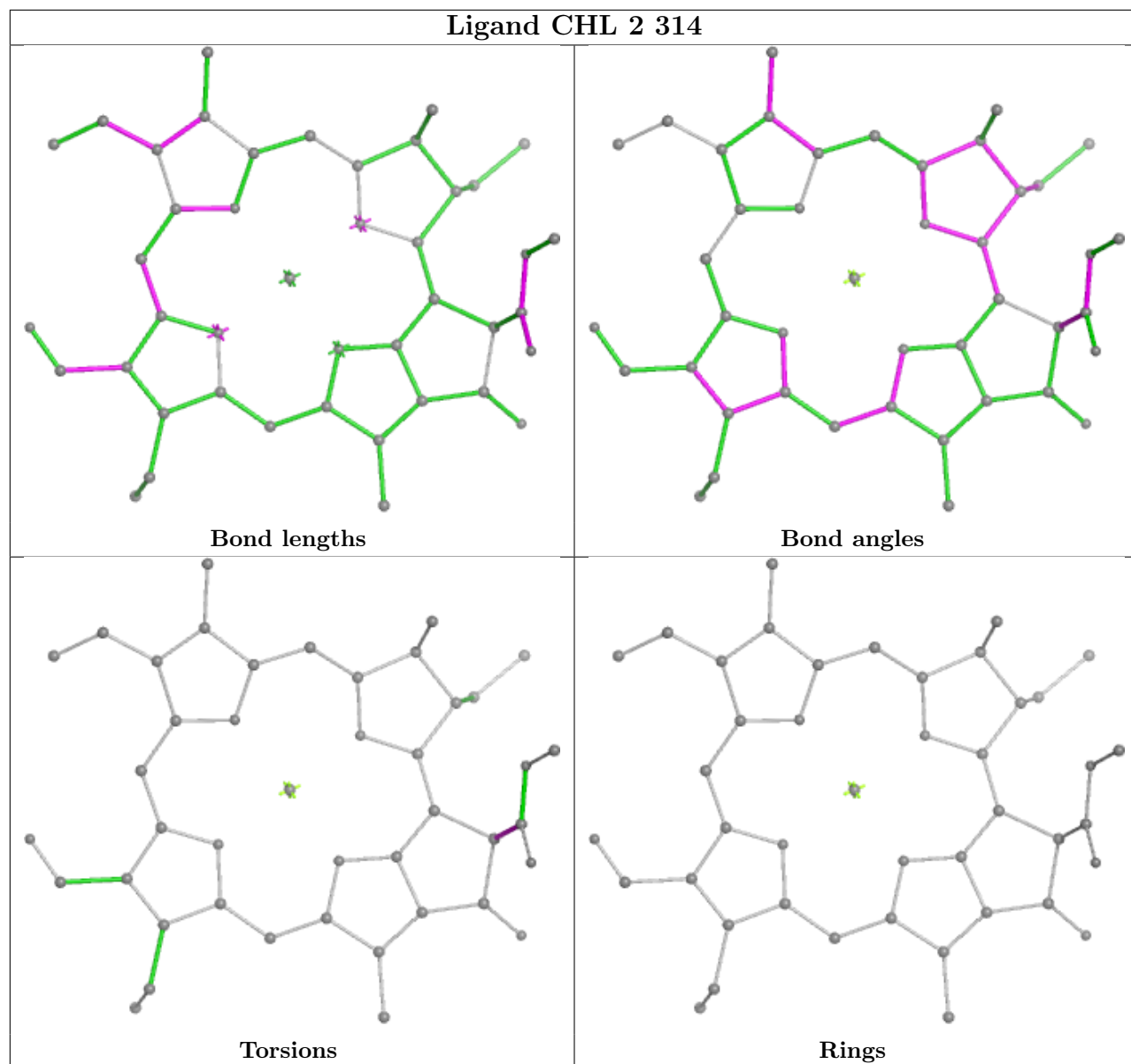


Ligand BCR B 847

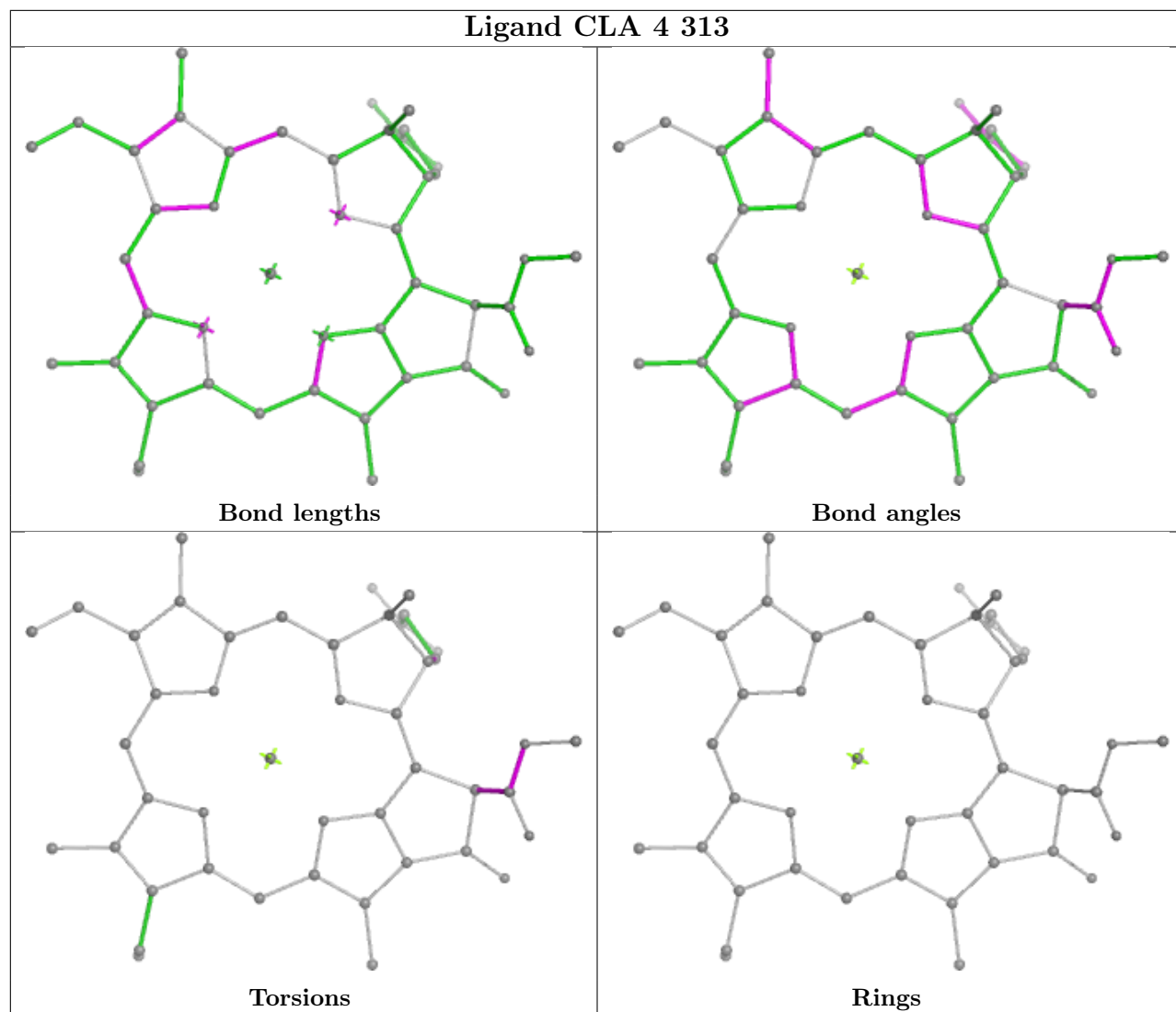


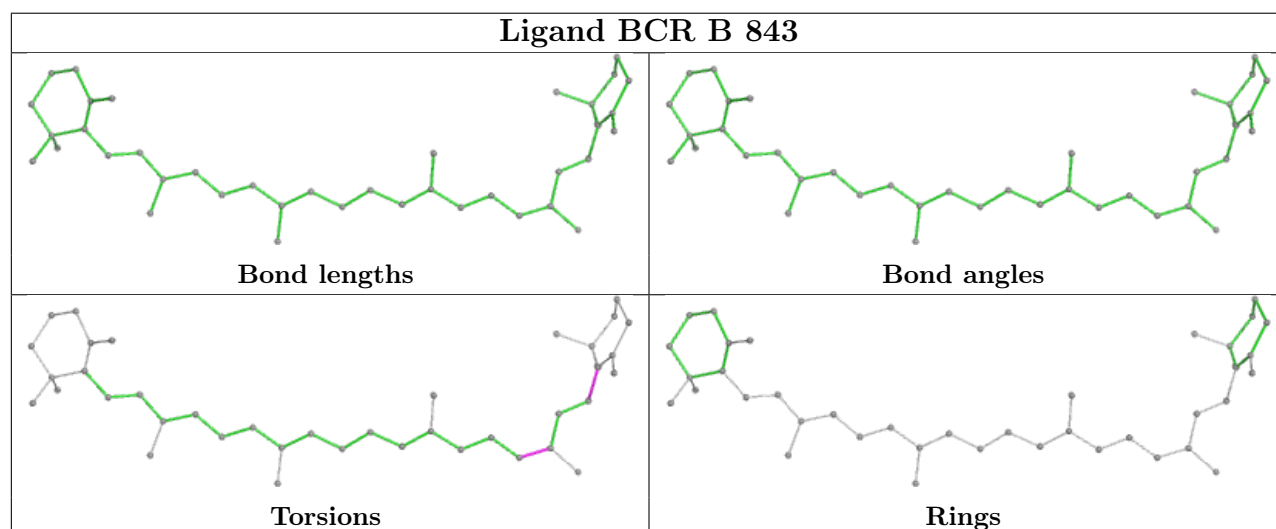
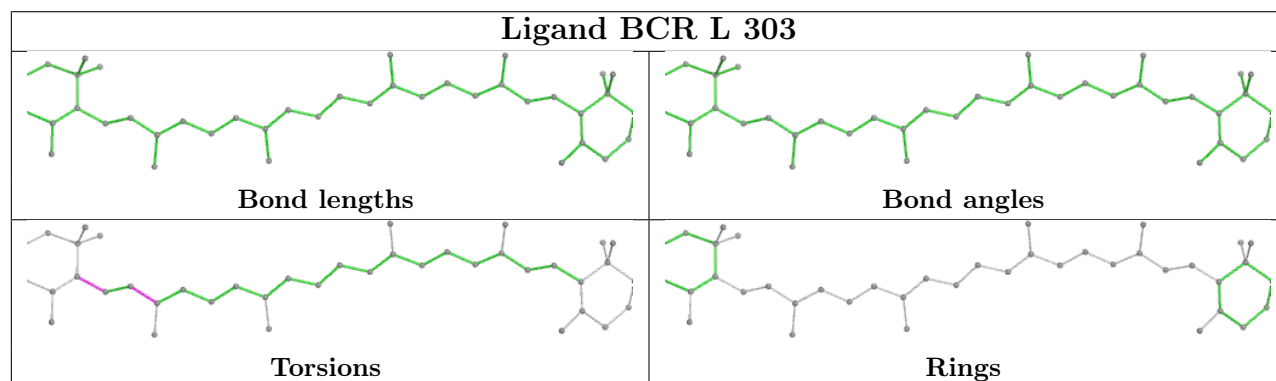
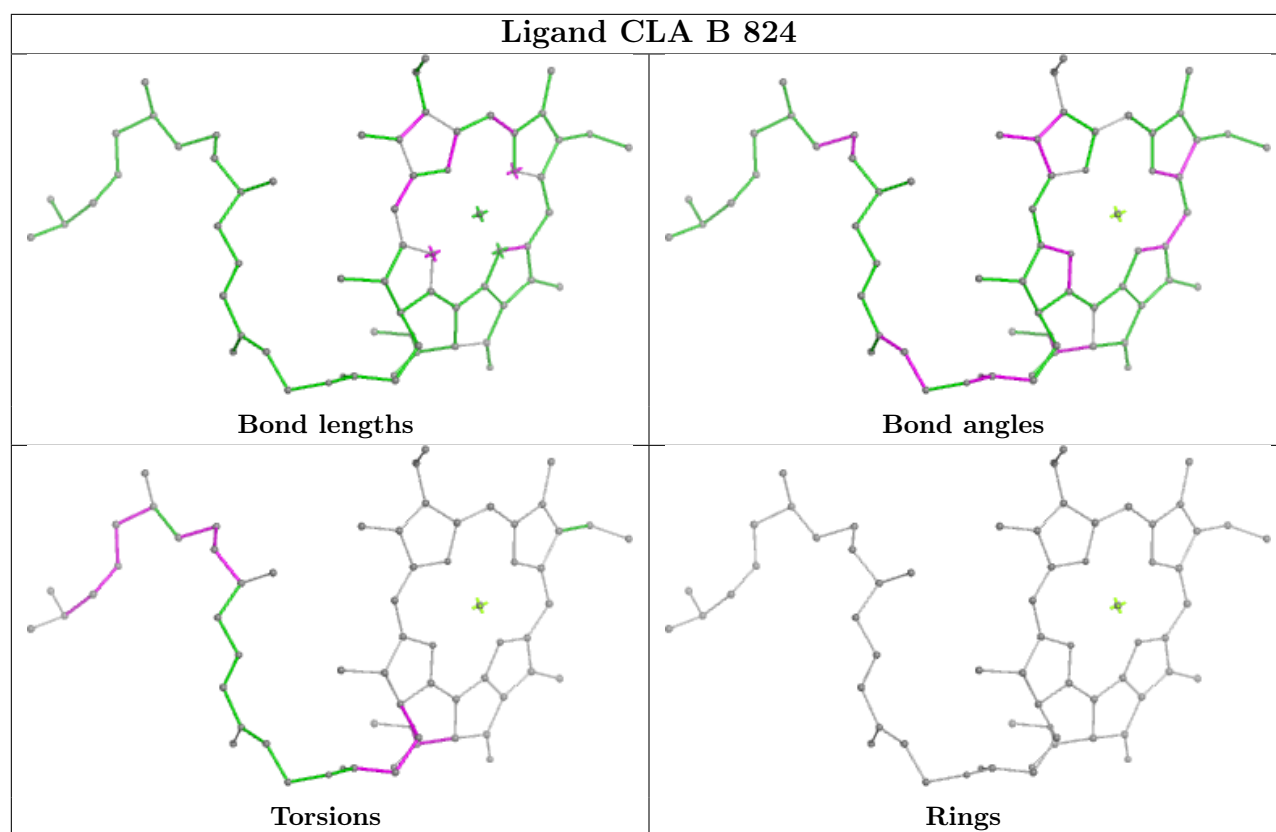


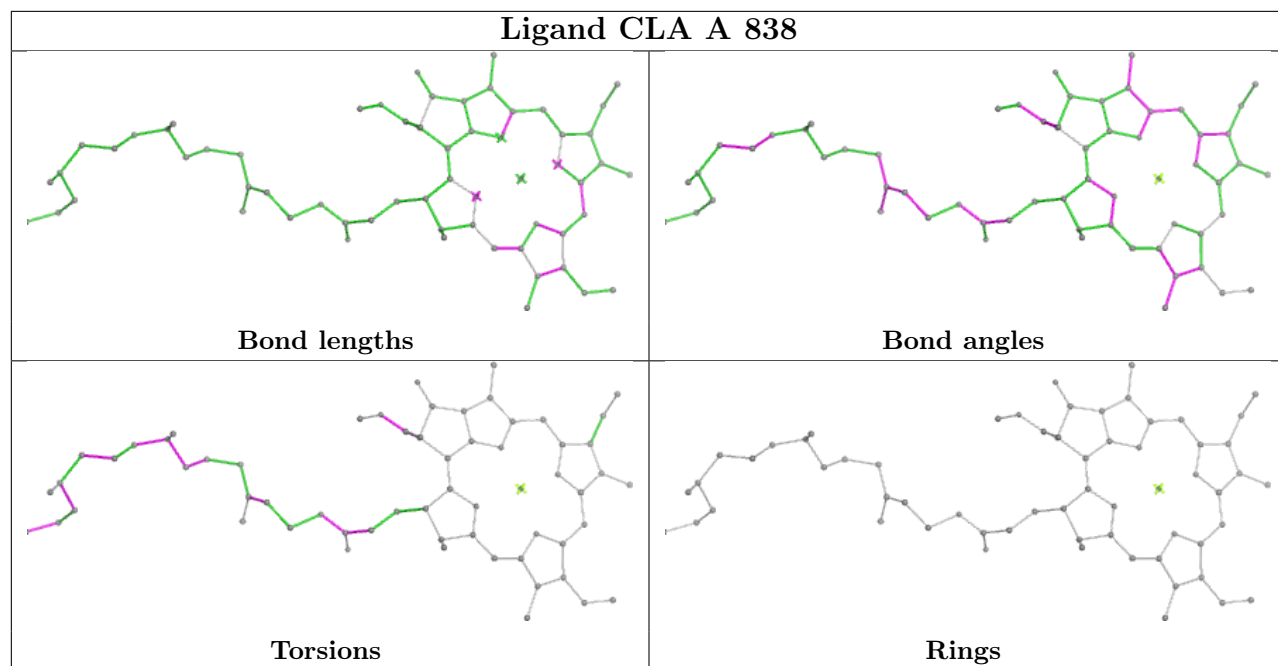
Ligand CHL 2 314



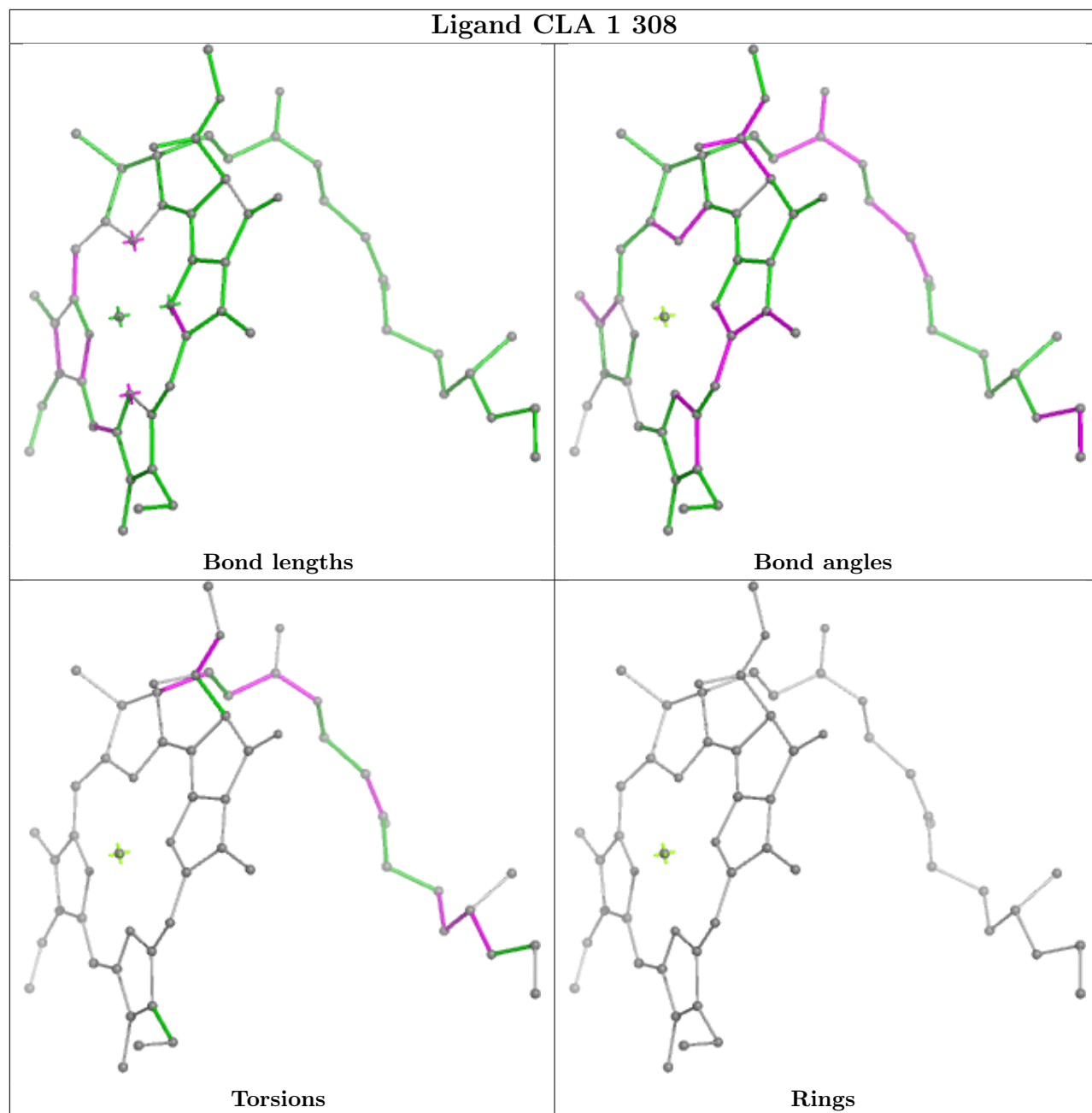
Ligand CLA 4 313



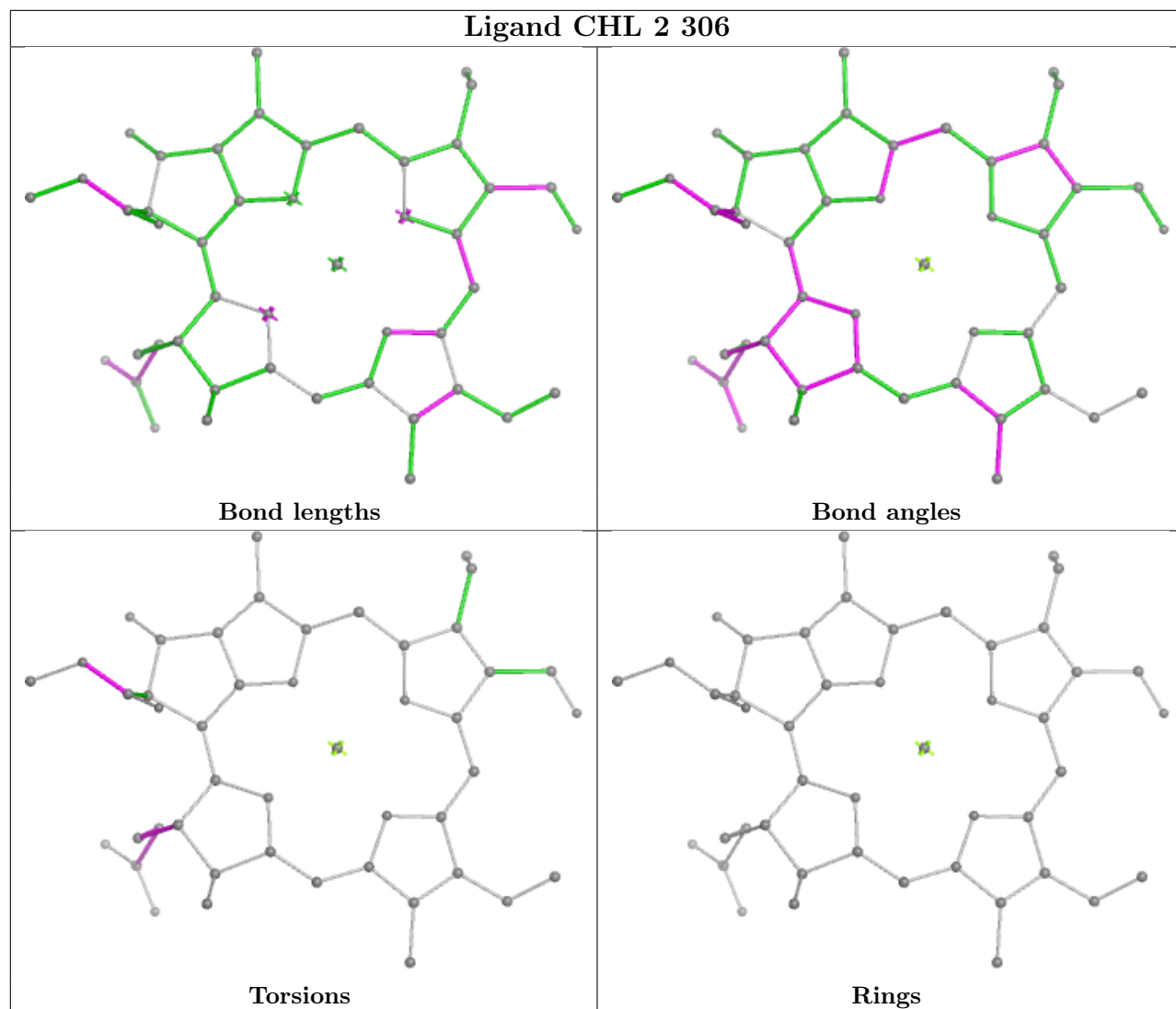




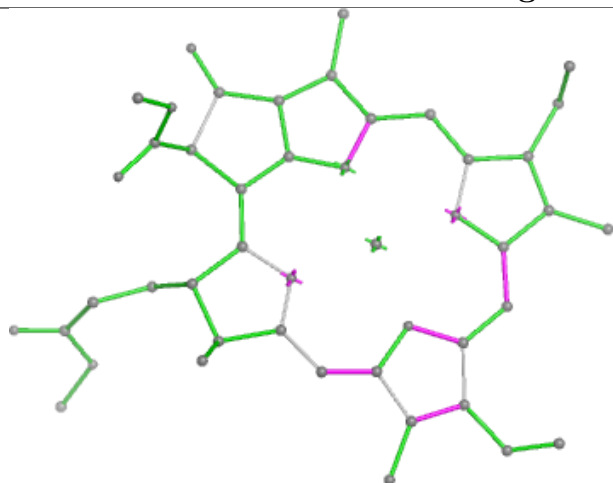
Ligand CLA 1 308



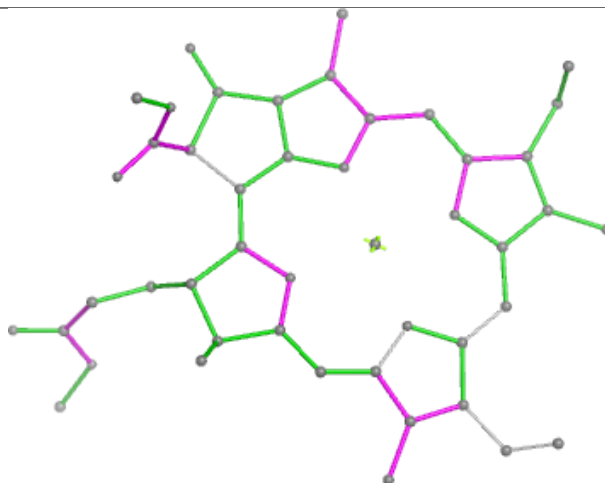
Ligand CHL 2 306



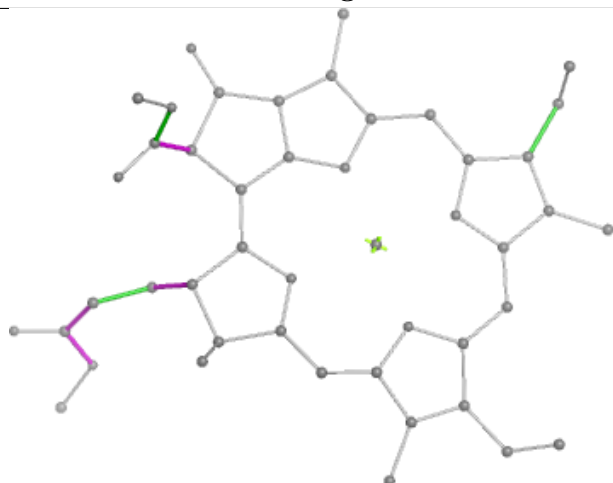
Ligand CLA 4 301



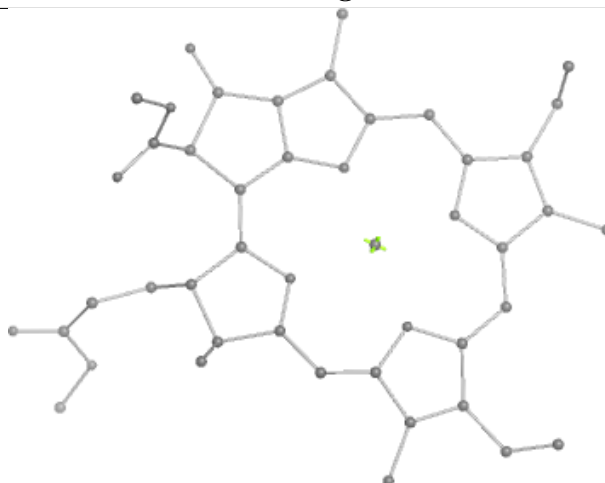
Bond lengths



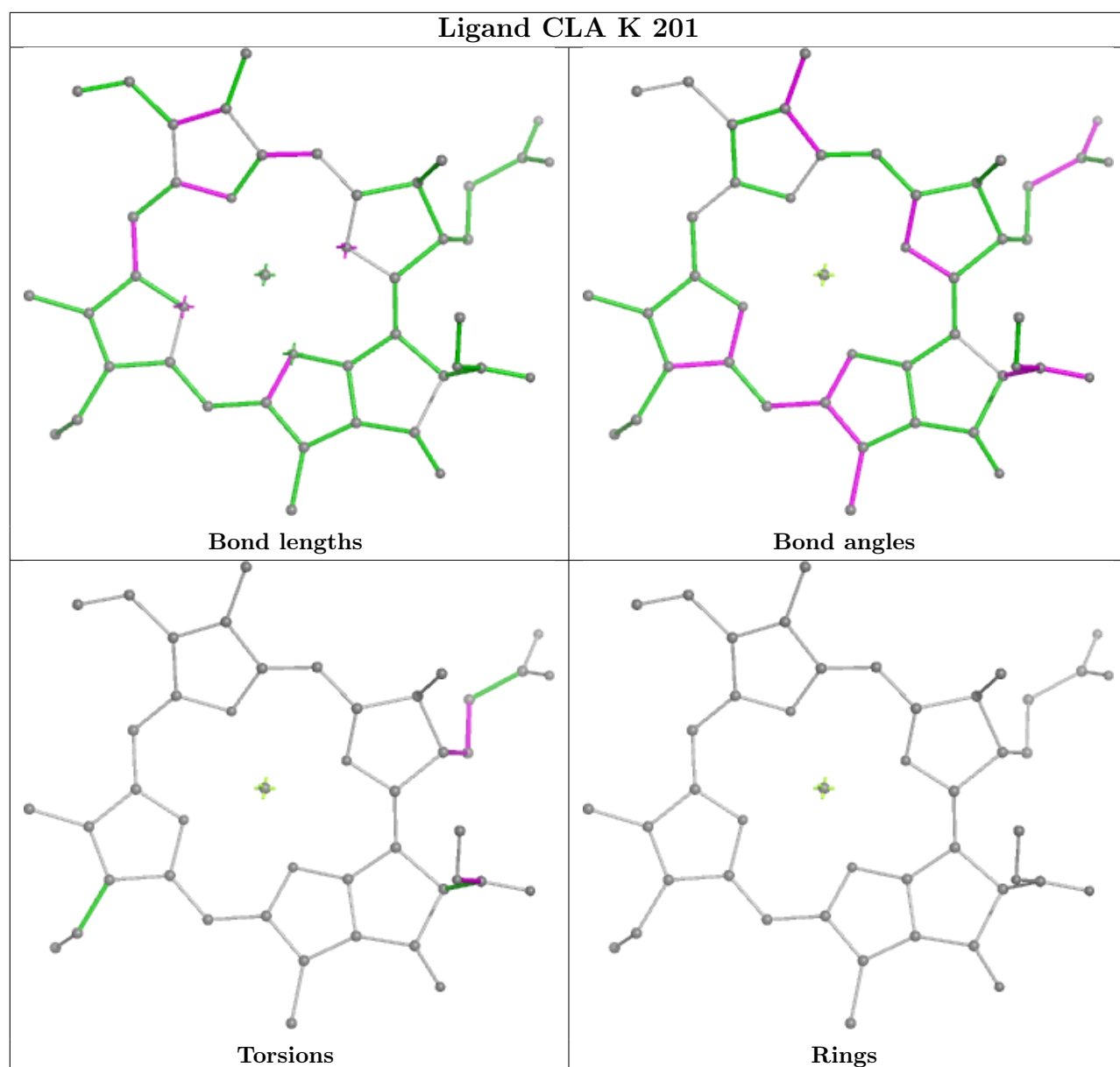
Bond angles

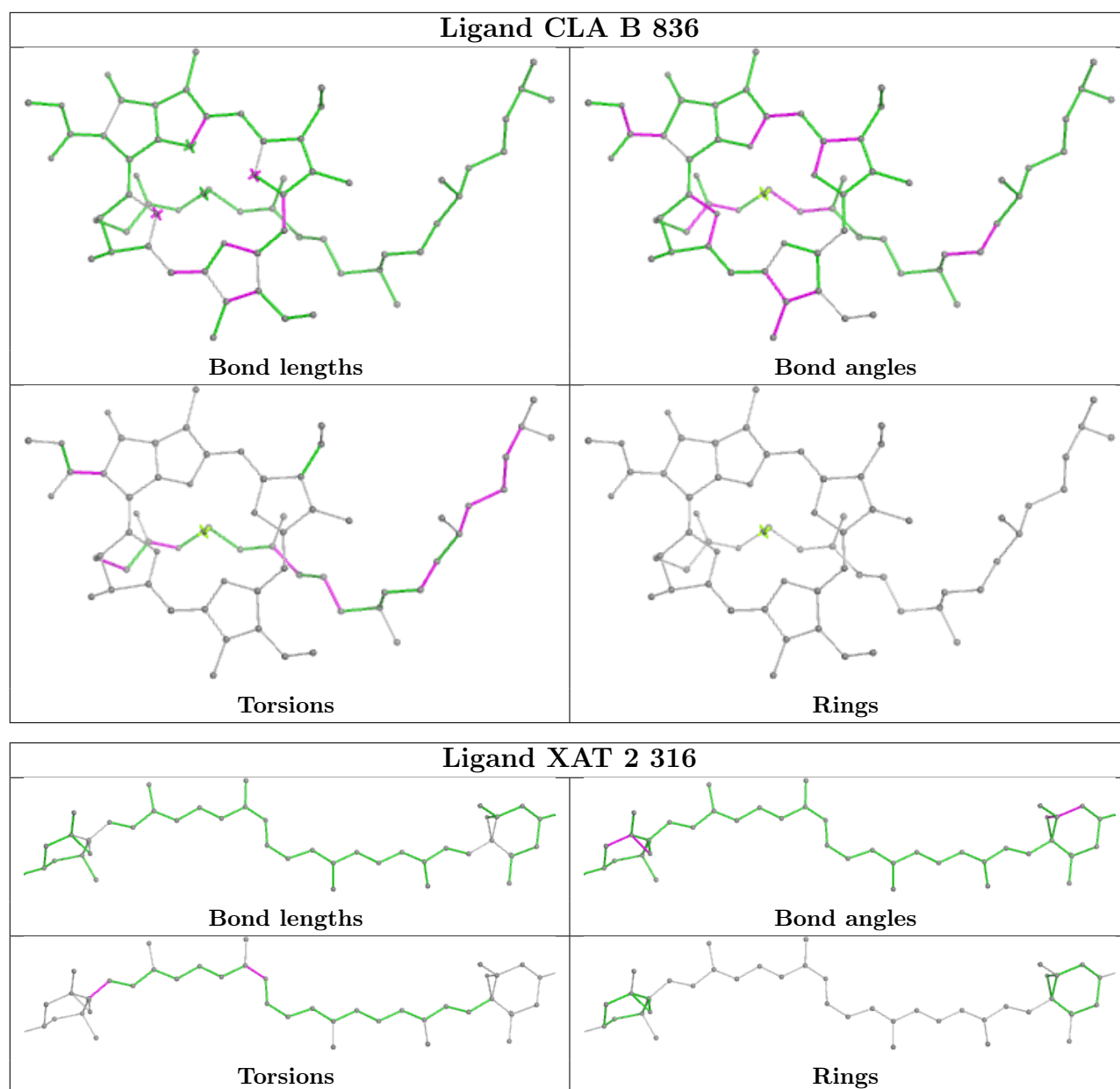


Torsions

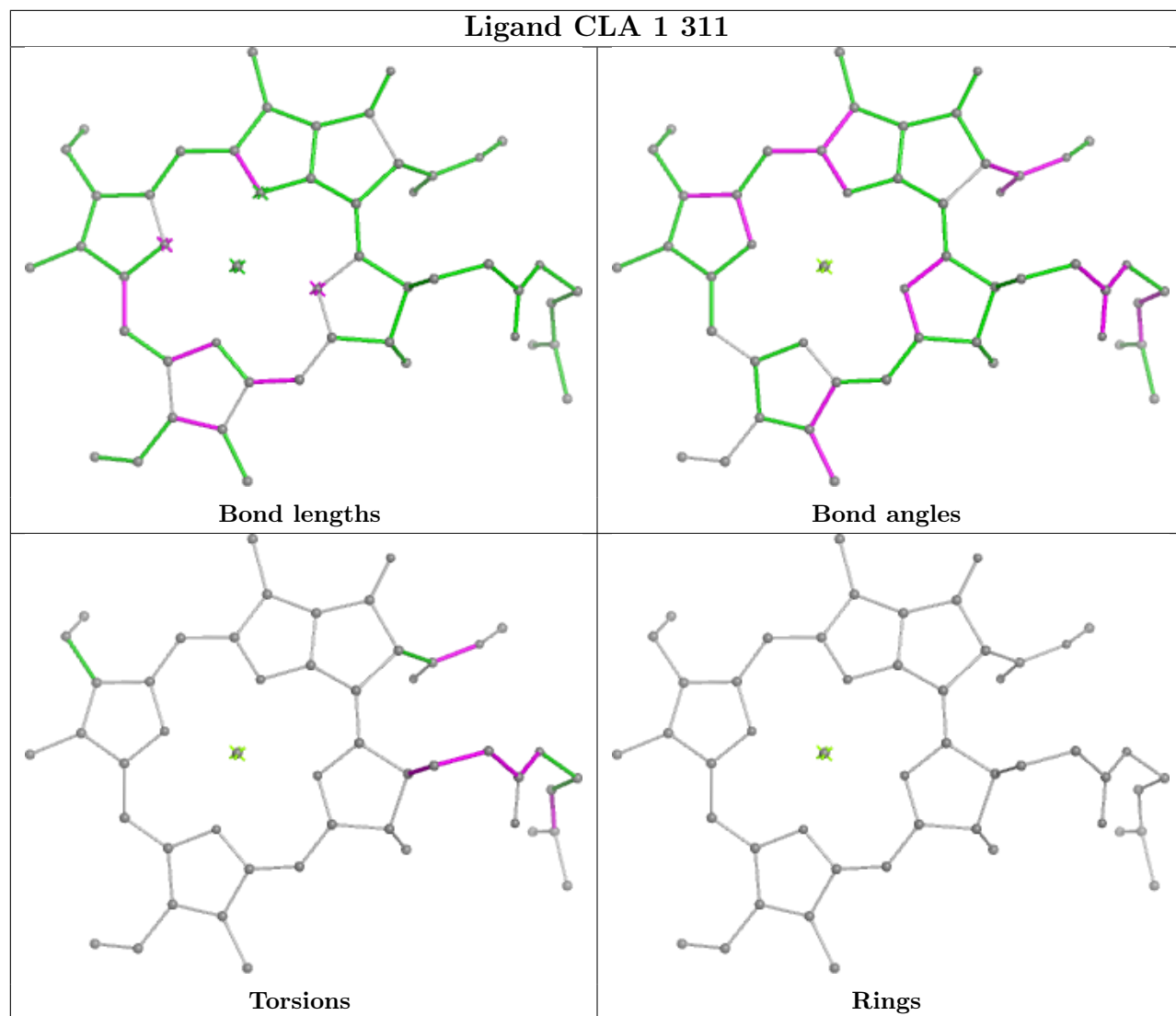


Rings

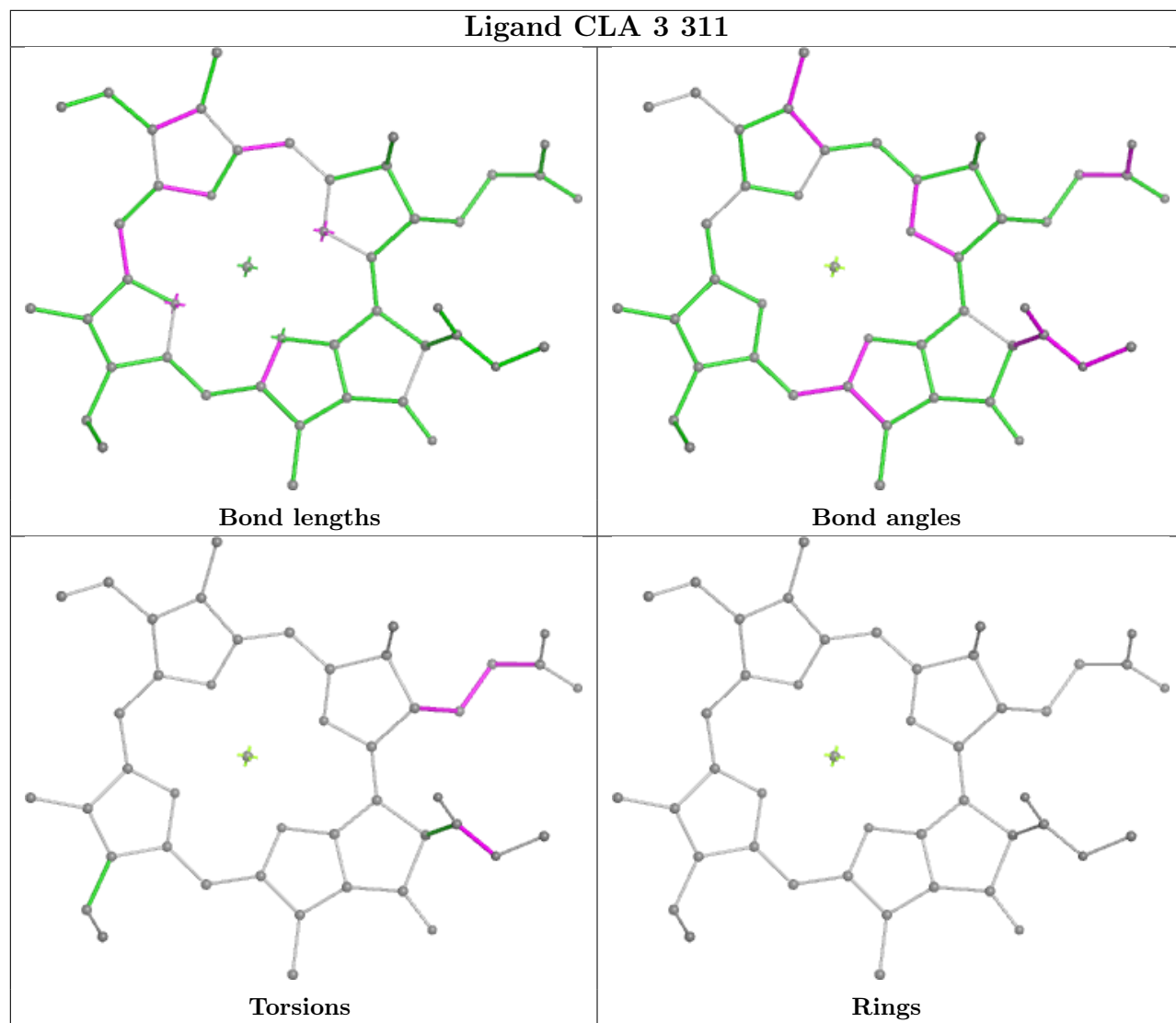


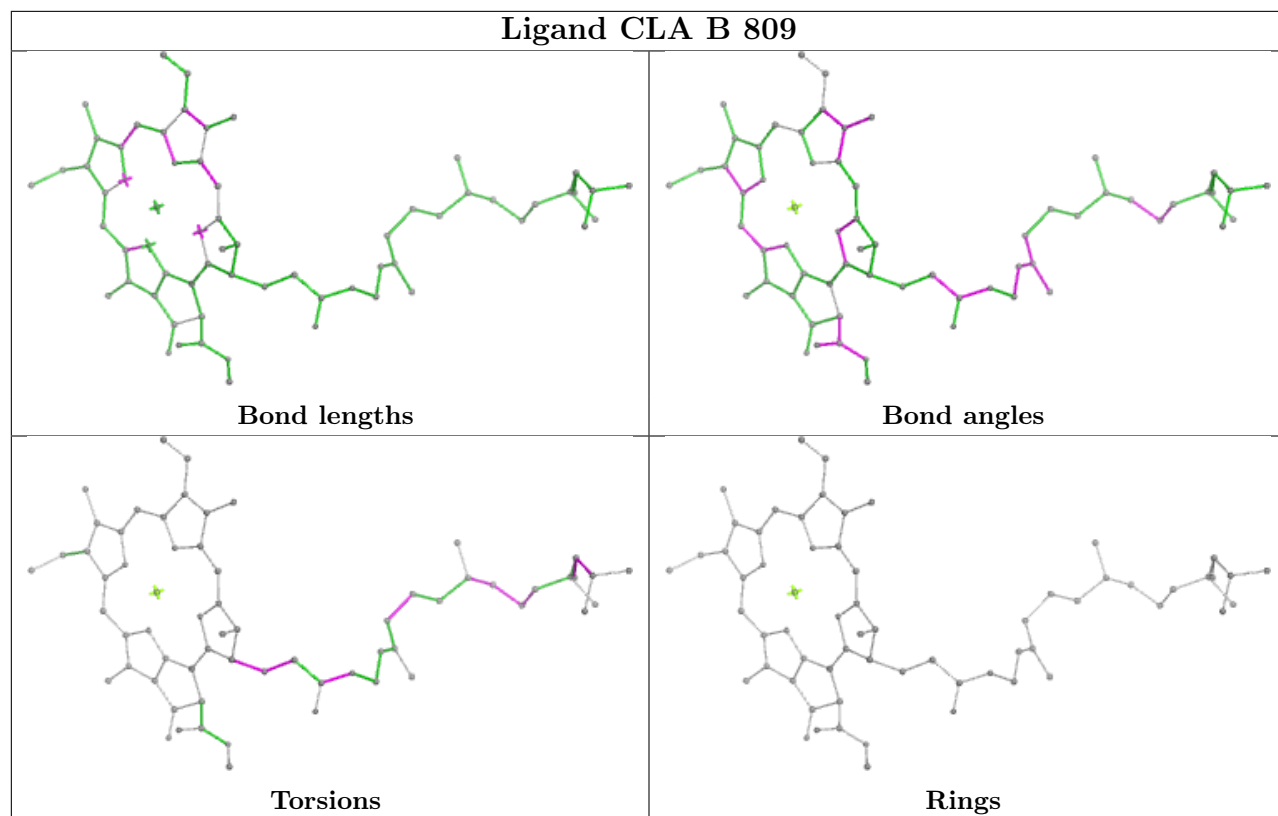


Ligand CLA 1 311

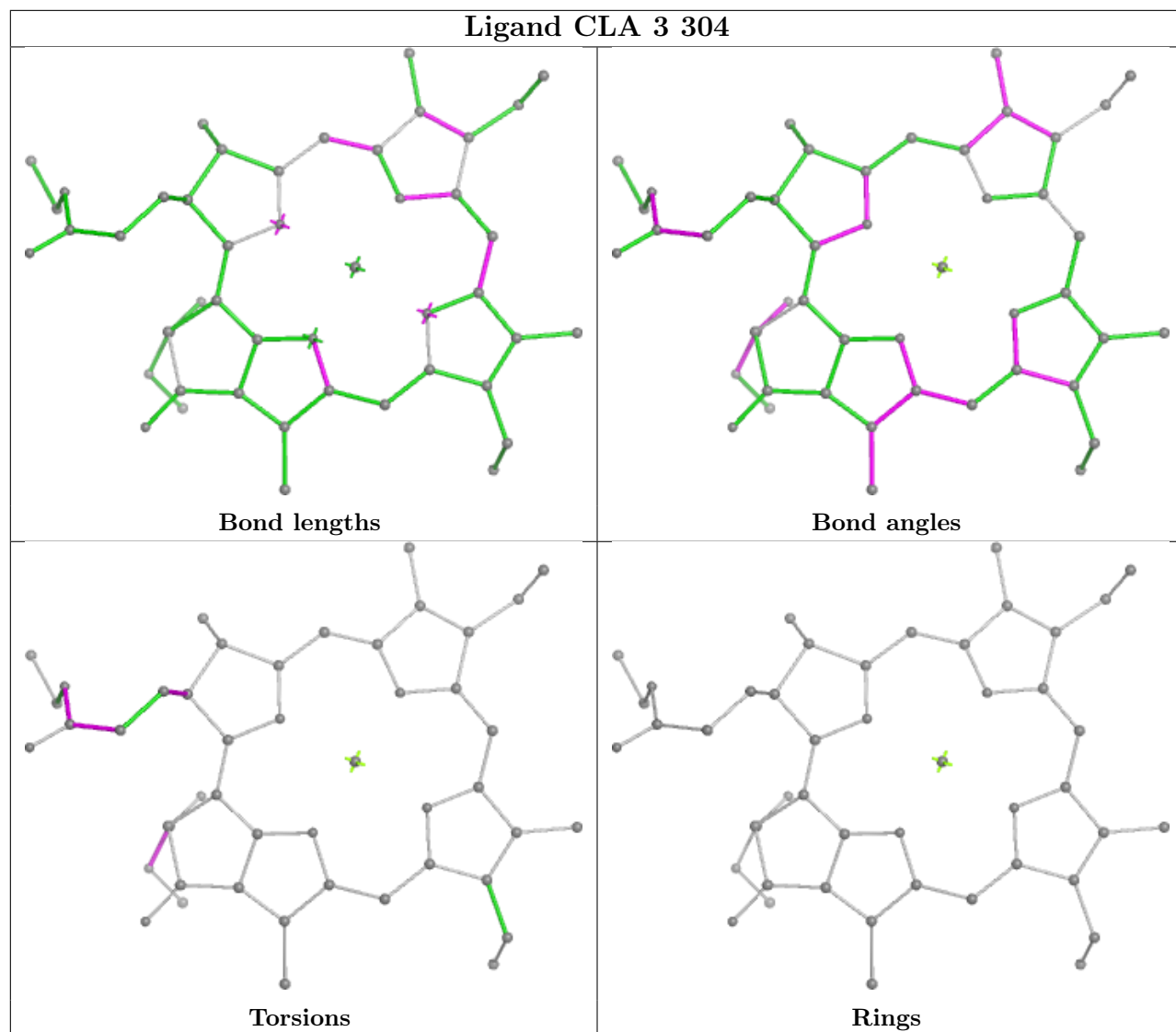


Ligand CLA 3 311

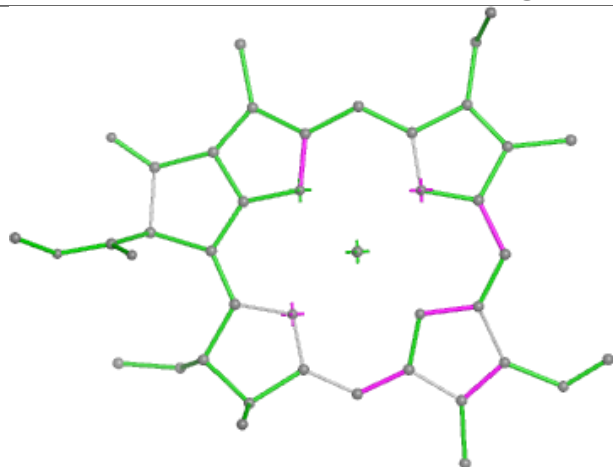




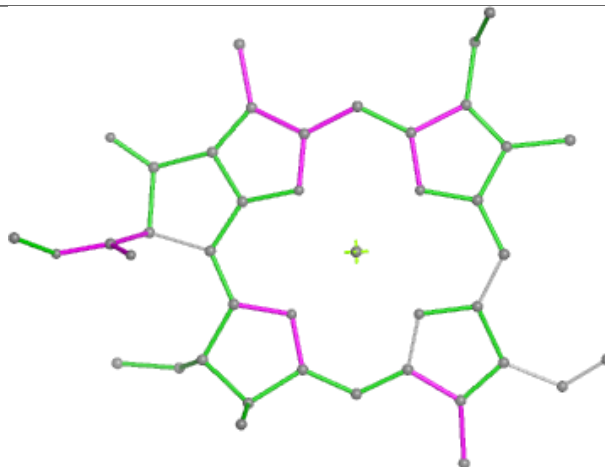
Ligand CLA 3 304



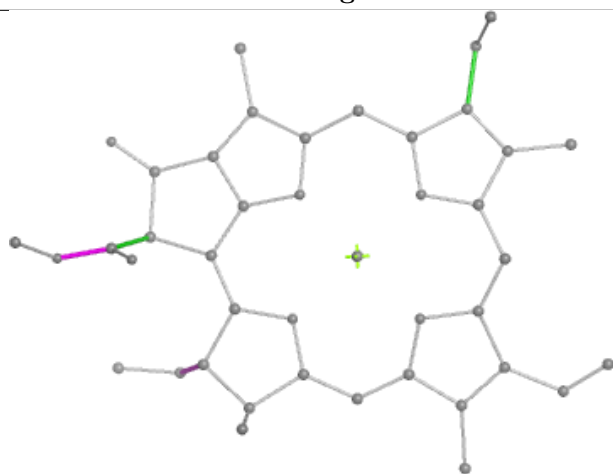
Ligand CLA 1 305



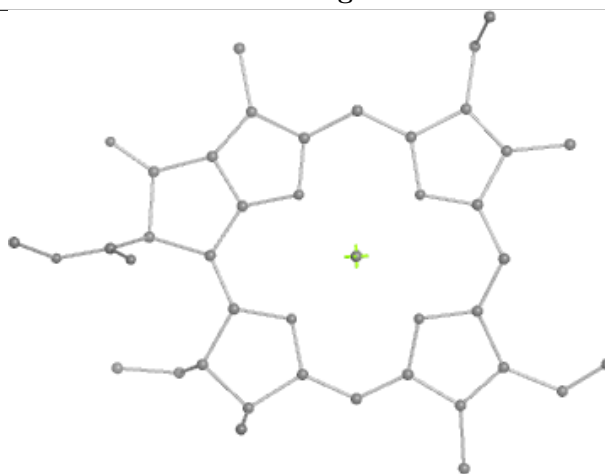
Bond lengths



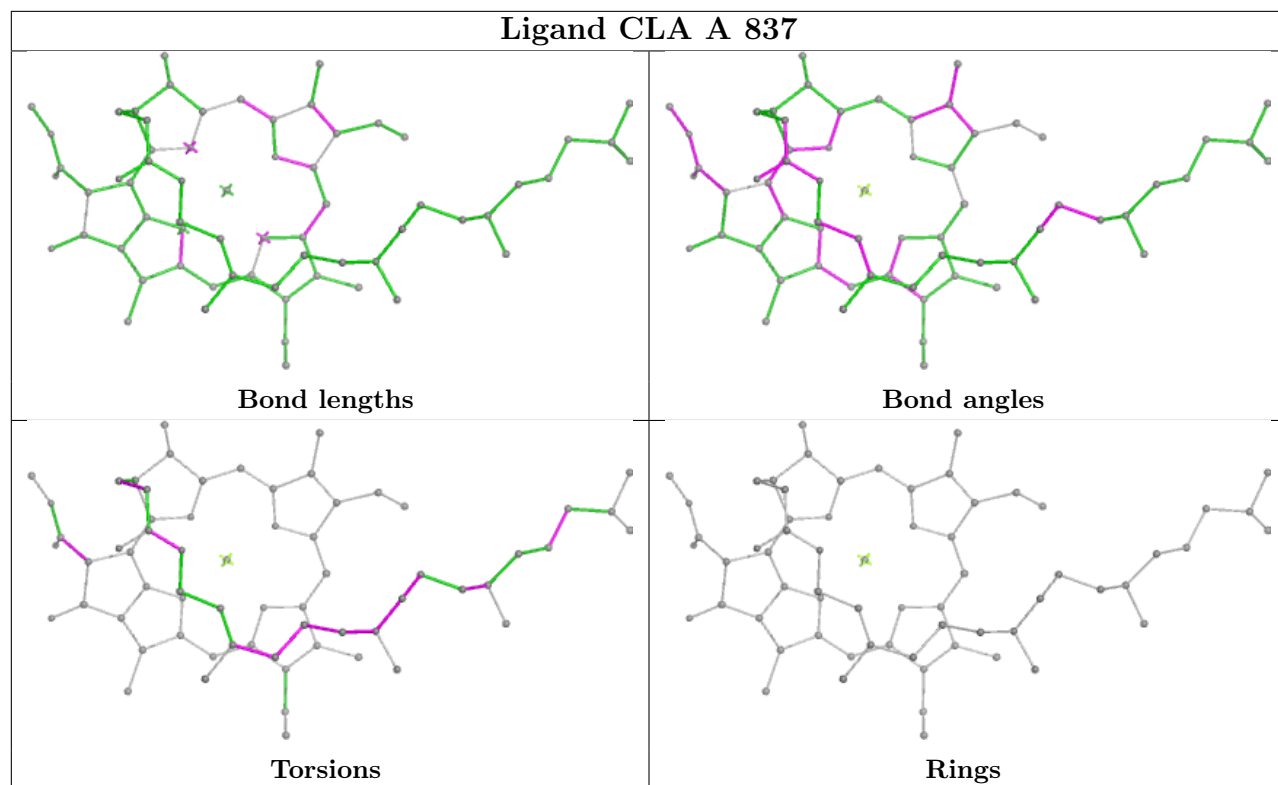
Bond angles

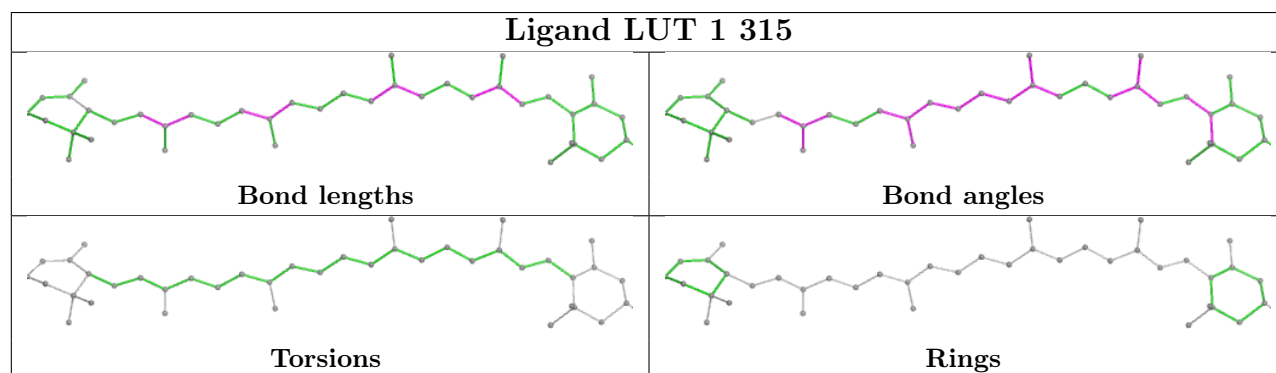
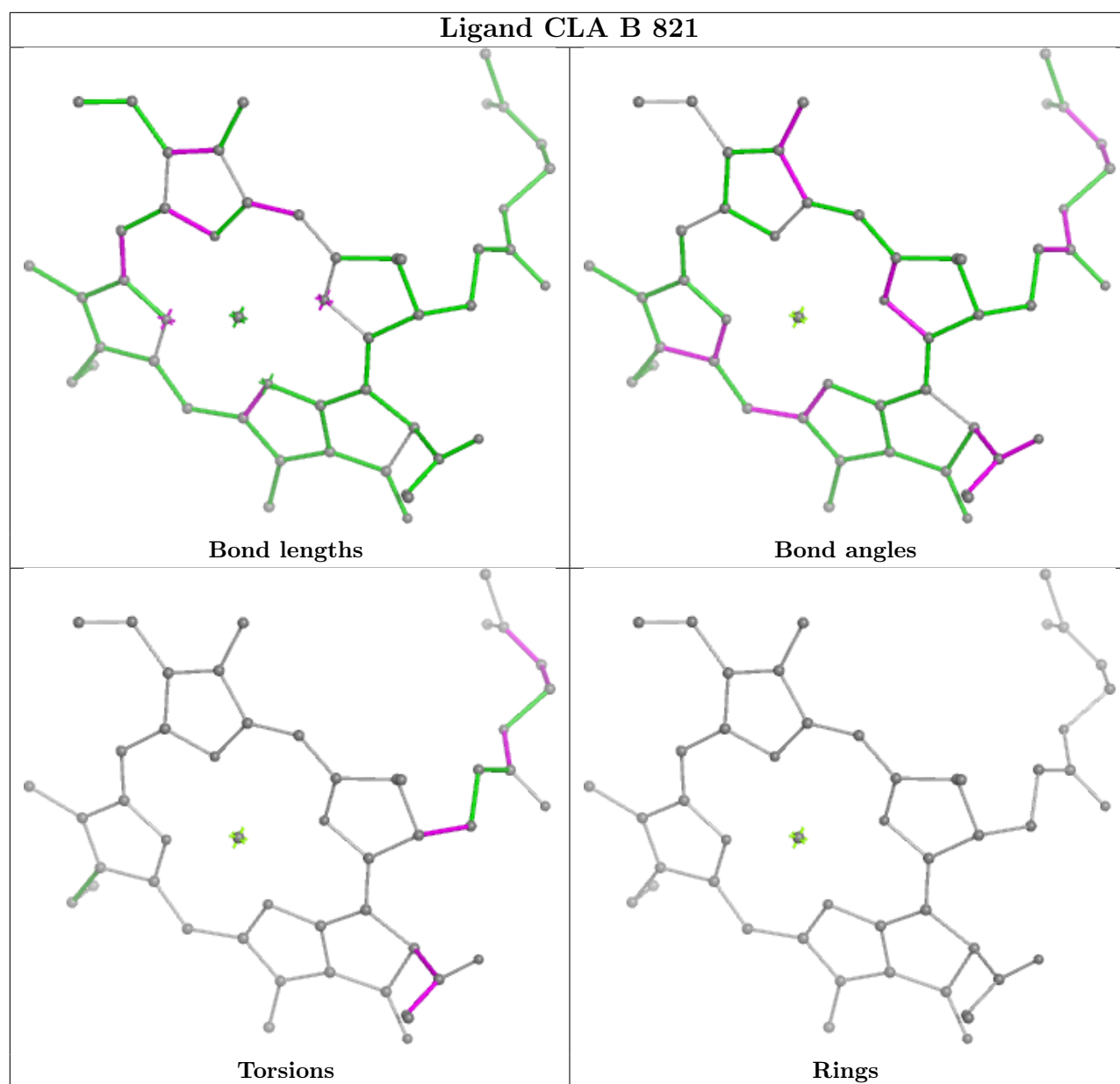


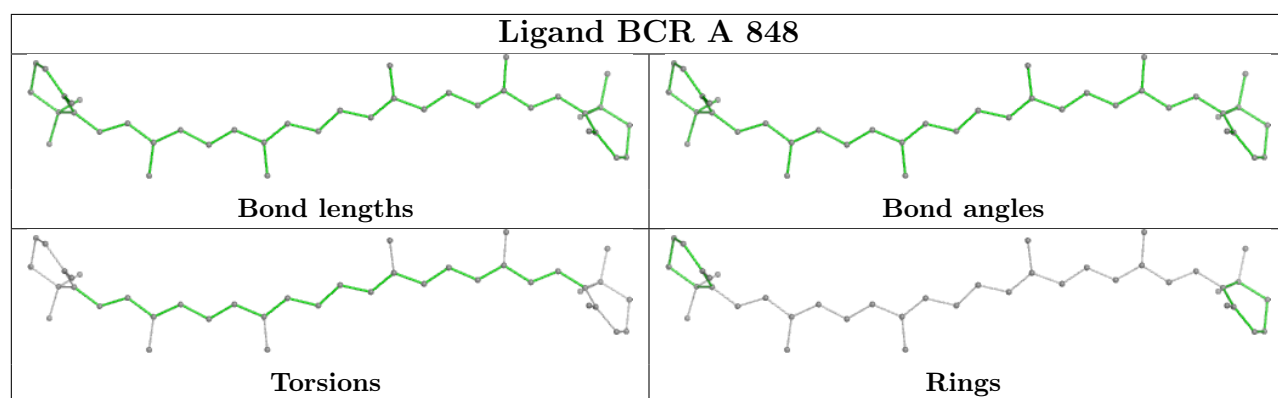
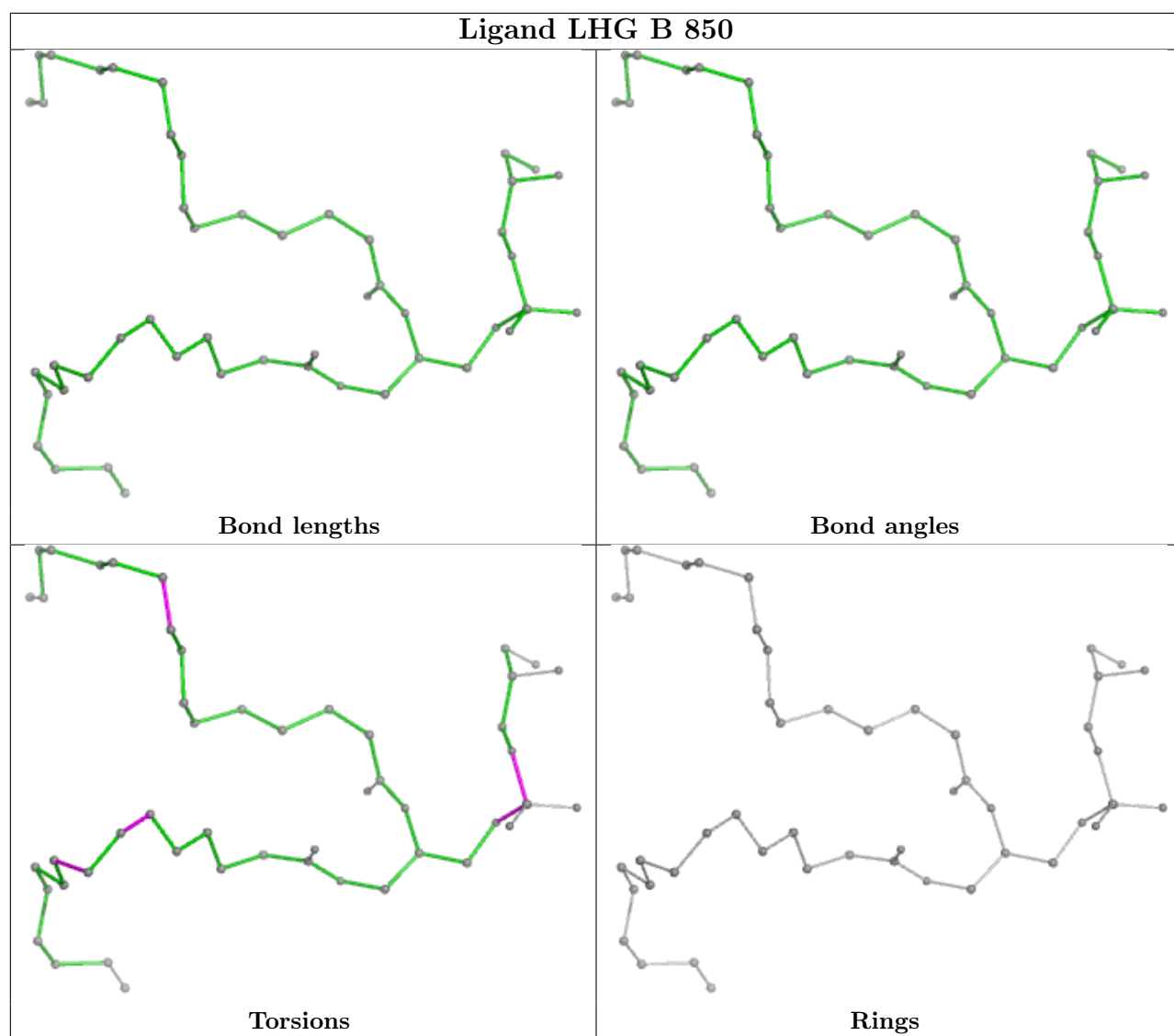
Torsions

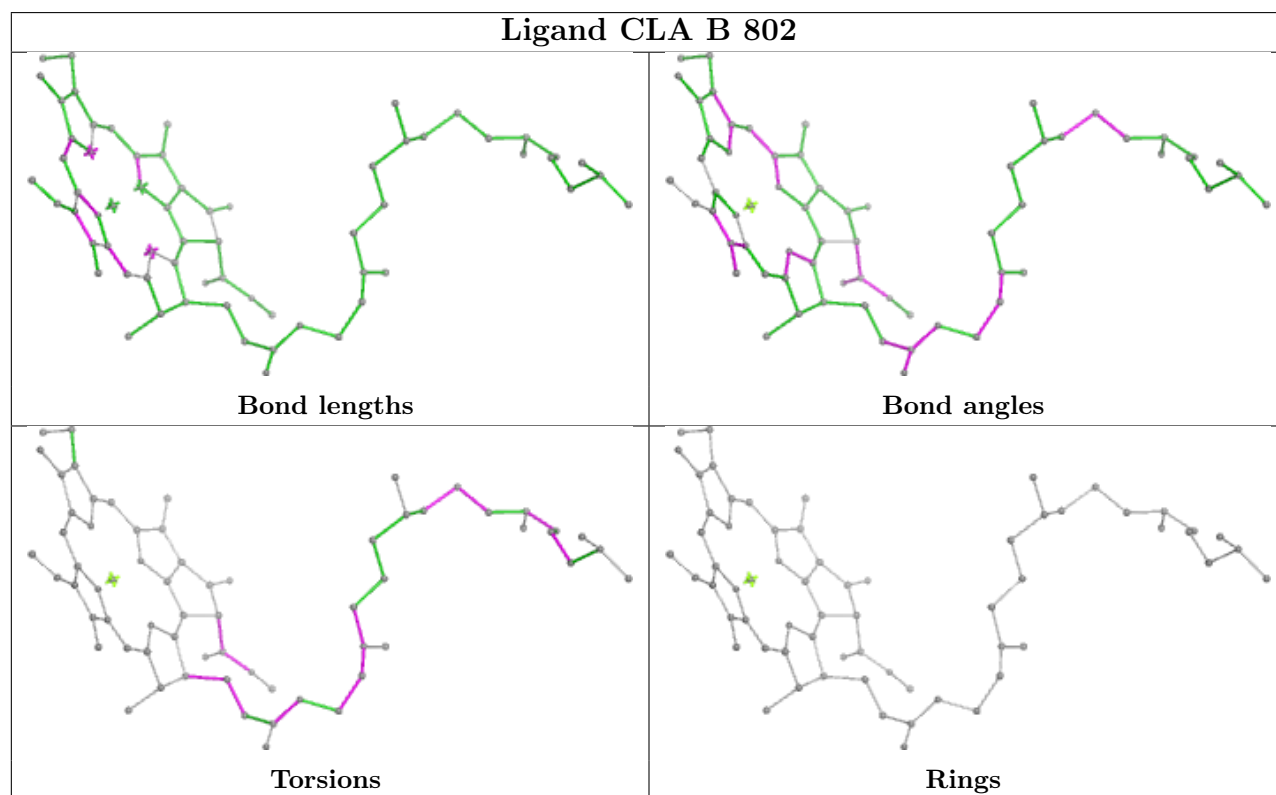
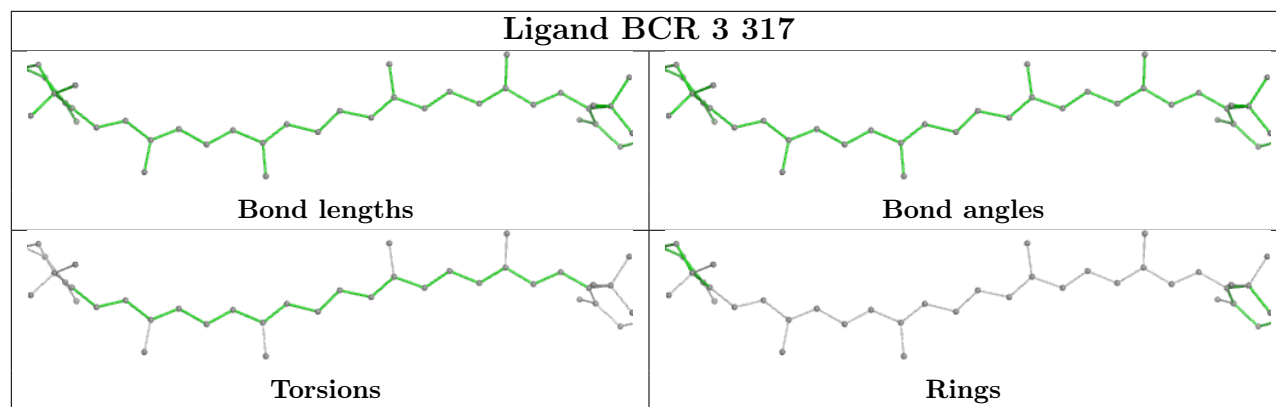


Rings

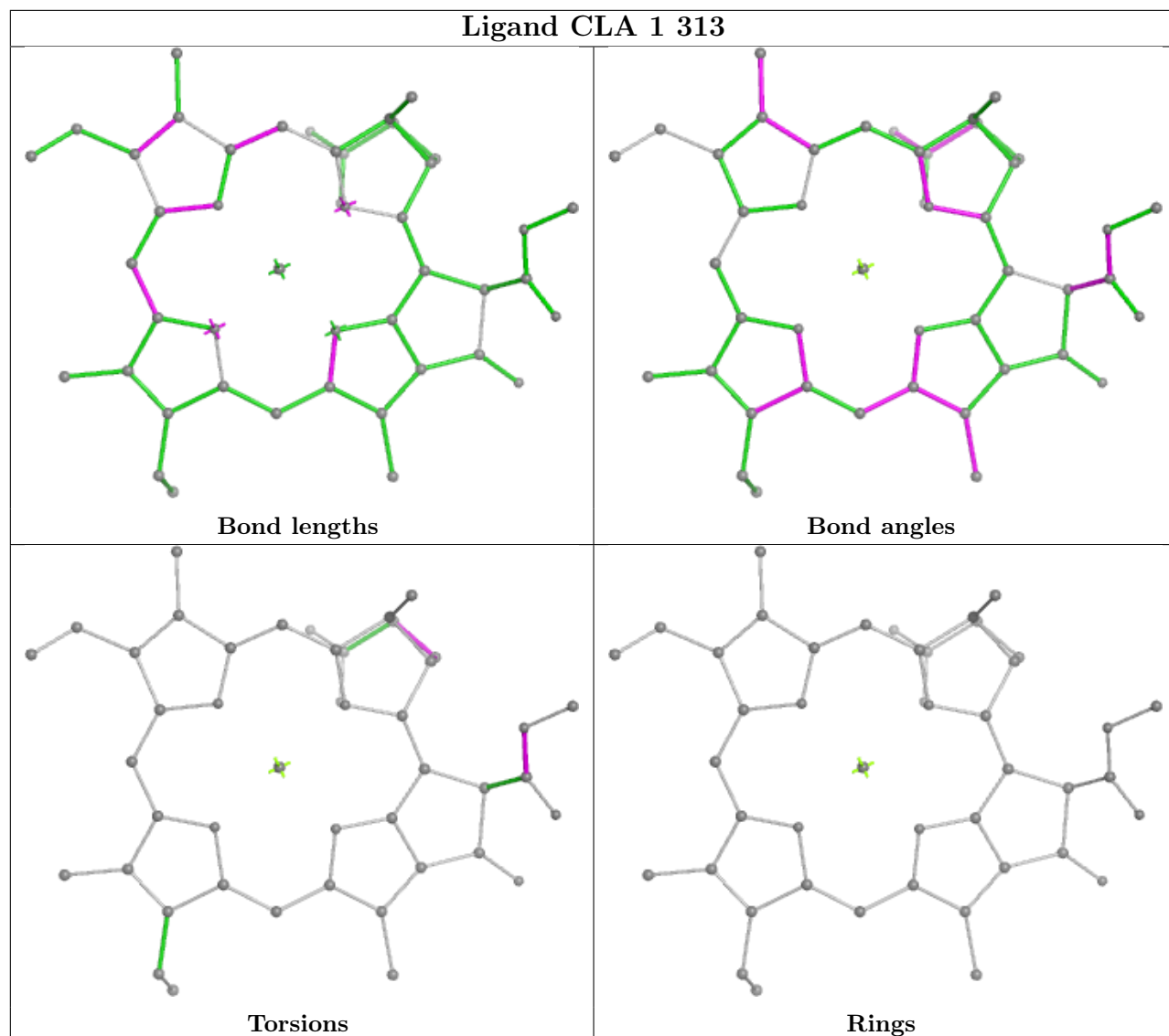




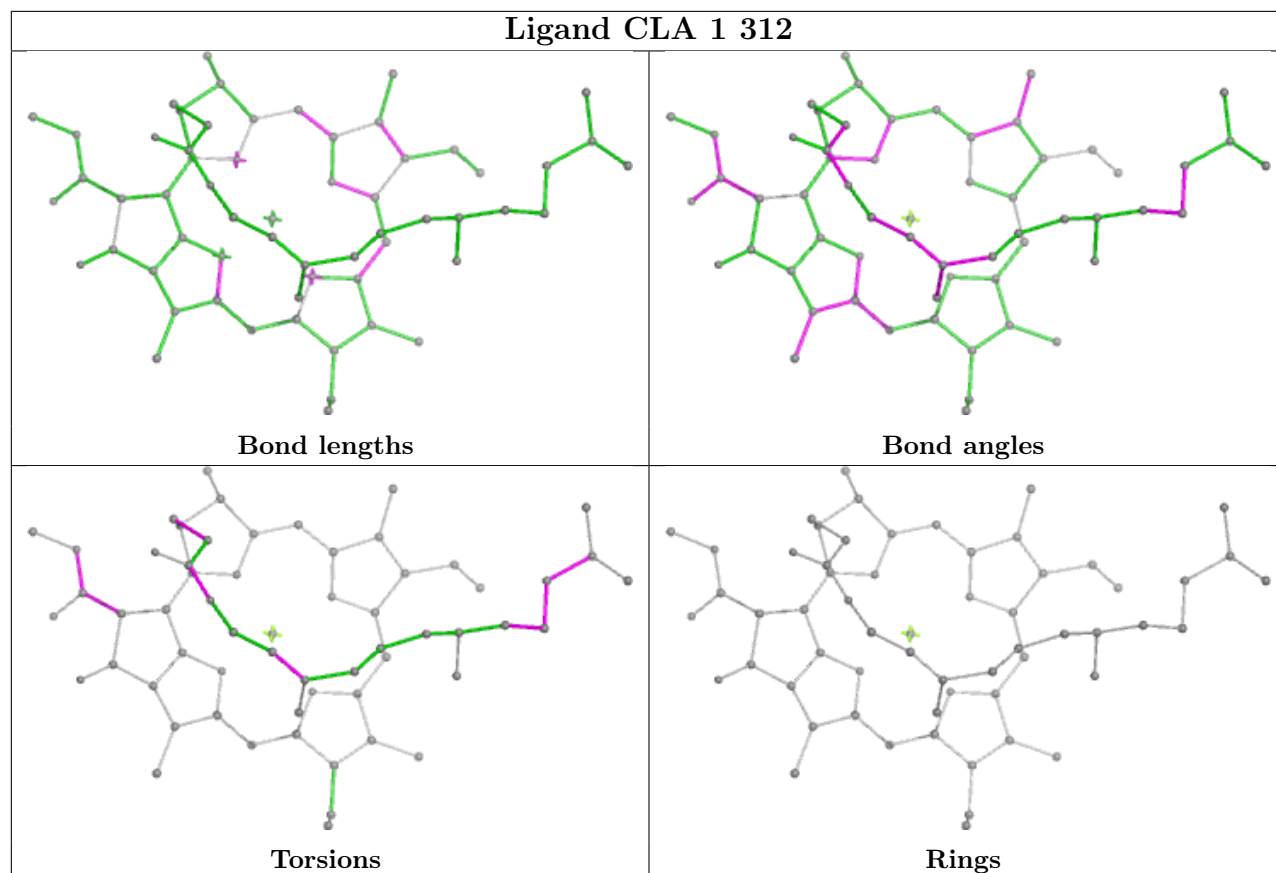




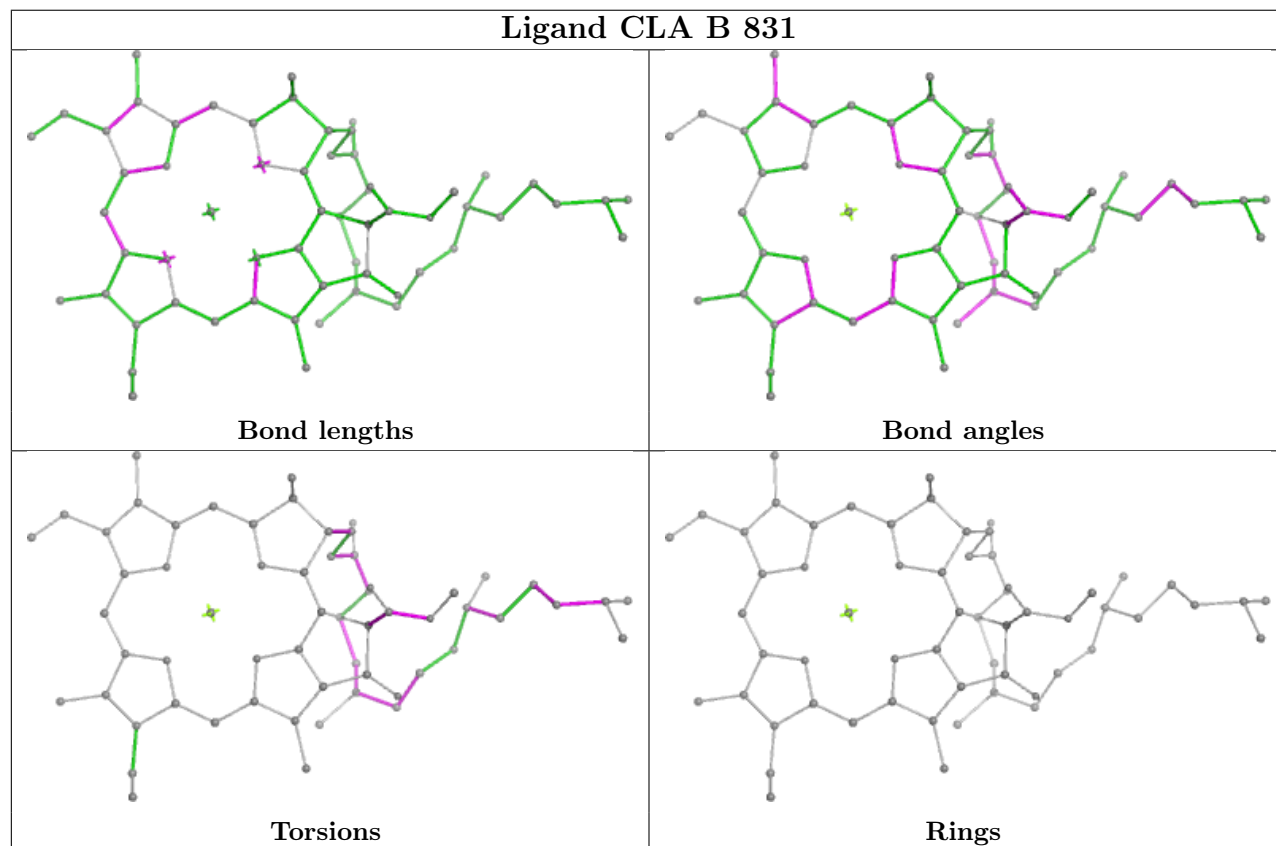
Ligand CLA 1 313



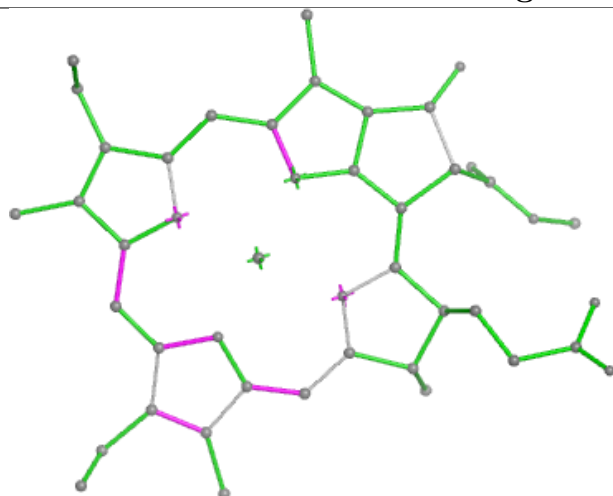
Ligand CLA 1 312



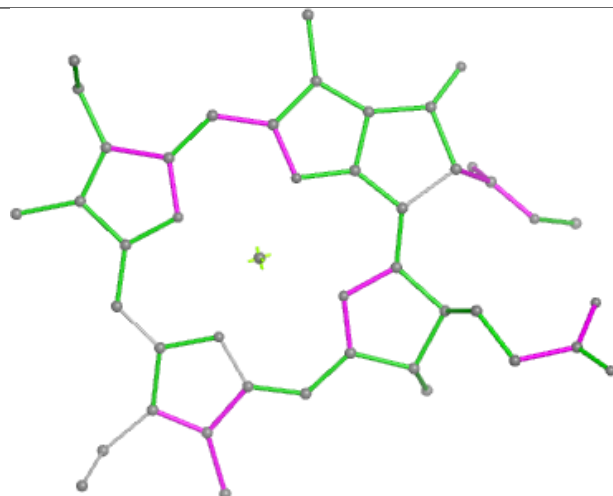
Ligand CLA B 831



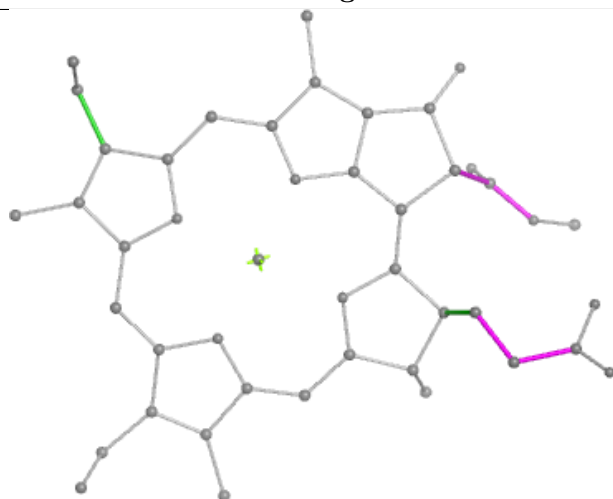
Ligand CLA F 302



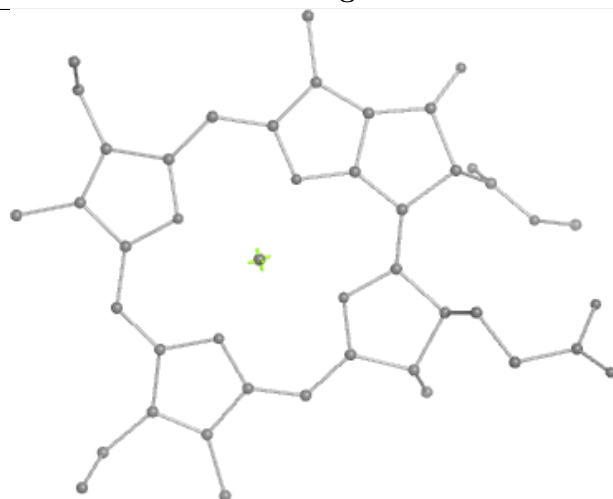
Bond lengths



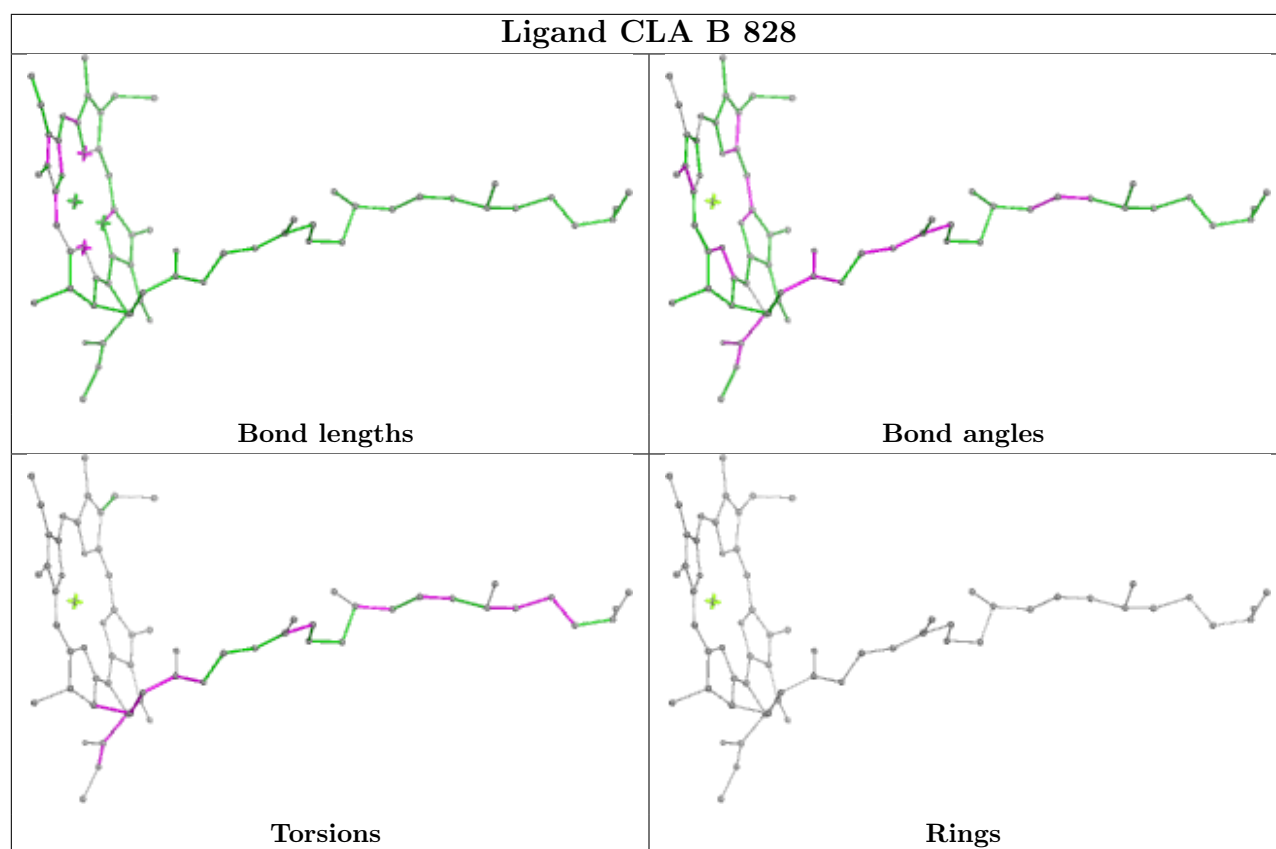
Bond angles



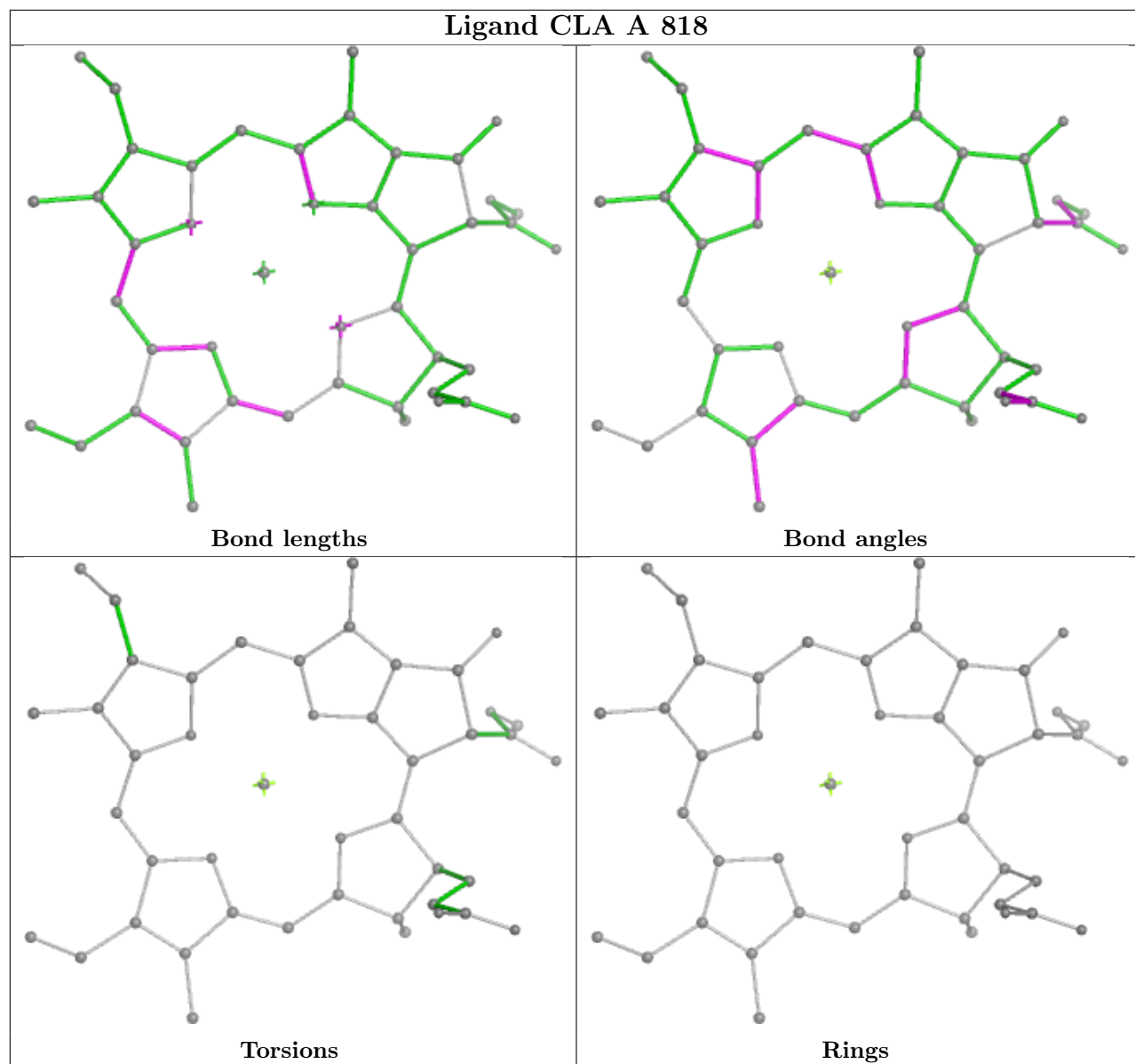
Torsions

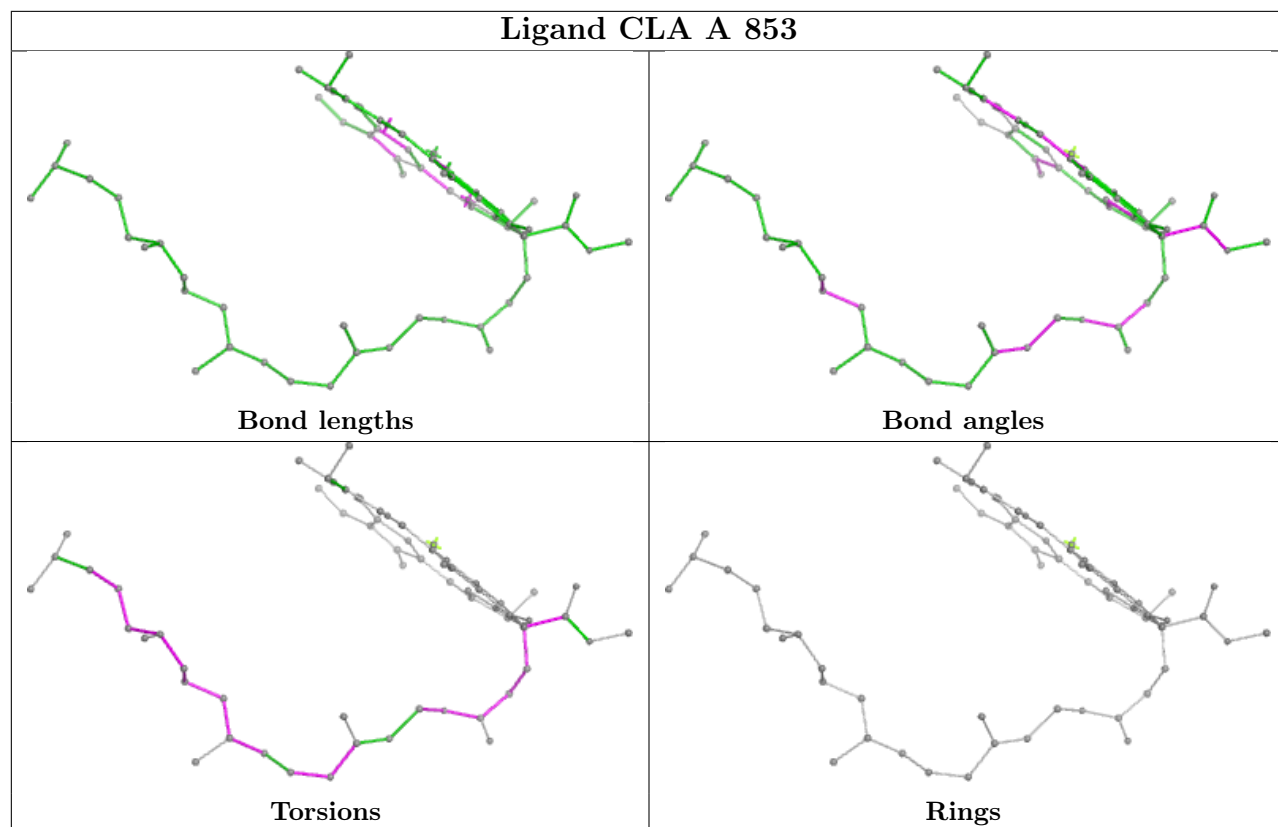


Rings

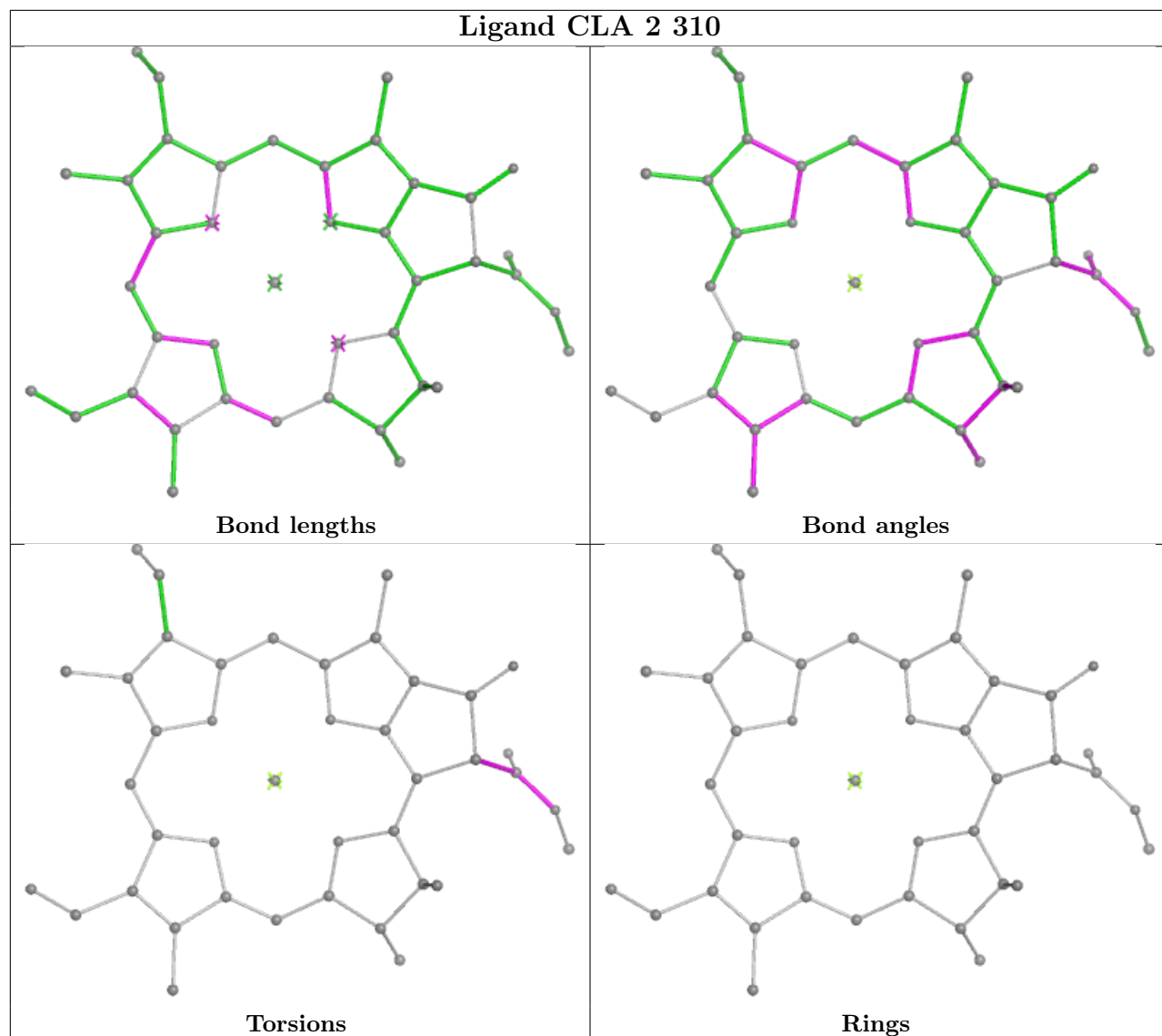


Ligand CLA A 818

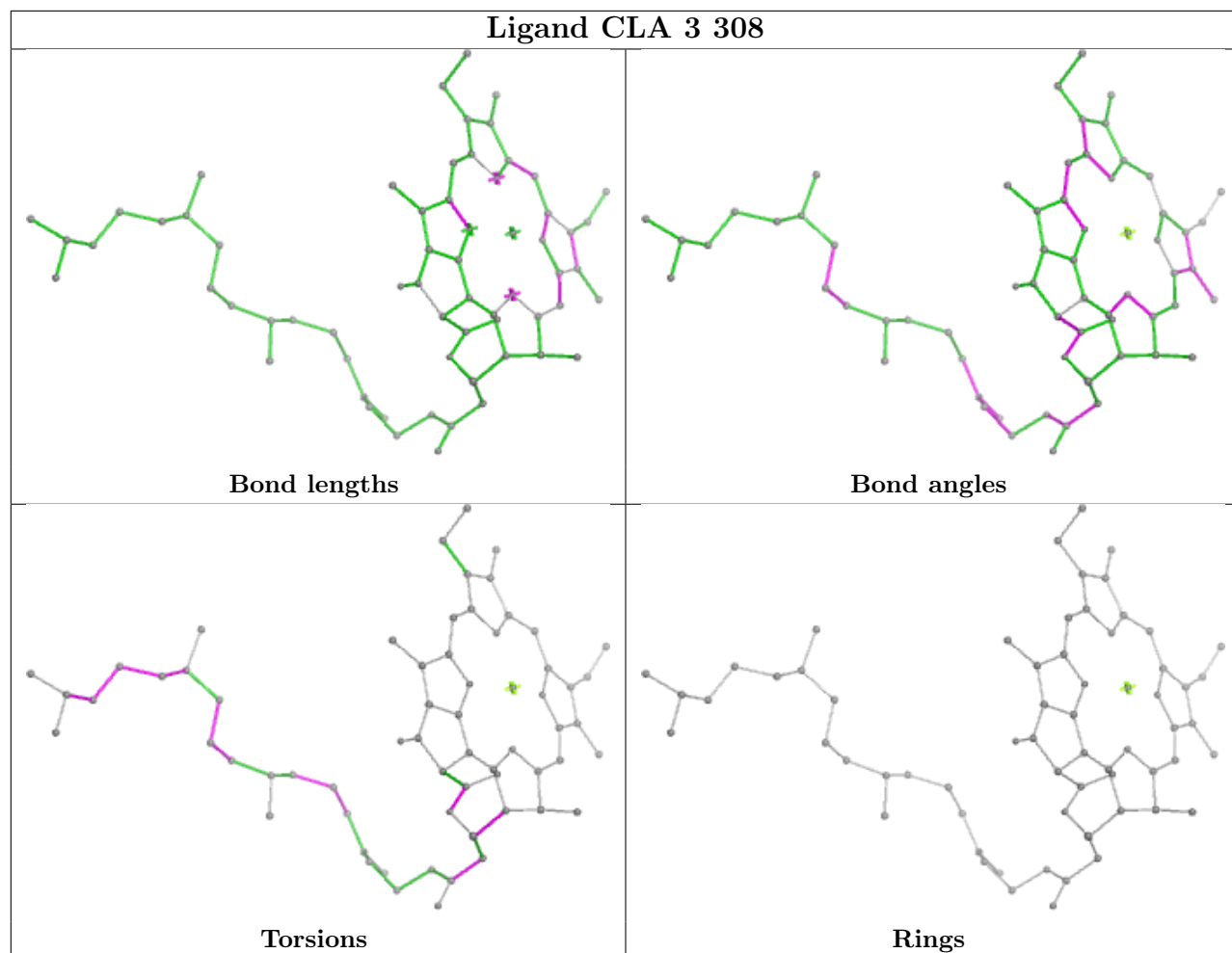




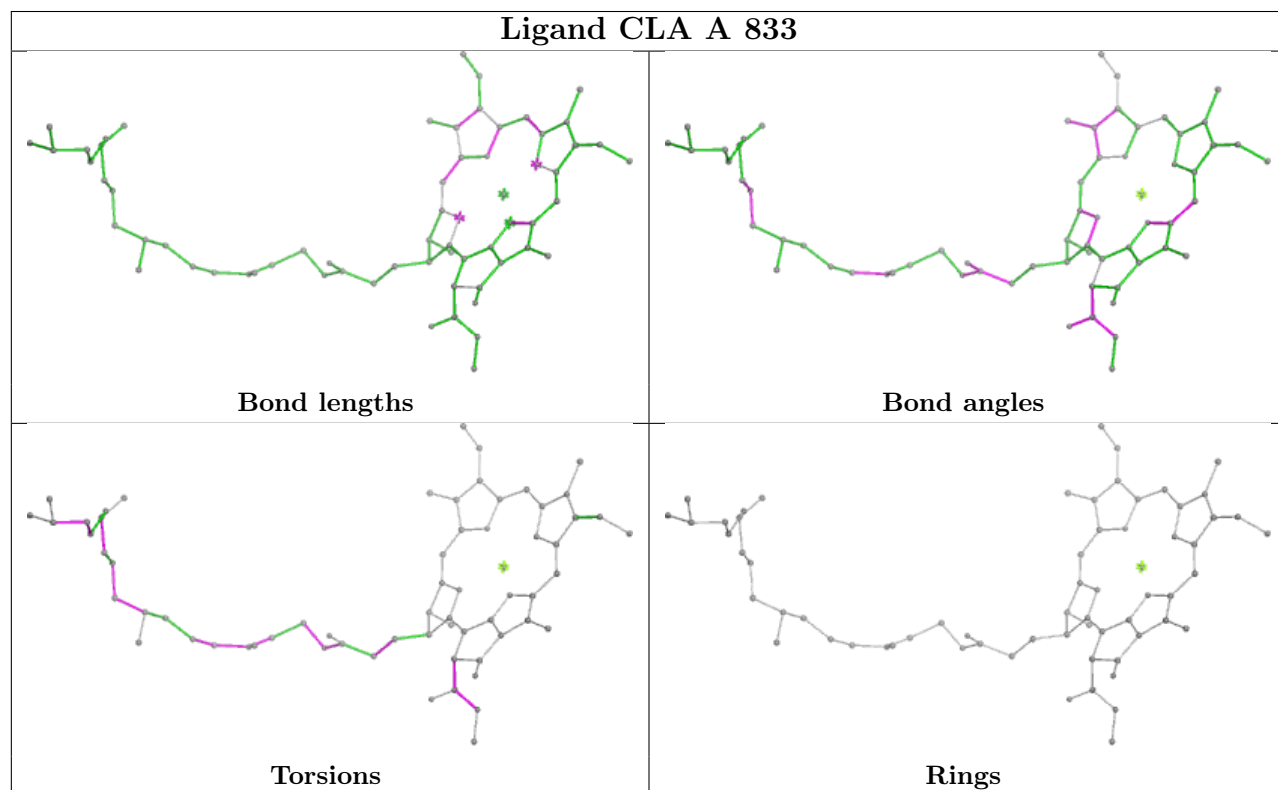
Ligand CLA 2 310

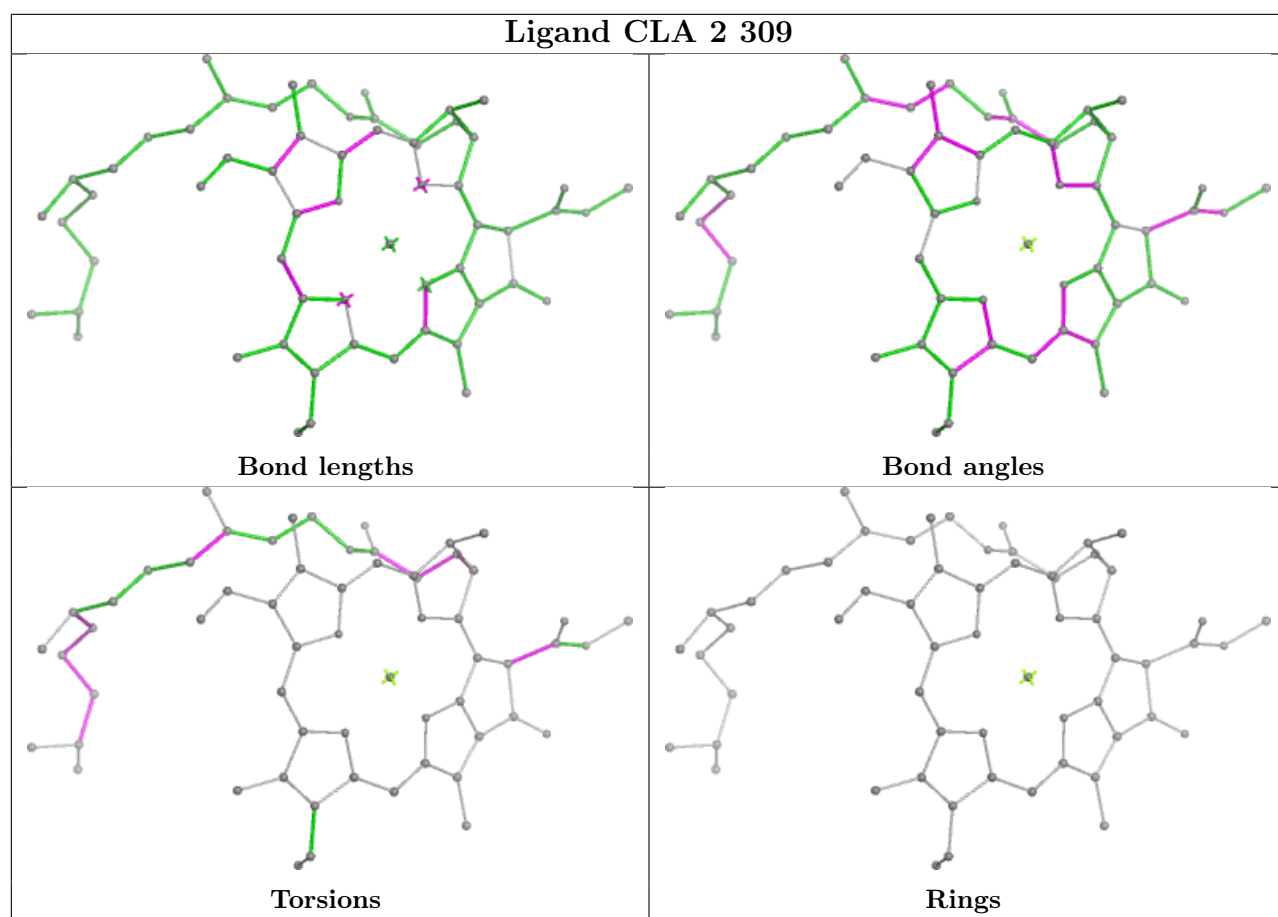


Ligand CLA 3 308

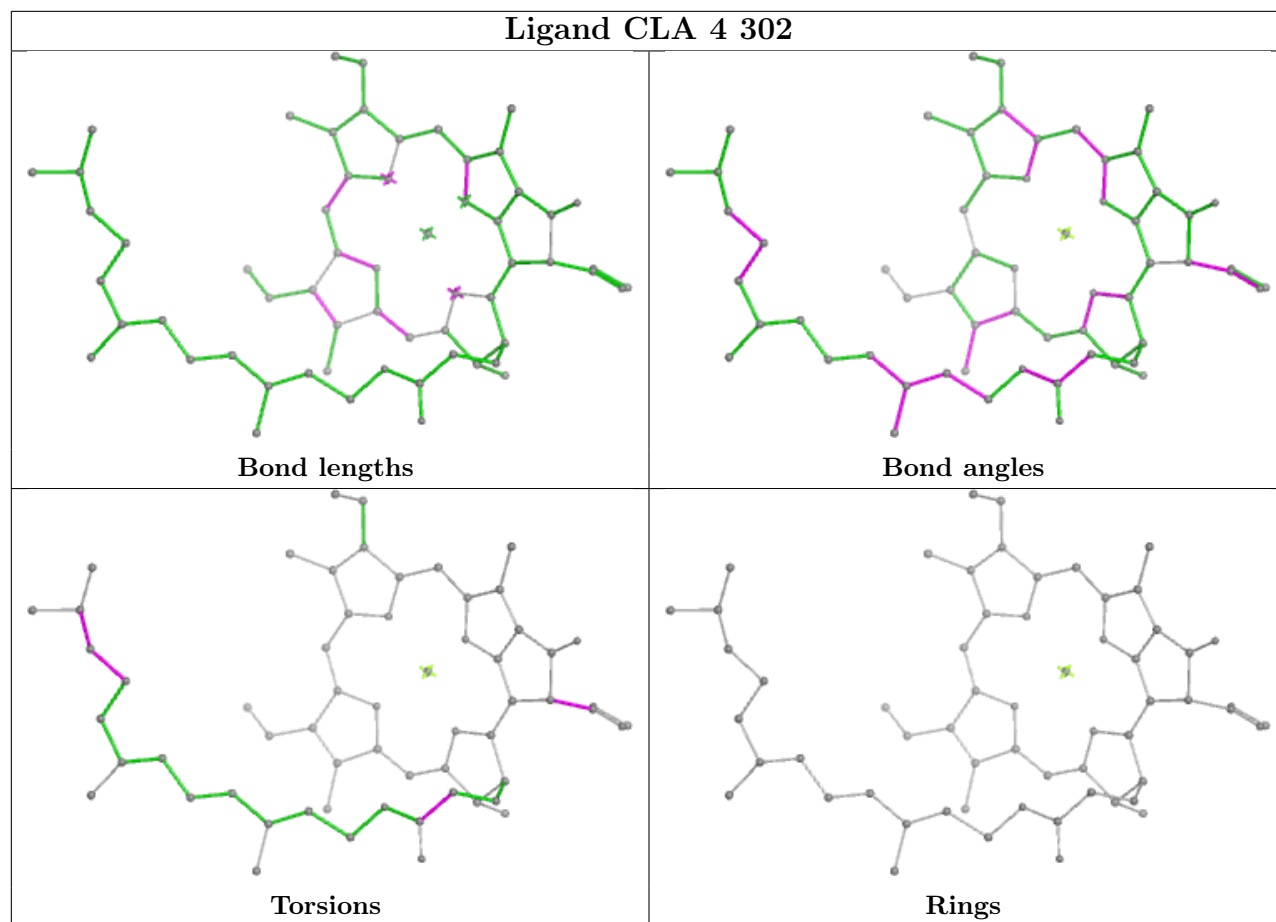


Ligand CLA A 833

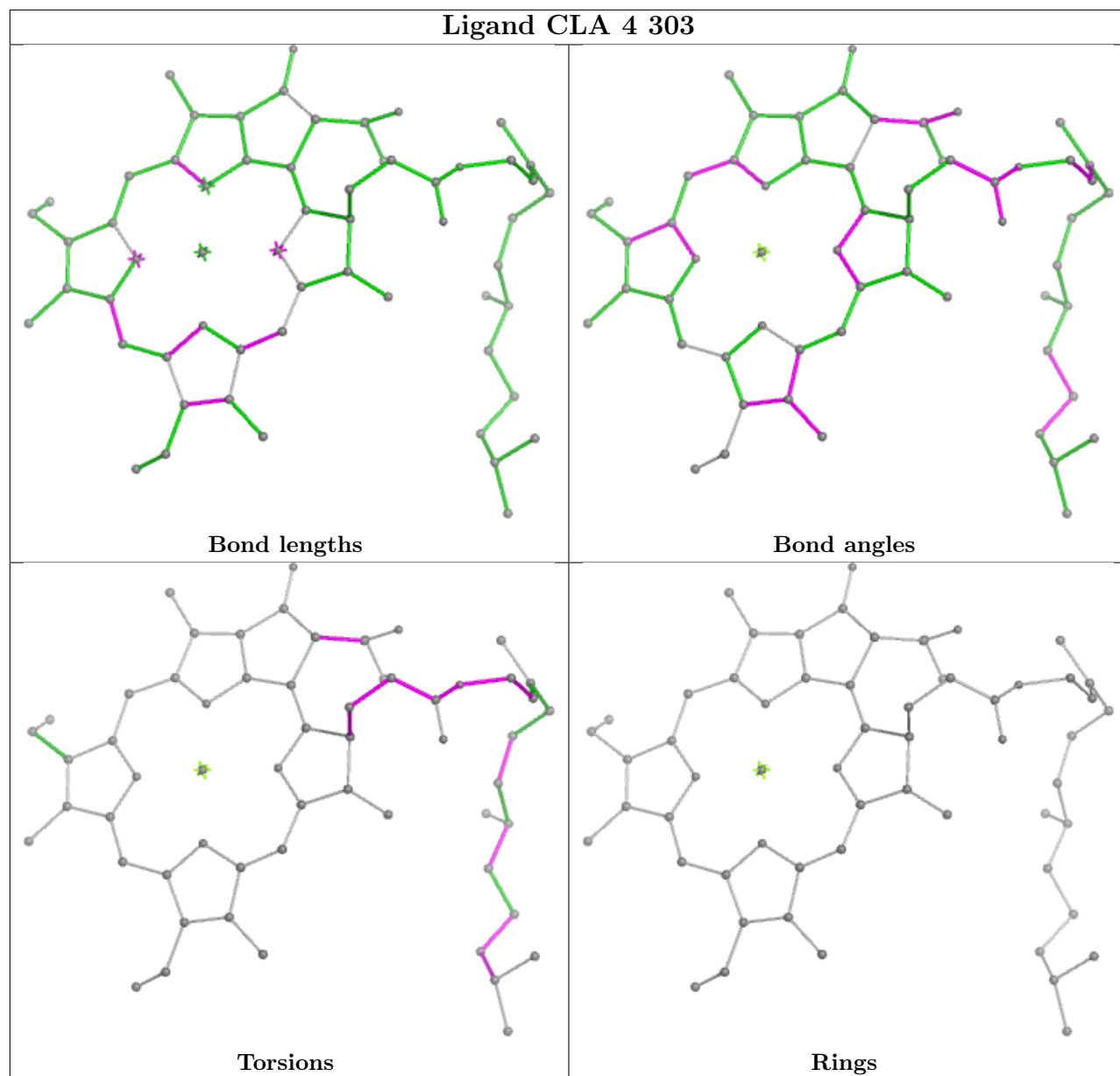


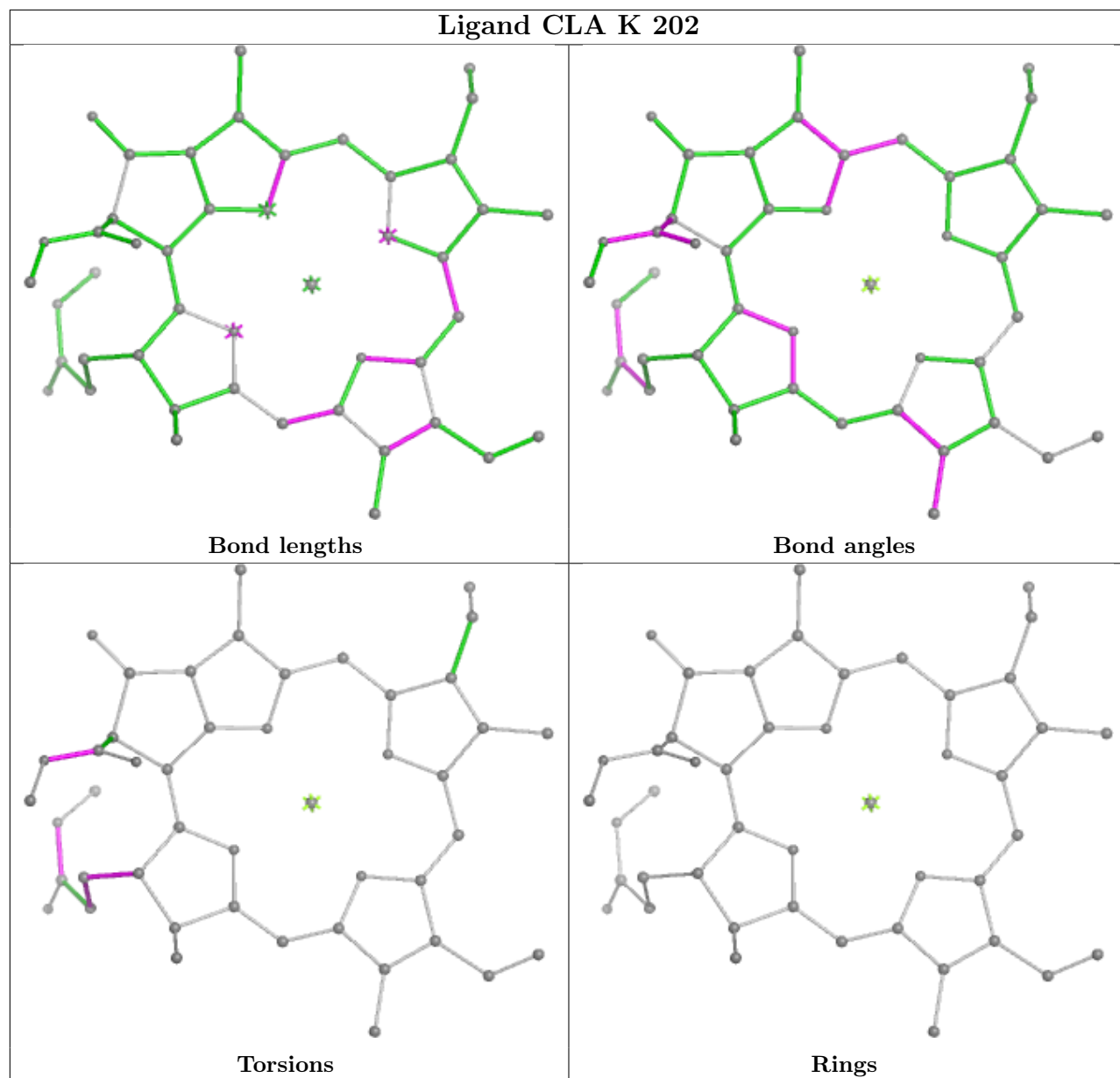


Ligand CLA 4 302

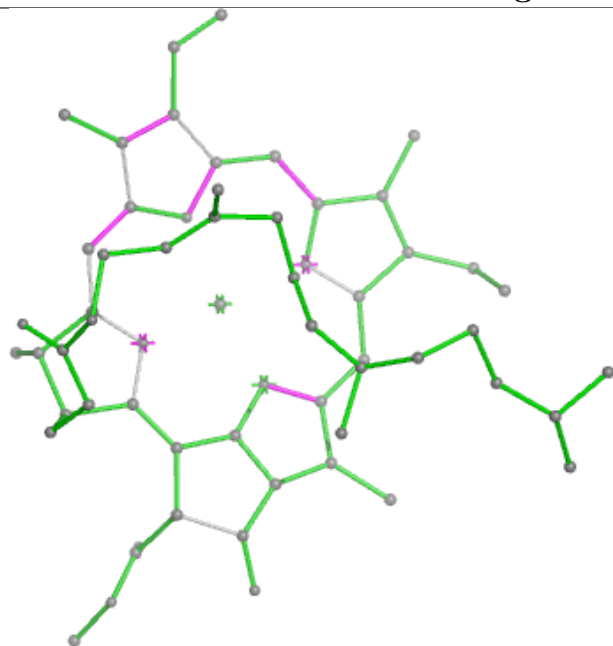


Ligand CLA 4 303

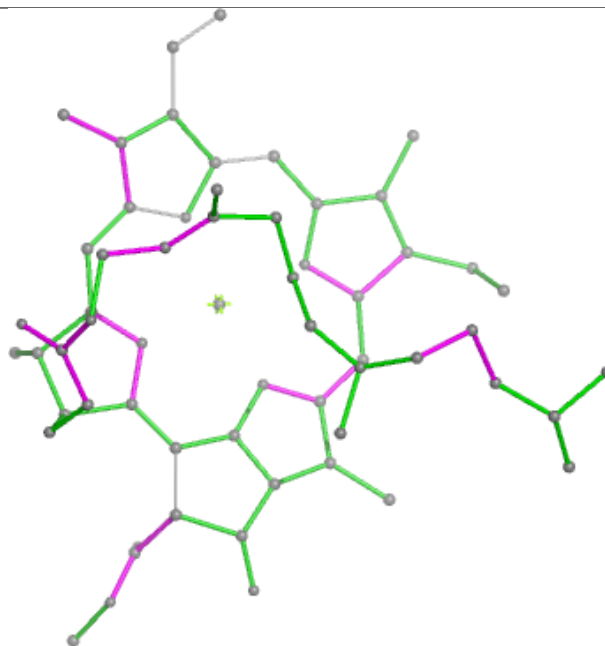




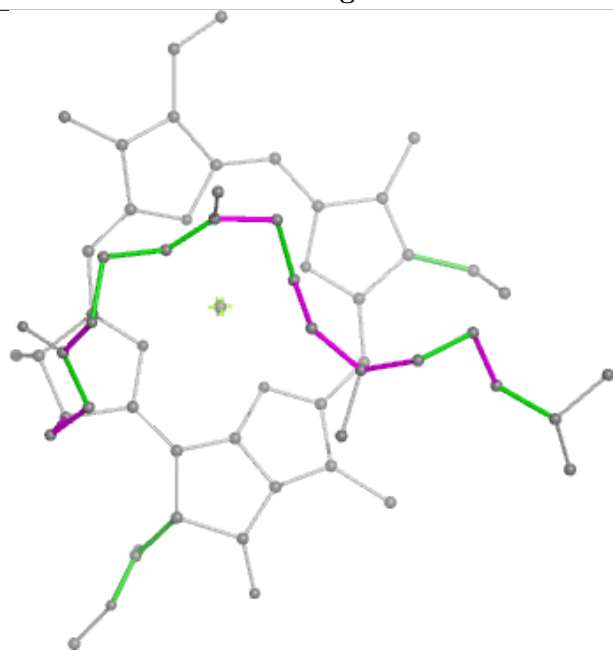
Ligand CLA B 827



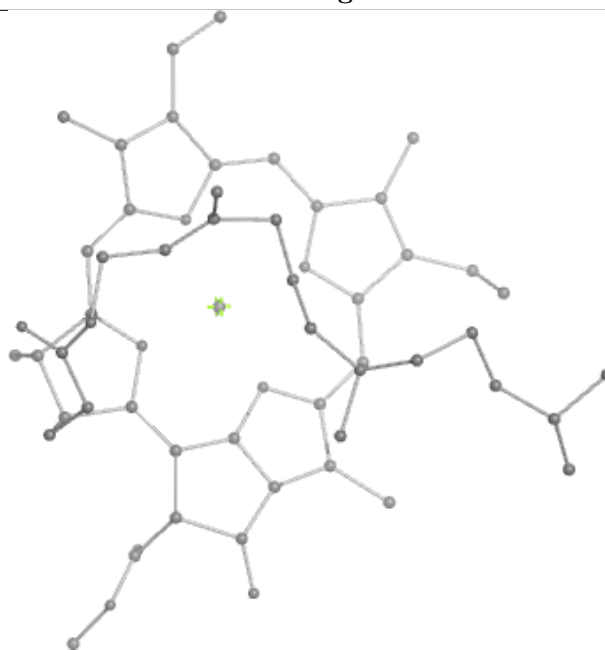
Bond lengths



Bond angles

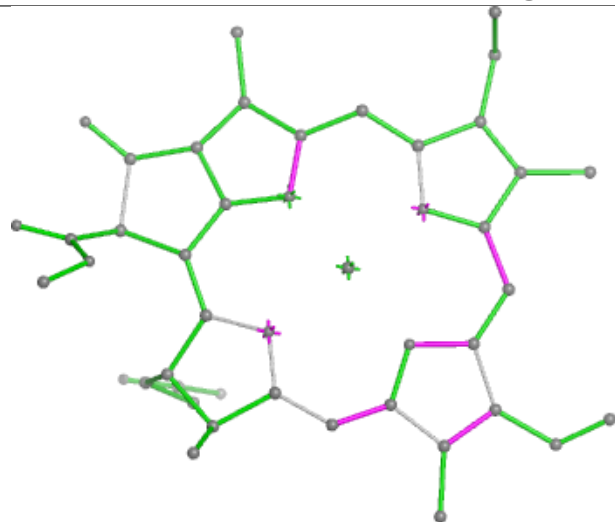


Torsions

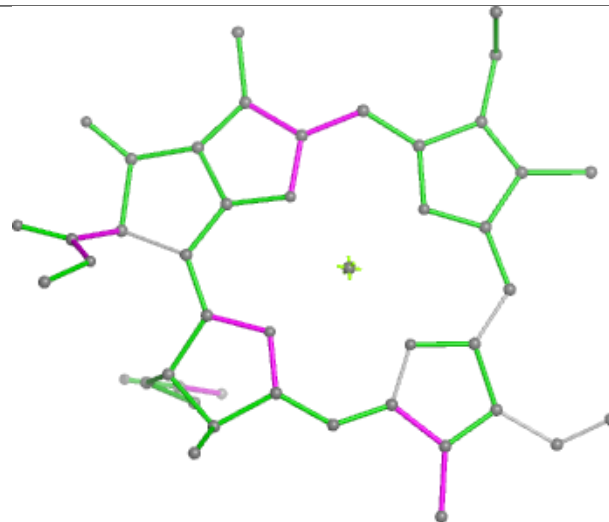


Rings

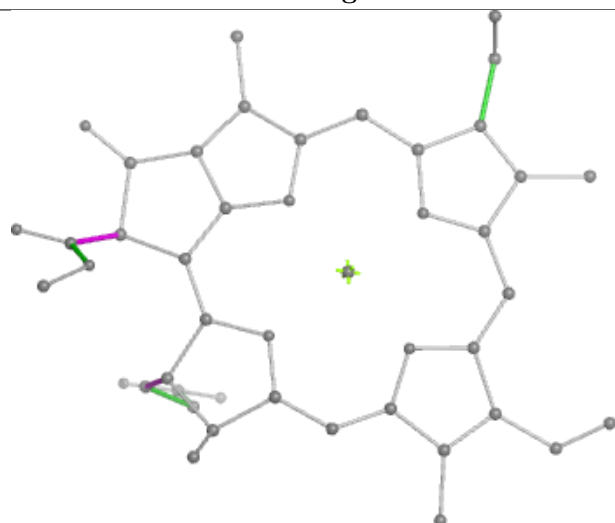
Ligand CLA 4 304



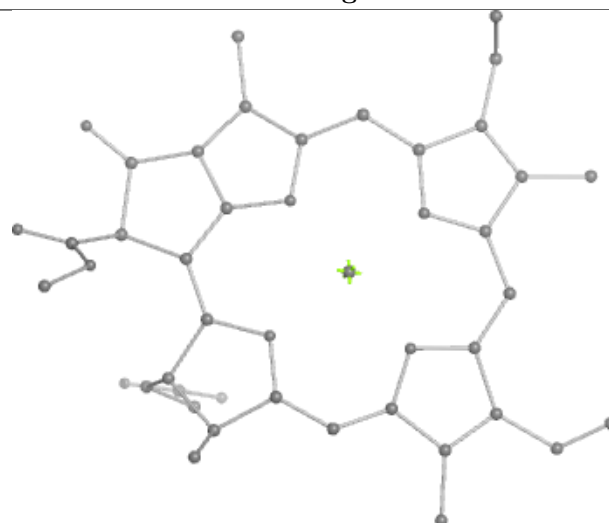
Bond lengths



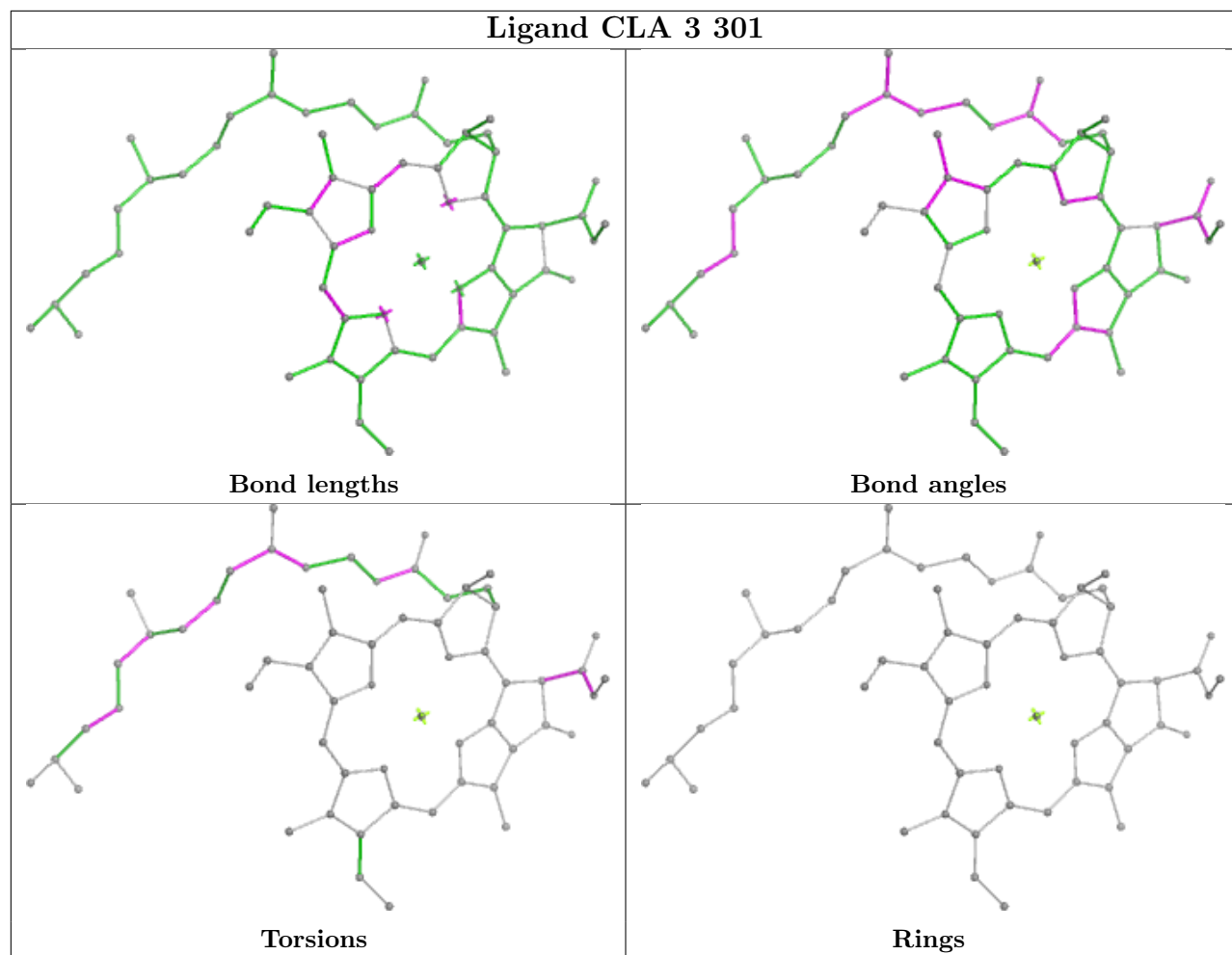
Bond angles

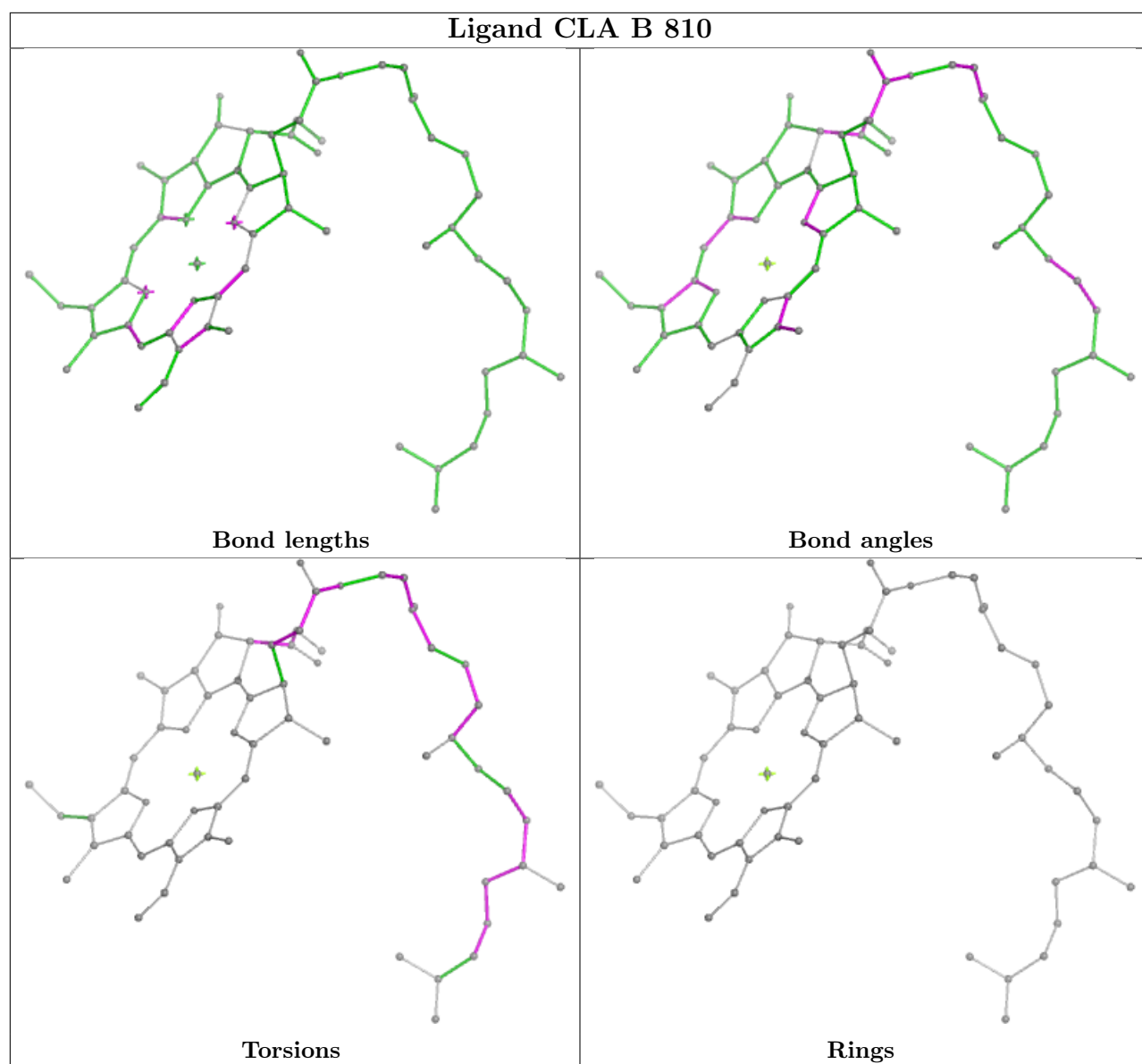


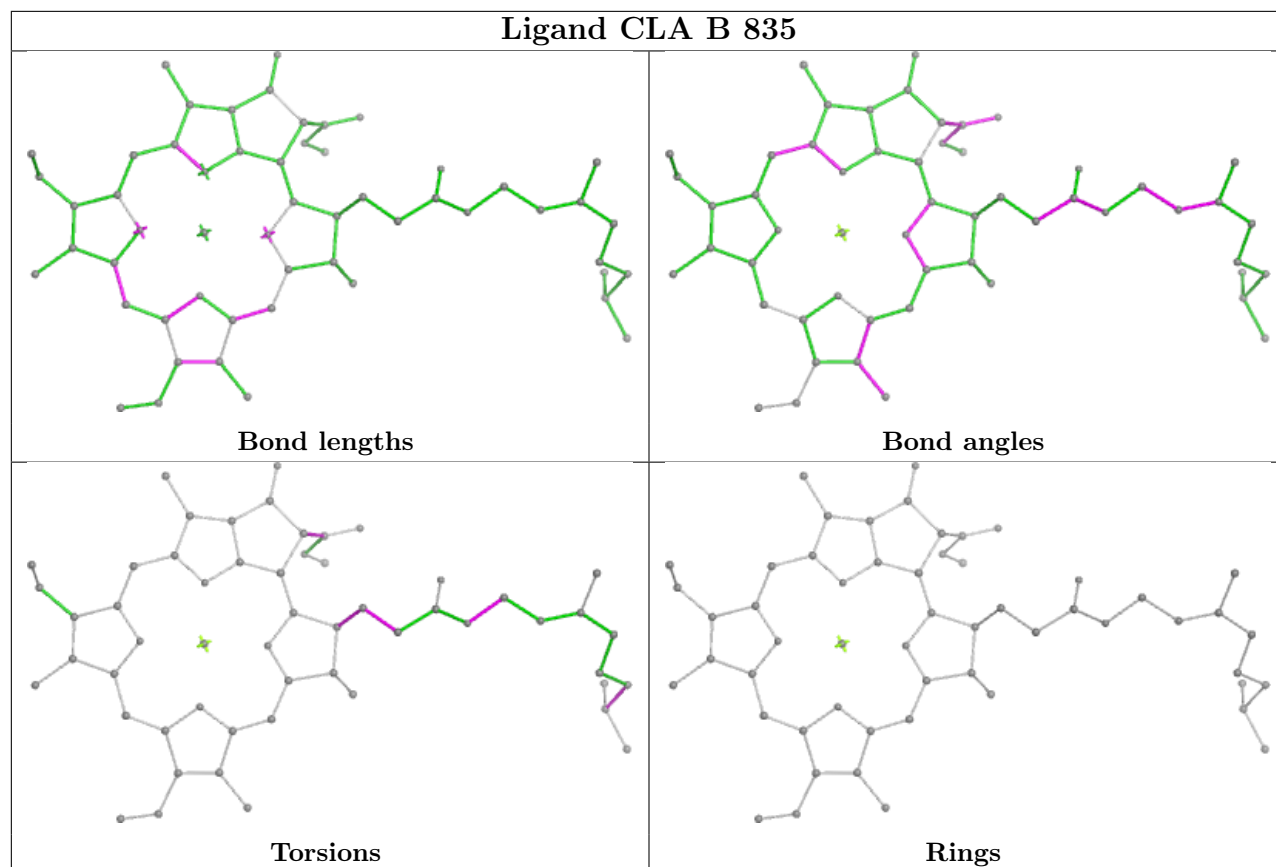
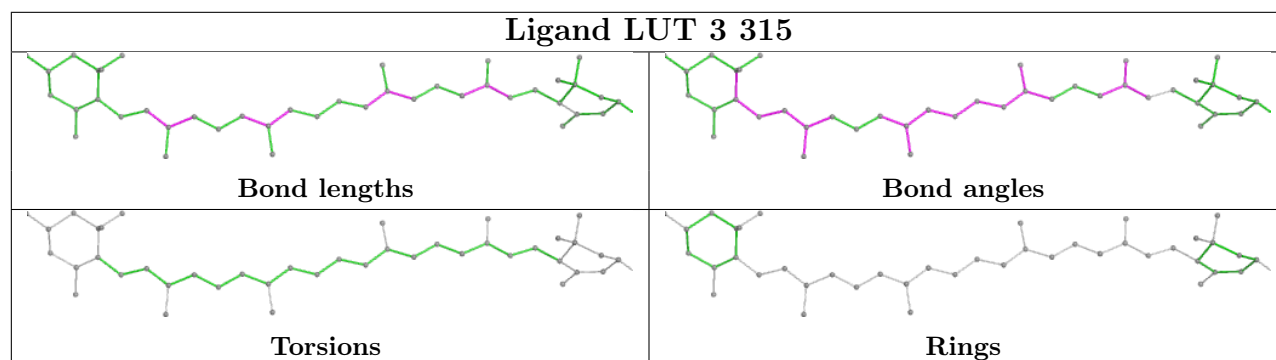
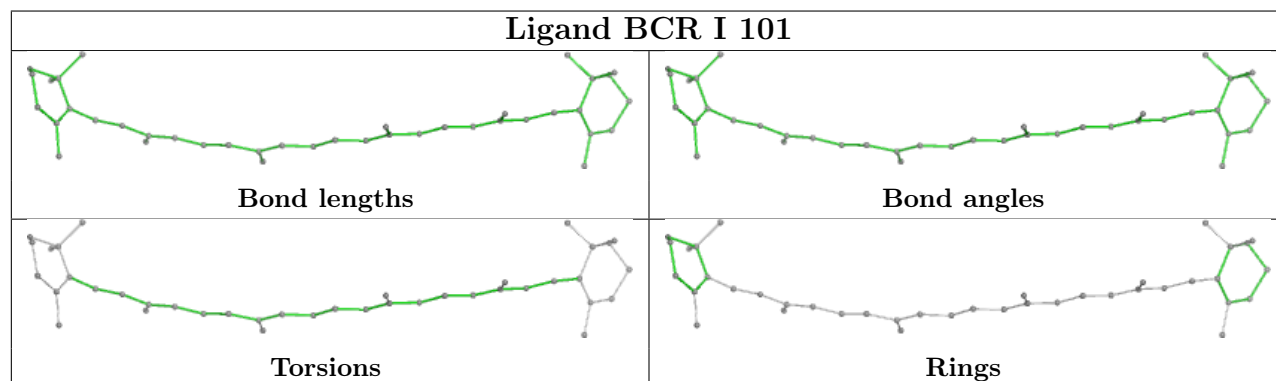
Torsions

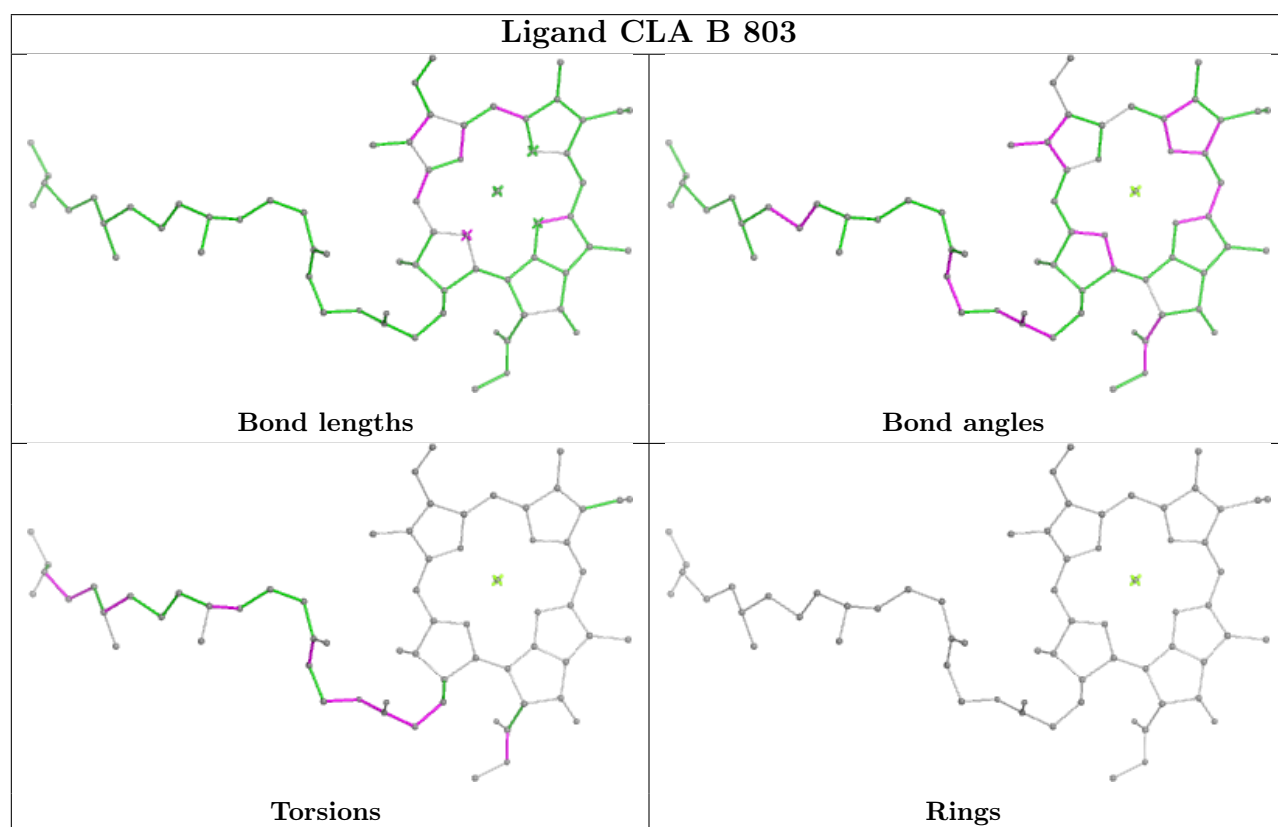
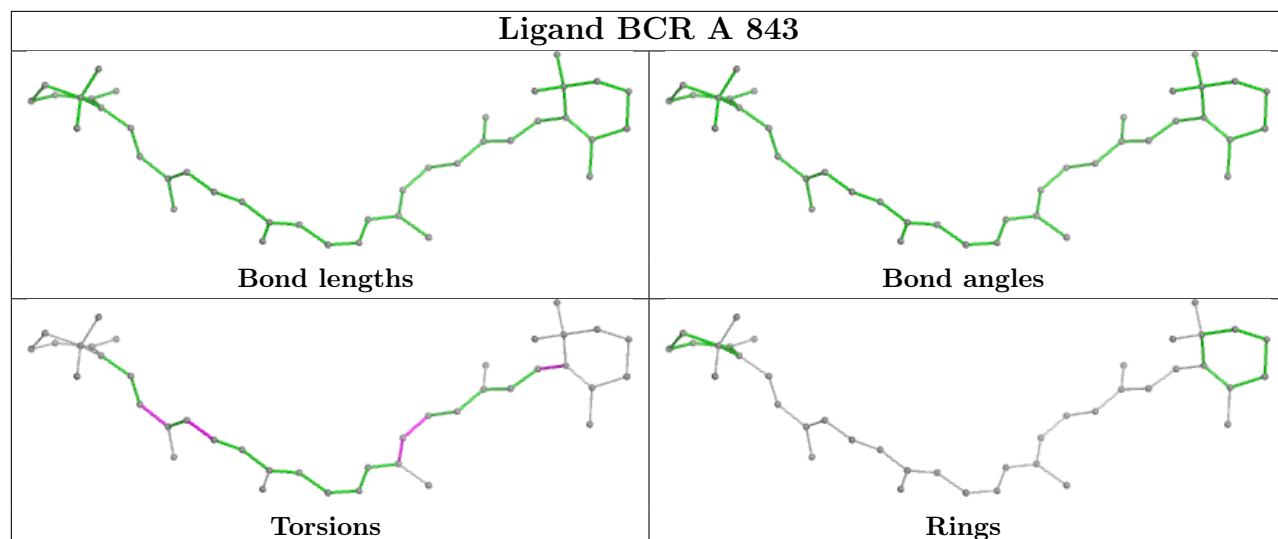


Rings

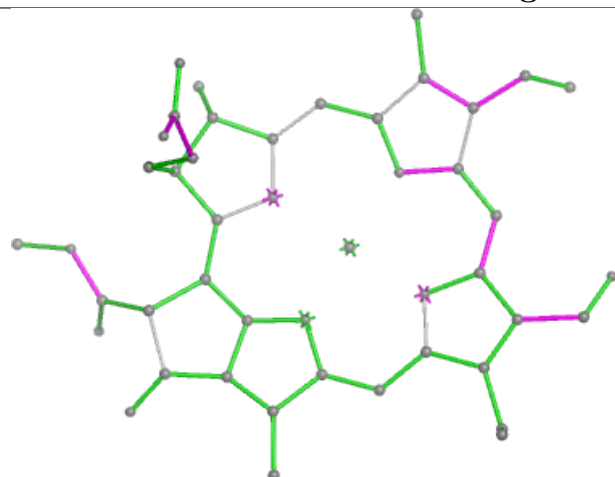




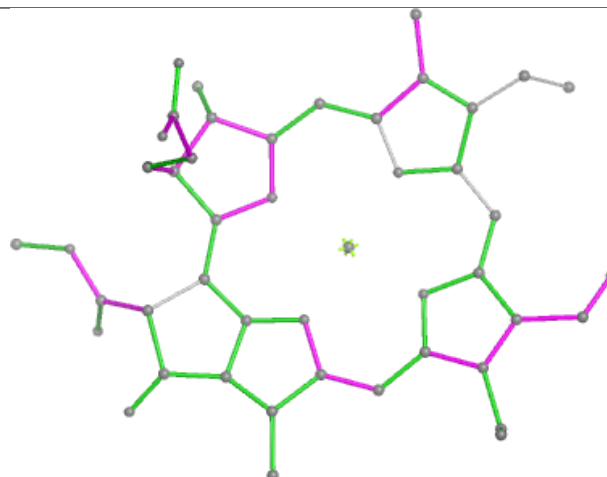
Ligand CLA B 835**Ligand LUT 3 315****Ligand BCR I 101**



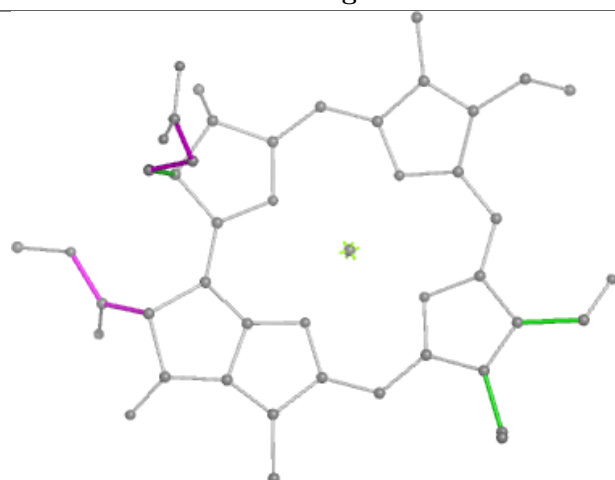
Ligand CHL 2 307



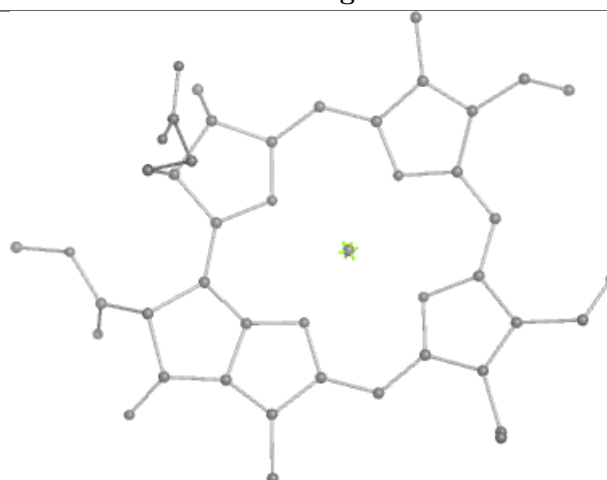
Bond lengths



Bond angles

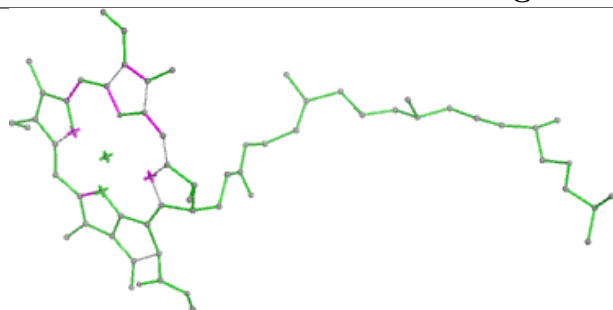


Torsions

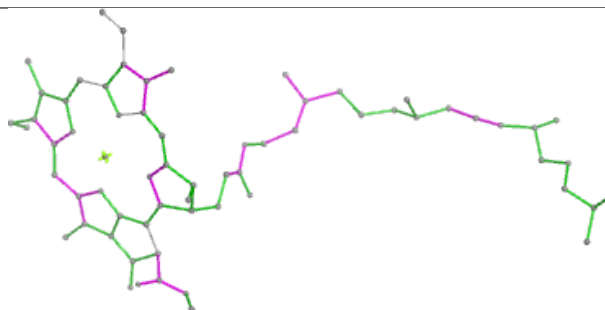


Rings

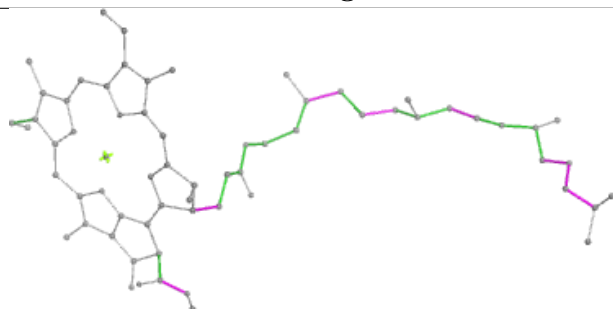
Ligand CLA A 819



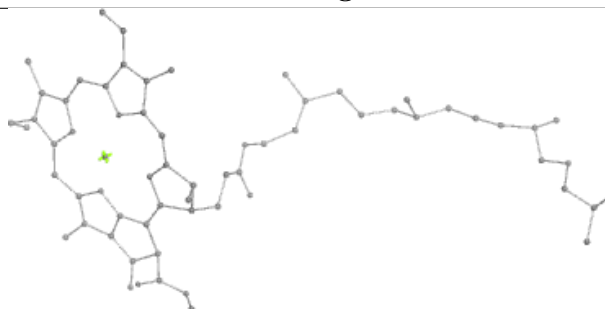
Bond lengths



Bond angles

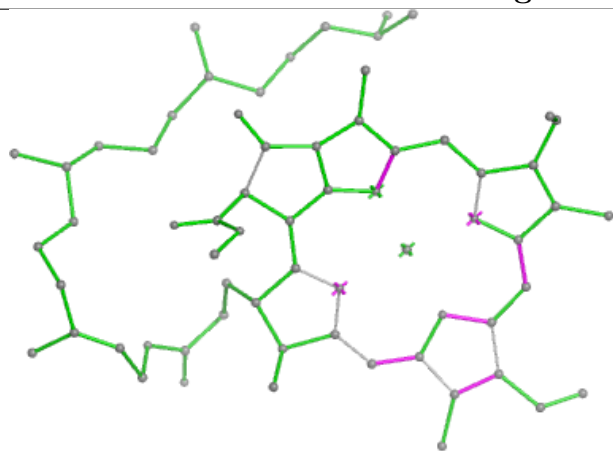


Torsions

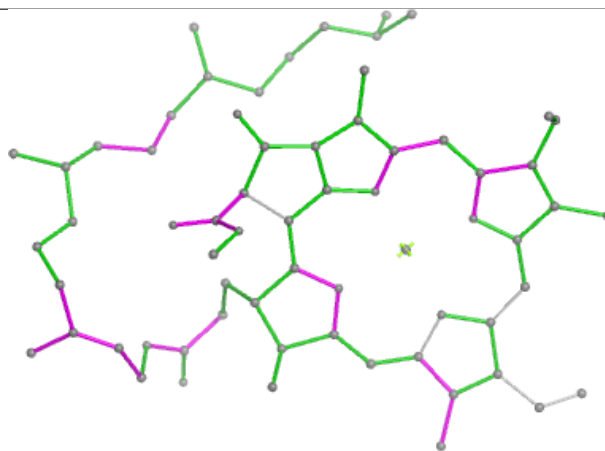


Rings

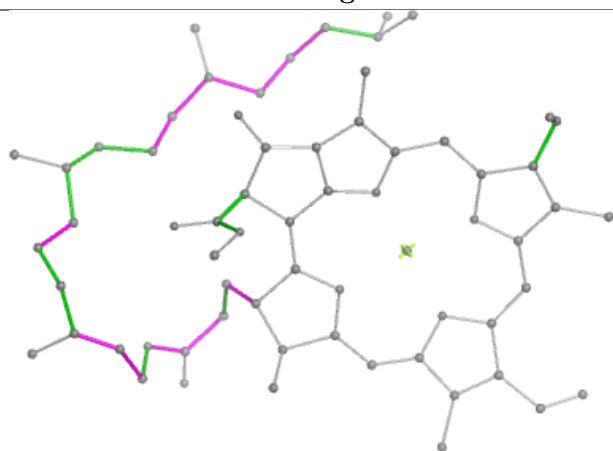
Ligand CLA B 805



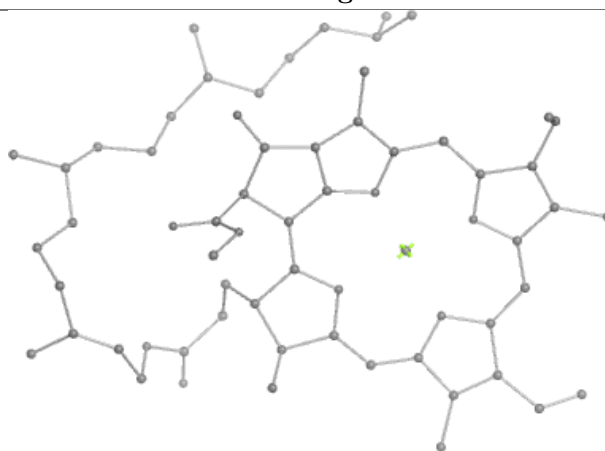
Bond lengths



Bond angles

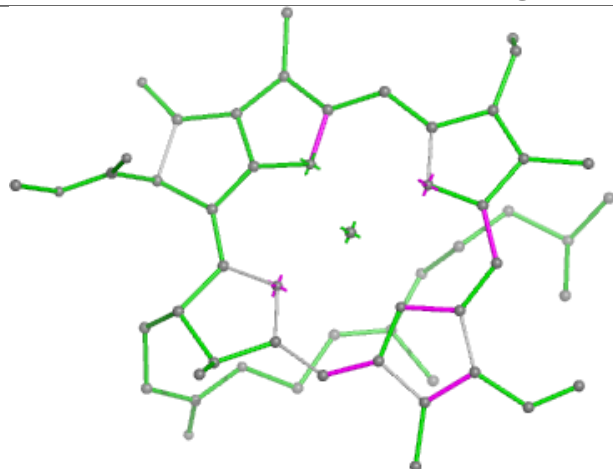


Torsions

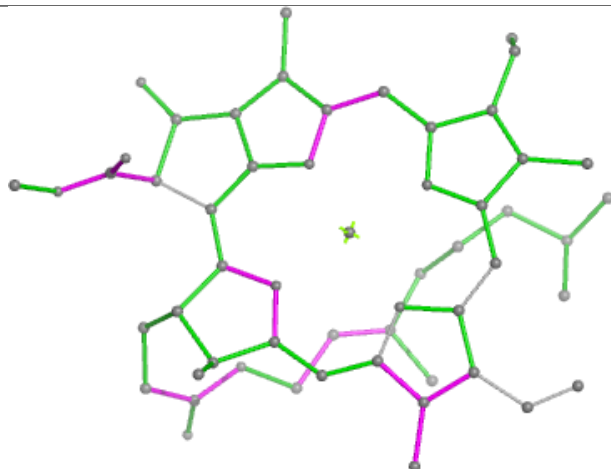


Rings

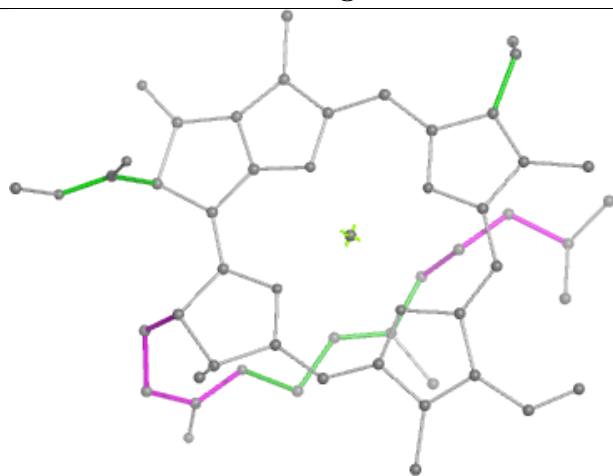
Ligand CLA A 816



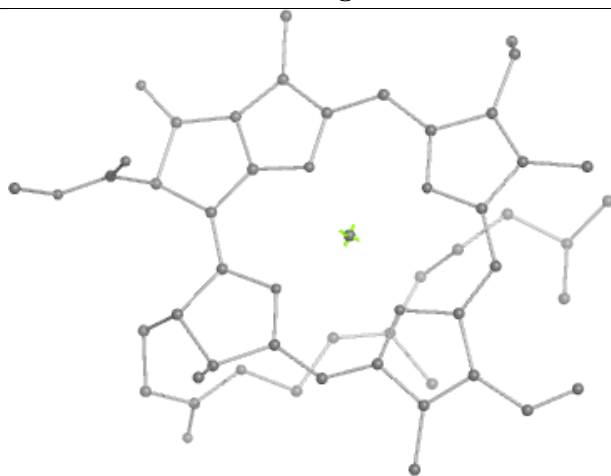
Bond lengths



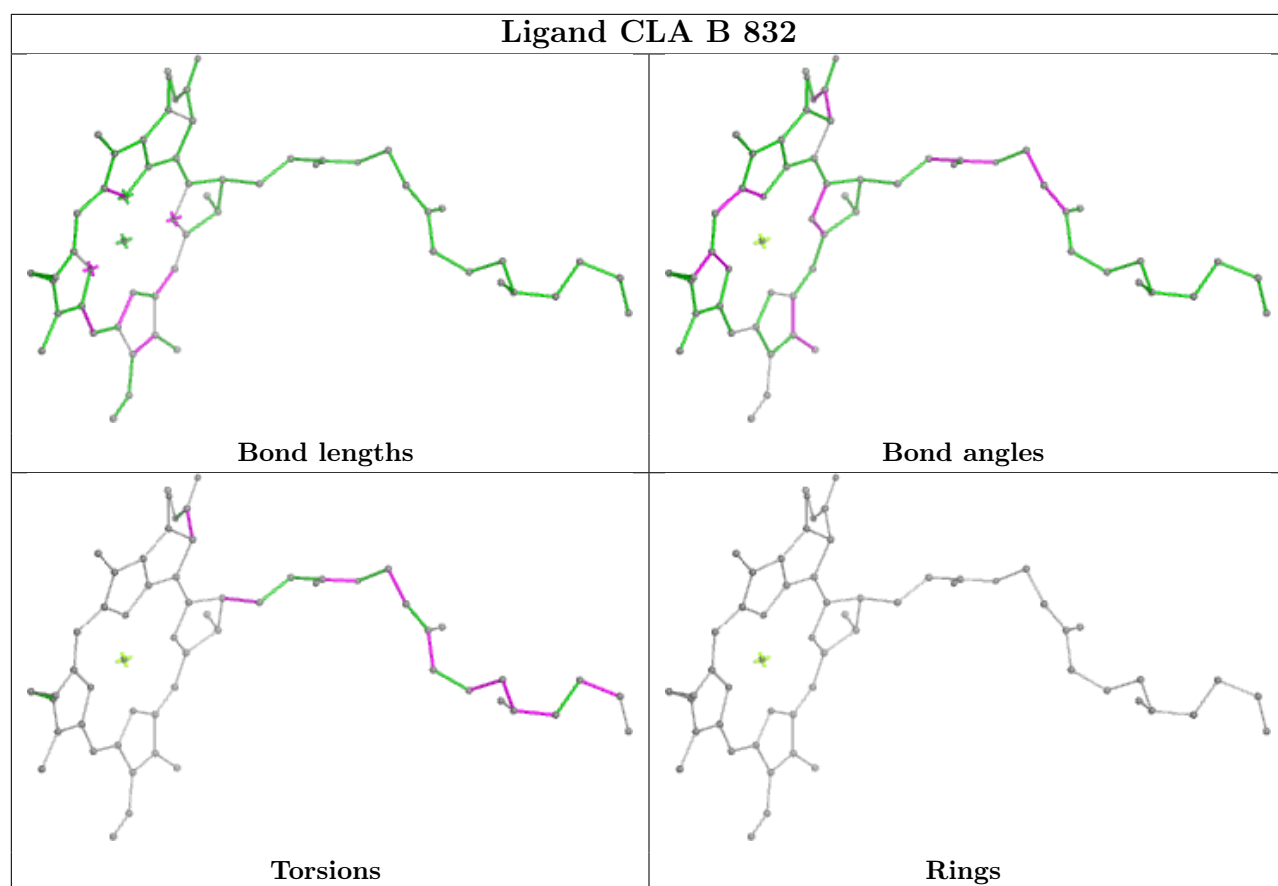
Bond angles



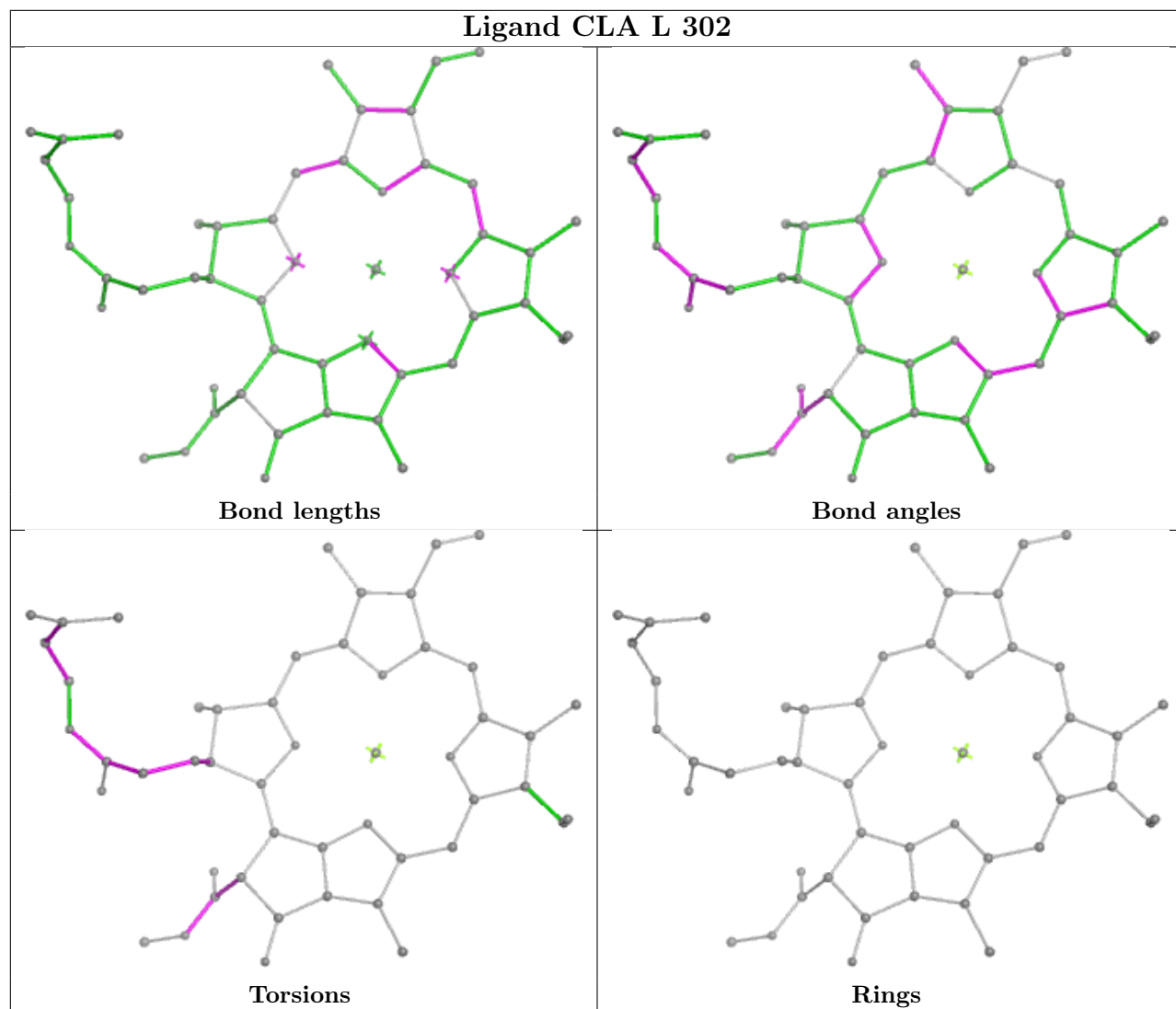
Torsions

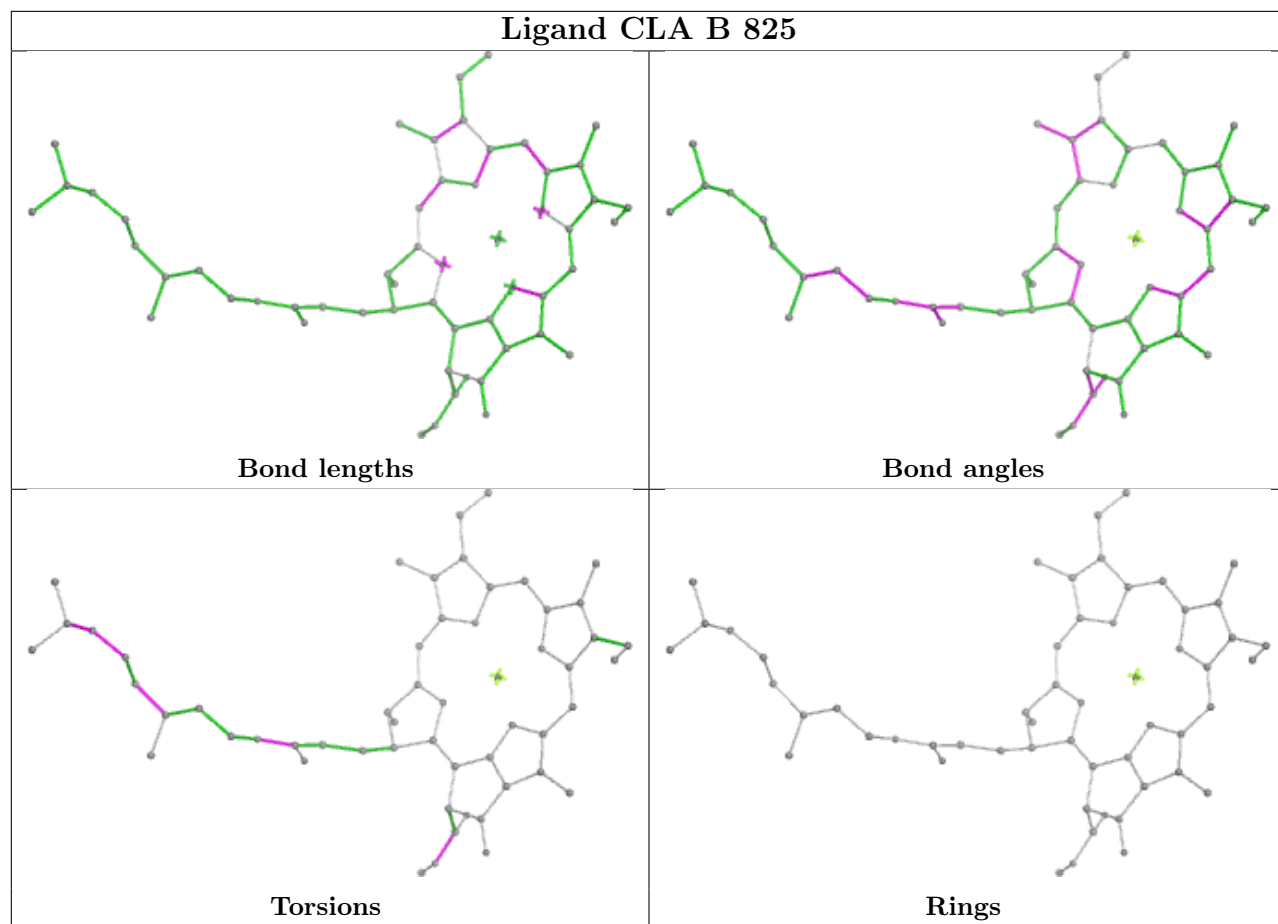


Rings

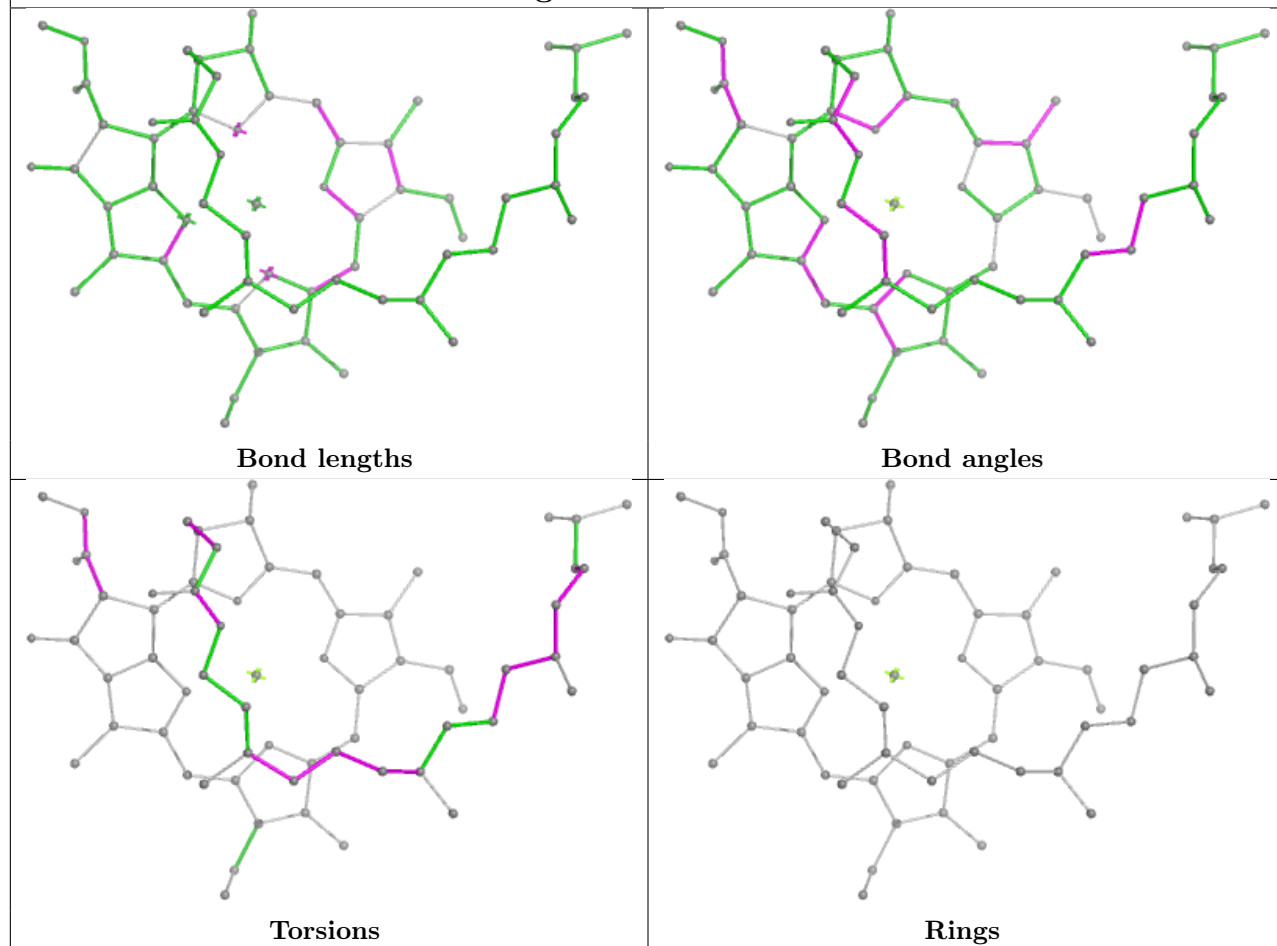


Ligand CLA L 302

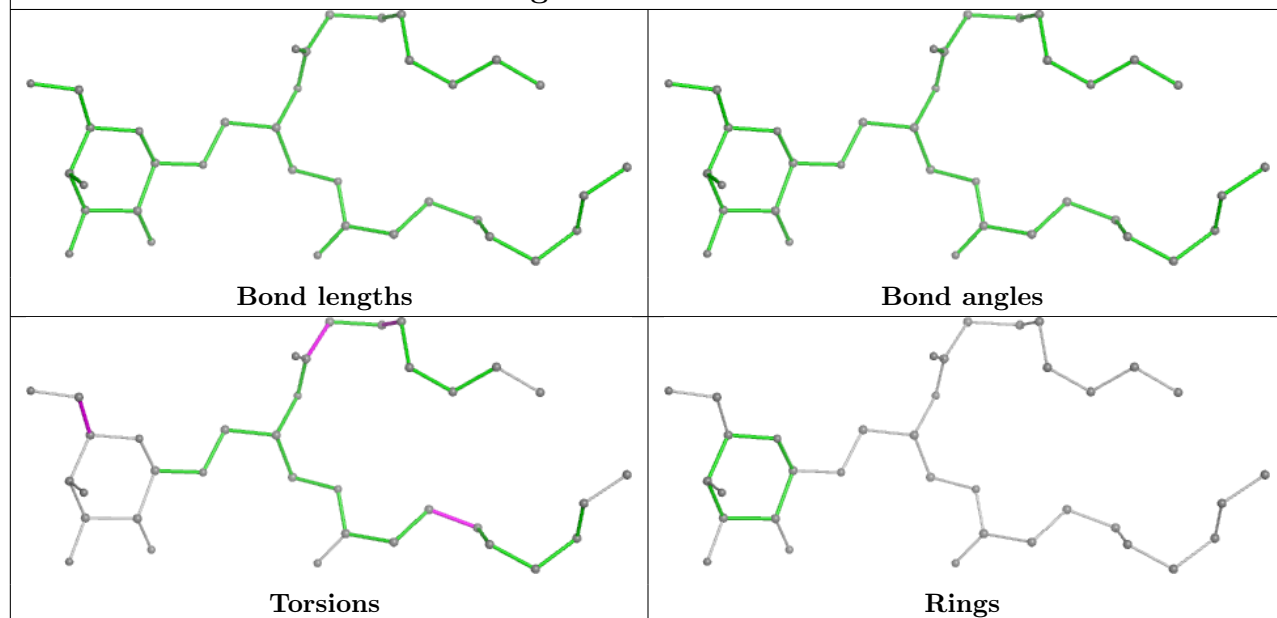




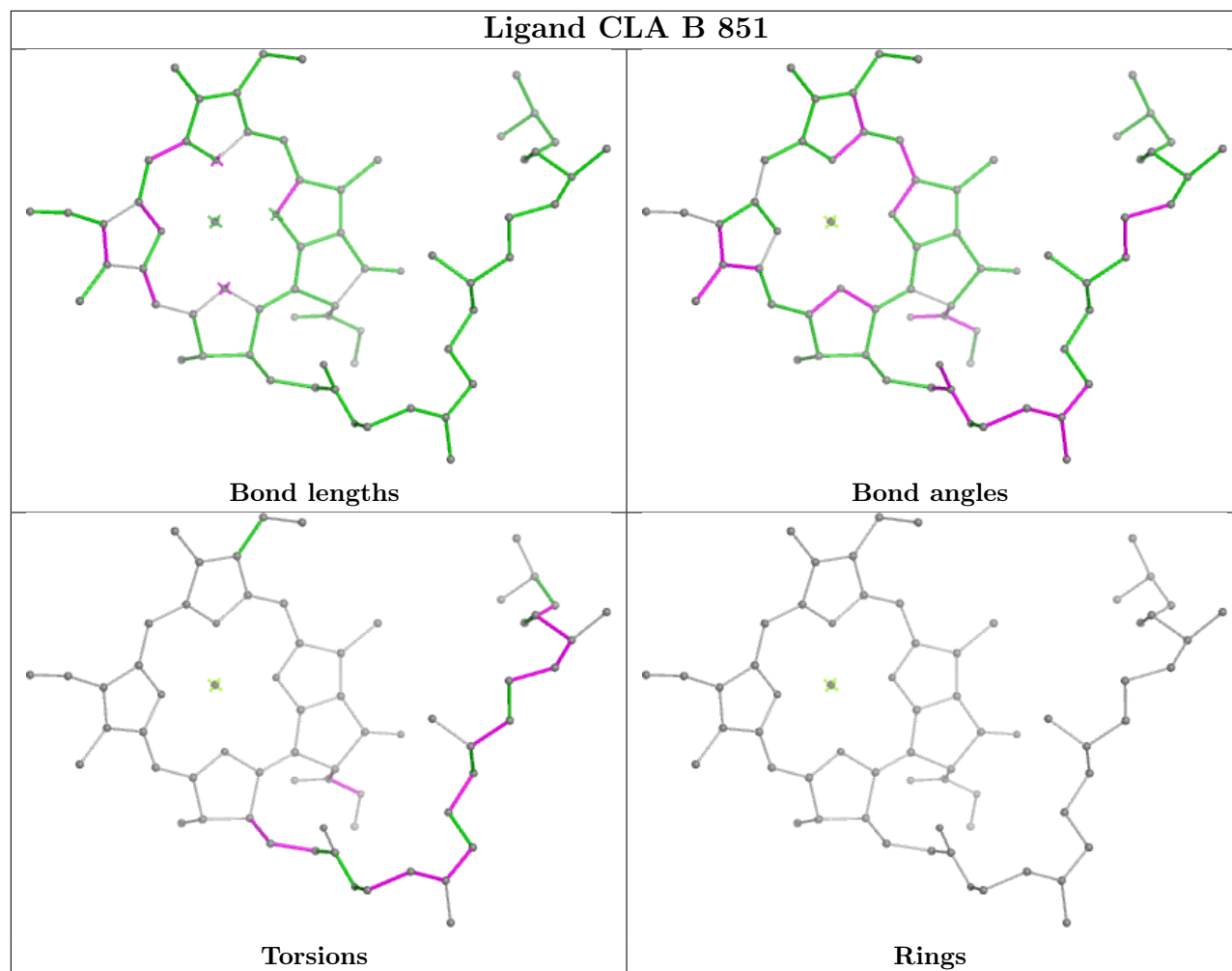
Ligand CLA 2 312



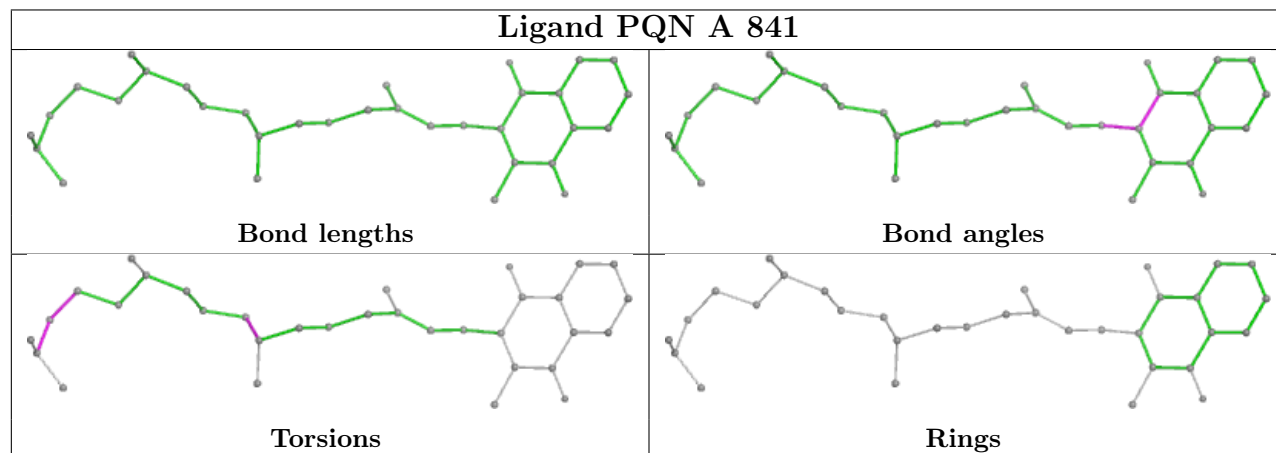
Ligand LMG 4 318



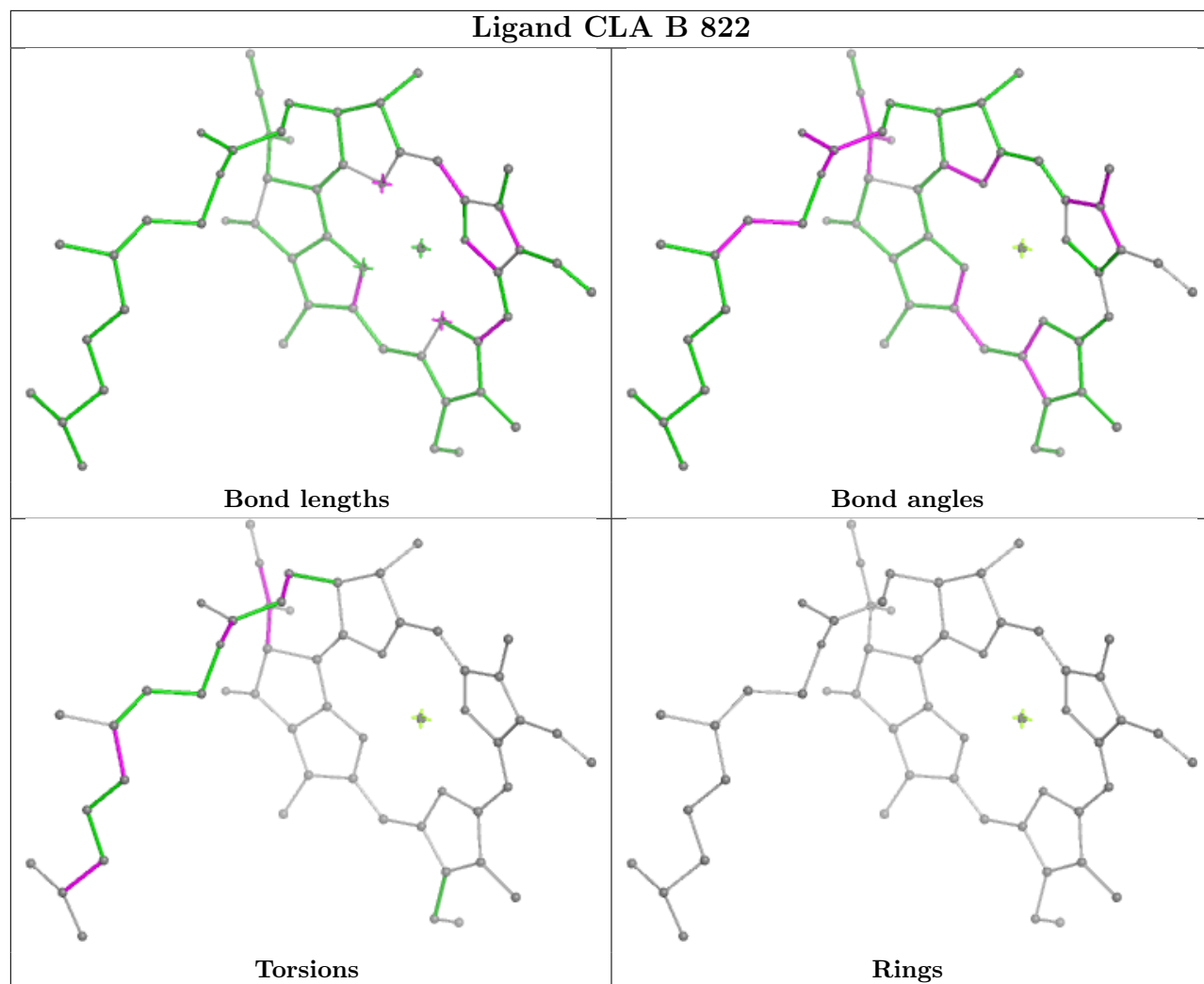
Ligand CLA B 851



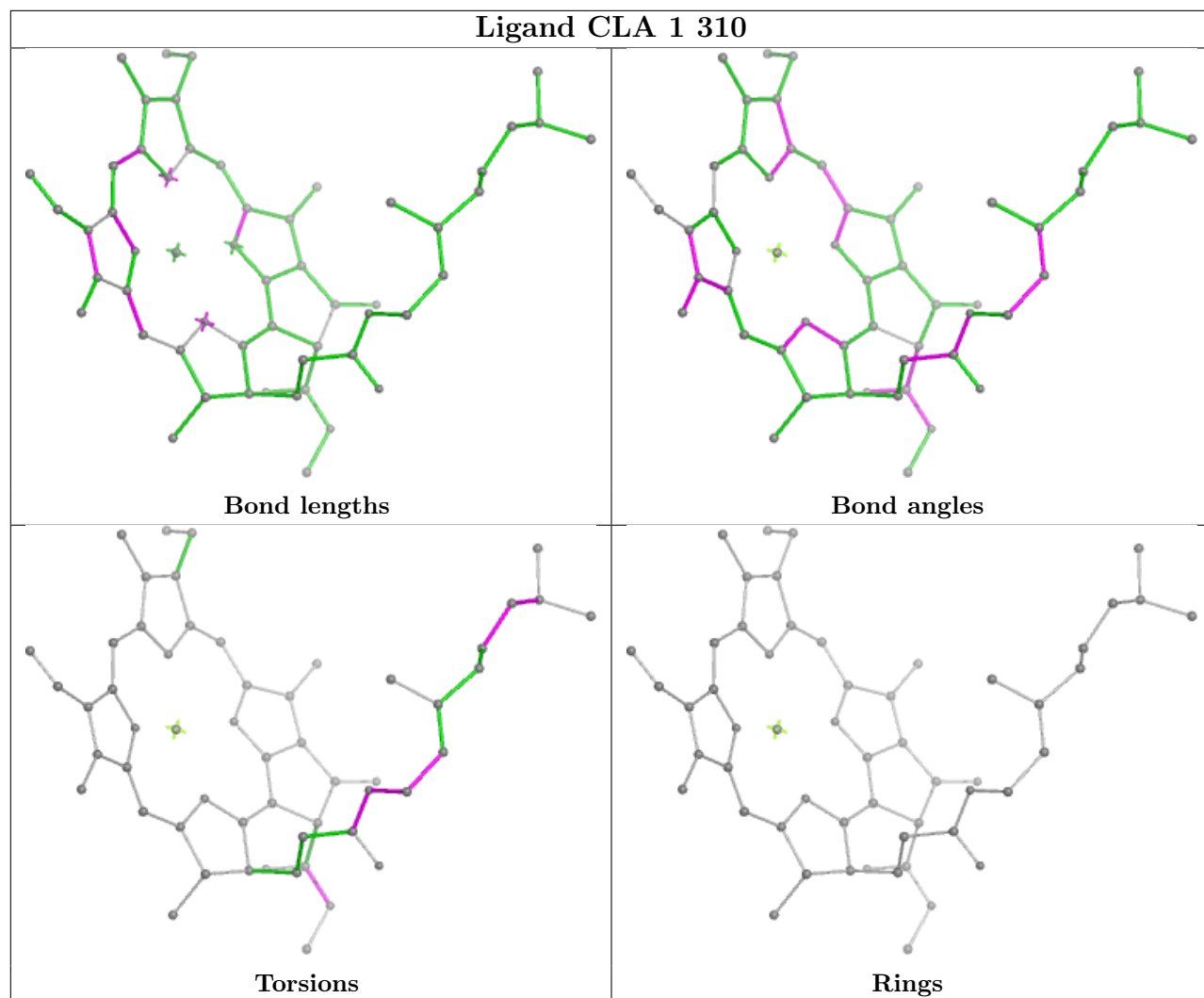
Ligand PQN A 841



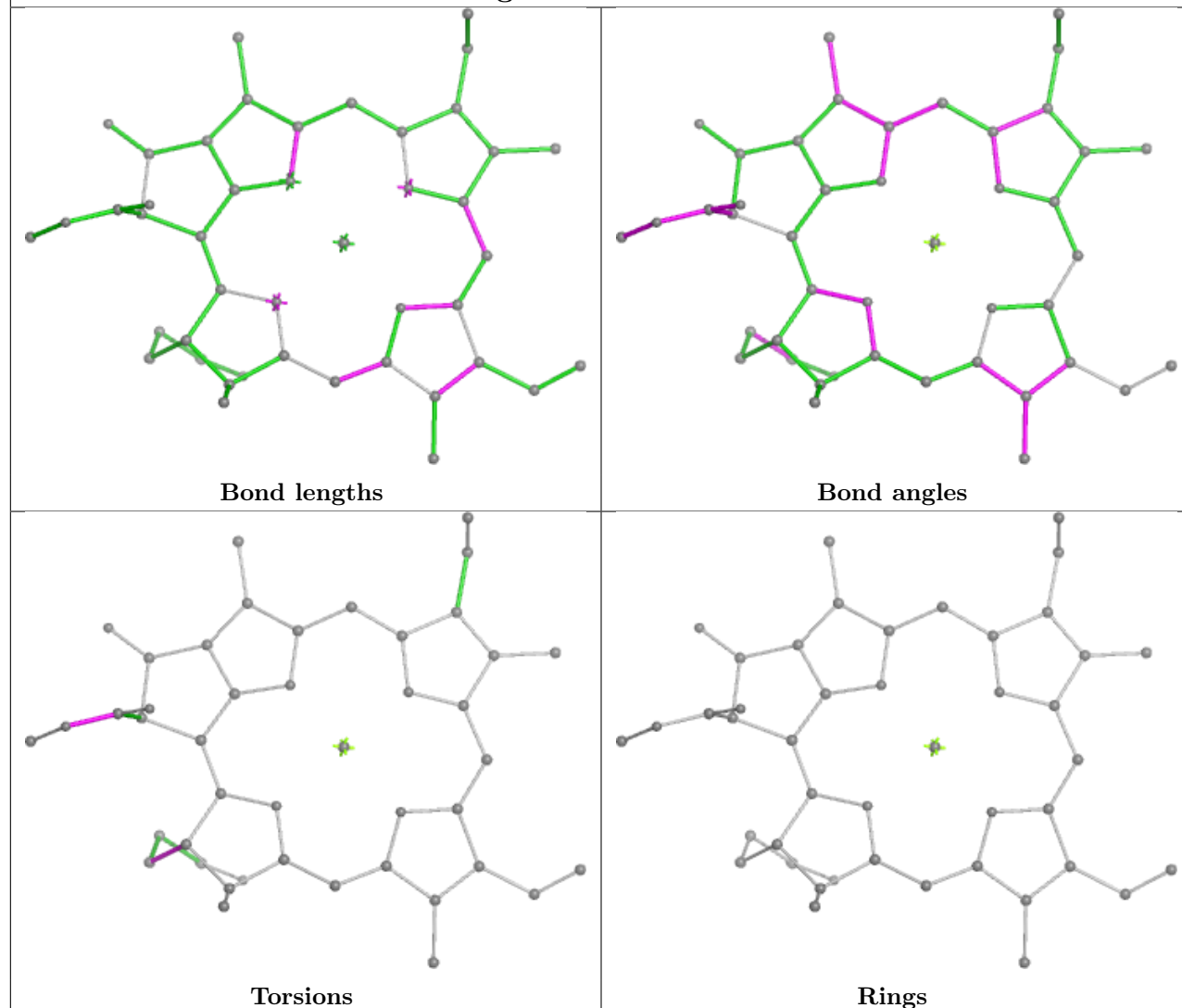
Ligand CLA B 822



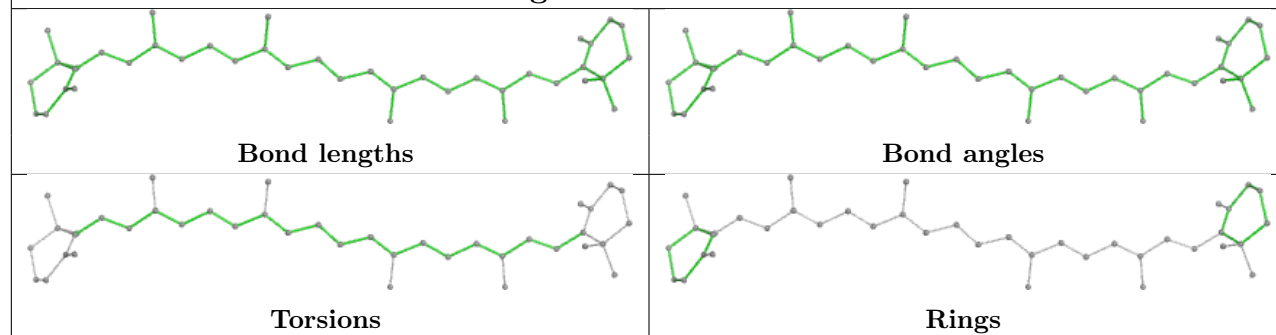
Ligand CLA 1 310



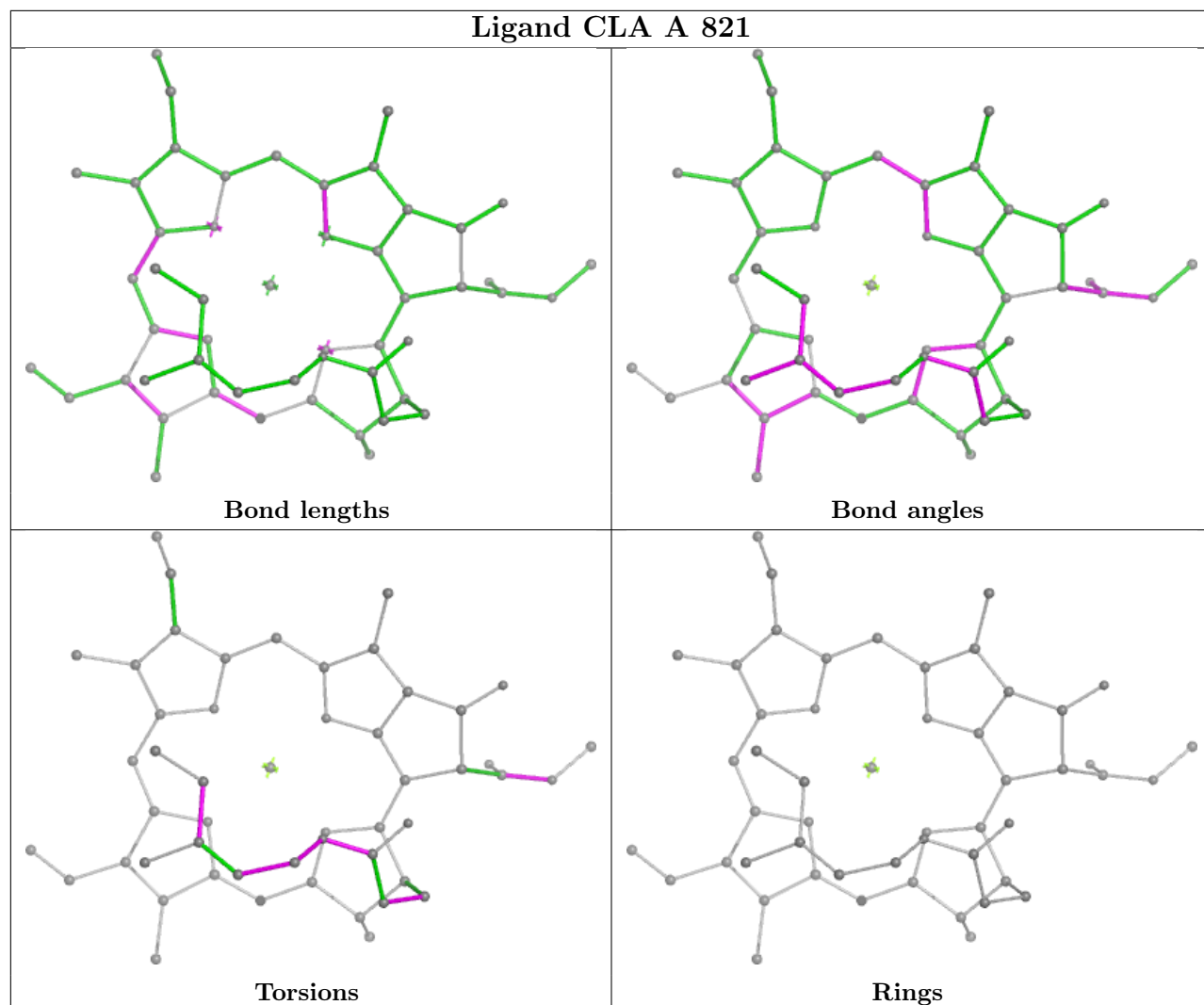
Ligand CLA 2 304



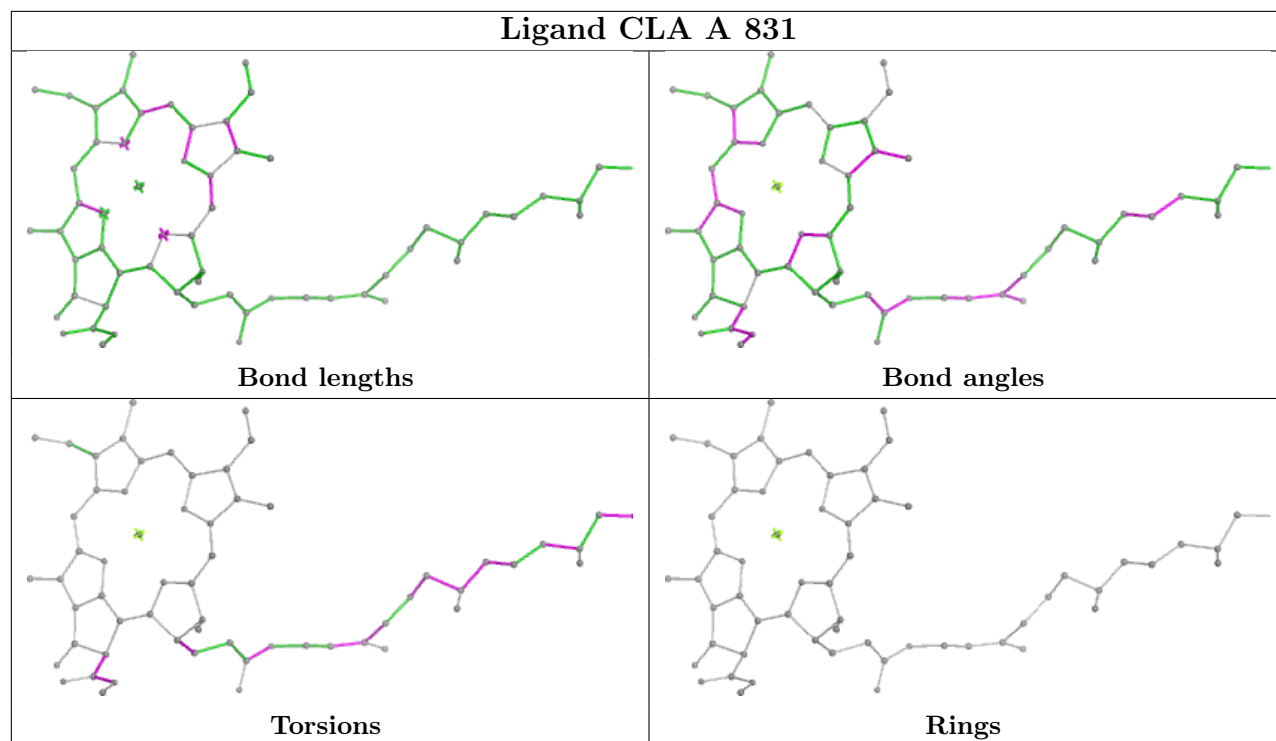
Ligand BCR A 846



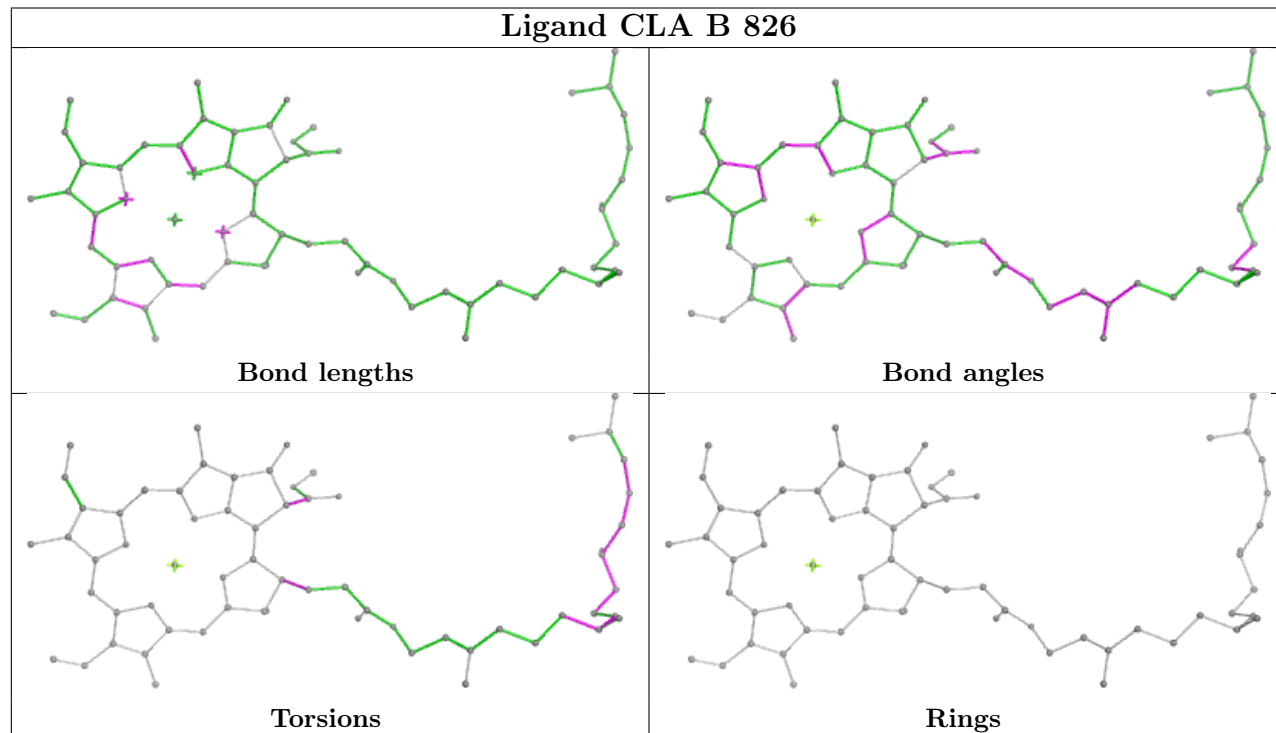
Ligand CLA A 821

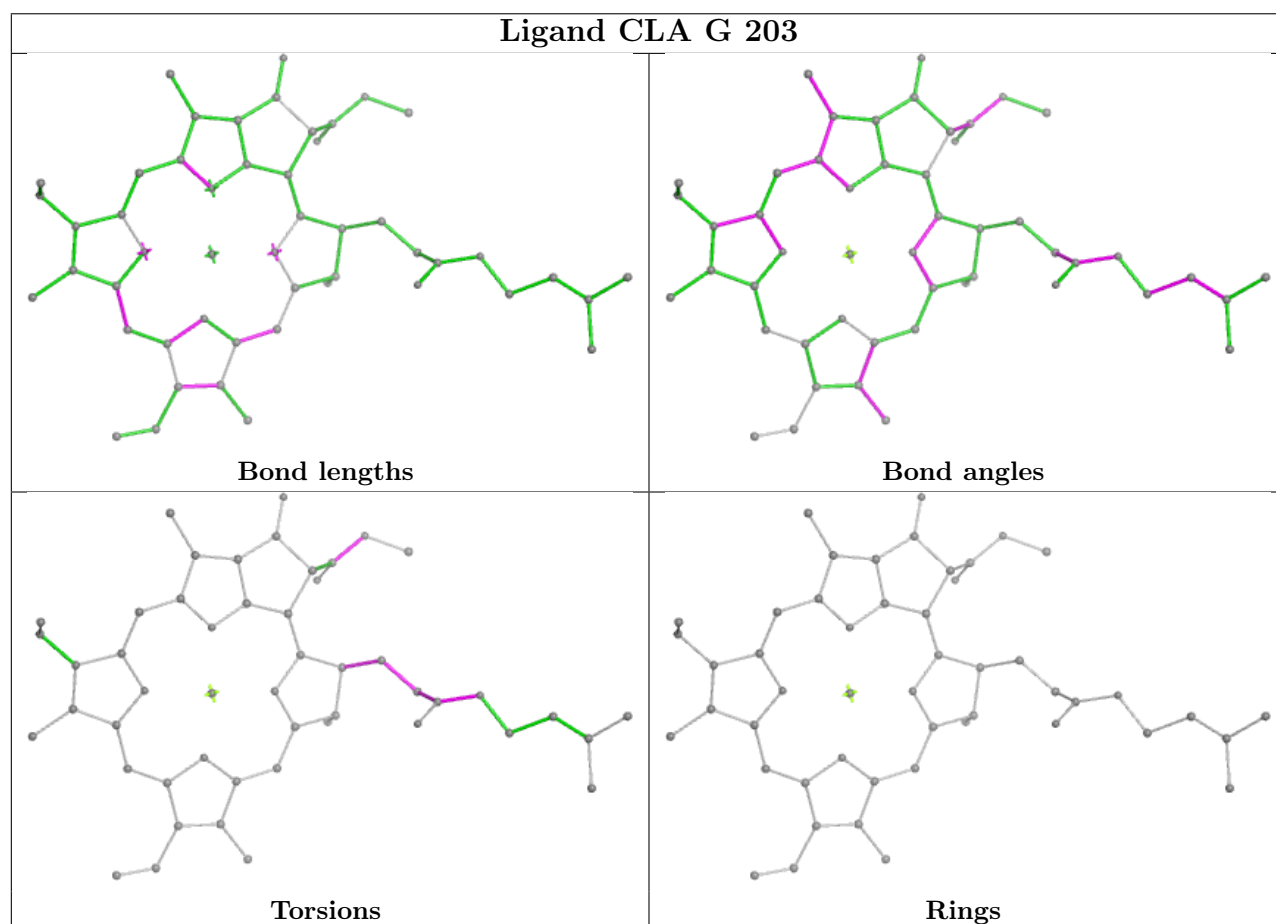
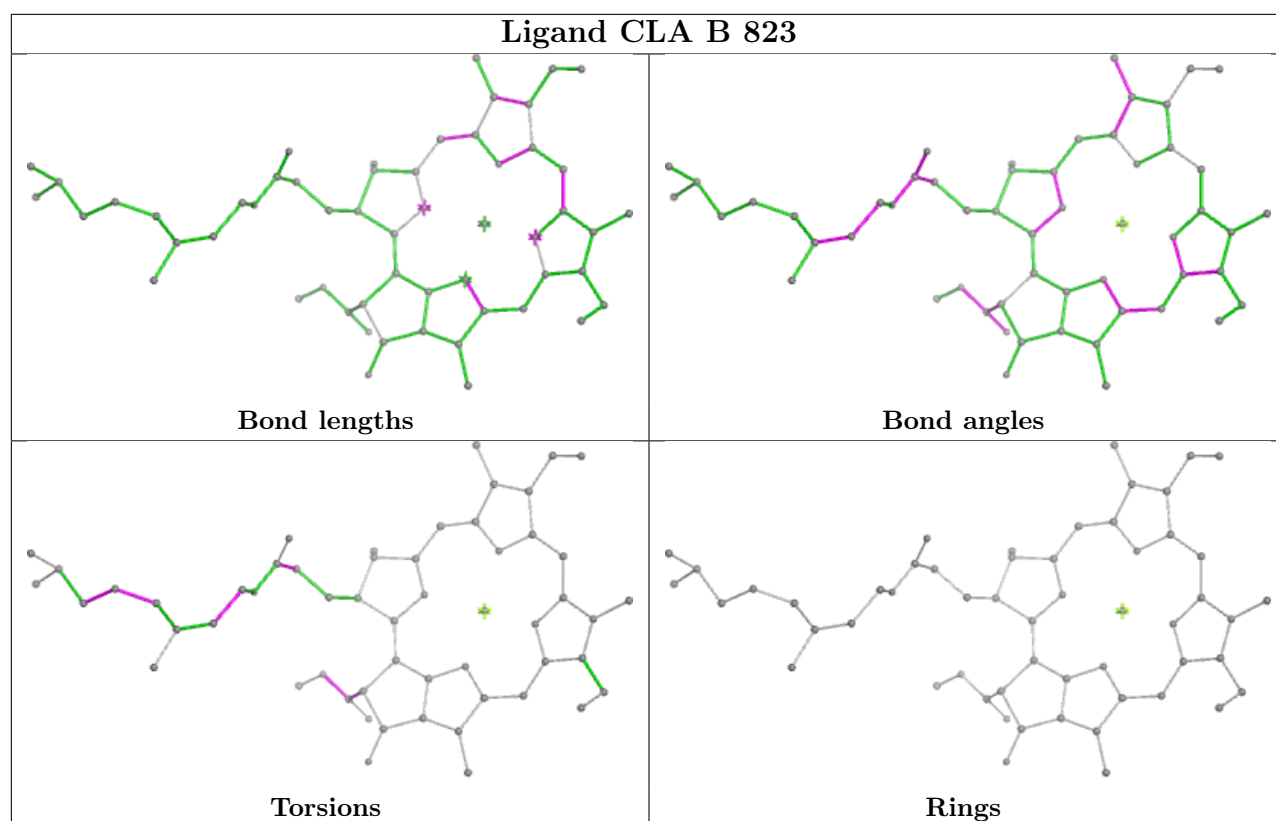


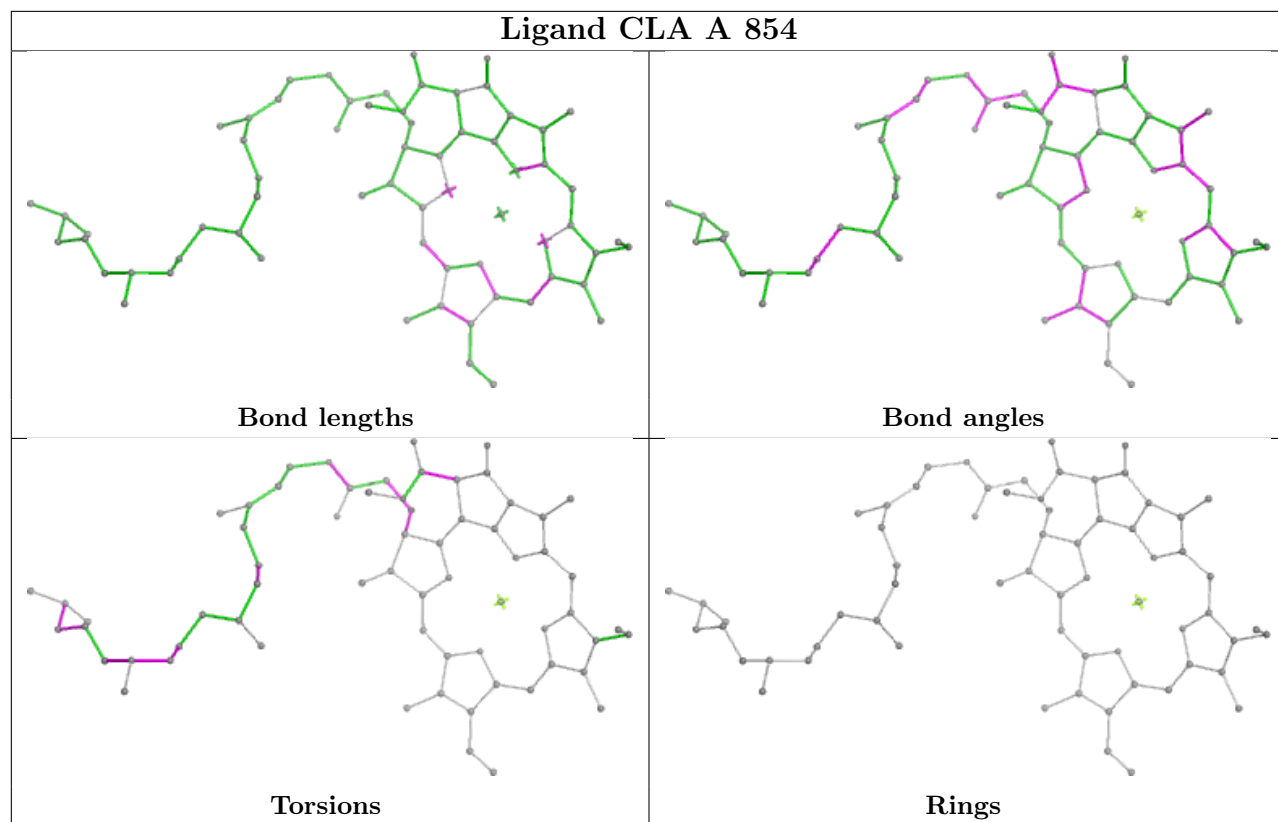
Ligand CLA A 831



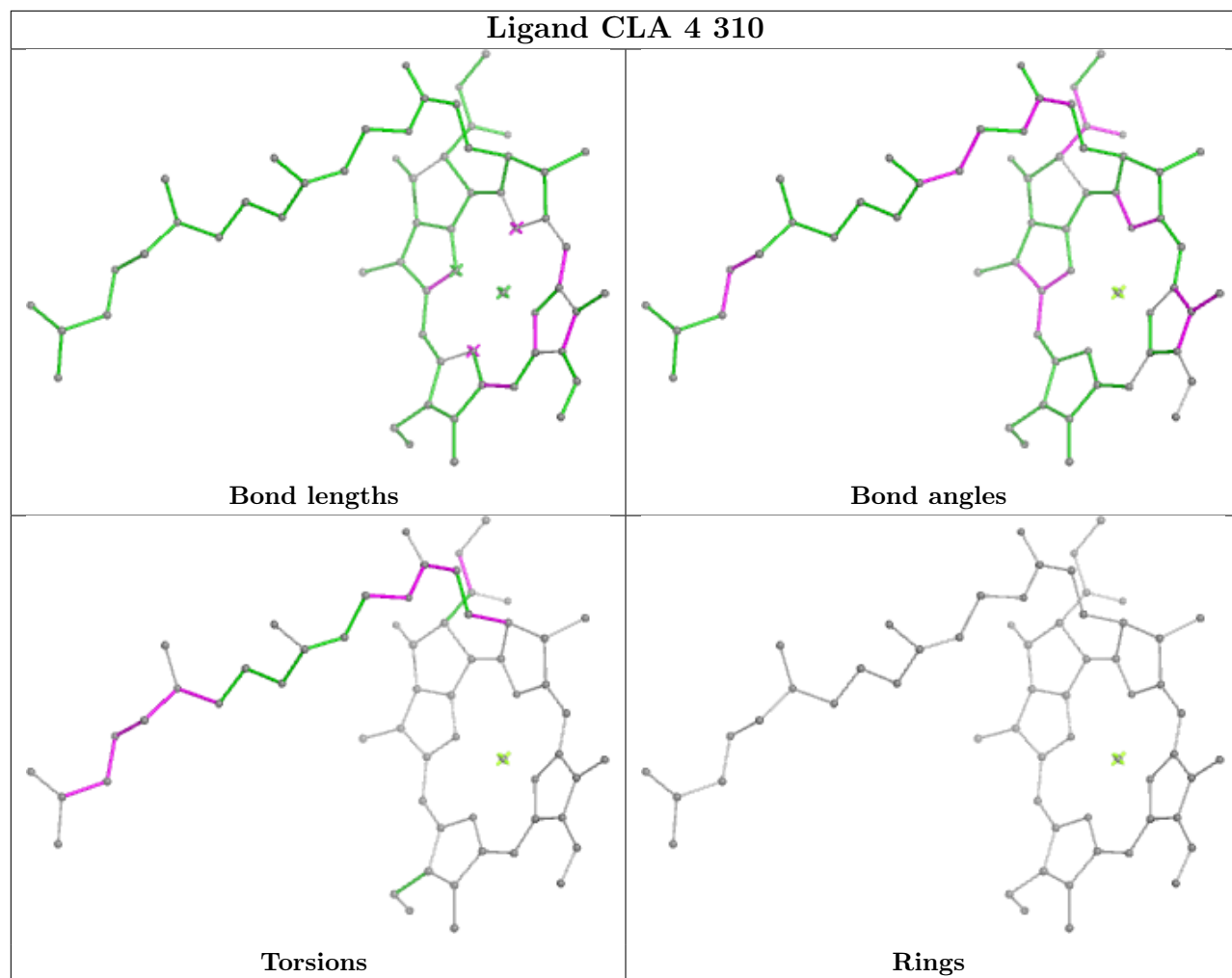
Ligand CLA B 826

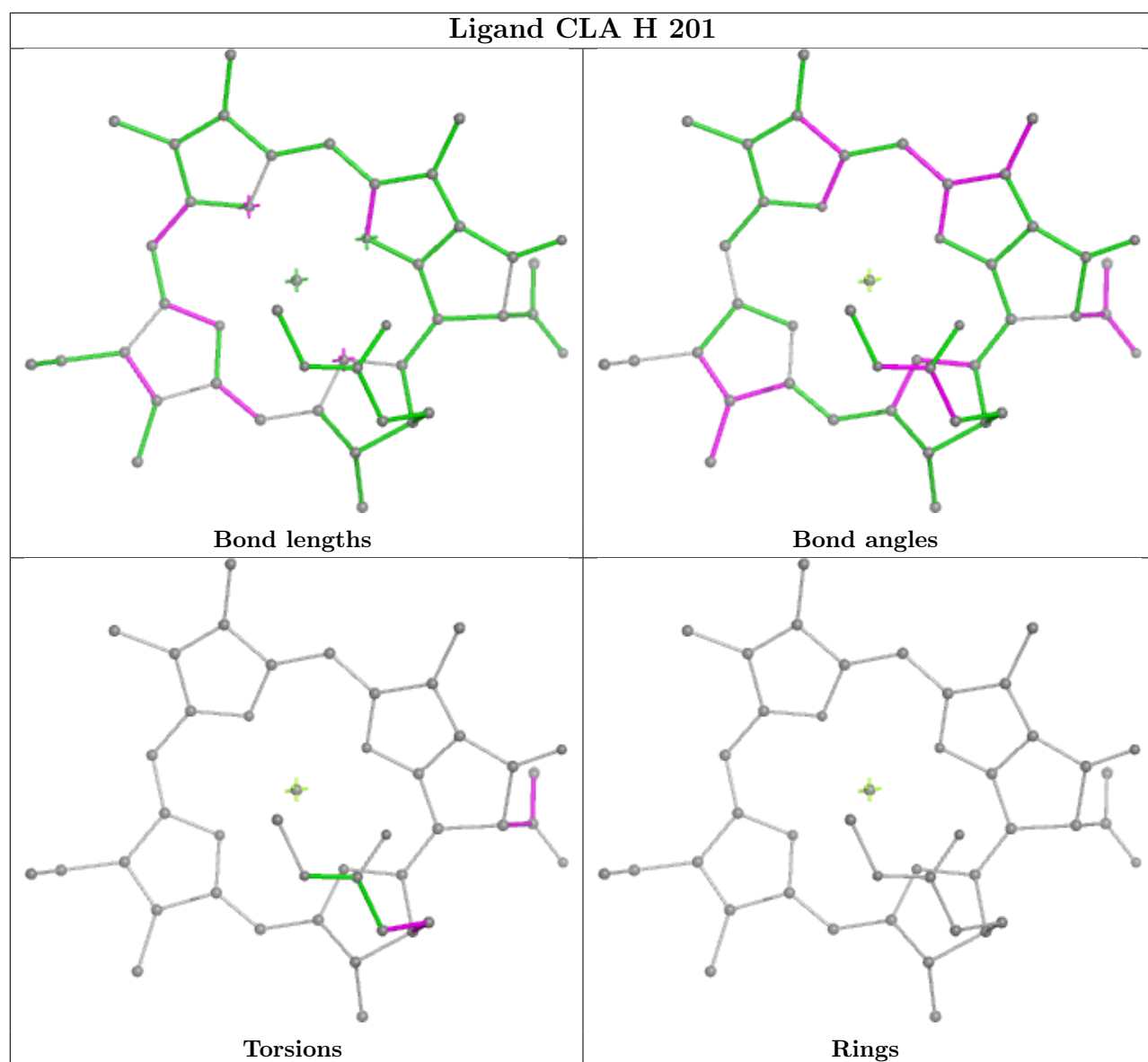




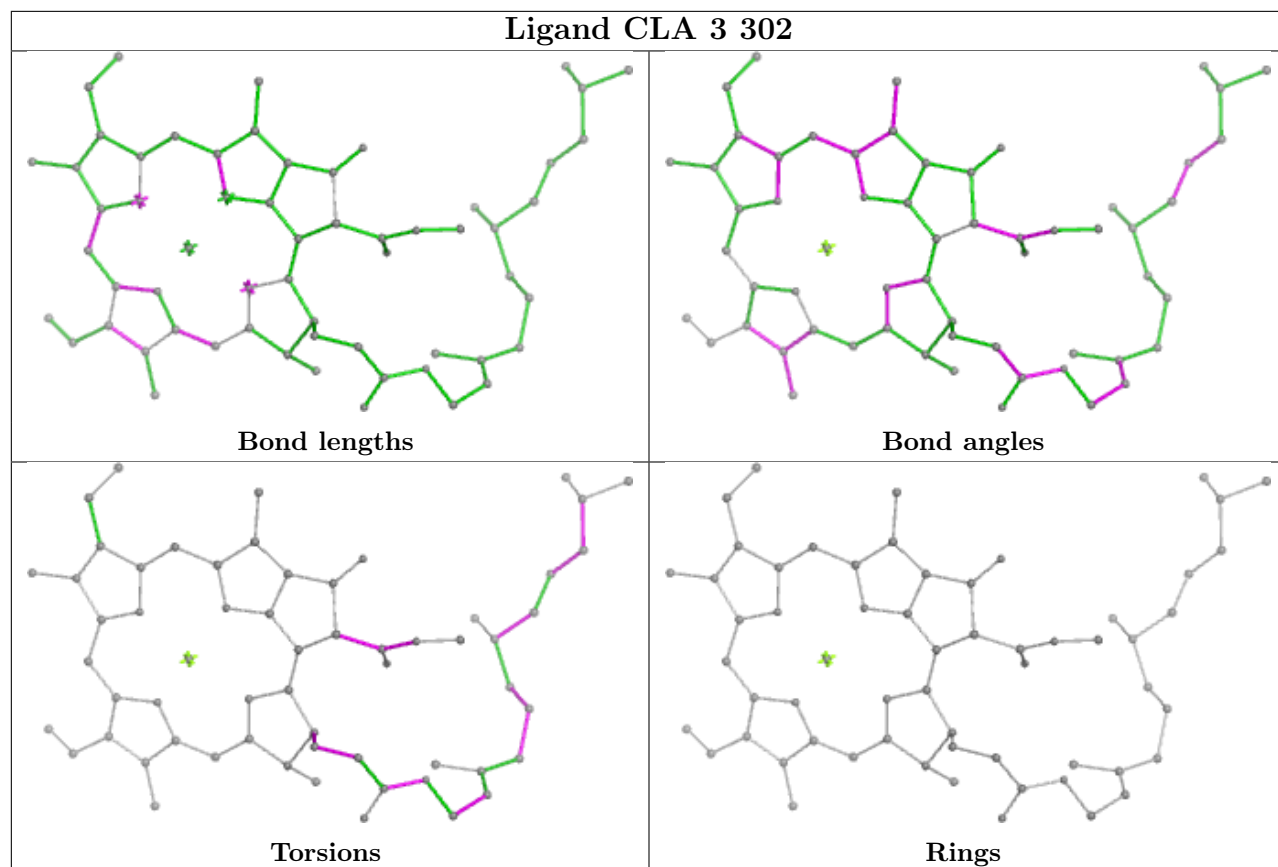


Ligand CLA 4 310

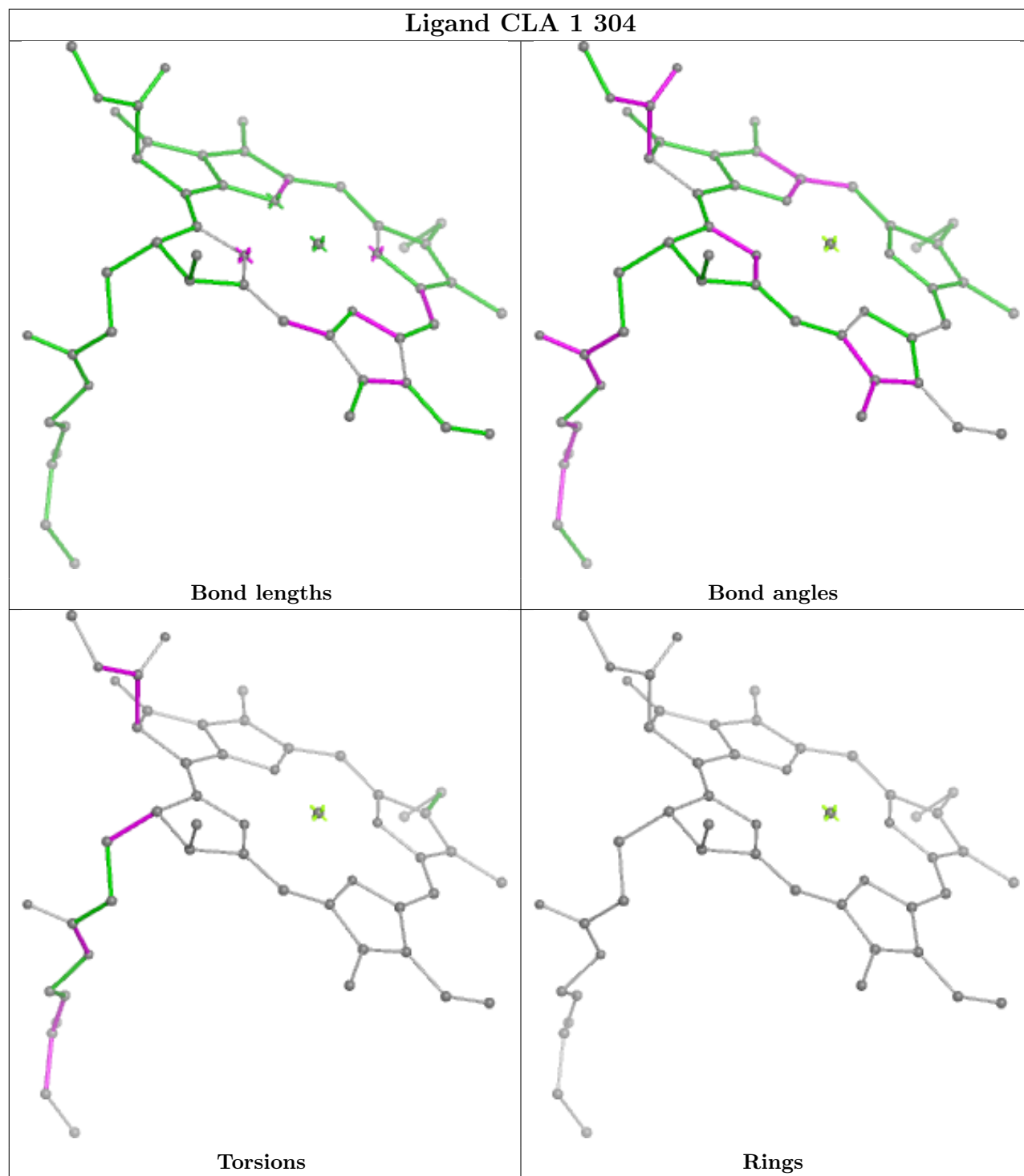




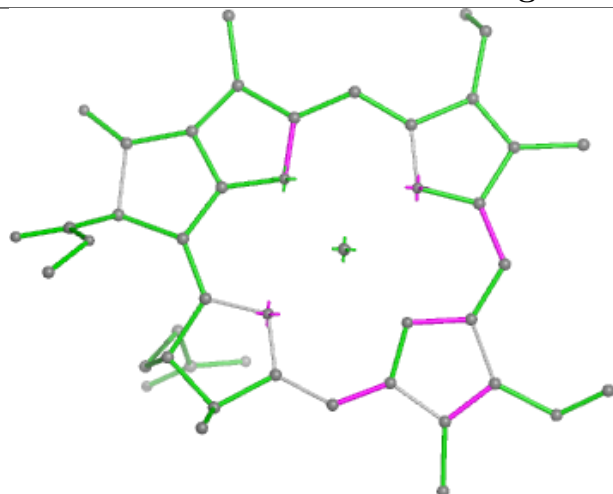
Ligand CLA 3 302



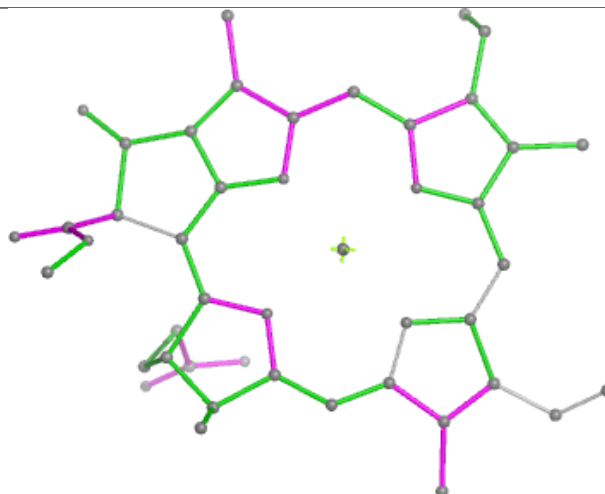
Ligand CLA 1 304



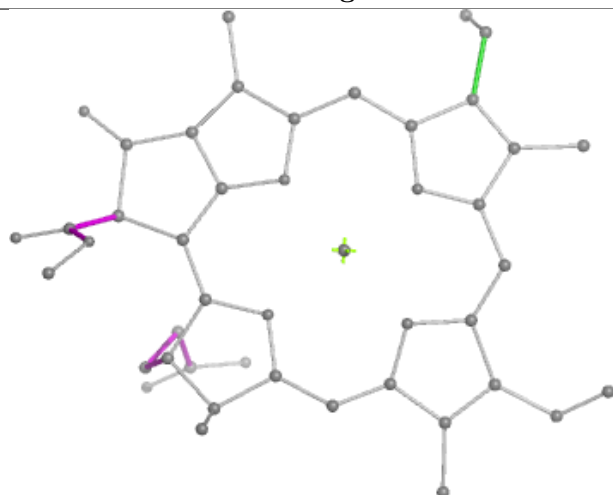
Ligand CLA 3 303



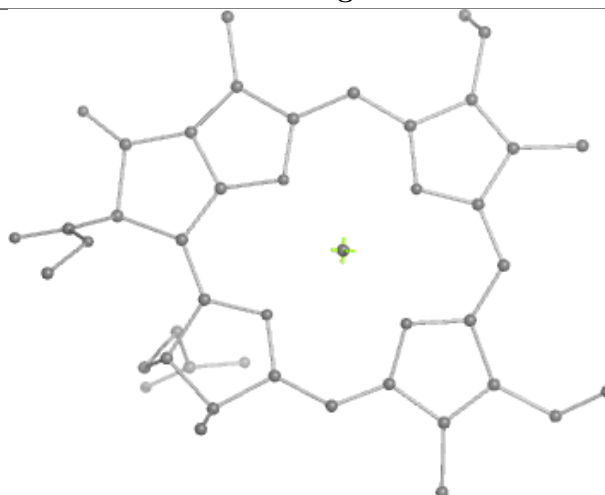
Bond lengths



Bond angles

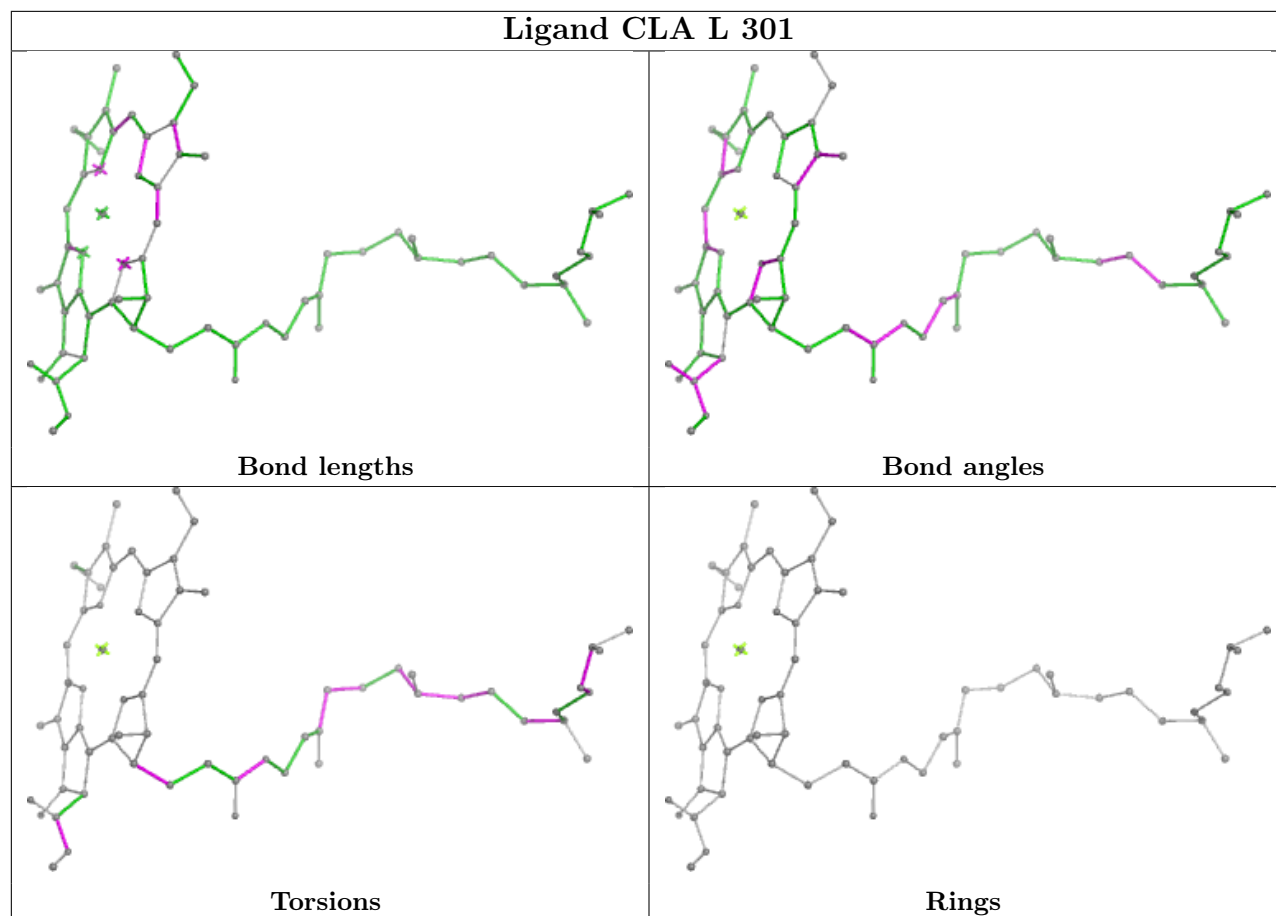


Torsions

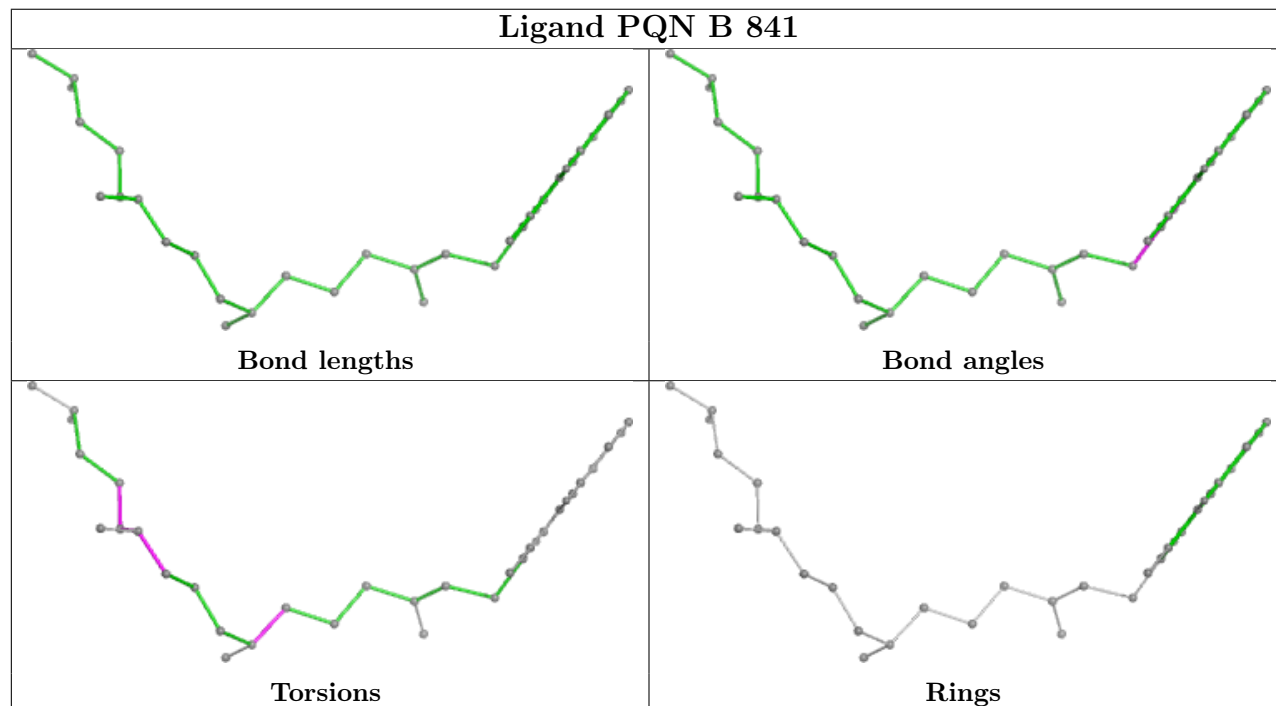


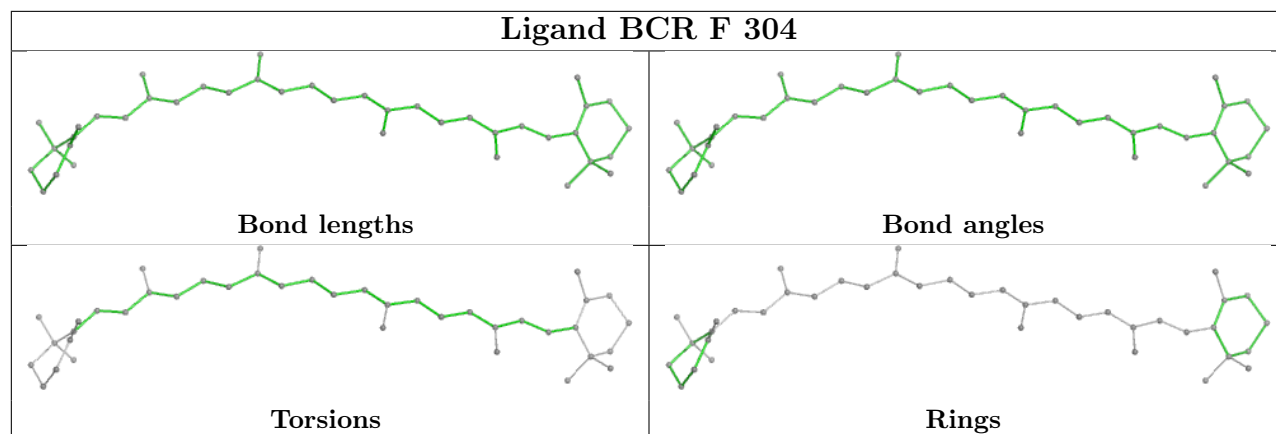
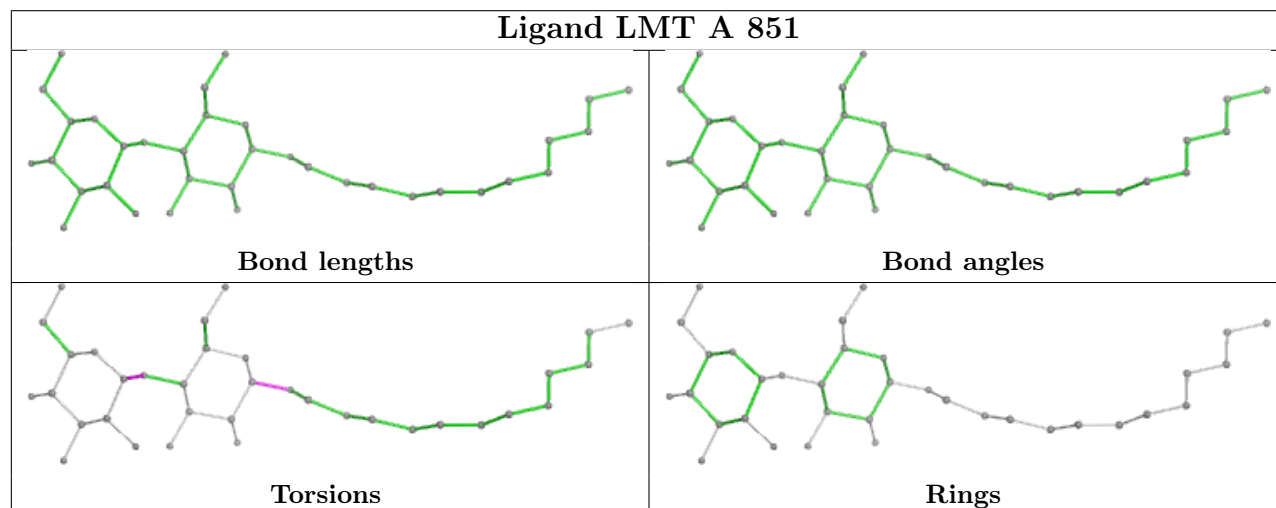
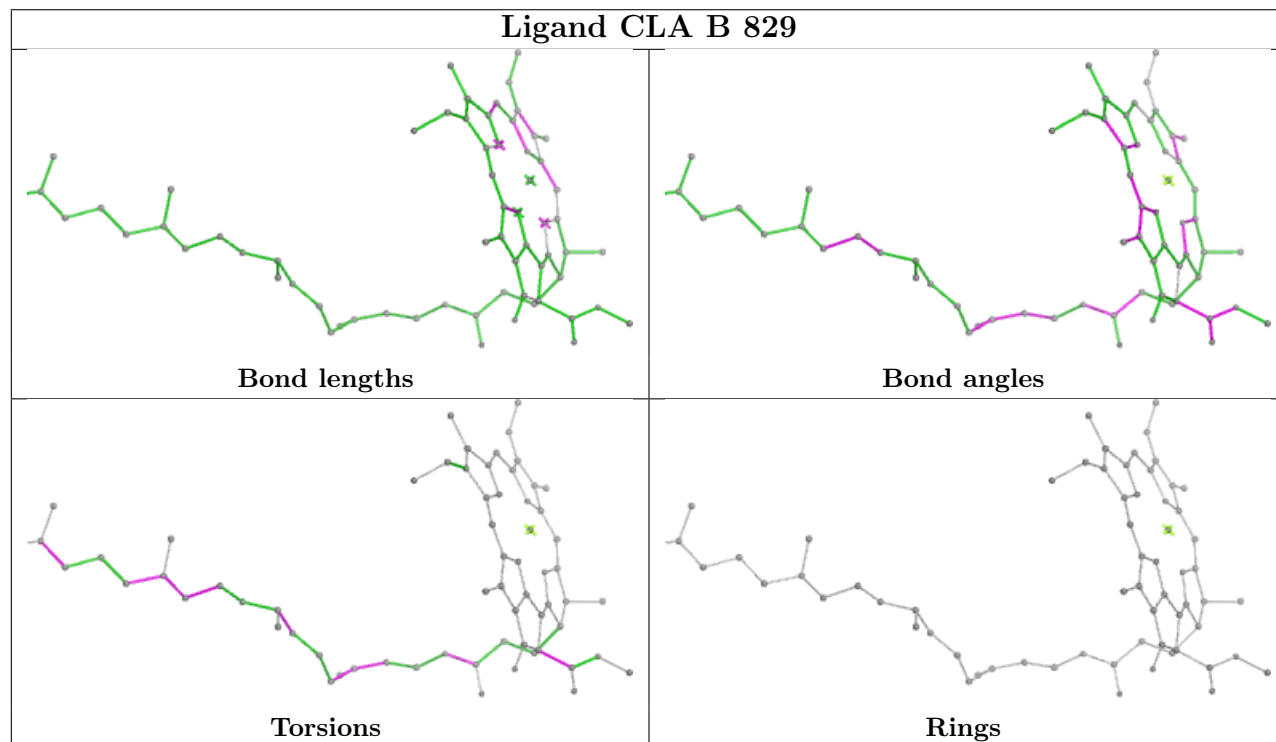
Rings

Ligand CLA L 301

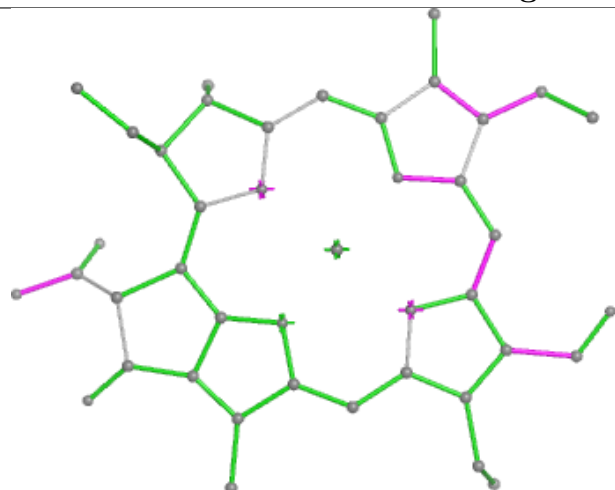


Ligand PQN B 841

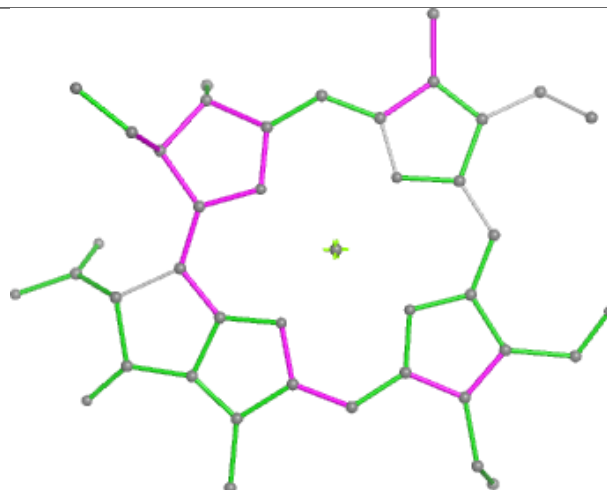


Ligand BCR F 304**Ligand LMT A 851****Ligand CLA B 829**

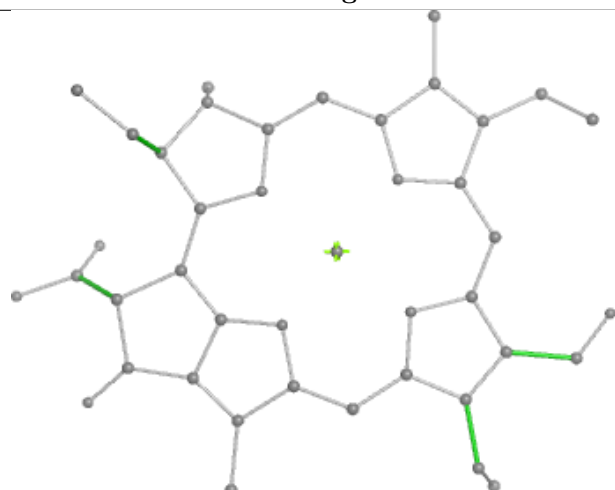
Ligand CHL 4 314



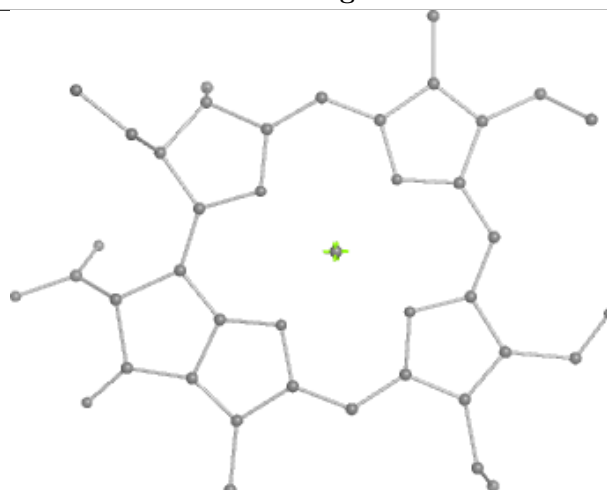
Bond lengths



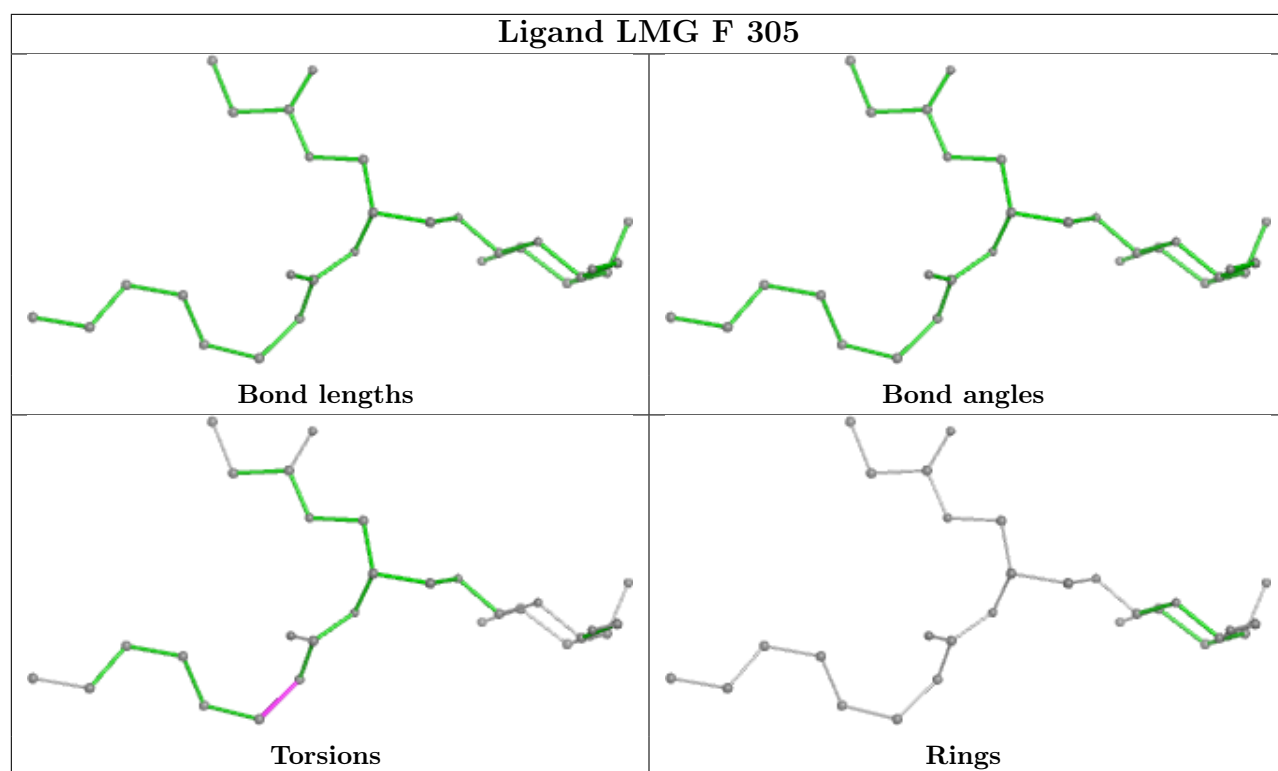
Bond angles



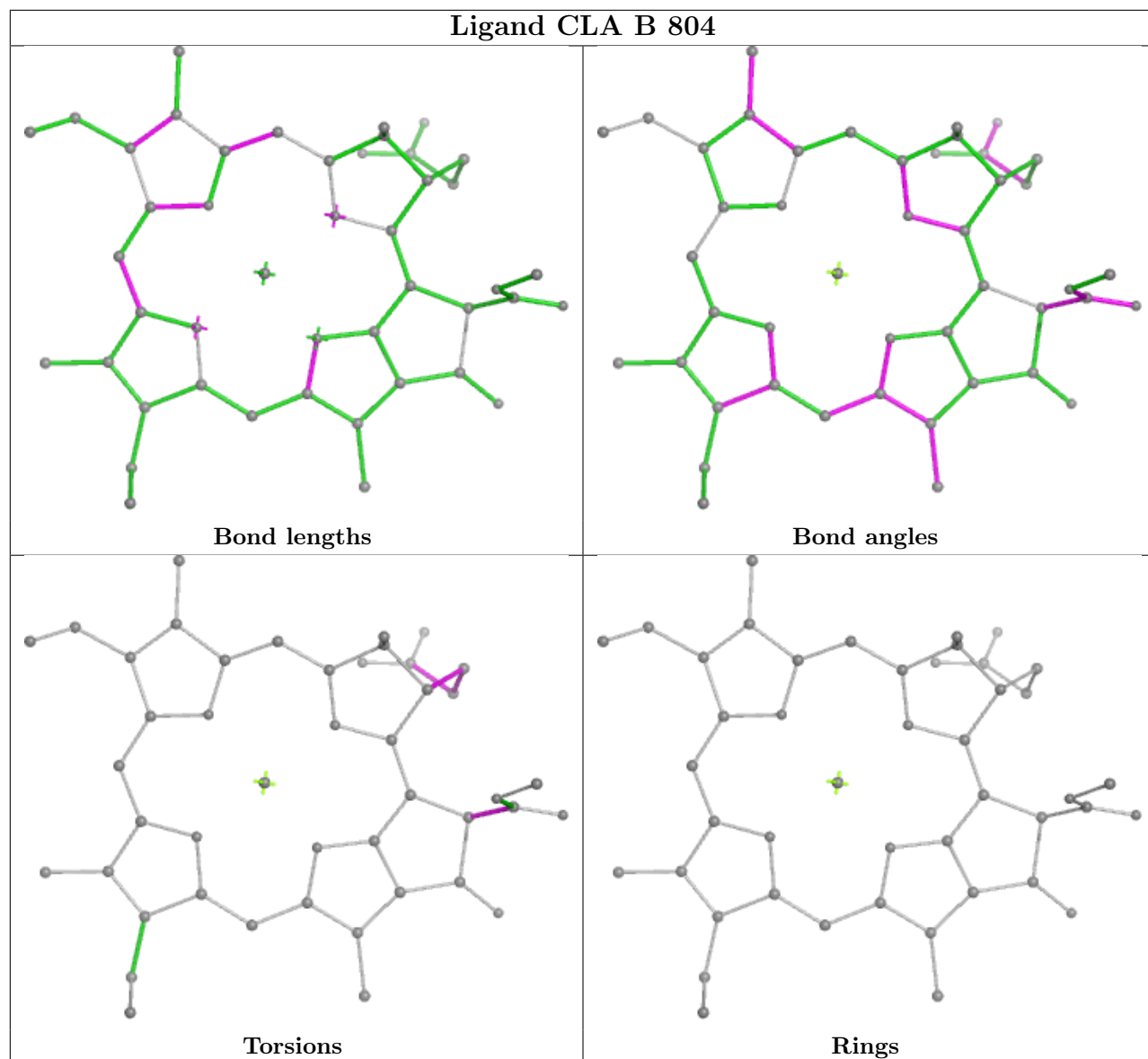
Torsions



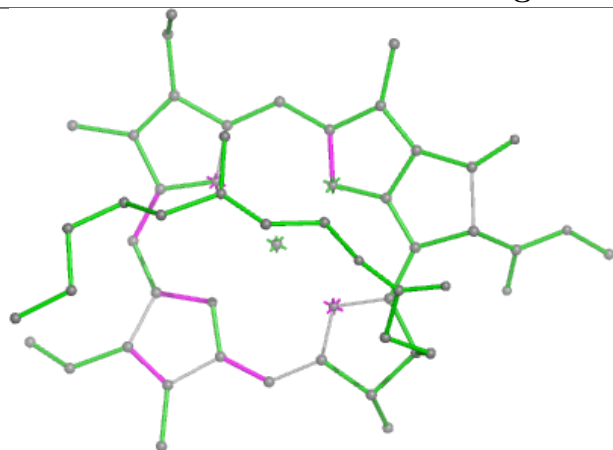
Rings



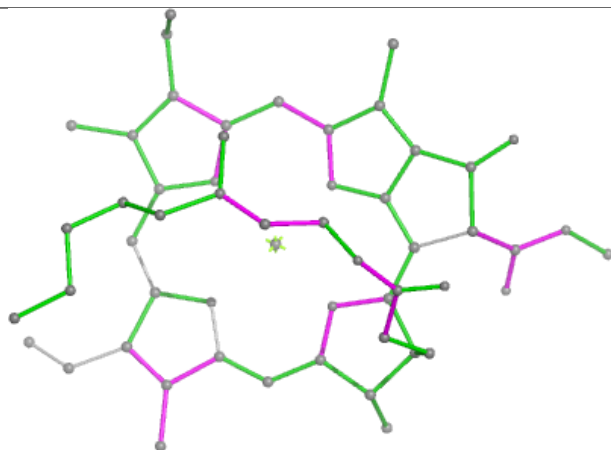
Ligand CLA B 804



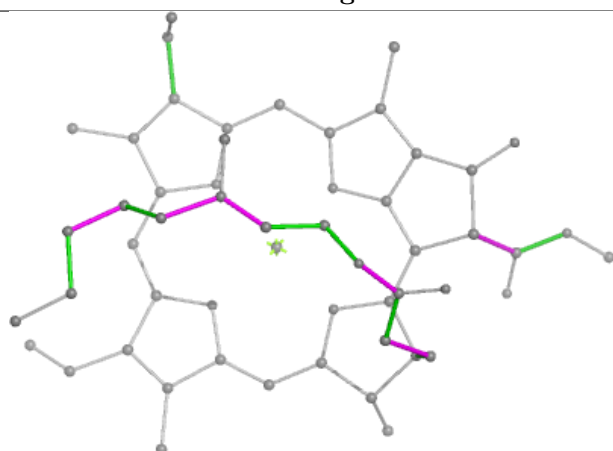
Ligand CLA A 810



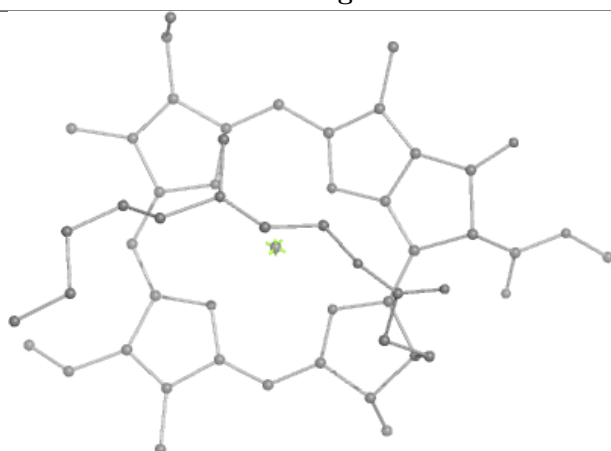
Bond lengths



Bond angles

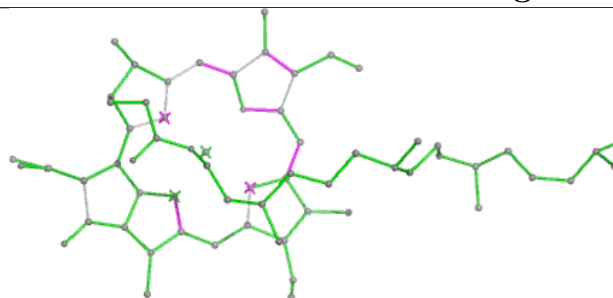


Torsions

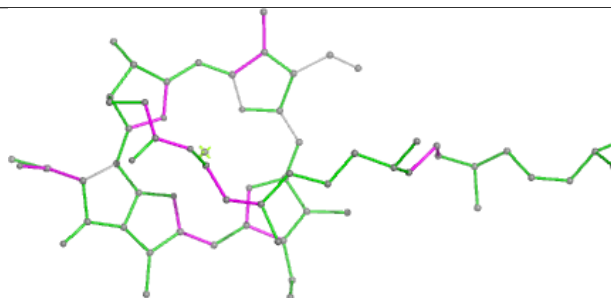


Rings

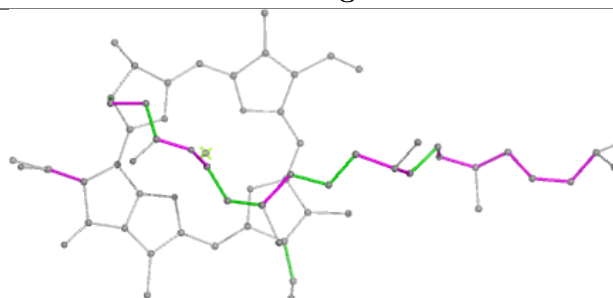
Ligand CLA A 835



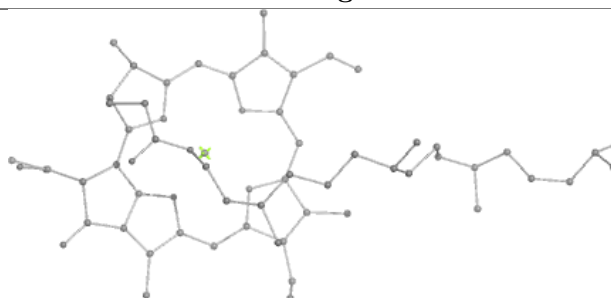
Bond lengths



Bond angles

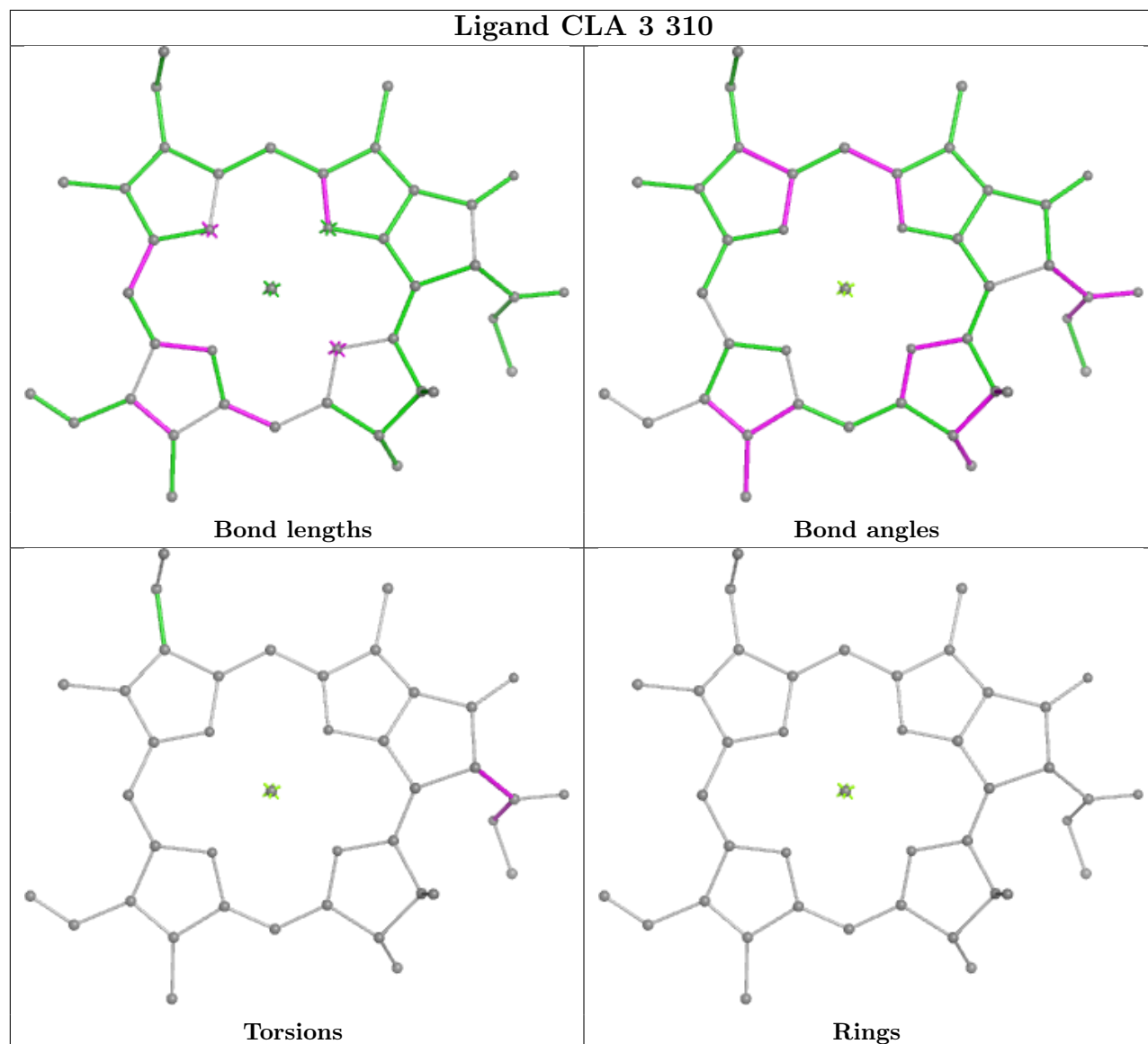


Torsions

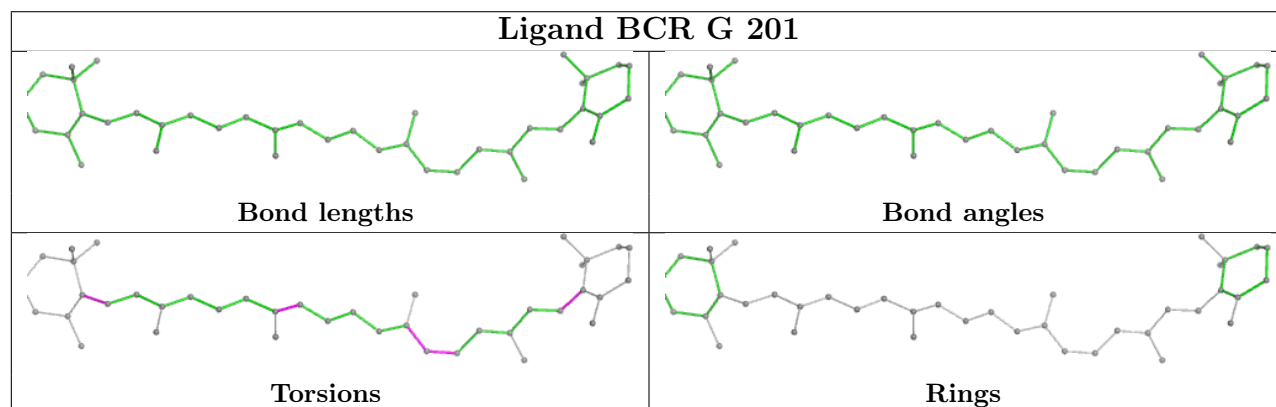


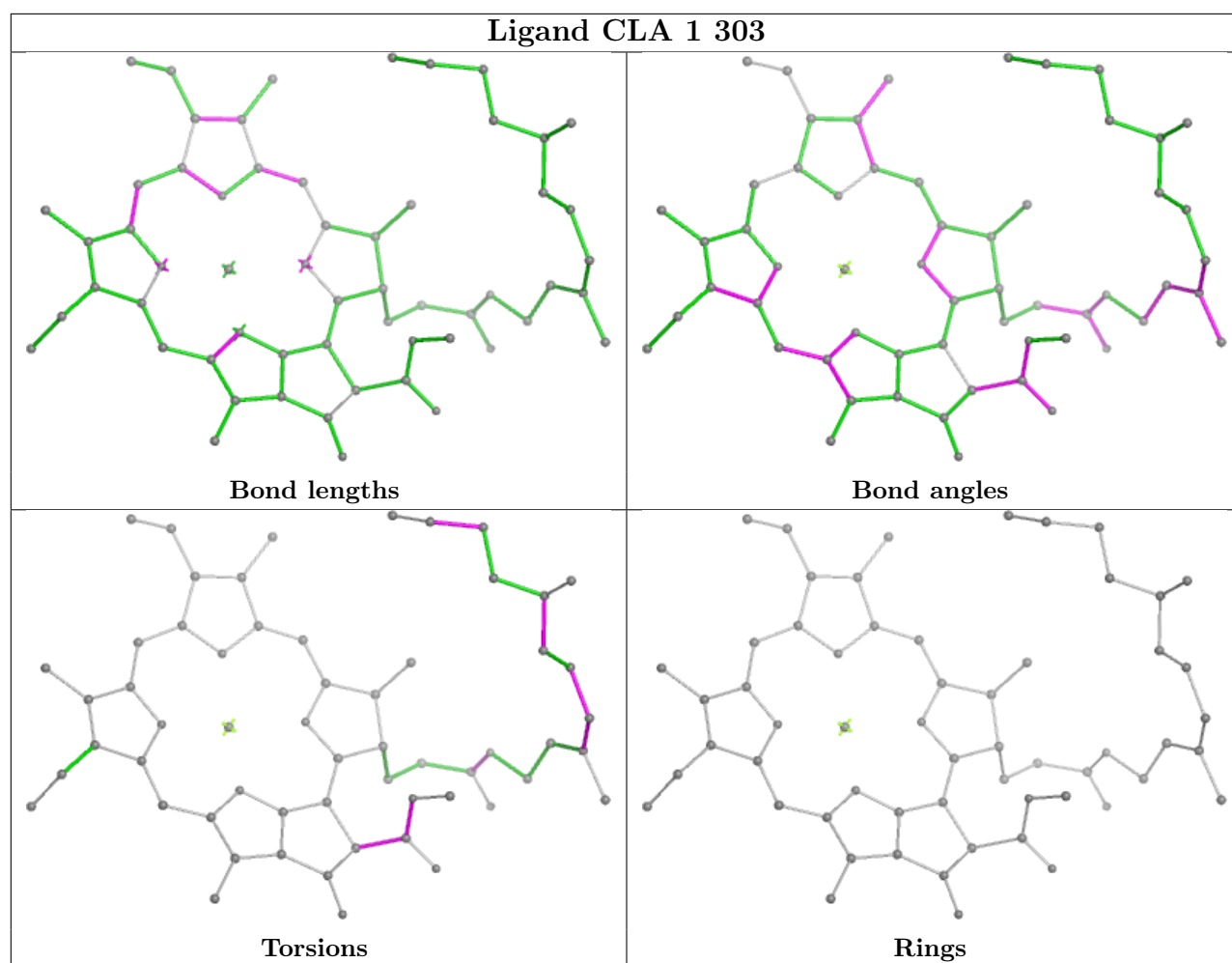
Rings

Ligand CLA 3 310

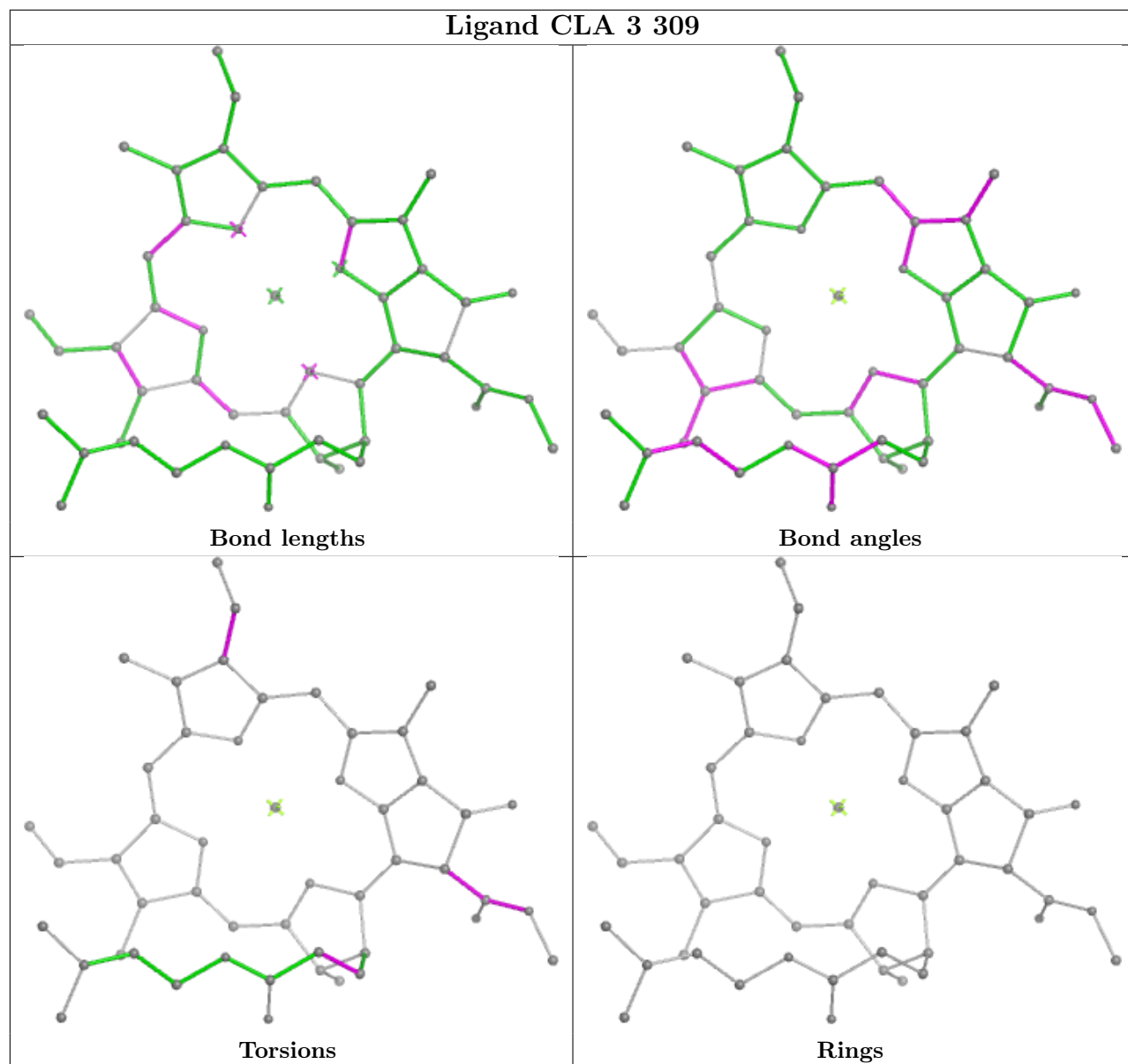


Ligand BCR G 201

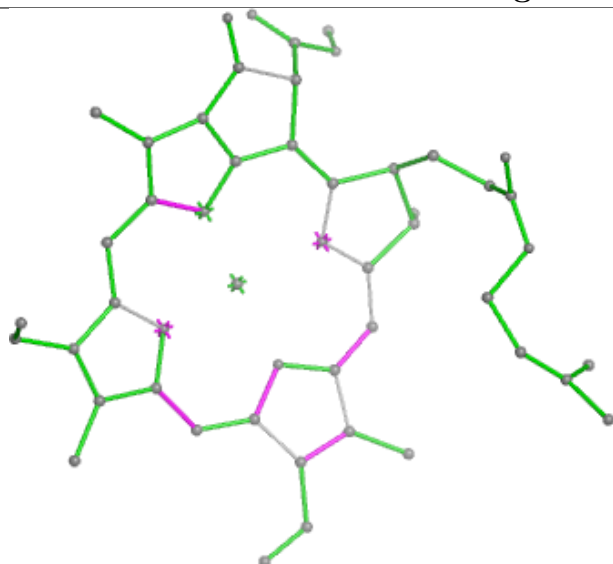




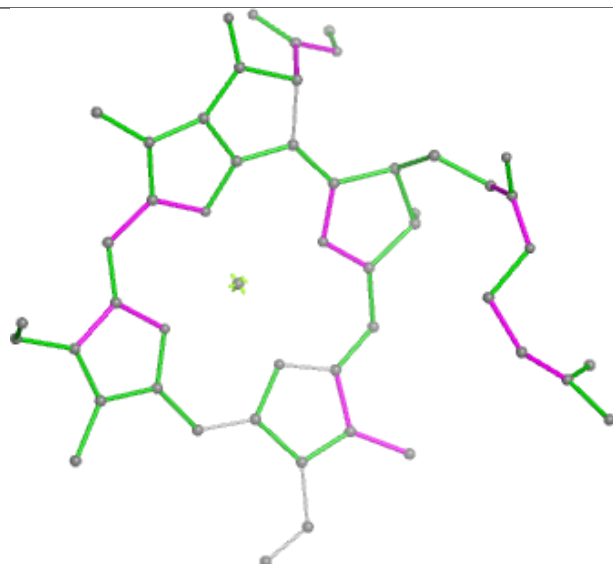
Ligand CLA 3 309



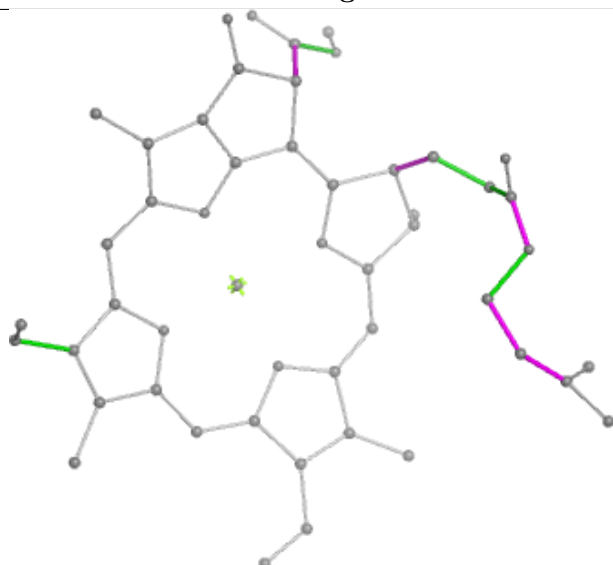
Ligand CLA A 813



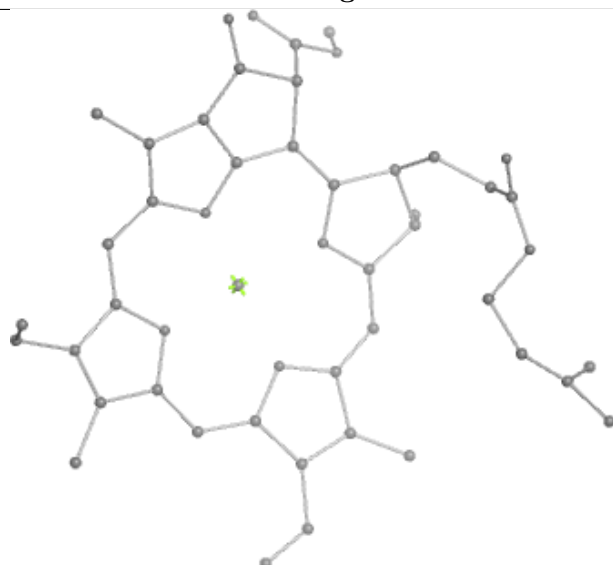
Bond lengths



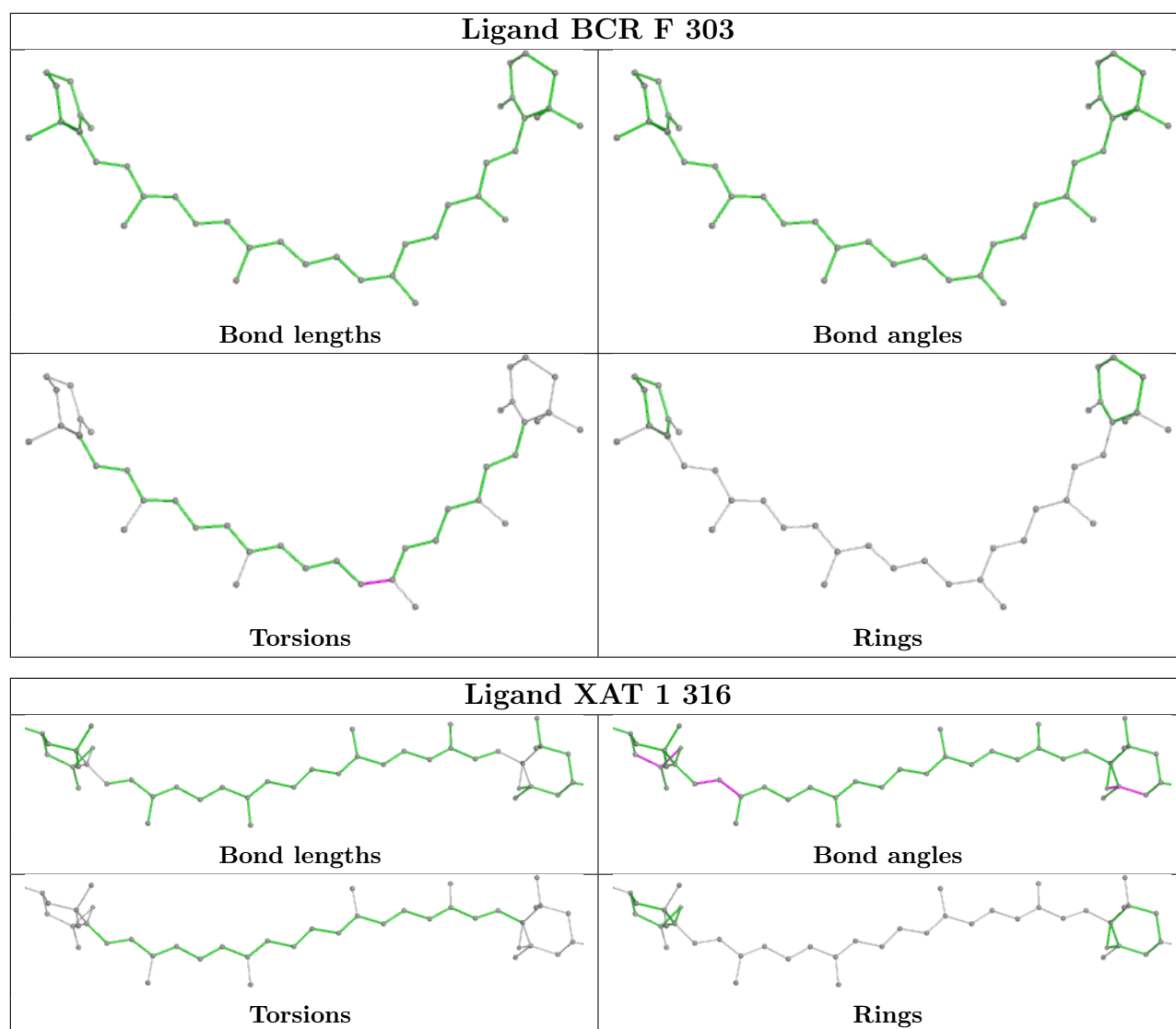
Bond angles



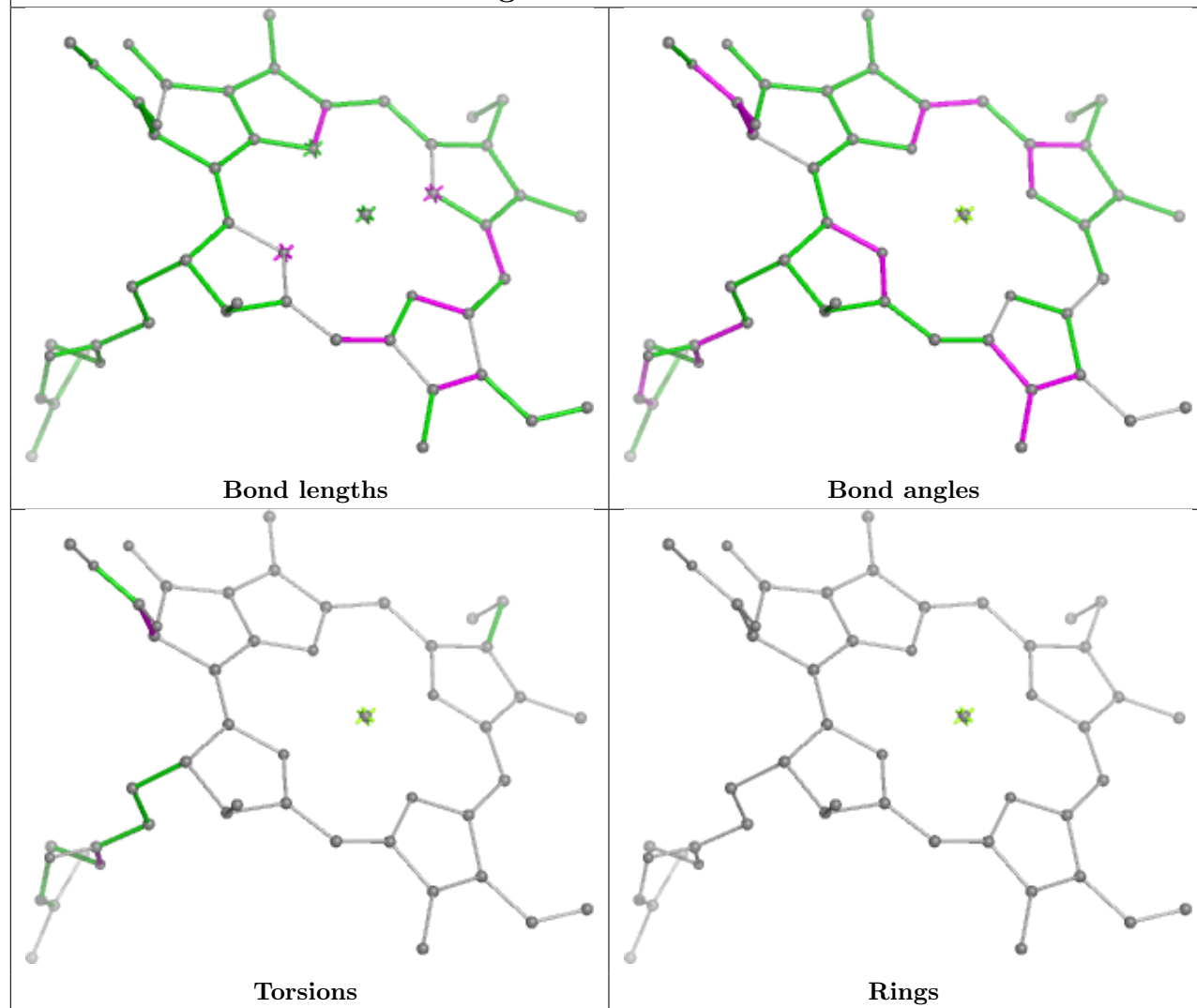
Torsions



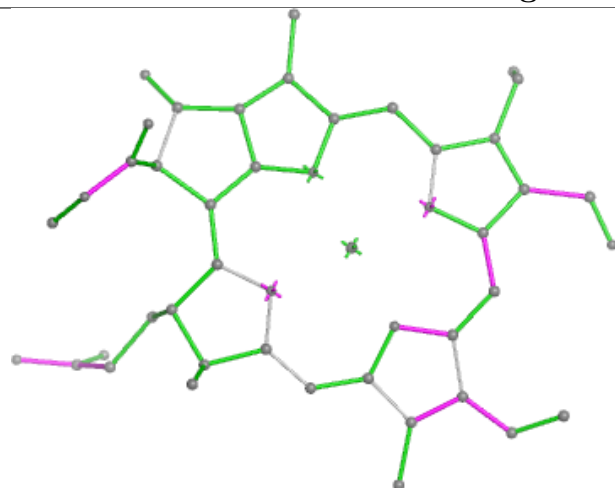
Rings



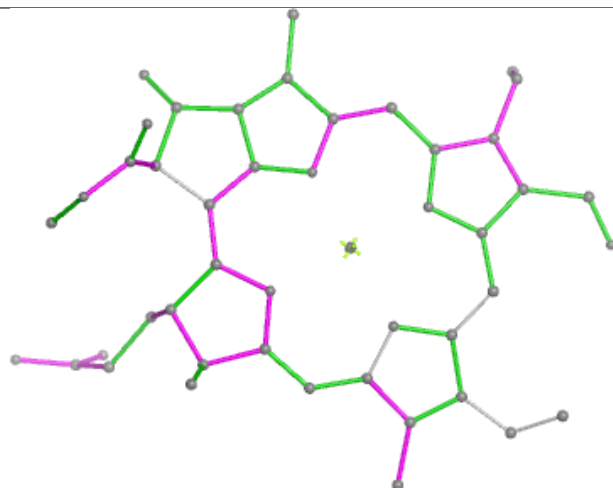
Ligand CLA A 805



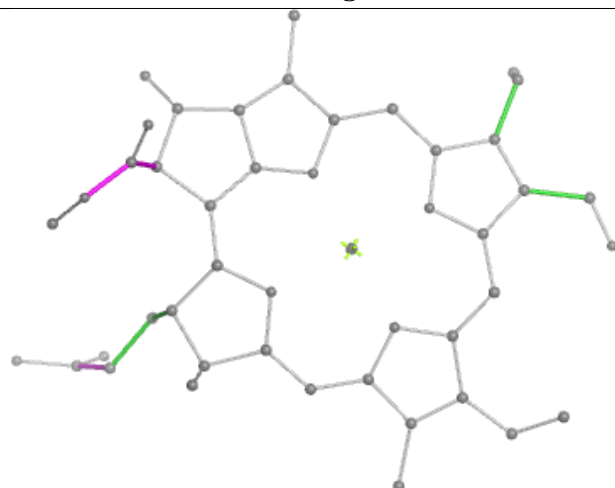
Ligand CHL 4 306



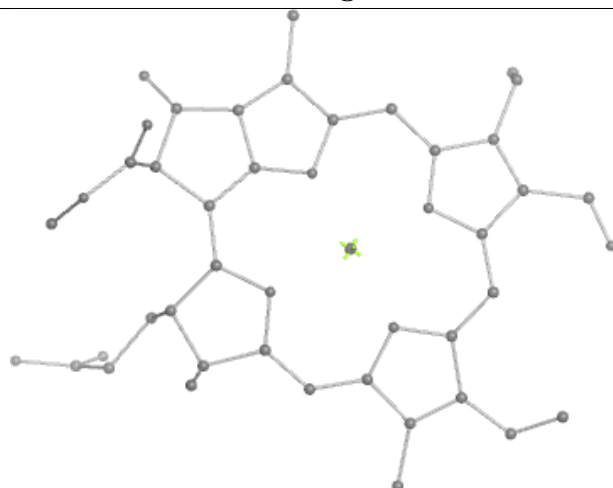
Bond lengths



Bond angles

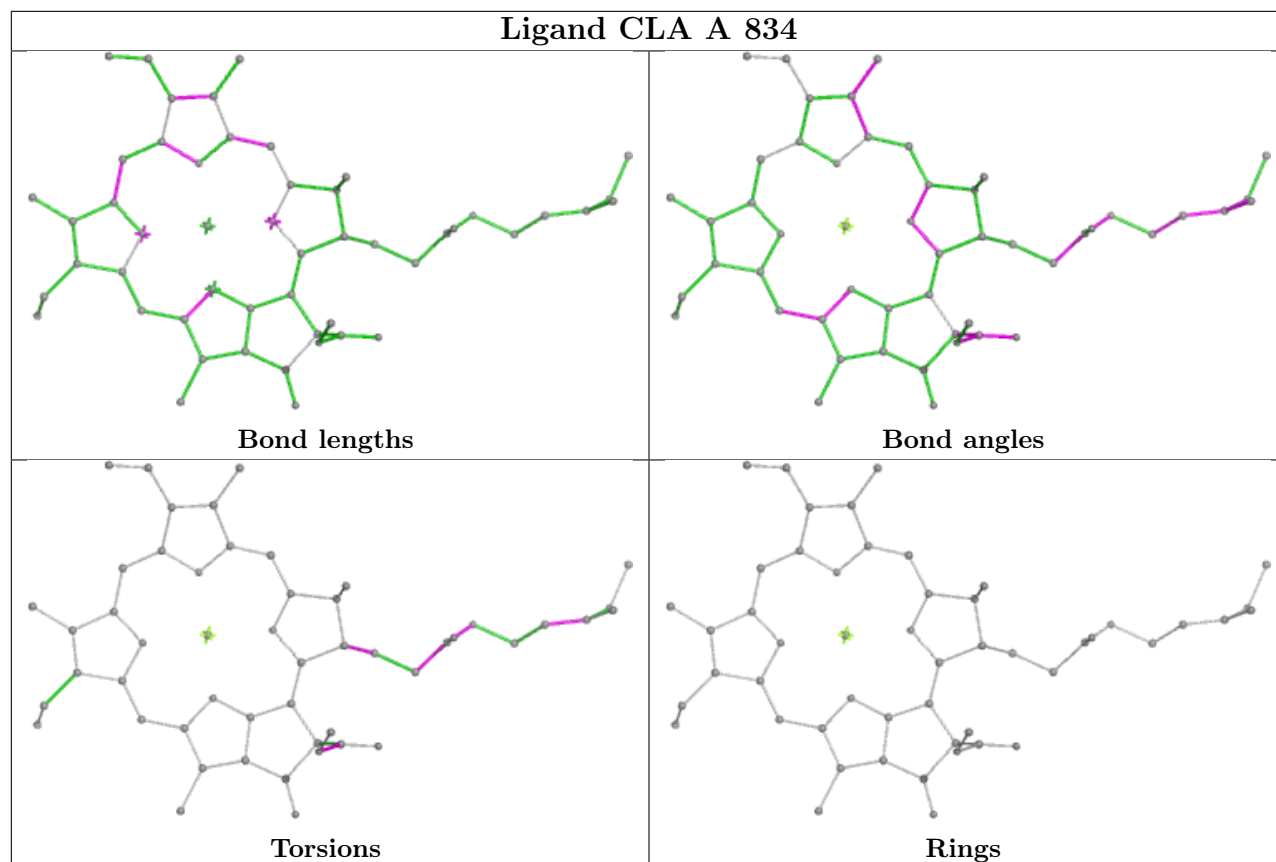


Torsions

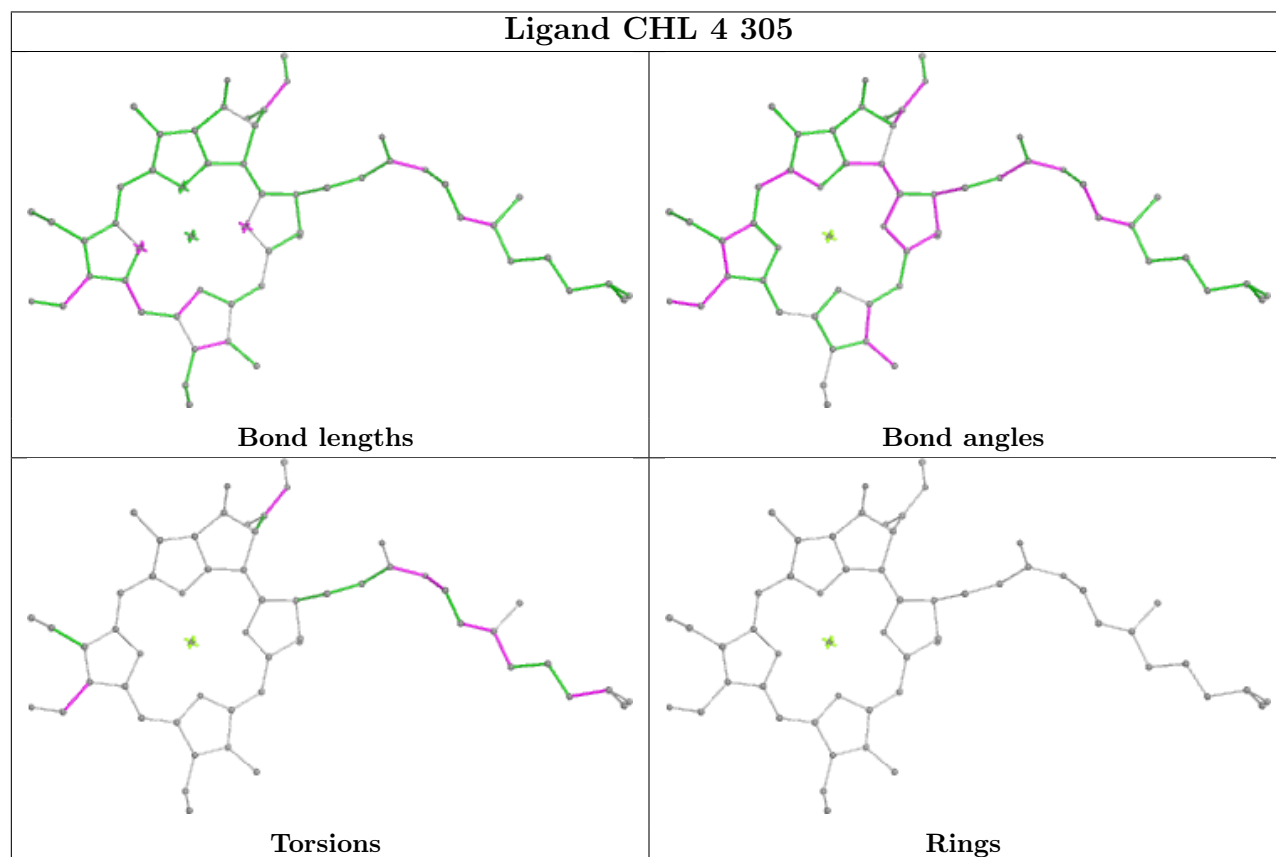


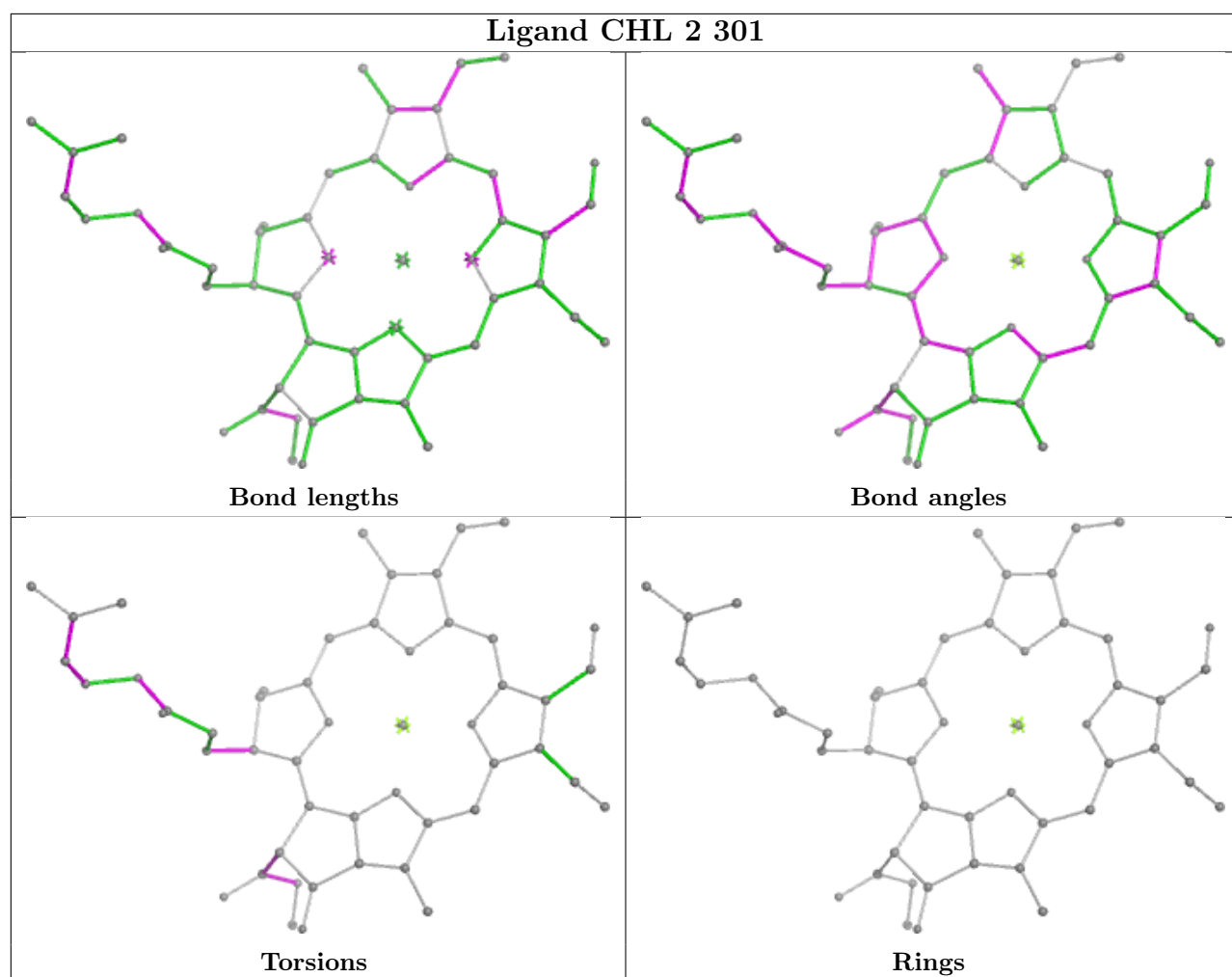
Rings

Ligand CLA A 834

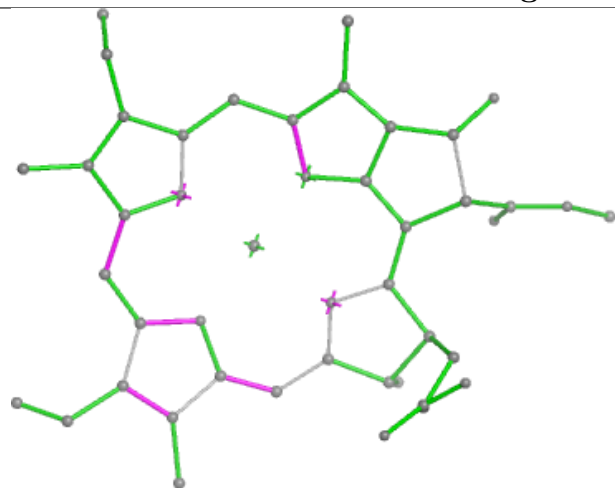


Ligand CHL 4 305

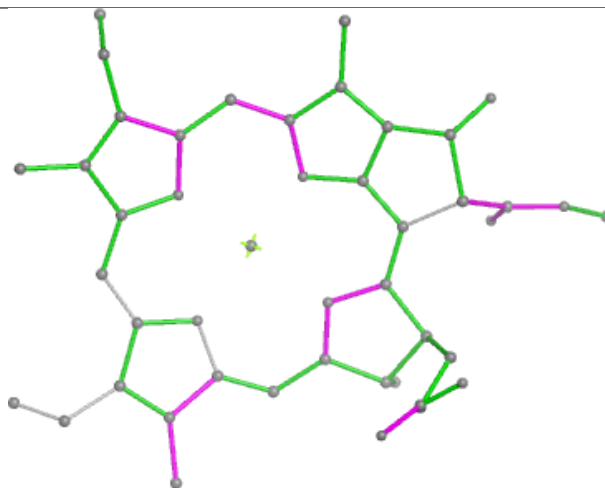




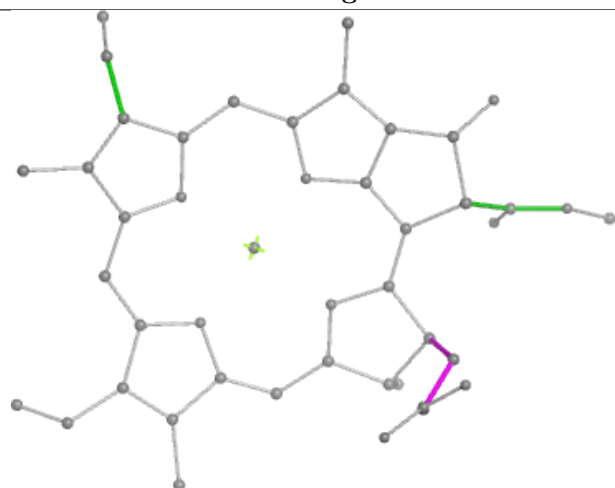
Ligand CLA 2 308



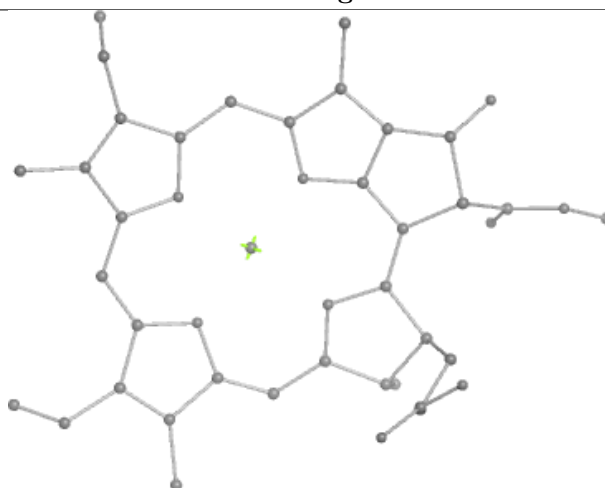
Bond lengths



Bond angles

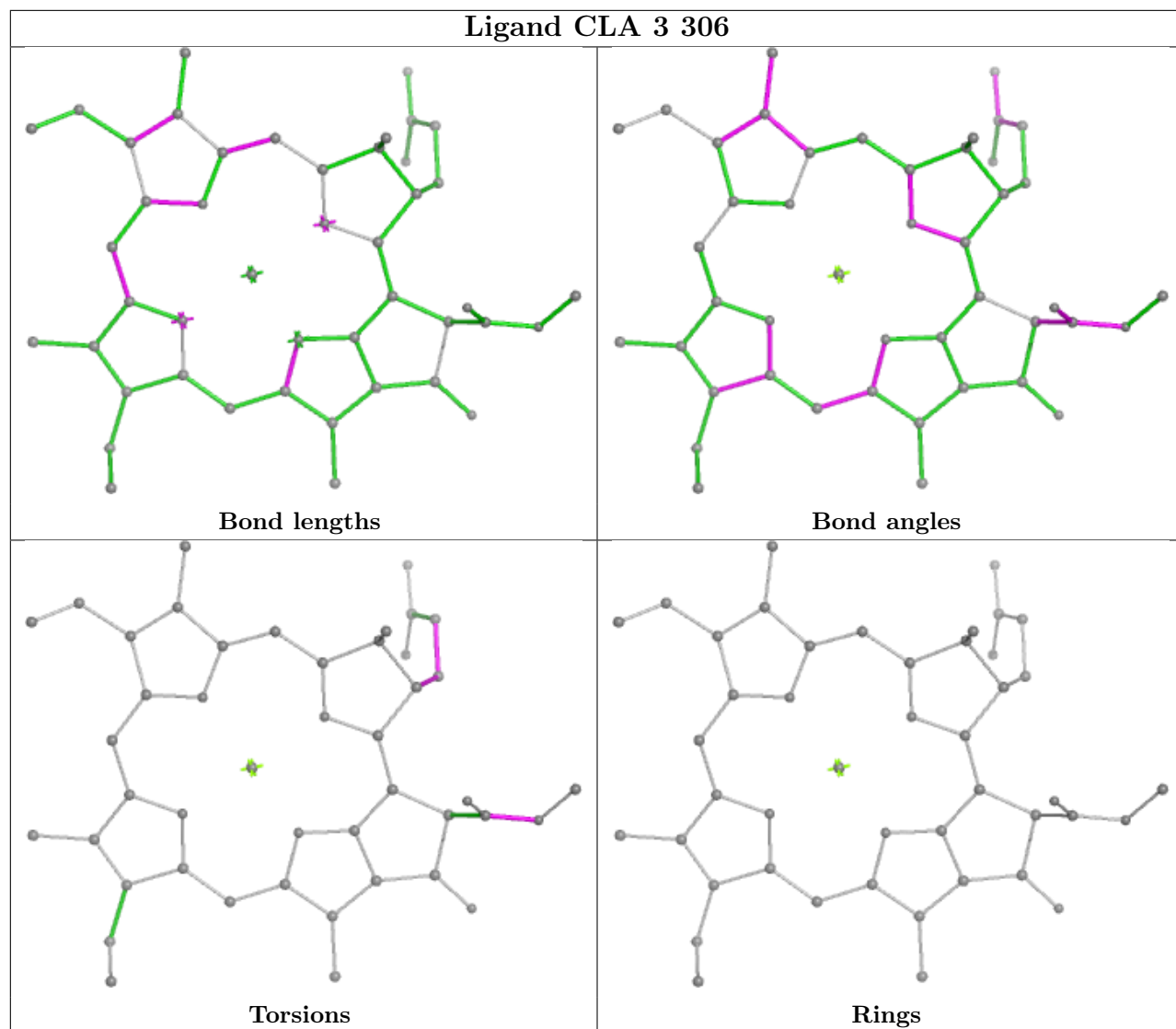


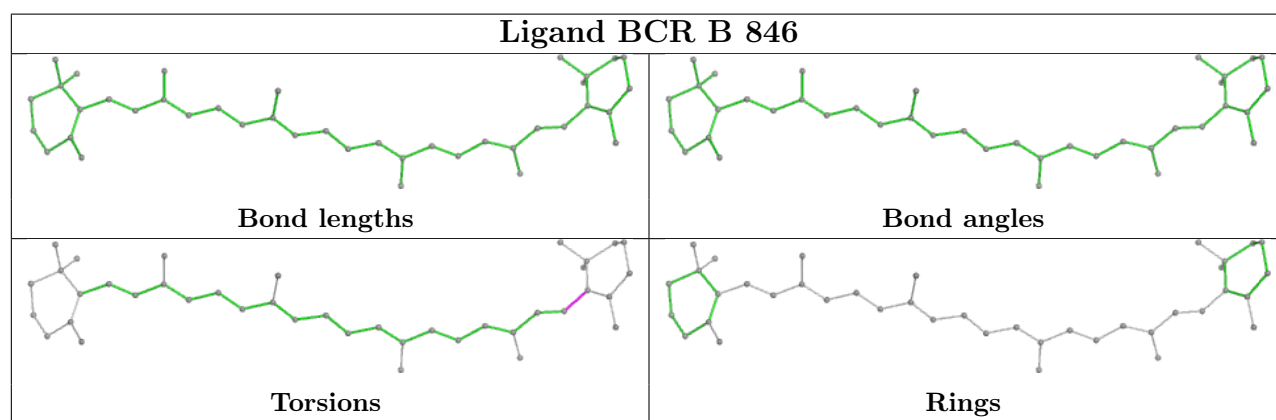
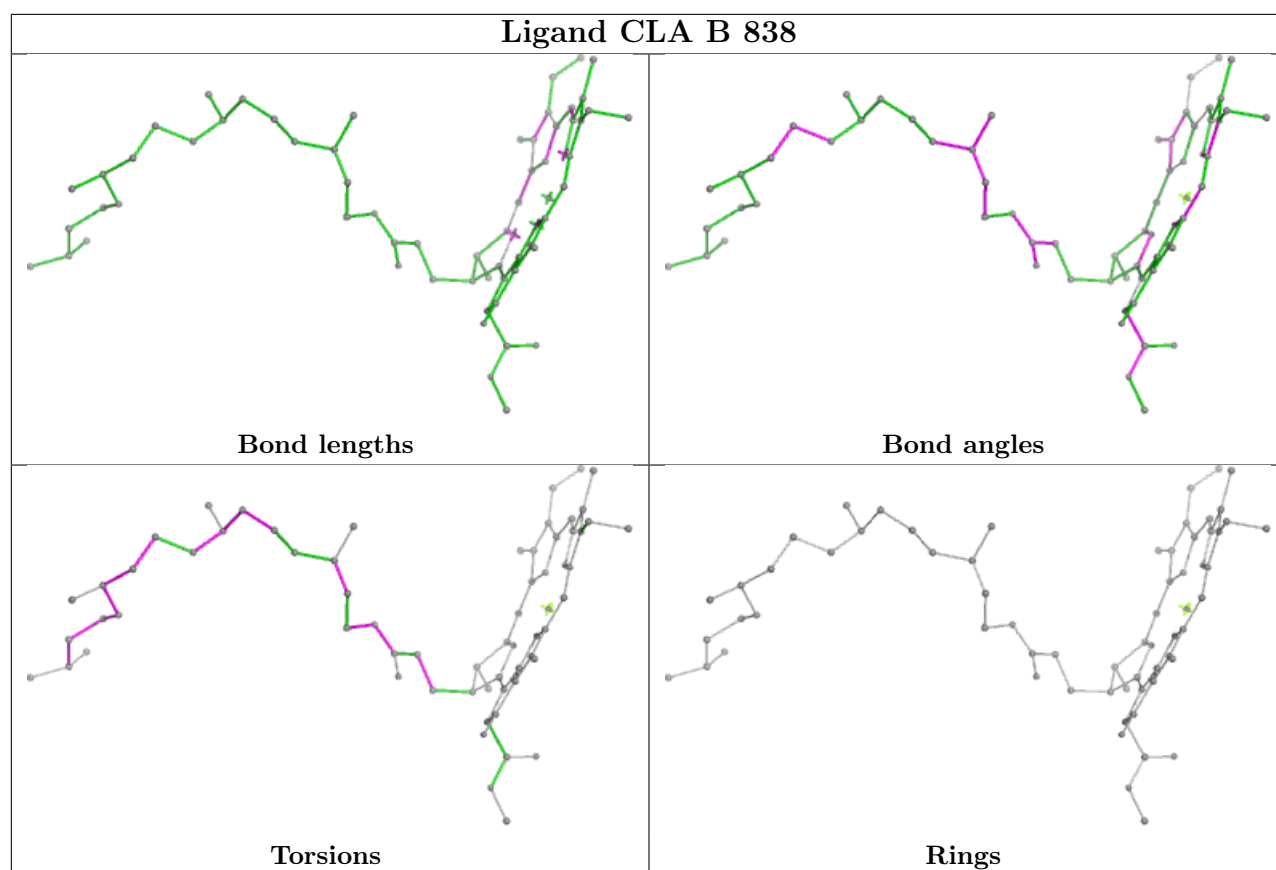
Torsions

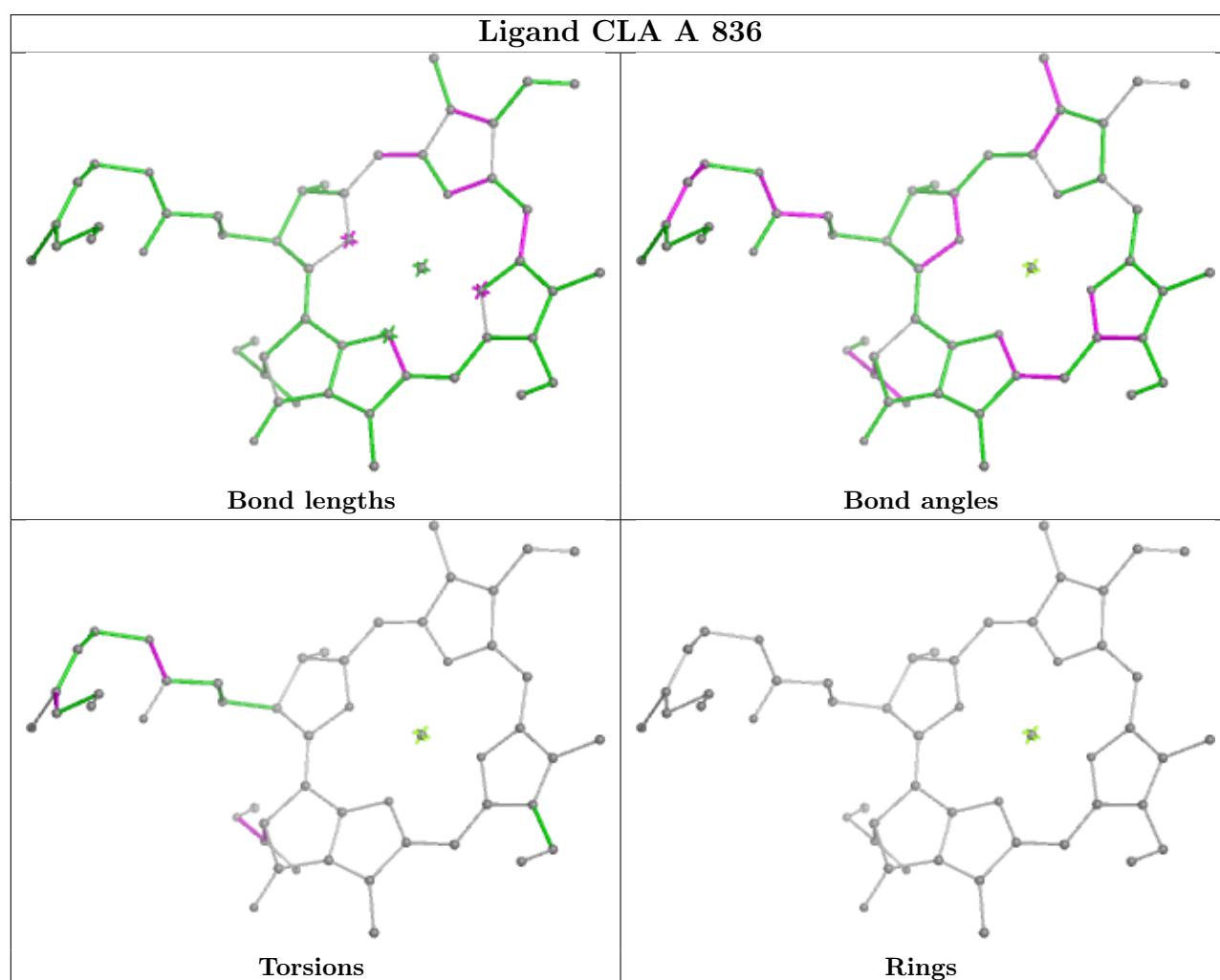
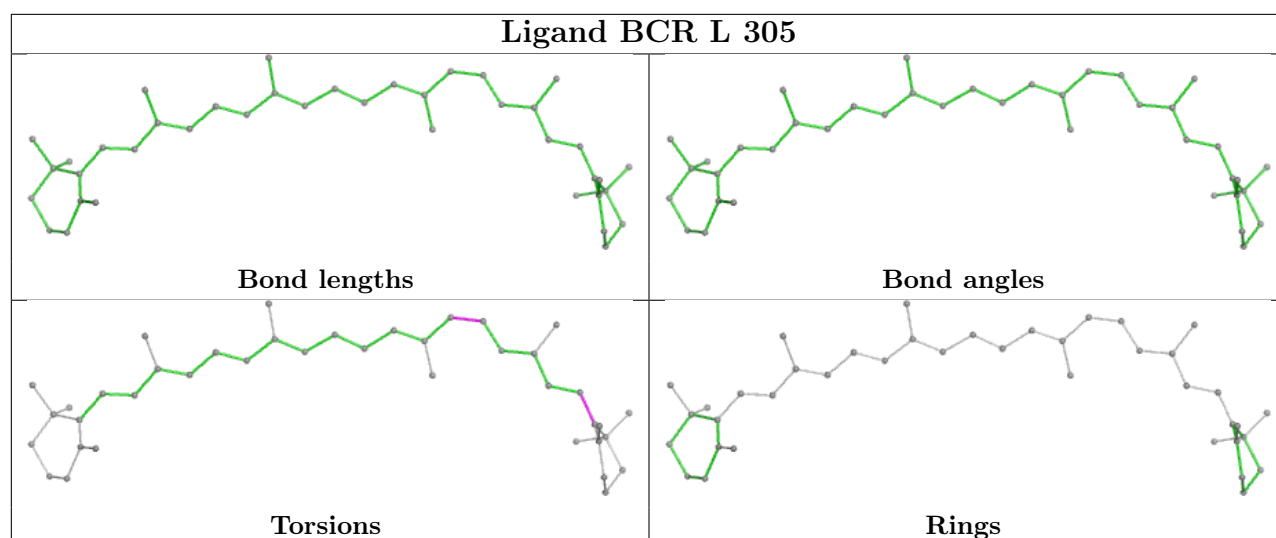


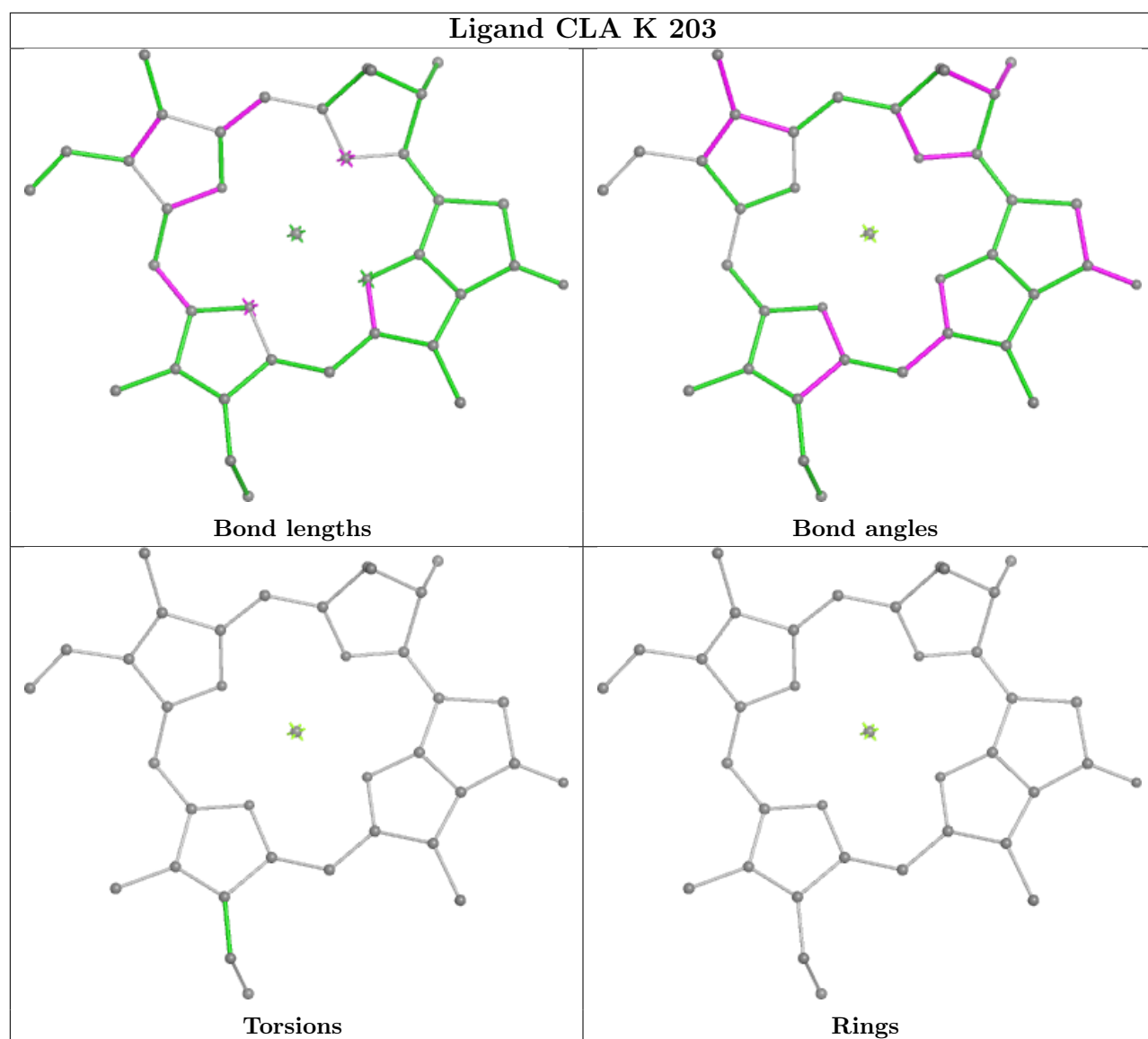
Rings

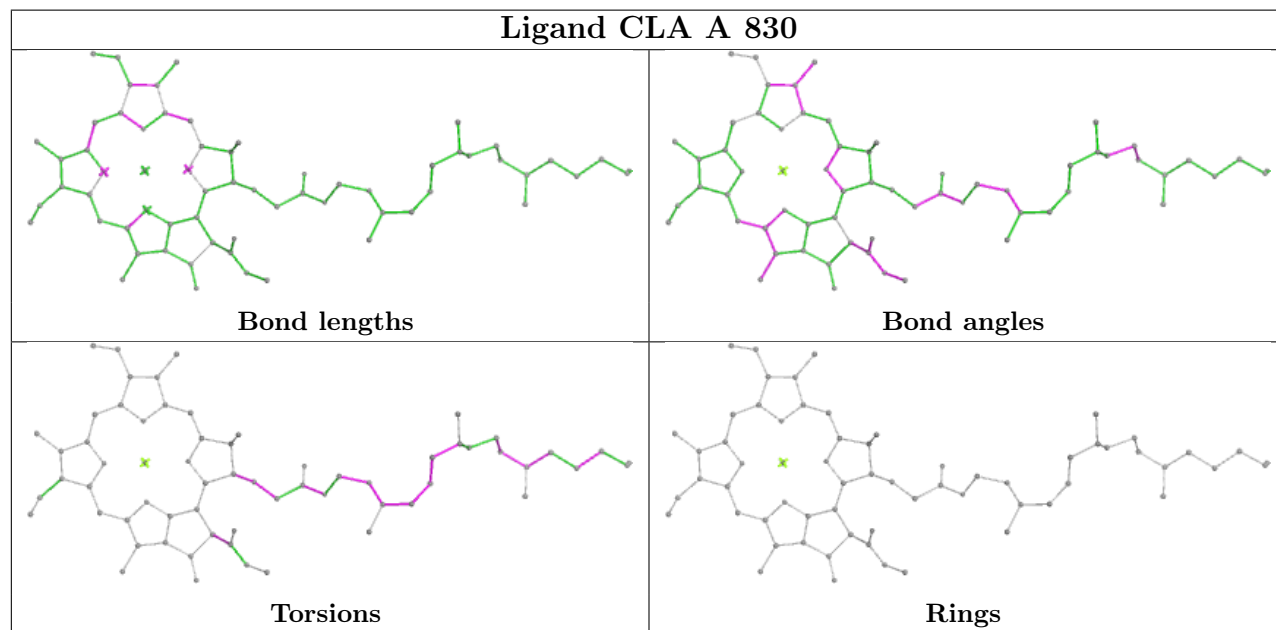
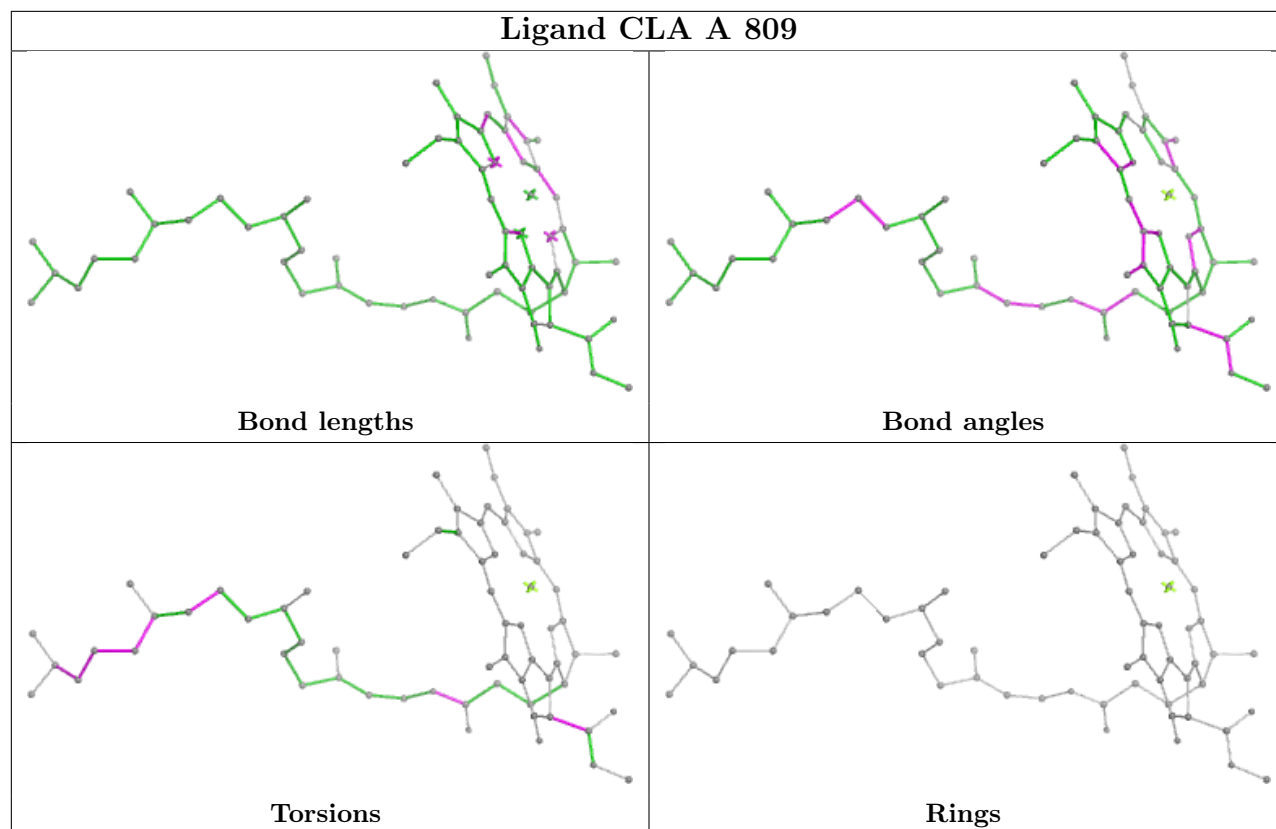
Ligand CLA 3 306



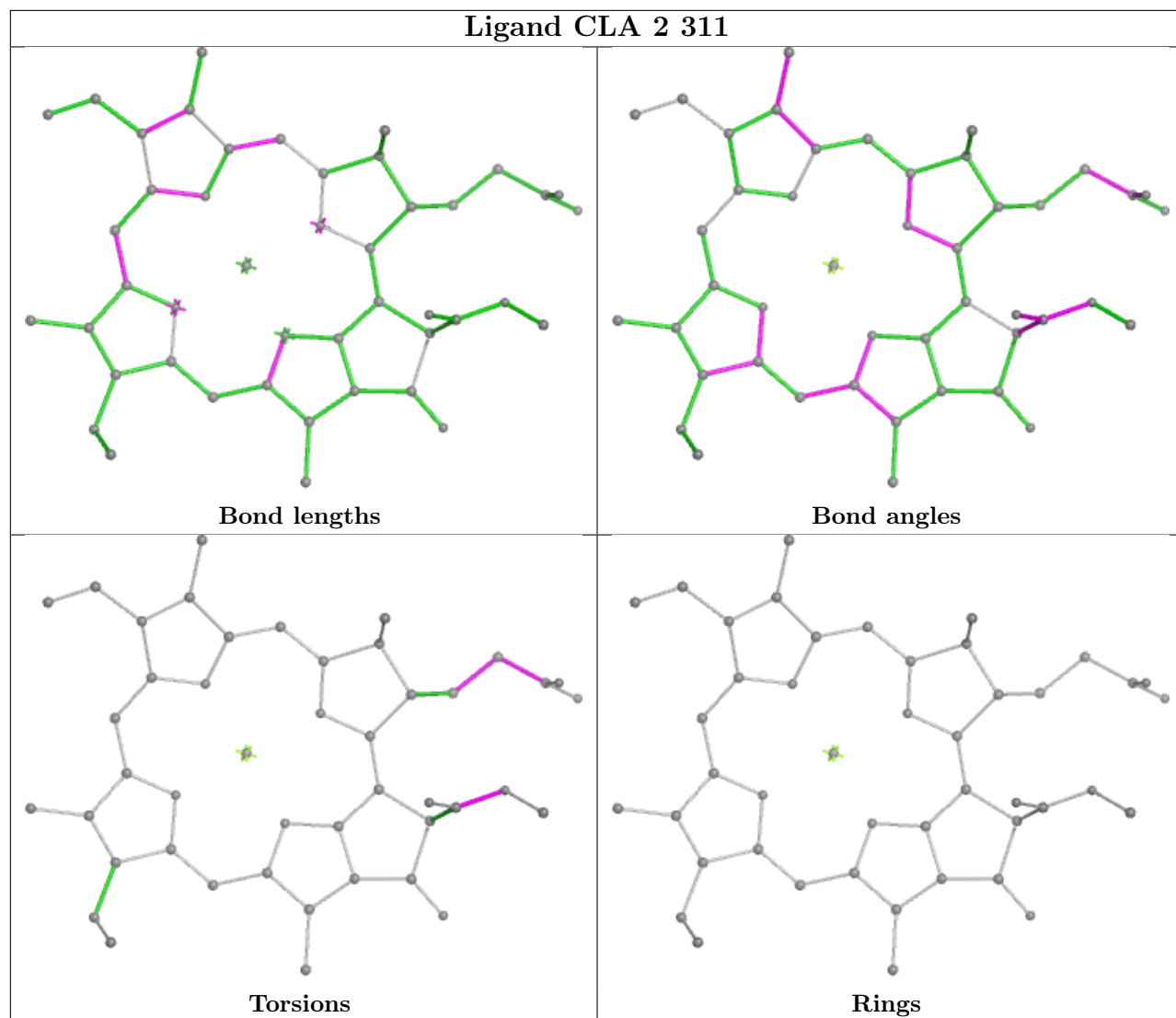




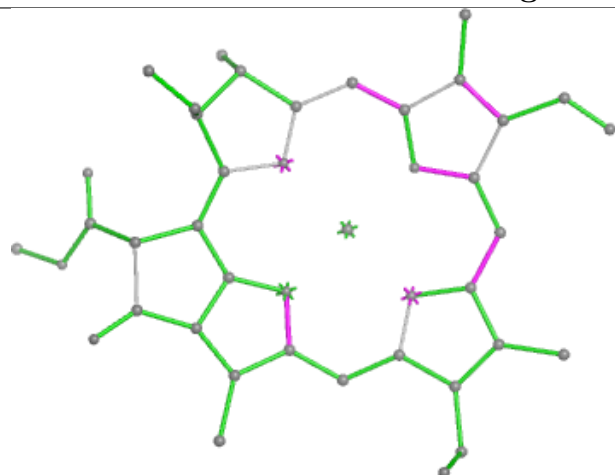




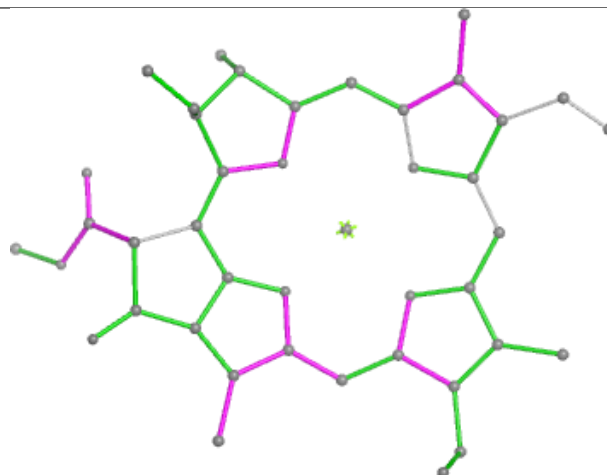
Ligand CLA 2 311



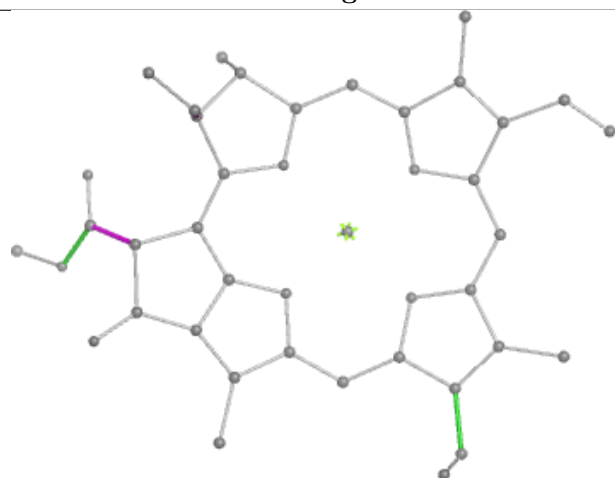
Ligand CLA J 102



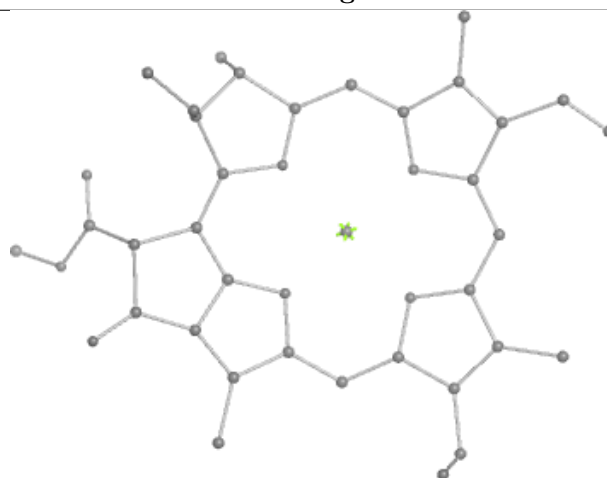
Bond lengths



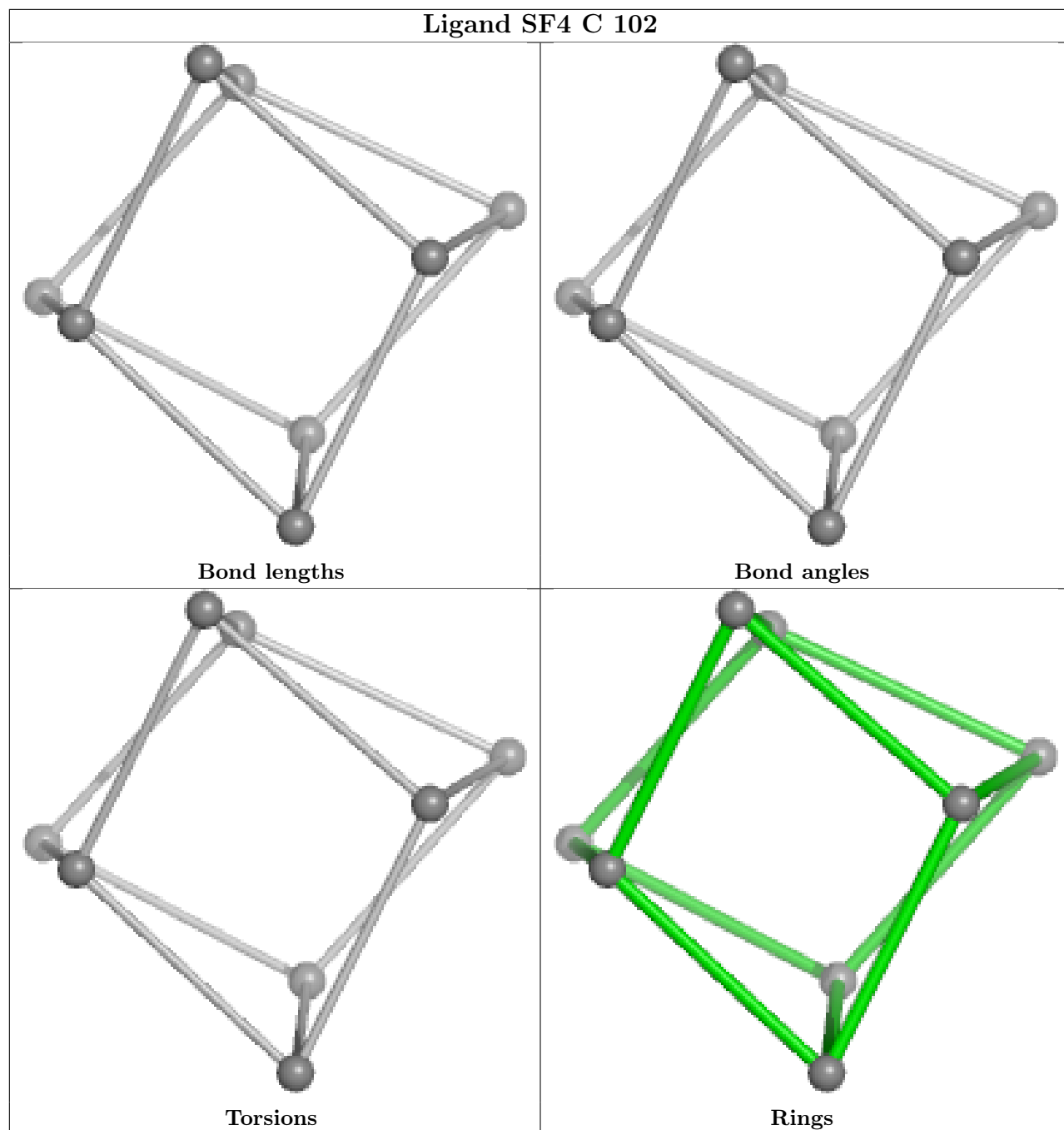
Bond angles

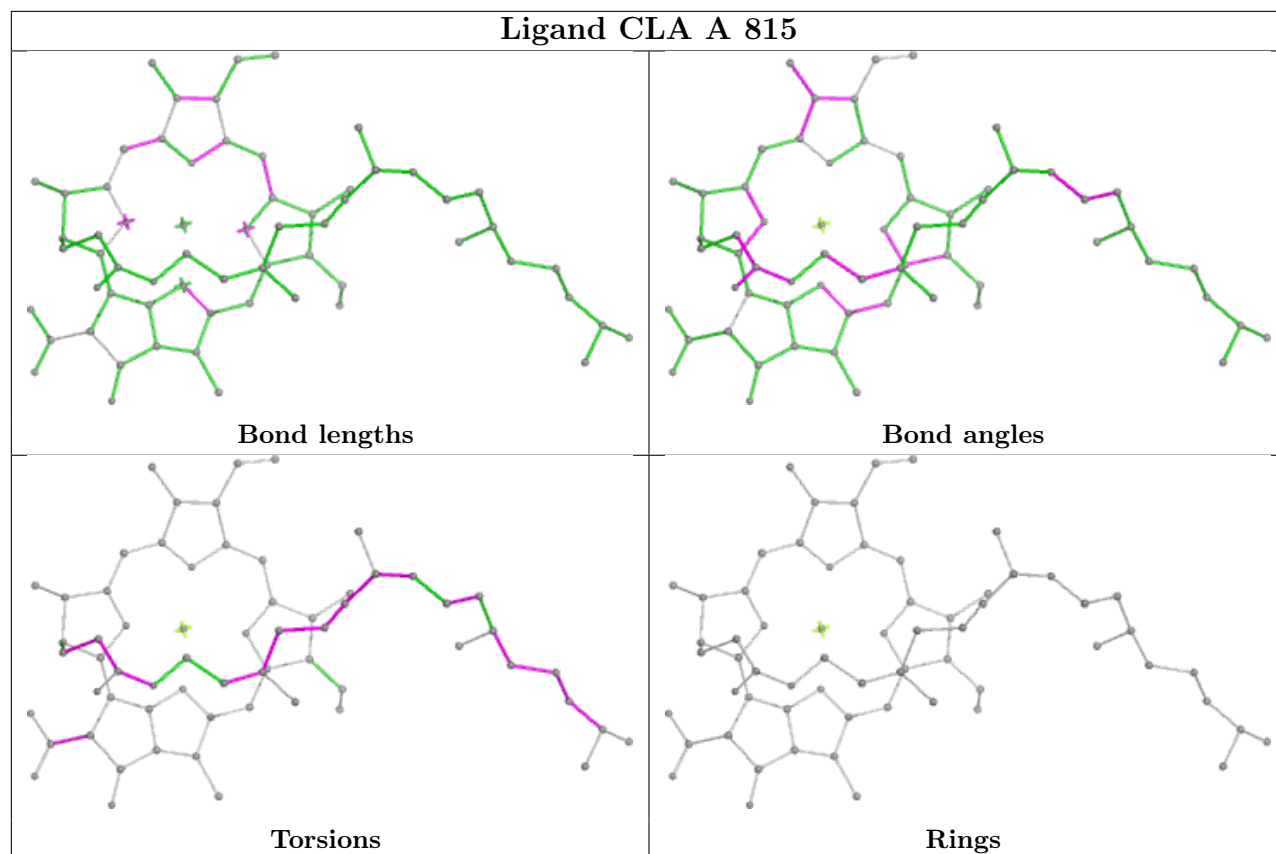
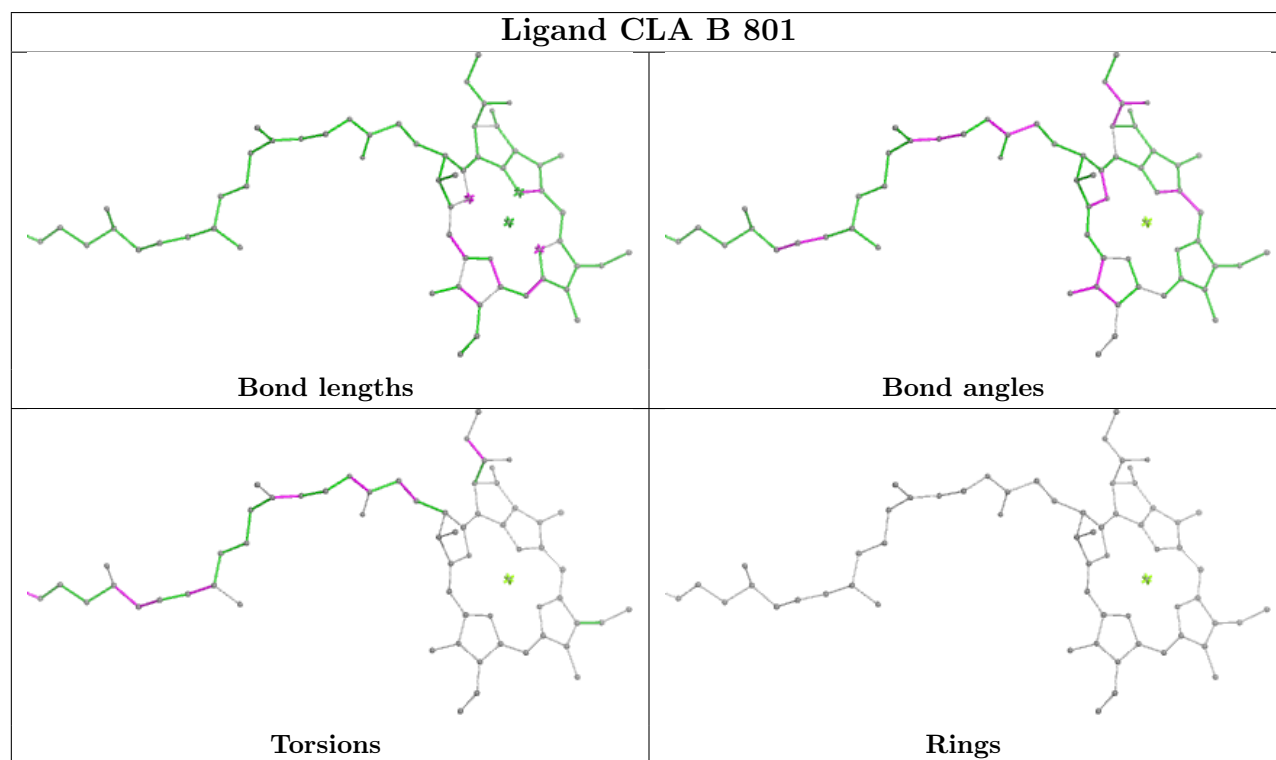


Torsions

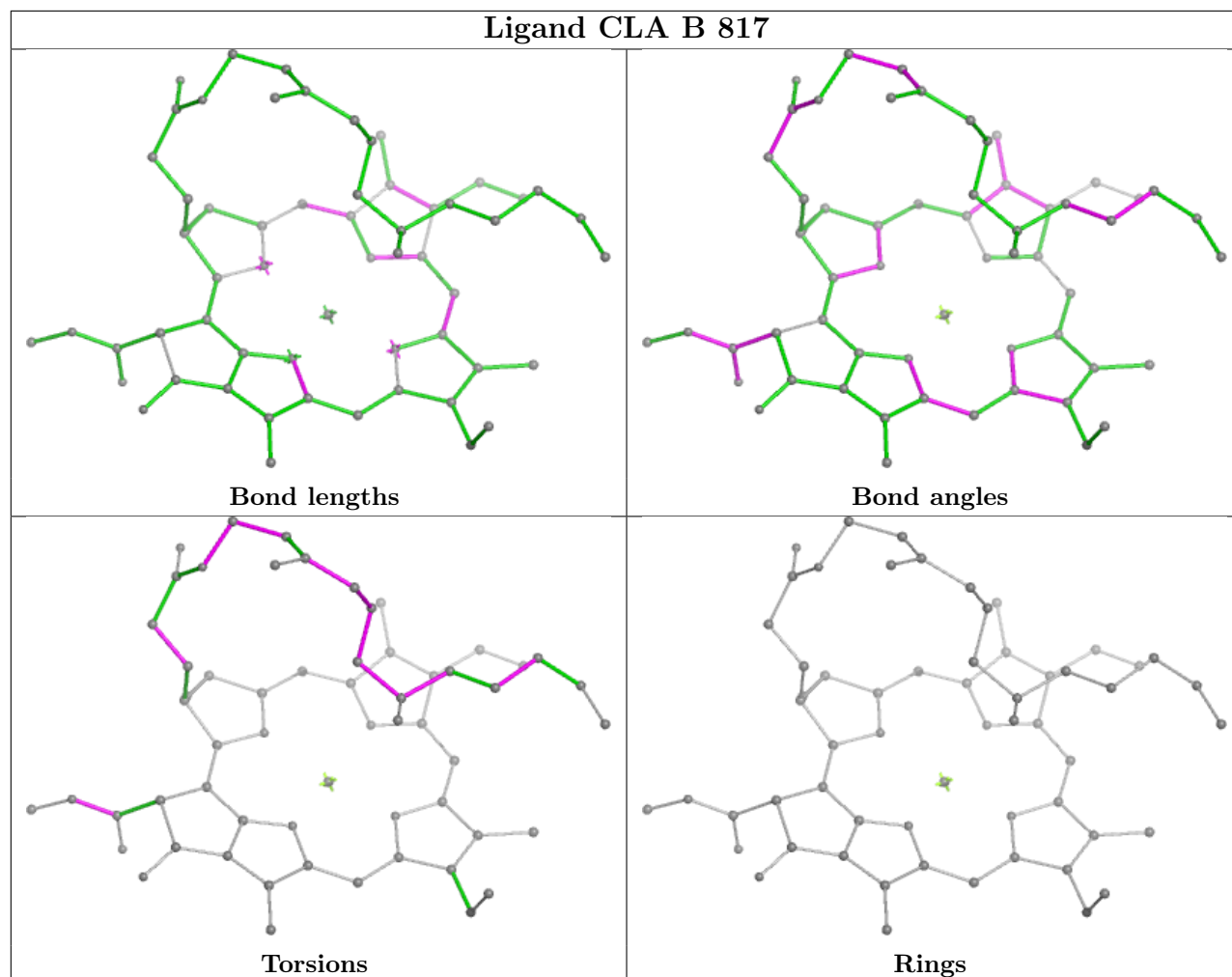


Rings

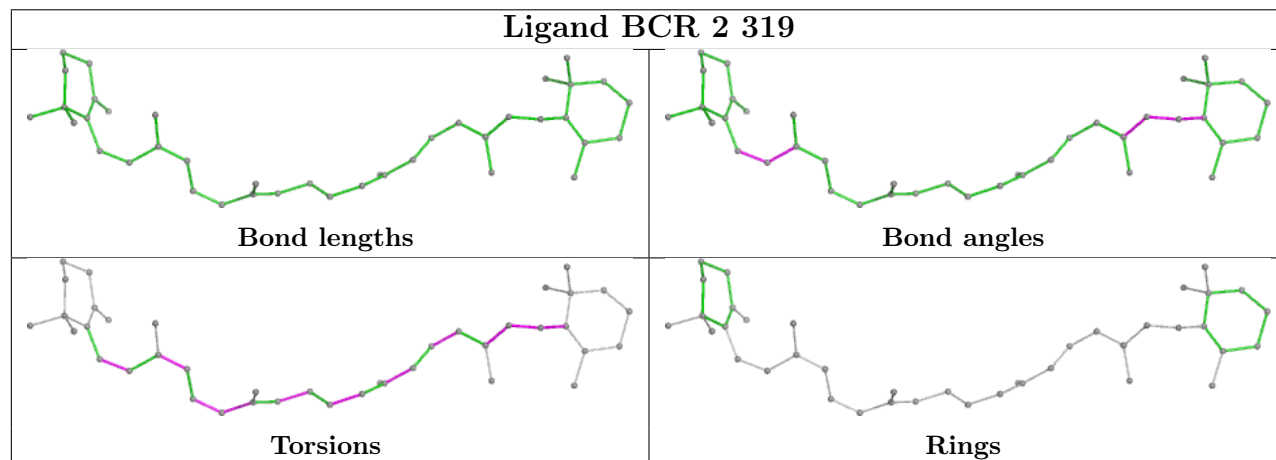


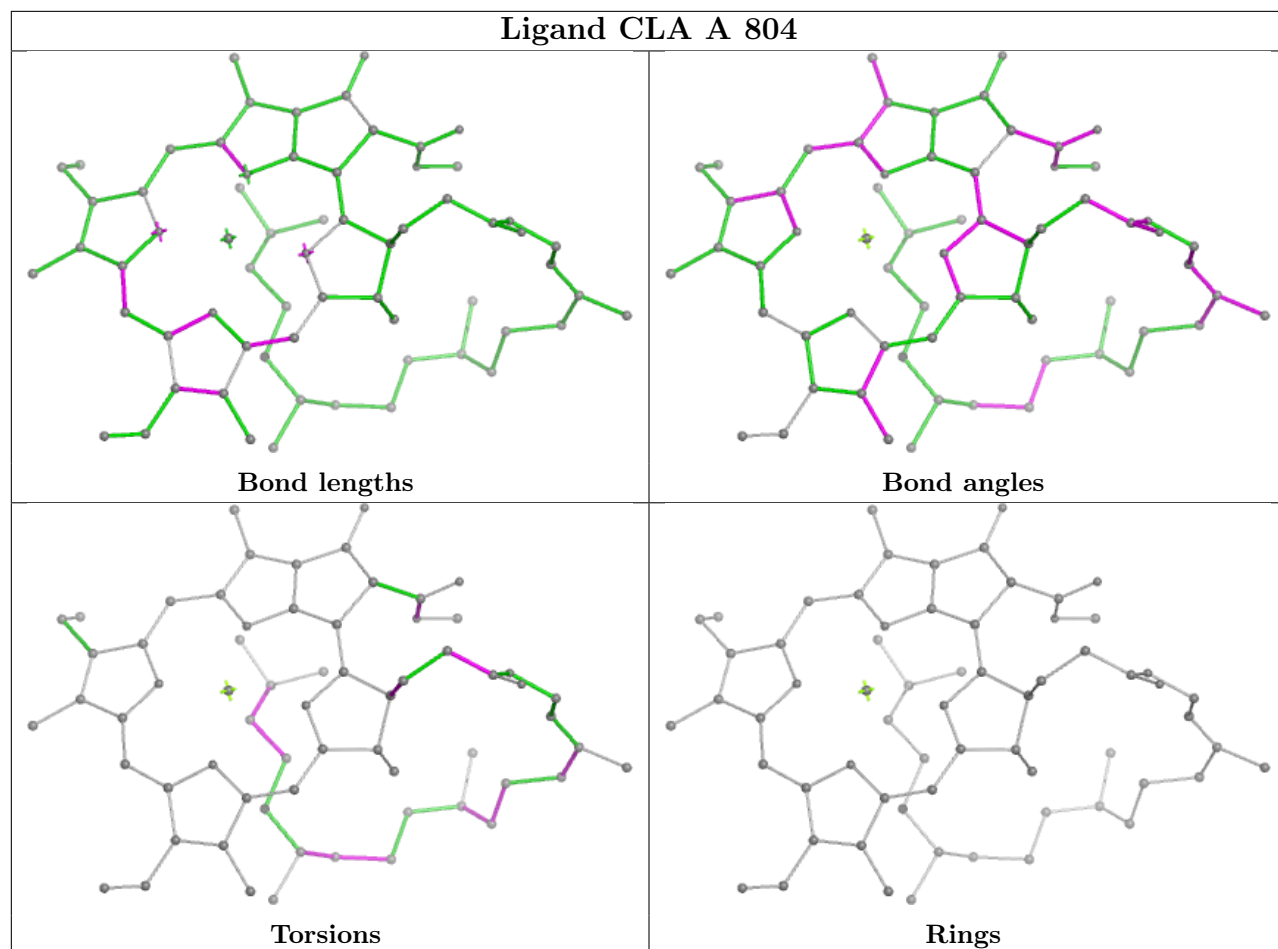
Ligand CLA A 815**Ligand CLA B 801**

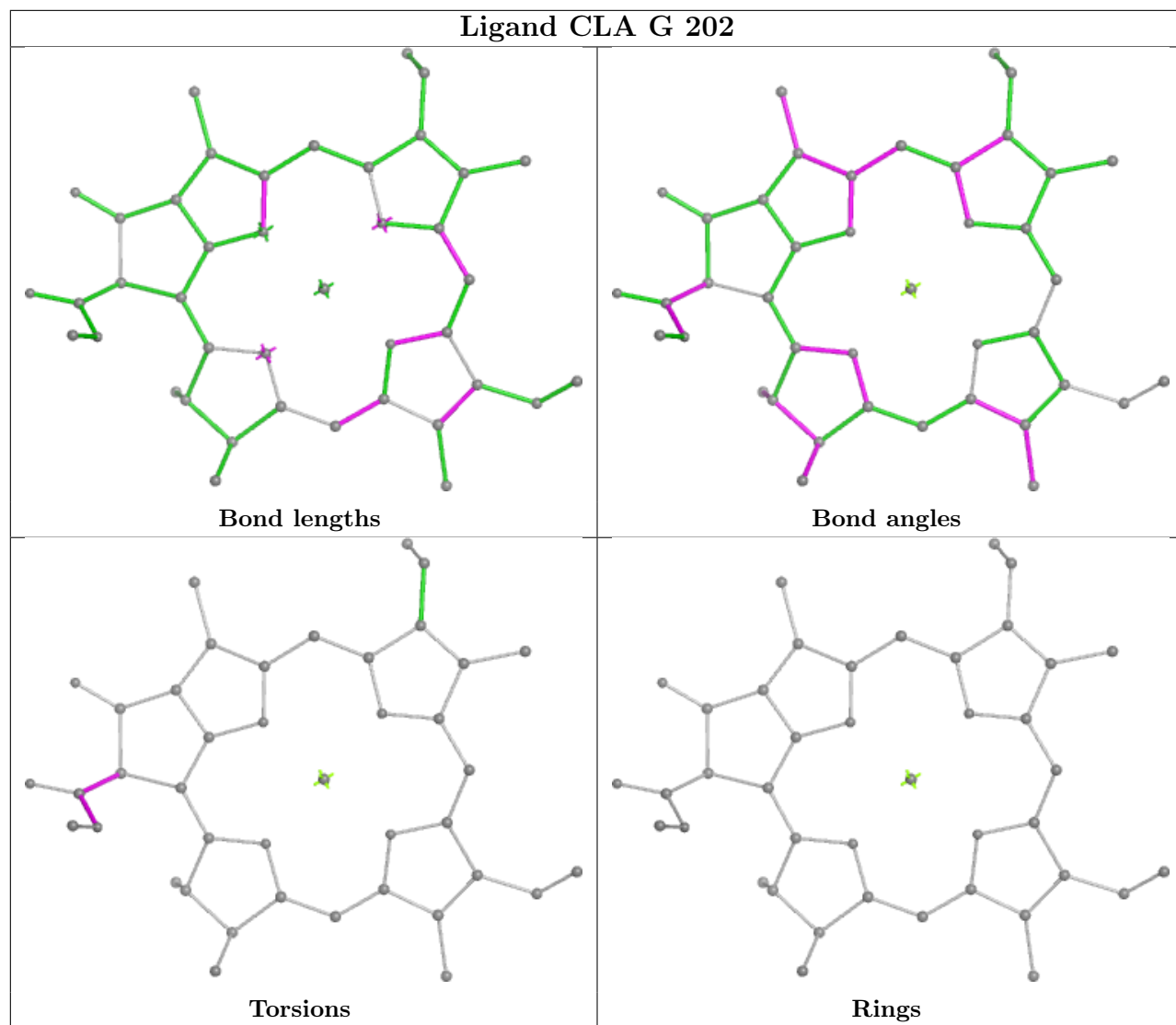
Ligand CLA B 817

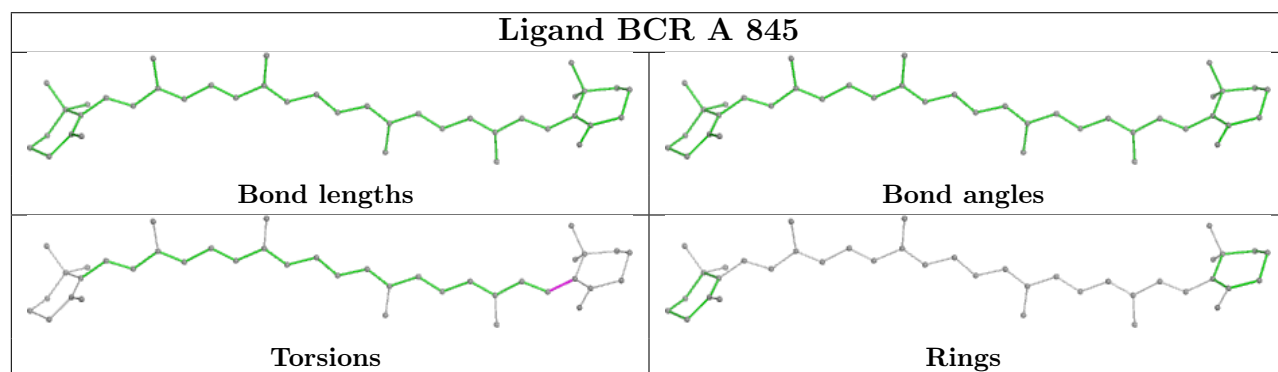
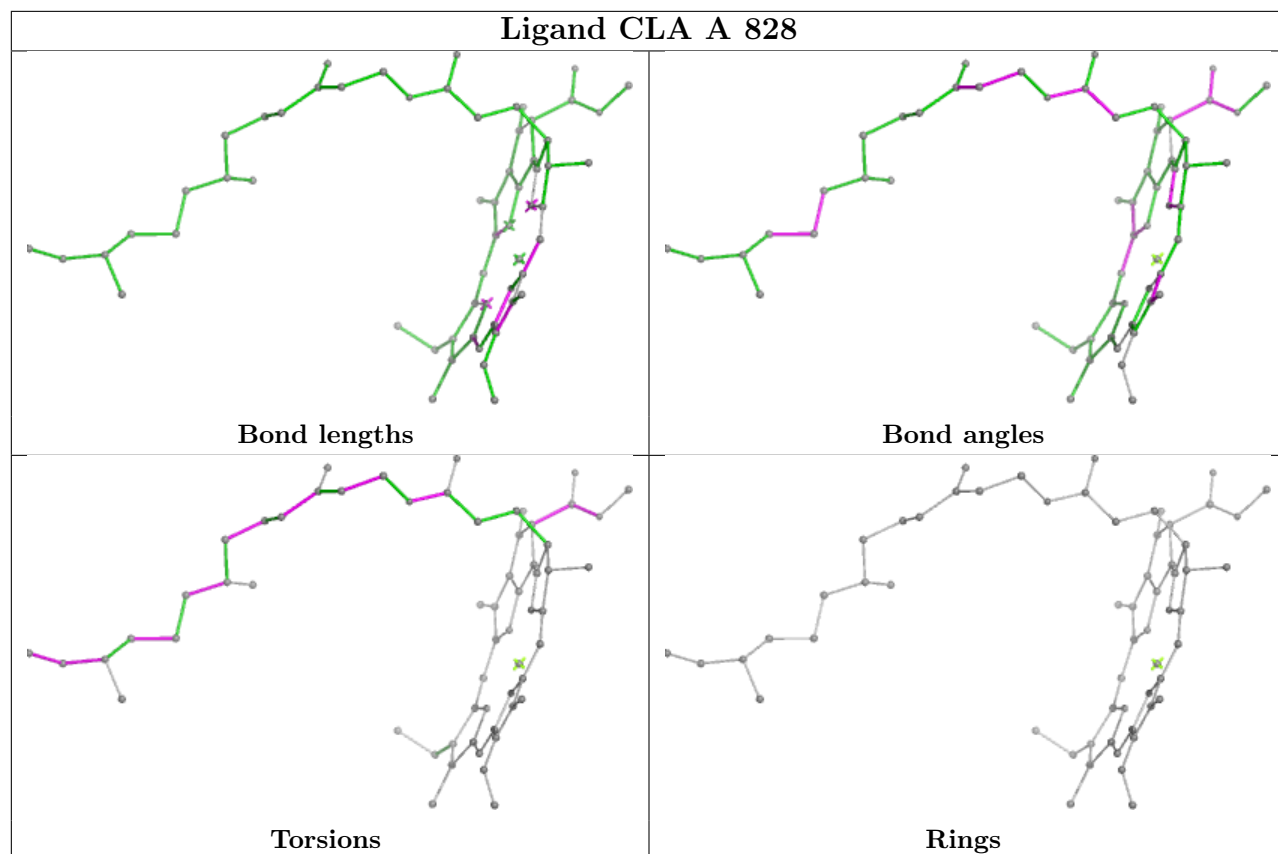


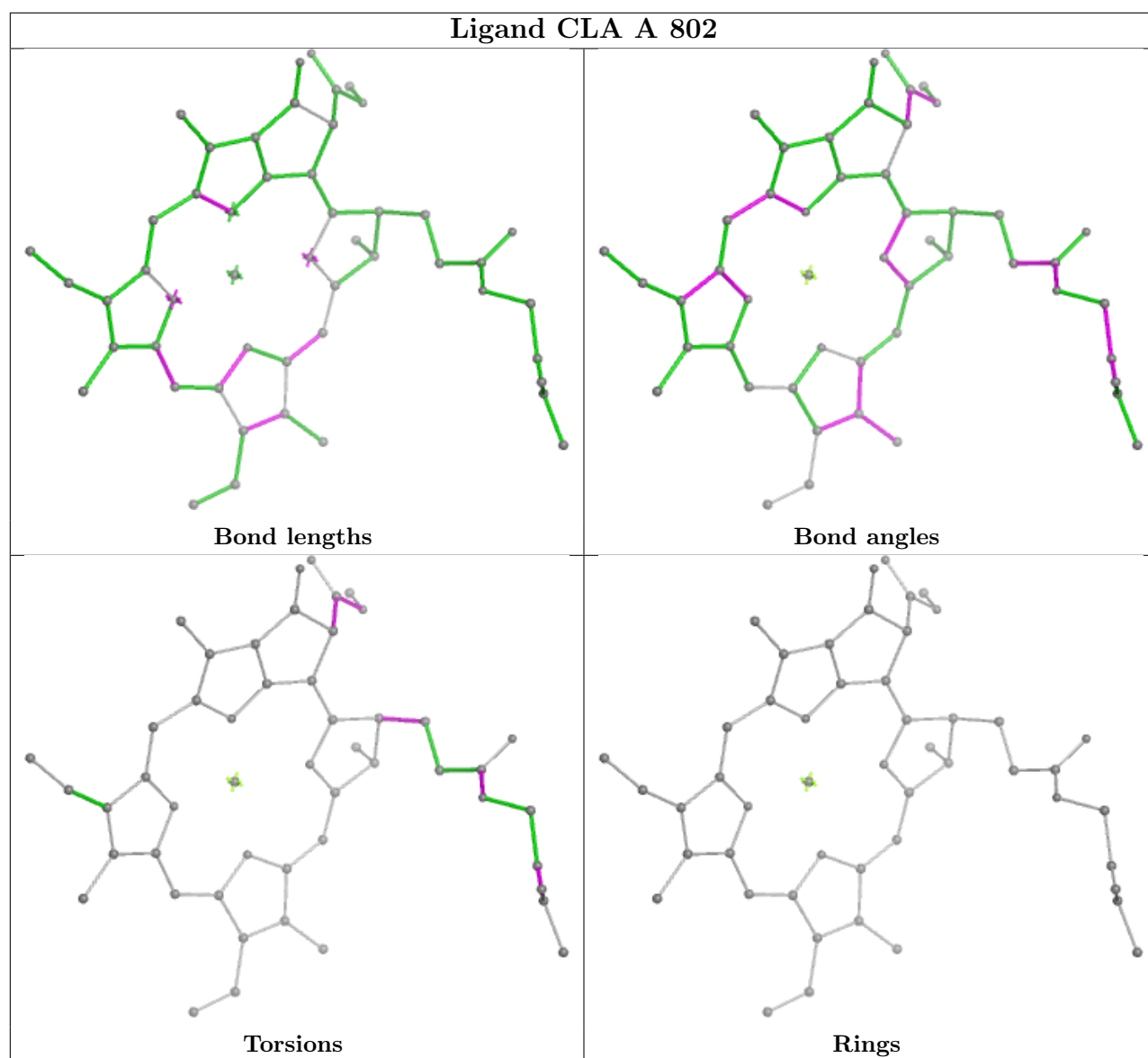
Ligand BCR 2 319



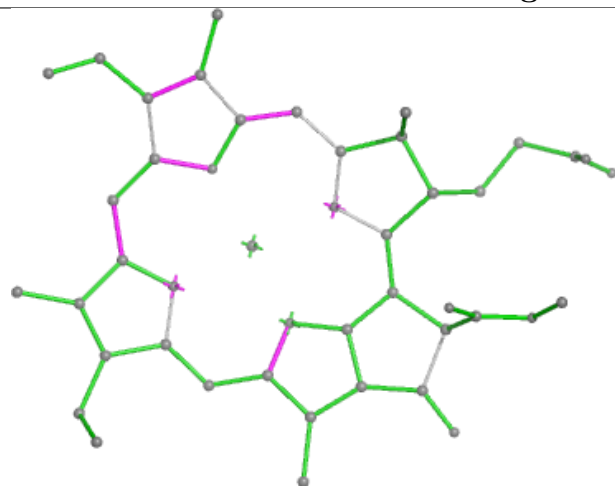




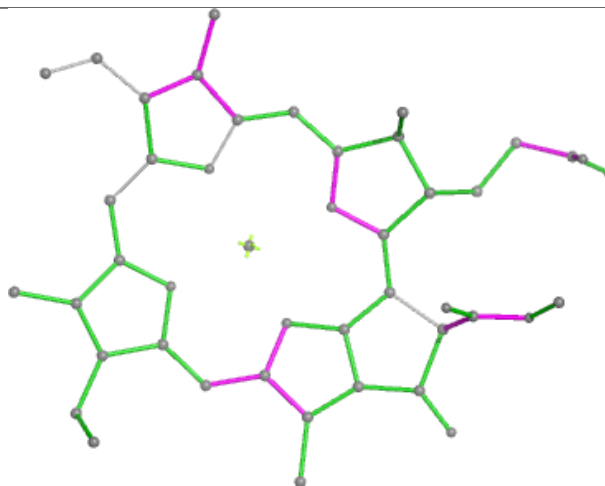




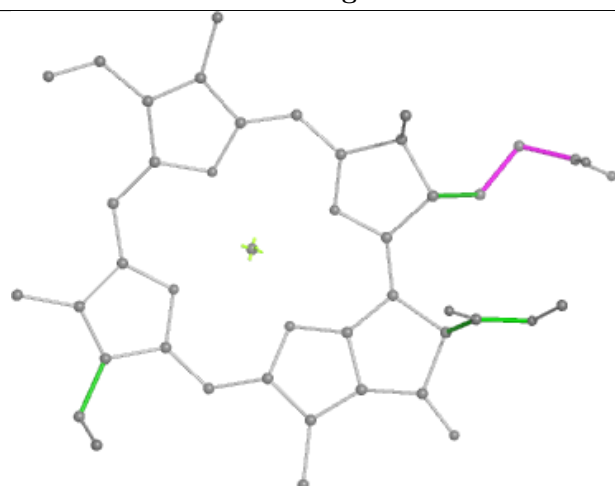
Ligand CLA 4 311



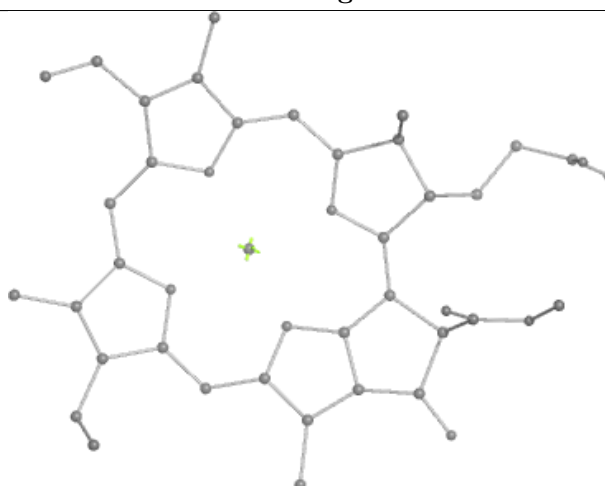
Bond lengths



Bond angles

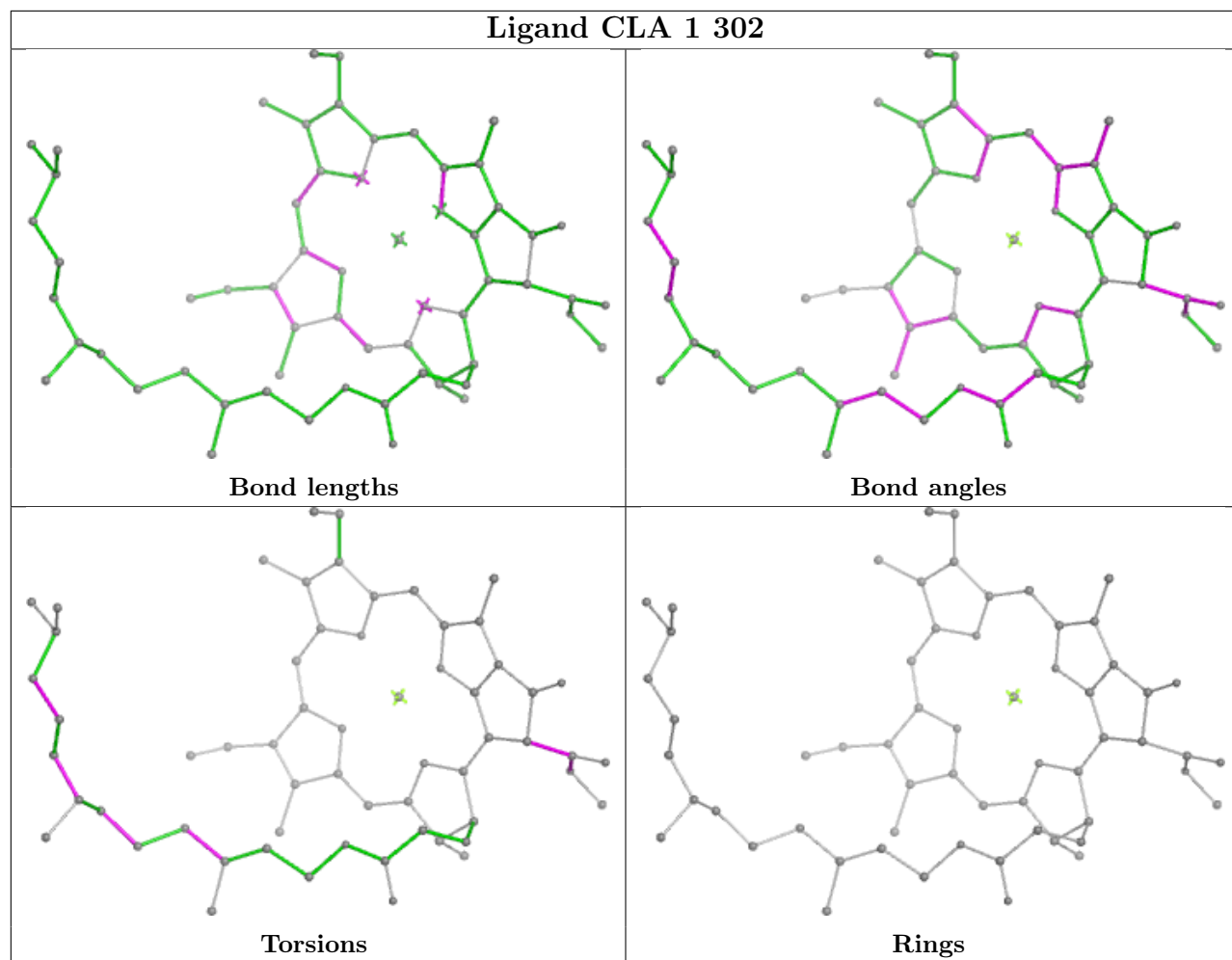


Torsions

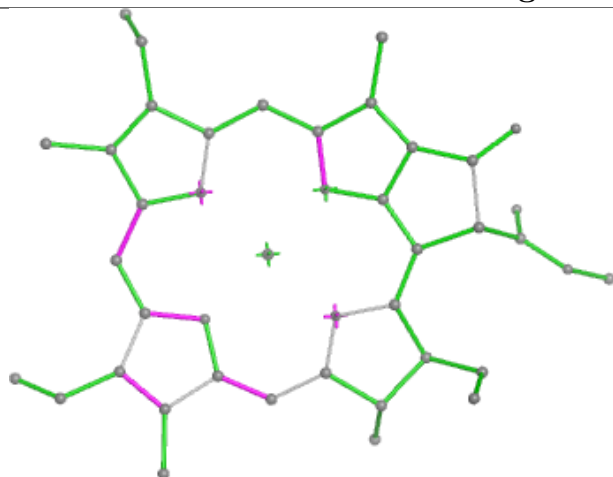


Rings

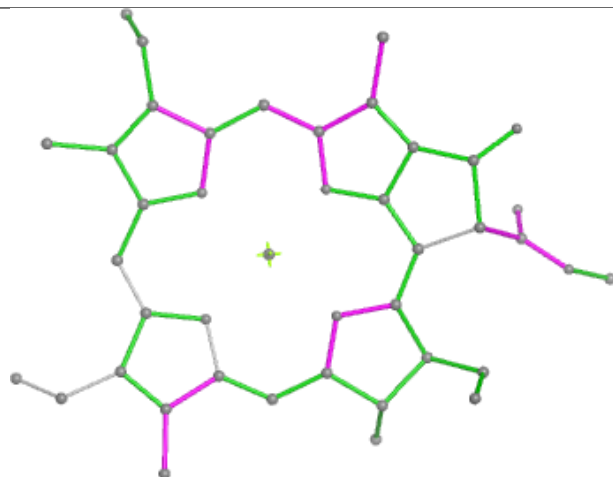
Ligand CLA 1 302



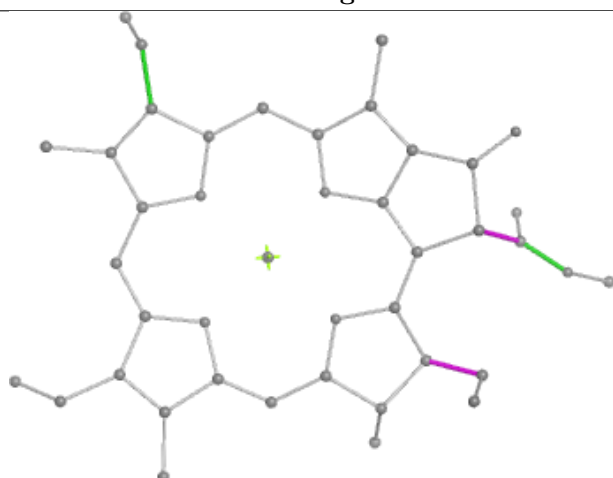
Ligand CLA 3 305



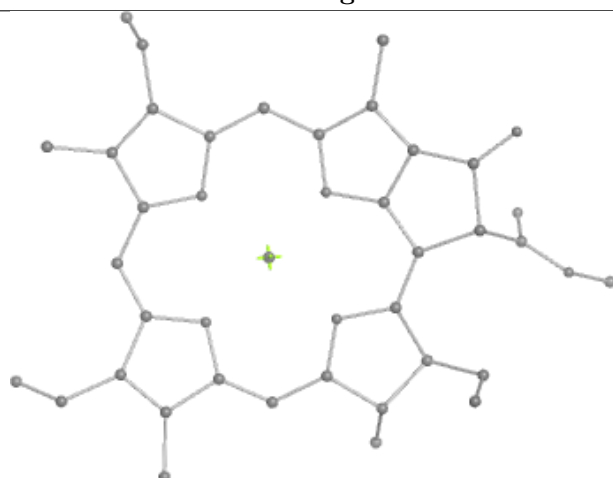
Bond lengths



Bond angles

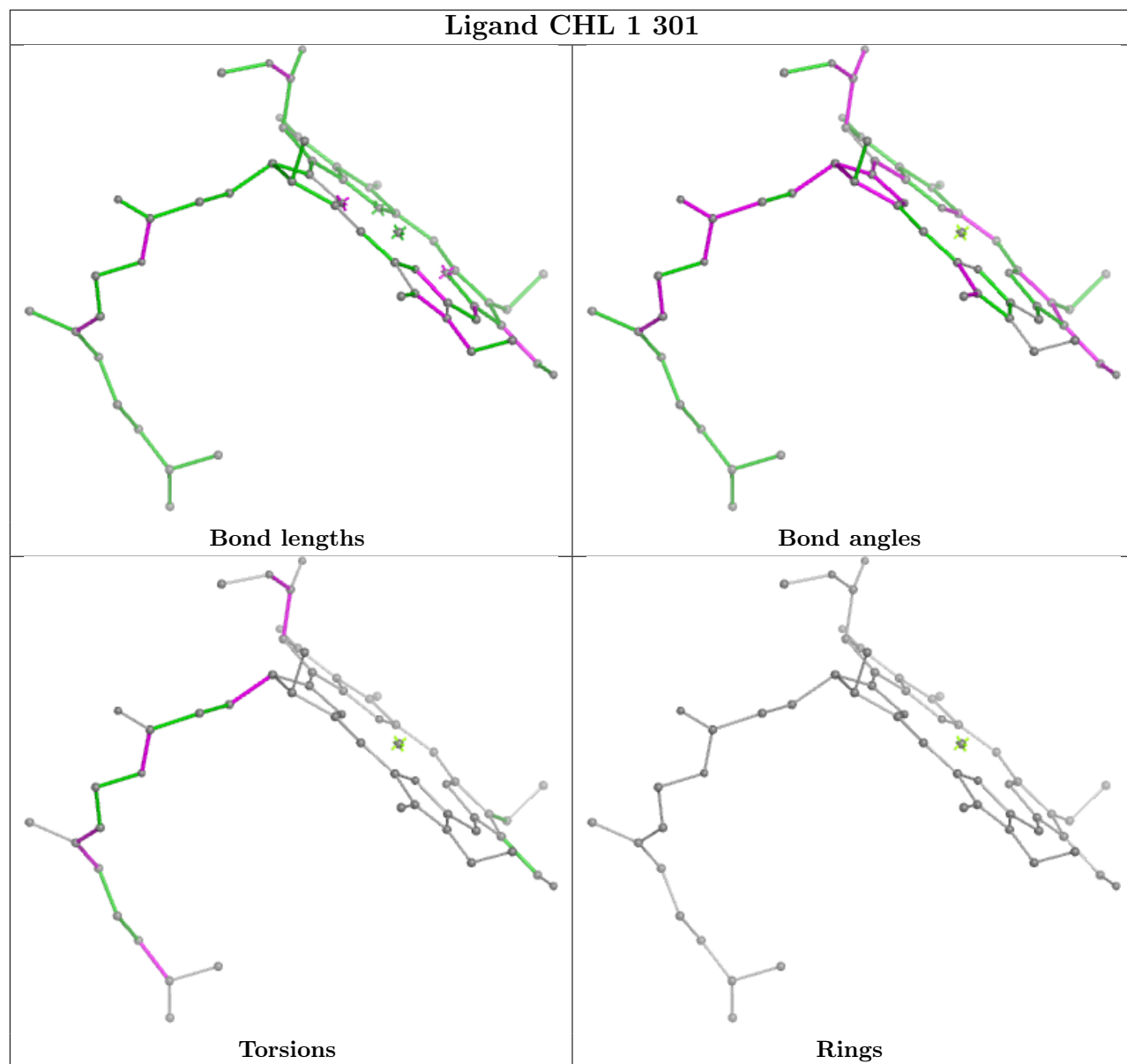


Torsions

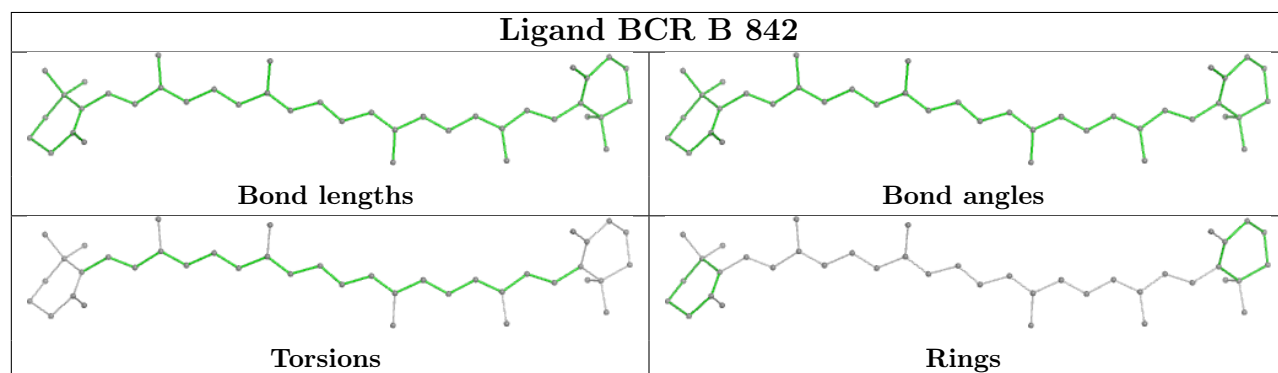


Rings

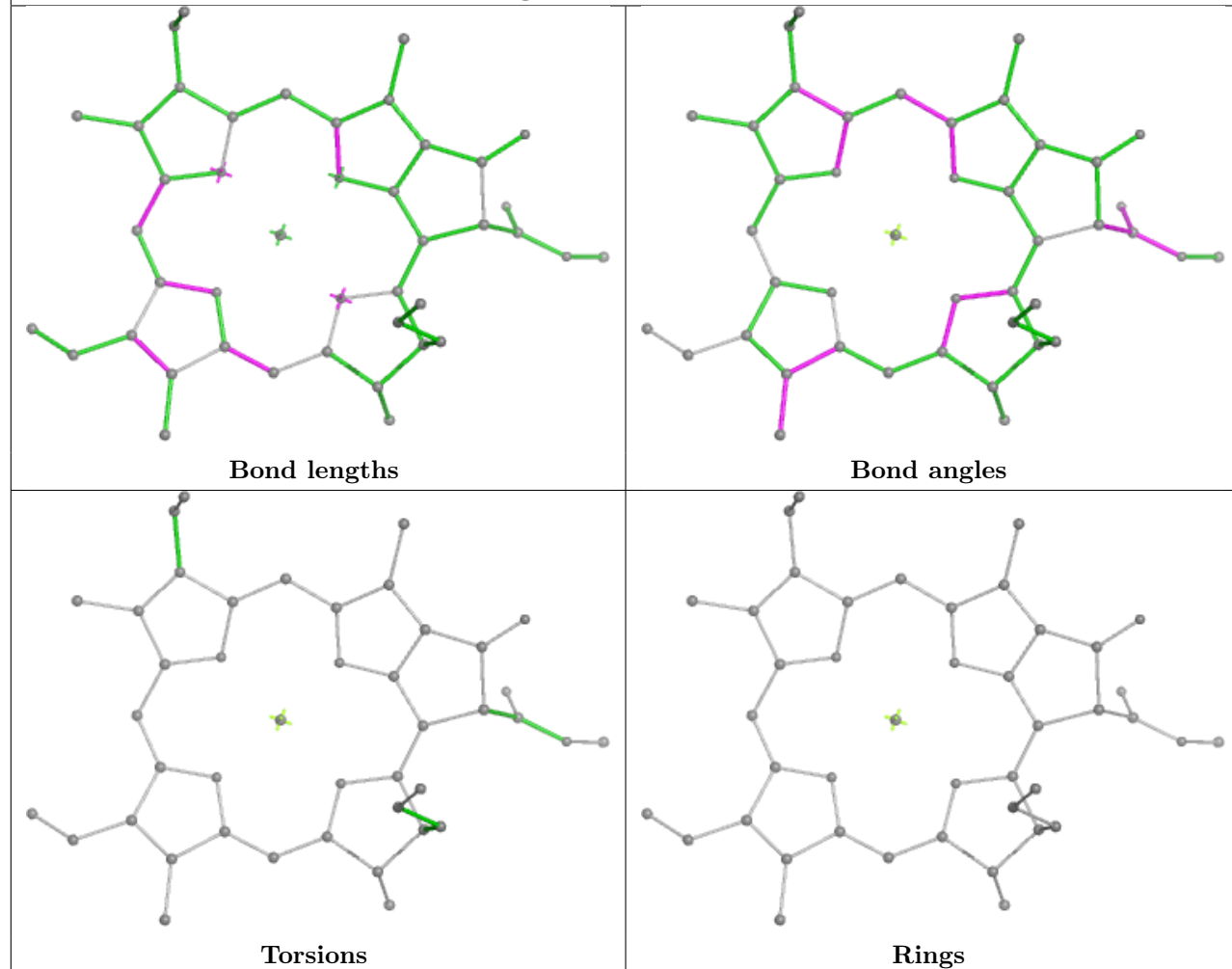
Ligand CHL 1 301



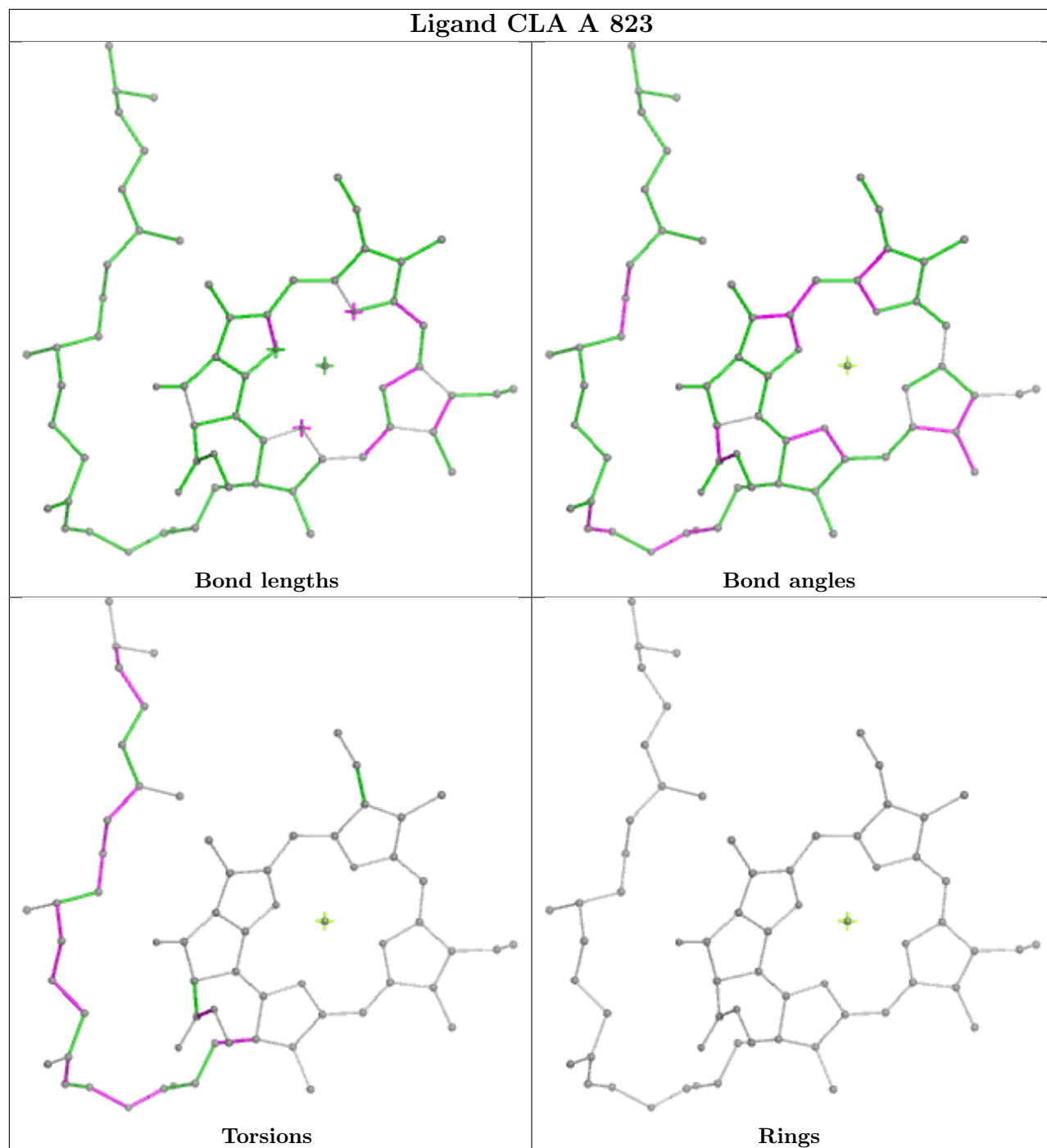
Ligand BCR B 842

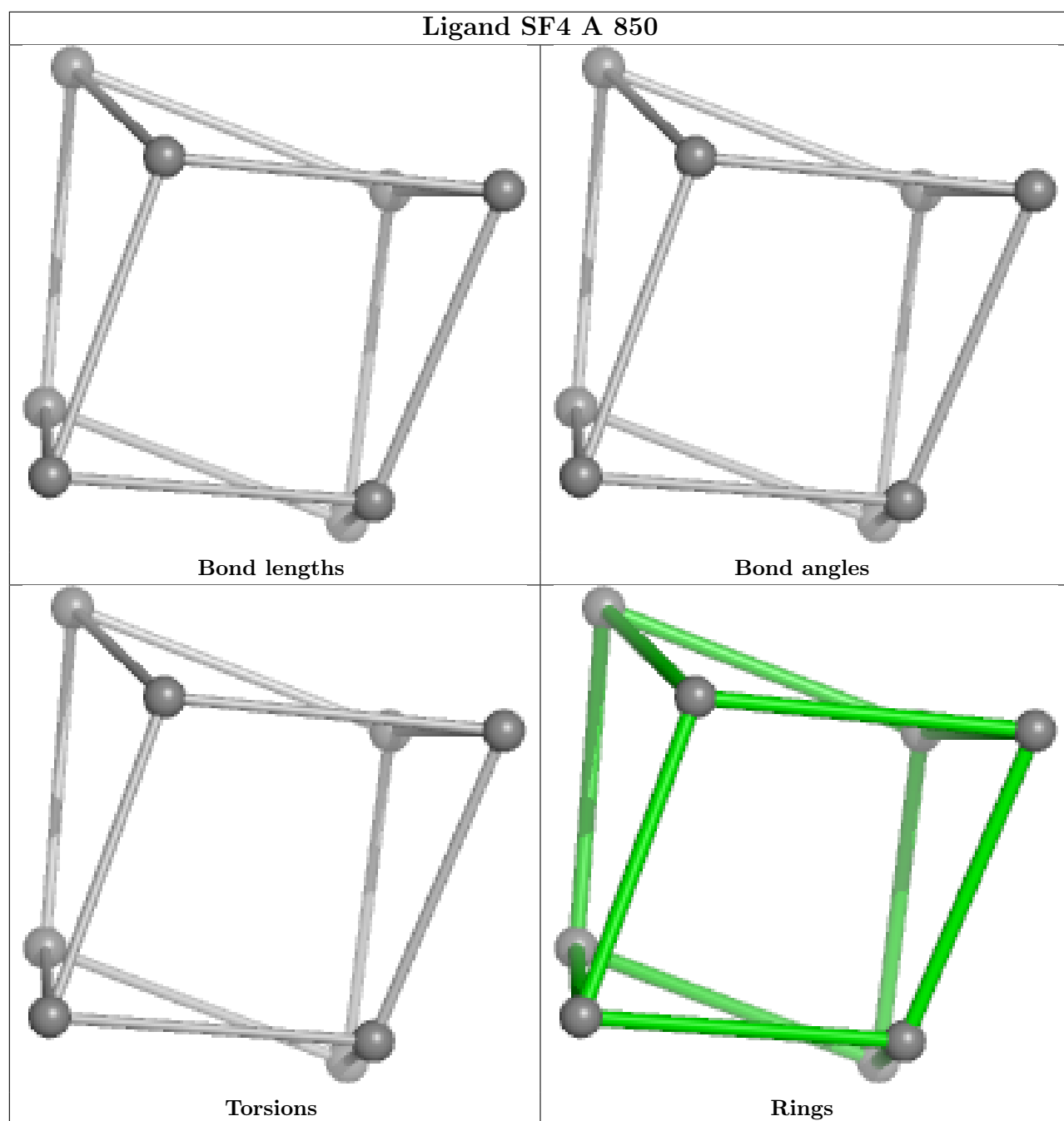


Ligand CLA 2 313

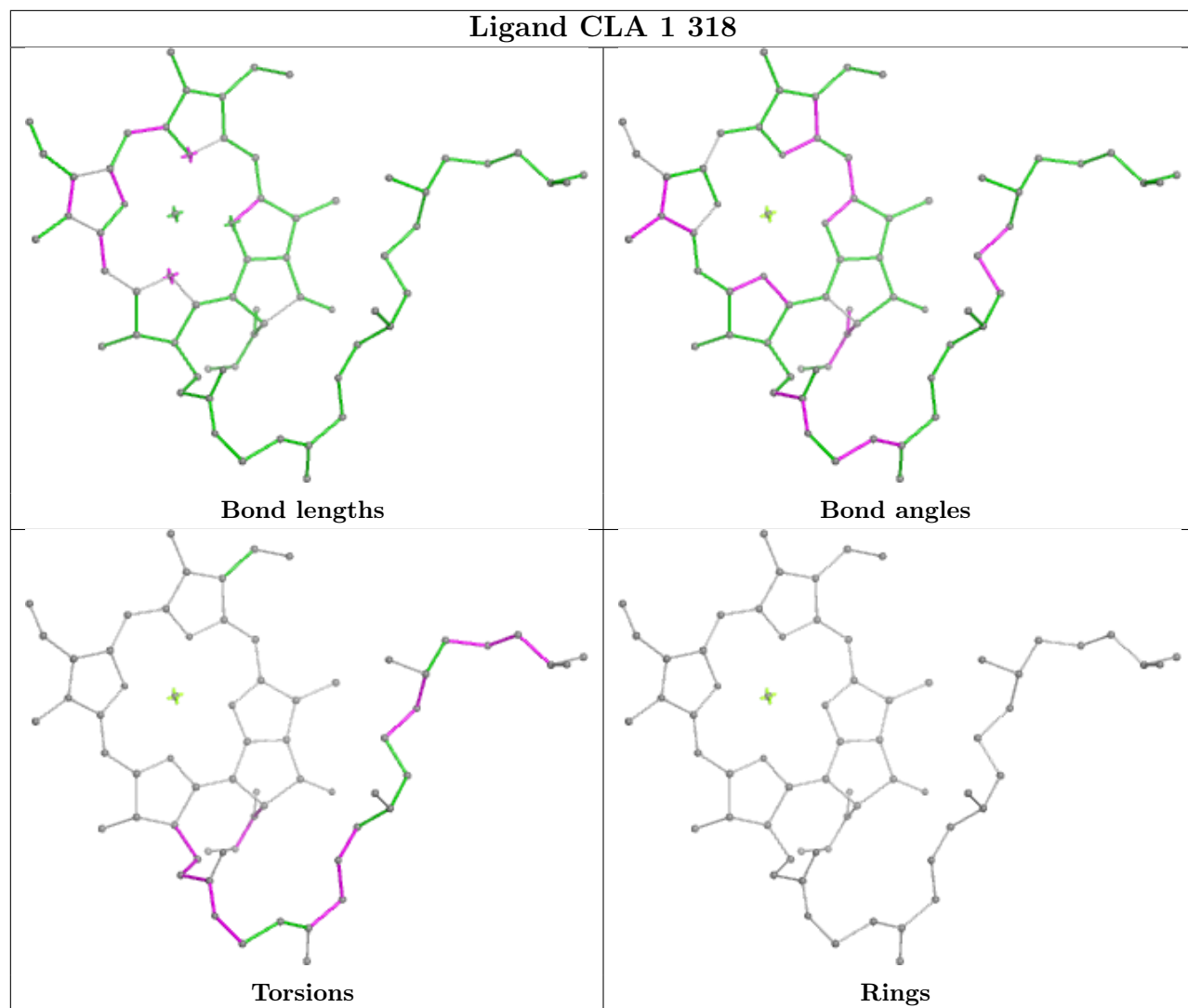


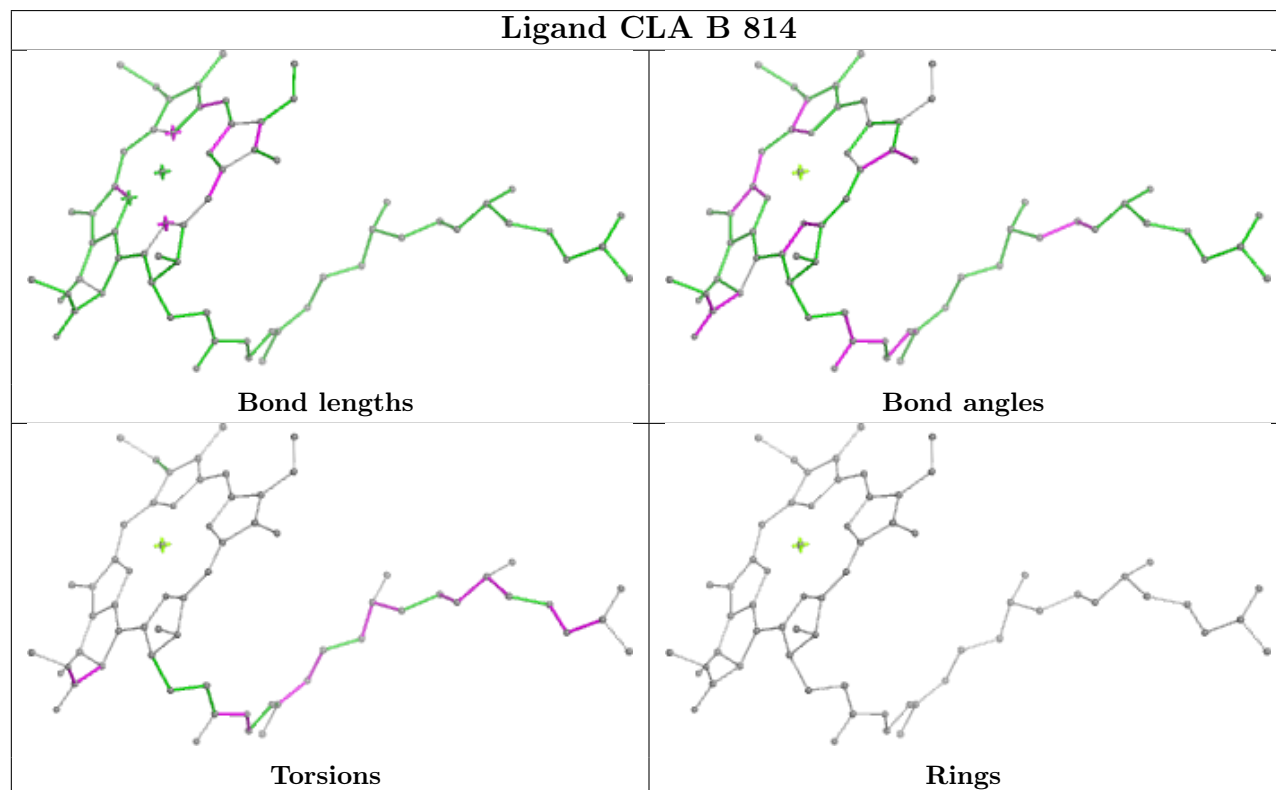
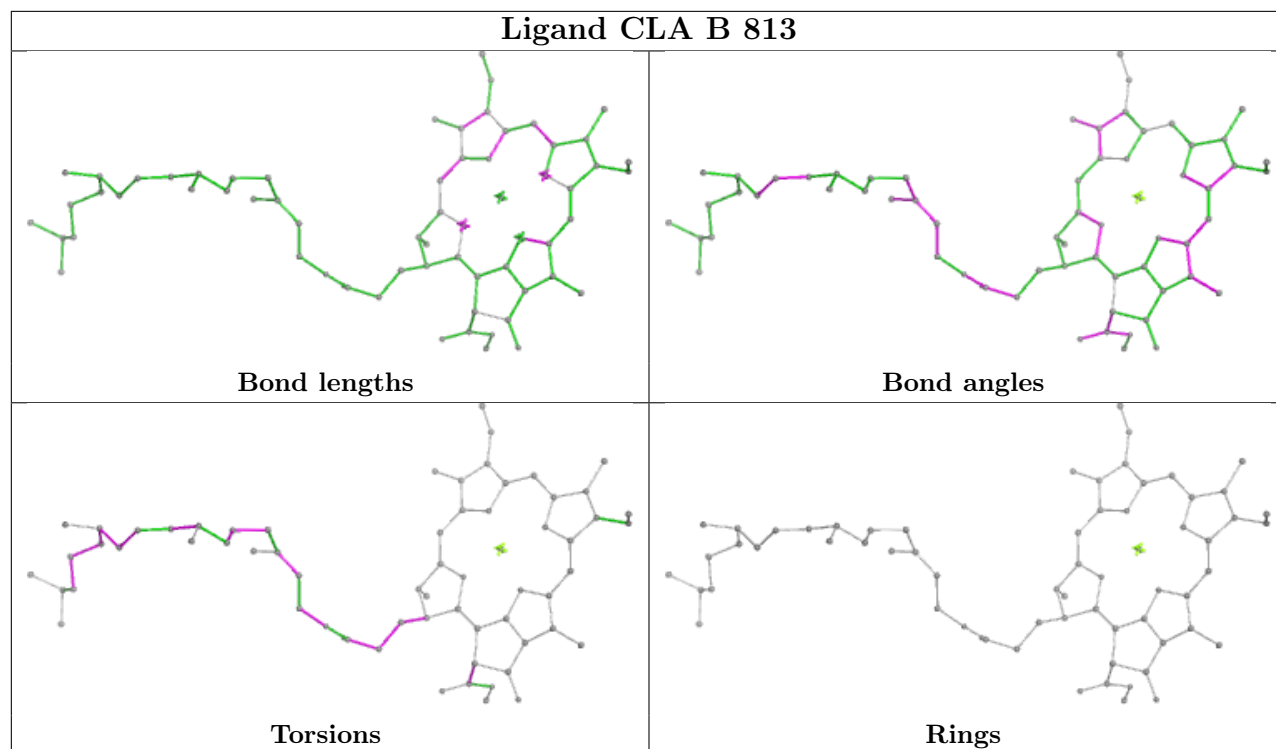
Ligand CLA A 823

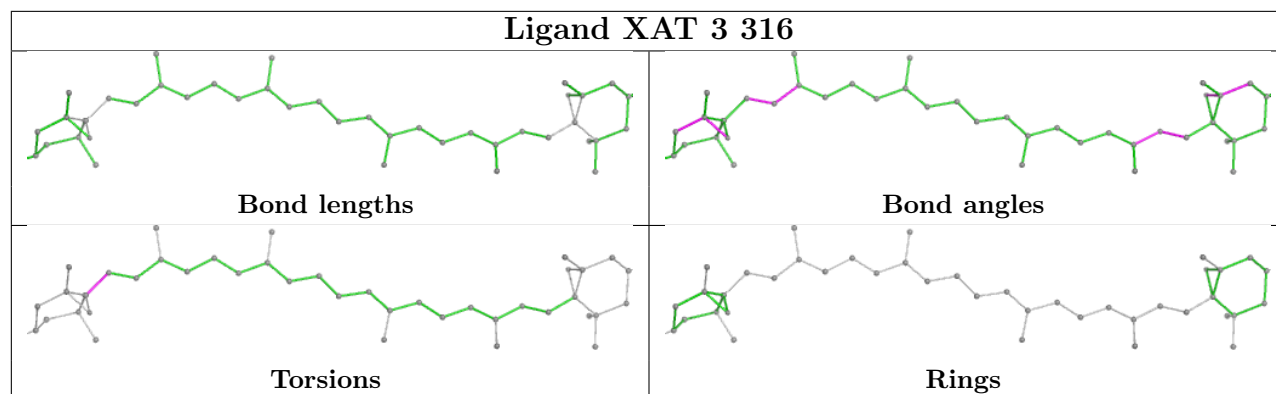
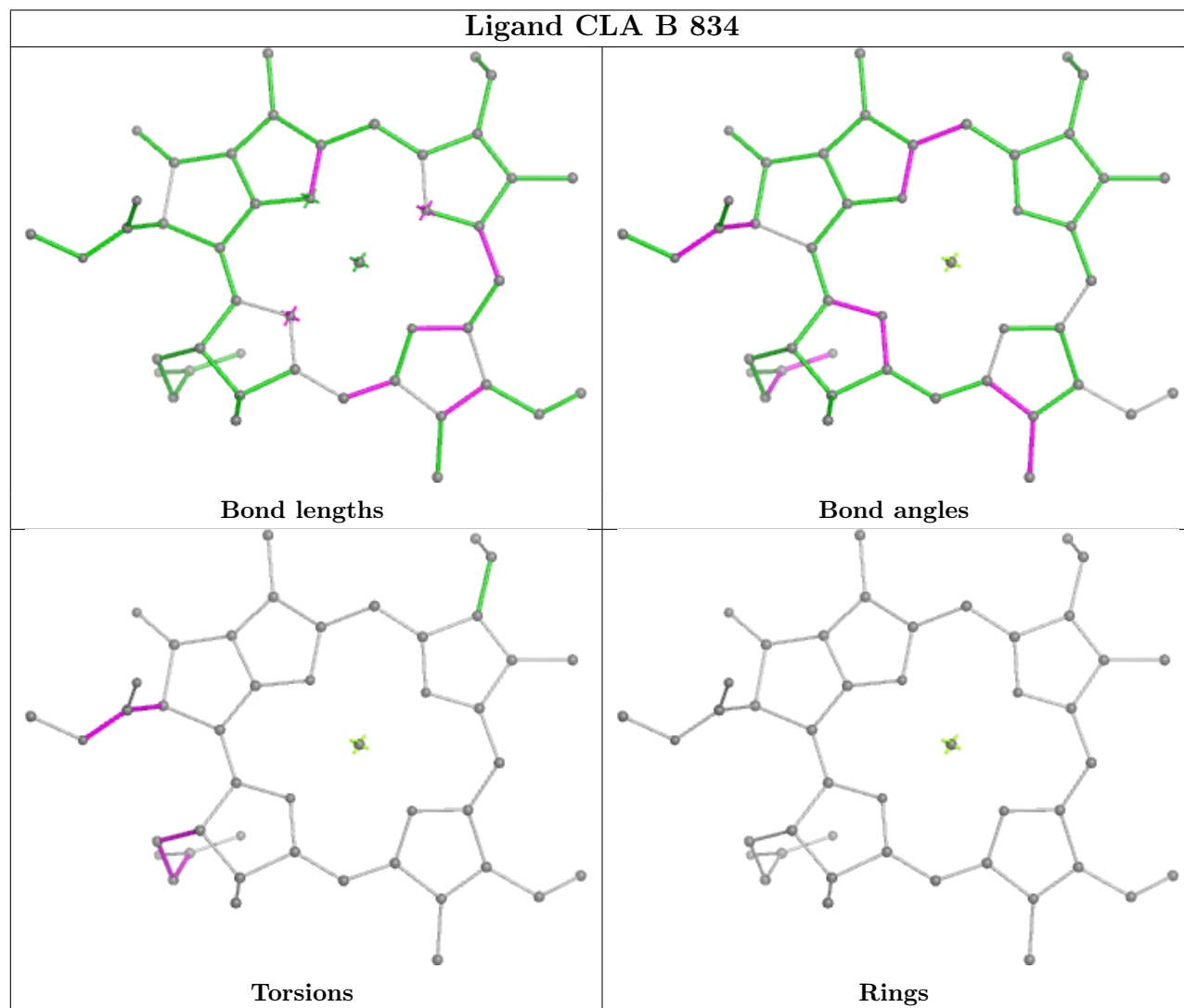




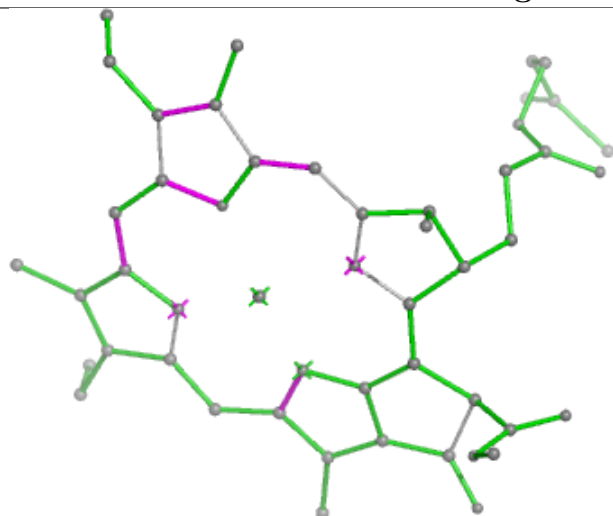
Ligand CLA 1 318



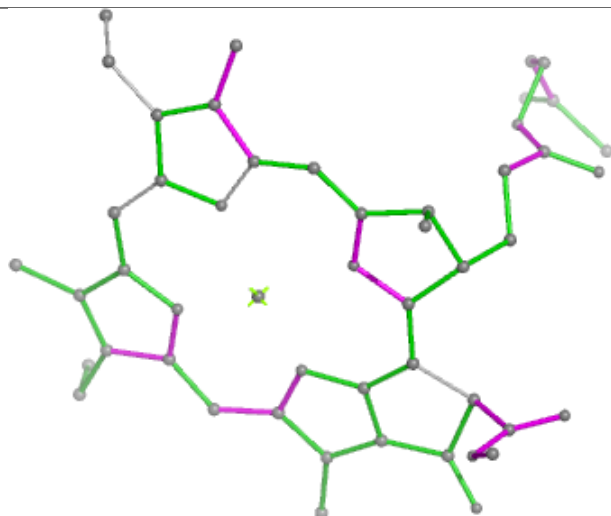


Ligand XAT 3 316**Ligand CLA B 834**

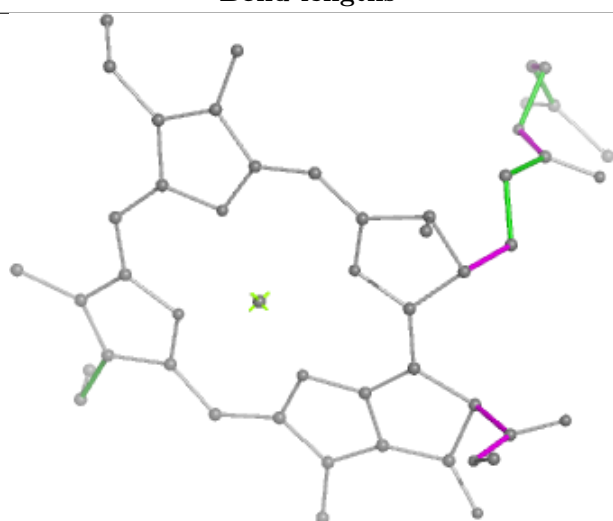
Ligand CLA B 830



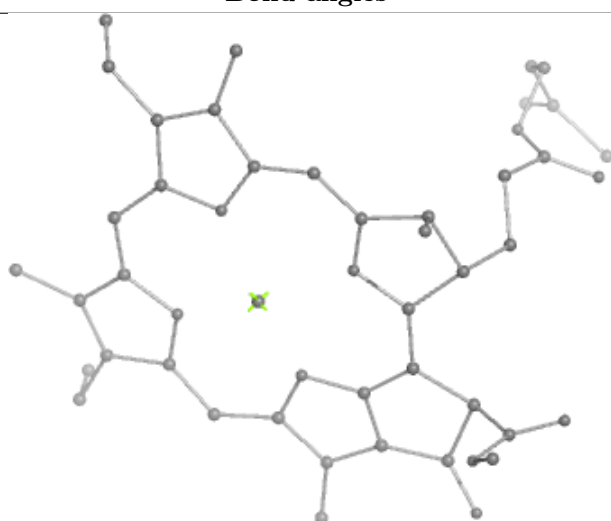
Bond lengths



Bond angles

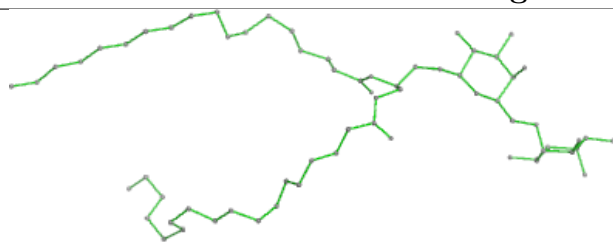


Torsions

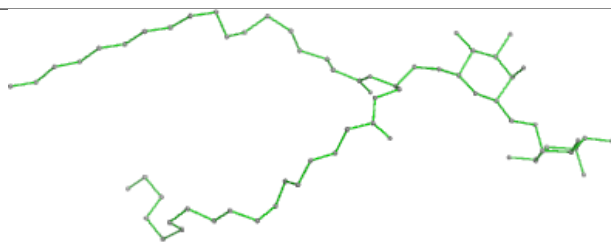


Rings

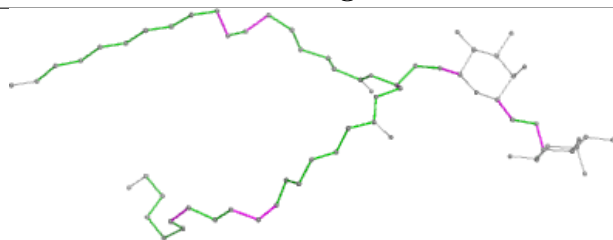
Ligand DGD B 848



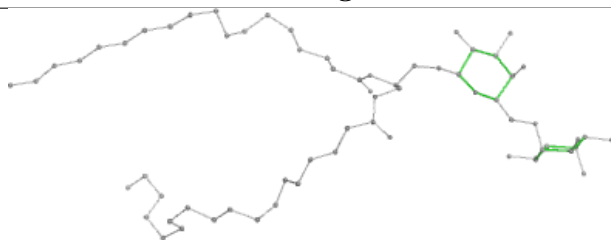
Bond lengths



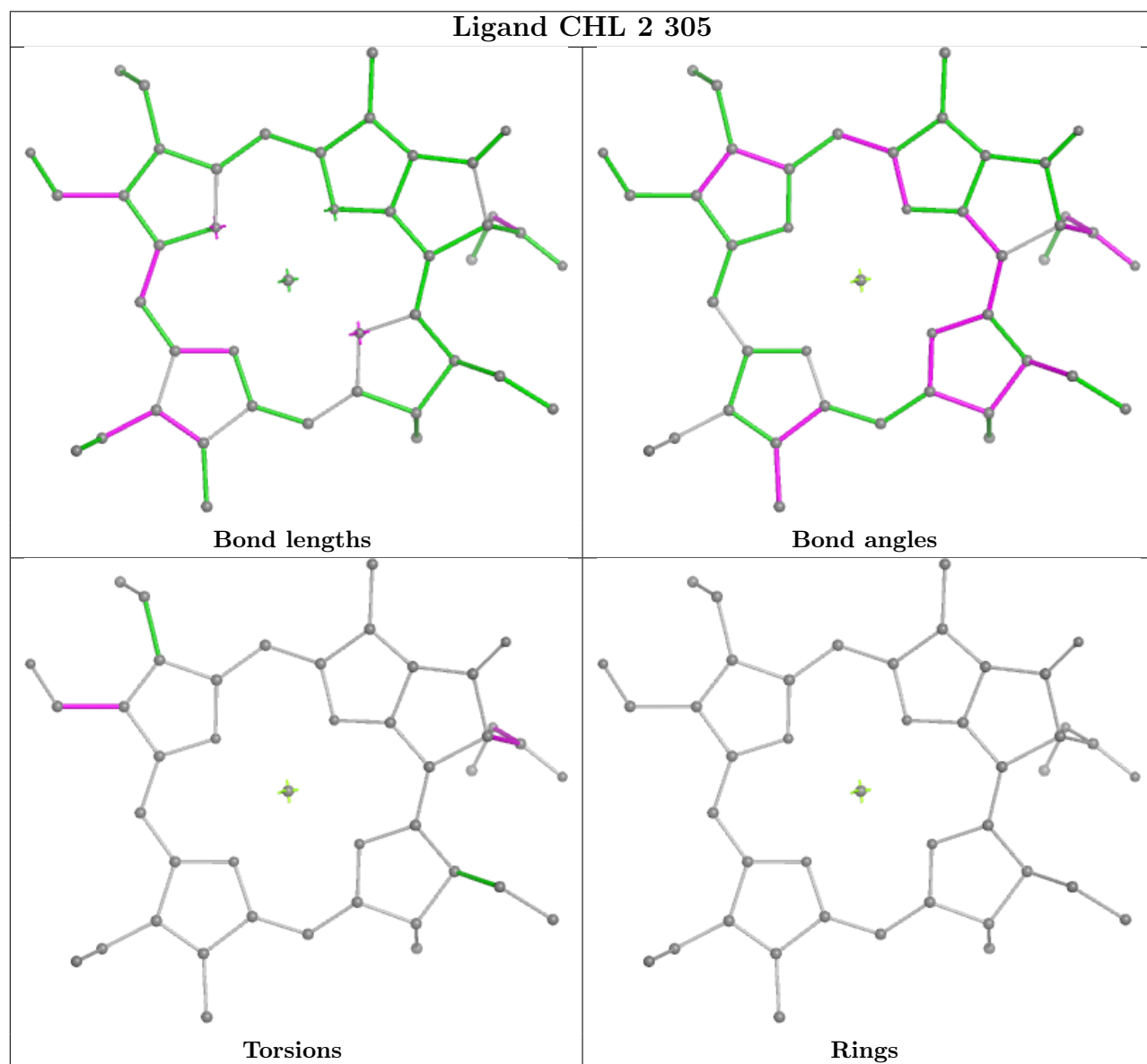
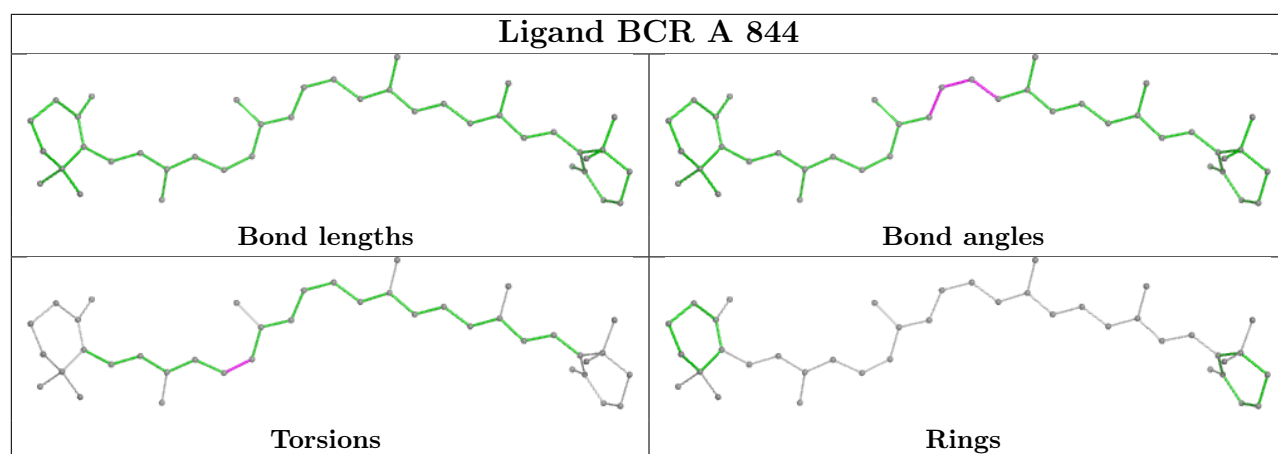
Bond angles

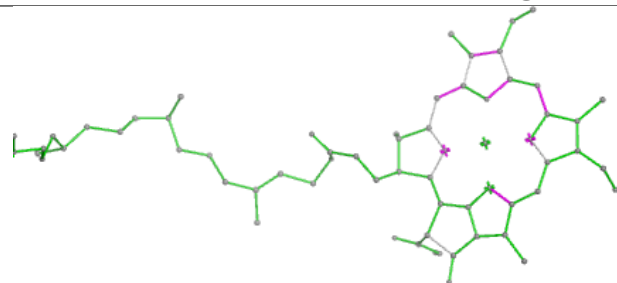


Torsions

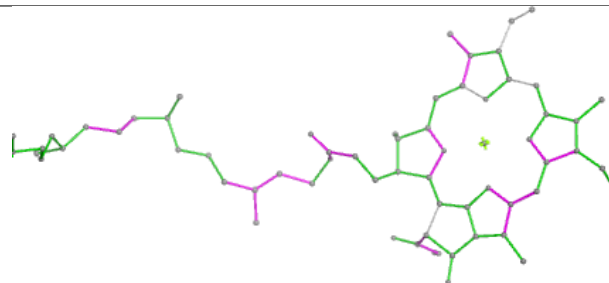


Rings

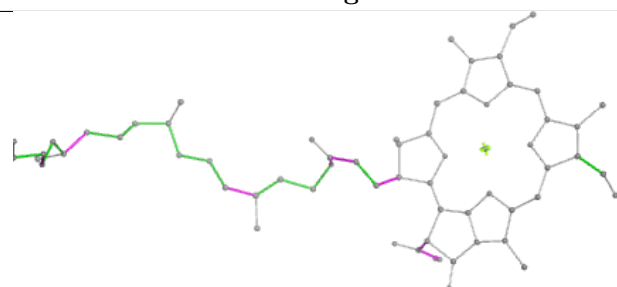


Ligand CLA A 803

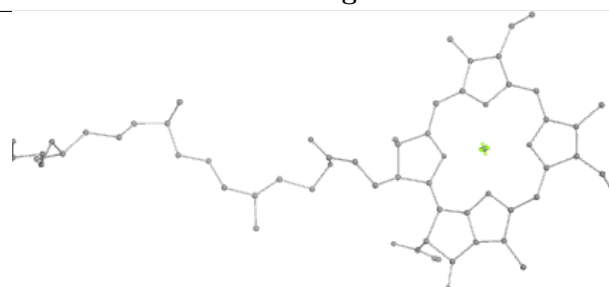
Bond lengths



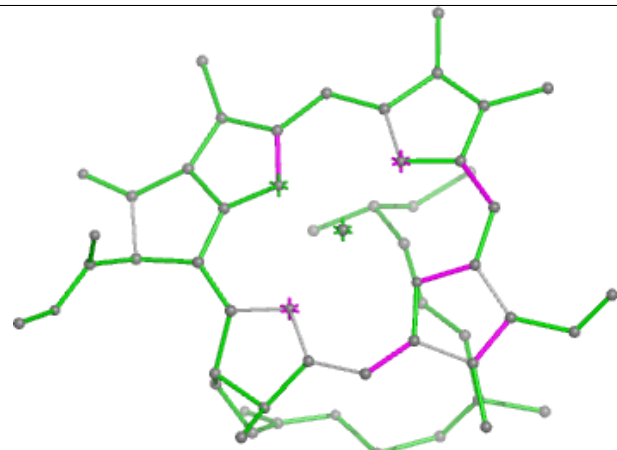
Bond angles



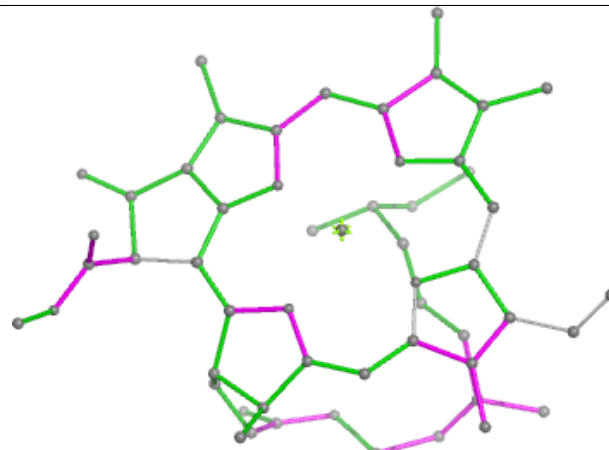
Torsions



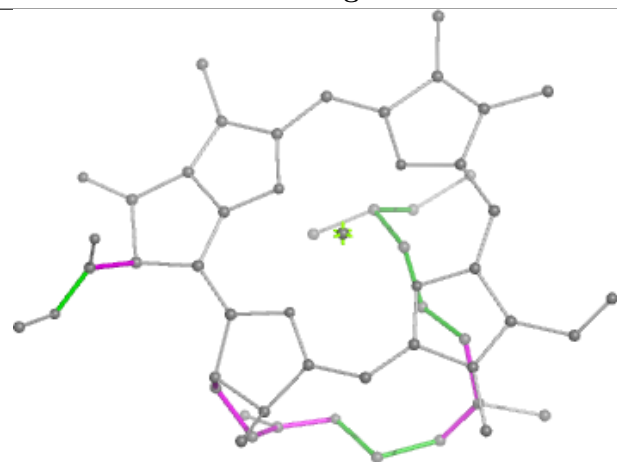
Rings

Ligand CLA H 202

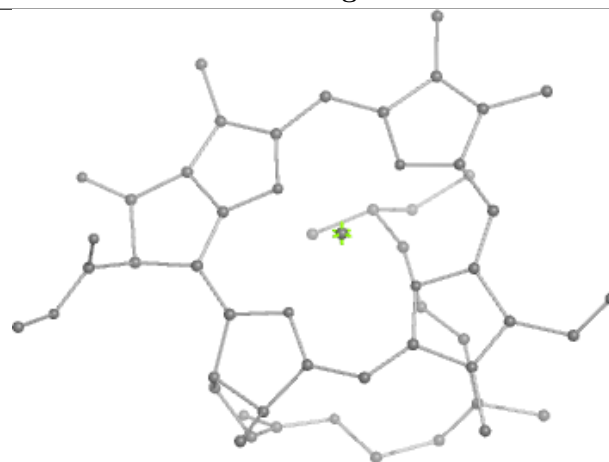
Bond lengths



Bond angles

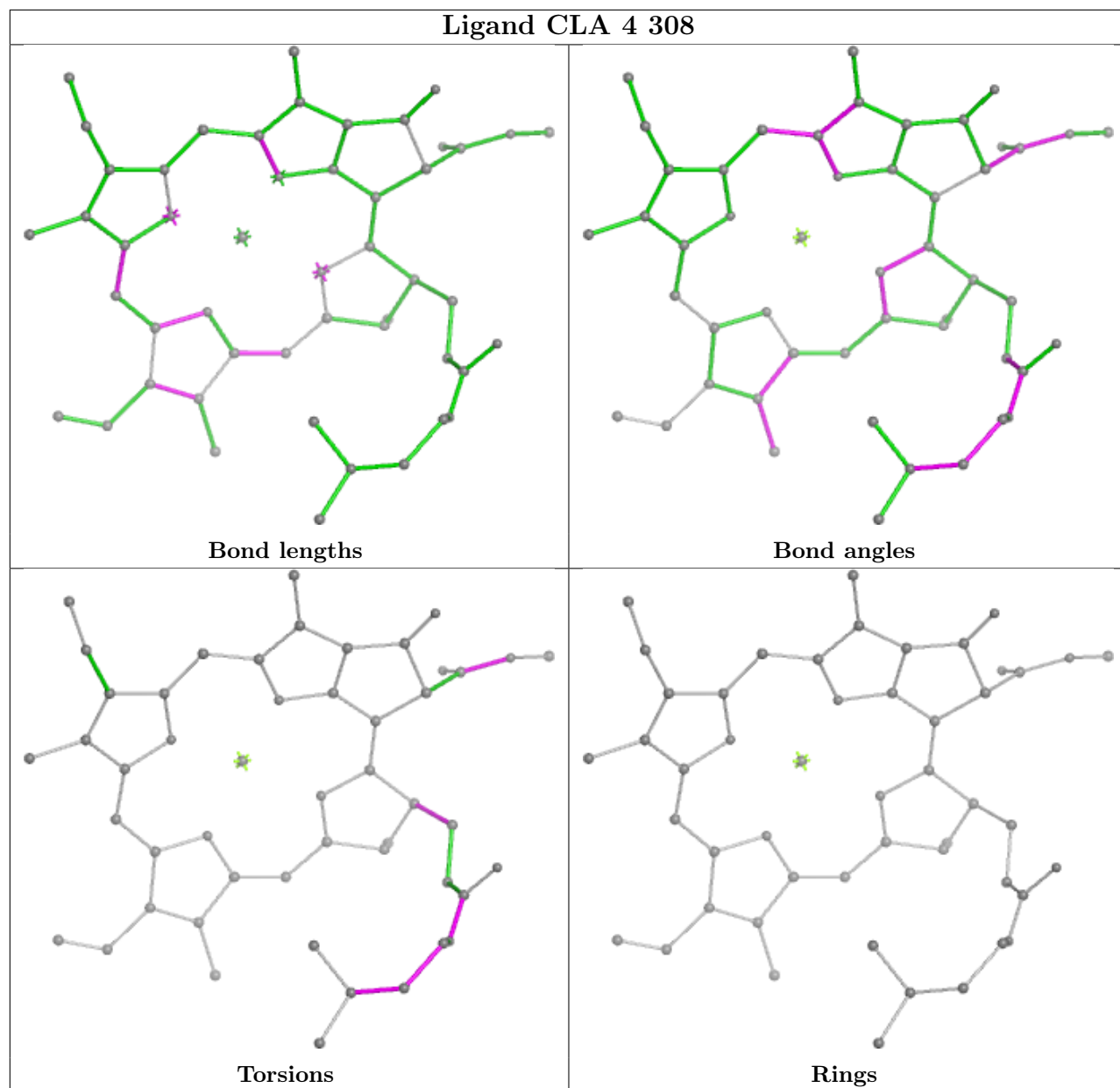


Torsions

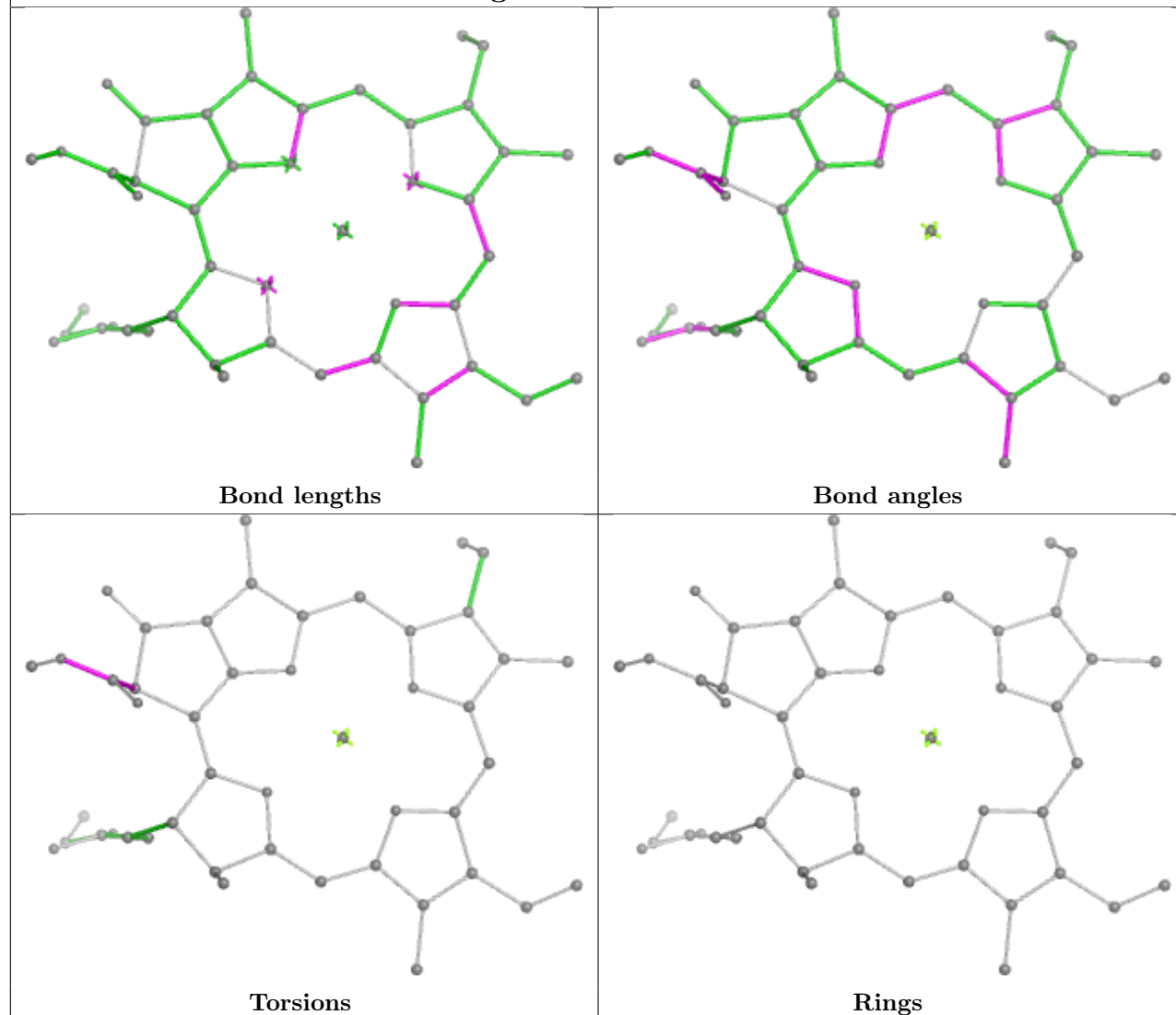


Rings

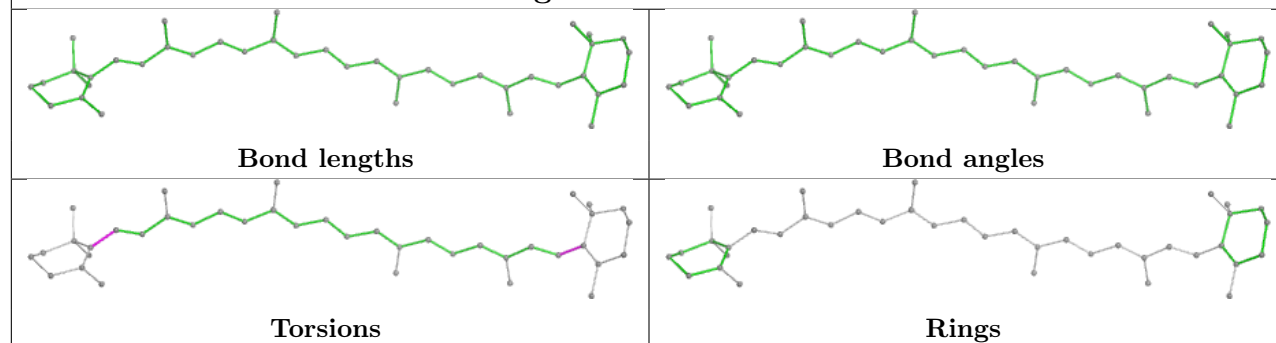
Ligand CLA 4 308

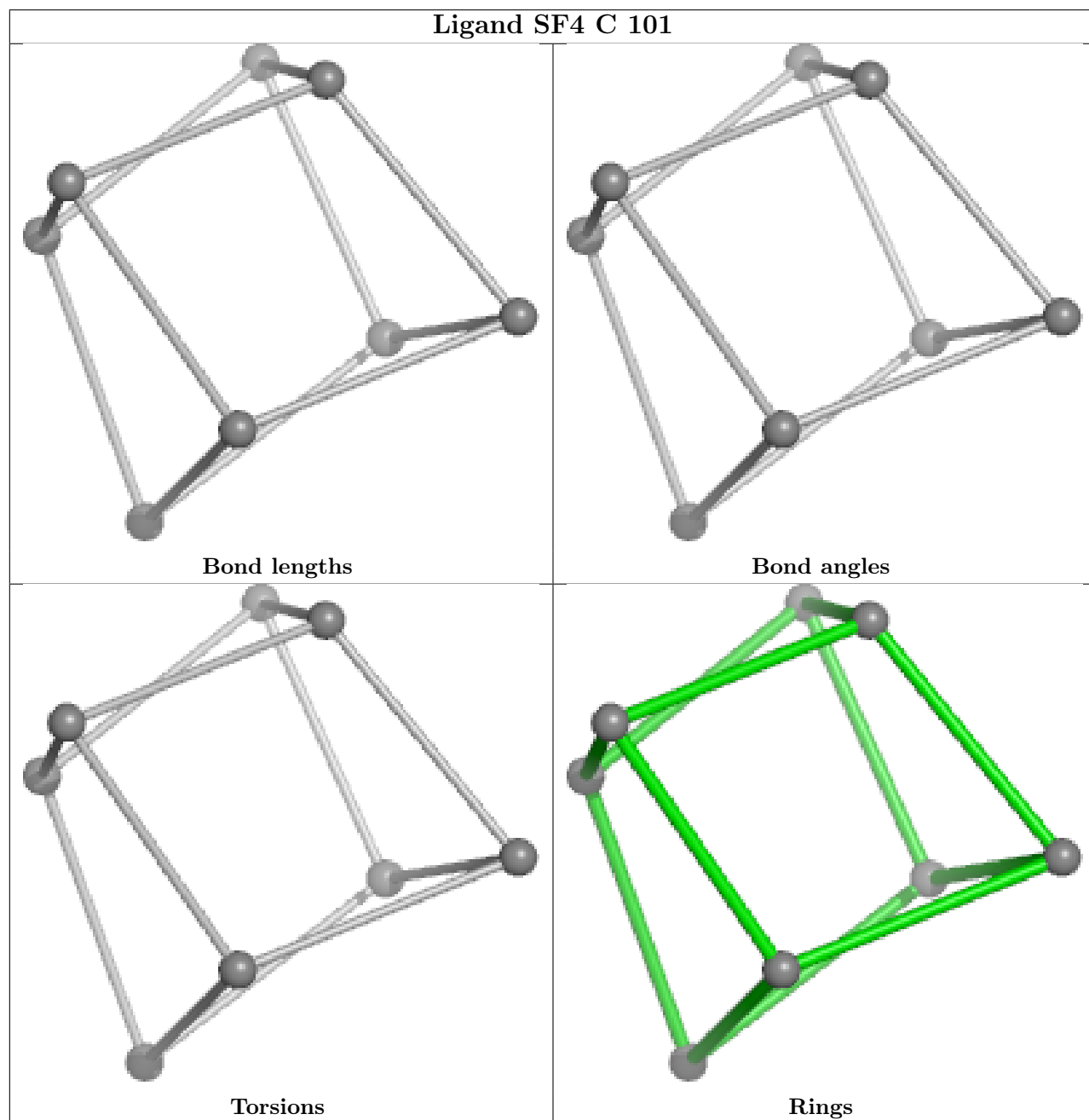
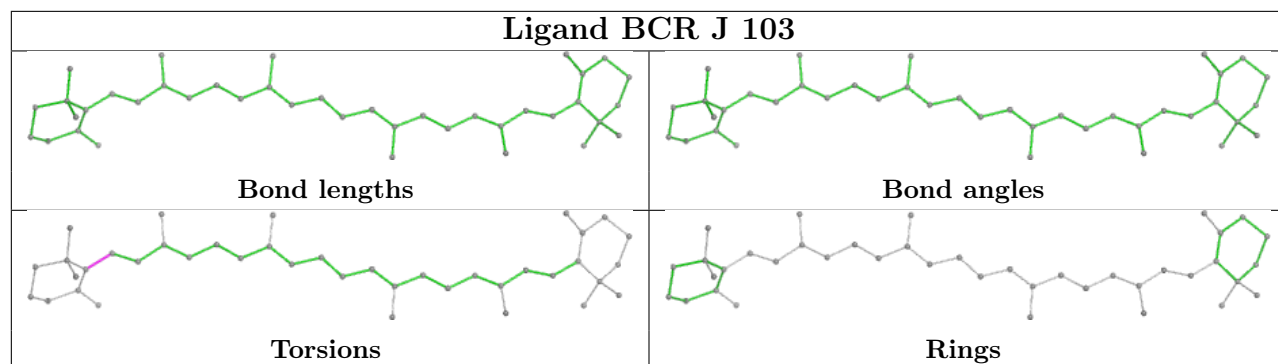


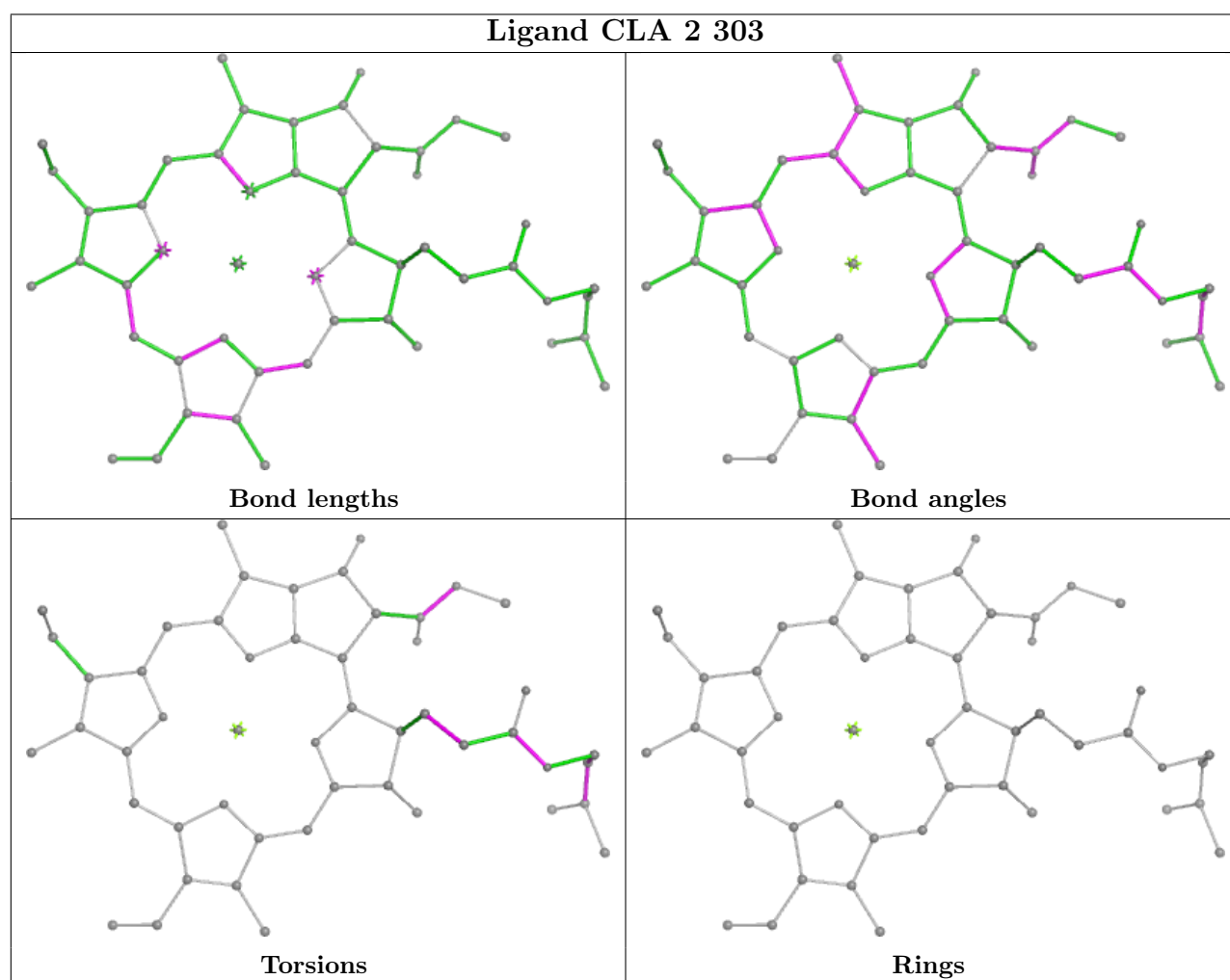
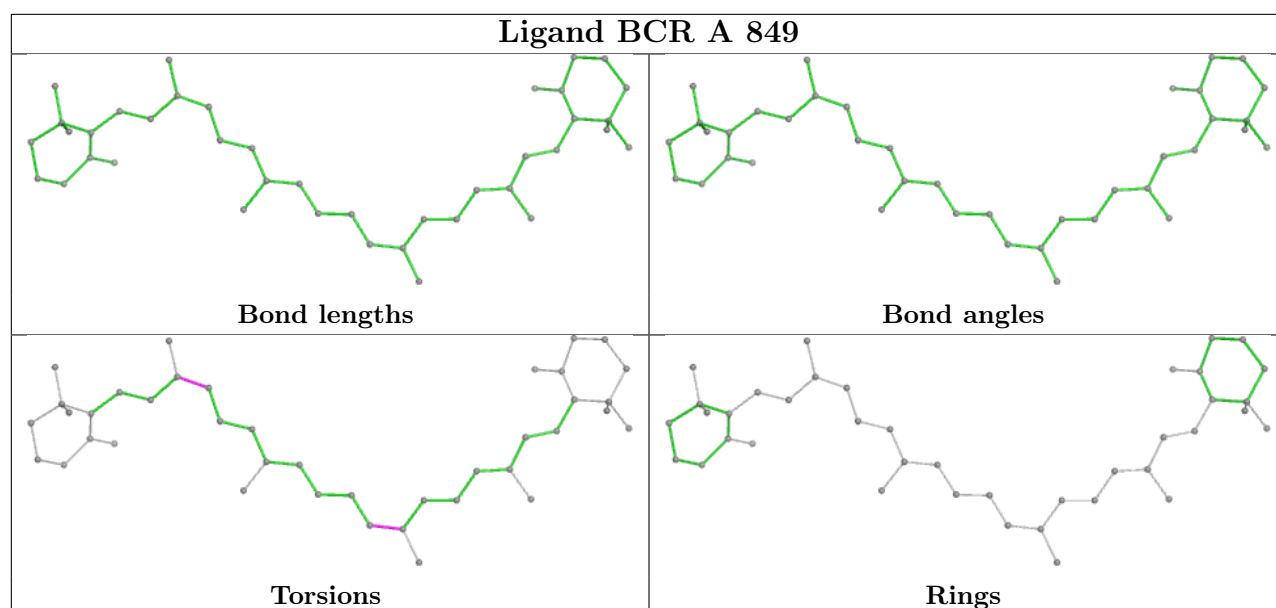
Ligand CLA B 837



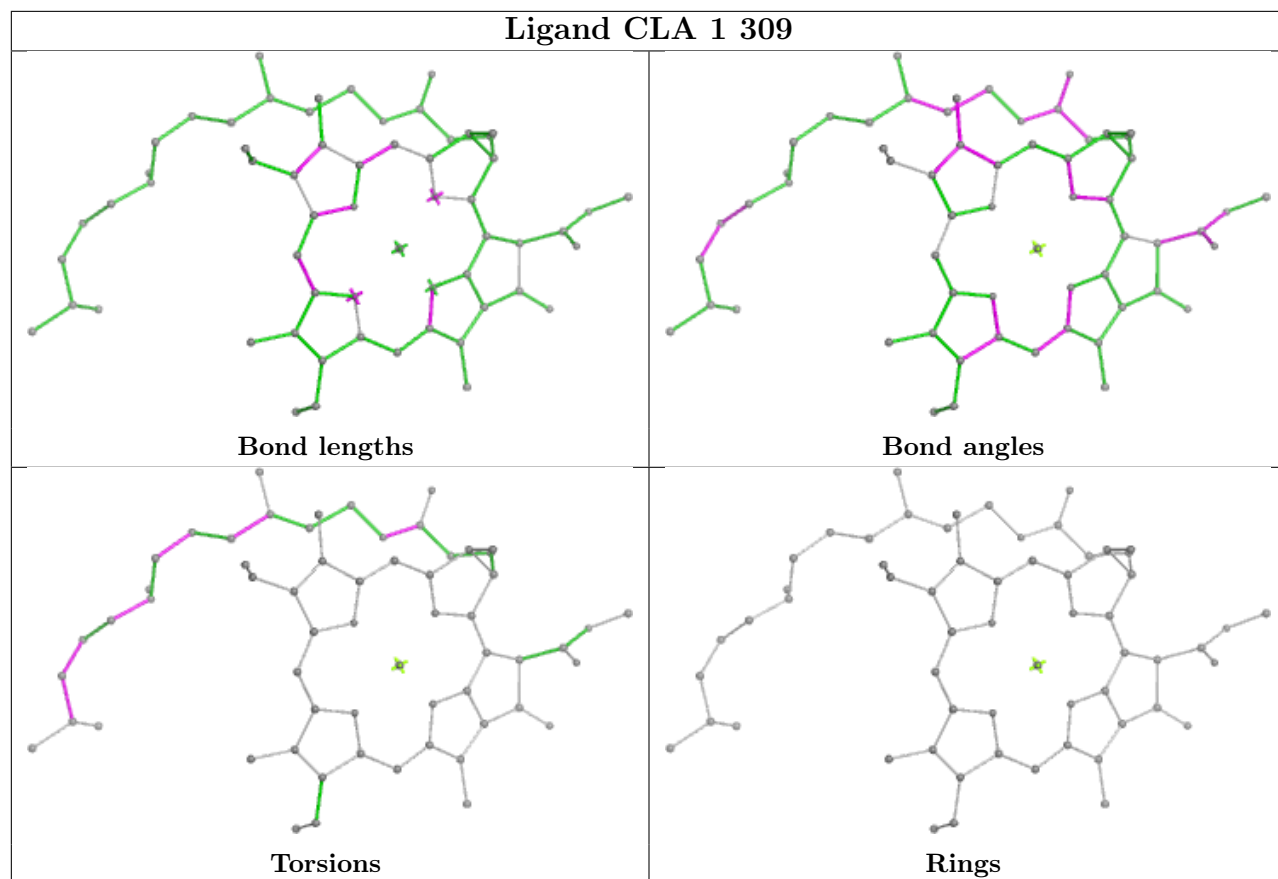
Ligand BCR J 104



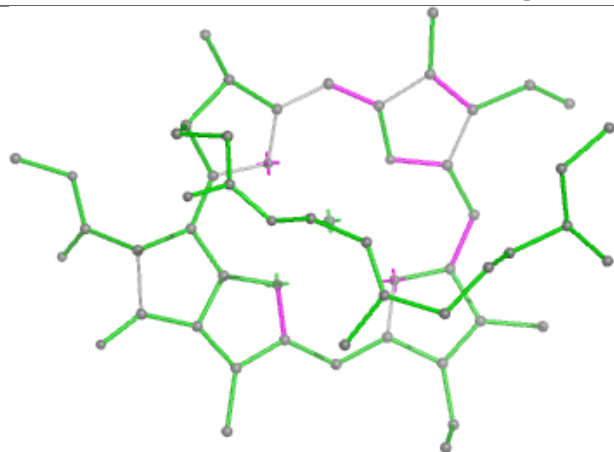




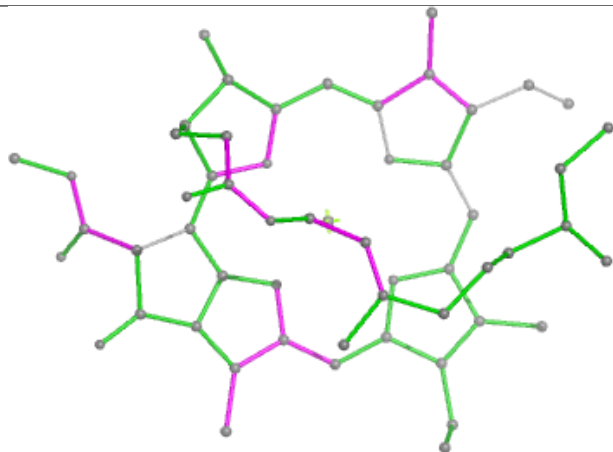
Ligand CLA 1 309



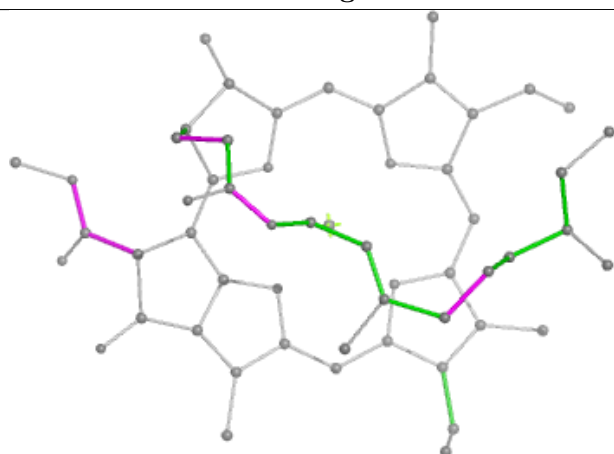
Ligand CLA 4 312



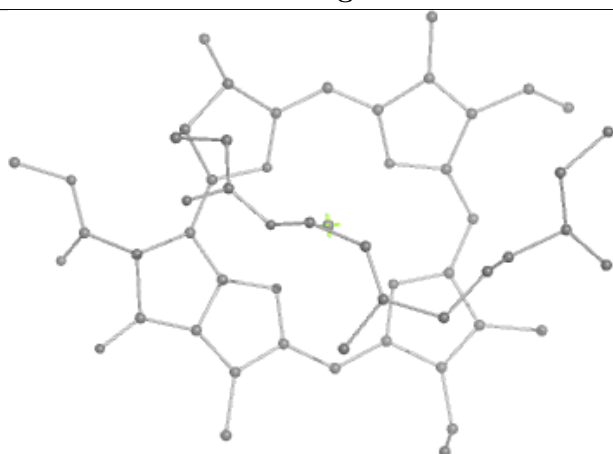
Bond lengths



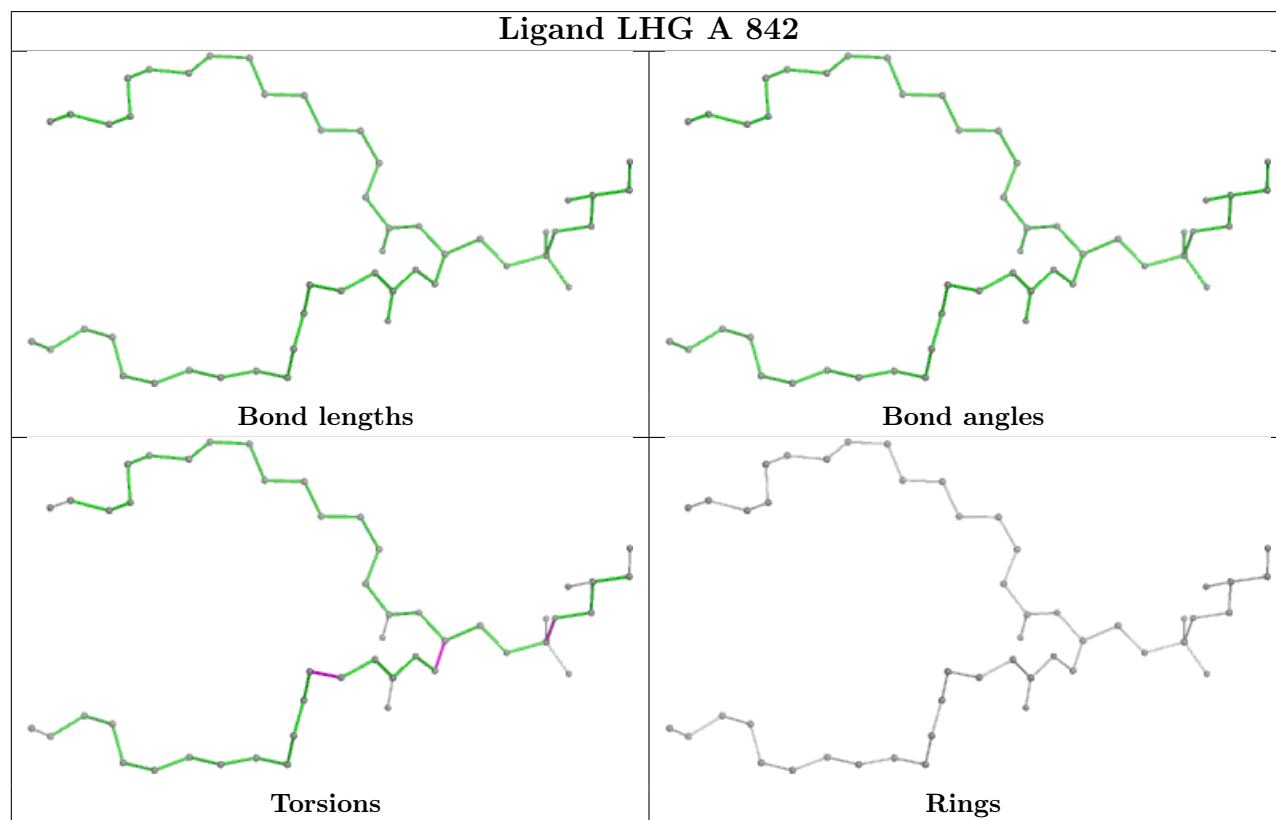
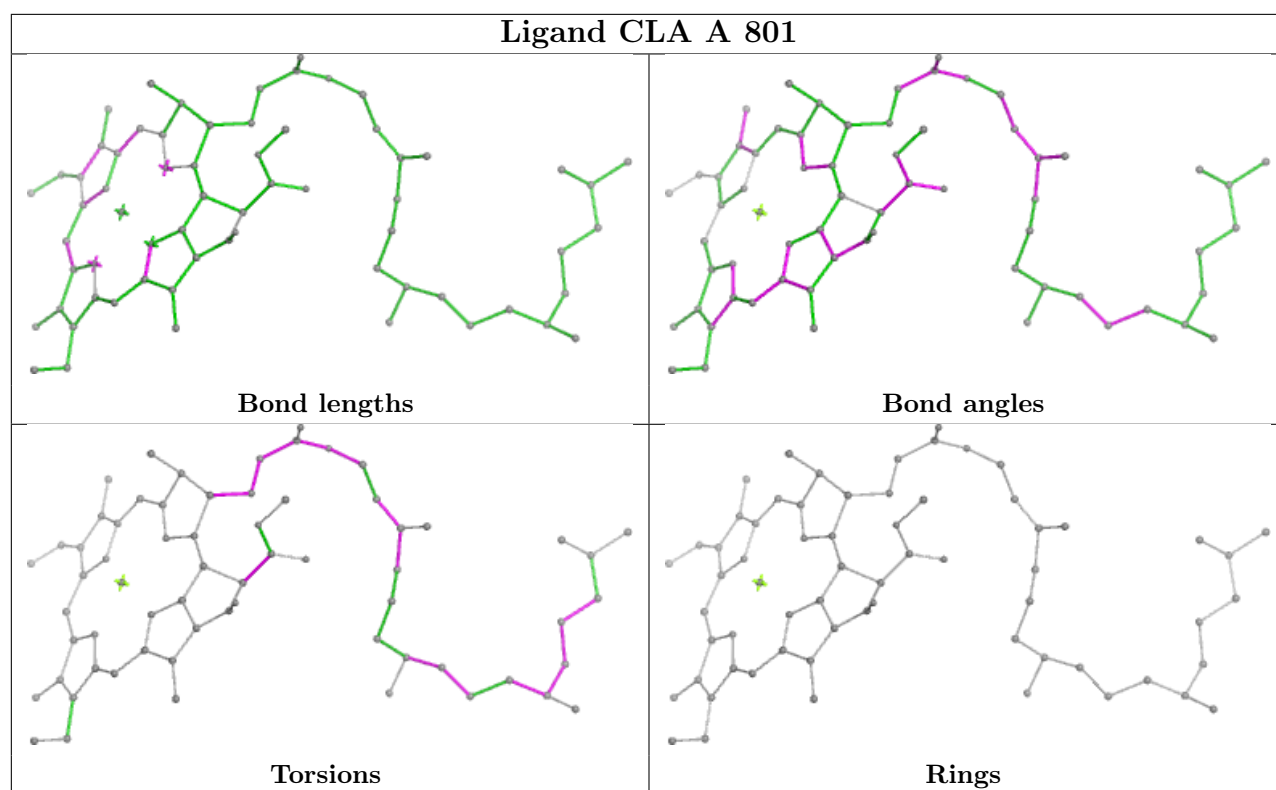
Bond angles



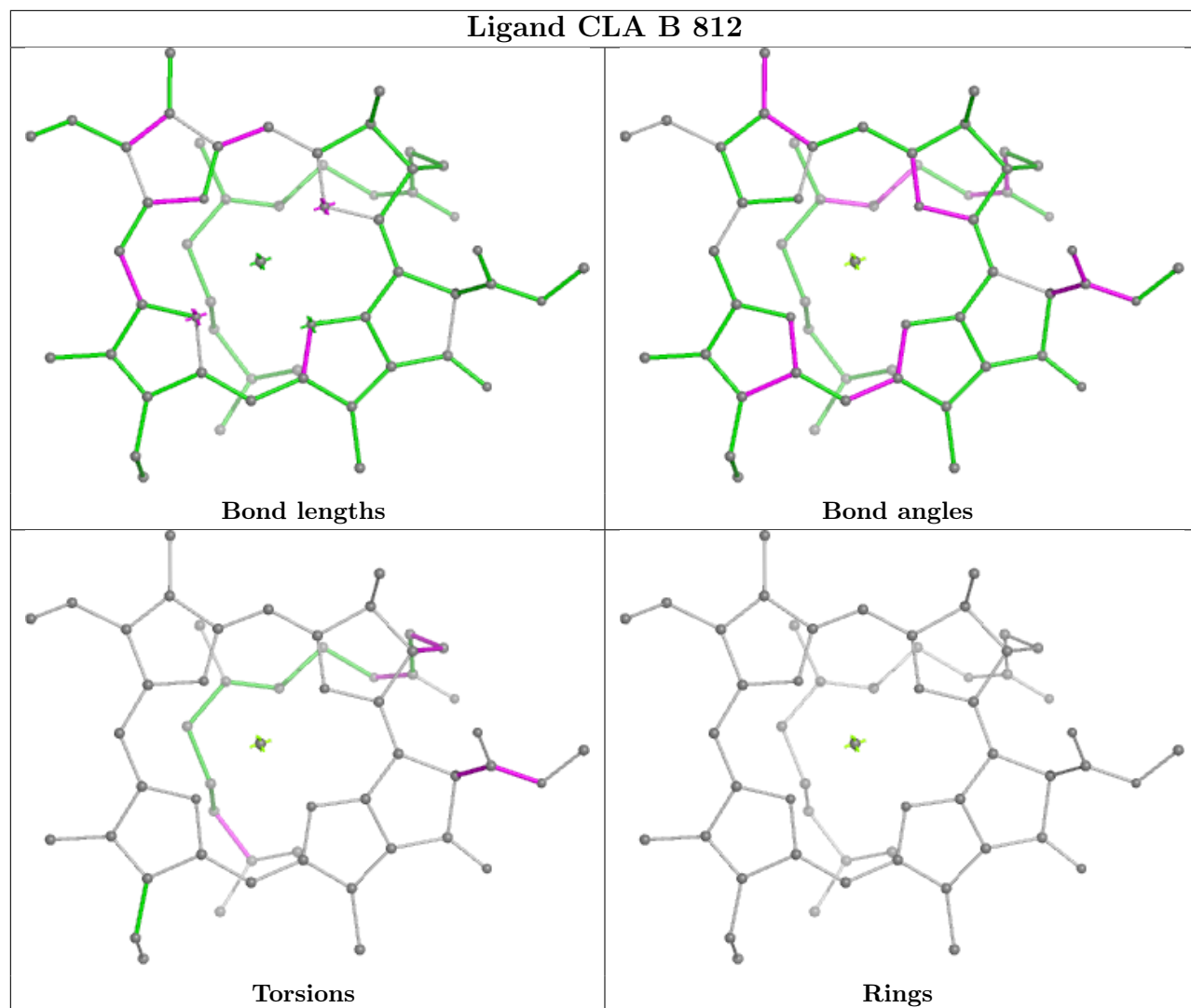
Torsions



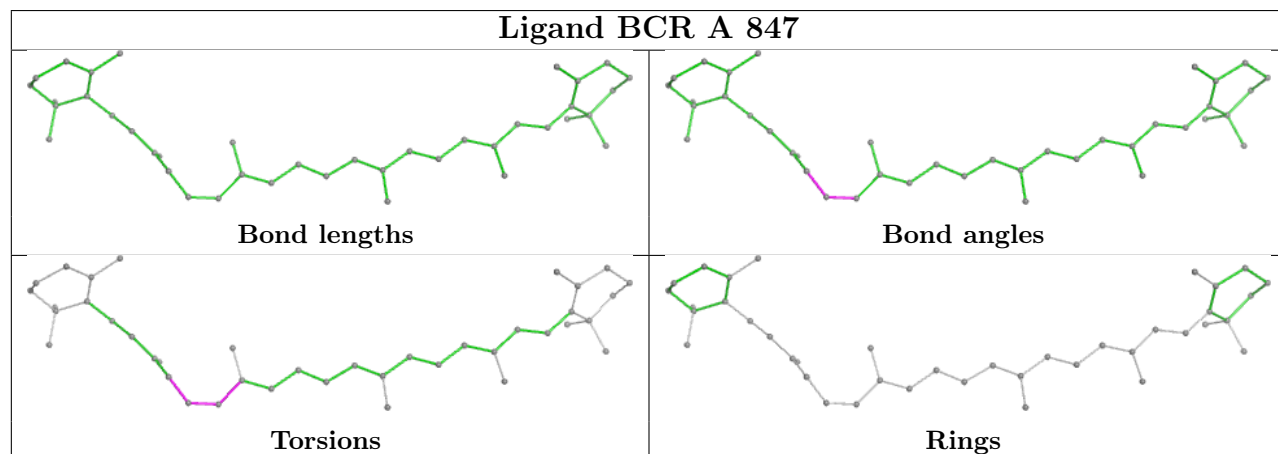
Rings



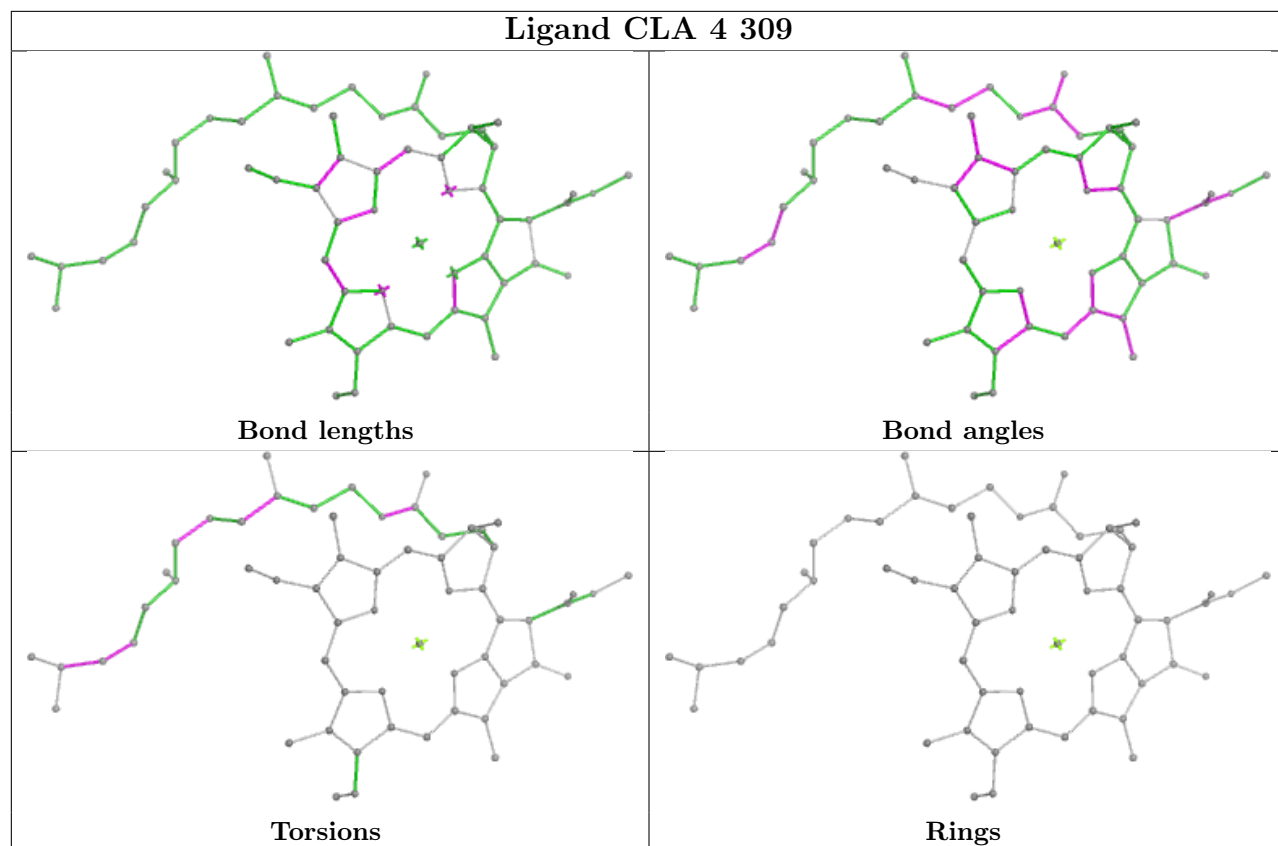
Ligand CLA B 812



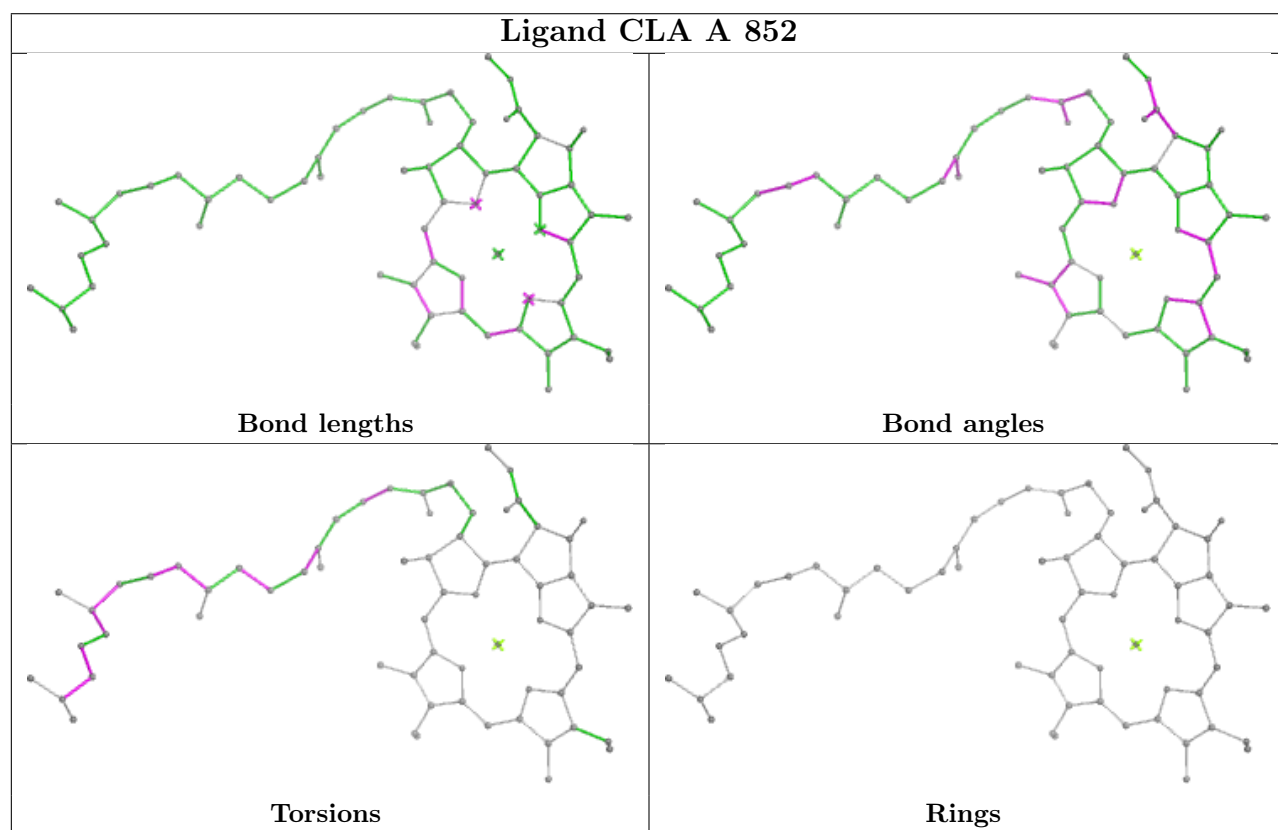
Ligand BCR A 847

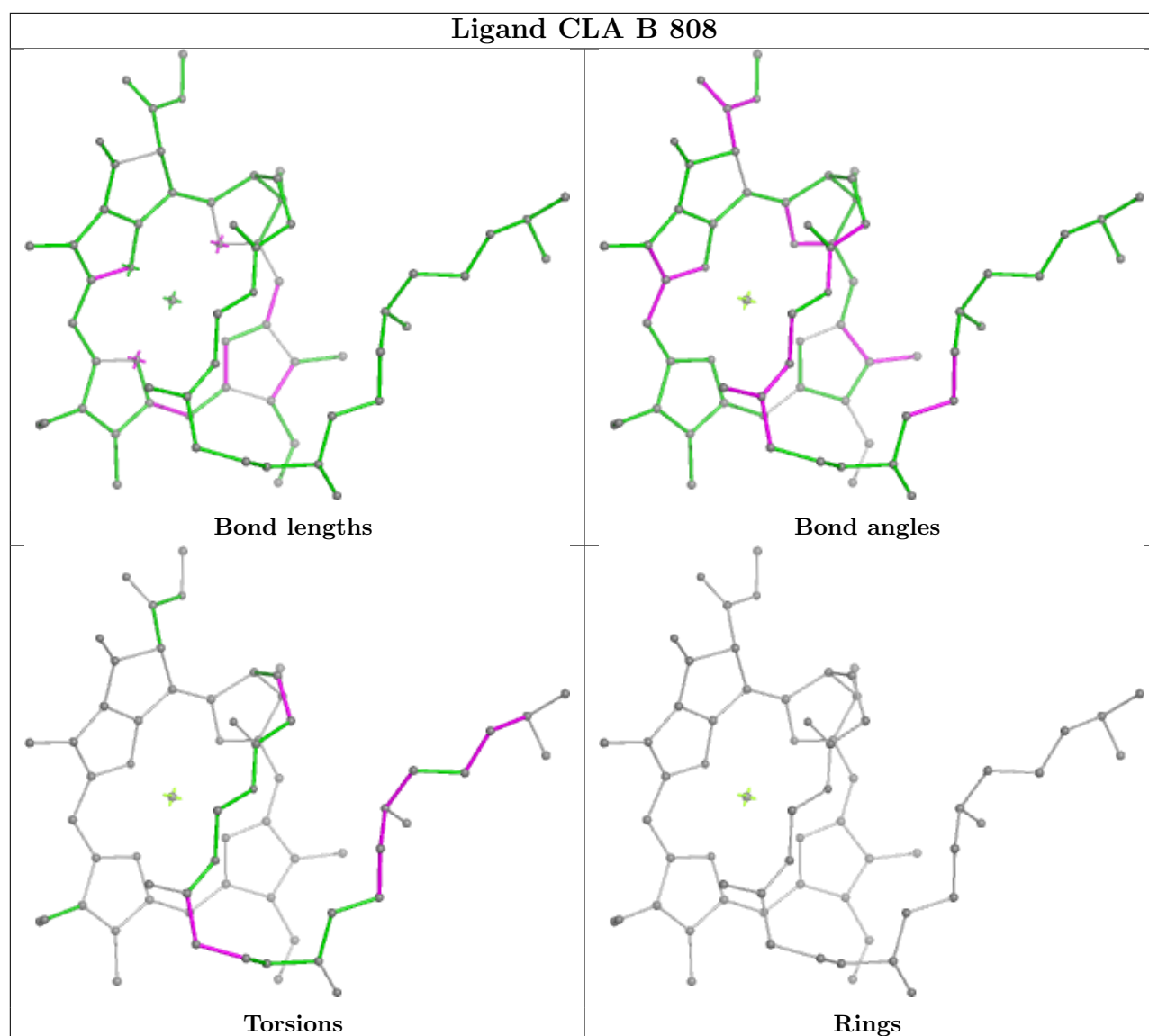


Ligand CLA 4 309



Ligand CLA A 852





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.

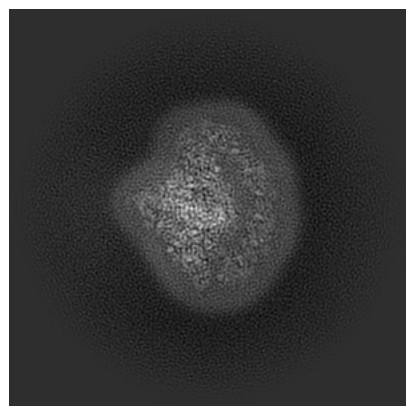
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51227. These allow visual inspection of the internal detail of the map and identification of artifacts.

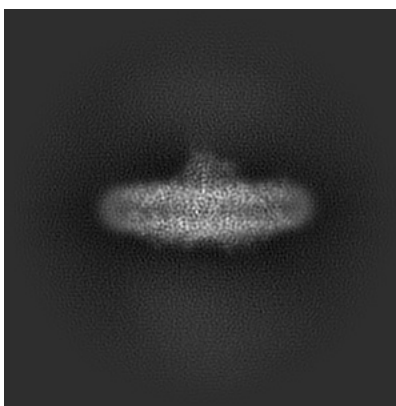
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

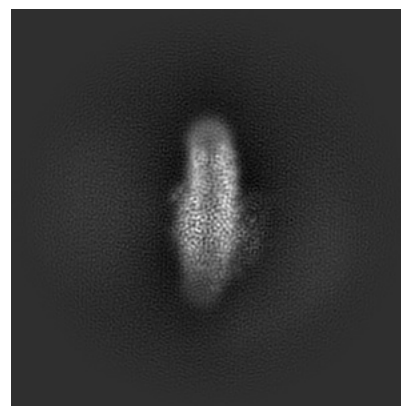
6.1.1 Primary map



X

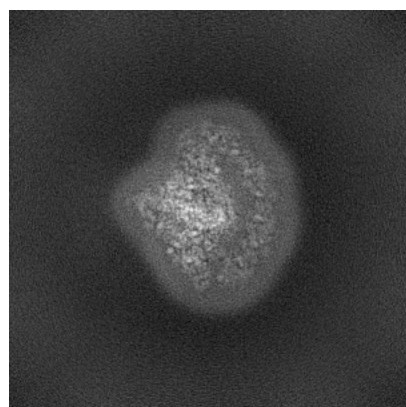


Y

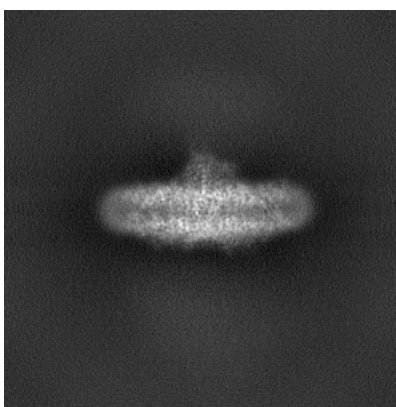


Z

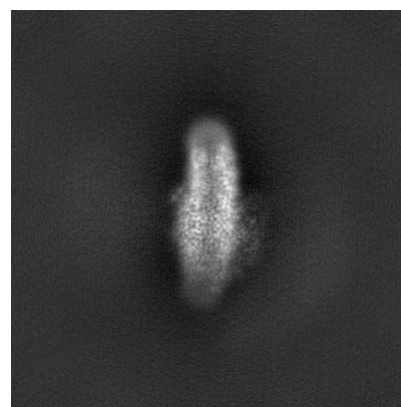
6.1.2 Raw map



X



Y

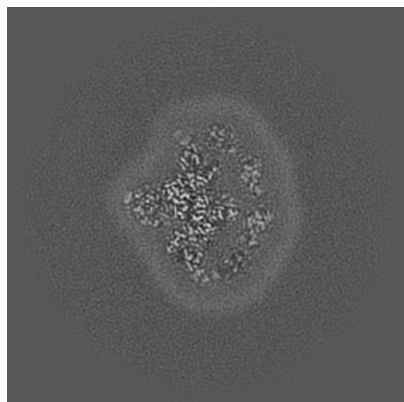


Z

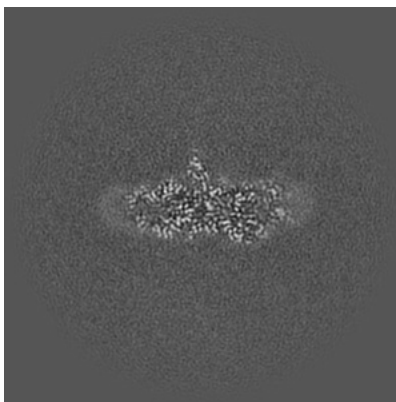
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

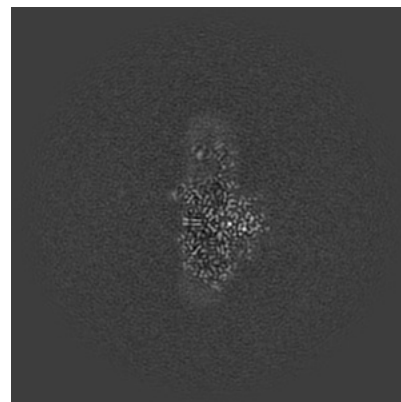
6.2.1 Primary map



X Index: 224

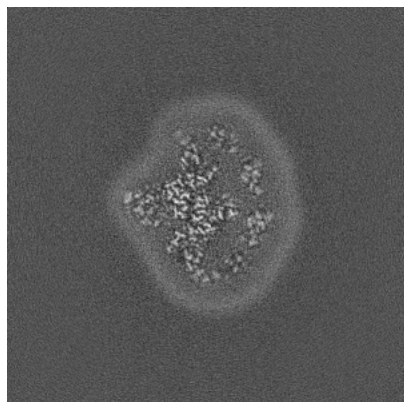


Y Index: 224

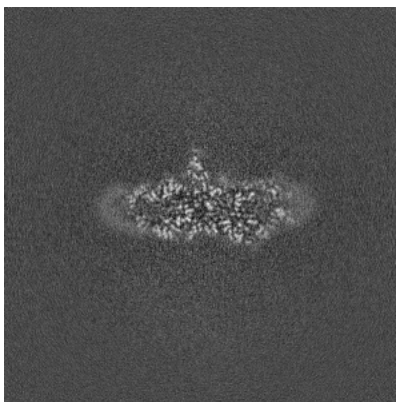


Z Index: 224

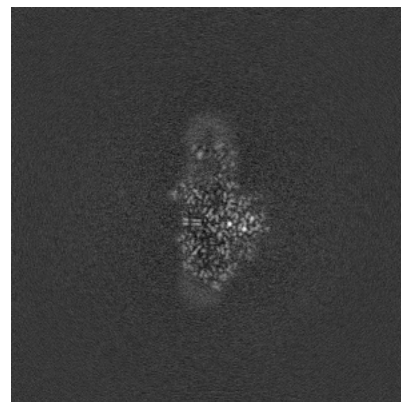
6.2.2 Raw map



X Index: 224



Y Index: 224

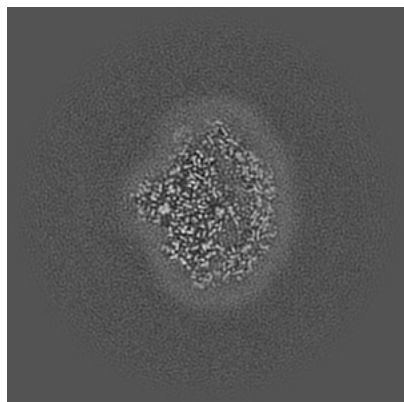


Z Index: 224

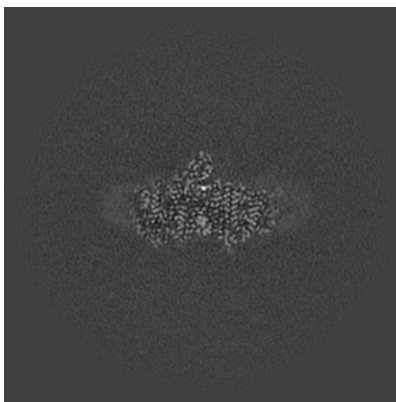
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

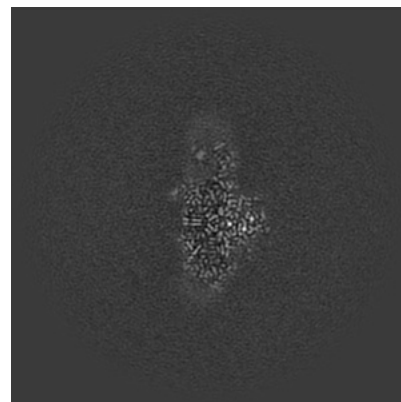
6.3.1 Primary map



X Index: 236

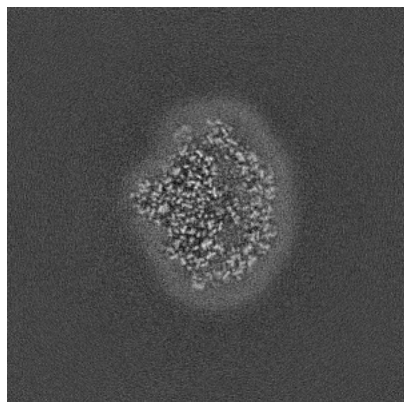


Y Index: 204

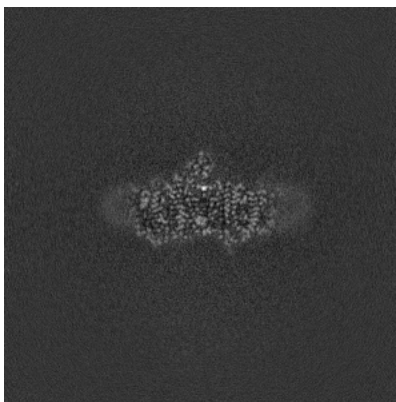


Z Index: 223

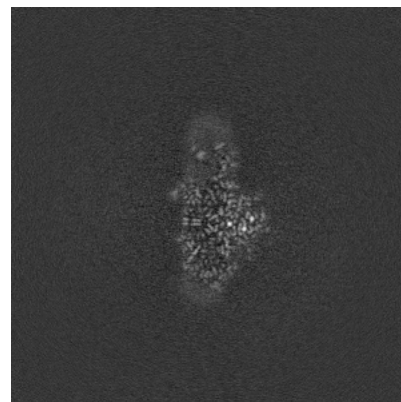
6.3.2 Raw map



X Index: 237



Y Index: 205

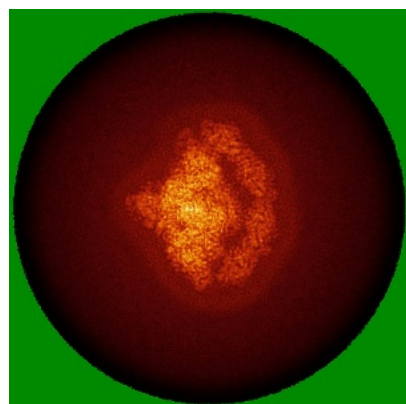


Z Index: 223

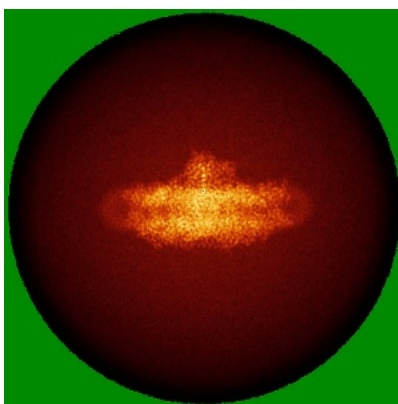
The images above show the largest variance slices of the map in three orthogonal directions.

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

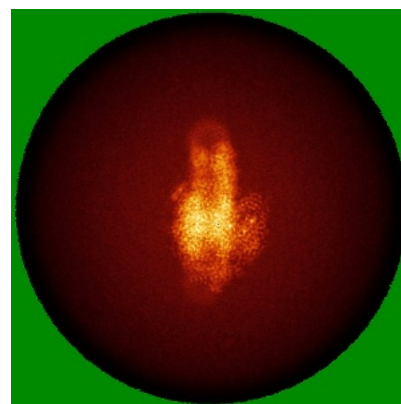
6.4.1 Primary map



X

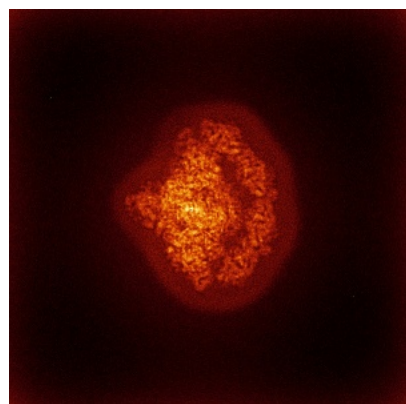


Y

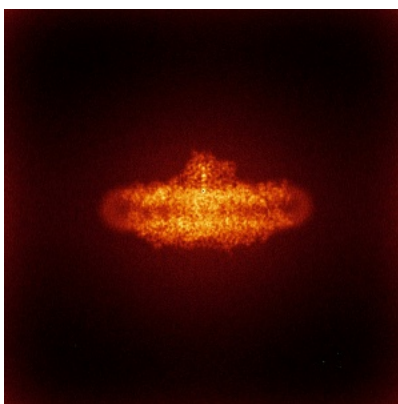


Z

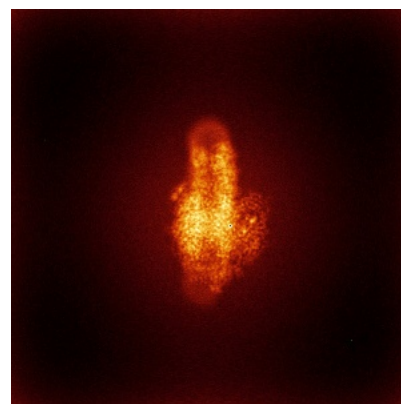
6.4.2 Raw map



X



Y

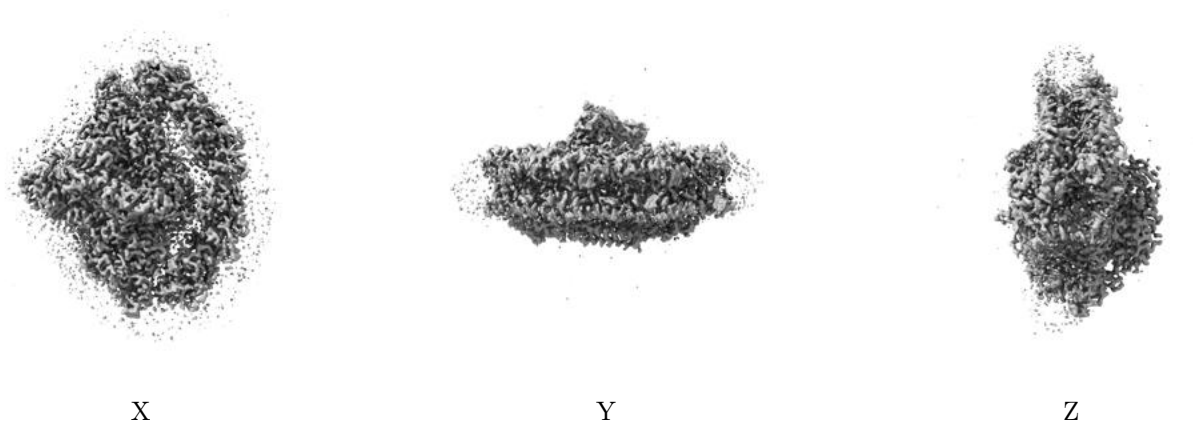


Z

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.

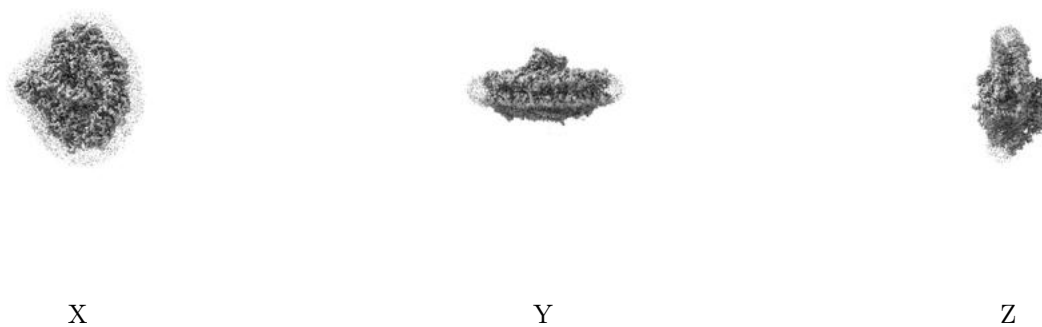
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

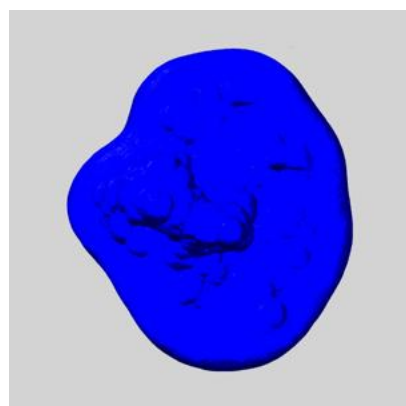
6.6 Mask visualisation [i](#)

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

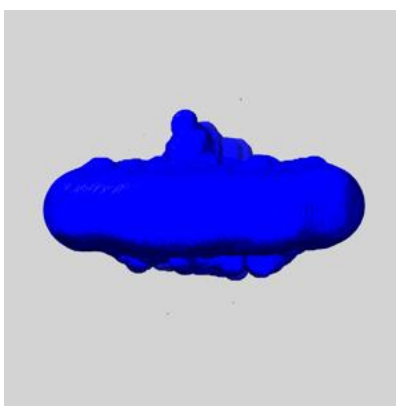
A mask typically either:

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

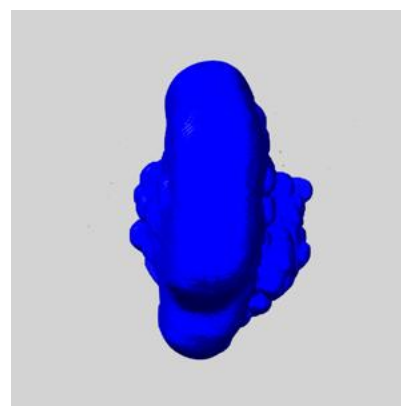
6.6.1 emd_51227_msk_1.map [i](#)



X



Y

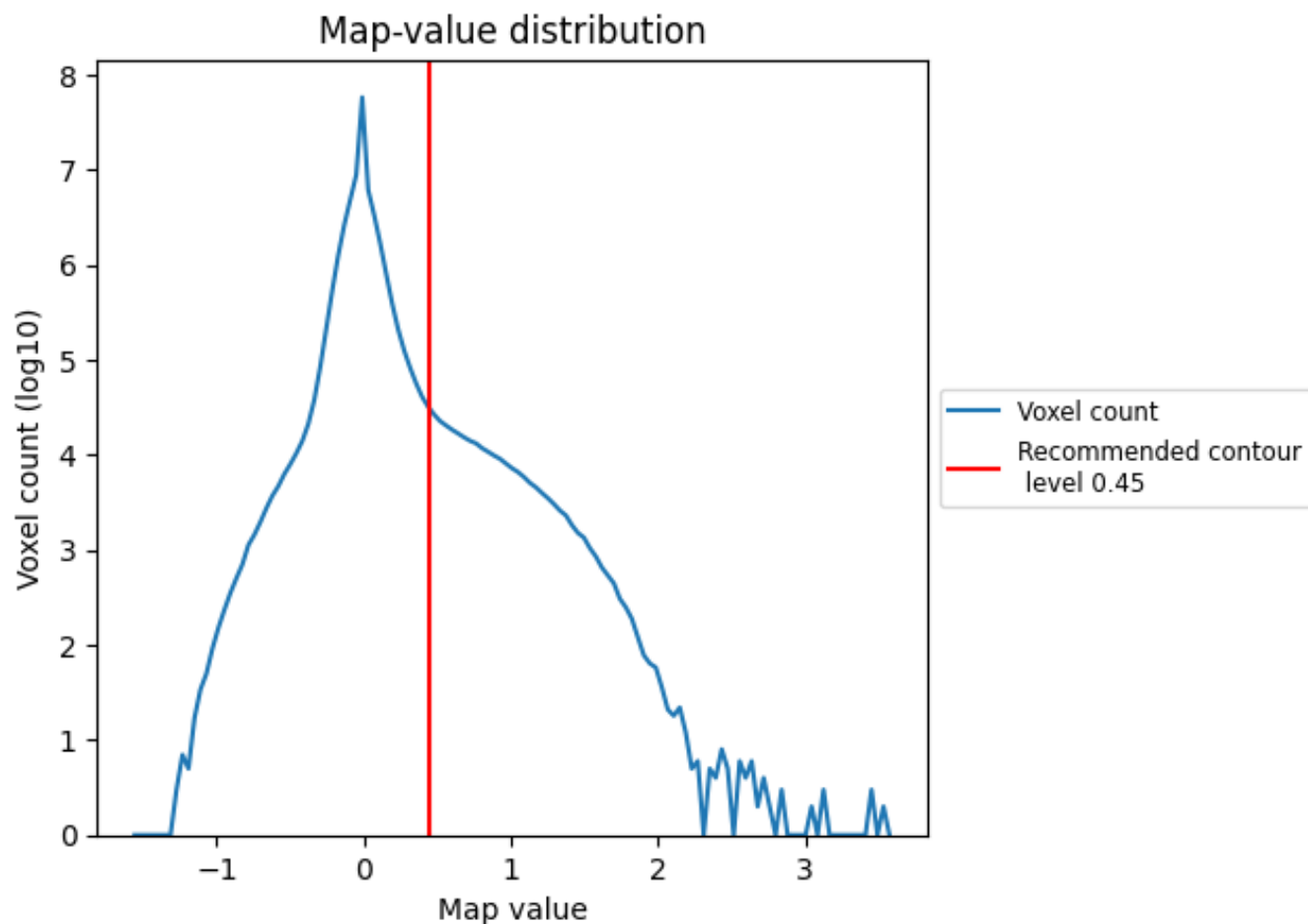


Z

7 Map analysis [i](#)

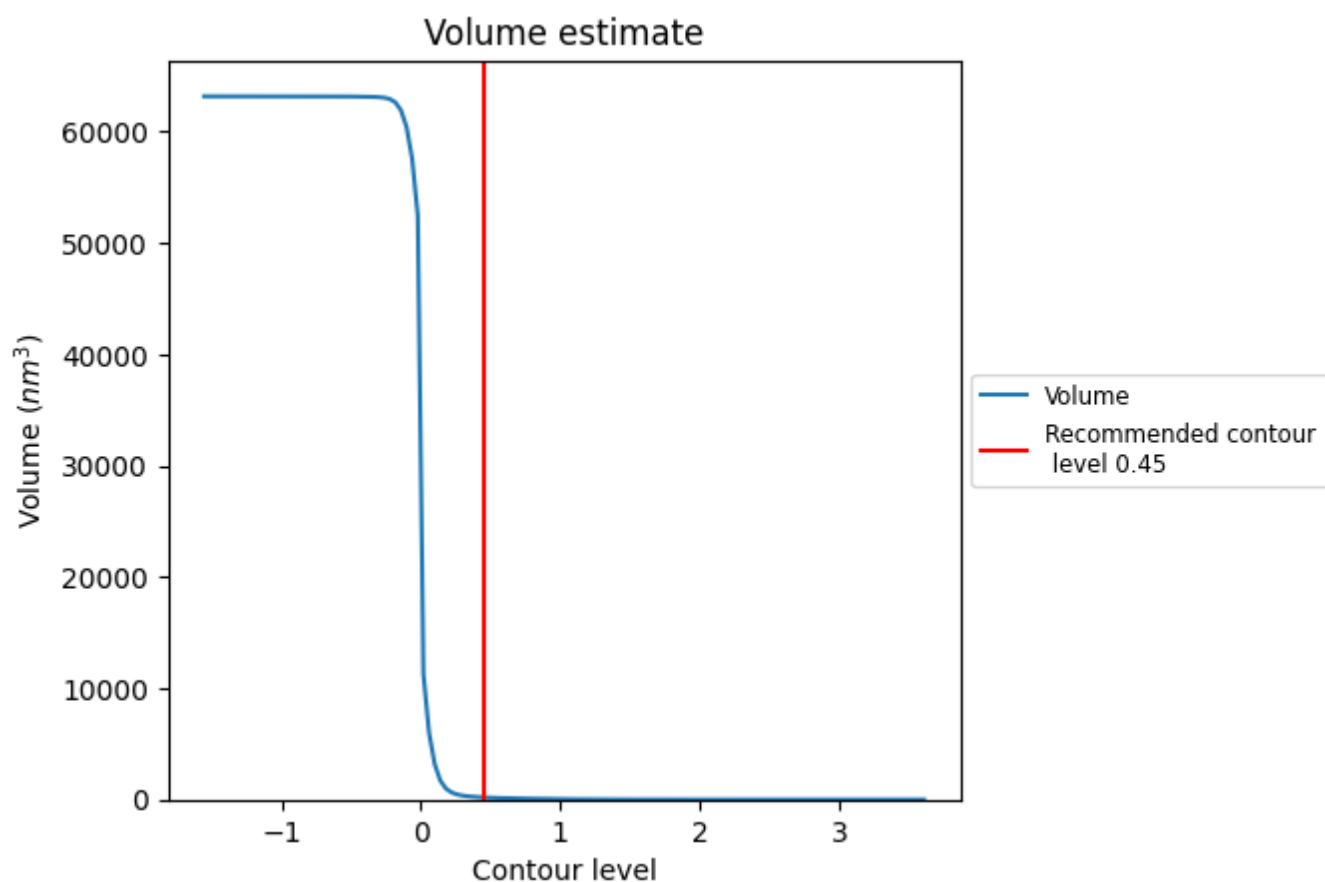
This section contains the results of statistical analysis of the map.

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.

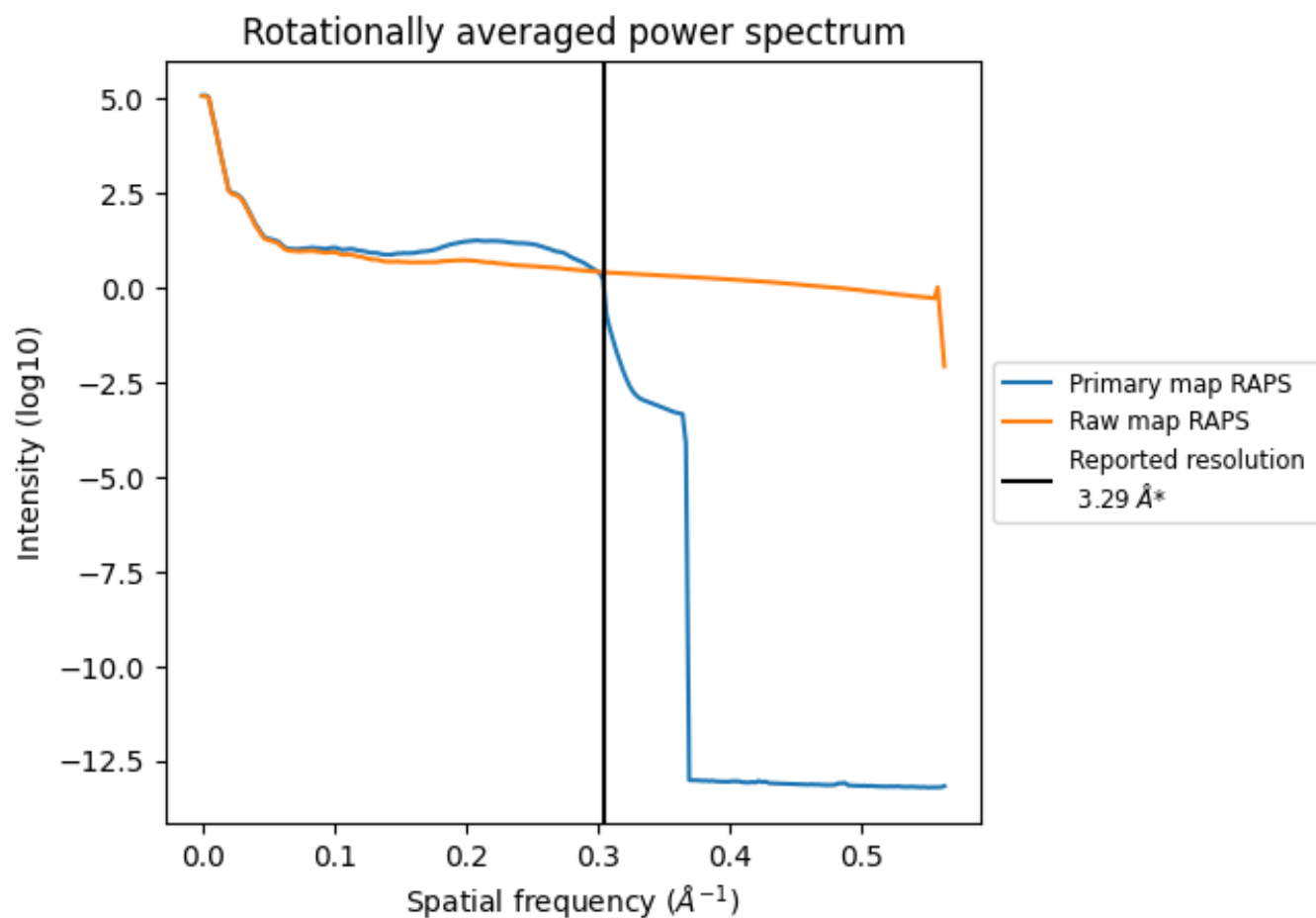
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm^3 ; this corresponds to an approximate mass of 174 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 ⓘ

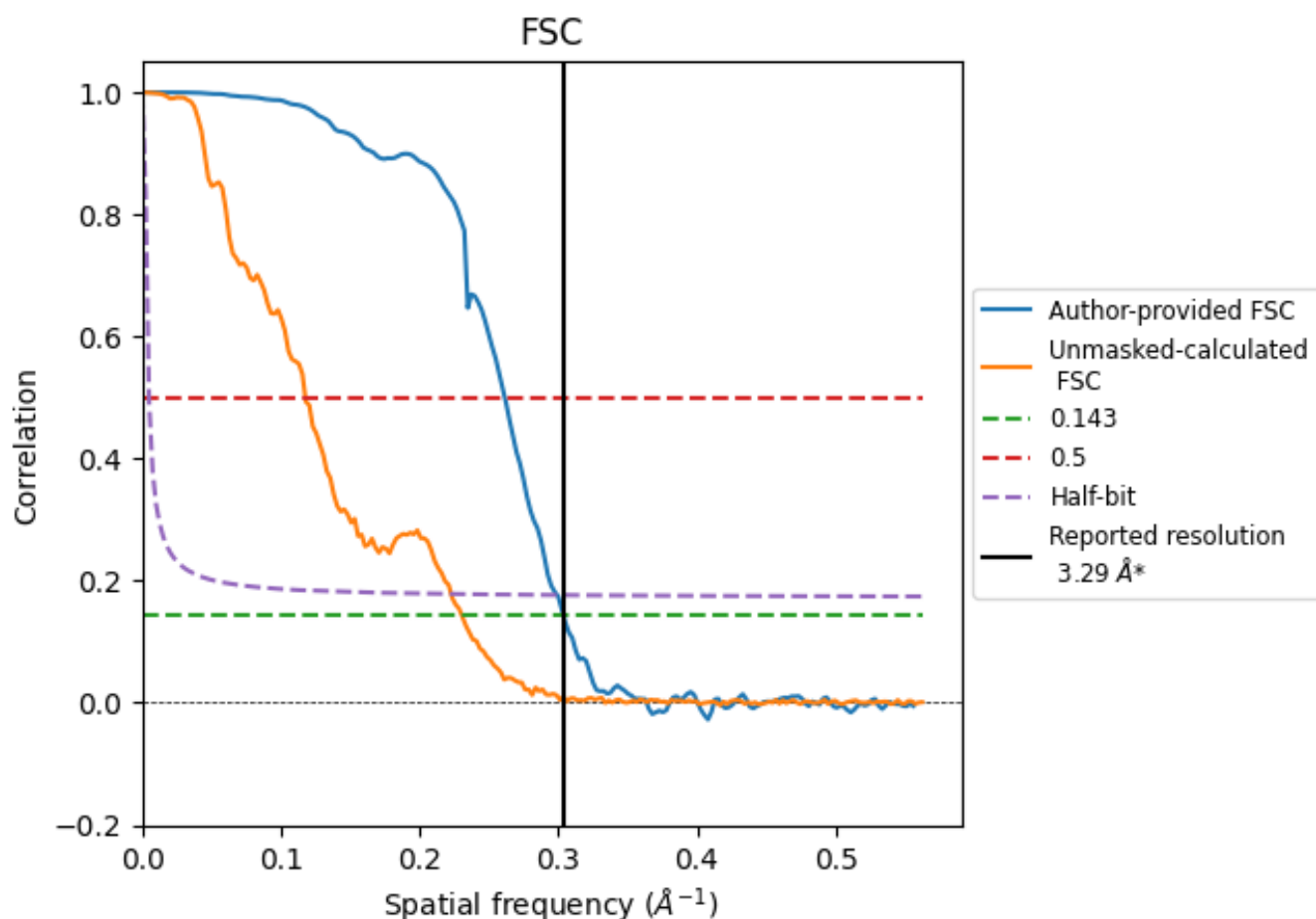


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.304 \AA^{-1}

8.2 Resolution estimates [i](#)

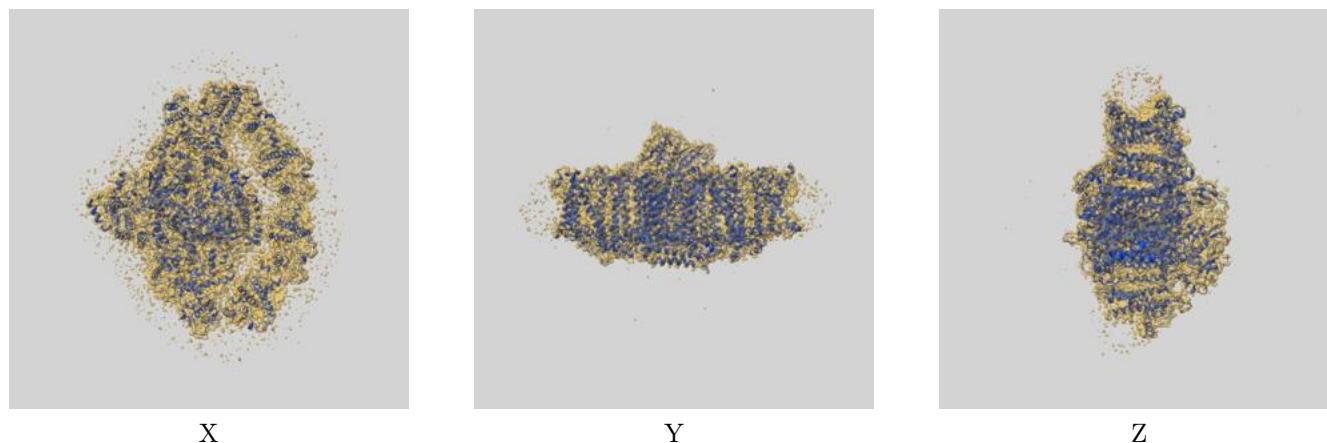
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	3.82	3.34
Unmasked-calculated*	4.34	8.50	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51227 and PDB model 9GC2. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



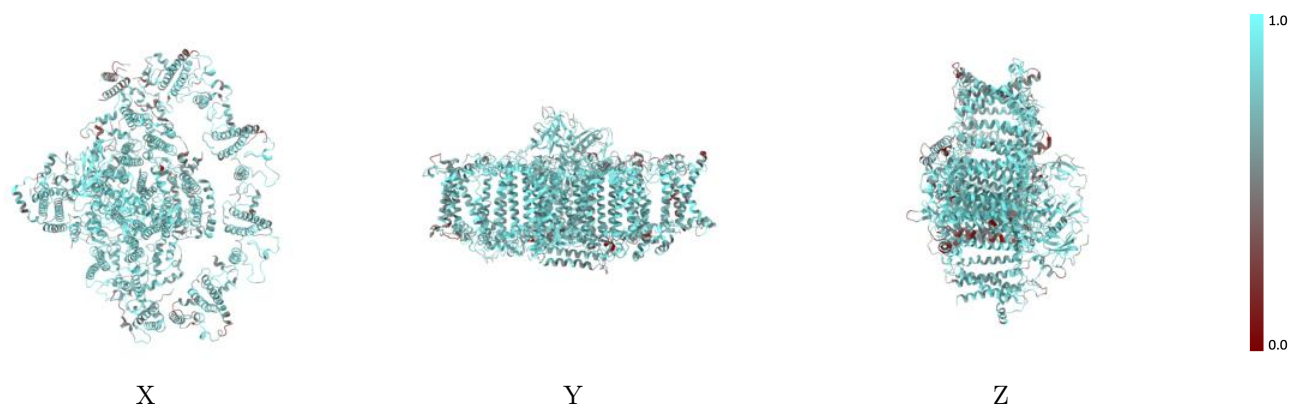
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



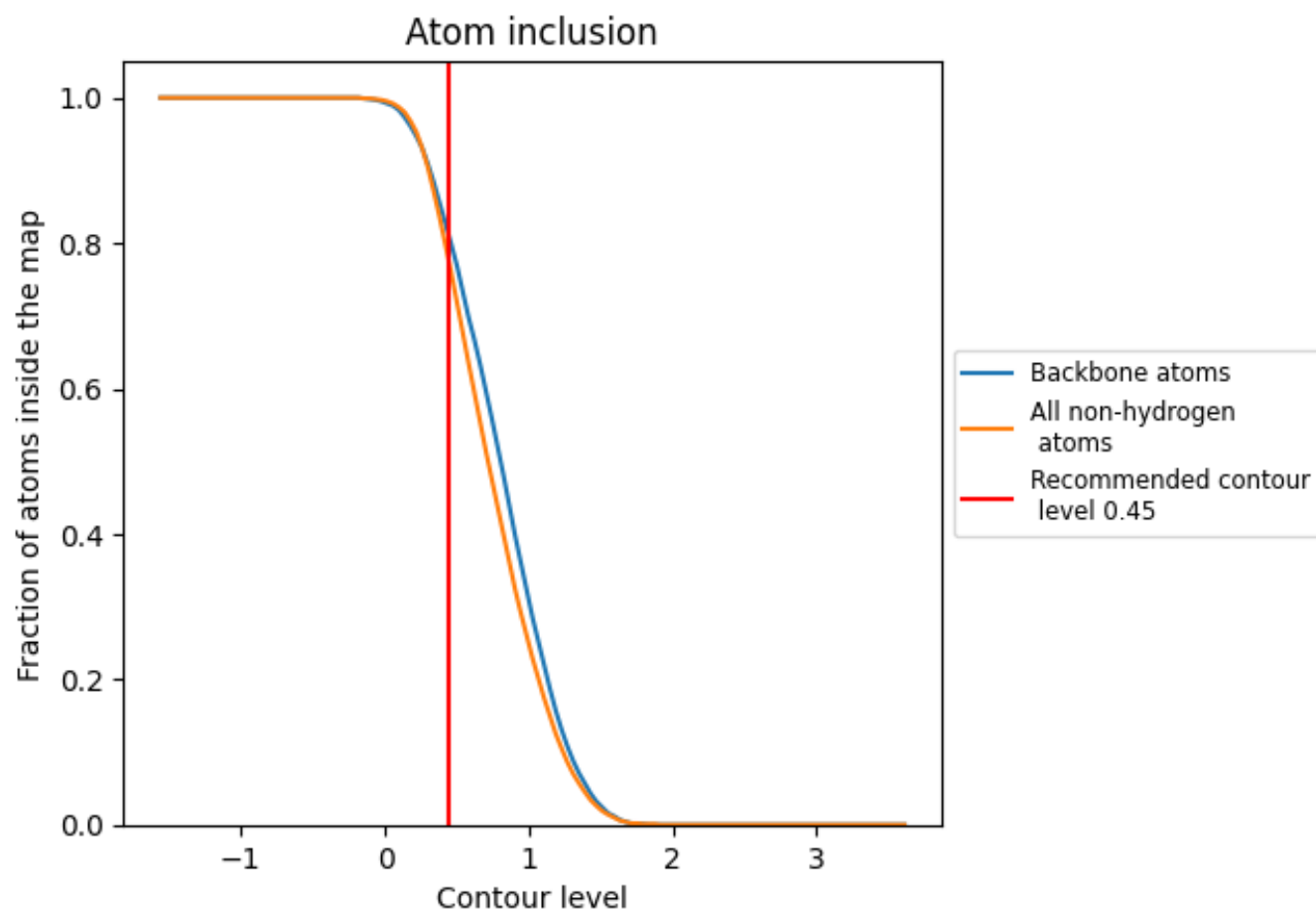
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7710	<div></div> 0.5350
1	<div></div> 0.6620	<div></div> 0.4900
2	<div></div> 0.7100	<div></div> 0.4990
3	<div></div> 0.7130	<div></div> 0.5060
4	<div></div> 0.7340	<div></div> 0.5160
A	<div></div> 0.8080	<div></div> 0.5540
B	<div></div> 0.8480	<div></div> 0.5650
C	<div></div> 0.8690	<div></div> 0.5520
D	<div></div> 0.7950	<div></div> 0.5440
E	<div></div> 0.7620	<div></div> 0.5410
F	<div></div> 0.7530	<div></div> 0.5280
G	<div></div> 0.6710	<div></div> 0.5110
H	<div></div> 0.7100	<div></div> 0.5250
I	<div></div> 0.7850	<div></div> 0.5400
J	<div></div> 0.6410	<div></div> 0.5130
K	<div></div> 0.4700	<div></div> 0.4390
L	<div></div> 0.7670	<div></div> 0.5330
N	<div></div> 0.2310	<div></div> 0.4100

