



Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 05:08 PM JST

PDB ID : 9WLS / pdb_00009wls
EMDB ID : EMD-66073
Title : PSI complex of A.thaliana isolated using DOC based Clear-Native-PAGE method
Authors : Kawamoto, A.; Seki, S.; Kurisu, G.
Deposited on : 2025-09-02
Resolution : 2.18 Å(reported)
Based on initial model : 8J7B

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:

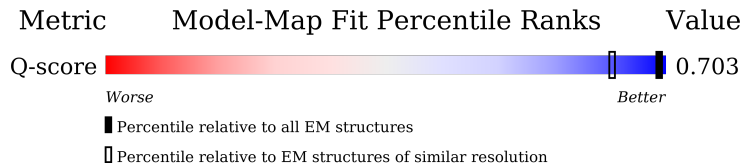
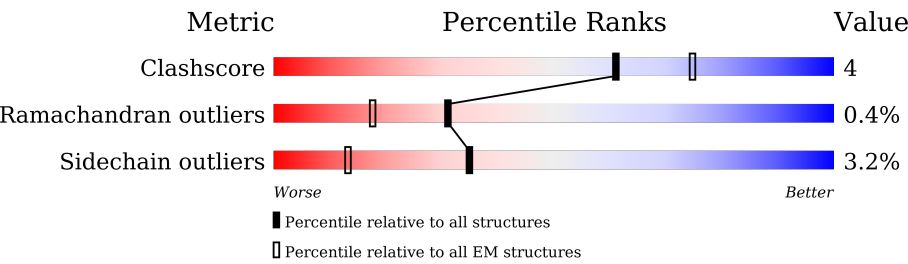
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.18 Å.

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



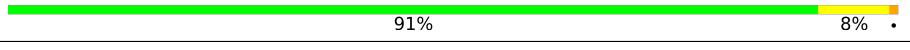
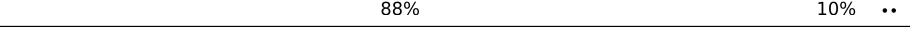
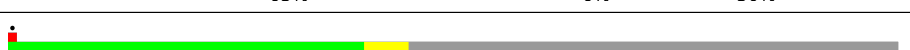
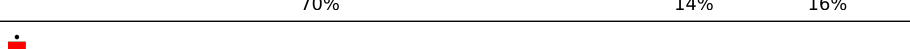
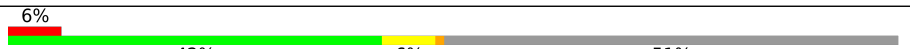
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2701 (1.70 - 2.68)

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	241	16% 71% 9% 20%
2	2	257	25% 72% 9% 19%
3	3	273	8% 73% 7% 19%
4	4	251	19% 74% 5% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	204	
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	
17	N	171	

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	601	X	-	-	-
18	CHL	2	316	X	-	-	-
18	CHL	3	303	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	612	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	312	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	4	317	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	846	X	-	-	-
19	CLA	A	850	X	-	-	-
19	CLA	A	851	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	841	X	-	-	-
19	CLA	B	843	X	-	-	-
19	CLA	B	844	X	-	-	-
19	CLA	B	845	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	H	201	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	L	304	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36141 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	209	Total	C	N	O	S	0	0
			1622	1061	264	293	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	221	Total	C	N	O	S	0	0
			1699	1112	276	306	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1550	1012	252	283	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	743	Total	C	N	O	S	0	0
			5851	3836	993	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
			5858	3845	998	1001	14		

- 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	143	Total	C	N	O	S	0	0
			1128	723	195	206	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O	S	0	0
			517	331	92	94			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	153	Total	C	N	O	S	0	0
			1211	791	207	210	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			763	495	125	143			

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	95	Total	C	N	O	S	0	0
			735	478	119	138			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	31	Total	C	N	O	S	0	0
			239	162	39	37	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
			338	230	51	56	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	64	Total	C	N	O	S	0	0
			447	286	73	85	3		

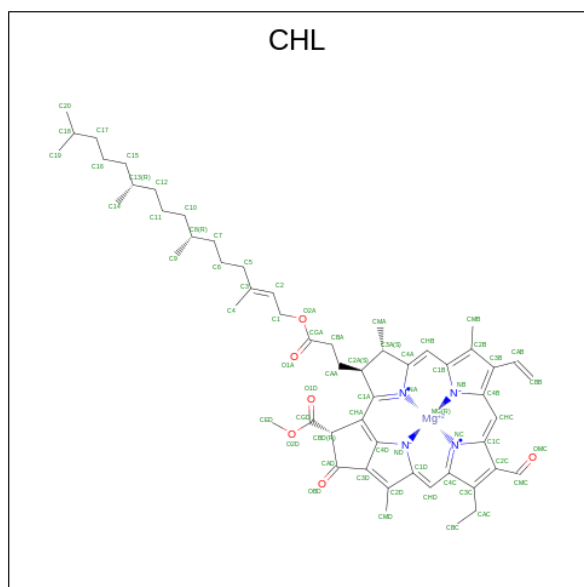
- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	150	Total	C	N	O	S	0	0
			1119	737	179	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	50	Total	C	N	O	S	0	0
			394	246	70	76	2		

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



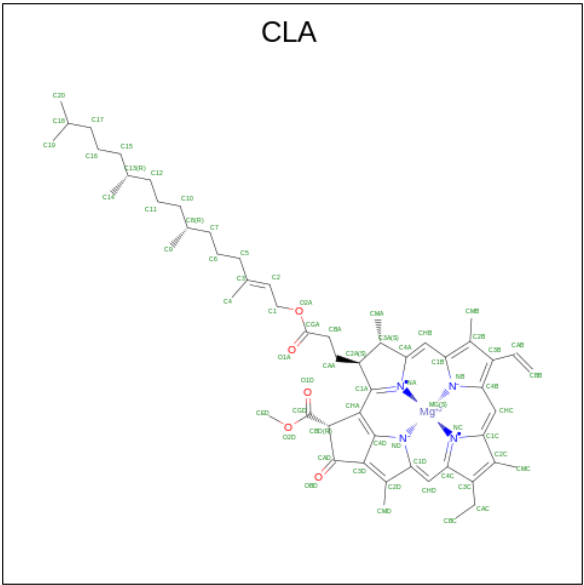
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			59	48	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			42	33	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
			59	48	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			51	40	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
			46	35	1	4	6	

- 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
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			51	41	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
			55	45	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			55	45	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
			62	52	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
			52	42	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
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			48	38	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
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
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
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			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
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	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
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			53	43	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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			58	48	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	
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	
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
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 60	C 50	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 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 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 42	C 34	Mg 1	N 4	O 3	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 52	C 42	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 51	C 41	Mg 1	N 4	O 5	0
19	B	1	Total 43	C 35	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
			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
			57	47	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	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
			43	35	1	4	3	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	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
			65	55	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
			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
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	F	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

Continued on next page...

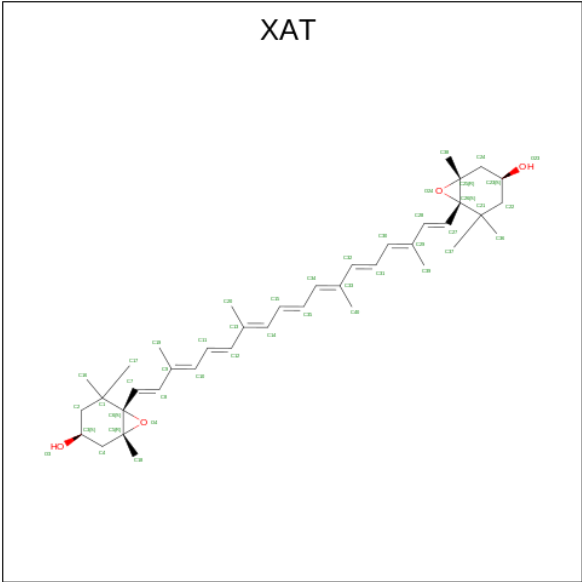
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

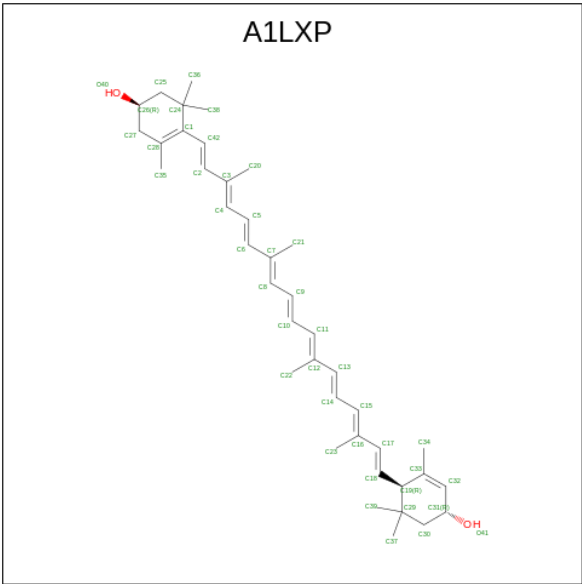
Mol	Chain	Residues	Atoms					AltConf
20	1	6	Total	C	Mg	N	O	0
			274	220	6	24	24	
20	2	7	Total	C	Mg	N	O	0
			291	234	7	28	22	
20	3	4	Total	C	Mg	N	O	0
			163	133	4	16	10	
20	4	8	Total	C	Mg	N	O	0
			354	284	8	32	30	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- 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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



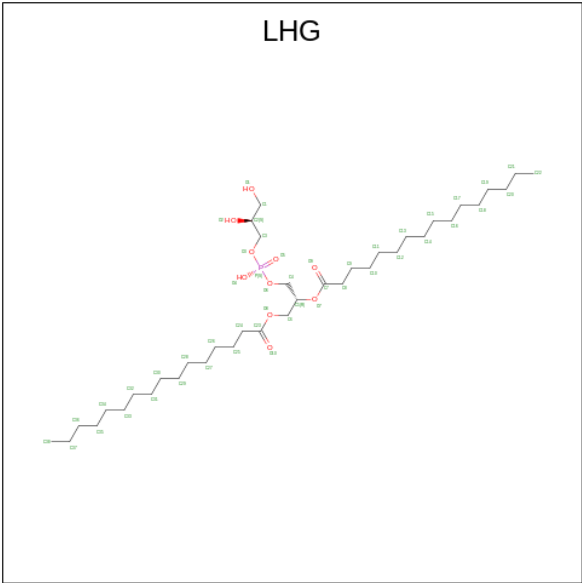
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			28	26	2	
21	2	1	Total	C	O	0
			44	40	4	

- Molecule 22 is Lutein (CCD ID: A1LXP) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	1	1	Total	C	O	0
			42	40	2	
22	2	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	J	1	Total	C	O	0
			42	40	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



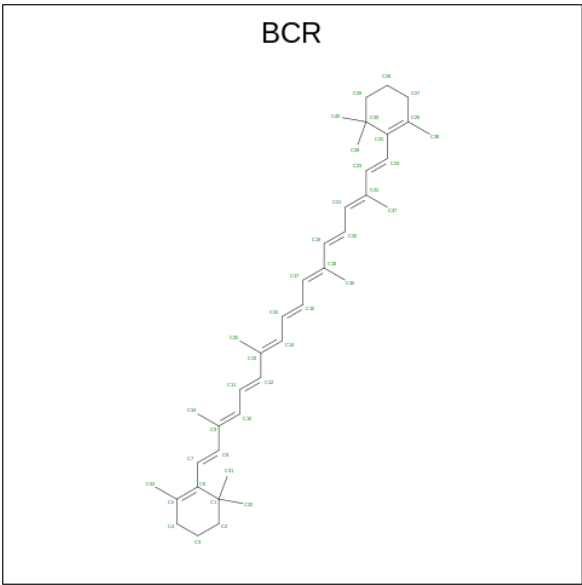
Mol	Chain	Residues	Atoms				AltConf
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			21	10	10	1	
23	2	1	Total	C	O	P	0
			45	34	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



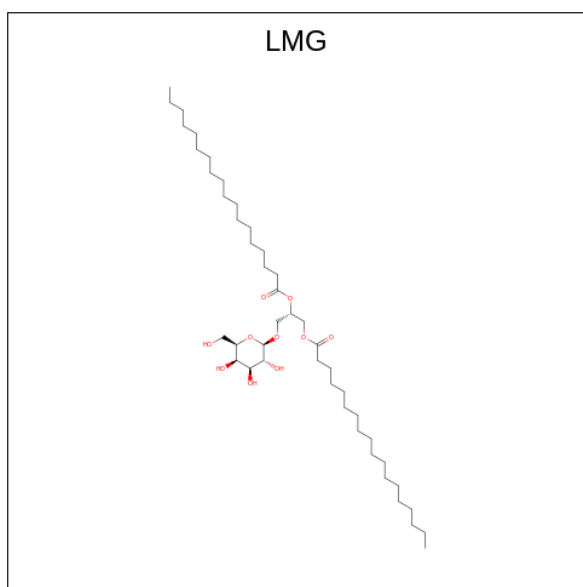
Mol	Chain	Residues	Atoms		AltConf
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			25	25	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

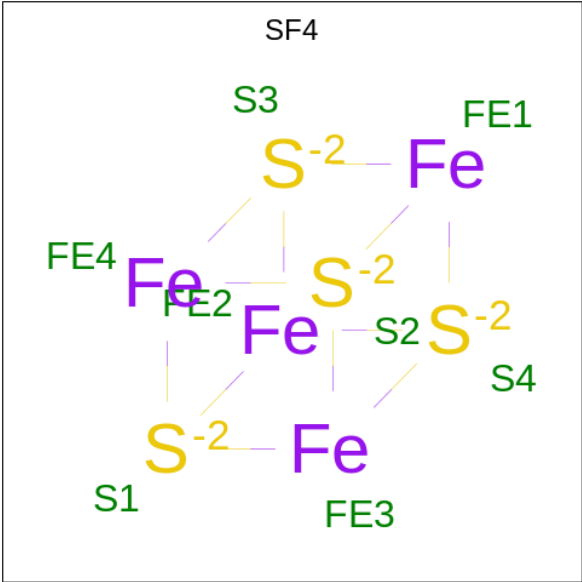
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C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



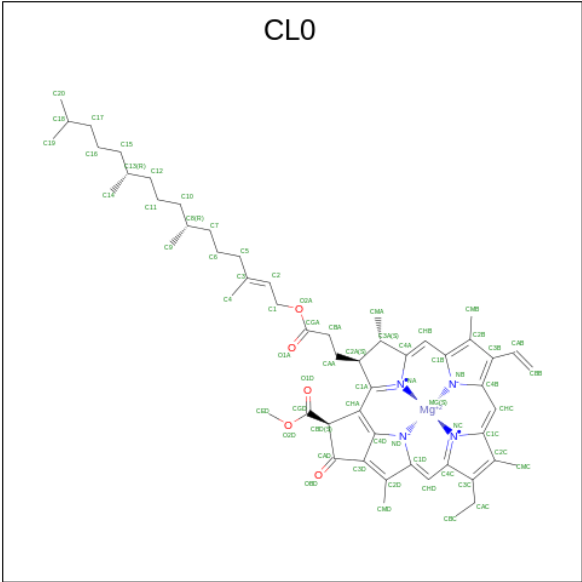
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			30	20	10	
25	F	1	Total	C	O	0
			30	20	10	
25	G	1	Total	C	O	0
			35	25	10	
25	J	1	Total	C	O	0
			41	31	10	
25	N	1	Total	C	O	0
			27	18	9	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



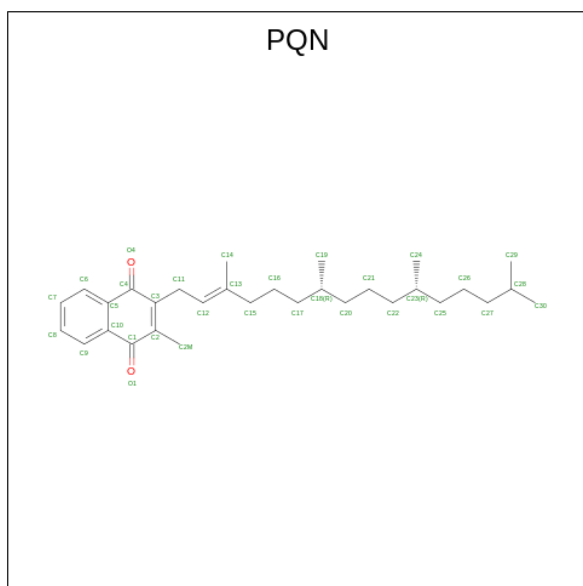
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



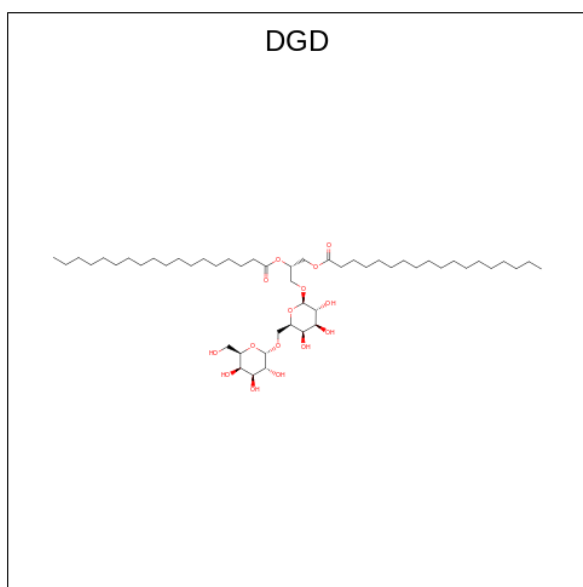
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			60	45	15	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	1	6	Total	O	0
			6	6	
30	2	12	Total	O	0
			12	12	
30	3	11	Total	O	0
			11	11	
30	4	3	Total	O	0
			3	3	
30	A	137	Total	O	0
			137	137	
30	B	177	Total	O	0
			177	177	
30	C	43	Total	O	0
			43	43	
30	D	29	Total	O	0
			29	29	
30	E	16	Total	O	0
			16	16	
30	F	6	Total	O	0
			6	6	
30	G	4	Total	O	0
			4	4	

Continued on next page...

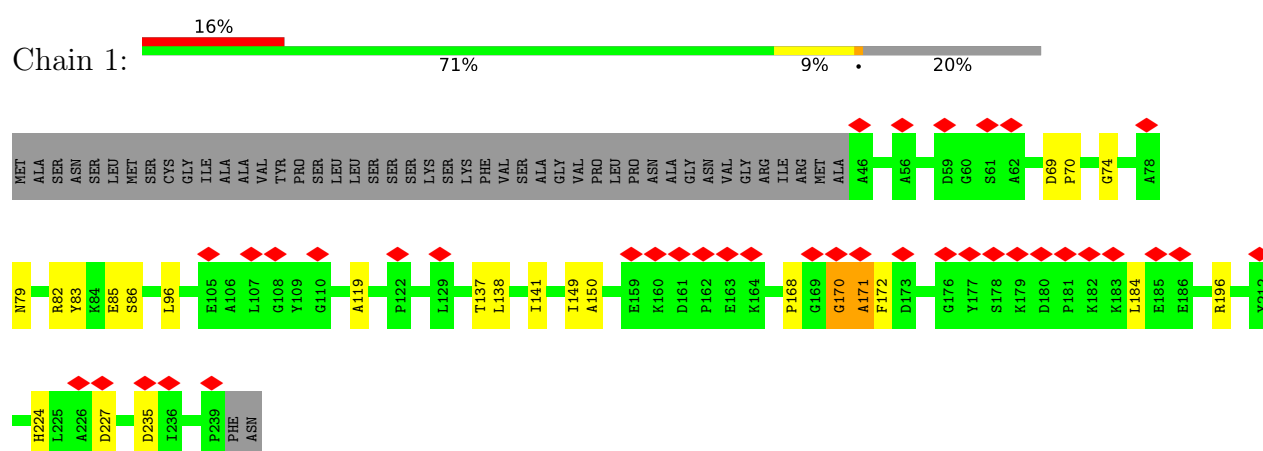
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
30	H	7	Total 7	O 7	0
30	I	1	Total 1	O 1	0
30	J	6	Total 6	O 6	0
30	K	2	Total 2	O 2	0
30	L	16	Total 16	O 16	0
30	N	4	Total 4	O 4	0

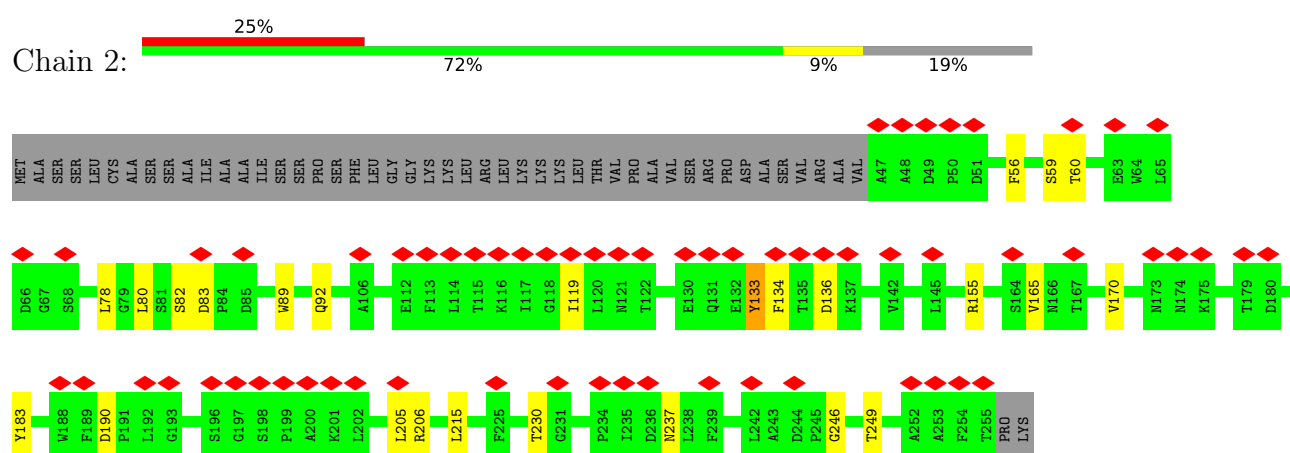
3 Residue-property plots

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

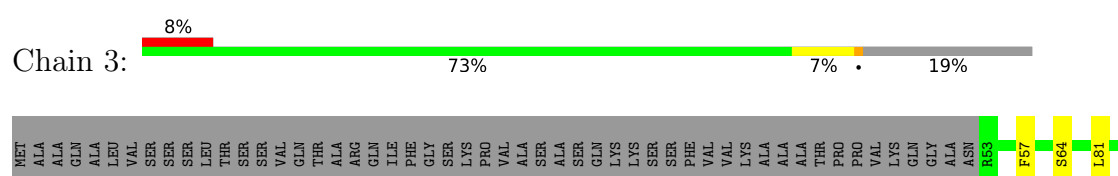
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic

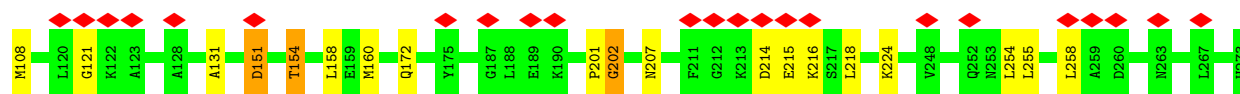


- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

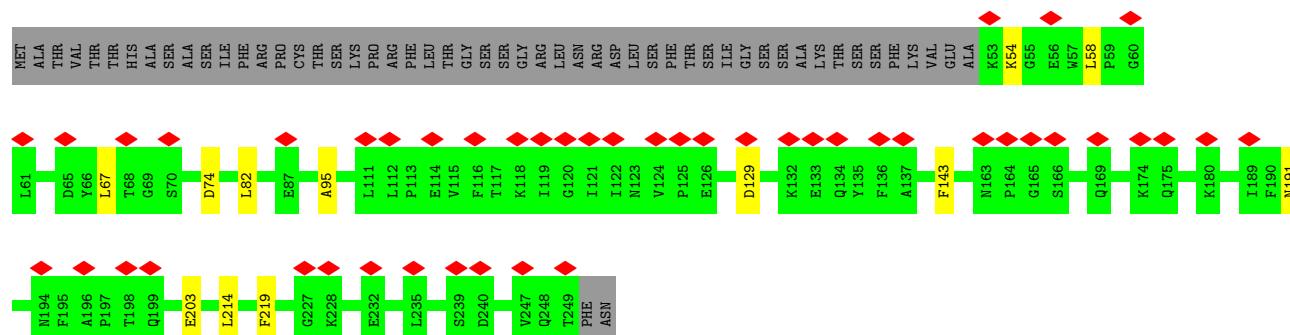
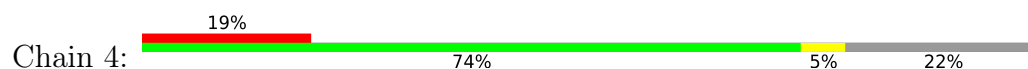


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

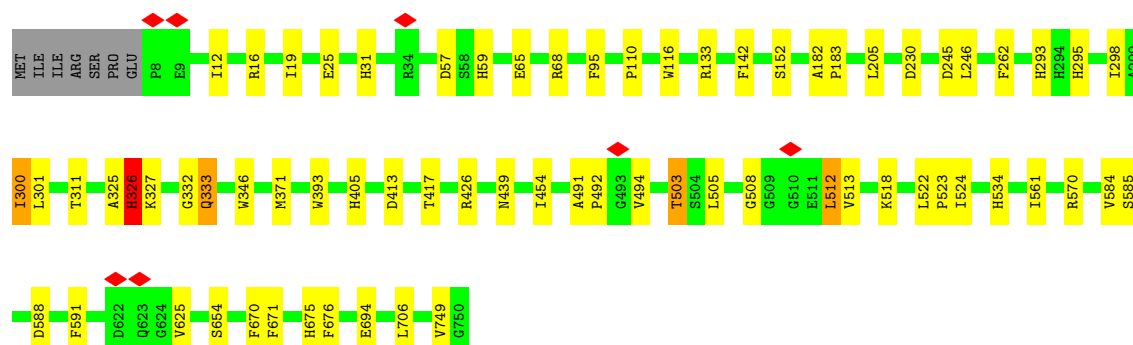
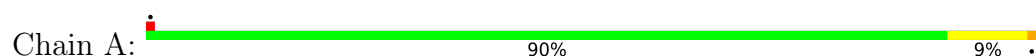




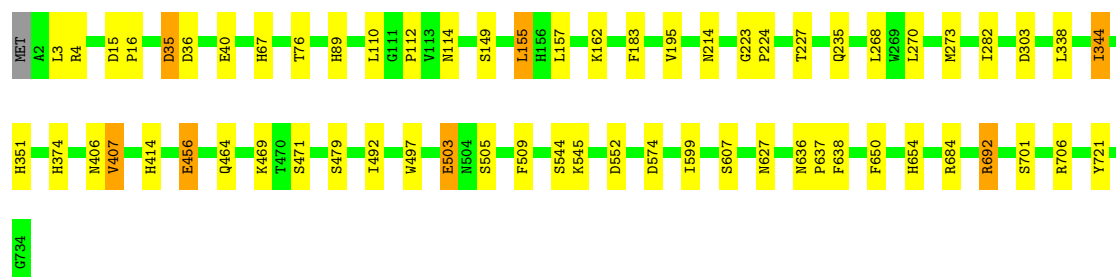
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center

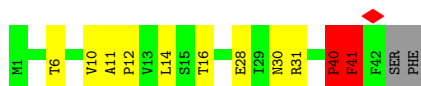




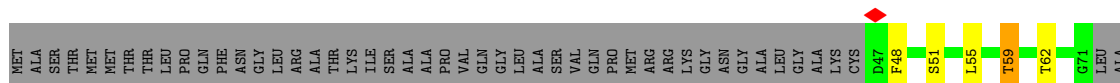
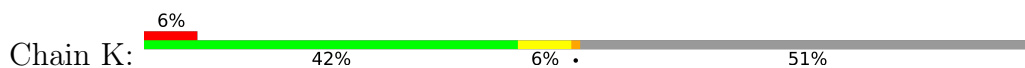
• Molecule 13: Photosystem I reaction center subunit VIII



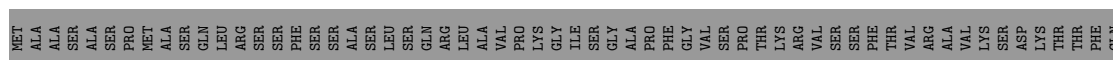
• Molecule 14: Photosystem I reaction center subunit IX



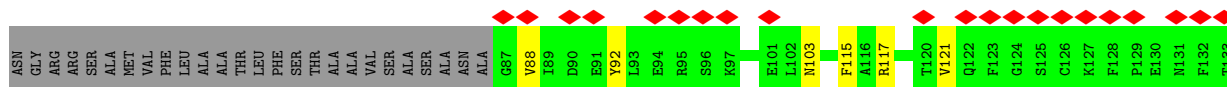
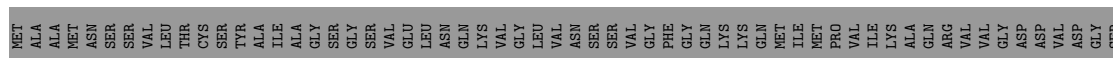
• Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic



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



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



C134	ASP
C135	LEU
Q136	ALA
	LYS
	GLN
	LYS
	LYS
	VAL
	PRO
	PHE
	ILE
	SER
	GLU
	ASP
	ILE
	ALA
	LEU
	GLU
	CYS
	GLU
	GLY
	LYS
	LYS
	ASP
	LYS
	TYR
	LYS
	CYS
	GLY
	SER
	ASN
	VAL
	PHE
	TRP
	LYS
	TRP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00994	Depositor
Map size ($\text{\AA}$)	264.6, 264.6, 264.6	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.675, 0.675, 0.675	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, A1LXP, SF4, CHL, UNL, BCR, LMG, CL0, DGD, LHG, CLA, PQN

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	0.55	0/1551	1.08	1/2117 (0.0%)
2	2	0.55	0/1680	1.14	2/2299 (0.1%)
3	3	0.55	0/1752	1.06	2/2382 (0.1%)
4	4	0.54	0/1598	1.08	2/2179 (0.1%)
5	A	0.89	0/6050	1.16	13/8254 (0.2%)
6	B	0.90	0/6069	1.22	24/8286 (0.3%)
7	C	0.88	0/628	1.46	7/852 (0.8%)
8	D	0.72	0/1157	1.24	4/1563 (0.3%)
9	E	0.67	0/528	1.05	0/715
10	F	0.72	0/1241	1.22	2/1675 (0.1%)
11	G	0.68	0/783	1.21	4/1061 (0.4%)
12	H	0.66	0/756	1.23	4/1024 (0.4%)
13	I	0.76	0/245	1.09	1/333 (0.3%)
14	J	0.69	0/348	1.20	5/474 (1.1%)
15	K	0.60	0/451	1.18	3/608 (0.5%)
16	L	0.74	0/1152	1.18	2/1572 (0.1%)
17	N	0.49	0/400	1.19	0/534
All	All	0.77	0/26389	1.18	76/35928 (0.2%)

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
2	2	0	1
5	A	0	5
7	C	0	2
9	E	0	1
10	F	0	1
14	J	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
16	L	0	1
All	All	0	12

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	326	HIS	CA-CB-CG	-10.49	103.31	113.80
6	B	4	ARG	N-CA-CB	-10.39	95.15	111.56
7	C	23	THR	OG1-CB-CG2	-9.60	90.10	109.30
6	B	407	VAL	N-CA-CB	-9.10	95.09	110.65
7	C	23	THR	CA-C-N	-8.74	109.78	123.24
7	C	23	THR	C-N-CA	-8.74	109.78	123.24
7	C	23	THR	O-C-N	-7.40	114.70	122.84
10	F	152	THR	CA-CB-OG1	-7.37	98.54	109.60
7	C	23	THR	CA-CB-OG1	7.31	120.57	109.60
5	A	405	HIS	CA-CB-CG	-7.27	106.53	113.80
5	A	671	PHE	CA-CB-CG	7.19	120.99	113.80
6	B	67	HIS	CA-CB-CG	-6.87	106.93	113.80
6	B	638	PHE	CA-CB-CG	-6.78	107.02	113.80
6	B	552	ASP	CA-CB-CG	6.73	119.33	112.60
5	A	670	PHE	CA-CB-CG	-6.64	107.16	113.80
6	B	40	GLU	N-CA-CB	6.62	119.88	109.82
12	H	70	GLN	CB-CA-C	-6.57	101.78	112.03
14	J	6	THR	CA-CB-OG1	-6.57	99.75	109.60
6	B	407	VAL	CB-CA-C	6.55	122.32	112.16
5	A	262	PHE	CA-CB-CG	-6.51	107.29	113.80
6	B	4	ARG	CB-CA-C	6.50	125.84	111.09
8	D	127	ARG	CD-NE-CZ	6.48	133.47	124.40
6	B	35	ASP	CA-CB-CG	6.35	118.95	112.60
11	G	93	LYS	N-CA-CB	-6.31	100.92	110.07
14	J	41	PHE	CA-CB-CG	6.31	120.11	113.80
12	H	52	TYR	N-CA-C	-6.27	104.07	111.03
7	C	23	THR	N-CA-C	-6.24	99.20	109.80
6	B	112	PRO	CB-CA-C	6.22	119.49	111.46
16	L	160	GLU	N-CA-CB	6.22	119.20	109.69
10	F	190	VAL	O-C-N	-6.21	115.66	120.07
2	2	83	ASP	CA-CB-CG	6.14	118.74	112.60
6	B	214	ASN	CB-CA-C	-6.06	101.21	111.02
6	B	15	ASP	CA-CB-CG	6.02	118.62	112.60
3	3	151	ASP	CA-CB-CG	5.99	118.58	112.60
16	L	203	THR	CA-CB-OG1	-5.98	100.63	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	650	PHE	CA-CB-CG	5.95	119.75	113.80
15	K	62	THR	CA-CB-OG1	-5.90	100.75	109.60
4	4	219	PHE	CA-CB-CG	5.88	119.68	113.80
15	K	102	THR	CA-CB-OG1	-5.79	100.91	109.60
15	K	59	THR	OG1-CB-CG2	-5.79	97.72	109.30
6	B	456	GLU	O-C-N	-5.75	116.18	121.30
14	J	30	ASN	CA-CB-CG	-5.72	106.88	112.60
6	B	76	THR	CA-CB-OG1	-5.72	101.02	109.60
6	B	545	LYS	CB-CA-C	5.71	121.64	110.67
5	A	57	ASP	CA-CB-CG	5.70	118.30	112.60
12	H	93	PHE	CA-CB-CG	-5.61	108.19	113.80
8	D	123	LEU	N-CA-CB	-5.57	101.17	110.80
6	B	227	THR	CA-CB-OG1	-5.47	101.40	109.60
14	J	16	THR	CA-CB-OG1	-5.43	101.45	109.60
8	D	167	TYR	CB-CA-C	5.37	118.00	109.52
5	A	524	ILE	CA-C-O	5.35	122.31	119.15
11	G	72	THR	OG1-CB-CG2	-5.34	98.61	109.30
6	B	654	HIS	CA-CB-CG	5.34	119.14	113.80
6	B	414	HIS	CA-CB-CG	5.30	119.10	113.80
12	H	52	TYR	N-CA-CB	5.30	117.66	109.98
7	C	24	ASP	CA-CB-CG	5.27	117.87	112.60
6	B	155	LEU	N-CA-CB	-5.25	102.40	110.01
14	J	40	PRO	CB-CA-C	5.25	120.22	111.56
6	B	692	ARG	CA-CB-CG	5.25	124.60	114.10
3	3	108	MET	CG-SD-CE	5.23	112.41	100.90
8	D	164	ASP	CA-CB-CG	5.22	117.82	112.60
13	I	11	PHE	CA-CB-CG	-5.20	108.60	113.80
6	B	627	ASN	CA-CB-CG	-5.18	107.42	112.60
5	A	295	HIS	CA-CB-CG	-5.16	108.64	113.80
11	G	93	LYS	CB-CA-C	5.15	119.03	110.90
2	2	136	ASP	CA-CB-CG	5.15	117.75	112.60
6	B	464	GLN	N-CA-CB	5.14	117.68	110.12
5	A	591	PHE	CA-CB-CG	5.10	118.90	113.80
5	A	293	HIS	CA-CB-CG	5.09	118.89	113.80
5	A	311	THR	CA-C-O	-5.09	116.87	119.77
11	G	89	GLU	CB-CA-C	5.09	118.95	110.90
5	A	59	HIS	CA-CB-CG	5.09	118.89	113.80
5	A	675	HIS	CA-CB-CG	5.09	118.89	113.80
4	4	143	PHE	N-CA-CB	5.06	117.52	109.82
1	1	227	ASP	CA-CB-CG	5.03	117.63	112.60
6	B	406	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	133	TYR	Peptide
5	A	16	ARG	Sidechain
5	A	326	HIS	Peptide
5	A	426	ARG	Sidechain
5	A	570	ARG	Sidechain
5	A	68	ARG	Sidechain
7	C	19	ARG	Sidechain
7	C	24	ASP	Mainchain
9	E	92	ARG	Sidechain
10	F	209	ARG	Sidechain
14	J	31	ARG	Sidechain
16	L	174	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1501	0	1476	14	0
2	2	1622	0	1562	8	0
3	3	1699	0	1665	8	0
4	4	1550	0	1490	9	0
5	A	5851	0	5706	41	0
6	B	5858	0	5649	24	0
7	C	615	0	592	3	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0
10	F	1211	0	1239	5	0
11	G	763	0	738	9	0
12	H	735	0	732	8	0
13	I	239	0	258	2	0
14	J	338	0	351	5	0
15	K	447	0	460	4	0
16	L	1119	0	1124	9	0
17	N	394	0	381	5	0
18	1	102	0	82	4	0
18	2	147	0	111	0	0
18	3	117	0	107	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	4	92	0	62	2	0
19	1	325	0	288	9	0
19	2	212	0	184	2	0
19	3	404	0	335	4	0
19	4	244	0	195	6	0
19	A	2378	0	2287	57	0
19	B	2326	0	2257	56	0
19	F	90	0	67	2	0
19	G	87	0	64	5	0
19	H	55	0	49	0	0
19	J	65	0	72	1	0
19	K	90	0	66	2	0
19	L	155	0	138	2	0
20	1	274	0	0	4	0
20	2	291	0	0	1	0
20	3	163	0	0	1	0
20	4	354	0	0	1	0
20	G	45	0	0	0	0
20	J	42	0	0	1	0
20	K	42	0	0	0	0
20	N	41	0	0	0	0
21	1	72	0	90	6	0
21	2	44	0	56	1	0
22	1	84	0	0	0	0
22	2	42	0	0	1	0
22	3	84	0	0	1	0
22	4	84	0	0	1	0
22	J	42	0	0	0	0
23	1	70	0	86	0	0
23	2	45	0	63	0	0
23	A	49	0	74	0	0
24	3	40	0	56	0	0
24	4	40	0	56	3	0
24	A	225	0	313	25	0
24	B	200	0	280	11	0
24	F	80	0	112	5	0
24	G	80	0	112	6	0
24	I	40	0	56	1	0
24	J	40	0	56	0	0
24	K	40	0	56	2	0
24	L	120	0	168	4	0
25	4	34	0	38	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	F	60	0	60	2	0
25	G	35	0	40	0	0
25	J	41	0	55	0	0
25	N	27	0	30	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	A	65	0	72	0	0
28	A	33	0	46	0	0
28	B	33	0	46	0	0
29	B	60	0	81	1	0
30	1	6	0	0	0	0
30	2	12	0	0	0	0
30	3	11	0	0	0	0
30	4	3	0	0	0	0
30	A	137	0	0	1	0
30	B	177	0	0	0	0
30	C	43	0	0	0	0
30	D	29	0	0	1	0
30	E	16	0	0	0	0
30	F	6	0	0	0	0
30	G	4	0	0	0	0
30	H	7	0	0	0	0
30	I	1	0	0	0	0
30	J	6	0	0	0	0
30	K	2	0	0	0	0
30	L	16	0	0	0	0
30	N	4	0	0	0	0
All	All	36141	0	33549	303	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 4.

All (303) 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)
12:H:51:LYS:HA	12:H:66:ASN:HB3	1.43	0.99
16:L:65:ILE:HB	16:L:73:SER:OG	1.66	0.95
19:1:602:CLA:O1A	21:1:615:XAT:H241	1.72	0.88
19:G:203:CLA:HBB1	24:G:205:BCR:H352	1.67	0.77
4:4:54:LYS:NZ	4:4:74:ASP:OD1	2.16	0.76
6:B:503:GLU:OE2	6:B:505:SER:OG	2.02	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:230:THR:HG21	2:2:237:ASN:OD1	1.89	0.73
9:E:97:PHE:CE2	9:E:98:LYS:HD3	2.25	0.71
24:A:845:BCR:H382	24:A:845:BCR:H23C	1.75	0.69
5:A:503:THR:OG1	19:A:821:CLA:O1A	2.03	0.69
11:G:69:SER:HA	19:G:203:CLA:O2A	1.93	0.69
19:B:844:CLA:H93	19:B:844:CLA:C3	2.24	0.68
19:A:819:CLA:H141	19:A:831:CLA:H202	1.74	0.68
11:G:115:TYR:O	11:G:119:LEU:HG	1.94	0.67
16:L:66:ASN:ND2	16:L:171:LEU:O	2.27	0.67
19:B:844:CLA:HAA1	19:B:844:CLA:HBD	1.75	0.67
1:1:168:PRO:O	20:1:609:UNL:OBD	2.13	0.66
4:4:82:LEU:HD13	19:4:317:CLA:H42	1.77	0.66
19:B:842:CLA:HMB1	19:B:842:CLA:HBB1	1.76	0.66
24:B:812:BCR:H313	24:B:813:BCR:H313	1.79	0.65
5:A:417:THR:HA	8:D:105:ILE:HG21	1.79	0.64
19:A:849:CLA:HBB1	19:A:849:CLA:HMB1	1.80	0.63
19:B:801:CLA:H191	19:B:806:CLA:H121	1.79	0.63
9:E:82:LYS:O	9:E:85:SER:OG	2.15	0.63
19:A:826:CLA:H112	19:A:833:CLA:H143	1.81	0.63
19:A:843:CLA:H43	19:L:304:CLA:H43	1.82	0.62
24:4:308:BCR:H23C	24:4:308:BCR:H403	1.81	0.61
16:L:67:GLY:O	16:L:69:PRO:HD3	1.98	0.61
5:A:110:PRO:HB3	5:A:142:PHE:CD2	2.35	0.61
19:A:808:CLA:H52	19:A:827:CLA:H2	1.81	0.61
6:B:503:GLU:CD	6:B:505:SER:HG	2.04	0.61
12:H:51:LYS:HA	12:H:66:ASN:CB	2.26	0.61
17:N:88:VAL:O	17:N:92:TYR:HD1	1.84	0.60
4:4:58:LEU:HD13	18:4:319:CHL:HMA3	1.83	0.60
6:B:721:TYR:HB2	19:B:819:CLA:HED2	1.83	0.60
5:A:512:LEU:HD12	5:A:512:LEU:C	2.27	0.59
5:A:298:ILE:CD1	19:A:821:CLA:HBC2	2.31	0.59
5:A:301:LEU:HD21	19:A:831:CLA:H201	1.84	0.59
19:B:818:CLA:H193	19:J:101:CLA:H193	1.85	0.58
19:A:813:CLA:HMB1	19:A:813:CLA:HBB1	1.86	0.58
19:B:806:CLA:HBB1	19:B:806:CLA:HMB3	1.86	0.57
4:4:191:ASN:OD1	22:4:306:A1LXP:O41	2.21	0.57
19:A:813:CLA:HBB1	19:A:813:CLA:CMB	2.34	0.57
11:G:68:ILE:O	11:G:72:THR:HG22	2.03	0.57
19:B:833:CLA:CMB	19:B:833:CLA:HBB1	2.34	0.57
4:4:67:LEU:HD22	19:4:317:CLA:HED1	1.86	0.56
13:I:34:ASN:O	13:I:35:LYS:C	2.48	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:852:BCR:H331	24:A:852:BCR:C8	2.36	0.56
19:F:303:CLA:HHC	19:F:303:CLA:HBB1	1.86	0.56
19:B:832:CLA:HMB1	19:B:832:CLA:HBB1	1.88	0.55
5:A:585:SER:OG	5:A:588:ASP:OD2	2.23	0.55
24:A:852:BCR:C19	15:K:111:THR:HG21	2.36	0.55
24:G:201:BCR:H362	24:G:205:BCR:H322	1.88	0.55
5:A:300:ILE:HD12	24:A:852:BCR:H352	1.90	0.54
1:1:69:ASP:OD2	1:1:74:GLY:N	2.34	0.54
12:H:117:TYR:CE1	12:H:121:ASN:ND2	2.75	0.54
29:B:817:DGD:HAW1	19:B:846:CLA:H112	1.89	0.54
19:B:844:CLA:H93	19:B:844:CLA:C2	2.39	0.53
5:A:371:MET:SD	5:A:503:THR:HG23	2.49	0.53
19:B:827:CLA:HHC	19:B:827:CLA:HBB1	1.89	0.53
3:3:201:PRO:O	3:3:202:GLY:O	2.27	0.53
6:B:35:ASP:O	6:B:36:ASP:HB2	2.07	0.53
20:1:604:UNL:O1A	21:1:618:XAT:H382	2.08	0.53
4:4:129:ASP:HA	18:4:313:CHL:HED3	1.90	0.53
5:A:12:ILE:HD11	19:A:815:CLA:O1A	2.09	0.53
6:B:497:TRP:CE3	19:B:834:CLA:H11	2.44	0.53
25:F:305:LMG:O9	25:F:305:LMG:HC72	2.07	0.53
11:G:72:THR:HG23	19:G:203:CLA:O2A	2.09	0.53
1:1:172:PHE:CD1	19:1:607:CLA:O1A	2.62	0.52
18:1:606:CHL:HED3	11:G:159:PHE:CZ	2.45	0.52
19:B:818:CLA:HBB1	19:B:818:CLA:HMB1	1.90	0.52
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.43	0.52
5:A:325:ALA:O	5:A:326:HIS:C	2.52	0.52
19:B:833:CLA:HBB1	19:B:833:CLA:HMB1	1.91	0.52
19:A:805:CLA:HMB3	19:A:805:CLA:HBB1	1.92	0.52
4:4:203:GLU:HG3	20:4:301:UNL:CED	2.40	0.51
19:A:851:CLA:H52	19:B:808:CLA:H43	1.92	0.51
19:A:802:CLA:H42	19:A:840:CLA:CMC	2.41	0.51
20:1:604:UNL:CHC	21:1:618:XAT:H362	2.41	0.51
19:A:834:CLA:HMB3	19:A:834:CLA:HBB1	1.91	0.51
18:1:601:CHL:CHB	19:4:311:CLA:HED2	2.41	0.51
24:B:812:BCR:C31	24:B:813:BCR:H313	2.40	0.51
19:B:829:CLA:HBB1	19:B:829:CLA:HMB3	1.93	0.51
24:A:804:BCR:H382	24:A:804:BCR:H23C	1.93	0.51
1:1:82:ARG:NH2	19:1:603:CLA:O1D	2.44	0.50
24:L:302:BCR:C8	24:L:302:BCR:H331	2.40	0.50
19:1:603:CLA:OBD	19:1:608:CLA:O1A	2.28	0.50
11:G:96:LEU:HD21	11:G:114:GLU:OE2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:95:THR:O	15:K:95:THR:HG23	2.12	0.50
8:D:110:THR:OG1	30:D:301:HOH:O	2.20	0.50
10:F:103:SER:HB2	10:F:105:PRO:HD2	1.93	0.50
10:F:100:ALA:O	10:F:103:SER:OG	2.22	0.50
2:2:56:PHE:O	2:2:59:SER:OG	2.20	0.50
5:A:413:ASP:OD2	30:A:901:HOH:O	2.20	0.50
24:A:852:BCR:H383	24:A:852:BCR:H23C	1.94	0.50
12:H:122:SER:OG	12:H:130:LYS:HE3	2.12	0.49
5:A:25:GLU:N	5:A:25:GLU:OE1	2.42	0.49
5:A:522:LEU:C	5:A:522:LEU:HD12	2.37	0.49
12:H:51:LYS:N	12:H:51:LYS:CD	2.76	0.49
15:K:55:LEU:O	15:K:59:THR:HG22	2.13	0.49
19:A:851:CLA:H43	19:A:851:CLA:O1A	2.13	0.49
19:B:832:CLA:HBB1	19:B:832:CLA:CMB	2.43	0.49
5:A:333:GLN:CA	5:A:333:GLN:OE1	2.60	0.49
6:B:270:LEU:HD23	6:B:273:MET:HE3	1.95	0.49
19:A:808:CLA:HMC2	19:A:831:CLA:H203	1.94	0.48
10:F:163:TRP:CD1	10:F:200:GLY:HA3	2.48	0.48
5:A:676:PHE:CG	24:A:845:BCR:H363	2.48	0.48
19:A:802:CLA:H43	19:A:840:CLA:C9	2.44	0.48
2:2:190:ASP:OD1	22:2:309:A1LXP:O41	2.32	0.48
6:B:456:GLU:OE1	10:F:137:HIS:HD2	1.96	0.48
1:1:170:GLY:O	1:1:171:ALA:CB	2.61	0.48
3:3:151:ASP:OD1	3:3:154:THR:HG22	2.13	0.48
19:B:806:CLA:C1A	19:B:806:CLA:CGA	2.92	0.48
6:B:223:GLY:O	6:B:224:PRO:C	2.55	0.48
19:1:602:CLA:C15	21:1:615:XAT:H393	2.44	0.48
6:B:157:LEU:O	6:B:162:LYS:HE3	2.14	0.48
5:A:116:TRP:CD2	19:A:810:CLA:HED3	2.49	0.48
1:1:83:TYR:OH	19:B:810:CLA:HMC1	2.14	0.47
6:B:469:LYS:HE3	6:B:509:PHE:O	2.14	0.47
19:B:801:CLA:H142	24:F:304:BCR:H333	1.95	0.47
16:L:65:ILE:O	16:L:68:ASP:N	2.35	0.47
24:L:301:BCR:H331	24:L:301:BCR:C8	2.44	0.47
24:L:302:BCR:H23C	24:L:302:BCR:H402	1.95	0.47
19:A:809:CLA:H91	19:A:840:CLA:H203	1.95	0.47
19:B:825:CLA:C1A	19:B:825:CLA:CGA	2.93	0.47
19:B:844:CLA:O1A	19:B:844:CLA:C9	2.62	0.47
19:B:803:CLA:HHC	19:B:803:CLA:HBB1	1.96	0.47
19:B:844:CLA:HAA1	19:B:844:CLA:CBD	2.42	0.47
19:3:304:CLA:H41	19:A:818:CLA:H191	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:812:BCR:H23C	24:B:812:BCR:H382	1.96	0.47
19:A:828:CLA:H41	19:A:828:CLA:H62	1.72	0.47
19:B:805:CLA:H43	19:F:303:CLA:HBB2	1.95	0.47
19:B:808:CLA:H191	19:B:827:CLA:H191	1.95	0.47
7:C:14:CYS:O	7:C:15:THR:OG1	2.27	0.47
20:1:604:UNL:C1C	21:1:618:XAT:H222	2.45	0.47
3:3:224:LYS:HD3	20:3:309:UNL:O1D	2.15	0.47
24:A:804:BCR:H331	24:A:804:BCR:C8	2.43	0.47
24:A:845:BCR:H23C	24:A:845:BCR:C38	2.44	0.47
16:L:212:LEU:CD1	16:L:212:LEU:N	2.78	0.47
17:N:121:VAL:HG23	25:N:201:LMG:HC4	1.97	0.47
3:3:81:LEU:HD13	18:3:303:CHL:H42	1.97	0.46
5:A:95:PHE:CE1	17:N:117:ARG:HD2	2.51	0.46
5:A:205:LEU:HD22	24:A:838:BCR:H361	1.98	0.46
6:B:183:PHE:HZ	19:B:841:CLA:H12	1.79	0.46
24:A:852:BCR:H331	24:A:852:BCR:HC8	1.96	0.46
19:B:804:CLA:HAA2	19:B:834:CLA:H141	1.97	0.46
5:A:676:PHE:CD2	24:A:845:BCR:H363	2.51	0.46
5:A:19:ILE:HD12	19:A:840:CLA:HED1	1.96	0.46
5:A:133:ARG:HB2	17:N:115:PHE:CE1	2.51	0.46
19:A:809:CLA:H143	19:B:818:CLA:H191	1.98	0.46
19:A:810:CLA:HBB1	19:A:810:CLA:HMB3	1.96	0.46
25:F:305:LMG:O9	25:F:305:LMG:C7	2.64	0.46
19:3:304:CLA:HHC	19:3:304:CLA:HBB1	1.98	0.46
6:B:636:ASN:HB2	6:B:637:PRO:CD	2.46	0.46
2:2:89:TRP:CE2	19:2:311:CLA:HED1	2.51	0.45
24:A:845:BCR:H331	24:A:845:BCR:C8	2.46	0.45
19:1:603:CLA:HBB1	21:1:615:XAT:C35	2.46	0.45
6:B:374:HIS:HE2	19:B:845:CLA:C1B	2.28	0.45
12:H:51:LYS:N	12:H:51:LYS:HE2	2.30	0.45
4:4:67:LEU:HD22	19:4:317:CLA:CED	2.46	0.45
3:3:121:GLY:HA3	3:3:131:ALA:HB1	1.98	0.45
5:A:694:GLU:OE2	6:B:544:SER:OG	2.21	0.45
19:A:849:CLA:HBB1	19:A:849:CLA:CMB	2.46	0.45
6:B:338:LEU:HD23	19:B:822:CLA:HED1	1.98	0.45
5:A:333:GLN:OE1	5:A:333:GLN:HA	2.16	0.45
1:1:149:ILE:O	1:1:150:ALA:C	2.59	0.45
5:A:491:ALA:N	5:A:492:PRO:HD2	2.32	0.45
16:L:75:GLU:OE1	16:L:75:GLU:HA	2.17	0.45
5:A:503:THR:HG21	19:A:831:CLA:HAB	1.99	0.45
19:A:809:CLA:HBA1	19:A:809:CLA:C4A	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:69:ASP:O	1:1:70:PRO:C	2.60	0.44
19:A:833:CLA:HMB1	19:A:833:CLA:HBB1	1.98	0.44
24:A:845:BCR:H24C	24:A:845:BCR:H371	1.77	0.44
24:B:813:BCR:H24C	24:B:813:BCR:H371	1.84	0.44
12:H:51:LYS:N	12:H:51:LYS:HD3	2.32	0.44
19:A:842:CLA:H62	19:A:842:CLA:H41	1.35	0.44
24:G:201:BCR:H383	24:G:201:BCR:H23C	1.97	0.44
19:A:802:CLA:H42	19:A:840:CLA:HMC1	2.00	0.44
6:B:268:LEU:HD13	19:B:834:CLA:HMA2	1.98	0.44
19:A:842:CLA:C1A	19:A:842:CLA:CGA	2.96	0.44
19:A:843:CLA:CBB	19:A:851:CLA:HBA2	2.48	0.44
12:H:51:LYS:HB2	12:H:58:TYR:HA	1.98	0.44
24:F:302:BCR:H20C	24:F:302:BCR:H361	1.89	0.44
19:A:805:CLA:HBB1	19:A:805:CLA:CMB	2.48	0.44
24:F:302:BCR:C8	24:F:302:BCR:H331	2.47	0.44
24:A:804:BCR:H24C	24:A:804:BCR:H371	1.86	0.44
19:A:807:CLA:HAA1	19:A:807:CLA:HBD	1.99	0.44
24:F:304:BCR:H24C	24:F:304:BCR:H371	1.87	0.44
1:1:85:GLU:O	1:1:86:SER:C	2.60	0.44
21:2:306:XAT:H183	20:2:317:UNL:C4B	2.48	0.44
19:B:808:CLA:H61	19:B:808:CLA:H41	1.71	0.44
9:E:87:VAL:O	9:E:100:VAL:HA	2.17	0.44
16:L:65:ILE:C	16:L:67:GLY:N	2.74	0.44
5:A:393:TRP:HB3	19:A:829:CLA:HMC3	2.00	0.43
24:4:308:BCR:H20C	24:4:308:BCR:H361	1.91	0.43
19:A:806:CLA:CHD	24:A:852:BCR:H382	2.48	0.43
6:B:456:GLU:OE1	10:F:137:HIS:CD2	2.70	0.43
19:B:818:CLA:H61	19:B:818:CLA:H41	1.66	0.43
24:K:201:BCR:H20C	24:K:201:BCR:H361	1.88	0.43
1:1:119:ALA:HB1	1:1:138:LEU:HD13	2.01	0.43
5:A:325:ALA:O	5:A:327:LYS:N	2.51	0.43
19:B:827:CLA:H62	19:B:827:CLA:H41	1.61	0.43
19:B:837:CLA:HBB1	19:B:837:CLA:HMB3	1.99	0.43
19:3:308:CLA:O2A	19:3:308:CLA:HED3	2.18	0.43
19:B:810:CLA:HMB1	19:B:810:CLA:HBB1	1.99	0.43
3:3:207:ASN:OD1	22:3:305:A1LXP:O41	2.37	0.43
5:A:561:ILE:HD12	5:A:584:VAL:HG21	1.99	0.43
19:A:851:CLA:HBD	19:A:851:CLA:HBA1	2.00	0.43
19:B:830:CLA:H111	19:B:830:CLA:H71	1.67	0.43
8:D:103:GLU:HA	8:D:116:MET:O	2.17	0.43
14:J:28:GLU:HG3	20:J:104:UNL:C1B	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:439:ASN:OD1	19:B:820:CLA:HED2	2.19	0.43
1:1:79:ASN:O	1:1:83:TYR:CD2	2.71	0.43
24:B:812:BCR:C32	19:B:845:CLA:C19	2.97	0.43
5:A:503:THR:HA	19:A:821:CLA:O1A	2.19	0.43
24:A:838:BCR:H361	24:A:838:BCR:H20C	1.85	0.43
19:B:802:CLA:HMB1	19:B:802:CLA:HBB1	2.00	0.43
16:L:117:GLY:HA2	19:L:303:CLA:HMA1	2.01	0.43
1:1:170:GLY:O	1:1:171:ALA:HB3	2.18	0.43
24:A:845:BCR:C38	24:A:845:BCR:C23	2.97	0.43
6:B:235:GLN:OE1	6:B:235:GLN:HA	2.19	0.43
18:1:601:CHL:HHB	19:4:311:CLA:HED2	2.00	0.43
24:B:816:BCR:H20C	24:B:816:BCR:H361	1.87	0.43
1:1:196:ARG:HD3	19:1:602:CLA:CHD	2.49	0.42
19:A:823:CLA:HBB1	19:A:823:CLA:HMB3	2.00	0.42
24:A:852:BCR:H371	24:A:852:BCR:H24C	1.81	0.42
5:A:505:LEU:HD11	5:A:513:VAL:HG23	2.01	0.42
19:K:203:CLA:HBC3	19:K:203:CLA:HHD	2.02	0.42
24:B:816:BCR:H24C	24:B:816:BCR:H371	1.91	0.42
8:D:72:THR:HG23	8:D:120:PRO:HB2	2.00	0.42
14:J:10:VAL:O	14:J:11:ALA:C	2.61	0.42
5:A:230:ASP:OD2	17:N:103:ASN:ND2	2.52	0.42
24:A:847:BCR:H24C	24:A:847:BCR:H371	1.91	0.42
19:A:833:CLA:HBB1	19:A:833:CLA:CMB	2.49	0.42
19:B:833:CLA:HMB1	19:B:833:CLA:CBB	2.49	0.42
19:A:814:CLA:H61	19:A:814:CLA:H2	1.76	0.42
19:B:829:CLA:HBB1	19:B:829:CLA:CMB	2.49	0.42
19:A:812:CLA:H112	19:A:812:CLA:H152	1.69	0.42
25:N:201:LMG:O7	25:N:201:LMG:HC1	2.20	0.42
5:A:522:LEU:HB2	5:A:523:PRO:HD2	2.01	0.42
11:G:135:TRP:CE2	24:G:201:BCR:H322	2.54	0.42
2:2:80:LEU:HD13	19:2:312:CLA:H42	2.01	0.42
24:4:308:BCR:H403	24:4:308:BCR:C23	2.47	0.42
19:A:819:CLA:CGA	19:A:819:CLA:H3A	2.50	0.42
19:A:851:CLA:H61	19:A:851:CLA:H41	1.69	0.42
24:B:813:BCR:HC8	24:B:813:BCR:H321	2.02	0.42
5:A:298:ILE:HD11	19:A:821:CLA:CBC	2.50	0.41
5:A:706:LEU:HD21	19:B:848:CLA:H3A	2.01	0.41
24:B:813:BCR:HC8	24:B:813:BCR:H311	2.02	0.41
24:B:815:BCR:H24C	24:B:815:BCR:H371	1.84	0.41
6:B:344:ILE:HD13	19:B:843:CLA:H43	2.02	0.41
5:A:346:TRP:HB3	19:A:814:CLA:HAC1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:804:BCR:C8	24:A:804:BCR:C33	2.98	0.41
19:B:840:CLA:HBB1	19:B:840:CLA:HMB3	2.02	0.41
2:2:183:TYR:CE1	2:2:206:ARG:HD2	2.54	0.41
24:A:852:BCR:C11	24:K:201:BCR:H333	2.50	0.41
6:B:89:HIS:CE1	6:B:114:ASN:HD22	2.39	0.41
19:B:809:CLA:H62	19:B:809:CLA:H41	1.87	0.41
19:B:825:CLA:HMB1	19:B:825:CLA:C14	2.50	0.41
2:2:183:TYR:CZ	2:2:206:ARG:HD2	2.55	0.41
6:B:338:LEU:CD2	19:B:822:CLA:HED1	2.50	0.41
3:3:172:GLN:OE1	3:3:172:GLN:HA	2.19	0.41
5:A:454:ILE:HG21	19:A:850:CLA:H92	2.02	0.41
6:B:351:HIS:ND1	19:B:834:CLA:OBD	2.49	0.41
19:B:833:CLA:CMB	19:B:833:CLA:CBB	2.99	0.41
7:C:22:PRO:C	8:D:132:LEU:HD23	2.45	0.41
13:I:17:LEU:C	13:I:20:PRO:HD2	2.46	0.41
4:4:95:ALA:N	19:4:318:CLA:HED2	2.36	0.41
8:D:105:ILE:HD12	8:D:115:ILE:HG12	2.03	0.41
1:1:224:HIS:CG	19:1:612:CLA:HAA2	2.56	0.41
24:A:804:BCR:H20C	24:A:804:BCR:H361	1.82	0.41
19:A:808:CLA:CMC	19:A:831:CLA:H203	2.51	0.41
19:A:813:CLA:C1A	19:A:813:CLA:CGA	2.99	0.41
19:A:813:CLA:CMD	19:K:203:CLA:HED2	2.51	0.41
19:B:820:CLA:H42	19:B:820:CLA:O1A	2.20	0.41
7:C:31:TRP:O	7:C:37:LYS:HA	2.20	0.41
19:3:301:CLA:H91	19:3:301:CLA:H111	1.97	0.41
5:A:327:LYS:HA	5:A:332:GLY:O	2.21	0.41
19:A:808:CLA:H203	24:A:847:BCR:H393	2.02	0.41
6:B:692:ARG:NH1	16:L:165:ILE:HD11	2.36	0.41
24:B:814:BCR:H371	24:B:814:BCR:H24C	1.83	0.41
19:B:830:CLA:H142	19:B:830:CLA:H112	1.67	0.41
11:G:69:SER:CA	19:G:203:CLA:O2A	2.65	0.41
14:J:14:LEU:HD12	14:J:14:LEU:HA	1.92	0.41
24:L:301:BCR:H20C	24:L:301:BCR:H361	1.88	0.41
25:N:201:LMG:H332	25:N:201:LMG:H301	1.89	0.41
19:1:605:CLA:HBB2	18:1:606:CHL:CBB	2.51	0.41
2:2:246:GLY:O	3:3:154:THR:HG21	2.21	0.41
19:G:203:CLA:HBB1	24:G:205:BCR:C35	2.45	0.41
24:I:101:BCR:H24C	24:I:101:BCR:H371	1.85	0.41
14:J:40:PRO:O	14:J:41:PHE:C	2.64	0.41
11:G:128:ASN:OD1	11:G:131:ASP:OD1	2.39	0.40
15:K:48:PHE:O	15:K:51:SER:OG	2.31	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:10:VAL:HG12	14:J:12:PRO:HD2	2.03	0.40
5:A:182:ALA:HA	5:A:183:PRO:HD3	1.95	0.40
5:A:534:HIS:CG	19:A:842:CLA:HED3	2.56	0.40
19:A:806:CLA:HHD	19:A:806:CLA:HBC2	2.03	0.40
19:A:819:CLA:H72	19:A:819:CLA:H111	1.82	0.40
19:A:829:CLA:H191	19:B:818:CLA:H121	2.02	0.40
19:B:824:CLA:CGA	19:B:824:CLA:C1A	3.00	0.40
24:G:201:BCR:C8	24:G:201:BCR:H331	2.51	0.40
19:A:826:CLA:H92	24:F:302:BCR:C20	2.51	0.40
24:A:841:BCR:H403	24:A:841:BCR:H23C	2.03	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	192/241 (80%)	182 (95%)	8 (4%)	2 (1%)	12	10
2	2	207/257 (80%)	192 (93%)	13 (6%)	2 (1%)	12	10
3	3	219/273 (80%)	208 (95%)	9 (4%)	2 (1%)	14	12
4	4	195/251 (78%)	183 (94%)	12 (6%)	0	100	100
5	A	741/750 (99%)	713 (96%)	24 (3%)	4 (0%)	24	25
6	B	731/734 (100%)	712 (97%)	18 (2%)	1 (0%)	48	55
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	139 (99%)	2 (1%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	151/221 (68%)	147 (97%)	4 (3%)	0	100	100
11	G	96/160 (60%)	94 (98%)	2 (2%)	0	100	100
12	H	93/145 (64%)	91 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	29/37 (78%)	27 (93%)	2 (7%)	0	100	100
14	J	40/44 (91%)	38 (95%)	1 (2%)	1 (2%)	4	2
15	K	60/130 (46%)	55 (92%)	5 (8%)	0	100	100
16	L	148/219 (68%)	142 (96%)	6 (4%)	0	100	100
17	N	48/171 (28%)	45 (94%)	3 (6%)	0	100	100
All	All	3231/4061 (80%)	3103 (96%)	116 (4%)	12 (0%)	31	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	171	ALA
3	3	202	GLY
1	1	170	GLY
5	A	31	HIS
5	A	503	THR
2	2	133	TYR
2	2	134	PHE
3	3	57	PHE
14	J	40	PRO
5	A	494	VAL
6	B	492	ILE
5	A	508	GLY

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	153/190 (80%)	148 (97%)	5 (3%)	33	42
2	2	166/205 (81%)	155 (93%)	11 (7%)	15	16
3	3	171/211 (81%)	160 (94%)	11 (6%)	16	16
4	4	161/210 (77%)	160 (99%)	1 (1%)	78	87
5	A	603/610 (99%)	592 (98%)	11 (2%)	51	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	599/600 (100%)	582 (97%)	17 (3%)	38	49
7	C	70/71 (99%)	68 (97%)	2 (3%)	37	47
8	D	121/170 (71%)	118 (98%)	3 (2%)	42	53
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	124/185 (67%)	118 (95%)	6 (5%)	23	27
11	G	82/133 (62%)	77 (94%)	5 (6%)	17	18
12	H	79/113 (70%)	76 (96%)	3 (4%)	29	37
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	37/39 (95%)	36 (97%)	1 (3%)	39	50
15	K	47/95 (50%)	46 (98%)	1 (2%)	47	59
16	L	116/174 (67%)	109 (94%)	7 (6%)	17	19
17	N	42/138 (30%)	42 (100%)	0	100	100
All	All	2655/3291 (81%)	2571 (97%)	84 (3%)	35	43

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	96	LEU
1	1	137	THR
1	1	141	ILE
1	1	184	LEU
1	1	235	ASP
2	2	60	THR
2	2	78	LEU
2	2	82	SER
2	2	92	GLN
2	2	119	ILE
2	2	155	ARG
2	2	165	VAL
2	2	170	VAL
2	2	205	LEU
2	2	215	LEU
2	2	249	THR
3	3	64	SER
3	3	154	THR
3	3	158	LEU
3	3	160	MET
3	3	214	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	215	GLU
3	3	216	LYS
3	3	218	LEU
3	3	254	LEU
3	3	255	LEU
3	3	258	LEU
4	4	214	LEU
5	A	65	GLU
5	A	152	SER
5	A	245	ASP
5	A	246	LEU
5	A	300	ILE
5	A	333	GLN
5	A	512	LEU
5	A	518	LYS
5	A	625	VAL
5	A	654	SER
5	A	749	VAL
6	B	3	LEU
6	B	16	PRO
6	B	110	LEU
6	B	149	SER
6	B	155	LEU
6	B	195	VAL
6	B	282	ILE
6	B	303	ASP
6	B	344	ILE
6	B	407	VAL
6	B	471	SER
6	B	479	SER
6	B	503	GLU
6	B	599	ILE
6	B	607	SER
6	B	684	ARG
6	B	701	SER
7	C	24	ASP
7	C	65	VAL
8	D	64	THR
8	D	105	ILE
8	D	145	THR
10	F	73	THR
10	F	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	F	101	PRO
10	F	114	GLU
10	F	167	VAL
10	F	184	LYS
11	G	63	SER
11	G	70	LEU
11	G	74	LEU
11	G	91	VAL
11	G	117	SER
12	H	51	LYS
12	H	55	LYS
12	H	126	VAL
14	J	41	PHE
15	K	93	LEU
16	L	73	SER
16	L	114	PHE
16	L	137	LEU
16	L	159	LYS
16	L	168	SER
16	L	212	LEU
16	L	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	208	GLN
1	1	220	ASN
2	2	121	ASN
2	2	131	GLN
2	2	174	ASN
3	3	228	ASN
3	3	252	GLN
4	4	151	HIS
4	4	194	ASN
5	A	418	ASN
5	A	623	GLN
6	B	10	GLN
6	B	14	GLN
6	B	114	ASN
6	B	210	ASN
6	B	630	GLN
7	C	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	E	127	ASN
10	F	137	HIS
11	G	99	GLN
13	I	34	ASN
15	K	54	ASN
15	K	126	ASN
17	N	122	GLN

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](#)

Of 206 ligands modelled in this entry, 29 are unknown - leaving 177 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	CLA	A	807	30	49,53,73	1.89	9 (18%)	59,89,113	1.42	10 (16%)
19	CLA	A	837	5	69,73,73	1.64	10 (14%)	83,113,113	1.66	10 (12%)
24	BCR	F	302	-	41,41,41	0.59	0	56,56,56	0.76	0
19	CLA	A	814	5	69,73,73	1.52	6 (8%)	83,113,113	1.64	17 (20%)
19	CLA	A	805	5	51,55,73	1.89	9 (17%)	61,91,113	1.47	7 (11%)
19	CLA	B	803	6	49,53,73	1.74	9 (18%)	59,89,113	1.78	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	G	202	30	46,50,73	1.96	10 (21%)	55,85,113	1.54	7 (12%)
19	CLA	3	312	3	46,50,73	1.90	9 (19%)	55,85,113	1.49	5 (9%)
19	CLA	A	823	30	69,73,73	1.57	8 (11%)	83,113,113	1.66	13 (15%)
22	A1LXP	J	102	-	42,43,43	0.41	0	51,60,60	0.80	1 (1%)
19	CLA	B	832	6	49,53,73	1.92	7 (14%)	59,89,113	2.13	14 (23%)
19	CLA	B	827	6	69,73,73	1.91	11 (15%)	83,113,113	1.52	11 (13%)
19	CLA	A	826	5	69,73,73	1.17	6 (8%)	83,113,113	1.55	9 (10%)
18	CHL	2	315	30	50,54,74	1.18	6 (12%)	56,90,114	1.97	12 (21%)
19	CLA	B	825	6	69,73,73	1.55	5 (7%)	83,113,113	1.60	9 (10%)
22	A1LXP	3	305	-	42,43,43	0.42	0	51,60,60	0.70	1 (1%)
24	BCR	G	205	-	41,41,41	0.54	0	56,56,56	0.52	0
19	CLA	B	830	6	69,73,73	1.46	6 (8%)	83,113,113	1.61	9 (10%)
19	CLA	H	201	12	59,63,73	1.61	10 (16%)	71,101,113	1.39	9 (12%)
19	CLA	B	836	30	60,64,73	1.76	8 (13%)	72,102,113	1.23	8 (11%)
27	CL0	A	830	5	69,73,73	1.65	6 (8%)	83,113,113	1.55	8 (9%)
19	CLA	3	302	3	56,60,73	1.89	8 (14%)	67,97,113	1.34	5 (7%)
19	CLA	A	815	5	49,53,73	1.75	9 (18%)	59,89,113	1.87	12 (20%)
19	CLA	A	840	19,5	69,73,73	1.57	8 (11%)	83,113,113	1.49	10 (12%)
19	CLA	B	823	6	69,73,73	1.14	7 (10%)	83,113,113	1.23	8 (9%)
19	CLA	B	838	6	49,53,73	1.65	11 (22%)	59,89,113	1.30	6 (10%)
19	CLA	4	318	4	49,53,73	2.34	7 (14%)	59,89,113	1.55	9 (15%)
24	BCR	K	201	-	41,41,41	0.42	0	56,56,56	0.51	0
19	CLA	A	816	5	54,58,73	1.82	7 (12%)	65,95,113	1.28	9 (13%)
19	CLA	A	825	5	46,50,73	2.01	8 (17%)	55,85,113	1.45	9 (16%)
19	CLA	A	828	5	69,73,73	1.57	10 (14%)	83,113,113	1.70	16 (19%)
19	CLA	A	832	5	49,53,73	2.07	7 (14%)	59,89,113	1.82	11 (18%)
19	CLA	F	303	10	46,50,73	1.82	8 (17%)	55,85,113	1.72	9 (16%)
18	CHL	1	606	1	47,51,74	1.45	4 (8%)	52,86,114	2.47	10 (19%)
24	BCR	B	816	-	41,41,41	0.55	0	56,56,56	0.74	1 (1%)
19	CLA	B	843	6	69,73,73	1.43	8 (11%)	83,113,113	1.36	10 (12%)
19	CLA	B	822	6	69,73,73	1.62	8 (11%)	83,113,113	1.22	7 (8%)
18	CHL	2	313	30	46,50,74	1.31	3 (6%)	51,85,114	2.16	14 (27%)
19	CLA	A	821	5	56,60,73	1.45	9 (16%)	67,97,113	1.42	8 (11%)
24	BCR	3	316	-	41,41,41	0.46	0	56,56,56	0.65	0
19	CLA	B	844	6	63,67,73	1.76	11 (17%)	75,105,113	1.55	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	307	4	49,53,73	2.37	5 (10%)	59,89,113	1.59	8 (13%)
19	CLA	B	847	6	54,58,73	1.46	9 (16%)	65,95,113	1.51	5 (7%)
19	CLA	1	612	1	59,63,73	2.04	8 (13%)	71,101,113	1.28	10 (14%)
28	PQN	A	839	-	34,34,34	0.41	0	42,45,45	0.74	1 (2%)
19	CLA	1	608	1	61,65,73	1.74	7 (11%)	73,103,113	1.17	7 (9%)
19	CLA	B	807	6	49,53,73	1.33	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	1	607	-	55,59,73	1.91	8 (14%)	66,96,113	1.33	4 (6%)
19	CLA	3	306	3	51,55,73	2.17	8 (15%)	61,91,113	1.51	9 (14%)
19	CLA	A	818	5	69,73,73	1.54	9 (13%)	83,113,113	1.56	13 (15%)
23	LHG	A	835	-	48,48,48	0.80	1 (2%)	51,54,54	1.43	7 (13%)
22	A1LXP	2	309	-	42,43,43	0.27	0	51,60,60	0.65	0
25	LMG	J	103	-	41,41,55	0.45	0	49,49,63	0.68	1 (2%)
26	SF4	A	803	6,5	0,12,12	-	-	-	-	-
19	CLA	B	826	6	69,73,73	1.15	5 (7%)	83,113,113	1.38	9 (10%)
19	CLA	A	836	5	49,53,73	1.62	7 (14%)	59,89,113	1.70	10 (16%)
19	CLA	B	834	6	69,73,73	1.10	4 (5%)	83,113,113	1.46	13 (15%)
24	BCR	B	813	-	41,41,41	0.75	1 (2%)	56,56,56	0.69	1 (1%)
21	XAT	2	306	-	39,47,47	0.31	0	54,74,74	1.02	2 (3%)
19	CLA	B	819	6	69,73,73	1.18	7 (10%)	83,113,113	1.11	6 (7%)
19	CLA	B	833	6	64,68,73	2.41	7 (10%)	77,107,113	1.51	11 (14%)
19	CLA	B	839	6	47,51,73	1.85	9 (19%)	56,86,113	1.64	8 (14%)
19	CLA	3	304	3	59,63,73	1.77	8 (13%)	71,101,113	1.46	10 (14%)
19	CLA	A	811	5	59,63,73	2.13	8 (13%)	71,101,113	1.31	9 (12%)
19	CLA	B	840	6	49,53,73	2.00	8 (16%)	59,89,113	1.93	12 (20%)
19	CLA	B	801	6	69,73,73	1.62	8 (11%)	83,113,113	1.48	9 (10%)
19	CLA	1	603	1	61,65,73	1.83	8 (13%)	73,103,113	1.53	9 (12%)
24	BCR	B	812	-	41,41,41	0.59	0	56,56,56	0.79	1 (1%)
19	CLA	B	818	30	69,73,73	1.28	6 (8%)	83,113,113	1.83	16 (19%)
19	CLA	F	306	30	52,56,73	1.59	7 (13%)	62,92,113	1.38	8 (12%)
19	CLA	A	833	-	69,73,73	1.58	10 (14%)	83,113,113	1.20	5 (6%)
24	BCR	A	838	-	41,41,41	0.63	1 (2%)	56,56,56	0.54	0
19	CLA	B	802	6	64,68,73	1.35	8 (12%)	77,107,113	1.40	8 (10%)
18	CHL	4	313	30	50,54,74	1.44	5 (10%)	56,90,114	2.02	11 (19%)
24	BCR	F	304	-	41,41,41	0.47	0	56,56,56	0.58	0
19	CLA	B	842	30	54,58,73	1.71	10 (18%)	65,95,113	1.66	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	845	6	69,73,73	1.49	8 (11%)	83,113,113	1.51	11 (13%)
19	CLA	B	806	6	69,73,73	1.37	5 (7%)	83,113,113	1.86	9 (10%)
19	CLA	B	828	6	55,59,73	1.73	6 (10%)	66,96,113	1.69	12 (18%)
24	BCR	A	845	-	41,41,41	0.51	0	56,56,56	0.65	0
24	BCR	A	804	-	41,41,41	0.65	0	56,56,56	0.70	2 (3%)
18	CHL	3	303	3	70,74,74	0.99	5 (7%)	80,114,114	1.95	13 (16%)
19	CLA	B	846	6	69,73,73	1.44	9 (13%)	83,113,113	1.42	9 (10%)
19	CLA	A	802	19,5	60,64,73	1.23	5 (8%)	72,102,113	1.65	12 (16%)
24	BCR	A	841	-	41,41,41	0.66	0	56,56,56	0.63	0
25	LMG	F	305	-	30,30,55	0.34	0	38,38,63	0.68	1 (2%)
22	A1LXP	4	303	-	42,43,43	0.78	3 (7%)	51,60,60	0.89	1 (1%)
19	CLA	4	317	4	61,65,73	1.90	9 (14%)	73,103,113	1.44	9 (12%)
19	CLA	2	310	2	59,63,73	2.12	6 (10%)	71,101,113	1.51	14 (19%)
19	CLA	G	203	11	49,53,73	1.73	11 (22%)	59,89,113	2.06	10 (16%)
19	CLA	1	602	1	64,68,73	1.67	9 (14%)	77,107,113	1.66	15 (19%)
26	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	A	829	5	69,73,73	1.38	8 (11%)	83,113,113	1.53	11 (13%)
23	LHG	1	617	20	48,48,48	0.35	0	51,54,54	0.79	2 (3%)
19	CLA	B	831	6	69,73,73	1.41	8 (11%)	83,113,113	1.49	9 (10%)
19	CLA	4	311	4	49,53,73	2.24	10 (20%)	59,89,113	1.58	11 (18%)
18	CHL	2	316	2	63,67,74	1.17	5 (7%)	71,105,114	2.04	10 (14%)
19	CLA	B	810	23	69,73,73	1.44	8 (11%)	83,113,113	1.22	6 (7%)
19	CLA	B	824	6	56,60,73	1.70	6 (10%)	67,97,113	1.70	10 (14%)
23	LHG	2	302	20	44,44,48	0.36	0	47,50,54	0.56	0
24	BCR	J	105	-	41,41,41	0.58	0	56,56,56	0.56	0
25	LMG	N	201	-	27,27,55	0.46	0	34,34,63	0.83	2 (5%)
19	CLA	B	808	30	69,73,73	1.19	7 (10%)	83,113,113	1.53	11 (13%)
18	CHL	3	315	30	55,59,74	1.29	7 (12%)	62,96,114	1.84	10 (16%)
19	CLA	B	809	6	69,73,73	1.21	10 (14%)	83,113,113	1.37	11 (13%)
22	A1LXP	4	306	-	42,43,43	0.38	0	51,60,60	0.66	0
19	CLA	A	817	30	53,57,73	1.41	7 (13%)	62,93,113	1.87	11 (17%)
23	LHG	1	620	19	20,20,48	0.59	0	23,26,54	0.81	0
19	CLA	L	303	30	49,53,73	1.70	7 (14%)	59,89,113	1.41	7 (11%)
22	A1LXP	1	619	-	42,43,43	0.44	0	51,60,60	0.57	0
19	CLA	B	848	6	49,53,73	2.21	10 (20%)	59,89,113	2.16	6 (10%)
22	A1LXP	1	616	-	42,43,43	0.58	1 (2%)	51,60,60	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	L	301	-	41,41,41	0.53	0	56,56,56	0.50	0
19	CLA	A	843	5	57,61,73	1.72	9 (15%)	68,98,113	1.73	12 (17%)
19	CLA	2	311	2	49,53,73	2.06	9 (18%)	59,89,113	1.47	8 (13%)
19	CLA	A	827	5	62,66,73	1.89	9 (14%)	74,104,113	1.38	11 (14%)
19	CLA	A	834	5	69,73,73	1.40	6 (8%)	83,113,113	1.42	7 (8%)
22	A1LXP	3	310	-	42,43,43	0.62	1 (2%)	51,60,60	1.02	3 (5%)
19	CLA	1	605	30	49,53,73	1.92	9 (18%)	59,89,113	1.36	8 (13%)
19	CLA	3	314	3	59,63,73	1.93	6 (10%)	71,101,113	1.37	9 (12%)
19	CLA	A	813	5	64,68,73	1.60	12 (18%)	77,107,113	1.85	10 (12%)
19	CLA	A	820	5	46,50,73	1.60	5 (10%)	55,85,113	1.50	8 (14%)
19	CLA	A	824	5	69,73,73	1.33	6 (8%)	83,113,113	1.23	5 (6%)
19	CLA	A	810	5	54,58,73	2.02	8 (14%)	65,95,113	1.69	11 (16%)
19	CLA	3	301	3	64,68,73	1.65	9 (14%)	77,107,113	1.36	10 (12%)
19	CLA	A	831	5	69,73,73	1.44	7 (10%)	83,113,113	1.37	10 (12%)
25	LMG	4	304	-	34,34,55	0.34	0	42,42,63	0.59	1 (2%)
24	BCR	4	308	-	41,41,41	0.35	0	56,56,56	0.56	0
19	CLA	A	819	5	69,73,73	1.38	8 (11%)	83,113,113	1.58	12 (14%)
19	CLA	A	848	5	54,58,73	1.72	9 (16%)	65,95,113	1.81	13 (20%)
19	CLA	A	849	5	54,58,73	1.58	10 (18%)	65,95,113	1.54	7 (10%)
28	PQN	B	811	-	34,34,34	0.60	0	42,45,45	0.96	2 (4%)
25	LMG	G	206	-	35,35,55	0.37	0	43,43,63	0.51	0
24	BCR	I	101	-	41,41,41	0.59	0	56,56,56	0.58	0
24	BCR	A	847	-	25,25,41	0.51	0	33,33,56	0.84	1 (3%)
19	CLA	A	801	30	59,63,73	1.84	10 (16%)	71,101,113	1.73	14 (19%)
19	CLA	B	835	6	61,65,73	1.50	6 (9%)	73,103,113	1.72	18 (24%)
19	CLA	L	304	16	69,73,73	1.29	6 (8%)	83,113,113	1.25	8 (9%)
19	CLA	A	850	30	69,73,73	1.13	6 (8%)	83,113,113	1.27	4 (4%)
19	CLA	3	308	30	49,53,73	1.43	7 (14%)	59,89,113	1.26	8 (13%)
19	CLA	B	841	30	60,64,73	1.42	10 (16%)	72,102,113	1.75	14 (19%)
19	CLA	A	822	5	57,61,73	1.64	8 (14%)	68,98,113	1.42	9 (13%)
19	CLA	J	101	5	69,73,73	1.75	8 (11%)	83,113,113	1.20	7 (8%)
19	CLA	K	203	30	49,53,73	2.01	10 (20%)	59,89,113	1.55	6 (10%)
25	LMG	F	301	-	30,30,55	0.36	0	38,38,63	0.48	0
18	CHL	4	319	4	50,54,74	1.27	6 (12%)	56,90,114	2.06	9 (16%)
19	CLA	2	312	2	66,70,73	2.01	7 (10%)	79,109,113	1.36	9 (11%)
19	CLA	L	305	16	49,53,73	2.38	6 (12%)	59,89,113	1.45	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	C	102	7	0,12,12	-	-	-		
24	BCR	G	201	-	41,41,41	0.83	2 (4%)	56,56,56	0.54	0
24	BCR	L	306	-	41,41,41	0.53	0	56,56,56	0.46	0
18	CHL	1	601	1	63,67,74	1.12	6 (9%)	71,105,114	1.93	8 (11%)
24	BCR	A	852	-	41,41,41	0.70	1 (2%)	56,56,56	0.73	1 (1%)
24	BCR	B	814	-	41,41,41	0.52	0	56,56,56	0.58	0
19	CLA	A	851	30	66,70,73	1.53	7 (10%)	79,109,113	1.62	13 (16%)
19	CLA	B	829	6	47,51,73	1.78	7 (14%)	56,86,113	1.60	9 (16%)
19	CLA	B	837	6	51,55,73	1.66	8 (15%)	61,91,113	1.59	12 (19%)
19	CLA	A	812	5	69,73,73	1.40	9 (13%)	83,113,113	1.25	10 (12%)
19	CLA	B	805	6	54,58,73	1.40	5 (9%)	65,95,113	1.55	5 (7%)
19	CLA	B	804	30	49,53,73	1.82	5 (10%)	59,89,113	1.44	10 (16%)
24	BCR	L	302	-	41,41,41	0.63	0	56,56,56	0.57	1 (1%)
24	BCR	B	815	-	41,41,41	0.59	1 (2%)	56,56,56	0.75	1 (1%)
19	CLA	3	307	30	52,56,73	1.71	9 (17%)	62,92,113	1.21	8 (12%)
19	CLA	B	820	-	69,73,73	1.75	9 (13%)	83,113,113	1.19	8 (9%)
21	XAT	1	615	-	39,47,47	0.44	0	54,74,74	1.65	5 (9%)
19	CLA	B	821	6	46,50,73	1.64	6 (13%)	55,85,113	2.04	10 (18%)
19	CLA	A	842	5	64,68,73	1.55	7 (10%)	77,107,113	1.69	15 (19%)
19	CLA	A	846	5	69,73,73	1.36	10 (14%)	83,113,113	1.60	15 (18%)
29	DGD	B	817	-	61,61,67	0.42	0	75,75,81	0.88	3 (4%)
19	CLA	A	806	5	46,50,73	2.21	9 (19%)	55,85,113	1.56	7 (12%)
19	CLA	K	202	15	49,53,73	1.82	10 (20%)	59,89,113	2.05	7 (11%)
19	CLA	4	314	4	56,60,73	2.17	7 (12%)	67,97,113	1.39	10 (14%)
19	CLA	A	808	30	69,73,73	1.37	6 (8%)	83,113,113	1.47	9 (10%)
21	XAT	1	618	-	25,29,47	0.42	0	33,43,74	1.54	2 (6%)
19	CLA	A	809	5	69,73,73	1.11	4 (5%)	83,113,113	1.71	15 (18%)
19	CLA	A	844	5	46,50,73	2.23	8 (17%)	55,85,113	1.52	9 (16%)
19	CLA	2	301	2	54,58,73	2.12	8 (14%)	65,95,113	1.34	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	807	30	-	0/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	837	5	1/1/15/20	12/39/115/115	-
24	BCR	F	302	-	-	0/29/63/63	0/2/2/2
19	CLA	A	814	5	1/1/15/20	12/39/115/115	-
19	CLA	A	805	5	-	1/18/94/115	-
19	CLA	B	803	6	-	0/15/91/115	-
19	CLA	A	809	5	1/1/15/20	7/39/115/115	-
19	CLA	G	202	30	-	3/12/88/115	-
19	CLA	3	312	3	-	3/12/88/115	-
19	CLA	A	823	30	-	8/39/115/115	-
22	A1LXP	J	102	-	-	3/29/67/67	0/2/2/2
19	CLA	B	832	6	-	6/15/91/115	-
19	CLA	B	827	6	1/1/15/20	10/39/115/115	-
19	CLA	A	826	5	1/1/15/20	9/39/115/115	-
18	CHL	2	315	30	-	10/17/93/117	-
19	CLA	B	825	6	1/1/15/20	12/39/115/115	-
22	A1LXP	3	305	-	-	2/29/67/67	0/2/2/2
24	BCR	G	205	-	-	4/29/63/63	0/2/2/2
19	CLA	B	830	6	1/1/15/20	20/39/115/115	-
19	CLA	H	201	12	1/1/13/20	8/27/103/115	-
19	CLA	B	836	30	1/1/13/20	1/29/105/115	-
27	CL0	A	830	5	-	2/39/115/115	-
19	CLA	A	840	19,5	1/1/15/20	12/39/115/115	-
19	CLA	3	302	3	-	9/24/100/115	-
19	CLA	A	815	5	-	3/15/91/115	-
19	CLA	B	838	6	-	3/15/91/115	-
19	CLA	4	318	4	-	5/15/91/115	-
24	BCR	K	201	-	-	4/29/63/63	0/2/2/2
19	CLA	A	828	5	1/1/15/20	17/39/115/115	-
19	CLA	A	816	5	-	2/21/97/115	-
19	CLA	A	825	5	-	10/12/88/115	-
19	CLA	A	832	5	-	0/15/91/115	-
19	CLA	F	303	10	-	2/12/88/115	-
18	CHL	1	606	1	-	5/14/90/117	-
24	BCR	B	816	-	-	0/29/63/63	0/2/2/2
19	CLA	B	843	6	1/1/15/20	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	822	6	1/1/15/20	13/39/115/115	-
18	CHL	2	313	30	-	6/12/88/117	-
19	CLA	A	821	5	-	7/24/100/115	-
24	BCR	3	316	-	-	4/29/63/63	0/2/2/2
19	CLA	B	844	6	1/1/13/20	7/32/108/115	-
19	CLA	4	307	4	-	5/15/91/115	-
19	CLA	B	847	6	-	3/21/97/115	-
19	CLA	1	612	1	1/1/13/20	4/27/103/115	-
28	PQN	A	839	-	-	4/23/43/43	0/2/2/2
19	CLA	1	608	1	1/1/13/20	10/30/106/115	-
19	CLA	B	807	6	-	2/15/91/115	-
19	CLA	1	607	-	-	7/23/99/115	-
19	CLA	A	818	5	1/1/15/20	14/39/115/115	-
19	CLA	3	306	3	-	3/18/94/115	-
23	LHG	A	835	-	-	17/53/53/53	-
22	A1LXP	2	309	-	-	2/29/67/67	0/2/2/2
25	LMG	J	103	-	-	16/36/56/70	0/1/1/1
26	SF4	A	803	6,5	-	-	0/6/5/5
19	CLA	B	826	6	1/1/15/20	14/39/115/115	-
19	CLA	A	836	5	-	5/15/91/115	-
19	CLA	B	834	6	1/1/15/20	9/39/115/115	-
24	BCR	B	813	-	-	6/29/63/63	0/2/2/2
21	XAT	2	306	-	-	1/31/93/93	0/4/4/4
19	CLA	B	819	6	1/1/15/20	9/39/115/115	-
19	CLA	B	833	6	1/1/14/20	7/33/109/115	-
19	CLA	B	839	6	-	2/13/89/115	-
19	CLA	3	304	3	1/1/13/20	5/27/103/115	-
19	CLA	A	811	5	1/1/13/20	2/27/103/115	-
19	CLA	B	840	6	-	2/15/91/115	-
19	CLA	B	801	6	1/1/15/20	10/39/115/115	-
19	CLA	1	603	1	1/1/13/20	12/30/106/115	-
24	BCR	B	812	-	-	4/29/63/63	0/2/2/2
19	CLA	B	818	30	1/1/15/20	17/39/115/115	-
19	CLA	F	306	30	-	3/19/95/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	833	-	1/1/15/20	6/39/115/115	-
24	BCR	A	838	-	-	2/29/63/63	0/2/2/2
19	CLA	B	802	6	1/1/14/20	7/33/109/115	-
18	CHL	4	313	30	-	4/17/93/117	-
24	BCR	F	304	-	-	2/29/63/63	0/2/2/2
19	CLA	B	842	30	-	4/21/97/115	-
19	CLA	B	845	6	1/1/15/20	4/39/115/115	-
19	CLA	B	806	6	1/1/15/20	9/39/115/115	-
19	CLA	B	828	6	-	10/23/99/115	-
24	BCR	A	845	-	-	4/29/63/63	0/2/2/2
24	BCR	A	804	-	-	1/29/63/63	0/2/2/2
18	CHL	3	303	3	1/1/15/21	14/41/117/117	-
19	CLA	B	846	6	1/1/15/20	12/39/115/115	-
19	CLA	A	802	19,5	1/1/13/20	6/29/105/115	-
24	BCR	A	841	-	-	4/29/63/63	0/2/2/2
25	LMG	F	305	-	-	7/24/44/70	0/1/1/1
22	A1LXP	4	303	-	-	0/29/67/67	0/2/2/2
19	CLA	4	317	4	1/1/13/20	4/30/106/115	-
19	CLA	2	310	2	1/1/13/20	8/27/103/115	-
19	CLA	G	203	11	-	7/15/91/115	-
19	CLA	1	602	1	1/1/14/20	15/33/109/115	-
26	SF4	C	101	7	-	-	0/6/5/5
19	CLA	A	829	5	1/1/15/20	6/39/115/115	-
23	LHG	1	617	20	-	25/53/53/53	-
19	CLA	B	831	6	1/1/15/20	15/39/115/115	-
19	CLA	4	311	4	-	2/15/91/115	-
18	CHL	2	316	2	1/1/13/21	10/33/109/117	-
19	CLA	B	810	23	1/1/15/20	14/39/115/115	-
19	CLA	B	824	6	-	1/24/100/115	-
23	LHG	2	302	20	-	20/49/49/53	-
24	BCR	J	105	-	-	2/29/63/63	0/2/2/2
25	LMG	N	201	-	-	5/20/40/70	0/1/1/1
19	CLA	B	808	30	1/1/15/20	10/39/115/115	-
18	CHL	3	315	30	-	8/23/99/117	-
19	CLA	B	809	6	1/1/15/20	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	A1LXP	4	306	-	-	2/29/67/67	0/2/2/2
19	CLA	A	817	30	-	5/20/96/115	-
23	LHG	1	620	19	-	2/23/23/53	-
19	CLA	L	303	30	-	2/15/91/115	-
22	A1LXP	1	619	-	-	2/29/67/67	0/2/2/2
19	CLA	B	848	6	-	1/15/91/115	-
22	A1LXP	1	616	-	-	0/29/67/67	0/2/2/2
24	BCR	L	301	-	-	1/29/63/63	0/2/2/2
19	CLA	A	843	5	-	1/25/101/115	-
19	CLA	2	311	2	-	0/15/91/115	-
19	CLA	A	827	5	1/1/13/20	4/31/107/115	-
19	CLA	A	834	5	1/1/15/20	8/39/115/115	-
22	A1LXP	3	310	-	-	0/29/67/67	0/2/2/2
19	CLA	1	605	30	-	8/15/91/115	-
19	CLA	3	314	3	1/1/13/20	2/27/103/115	-
19	CLA	A	813	5	1/1/14/20	6/33/109/115	-
19	CLA	A	824	5	1/1/15/20	11/39/115/115	-
19	CLA	A	820	5	-	4/12/88/115	-
19	CLA	A	810	5	-	0/21/97/115	-
19	CLA	3	301	3	1/1/14/20	7/33/109/115	-
19	CLA	A	831	5	1/1/15/20	12/39/115/115	-
25	LMG	4	304	-	-	7/29/49/70	0/1/1/1
24	BCR	4	308	-	-	6/29/63/63	0/2/2/2
19	CLA	A	819	5	1/1/15/20	7/39/115/115	-
19	CLA	A	848	5	-	2/21/97/115	-
19	CLA	A	849	5	-	1/21/97/115	-
28	PQN	B	811	-	-	5/23/43/43	0/2/2/2
25	LMG	G	206	-	-	7/30/50/70	0/1/1/1
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
24	BCR	A	847	-	-	2/18/35/63	0/1/1/2
19	CLA	A	801	30	1/1/13/20	2/27/103/115	-
19	CLA	B	835	6	1/1/13/20	3/30/106/115	-
19	CLA	L	304	16	1/1/15/20	9/39/115/115	-
19	CLA	A	850	30	1/1/15/20	6/39/115/115	-
19	CLA	3	308	30	-	0/15/91/115	-
19	CLA	B	841	30	1/1/13/20	5/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	J	101	5	1/1/15/20	9/39/115/115	-
19	CLA	A	822	5	-	10/25/101/115	-
19	CLA	K	203	30	-	6/15/91/115	-
25	LMG	F	301	-	-	2/25/45/70	0/1/1/1
18	CHL	4	319	4	-	7/17/93/117	-
19	CLA	2	312	2	1/1/14/20	15/36/112/115	-
19	CLA	L	305	16	-	0/15/91/115	-
26	SF4	C	102	7	-	-	0/6/5/5
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
24	BCR	L	306	-	-	3/29/63/63	0/2/2/2
18	CHL	1	601	1	1/1/13/21	11/33/109/117	-
24	BCR	A	852	-	-	2/29/63/63	0/2/2/2
24	BCR	B	814	-	-	2/29/63/63	0/2/2/2
19	CLA	A	851	30	1/1/14/20	12/36/112/115	-
19	CLA	B	829	6	-	3/13/89/115	-
19	CLA	B	837	6	-	1/18/94/115	-
19	CLA	A	812	5	1/1/15/20	10/39/115/115	-
19	CLA	B	805	6	-	1/21/97/115	-
19	CLA	B	804	30	-	0/15/91/115	-
24	BCR	L	302	-	-	0/29/63/63	0/2/2/2
24	BCR	B	815	-	-	4/29/63/63	0/2/2/2
19	CLA	3	307	30	-	3/19/95/115	-
19	CLA	B	820	-	1/1/15/20	9/39/115/115	-
21	XAT	1	615	-	-	0/31/93/93	0/4/4/4
19	CLA	B	821	6	-	4/12/88/115	-
19	CLA	A	842	5	1/1/14/20	8/33/109/115	-
19	CLA	A	846	5	1/1/15/20	8/39/115/115	-
29	DGD	B	817	-	-	16/49/89/95	0/2/2/2
19	CLA	A	806	5	-	7/12/88/115	-
19	CLA	K	202	15	-	7/15/91/115	-
19	CLA	4	314	4	-	2/24/100/115	-
19	CLA	A	808	30	1/1/15/20	7/39/115/115	-
21	XAT	1	618	-	-	0/21/52/93	0/2/2/4
19	CLA	B	823	6	1/1/15/20	9/39/115/115	-
19	CLA	A	844	5	-	2/12/88/115	-
19	CLA	2	301	2	-	7/21/97/115	-

All (984) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	312	CLA	C4B-NB	12.65	1.53	1.37
19	4	307	CLA	C4B-NB	11.36	1.51	1.37
19	A	844	CLA	C4B-NB	10.87	1.51	1.37
19	3	314	CLA	C4B-NB	10.35	1.50	1.37
19	B	833	CLA	C1B-NB	10.34	1.50	1.37
19	B	801	CLA	C4B-NB	10.25	1.50	1.37
19	2	311	CLA	C4B-NB	10.17	1.50	1.37
19	3	306	CLA	C4B-NB	10.13	1.50	1.37
19	4	318	CLA	C4B-NB	10.08	1.50	1.37
19	2	310	CLA	C4B-NB	9.73	1.49	1.37
19	A	825	CLA	C4B-NB	9.55	1.49	1.37
19	L	305	CLA	C4B-NB	9.49	1.49	1.37
19	1	603	CLA	C4B-NB	9.40	1.49	1.37
19	B	825	CLA	C4B-NB	9.36	1.49	1.37
19	2	301	CLA	C4B-NB	9.35	1.49	1.37
19	1	612	CLA	C4B-NB	9.31	1.49	1.37
19	A	816	CLA	C4B-NB	9.28	1.49	1.37
19	B	848	CLA	C4B-NB	9.28	1.49	1.37
19	4	314	CLA	C4B-NB	9.25	1.49	1.37
19	A	827	CLA	C4B-NB	9.23	1.49	1.37
19	4	311	CLA	C4B-NB	9.22	1.49	1.37
19	3	304	CLA	C4B-NB	9.17	1.49	1.37
19	A	811	CLA	C4B-NB	9.15	1.49	1.37
19	1	608	CLA	C4B-NB	9.11	1.49	1.37
19	1	605	CLA	C4B-NB	8.91	1.48	1.37
19	4	317	CLA	C4B-NB	8.90	1.48	1.37
19	B	836	CLA	C4B-NB	8.83	1.48	1.37
19	B	820	CLA	C4B-NB	8.77	1.48	1.37
19	B	827	CLA	C4B-NB	8.75	1.48	1.37
19	A	848	CLA	C4B-NB	8.74	1.48	1.37
19	G	202	CLA	C4B-NB	8.67	1.48	1.37
19	K	203	CLA	C4B-NB	8.62	1.48	1.37
19	L	305	CLA	MG-NB	-8.39	1.89	2.05
19	3	301	CLA	C4B-NB	8.27	1.48	1.37
19	1	602	CLA	C4B-NB	8.20	1.47	1.37
19	L	303	CLA	C4B-NB	8.18	1.47	1.37
19	B	840	CLA	C4B-NB	8.15	1.47	1.37
19	B	822	CLA	C4B-NB	8.10	1.47	1.37
19	A	806	CLA	C4B-NB	8.07	1.47	1.37
19	B	833	CLA	C4B-NB	7.99	1.47	1.37
19	B	843	CLA	C4B-NB	7.97	1.47	1.37
19	A	811	CLA	MG-ND	-7.87	1.90	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	607	CLA	C4B-NB	7.76	1.47	1.37
19	4	307	CLA	C1D-ND	7.72	1.47	1.37
27	A	830	CL0	MG-NA	7.69	2.24	2.06
19	A	832	CLA	C1B-NB	7.67	1.47	1.37
19	A	810	CLA	C1D-ND	7.61	1.47	1.37
18	4	313	CHL	C4B-NB	7.57	1.47	1.37
19	B	804	CLA	C4B-NB	7.55	1.47	1.37
19	2	310	CLA	C1D-ND	7.55	1.47	1.37
19	3	307	CLA	C4B-NB	7.54	1.47	1.37
19	A	823	CLA	C4B-NB	7.50	1.47	1.37
19	A	843	CLA	C1D-ND	7.43	1.46	1.37
19	B	845	CLA	C4B-NB	7.42	1.46	1.37
19	B	829	CLA	C4B-NB	7.36	1.46	1.37
27	A	830	CL0	MG-NC	7.36	2.23	2.06
19	3	312	CLA	C4B-NB	7.35	1.46	1.37
19	A	811	CLA	C1B-NB	7.33	1.46	1.37
19	A	831	CLA	C4B-NB	7.31	1.46	1.37
19	J	101	CLA	C4B-NB	7.28	1.46	1.37
19	A	801	CLA	C4B-NB	7.26	1.46	1.37
19	B	833	CLA	MG-ND	-7.26	1.91	2.05
19	F	303	CLA	C4B-NB	7.23	1.46	1.37
19	A	837	CLA	C1D-ND	7.21	1.46	1.37
19	B	810	CLA	C4B-NB	7.20	1.46	1.37
18	1	606	CHL	C4B-NB	7.12	1.46	1.37
19	4	318	CLA	C1D-ND	7.11	1.46	1.37
19	B	827	CLA	MG-ND	-7.10	1.91	2.05
19	L	305	CLA	C1D-ND	7.09	1.46	1.37
19	B	833	CLA	C1D-ND	7.09	1.46	1.37
19	B	822	CLA	C1D-ND	7.07	1.46	1.37
19	A	805	CLA	C1D-ND	7.05	1.46	1.37
19	A	832	CLA	C4B-NB	7.05	1.46	1.37
19	A	806	CLA	C1B-NB	7.00	1.46	1.37
19	B	832	CLA	C4B-NB	6.97	1.46	1.37
19	B	830	CLA	C1D-ND	6.91	1.46	1.37
19	4	307	CLA	C1B-NB	6.85	1.46	1.37
19	F	306	CLA	C4B-NB	6.84	1.46	1.37
19	B	821	CLA	C4B-NB	6.82	1.46	1.37
19	B	839	CLA	C4B-NB	6.81	1.46	1.37
19	2	301	CLA	C1D-ND	6.78	1.46	1.37
19	4	318	CLA	C1B-NB	6.76	1.46	1.37
19	A	814	CLA	C1B-NB	6.76	1.46	1.37
19	B	828	CLA	MG-NB	-6.62	1.92	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	848	CLA	MG-NB	-6.61	1.92	2.05
19	B	806	CLA	MG-NB	-6.59	1.92	2.05
19	A	824	CLA	C4B-NB	6.56	1.45	1.37
19	3	306	CLA	C1D-ND	6.56	1.45	1.37
19	B	828	CLA	C4B-NB	6.54	1.45	1.37
19	4	314	CLA	MG-NB	-6.49	1.92	2.05
19	3	302	CLA	C4B-NB	6.48	1.45	1.37
19	A	810	CLA	MG-NB	-6.47	1.93	2.05
19	A	840	CLA	C1B-NB	6.44	1.45	1.37
19	K	202	CLA	C4B-NB	6.33	1.45	1.37
19	A	842	CLA	C1D-ND	6.31	1.45	1.37
19	1	612	CLA	MG-NB	-6.31	1.93	2.05
19	A	801	CLA	C1D-ND	6.26	1.45	1.37
19	B	842	CLA	C1B-NB	6.19	1.45	1.37
19	B	833	CLA	MG-NB	-6.18	1.93	2.05
19	A	840	CLA	MG-ND	-6.16	1.93	2.05
19	B	820	CLA	MG-ND	-6.15	1.93	2.05
19	B	844	CLA	C1B-NB	6.14	1.45	1.37
19	4	314	CLA	C1D-ND	6.14	1.45	1.37
19	J	101	CLA	C1B-NB	6.12	1.45	1.37
19	B	830	CLA	C4B-NB	6.07	1.45	1.37
19	A	805	CLA	C1B-NB	6.01	1.45	1.37
19	A	813	CLA	C4B-NB	5.98	1.45	1.37
19	A	833	CLA	MG-ND	-5.97	1.94	2.05
19	A	851	CLA	MG-NB	-5.93	1.94	2.05
19	A	817	CLA	C4B-NB	5.92	1.45	1.37
19	4	314	CLA	C1B-NB	5.89	1.45	1.37
19	A	815	CLA	C4B-NB	5.89	1.45	1.37
19	B	840	CLA	MG-NB	-5.85	1.94	2.05
19	1	607	CLA	MG-ND	-5.85	1.94	2.05
19	A	814	CLA	MG-NB	-5.84	1.94	2.05
19	A	836	CLA	C4B-NB	5.82	1.44	1.37
19	B	803	CLA	C4B-NB	5.82	1.44	1.37
19	4	311	CLA	C1D-ND	5.82	1.44	1.37
19	A	810	CLA	C4B-NB	5.81	1.44	1.37
18	2	313	CHL	C4B-NB	5.77	1.44	1.37
19	B	804	CLA	C1D-ND	5.76	1.44	1.37
19	A	822	CLA	C4B-NB	5.76	1.44	1.37
19	4	317	CLA	C1D-ND	5.75	1.44	1.37
19	A	834	CLA	C1D-ND	5.75	1.44	1.37
19	B	832	CLA	MG-ND	-5.74	1.94	2.05
19	B	831	CLA	C1B-NB	5.71	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	MG-ND	-5.71	1.94	2.05
19	B	848	CLA	MG-ND	-5.70	1.94	2.05
19	1	602	CLA	C1D-ND	5.66	1.44	1.37
19	B	835	CLA	C4B-NB	5.65	1.44	1.37
19	3	302	CLA	C1D-ND	5.63	1.44	1.37
19	J	101	CLA	MG-NB	-5.62	1.94	2.05
19	K	203	CLA	MG-ND	-5.61	1.94	2.05
19	A	837	CLA	MG-ND	-5.58	1.94	2.05
19	A	829	CLA	C1C-C2C	5.58	1.55	1.44
19	B	832	CLA	MG-NB	-5.55	1.94	2.05
19	B	824	CLA	C4B-NB	5.55	1.44	1.37
19	G	203	CLA	C4B-NB	5.55	1.44	1.37
19	A	840	CLA	C4B-NB	5.54	1.44	1.37
19	4	311	CLA	MG-ND	-5.54	1.94	2.05
19	A	808	CLA	MG-NB	-5.54	1.94	2.05
19	1	603	CLA	MG-NB	-5.53	1.94	2.05
19	B	824	CLA	MG-NB	-5.53	1.94	2.05
19	B	837	CLA	MG-ND	-5.52	1.94	2.05
19	A	818	CLA	C4B-NB	5.51	1.44	1.37
19	3	312	CLA	C1B-NB	5.50	1.44	1.37
19	B	836	CLA	MG-ND	-5.49	1.94	2.05
19	A	806	CLA	MG-NB	-5.47	1.94	2.05
19	A	809	CLA	C1D-ND	5.45	1.44	1.37
19	L	304	CLA	C4B-NB	5.44	1.44	1.37
19	3	302	CLA	MG-NB	-5.43	1.95	2.05
19	B	837	CLA	C1D-ND	5.43	1.44	1.37
19	K	202	CLA	MG-NB	-5.43	1.95	2.05
19	B	838	CLA	MG-NB	-5.41	1.95	2.05
19	H	201	CLA	MG-ND	-5.41	1.95	2.05
18	2	316	CHL	C4B-NB	5.40	1.44	1.37
19	3	314	CLA	C1D-ND	5.37	1.44	1.37
19	3	302	CLA	C1B-NB	5.36	1.44	1.37
19	2	310	CLA	MG-NB	-5.35	1.95	2.05
19	A	810	CLA	MG-ND	-5.35	1.95	2.05
19	B	831	CLA	C4B-NB	5.33	1.44	1.37
19	A	818	CLA	C1C-NC	-5.32	1.29	1.37
18	1	601	CHL	C4B-NB	5.31	1.44	1.37
19	A	821	CLA	C4B-NB	5.31	1.44	1.37
19	1	607	CLA	C1C-C2C	5.28	1.54	1.44
19	B	809	CLA	C4B-NB	5.27	1.44	1.37
19	A	827	CLA	MG-ND	-5.26	1.95	2.05
19	B	835	CLA	MG-NB	-5.26	1.95	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	301	CLA	C1B-NB	5.25	1.44	1.37
19	A	819	CLA	C1B-NB	5.23	1.44	1.37
19	3	306	CLA	MG-ND	-5.22	1.95	2.05
19	A	828	CLA	MG-NB	-5.22	1.95	2.05
19	3	301	CLA	C1D-ND	5.20	1.44	1.37
19	1	605	CLA	MG-NB	-5.18	1.95	2.05
19	A	820	CLA	MG-NB	-5.18	1.95	2.05
19	1	612	CLA	C1B-NB	5.17	1.44	1.37
18	3	303	CHL	C4B-NB	5.15	1.44	1.37
19	K	203	CLA	C1C-C2C	5.14	1.54	1.44
19	1	608	CLA	MG-NB	-5.13	1.95	2.05
19	A	846	CLA	MG-NB	-5.13	1.95	2.05
19	B	827	CLA	C1B-NB	5.10	1.44	1.37
19	A	844	CLA	C1D-ND	5.10	1.44	1.37
19	B	805	CLA	MG-NB	-5.10	1.95	2.05
19	B	847	CLA	C4B-NB	5.10	1.44	1.37
19	A	822	CLA	C1D-ND	5.09	1.44	1.37
19	A	823	CLA	MG-ND	-5.09	1.95	2.05
19	B	844	CLA	C1D-ND	5.09	1.44	1.37
19	B	825	CLA	C1C-NC	5.08	1.45	1.37
18	3	315	CHL	C4B-NB	5.06	1.44	1.37
19	J	101	CLA	MG-NC	-5.05	1.94	2.06
19	1	612	CLA	C1D-ND	5.04	1.44	1.37
19	A	812	CLA	C1D-ND	5.04	1.44	1.37
19	A	827	CLA	C1D-ND	5.01	1.43	1.37
19	B	824	CLA	C1D-ND	5.01	1.43	1.37
19	A	813	CLA	MG-NB	-4.98	1.95	2.05
19	B	846	CLA	C1D-ND	4.96	1.43	1.37
19	B	829	CLA	C1B-NB	4.95	1.43	1.37
19	A	849	CLA	MG-NB	-4.95	1.96	2.05
19	A	828	CLA	C4B-NB	4.93	1.43	1.37
19	4	311	CLA	C1B-NB	4.90	1.43	1.37
19	A	822	CLA	C1B-NB	4.88	1.43	1.37
19	A	814	CLA	C1D-ND	4.88	1.43	1.37
19	A	836	CLA	MG-NB	-4.86	1.96	2.05
19	B	834	CLA	C4B-NB	4.86	1.43	1.37
19	B	804	CLA	MG-ND	-4.86	1.96	2.05
19	L	304	CLA	MG-NB	-4.85	1.96	2.05
19	A	823	CLA	C1B-NB	4.84	1.43	1.37
19	B	845	CLA	C1D-ND	4.84	1.43	1.37
19	A	833	CLA	C1D-ND	4.83	1.43	1.37
18	2	315	CHL	C4B-NB	4.82	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	202	CLA	MG-ND	-4.81	1.96	2.05
19	A	842	CLA	CBB-CAB	-4.80	1.06	1.30
18	4	319	CHL	C4B-NB	4.79	1.43	1.37
19	3	304	CLA	C1D-ND	4.79	1.43	1.37
19	B	842	CLA	MG-NB	-4.77	1.96	2.05
19	3	314	CLA	MG-ND	-4.76	1.96	2.05
19	2	310	CLA	C1B-NB	4.75	1.43	1.37
19	2	311	CLA	C1D-ND	4.75	1.43	1.37
19	B	827	CLA	C1C-C2C	4.73	1.53	1.44
19	3	307	CLA	C1D-ND	4.72	1.43	1.37
19	4	317	CLA	MG-NA	-4.72	1.95	2.06
19	F	303	CLA	MG-NB	-4.71	1.96	2.05
19	A	815	CLA	MG-ND	-4.69	1.96	2.05
19	A	819	CLA	C1D-ND	4.68	1.43	1.37
19	A	820	CLA	C4B-NB	4.66	1.43	1.37
19	A	807	CLA	MG-NB	-4.66	1.96	2.05
19	B	826	CLA	C1C-NC	-4.65	1.30	1.37
19	B	802	CLA	MG-ND	-4.63	1.96	2.05
19	A	842	CLA	C4B-NB	4.61	1.43	1.37
19	B	806	CLA	C4B-NB	4.61	1.43	1.37
19	B	840	CLA	MG-NC	-4.60	1.95	2.06
19	A	828	CLA	C1B-NB	4.60	1.43	1.37
19	3	306	CLA	MG-NB	-4.59	1.96	2.05
19	1	607	CLA	MG-NB	-4.59	1.96	2.05
19	B	846	CLA	C4B-NB	4.55	1.43	1.37
19	2	310	CLA	MG-ND	-4.55	1.96	2.05
19	B	803	CLA	MG-NC	-4.53	1.95	2.06
19	A	851	CLA	C1C-NC	-4.53	1.31	1.37
19	A	818	CLA	C1C-C2C	4.52	1.53	1.44
19	G	202	CLA	C1B-NB	4.52	1.43	1.37
19	3	302	CLA	MG-ND	-4.52	1.96	2.05
19	A	828	CLA	MG-ND	-4.51	1.96	2.05
19	B	818	CLA	C4B-NB	4.51	1.43	1.37
19	H	201	CLA	MG-NB	-4.50	1.96	2.05
19	B	841	CLA	C1C-C2C	4.50	1.53	1.44
19	A	843	CLA	MG-ND	-4.50	1.96	2.05
19	B	805	CLA	C4B-NB	4.49	1.43	1.37
19	4	311	CLA	MG-NB	-4.49	1.96	2.05
19	B	833	CLA	MG-NC	-4.48	1.95	2.06
19	B	802	CLA	MG-NB	-4.47	1.96	2.05
19	B	828	CLA	MG-NC	-4.47	1.95	2.06
19	B	808	CLA	C4B-NB	4.46	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	202	CLA	C1D-ND	4.45	1.43	1.37
19	A	807	CLA	MG-NA	-4.45	1.95	2.06
19	A	833	CLA	C4B-NB	4.44	1.43	1.37
19	A	829	CLA	C1D-ND	4.44	1.43	1.37
19	A	808	CLA	C1D-ND	4.43	1.43	1.37
19	G	203	CLA	C1B-NB	4.43	1.43	1.37
19	B	846	CLA	MG-NB	-4.42	1.97	2.05
19	G	203	CLA	MG-NB	-4.42	1.97	2.05
19	F	306	CLA	C1C-C2C	4.42	1.53	1.44
19	A	801	CLA	C1B-NB	4.42	1.43	1.37
19	A	832	CLA	MG-NC	-4.42	1.95	2.06
19	2	301	CLA	MG-NB	-4.41	1.97	2.05
19	B	839	CLA	C3A-C2A	-4.39	1.42	1.54
19	B	821	CLA	MG-NC	-4.39	1.95	2.06
19	3	308	CLA	C4B-NB	4.38	1.43	1.37
19	A	848	CLA	C1D-ND	4.38	1.43	1.37
19	A	849	CLA	MG-ND	-4.36	1.97	2.05
19	B	803	CLA	C1B-NB	4.35	1.43	1.37
19	A	851	CLA	MG-ND	-4.35	1.97	2.05
19	B	810	CLA	C1B-NB	4.33	1.43	1.37
19	A	806	CLA	C1D-ND	4.33	1.43	1.37
19	2	312	CLA	MG-NB	-4.33	1.97	2.05
19	A	808	CLA	C4B-NB	4.31	1.43	1.37
19	A	805	CLA	MG-NB	-4.30	1.97	2.05
19	A	829	CLA	CHD-C1D	4.30	1.46	1.38
19	A	819	CLA	C1C-NC	-4.30	1.31	1.37
19	A	801	CLA	MG-NB	-4.29	1.97	2.05
19	B	836	CLA	C1D-ND	4.27	1.43	1.37
19	A	828	CLA	C1D-ND	4.25	1.43	1.37
19	B	820	CLA	C1C-C2C	4.24	1.52	1.44
19	3	301	CLA	MG-NB	-4.24	1.97	2.05
19	A	832	CLA	MG-NA	-4.24	1.96	2.06
19	1	605	CLA	MG-ND	-4.23	1.97	2.05
19	G	202	CLA	MG-NB	-4.22	1.97	2.05
19	A	825	CLA	C1B-NB	4.22	1.43	1.37
19	A	812	CLA	MG-ND	-4.22	1.97	2.05
19	A	818	CLA	C1B-NB	4.22	1.43	1.37
19	B	844	CLA	MG-NB	-4.20	1.97	2.05
19	2	301	CLA	MG-ND	-4.19	1.97	2.05
19	B	844	CLA	MG-ND	-4.19	1.97	2.05
19	3	314	CLA	MG-NC	-4.18	1.96	2.06
19	A	807	CLA	C1D-ND	4.18	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	824	CLA	MG-ND	-4.17	1.97	2.05
19	A	805	CLA	C4B-NB	4.16	1.42	1.37
19	1	602	CLA	MG-ND	-4.16	1.97	2.05
19	A	837	CLA	MG-NC	-4.15	1.96	2.06
18	4	319	CHL	C1B-C2B	4.15	1.53	1.43
19	A	833	CLA	MG-NB	-4.15	1.97	2.05
19	A	833	CLA	C1B-NB	4.15	1.42	1.37
19	B	819	CLA	C1C-C2C	4.15	1.52	1.44
19	B	829	CLA	MG-NB	-4.14	1.97	2.05
19	A	822	CLA	C1C-C2C	4.13	1.52	1.44
19	4	317	CLA	C1B-NB	4.12	1.42	1.37
19	B	842	CLA	C4B-NB	4.12	1.42	1.37
19	A	844	CLA	MG-NA	-4.11	1.96	2.06
19	4	317	CLA	MG-NB	-4.10	1.97	2.05
19	B	840	CLA	MG-ND	-4.08	1.97	2.05
19	A	815	CLA	MG-NB	-4.08	1.97	2.05
19	F	303	CLA	C1D-ND	4.08	1.42	1.37
19	A	806	CLA	C1C-C2C	4.08	1.52	1.44
19	4	314	CLA	MG-ND	-4.07	1.97	2.05
19	3	312	CLA	MG-NC	-4.07	1.96	2.06
19	2	312	CLA	C1D-ND	4.05	1.42	1.37
19	F	306	CLA	MG-NB	-4.05	1.97	2.05
19	H	201	CLA	C4B-NB	4.04	1.42	1.37
19	B	832	CLA	C1D-ND	4.04	1.42	1.37
19	1	612	CLA	MG-NC	-4.03	1.96	2.06
19	A	832	CLA	C1C-C2C	4.03	1.52	1.44
19	B	805	CLA	CHD-C1D	4.03	1.46	1.38
19	A	819	CLA	C4B-NB	4.03	1.42	1.37
19	A	816	CLA	C1B-NB	4.02	1.42	1.37
19	1	608	CLA	C1D-ND	4.01	1.42	1.37
19	B	844	CLA	O2A-C1	4.01	1.57	1.46
19	A	849	CLA	C1C-NC	-4.00	1.31	1.37
19	A	826	CLA	MG-NC	-4.00	1.96	2.06
19	1	608	CLA	MG-ND	-4.00	1.97	2.05
19	3	307	CLA	MG-ND	-4.00	1.97	2.05
19	A	843	CLA	C1B-NB	4.00	1.42	1.37
19	2	312	CLA	C1C-C2C	4.00	1.52	1.44
19	L	303	CLA	MG-NB	-3.99	1.97	2.05
19	B	847	CLA	C1C-C2C	3.99	1.52	1.44
19	B	846	CLA	MG-NA	3.98	2.15	2.06
19	B	835	CLA	C1B-NB	3.98	1.42	1.37
19	A	817	CLA	MG-ND	-3.94	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	832	CLA	C1D-ND	3.94	1.42	1.37
19	B	824	CLA	MG-ND	-3.93	1.98	2.05
19	4	318	CLA	MG-NB	-3.91	1.98	2.05
19	B	831	CLA	C3A-C2A	-3.91	1.43	1.54
19	A	810	CLA	C1B-NB	3.90	1.42	1.37
19	3	312	CLA	MG-ND	-3.89	1.98	2.05
19	2	311	CLA	C1C-C2C	3.89	1.52	1.44
19	H	201	CLA	C1C-C2C	3.89	1.52	1.44
19	A	812	CLA	C4B-NB	3.88	1.42	1.37
19	A	807	CLA	C4B-NB	3.88	1.42	1.37
19	A	820	CLA	MG-ND	-3.87	1.98	2.05
19	1	607	CLA	C1D-ND	3.87	1.42	1.37
19	A	825	CLA	MG-NA	-3.87	1.97	2.06
19	A	807	CLA	C1C-NC	-3.85	1.32	1.37
19	3	308	CLA	MG-ND	-3.85	1.98	2.05
19	4	318	CLA	C1C-C2C	3.84	1.52	1.44
19	B	841	CLA	C4B-NB	3.83	1.42	1.37
19	A	802	CLA	C1B-NB	3.83	1.42	1.37
19	1	603	CLA	MG-ND	-3.82	1.98	2.05
19	A	801	CLA	MG-ND	-3.82	1.98	2.05
19	B	801	CLA	MG-NB	-3.80	1.98	2.05
19	B	839	CLA	MG-NB	-3.79	1.98	2.05
19	B	818	CLA	MG-NB	-3.79	1.98	2.05
19	A	842	CLA	MG-NC	-3.79	1.97	2.06
19	A	834	CLA	C4B-NB	3.79	1.42	1.37
19	A	846	CLA	C1C-NC	3.79	1.43	1.37
19	F	303	CLA	C1B-NB	3.78	1.42	1.37
19	A	827	CLA	C1C-NC	3.78	1.43	1.37
19	A	813	CLA	MG-ND	-3.77	1.98	2.05
19	B	819	CLA	C1D-ND	3.77	1.42	1.37
27	A	830	CL0	CHD-C4C	3.77	1.47	1.39
19	B	835	CLA	C1D-ND	3.76	1.42	1.37
19	B	831	CLA	C1C-C2C	3.76	1.51	1.44
19	B	841	CLA	MG-NB	-3.76	1.98	2.05
19	A	843	CLA	C4B-NB	3.75	1.42	1.37
19	B	839	CLA	MG-ND	-3.75	1.98	2.05
19	B	810	CLA	MG-NB	-3.75	1.98	2.05
19	B	839	CLA	C1D-ND	3.75	1.42	1.37
19	B	823	CLA	C1D-ND	3.75	1.42	1.37
19	3	302	CLA	MG-NC	-3.74	1.97	2.06
19	A	802	CLA	MG-NB	-3.74	1.98	2.05
19	A	820	CLA	MG-NC	-3.74	1.97	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	830	CL0	C1D-ND	3.74	1.42	1.37
19	1	612	CLA	MG-ND	-3.74	1.98	2.05
19	B	845	CLA	MG-NB	-3.74	1.98	2.05
19	1	603	CLA	C1D-ND	3.73	1.42	1.37
19	1	603	CLA	C1C-C2C	3.72	1.51	1.44
19	L	305	CLA	C1B-NB	3.71	1.42	1.37
19	A	831	CLA	MG-ND	-3.71	1.98	2.05
19	A	813	CLA	C1D-ND	3.69	1.42	1.37
19	4	317	CLA	C1C-C2C	3.69	1.51	1.44
19	G	203	CLA	MG-NC	-3.69	1.97	2.06
19	A	846	CLA	MG-NC	-3.68	1.97	2.06
19	A	806	CLA	MG-NC	-3.68	1.97	2.06
19	2	312	CLA	C1C-NC	3.68	1.43	1.37
19	B	837	CLA	C4B-NB	3.67	1.42	1.37
19	B	818	CLA	C1B-NB	3.67	1.42	1.37
19	A	815	CLA	C3A-C2A	-3.66	1.44	1.54
19	B	847	CLA	MG-NB	-3.66	1.98	2.05
19	A	818	CLA	C1D-ND	3.65	1.42	1.37
19	A	844	CLA	C1C-C2C	3.65	1.51	1.44
19	B	821	CLA	C1C-C2C	3.65	1.51	1.44
19	A	834	CLA	MG-ND	-3.63	1.98	2.05
19	A	851	CLA	C1C-C2C	3.63	1.51	1.44
19	B	826	CLA	C1D-ND	3.62	1.42	1.37
19	B	838	CLA	C1C-C2C	3.62	1.51	1.44
19	B	807	CLA	MG-NC	-3.61	1.97	2.06
19	F	306	CLA	MG-NC	-3.61	1.97	2.06
19	B	837	CLA	C1B-NB	3.60	1.42	1.37
19	B	806	CLA	C1B-NB	3.59	1.42	1.37
19	B	803	CLA	MG-ND	-3.59	1.98	2.05
19	3	314	CLA	C1B-NB	3.59	1.42	1.37
19	A	824	CLA	C1D-ND	3.58	1.42	1.37
19	J	101	CLA	MG-ND	-3.58	1.98	2.05
19	2	310	CLA	MG-NC	-3.56	1.97	2.06
19	B	806	CLA	C1D-ND	3.56	1.42	1.37
19	B	841	CLA	C1C-NC	-3.55	1.32	1.37
19	B	802	CLA	CHC-C1C	-3.55	1.31	1.38
19	A	825	CLA	MG-NB	-3.54	1.98	2.05
19	B	838	CLA	C4B-NB	3.54	1.42	1.37
19	3	306	CLA	C1B-NB	3.54	1.42	1.37
18	1	601	CHL	C1B-C2B	3.53	1.51	1.43
19	2	311	CLA	MG-ND	-3.53	1.98	2.05
19	1	602	CLA	MG-NC	-3.52	1.97	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	308	CLA	MG-NB	-3.50	1.98	2.05
19	B	823	CLA	MG-ND	-3.50	1.98	2.05
19	H	201	CLA	C1D-ND	3.50	1.42	1.37
19	1	605	CLA	C1D-ND	3.49	1.42	1.37
19	A	831	CLA	C1D-ND	3.48	1.42	1.37
19	B	803	CLA	MG-NB	-3.48	1.98	2.05
19	A	816	CLA	CBC-CAC	-3.47	1.36	1.51
19	A	807	CLA	CBB-CAB	-3.47	1.13	1.30
19	A	827	CLA	C1B-NB	3.46	1.42	1.37
19	3	301	CLA	MG-NC	-3.46	1.98	2.06
19	B	820	CLA	CHD-C1D	3.46	1.45	1.38
19	A	826	CLA	MG-NB	-3.45	1.98	2.05
19	A	825	CLA	C1D-ND	3.45	1.42	1.37
19	3	304	CLA	C1C-C2C	3.45	1.51	1.44
19	A	834	CLA	CHD-C1D	3.44	1.45	1.38
19	A	811	CLA	CHD-C1D	3.43	1.45	1.38
19	A	801	CLA	C1C-C2C	3.43	1.51	1.44
19	3	304	CLA	MG-NA	-3.43	1.98	2.06
19	B	824	CLA	C3A-C2A	-3.43	1.44	1.54
27	A	830	CL0	C3D-C2D	3.43	1.48	1.39
19	A	826	CLA	C4B-NB	3.42	1.42	1.37
19	A	809	CLA	C1C-C2C	3.42	1.51	1.44
19	A	844	CLA	MG-NB	-3.41	1.99	2.05
19	B	842	CLA	C1C-NC	-3.41	1.32	1.37
19	A	846	CLA	C4B-NB	3.40	1.42	1.37
19	2	311	CLA	C1B-NB	3.40	1.42	1.37
19	A	828	CLA	C1C-NC	-3.39	1.32	1.37
19	B	823	CLA	C1B-NB	3.39	1.42	1.37
19	A	812	CLA	MG-NB	-3.39	1.99	2.05
19	B	802	CLA	C1D-ND	3.38	1.41	1.37
19	A	837	CLA	C4B-NB	3.38	1.41	1.37
19	4	311	CLA	C1C-C2C	3.38	1.51	1.44
19	A	844	CLA	MG-ND	-3.37	1.99	2.05
19	B	834	CLA	MG-ND	-3.36	1.99	2.05
19	L	304	CLA	C1D-ND	3.36	1.41	1.37
19	A	850	CLA	C4B-NB	3.35	1.41	1.37
19	B	804	CLA	MG-NB	-3.34	1.99	2.05
19	A	816	CLA	MG-ND	-3.34	1.99	2.05
19	B	820	CLA	C1D-ND	3.33	1.41	1.37
19	B	829	CLA	MG-ND	-3.33	1.99	2.05
19	4	307	CLA	C1C-C2C	3.33	1.51	1.44
19	1	602	CLA	MG-NB	-3.33	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	827	CLA	MG-NB	-3.32	1.99	2.05
19	A	811	CLA	C1D-ND	3.32	1.41	1.37
19	B	843	CLA	C3D-C4D	-3.32	1.36	1.44
19	A	813	CLA	C3A-C2A	-3.32	1.45	1.54
19	A	849	CLA	C4B-NB	3.32	1.41	1.37
19	H	201	CLA	MG-NA	-3.31	1.98	2.06
19	A	843	CLA	C1C-C2C	3.31	1.51	1.44
18	1	606	CHL	C1B-C2B	3.30	1.51	1.43
19	B	839	CLA	C1B-NB	3.30	1.41	1.37
19	A	840	CLA	C1D-ND	3.30	1.41	1.37
19	A	816	CLA	C1D-ND	3.29	1.41	1.37
19	B	836	CLA	C1C-C2C	3.27	1.50	1.44
19	3	308	CLA	C1D-ND	3.27	1.41	1.37
19	A	832	CLA	MG-NB	-3.27	1.99	2.05
19	G	202	CLA	C1D-ND	3.27	1.41	1.37
19	A	837	CLA	C1B-NB	3.27	1.41	1.37
19	A	812	CLA	C1C-NC	-3.26	1.32	1.37
19	4	314	CLA	MG-NC	-3.26	1.98	2.06
19	K	203	CLA	MG-NB	-3.25	1.99	2.05
19	2	311	CLA	MG-NB	-3.25	1.99	2.05
19	B	808	CLA	MG-ND	-3.25	1.99	2.05
19	B	838	CLA	MG-ND	-3.25	1.99	2.05
19	3	308	CLA	MG-NA	-3.24	1.98	2.06
19	4	314	CLA	C1C-C2C	3.24	1.50	1.44
24	B	813	BCR	C7-C6	3.23	1.56	1.45
19	A	848	CLA	MG-NC	-3.22	1.98	2.06
19	A	850	CLA	CHC-C4B	3.22	1.46	1.39
19	1	608	CLA	MG-NA	-3.22	1.98	2.06
19	B	803	CLA	C4C-C3C	-3.22	1.39	1.45
19	3	312	CLA	MG-NB	-3.21	1.99	2.05
19	A	825	CLA	MG-ND	-3.21	1.99	2.05
19	B	832	CLA	C1B-NB	3.21	1.41	1.37
19	A	823	CLA	MG-NB	-3.20	1.99	2.05
19	B	821	CLA	MG-ND	-3.20	1.99	2.05
19	3	304	CLA	MG-ND	-3.20	1.99	2.05
19	B	828	CLA	C1C-C2C	3.19	1.50	1.44
19	A	849	CLA	CBC-CAC	-3.19	1.37	1.51
19	B	808	CLA	CHD-C1D	3.19	1.44	1.38
19	1	603	CLA	C1B-NB	3.17	1.41	1.37
19	G	202	CLA	C1C-C2C	3.16	1.50	1.44
19	2	301	CLA	C1C-C2C	3.16	1.50	1.44
19	3	307	CLA	MG-NB	-3.15	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	301	CLA	MG-NA	-3.14	1.98	2.06
19	A	828	CLA	C3D-C4D	-3.14	1.37	1.44
19	A	836	CLA	MG-NA	-3.13	1.98	2.06
18	3	315	CHL	C2C-C1C	3.13	1.51	1.44
19	B	810	CLA	C1D-ND	3.12	1.41	1.37
19	B	844	CLA	C1C-C2C	3.12	1.50	1.44
19	L	305	CLA	MG-ND	-3.12	1.99	2.05
19	B	825	CLA	MG-NC	-3.12	1.98	2.06
19	A	821	CLA	C1D-ND	3.11	1.41	1.37
19	A	806	CLA	MG-ND	-3.11	1.99	2.05
19	H	201	CLA	MG-NC	-3.10	1.98	2.06
19	A	821	CLA	MG-NA	3.10	2.13	2.06
19	B	838	CLA	C1B-NB	3.10	1.41	1.37
19	A	815	CLA	C1D-ND	3.09	1.41	1.37
19	B	844	CLA	C3A-C2A	-3.08	1.45	1.54
19	A	851	CLA	C3D-C4D	-3.07	1.37	1.44
19	A	802	CLA	C1C-NC	-3.07	1.33	1.37
19	3	312	CLA	C1D-ND	3.06	1.41	1.37
19	A	836	CLA	MG-NC	-3.05	1.99	2.06
19	B	842	CLA	MG-NC	-3.05	1.99	2.06
19	A	846	CLA	CHC-C1C	-3.05	1.32	1.38
19	3	302	CLA	C1C-C2C	3.04	1.50	1.44
18	2	313	CHL	C3A-C2A	-3.04	1.51	1.54
19	B	808	CLA	MG-NB	-3.04	1.99	2.05
19	A	821	CLA	CBB-CAB	-3.03	1.15	1.30
19	B	842	CLA	MG-NA	3.03	2.13	2.06
19	B	846	CLA	C1B-NB	3.03	1.41	1.37
19	B	848	CLA	C1C-NC	-3.03	1.33	1.37
19	A	837	CLA	MG-NB	-3.02	1.99	2.05
19	G	203	CLA	MG-ND	-3.01	1.99	2.05
19	K	203	CLA	C1D-ND	3.01	1.41	1.37
19	A	840	CLA	C1C-NC	3.01	1.42	1.37
19	B	842	CLA	C1D-ND	3.01	1.41	1.37
19	A	829	CLA	MG-NB	-3.00	1.99	2.05
19	A	848	CLA	MG-ND	-3.00	1.99	2.05
19	A	817	CLA	MG-NC	-3.00	1.99	2.06
19	3	301	CLA	C1C-C2C	3.00	1.50	1.44
19	3	307	CLA	C1B-NB	2.99	1.41	1.37
19	G	203	CLA	C1D-ND	2.99	1.41	1.37
19	L	305	CLA	MG-NA	-2.98	1.99	2.06
19	G	202	CLA	MG-ND	-2.98	1.99	2.05
19	A	820	CLA	C1B-NB	2.98	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	841	CLA	C3A-C2A	2.98	1.62	1.54
19	K	203	CLA	C1B-NB	2.97	1.41	1.37
19	A	831	CLA	MG-NB	-2.97	1.99	2.05
19	B	807	CLA	MG-ND	-2.97	1.99	2.05
19	B	827	CLA	OBD-CAD	-2.97	1.17	1.22
19	1	612	CLA	C1C-C2C	2.97	1.50	1.44
19	B	834	CLA	MG-NC	-2.96	1.99	2.06
19	A	831	CLA	C1B-NB	2.95	1.41	1.37
19	H	201	CLA	C1B-NB	2.95	1.41	1.37
19	A	819	CLA	MG-ND	-2.95	1.99	2.05
19	A	818	CLA	MG-ND	-2.94	2.00	2.05
19	B	810	CLA	MG-ND	-2.94	2.00	2.05
19	F	306	CLA	C1B-NB	2.93	1.41	1.37
19	A	813	CLA	C1B-NB	2.92	1.41	1.37
19	L	303	CLA	C1D-ND	2.92	1.41	1.37
19	A	843	CLA	MG-NC	-2.92	1.99	2.06
19	B	843	CLA	C1C-C2C	2.91	1.50	1.44
19	A	822	CLA	C1D-C2D	-2.91	1.39	1.45
19	B	843	CLA	CBB-CAB	-2.90	1.15	1.30
19	A	846	CLA	C1D-ND	2.90	1.41	1.37
19	J	101	CLA	C1D-ND	2.90	1.41	1.37
19	A	826	CLA	MG-NA	2.90	2.13	2.06
19	B	807	CLA	OBD-CAD	-2.90	1.17	1.22
19	B	810	CLA	C1D-C2D	-2.89	1.39	1.45
19	A	833	CLA	C1C-NC	2.89	1.42	1.37
19	A	829	CLA	C3A-C2A	-2.89	1.46	1.54
19	A	814	CLA	MG-ND	-2.88	2.00	2.05
19	A	808	CLA	MG-ND	-2.87	2.00	2.05
18	4	313	CHL	C1B-C2B	2.87	1.50	1.43
19	A	850	CLA	C4C-C3C	-2.87	1.40	1.45
19	B	843	CLA	C1D-C2D	-2.87	1.39	1.45
18	2	316	CHL	C1B-C2B	2.87	1.50	1.43
19	B	838	CLA	C1C-NC	-2.87	1.33	1.37
19	B	822	CLA	C1B-NB	2.86	1.41	1.37
19	B	818	CLA	MG-NA	2.86	2.13	2.06
19	B	830	CLA	C1C-C2C	2.86	1.50	1.44
19	B	804	CLA	MG-NC	-2.86	1.99	2.06
19	F	303	CLA	MG-ND	-2.85	2.00	2.05
19	B	831	CLA	MG-NB	-2.85	2.00	2.05
19	B	823	CLA	C3A-C2A	-2.85	1.46	1.54
19	A	818	CLA	C3A-C2A	-2.85	1.46	1.54
19	B	839	CLA	C1D-C2D	-2.85	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	C1C-NC	-2.84	1.33	1.37
19	A	834	CLA	C1D-C2D	-2.84	1.39	1.45
19	2	311	CLA	MG-NA	-2.83	1.99	2.06
19	B	802	CLA	C1C-C2C	2.83	1.50	1.44
19	B	809	CLA	CHC-C4B	2.83	1.45	1.39
19	B	848	CLA	C1B-NB	2.82	1.41	1.37
19	A	827	CLA	C3A-C2A	2.82	1.62	1.54
19	B	841	CLA	O2A-C1	2.82	1.54	1.46
19	B	840	CLA	C1D-ND	2.82	1.41	1.37
19	B	803	CLA	C3B-C2B	-2.82	1.31	1.41
19	A	844	CLA	C1B-NB	2.82	1.41	1.37
19	B	832	CLA	MG-NC	-2.81	1.99	2.06
24	G	201	BCR	C7-C6	2.81	1.55	1.45
19	A	821	CLA	C1D-C2D	-2.81	1.39	1.45
19	A	805	CLA	MG-ND	-2.81	2.00	2.05
19	B	829	CLA	CHD-C1D	2.81	1.43	1.38
19	A	815	CLA	CHC-C1C	-2.81	1.32	1.38
19	B	844	CLA	CBA-CGA	-2.80	1.42	1.50
19	B	848	CLA	MG-NC	-2.79	1.99	2.06
18	2	316	CHL	CHD-C1D	2.79	1.43	1.38
19	G	203	CLA	C1D-C2D	-2.79	1.39	1.45
19	B	836	CLA	C1B-NB	2.78	1.41	1.37
19	B	822	CLA	CHD-C1D	2.78	1.43	1.38
19	A	831	CLA	C3D-C4D	-2.78	1.37	1.44
19	L	303	CLA	MG-NC	-2.78	1.99	2.06
19	4	311	CLA	MG-NA	-2.78	1.99	2.06
19	B	803	CLA	C1D-ND	2.77	1.41	1.37
19	B	846	CLA	C1C-NC	-2.77	1.33	1.37
19	2	312	CLA	MG-NA	-2.77	1.99	2.06
19	A	833	CLA	MG-NC	-2.77	1.99	2.06
18	1	606	CHL	C2C-C1C	2.76	1.50	1.44
19	G	202	CLA	C1C-NC	2.75	1.41	1.37
19	A	821	CLA	MG-NC	-2.75	1.99	2.06
19	B	845	CLA	CBC-CAC	-2.74	1.39	1.51
19	2	312	CLA	MG-ND	-2.74	2.00	2.05
19	3	314	CLA	C1C-C2C	2.74	1.49	1.44
19	B	837	CLA	C1C-C2C	2.74	1.49	1.44
19	A	821	CLA	C1B-NB	2.73	1.41	1.37
19	A	808	CLA	C1C-C2C	2.73	1.49	1.44
19	B	847	CLA	CHD-C4C	-2.73	1.33	1.39
19	A	811	CLA	MG-NB	-2.73	2.00	2.05
19	B	830	CLA	MG-NA	2.72	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	607	CLA	C1D-C2D	-2.72	1.40	1.45
19	L	303	CLA	C1D-C2D	-2.72	1.40	1.45
19	A	850	CLA	C3D-C4D	-2.71	1.38	1.44
19	B	827	CLA	C3D-C4D	-2.71	1.38	1.44
19	1	612	CLA	MG-NA	-2.68	1.99	2.06
19	B	801	CLA	C1B-NB	2.68	1.41	1.37
19	B	844	CLA	C1C-NC	-2.68	1.33	1.37
19	1	605	CLA	MG-NA	-2.67	1.99	2.06
19	A	823	CLA	C1D-C2D	-2.67	1.40	1.45
19	A	818	CLA	MG-NB	-2.67	2.00	2.05
18	3	315	CHL	C1D-C2D	-2.66	1.40	1.45
19	B	809	CLA	MG-NC	-2.66	2.00	2.06
19	3	312	CLA	C1C-C2C	2.65	1.49	1.44
19	A	818	CLA	MG-NA	2.65	2.12	2.06
19	A	819	CLA	OBD-CAD	-2.65	1.17	1.22
19	B	810	CLA	C3D-C4D	-2.64	1.38	1.44
19	A	813	CLA	MG-NC	-2.64	2.00	2.06
19	K	202	CLA	CHC-C1C	-2.64	1.33	1.38
18	2	316	CHL	C3D-C4D	-2.64	1.38	1.44
19	4	311	CLA	MG-NC	-2.64	2.00	2.06
19	A	822	CLA	C3A-C2A	-2.63	1.47	1.54
19	A	849	CLA	C1B-NB	2.62	1.41	1.37
19	3	301	CLA	MG-ND	-2.62	2.00	2.05
19	A	819	CLA	MG-NB	-2.62	2.00	2.05
19	B	823	CLA	C3D-C4D	-2.62	1.38	1.44
19	A	824	CLA	MG-NB	-2.62	2.00	2.05
18	1	606	CHL	C1B-NB	-2.62	1.34	1.37
19	3	307	CLA	MG-NC	-2.62	2.00	2.06
19	B	807	CLA	C1C-C2C	2.61	1.49	1.44
19	B	846	CLA	C1C-C2C	2.61	1.49	1.44
19	A	805	CLA	MG-NC	-2.60	2.00	2.06
19	B	847	CLA	C3A-C2A	-2.60	1.47	1.54
19	A	814	CLA	C4B-NB	2.60	1.41	1.37
19	B	830	CLA	MG-NB	-2.60	2.00	2.05
19	A	833	CLA	C1D-C2D	-2.60	1.40	1.45
19	F	303	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	851	CLA	CBB-CAB	-2.59	1.17	1.30
19	1	607	CLA	MG-NC	-2.59	2.00	2.06
19	4	317	CLA	C1C-NC	2.59	1.41	1.37
19	B	831	CLA	C1D-ND	2.59	1.41	1.37
19	A	850	CLA	CHD-C1D	2.58	1.43	1.38
19	A	833	CLA	CHC-C4B	2.58	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	839	CLA	C3D-C2D	2.58	1.46	1.39
19	L	304	CLA	CHC-C4B	2.57	1.45	1.39
19	A	817	CLA	MG-NA	-2.57	2.00	2.06
19	A	807	CLA	MG-NC	-2.57	2.00	2.06
19	A	829	CLA	C1C-NC	-2.57	1.34	1.37
18	4	313	CHL	C2C-C1C	2.57	1.50	1.44
19	G	203	CLA	C3D-C4D	-2.56	1.38	1.44
19	L	303	CLA	C3D-C4D	-2.56	1.38	1.44
19	2	301	CLA	MG-NC	-2.56	2.00	2.06
19	2	301	CLA	MG-NA	-2.56	2.00	2.06
19	A	827	CLA	CHD-C1D	2.56	1.43	1.38
19	3	307	CLA	C1C-C2C	2.56	1.49	1.44
19	2	311	CLA	MG-NC	-2.56	2.00	2.06
19	B	818	CLA	CHD-C1D	2.55	1.43	1.38
18	3	303	CHL	C1B-C2B	2.55	1.49	1.43
19	A	828	CLA	CAA-CBA	-2.54	1.44	1.52
19	K	202	CLA	MG-NC	-2.54	2.00	2.06
19	A	811	CLA	C1D-C2D	-2.53	1.40	1.45
19	A	833	CLA	CHD-C1D	2.53	1.43	1.38
19	B	822	CLA	MG-NB	-2.53	2.00	2.05
19	B	802	CLA	C4B-NB	2.52	1.40	1.37
19	L	303	CLA	C1C-C2C	2.51	1.49	1.44
19	K	202	CLA	C3A-C2A	-2.51	1.47	1.54
19	4	318	CLA	MG-NA	-2.50	2.00	2.06
19	B	845	CLA	MG-ND	-2.50	2.00	2.05
19	B	809	CLA	C1D-C2D	-2.50	1.40	1.45
19	B	819	CLA	MG-NA	2.50	2.12	2.06
19	G	202	CLA	MG-NA	-2.49	2.00	2.06
19	K	203	CLA	C1D-C2D	-2.49	1.40	1.45
19	A	836	CLA	CHD-C1D	2.49	1.43	1.38
19	1	602	CLA	C3D-C4D	-2.49	1.38	1.44
19	A	846	CLA	C3D-C2D	2.49	1.45	1.39
19	J	101	CLA	C1D-C2D	-2.49	1.40	1.45
19	B	821	CLA	MG-NB	-2.48	2.00	2.05
19	B	826	CLA	MG-ND	-2.48	2.00	2.05
18	2	316	CHL	C1D-C2D	-2.47	1.40	1.45
19	A	815	CLA	C1C-C2C	2.47	1.49	1.44
19	A	813	CLA	C1C-C2C	2.47	1.49	1.44
19	A	823	CLA	C3A-C2A	-2.47	1.47	1.54
19	B	802	CLA	OBD-CAD	-2.47	1.18	1.22
19	F	303	CLA	MG-NC	-2.46	2.00	2.06
19	A	805	CLA	CBC-CAC	-2.46	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	823	CLA	CHD-C1D	2.46	1.43	1.38
19	B	848	CLA	CHD-C1D	2.45	1.43	1.38
19	B	801	CLA	C3D-C4D	-2.45	1.38	1.44
19	A	822	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	829	CLA	C3D-C4D	-2.45	1.38	1.44
24	A	852	BCR	C24-C25	2.45	1.53	1.45
19	F	303	CLA	C1D-C2D	-2.44	1.40	1.45
19	A	805	CLA	CHD-C1D	2.44	1.43	1.38
19	B	801	CLA	C1D-C2D	-2.44	1.40	1.45
19	B	822	CLA	MG-ND	-2.44	2.01	2.05
19	A	849	CLA	C1D-C2D	-2.44	1.40	1.45
19	A	817	CLA	C1D-C2D	-2.43	1.40	1.45
19	B	841	CLA	CHD-C4C	-2.43	1.33	1.39
19	A	821	CLA	MG-ND	-2.43	2.01	2.05
19	B	843	CLA	C1B-C2B	-2.43	1.37	1.43
19	B	819	CLA	C1C-NC	2.43	1.41	1.37
24	A	838	BCR	C24-C25	2.43	1.53	1.45
19	A	836	CLA	C3D-C4D	-2.43	1.38	1.44
19	A	837	CLA	CBC-CAC	-2.42	1.40	1.51
19	1	602	CLA	C1B-NB	2.42	1.40	1.37
19	A	813	CLA	C1D-C2D	-2.42	1.40	1.45
19	B	820	CLA	MG-NB	-2.40	2.01	2.05
19	B	809	CLA	C1C-C2C	2.40	1.49	1.44
19	B	837	CLA	C3D-C4D	-2.40	1.38	1.44
19	B	827	CLA	CHD-C4C	-2.39	1.33	1.39
19	B	847	CLA	CHD-C1D	2.39	1.43	1.38
19	B	828	CLA	MG-ND	-2.39	2.01	2.05
19	K	202	CLA	C1B-NB	2.38	1.40	1.37
19	A	848	CLA	MG-NA	-2.38	2.00	2.06
19	B	809	CLA	CHC-C1C	-2.38	1.33	1.38
19	B	835	CLA	OBD-CAD	-2.38	1.18	1.22
22	4	303	A1LXP	C29-C19	2.38	1.63	1.56
19	B	827	CLA	C3A-C2A	-2.38	1.47	1.54
19	A	837	CLA	C1A-CHA	-2.38	1.33	1.43
19	4	317	CLA	MG-NC	-2.38	2.00	2.06
19	B	805	CLA	C3D-C4D	-2.38	1.38	1.44
19	A	826	CLA	C3B-C2B	-2.38	1.33	1.41
19	B	848	CLA	CHC-C1C	-2.37	1.33	1.38
19	B	819	CLA	C1D-C2D	-2.37	1.40	1.45
19	A	808	CLA	C3A-C2A	-2.37	1.47	1.54
19	A	819	CLA	C3A-C2A	-2.37	1.47	1.54
19	A	846	CLA	MG-ND	-2.37	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	849	CLA	C1D-ND	2.36	1.40	1.37
19	B	836	CLA	C3D-C4D	-2.36	1.38	1.44
19	K	203	CLA	MG-NA	-2.36	2.00	2.06
19	B	845	CLA	C1C-C2C	2.36	1.49	1.44
19	B	839	CLA	C1C-NC	2.36	1.41	1.37
19	B	803	CLA	CBB-CAB	-2.35	1.18	1.30
19	A	848	CLA	C3A-C2A	-2.35	1.47	1.54
19	B	848	CLA	MG-NA	-2.34	2.00	2.06
19	3	308	CLA	MG-NC	-2.34	2.00	2.06
19	A	827	CLA	MG-NB	-2.34	2.01	2.05
19	B	846	CLA	C1D-C2D	-2.34	1.40	1.45
18	3	315	CHL	C1B-C2B	2.34	1.48	1.43
19	A	828	CLA	C1D-C2D	-2.34	1.40	1.45
19	A	840	CLA	CHD-C4C	-2.34	1.33	1.39
22	4	303	A1LXP	C30-C31	2.33	1.56	1.53
19	A	836	CLA	CBC-CAC	-2.33	1.41	1.51
19	B	823	CLA	CBB-CAB	-2.33	1.18	1.30
19	B	808	CLA	C1D-ND	2.33	1.40	1.37
19	B	838	CLA	MG-NC	-2.33	2.00	2.06
22	1	616	A1LXP	C30-C31	-2.33	1.49	1.53
19	K	203	CLA	CBC-CAC	-2.32	1.41	1.51
18	2	315	CHL	C1B-C2B	2.32	1.48	1.43
19	B	829	CLA	CBC-CAC	-2.32	1.41	1.51
19	A	806	CLA	C3D-C2D	2.32	1.45	1.39
19	A	831	CLA	CHC-C4B	2.32	1.44	1.39
19	1	605	CLA	C1C-NC	2.31	1.41	1.37
19	A	816	CLA	CHB-C1B	2.31	1.44	1.39
19	3	304	CLA	C1B-NB	2.31	1.40	1.37
19	A	842	CLA	CHC-C4B	-2.31	1.34	1.39
19	1	602	CLA	C1C-C2C	2.31	1.49	1.44
19	B	807	CLA	CHC-C1C	-2.31	1.33	1.38
19	A	840	CLA	CHC-C4B	2.31	1.44	1.39
23	A	835	LHG	P-O6	-2.31	1.50	1.59
19	B	841	CLA	C1D-ND	2.30	1.40	1.37
19	B	847	CLA	C1D-C2D	-2.30	1.40	1.45
19	B	809	CLA	MG-NB	-2.30	2.01	2.05
18	4	319	CHL	C2C-C1C	2.30	1.49	1.44
19	K	202	CLA	C1D-C2D	-2.30	1.40	1.45
19	1	608	CLA	C1C-C2C	2.30	1.49	1.44
19	B	838	CLA	C3D-C4D	-2.30	1.39	1.44
19	B	809	CLA	C1D-ND	2.29	1.40	1.37
19	A	801	CLA	C2A-C1A	-2.29	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	813	CLA	CHC-C1C	-2.29	1.33	1.38
19	B	843	CLA	MG-ND	-2.29	2.01	2.05
19	4	311	CLA	CHD-C1D	2.29	1.42	1.38
18	2	313	CHL	C1B-NB	-2.29	1.35	1.37
19	A	848	CLA	OBD-CAD	-2.29	1.18	1.22
19	B	845	CLA	C1B-NB	2.28	1.40	1.37
19	B	824	CLA	C1A-CHA	-2.28	1.33	1.43
19	B	801	CLA	MG-ND	-2.28	2.01	2.05
18	3	303	CHL	C1B-NB	-2.28	1.35	1.37
19	A	843	CLA	C3D-C2D	2.28	1.45	1.39
19	B	838	CLA	C1D-C2D	-2.28	1.40	1.45
18	1	601	CHL	C1C-NC	-2.28	1.34	1.37
19	B	808	CLA	OBD-CAD	-2.27	1.18	1.22
18	4	319	CHL	C3B-C4B	2.27	1.48	1.42
19	1	607	CLA	C1B-NB	2.27	1.40	1.37
19	B	808	CLA	C1C-C2C	2.27	1.49	1.44
19	A	813	CLA	C3D-C4D	-2.26	1.39	1.44
19	4	307	CLA	MG-ND	-2.26	2.01	2.05
19	A	848	CLA	C3B-C2B	-2.26	1.33	1.41
18	3	315	CHL	C1C-NC	-2.26	1.34	1.37
19	B	834	CLA	MG-NA	2.25	2.11	2.06
19	A	801	CLA	C3D-C4D	-2.25	1.39	1.44
19	G	203	CLA	C1C-C2C	2.25	1.48	1.44
19	A	809	CLA	C3A-C2A	-2.24	1.48	1.54
22	4	303	A1LXP	C42-C1	2.24	1.53	1.45
19	F	306	CLA	MG-ND	-2.24	2.01	2.05
19	B	830	CLA	C3D-C2D	2.24	1.45	1.39
19	J	101	CLA	C3D-C4D	-2.24	1.39	1.44
19	A	811	CLA	MG-NC	-2.24	2.01	2.06
19	A	812	CLA	C1B-NB	2.24	1.40	1.37
19	B	807	CLA	CHC-C4B	2.24	1.44	1.39
19	3	304	CLA	C3A-C2A	-2.23	1.48	1.54
19	B	810	CLA	C1C-C2C	2.23	1.48	1.44
18	2	315	CHL	C2C-C1C	2.23	1.49	1.44
18	4	319	CHL	C1D-C2D	-2.23	1.40	1.45
19	B	807	CLA	C1B-NB	2.23	1.40	1.37
19	A	827	CLA	CBB-CAB	-2.23	1.19	1.30
19	3	301	CLA	C3D-C4D	-2.23	1.39	1.44
19	A	842	CLA	CHB-C1B	2.23	1.44	1.39
19	A	850	CLA	C1D-ND	2.23	1.40	1.37
19	1	608	CLA	MG-NC	-2.22	2.01	2.06
19	B	805	CLA	C1C-NC	-2.22	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	848	CLA	C3A-C2A	-2.22	1.48	1.54
19	B	802	CLA	C1B-NB	2.22	1.40	1.37
19	A	801	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	825	CLA	MG-NC	-2.22	2.01	2.06
19	3	312	CLA	C1C-NC	2.21	1.41	1.37
19	A	846	CLA	C1D-C2D	-2.20	1.41	1.45
19	A	814	CLA	C3A-C2A	2.20	1.60	1.54
19	1	605	CLA	C1C-C2C	2.20	1.48	1.44
19	2	311	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	805	CLA	C3D-C4D	-2.20	1.39	1.44
19	3	306	CLA	MG-NC	-2.20	2.01	2.06
19	A	825	CLA	C1D-C2D	-2.19	1.41	1.45
19	B	825	CLA	C1D-C2D	-2.19	1.41	1.45
19	A	826	CLA	C1C-NC	2.19	1.41	1.37
19	A	842	CLA	C2A-C1A	-2.19	1.47	1.52
18	3	315	CHL	C3D-C4D	-2.19	1.39	1.44
19	B	840	CLA	CHC-C1C	-2.18	1.34	1.38
19	A	848	CLA	C3D-C2D	2.18	1.45	1.39
19	B	836	CLA	C1D-C2D	-2.18	1.41	1.45
19	F	306	CLA	C3A-C2A	2.18	1.60	1.54
19	A	801	CLA	C1B-C2B	-2.17	1.38	1.43
19	B	838	CLA	CHD-C1D	2.17	1.42	1.38
19	H	201	CLA	CHD-C4C	-2.17	1.34	1.39
19	A	806	CLA	C1D-C2D	-2.17	1.41	1.45
19	B	832	CLA	C4C-C3C	-2.17	1.41	1.45
19	B	836	CLA	C3D-C2D	2.17	1.45	1.39
19	B	822	CLA	C1C-C2C	2.16	1.48	1.44
19	A	812	CLA	MG-NC	2.16	2.11	2.06
19	B	822	CLA	C1D-C2D	-2.16	1.41	1.45
19	A	817	CLA	C3D-C4D	-2.16	1.39	1.44
19	B	845	CLA	CHD-C4C	-2.16	1.34	1.39
19	A	849	CLA	MG-NC	-2.16	2.01	2.06
19	B	809	CLA	C3D-C4D	-2.16	1.39	1.44
19	B	828	CLA	C1D-ND	2.16	1.40	1.37
19	A	816	CLA	MG-NA	2.15	2.11	2.06
19	B	847	CLA	MG-NC	-2.15	2.01	2.06
19	B	840	CLA	C1D-C2D	-2.15	1.41	1.45
19	B	809	CLA	C3B-C2B	-2.15	1.33	1.41
19	G	202	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	812	CLA	C3A-C2A	-2.14	1.48	1.54
19	B	844	CLA	CBC-CAC	-2.14	1.41	1.51
19	K	202	CLA	CHD-C4C	-2.14	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	806	CLA	MG-NA	-2.14	2.01	2.06
19	4	311	CLA	C3D-C4D	-2.13	1.39	1.44
19	K	203	CLA	C3D-C4D	-2.13	1.39	1.44
19	B	823	CLA	C1D-C2D	-2.13	1.41	1.45
22	3	310	A1LXP	C30-C31	-2.13	1.49	1.53
19	H	201	CLA	C1D-C2D	-2.13	1.41	1.45
19	A	807	CLA	C1D-C2D	-2.13	1.41	1.45
19	A	824	CLA	C1B-NB	2.13	1.40	1.37
18	1	601	CHL	C1D-C2D	-2.13	1.41	1.45
19	1	603	CLA	C3A-C2A	-2.12	1.48	1.54
19	B	818	CLA	C1D-C2D	-2.12	1.41	1.45
19	B	821	CLA	CHD-C4C	-2.12	1.34	1.39
19	A	821	CLA	C3D-C4D	-2.12	1.39	1.44
19	A	815	CLA	MG-NC	-2.12	2.01	2.06
19	L	304	CLA	CHD-C4C	-2.12	1.34	1.39
19	B	825	CLA	CHC-C4B	2.11	1.44	1.39
19	A	809	CLA	MG-NC	-2.11	2.01	2.06
19	B	820	CLA	C2A-C1A	-2.11	1.47	1.52
19	A	813	CLA	CBC-CAC	-2.11	1.42	1.51
18	4	319	CHL	C3D-C4D	-2.11	1.39	1.44
19	A	802	CLA	CHC-C4B	2.11	1.44	1.39
18	4	313	CHL	C3D-C4D	-2.11	1.39	1.44
19	A	815	CLA	CBC-CAC	-2.10	1.42	1.51
19	B	826	CLA	CHB-C1B	2.10	1.44	1.39
19	B	846	CLA	O2D-CGD	-2.10	1.28	1.33
19	B	837	CLA	C3D-C2D	2.10	1.44	1.39
19	A	812	CLA	CHB-C1B	2.10	1.44	1.39
19	G	203	CLA	CBB-CAB	-2.10	1.19	1.30
19	A	829	CLA	C1B-NB	2.10	1.40	1.37
19	3	304	CLA	CHC-C1C	-2.09	1.34	1.38
18	3	303	CHL	C1D-ND	2.09	1.40	1.37
19	A	802	CLA	C4B-NB	2.09	1.40	1.37
18	1	601	CHL	C3D-C4D	-2.09	1.39	1.44
18	4	313	CHL	CHC-C1C	2.09	1.42	1.38
19	B	844	CLA	CAA-CBA	-2.09	1.46	1.52
19	B	826	CLA	C3B-C2B	-2.09	1.34	1.41
19	B	842	CLA	CHD-C1D	2.09	1.42	1.38
19	3	307	CLA	C3D-C4D	-2.09	1.39	1.44
19	A	817	CLA	C1C-NC	2.08	1.40	1.37
19	B	827	CLA	MG-NC	-2.08	2.01	2.06
18	3	315	CHL	CHD-C1D	2.08	1.42	1.38
19	B	820	CLA	C1B-NB	-2.08	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	835	CLA	MG-NC	-2.08	2.01	2.06
19	B	819	CLA	C2A-C1A	-2.08	1.47	1.52
19	A	810	CLA	CHD-C1D	2.08	1.42	1.38
19	3	312	CLA	C3D-C4D	-2.08	1.39	1.44
19	A	837	CLA	CHD-C1D	2.08	1.42	1.38
19	3	308	CLA	C1D-C2D	-2.07	1.41	1.45
19	G	203	CLA	C3A-C2A	-2.07	1.48	1.54
19	B	819	CLA	CHB-C1B	2.07	1.44	1.39
19	A	810	CLA	C1D-C2D	-2.07	1.41	1.45
19	A	843	CLA	C3D-C4D	-2.07	1.39	1.44
19	A	824	CLA	C3D-C4D	-2.06	1.39	1.44
19	B	801	CLA	C3A-C2A	-2.06	1.48	1.54
18	2	315	CHL	CHD-C1D	2.06	1.42	1.38
19	B	842	CLA	CHB-C1B	2.06	1.44	1.39
19	B	841	CLA	MG-NC	-2.06	2.01	2.06
19	L	304	CLA	C3D-C2D	2.06	1.44	1.39
19	A	849	CLA	C3D-C4D	-2.06	1.39	1.44
19	1	602	CLA	C1D-C2D	-2.06	1.41	1.45
19	A	844	CLA	C1D-C2D	-2.06	1.41	1.45
19	B	837	CLA	C1D-C2D	-2.06	1.41	1.45
19	1	603	CLA	C3D-C4D	-2.06	1.39	1.44
19	B	847	CLA	C1D-ND	-2.05	1.35	1.37
19	B	841	CLA	C1D-C2D	-2.05	1.41	1.45
19	A	823	CLA	C3D-C4D	-2.05	1.39	1.44
19	G	202	CLA	MG-NC	-2.05	2.01	2.06
19	3	301	CLA	C1D-C2D	-2.05	1.41	1.45
27	A	830	CL0	C4B-NB	-2.04	1.35	1.37
19	A	837	CLA	CHD-C4C	-2.04	1.34	1.39
19	A	810	CLA	CBB-CAB	-2.04	1.20	1.30
19	A	843	CLA	MG-NB	-2.04	2.01	2.05
19	B	827	CLA	CHD-C1D	2.04	1.42	1.38
19	A	822	CLA	MG-ND	-2.04	2.01	2.05
18	2	315	CHL	C1C-NC	-2.03	1.34	1.37
19	4	317	CLA	C1D-C2D	-2.03	1.41	1.45
19	B	820	CLA	C3B-C2B	-2.03	1.34	1.41
19	B	831	CLA	CBC-CAC	-2.03	1.42	1.51
18	1	601	CHL	C3D-C2D	2.03	1.44	1.39
19	A	846	CLA	CHC-C4B	2.03	1.44	1.39
19	3	307	CLA	C1D-C2D	-2.03	1.41	1.45
19	B	843	CLA	CHD-C1D	2.03	1.42	1.38
19	A	851	CLA	C3B-C2B	-2.03	1.34	1.41
19	A	829	CLA	MG-NA	2.02	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	605	CLA	MG-NC	-2.02	2.01	2.06
19	B	833	CLA	C4C-C3C	-2.02	1.41	1.45
19	A	828	CLA	C1C-C2C	2.02	1.48	1.44
19	B	831	CLA	OBD-CAD	-2.02	1.19	1.22
19	3	306	CLA	C1D-C2D	-2.02	1.41	1.45
24	B	815	BCR	C16-C15	-2.02	1.30	1.36
18	3	303	CHL	CHC-C1C	2.02	1.42	1.38
18	2	315	CHL	C3D-C4D	-2.02	1.39	1.44
19	1	605	CLA	C3D-C4D	-2.02	1.39	1.44
19	3	306	CLA	MG-NA	-2.02	2.01	2.06
19	B	840	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	838	CLA	CBB-CAB	-2.01	1.20	1.30
24	G	201	BCR	C24-C25	2.01	1.52	1.45
19	3	302	CLA	C1D-C2D	-2.01	1.41	1.45
19	B	801	CLA	C1C-NC	-2.00	1.34	1.37
19	4	318	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	842	CLA	C1D-C2D	-2.00	1.41	1.45
19	A	840	CLA	C1C-C2C	2.00	1.48	1.44

All (1273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	606	CHL	C4A-NA-C1A	13.18	112.63	106.71
19	G	203	CLA	C4A-NA-C1A	-12.86	100.92	106.71
18	2	316	CHL	C4A-NA-C1A	12.82	112.47	106.71
19	K	202	CLA	C4A-NA-C1A	-12.13	101.25	106.71
19	A	813	CLA	C4A-NA-C1A	-12.08	101.28	106.71
19	B	848	CLA	C4A-NA-C1A	-12.02	101.30	106.71
18	4	319	CHL	C4A-NA-C1A	11.59	111.92	106.71
18	1	601	CHL	C4A-NA-C1A	11.24	111.76	106.71
18	3	303	CHL	C4A-NA-C1A	9.99	111.20	106.71
19	B	832	CLA	C4A-NA-C1A	-9.74	102.33	106.71
19	A	837	CLA	C4A-NA-C1A	-9.58	102.40	106.71
19	B	806	CLA	C1-C2-C3	9.55	142.56	126.04
19	A	817	CLA	C4A-NA-C1A	-9.39	102.48	106.71
18	4	313	CHL	C4A-NA-C1A	8.84	110.68	106.71
18	3	315	CHL	C4A-NA-C1A	8.79	110.66	106.71
19	A	828	CLA	C4A-NA-C1A	-8.77	102.77	106.71
19	B	824	CLA	C4A-NA-C1A	-8.66	102.81	106.71
19	A	810	CLA	C4A-NA-C1A	-8.41	102.92	106.71
19	B	827	CLA	C4A-NA-C1A	-8.40	102.93	106.71
18	2	315	CHL	C4A-NA-C1A	8.39	110.48	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	823	CLA	C4A-NA-C1A	-8.28	102.98	106.71
18	2	313	CHL	C4A-NA-C1A	8.25	110.42	106.71
27	A	830	CL0	C4A-NA-C1A	8.23	110.41	106.71
21	1	615	XAT	O4-C5-C4	-8.00	107.37	113.38
19	B	847	CLA	C4A-NA-C1A	-7.97	103.12	106.71
19	B	821	CLA	C4A-NA-C1A	-7.84	103.18	106.71
19	B	828	CLA	C4A-NA-C1A	-7.82	103.19	106.71
19	B	806	CLA	C4A-NA-C1A	-7.81	103.20	106.71
19	A	848	CLA	C4A-NA-C1A	-7.78	103.21	106.71
19	A	826	CLA	C4A-NA-C1A	-7.74	103.22	106.71
19	B	808	CLA	C4A-NA-C1A	-7.62	103.28	106.71
19	B	805	CLA	C4A-NA-C1A	-7.58	103.30	106.71
19	F	303	CLA	C4A-NA-C1A	-7.56	103.31	106.71
19	A	840	CLA	CHD-C1D-ND	-7.55	117.51	124.45
19	B	842	CLA	CHD-C1D-ND	-7.48	117.58	124.45
19	A	851	CLA	C4A-NA-C1A	-7.38	103.39	106.71
19	B	840	CLA	C4A-NA-C1A	-7.38	103.39	106.71
19	A	829	CLA	CHD-C1D-ND	-7.38	117.67	124.45
19	K	203	CLA	C4A-NA-C1A	-7.32	103.42	106.71
19	B	839	CLA	C4A-NA-C1A	-7.26	103.44	106.71
19	A	809	CLA	CHD-C1D-ND	-7.24	117.80	124.45
19	A	801	CLA	C1-C2-C3	-7.19	113.61	126.04
19	3	306	CLA	C4A-NA-C1A	-7.09	103.52	106.71
19	B	818	CLA	O2A-C1-C2	7.09	127.27	108.64
19	A	849	CLA	C4A-NA-C1A	-7.04	103.54	106.71
19	3	312	CLA	C4A-NA-C1A	-6.95	103.58	106.71
19	B	835	CLA	CHD-C1D-ND	-6.95	118.07	124.45
19	A	843	CLA	C4A-NA-C1A	-6.93	103.59	106.71
19	B	825	CLA	CHD-C1D-ND	-6.91	118.10	124.45
19	B	803	CLA	CHD-C1D-ND	-6.90	118.11	124.45
19	1	603	CLA	C4A-NA-C1A	-6.86	103.62	106.71
19	4	311	CLA	C4A-NA-C1A	-6.86	103.62	106.71
19	A	814	CLA	CHD-C1D-ND	-6.81	118.20	124.45
19	B	826	CLA	C4A-NA-C1A	-6.79	103.66	106.71
19	A	815	CLA	C4A-NA-C1A	-6.74	103.67	106.71
19	B	830	CLA	C4A-NA-C1A	-6.69	103.70	106.71
19	B	801	CLA	C4A-NA-C1A	-6.66	103.71	106.71
19	A	842	CLA	CHD-C1D-ND	-6.64	118.35	124.45
19	A	842	CLA	C4A-NA-C1A	-6.63	103.73	106.71
19	B	818	CLA	CHD-C1D-ND	-6.50	118.48	124.45
19	3	302	CLA	C4A-NA-C1A	-6.49	103.79	106.71
19	B	845	CLA	CHD-C1D-ND	-6.49	118.49	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	CHD-C1D-ND	-6.48	118.50	124.45
19	A	834	CLA	C1-C2-C3	-6.47	114.85	126.04
19	A	802	CLA	C4A-NA-C1A	-6.36	103.84	106.71
19	2	312	CLA	C4A-NA-C1A	-6.35	103.85	106.71
19	A	808	CLA	C4A-NA-C1A	-6.33	103.86	106.71
19	A	848	CLA	CHD-C1D-ND	-6.30	118.67	124.45
19	A	819	CLA	C4A-NA-C1A	-6.30	103.88	106.71
19	A	832	CLA	CHD-C1D-ND	-6.27	118.69	124.45
19	B	846	CLA	CHD-C1D-ND	-6.26	118.70	124.45
19	B	834	CLA	CHD-C1D-ND	-6.19	118.77	124.45
19	B	809	CLA	CHD-C1D-ND	-6.16	118.80	124.45
19	B	844	CLA	C4A-NA-C1A	-6.15	103.94	106.71
19	B	830	CLA	CHD-C1D-ND	-6.10	118.84	124.45
19	A	820	CLA	CHD-C1D-ND	-6.05	118.89	124.45
19	B	829	CLA	C4A-NA-C1A	-6.03	104.00	106.71
18	1	601	CHL	C2B-C1B-NB	-6.03	106.19	110.23
19	A	846	CLA	CHD-C1D-ND	-6.00	118.94	124.45
19	B	840	CLA	CHD-C1D-ND	-5.98	118.96	124.45
19	A	827	CLA	CHD-C1D-ND	-5.96	118.97	124.45
19	A	844	CLA	C4A-NA-C1A	-5.96	104.03	106.71
19	B	845	CLA	C4A-NA-C1A	-5.96	104.03	106.71
19	L	303	CLA	C4A-NA-C1A	-5.95	104.03	106.71
19	3	304	CLA	C4A-NA-C1A	-5.93	104.04	106.71
19	A	826	CLA	CHD-C1D-ND	-5.87	119.06	124.45
19	B	823	CLA	C4A-NA-C1A	-5.85	104.07	106.71
19	A	831	CLA	CHD-C1D-ND	-5.84	119.09	124.45
19	B	810	CLA	C4A-NA-C1A	-5.83	104.08	106.71
19	A	836	CLA	CHD-C1D-ND	-5.83	119.09	124.45
19	B	844	CLA	CHD-C1D-ND	-5.79	119.13	124.45
19	1	607	CLA	C4A-NA-C1A	-5.78	104.11	106.71
19	B	846	CLA	C4A-NA-C1A	-5.78	104.11	106.71
23	A	835	LHG	O6-P-O5	5.78	131.64	109.07
19	G	202	CLA	CHD-C1D-ND	-5.77	119.15	124.45
19	A	817	CLA	CHD-C1D-ND	-5.76	119.16	124.45
19	F	306	CLA	CHD-C1D-ND	-5.76	119.16	124.45
19	1	602	CLA	C1-C2-C3	-5.76	116.08	126.04
19	B	821	CLA	CHD-C1D-ND	-5.70	119.21	124.45
19	B	831	CLA	C4A-NA-C1A	-5.65	104.17	106.71
19	B	848	CLA	CHD-C1D-ND	-5.63	119.28	124.45
18	3	303	CHL	CHD-C1D-ND	-5.63	119.28	124.45
18	1	606	CHL	C2B-C1B-NB	-5.63	106.46	110.23
19	4	307	CLA	C4A-NA-C1A	-5.62	104.18	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	802	CLA	CHD-C1D-ND	-5.61	119.30	124.45
19	A	808	CLA	CHD-C1D-ND	-5.60	119.31	124.45
21	1	618	XAT	C27-C28-C29	5.59	134.20	125.53
19	B	807	CLA	C4A-NA-C1A	-5.56	104.20	106.71
19	A	805	CLA	CHD-C1D-ND	-5.52	119.38	124.45
19	A	819	CLA	CHD-C1D-ND	-5.52	119.39	124.45
19	A	818	CLA	O2A-C1-C2	-5.50	94.18	108.64
19	4	317	CLA	CHD-C1D-ND	-5.46	119.43	124.45
19	4	318	CLA	CHD-C1D-ND	-5.46	119.43	124.45
19	A	850	CLA	CHD-C1D-ND	-5.46	119.44	124.45
19	B	848	CLA	C2C-C1C-NC	5.46	115.08	109.97
19	B	821	CLA	CAA-C2A-C1A	-5.42	100.14	112.14
19	B	833	CLA	C1D-ND-C4D	-5.41	102.49	106.33
19	2	301	CLA	C4A-NA-C1A	-5.40	104.28	106.71
19	L	305	CLA	C4A-NA-C1A	-5.40	104.28	106.71
19	A	823	CLA	CHD-C1D-ND	-5.40	119.49	124.45
19	3	314	CLA	C4A-NA-C1A	-5.39	104.28	106.71
19	B	831	CLA	CHD-C1D-ND	-5.39	119.50	124.45
18	3	315	CHL	C3B-C4B-NB	-5.36	105.54	110.52
19	A	806	CLA	CHD-C1D-ND	-5.36	119.53	124.45
19	A	806	CLA	C4A-NA-C1A	-5.32	104.32	106.71
19	A	814	CLA	C4A-NA-C1A	-5.31	104.32	106.71
19	4	317	CLA	C1D-ND-C4D	-5.29	102.58	106.33
19	4	307	CLA	C1D-ND-C4D	-5.28	102.59	106.33
19	A	834	CLA	CHD-C1D-ND	-5.27	119.61	124.45
19	B	825	CLA	C4A-NA-C1A	-5.25	104.34	106.71
18	1	606	CHL	C3B-C4B-NB	-5.25	105.64	110.52
19	A	850	CLA	C4A-NA-C1A	-5.22	104.36	106.71
18	3	303	CHL	C3B-C4B-NB	-5.21	105.68	110.52
19	A	836	CLA	C4A-NA-C1A	-5.21	104.36	106.71
19	B	841	CLA	CHD-C1D-ND	-5.20	119.67	124.45
19	B	832	CLA	CHD-C1D-ND	-5.20	119.68	124.45
19	B	836	CLA	CHD-C1D-ND	-5.19	119.68	124.45
21	2	306	XAT	O24-C25-C24	-5.19	109.48	113.38
19	3	301	CLA	C4A-NA-C1A	-5.19	104.37	106.71
19	3	314	CLA	CHD-C1D-ND	-5.19	119.69	124.45
19	B	801	CLA	C2C-C1C-NC	5.17	114.82	109.97
19	4	318	CLA	C4A-NA-C1A	-5.17	104.38	106.71
19	B	803	CLA	C1D-ND-C4D	-5.15	102.67	106.33
19	B	843	CLA	C4A-NA-C1A	-5.13	104.40	106.71
19	2	311	CLA	C4A-NA-C1A	-5.11	104.41	106.71
21	1	615	XAT	O24-C25-C24	-5.09	109.56	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	812	CLA	CHD-C1D-ND	-5.08	119.78	124.45
19	B	826	CLA	CHD-C1D-ND	-5.08	119.79	124.45
19	A	849	CLA	C2C-C1C-NC	5.07	114.72	109.97
19	B	835	CLA	C1D-ND-C4D	-5.06	102.74	106.33
19	A	801	CLA	C1D-ND-C4D	-5.06	102.74	106.33
19	A	836	CLA	CAA-C2A-C1A	-5.06	95.40	111.97
19	B	837	CLA	C2C-C1C-NC	5.05	114.70	109.97
19	A	846	CLA	C4A-NA-C1A	-5.04	104.44	106.71
19	A	840	CLA	C4A-NA-C1A	-5.04	104.44	106.71
19	B	806	CLA	CHD-C1D-ND	-5.04	119.82	124.45
19	A	837	CLA	CHD-C1D-ND	-5.02	119.84	124.45
19	B	802	CLA	C1-C2-C3	-4.99	117.42	126.04
19	2	311	CLA	CHD-C1D-ND	-4.99	119.87	124.45
18	2	315	CHL	C3B-C4B-NB	-4.98	105.89	110.52
19	A	821	CLA	CHD-C1D-ND	-4.98	119.88	124.45
19	A	811	CLA	C4A-NA-C1A	-4.97	104.47	106.71
19	B	832	CLA	C2C-C1C-NC	4.95	114.61	109.97
21	1	618	XAT	O24-C25-C24	-4.95	109.67	113.38
19	A	814	CLA	C2C-C1C-NC	4.95	114.61	109.97
19	A	818	CLA	C4D-CHA-C1A	4.94	127.27	121.25
19	A	851	CLA	C2C-C1C-NC	4.94	114.60	109.97
19	A	816	CLA	CHD-C1D-ND	-4.88	119.97	124.45
19	B	833	CLA	CHD-C1D-ND	-4.86	119.98	124.45
19	4	307	CLA	CHD-C1D-ND	-4.86	119.99	124.45
19	B	802	CLA	CHD-C1D-ND	-4.85	119.99	124.45
19	A	832	CLA	CHB-C1B-NB	-4.83	119.14	124.26
19	A	809	CLA	C1-C2-C3	-4.83	117.69	126.04
19	B	803	CLA	C4A-NA-C1A	-4.83	104.53	106.71
19	K	202	CLA	C2C-C1C-NC	4.82	114.49	109.97
19	3	312	CLA	CHD-C1D-ND	-4.82	120.02	124.45
19	B	837	CLA	C4A-NA-C1A	-4.81	104.54	106.71
18	4	313	CHL	CHD-C1D-ND	-4.81	120.04	124.45
19	B	822	CLA	CHD-C1D-ND	-4.81	120.04	124.45
18	2	316	CHL	C2B-C1B-NB	-4.80	107.01	110.23
19	A	822	CLA	CHD-C1D-ND	-4.78	120.06	124.45
18	4	313	CHL	C3B-C4B-NB	-4.77	106.09	110.52
19	A	825	CLA	CHD-C1D-ND	-4.77	120.07	124.45
19	A	833	CLA	C4A-NA-C1A	-4.76	104.56	106.71
19	A	805	CLA	CHB-C1B-NB	-4.75	119.23	124.26
21	1	615	XAT	C7-C8-C9	4.75	132.89	125.53
19	L	304	CLA	CHD-C1D-ND	-4.74	120.10	124.45
19	G	202	CLA	C1D-ND-C4D	-4.74	102.97	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	301	CLA	CHB-C1B-NB	-4.72	119.26	124.26
19	B	827	CLA	CHD-C1D-ND	-4.72	120.12	124.45
19	B	838	CLA	C4A-NA-C1A	-4.72	104.59	106.71
19	B	832	CLA	CAA-C2A-C1A	-4.71	96.55	111.97
19	4	314	CLA	CHD-C1D-ND	-4.69	120.15	124.45
19	A	832	CLA	C1D-ND-C4D	-4.67	103.02	106.33
19	B	819	CLA	CHD-C1D-ND	-4.67	120.16	124.45
19	B	801	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	4	314	CLA	C4A-NA-C1A	-4.65	104.62	106.71
19	1	608	CLA	C4A-NA-C1A	-4.63	104.63	106.71
19	B	841	CLA	O2A-C1-C2	4.62	120.79	108.64
19	B	808	CLA	CHD-C1D-ND	-4.61	120.21	124.45
23	A	835	LHG	O4-P-O6	-4.61	86.33	107.75
18	2	313	CHL	C3B-C4B-NB	-4.61	106.24	110.52
19	A	821	CLA	CAA-CBA-CGA	-4.60	99.81	113.25
19	A	813	CLA	C2C-C1C-NC	4.59	114.27	109.97
19	B	825	CLA	CHB-C1B-NB	-4.58	119.41	124.26
19	B	805	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	B	825	CLA	C1D-ND-C4D	-4.56	103.10	106.33
18	2	313	CHL	CHD-C1D-ND	-4.55	120.27	124.45
18	3	303	CHL	C4D-CHA-C1A	4.55	126.79	121.25
19	A	819	CLA	C1D-ND-C4D	-4.55	103.10	106.33
19	L	304	CLA	C4A-NA-C1A	-4.53	104.67	106.71
19	B	842	CLA	C1D-ND-C4D	-4.52	103.12	106.33
27	A	830	CL0	CHC-C4B-NB	4.52	129.04	124.26
19	B	837	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
19	A	843	CLA	CHB-C1B-NB	-4.50	119.49	124.26
19	1	612	CLA	CHD-C1D-ND	-4.50	120.32	124.45
19	B	843	CLA	C3B-C4B-NB	-4.48	106.36	110.52
19	B	841	CLA	C4A-NA-C1A	-4.48	104.69	106.71
19	A	831	CLA	C4A-NA-C1A	-4.47	104.70	106.71
18	2	313	CHL	C4D-CHA-C1A	4.45	126.66	121.25
18	2	315	CHL	CHD-C1D-ND	-4.43	120.38	124.45
19	B	831	CLA	O2A-C1-C2	-4.38	97.12	108.64
19	H	201	CLA	C4A-NA-C1A	-4.37	104.74	106.71
19	A	842	CLA	C1D-ND-C4D	-4.36	103.24	106.33
19	A	801	CLA	C4A-NA-C1A	-4.36	104.75	106.71
19	1	602	CLA	C4A-NA-C1A	-4.36	104.75	106.71
19	A	808	CLA	C1D-ND-C4D	-4.35	103.24	106.33
19	A	819	CLA	C1-C2-C3	-4.35	118.52	126.04
19	1	608	CLA	CHD-C1D-ND	-4.34	120.47	124.45
19	A	818	CLA	CHD-C1D-ND	-4.32	120.48	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	843	CLA	CHC-C4B-NB	-4.31	119.69	124.26
18	4	313	CHL	C2B-C1B-NB	-4.30	107.35	110.23
19	A	809	CLA	C4A-NA-C1A	-4.29	104.78	106.71
19	A	833	CLA	CHD-C1D-ND	-4.29	120.52	124.45
19	1	603	CLA	CHD-C1D-ND	-4.28	120.52	124.45
19	A	849	CLA	CHD-C1D-ND	-4.27	120.53	124.45
19	A	802	CLA	O2A-C1-C2	4.26	119.84	108.64
19	B	804	CLA	CHD-C1D-ND	-4.26	120.54	124.45
19	A	824	CLA	CHB-C1B-NB	-4.25	119.75	124.26
19	3	301	CLA	CHD-C1D-ND	-4.25	120.55	124.45
19	A	823	CLA	CMC-C2C-C1C	4.25	131.51	125.04
19	B	845	CLA	C1D-ND-C4D	-4.23	103.33	106.33
19	A	815	CLA	CMC-C2C-C1C	4.23	131.49	125.04
19	B	820	CLA	CHD-C1D-ND	-4.23	120.57	124.45
19	B	829	CLA	C2C-C1C-NC	4.22	113.93	109.97
19	B	836	CLA	C4A-NA-C1A	-4.22	104.81	106.71
19	A	851	CLA	O2A-C1-C2	4.21	119.71	108.64
19	B	840	CLA	CMC-C2C-C1C	4.20	131.44	125.04
19	A	832	CLA	C2A-C3A-C4A	4.20	108.65	101.87
19	B	838	CLA	CHD-C1D-ND	-4.20	120.59	124.45
18	3	315	CHL	CHD-C1D-ND	-4.19	120.61	124.45
19	2	310	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
19	A	811	CLA	CHD-C1D-ND	-4.18	120.62	124.45
19	4	318	CLA	C1D-ND-C4D	-4.16	103.38	106.33
19	3	304	CLA	CHB-C1B-NB	-4.16	119.85	124.26
19	A	818	CLA	C4A-NA-C1A	-4.16	104.84	106.71
19	G	202	CLA	C4A-NA-C1A	-4.15	104.84	106.71
19	H	201	CLA	CMC-C2C-C1C	4.14	131.34	125.04
19	1	602	CLA	O2A-C1-C2	4.13	119.48	108.64
19	B	808	CLA	C2C-C1C-NC	4.12	113.83	109.97
19	B	824	CLA	C1-C2-C3	-4.11	118.93	126.04
18	2	315	CHL	C2B-C1B-NB	-4.11	107.48	110.23
19	B	818	CLA	C2C-C1C-NC	4.10	113.81	109.97
19	A	809	CLA	CHB-C1B-NB	-4.10	119.92	124.26
19	B	833	CLA	C4A-NA-C1A	-4.10	104.86	106.71
19	F	303	CLA	CHD-C1D-ND	-4.09	120.69	124.45
19	A	822	CLA	C4A-NA-C1A	-4.09	104.87	106.71
18	3	303	CHL	C2B-C1B-NB	-4.08	107.50	110.23
19	K	202	CLA	CHA-C1A-NA	-4.06	117.10	126.40
19	B	807	CLA	CHD-C1D-ND	-4.06	120.72	124.45
19	1	602	CLA	CHD-C1D-ND	-4.05	120.73	124.45
19	B	842	CLA	C2D-C1D-ND	4.05	113.09	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	839	CLA	CHD-C1D-ND	-4.05	120.74	124.45
19	A	809	CLA	C1D-ND-C4D	-4.04	103.47	106.33
19	1	612	CLA	C4A-NA-C1A	-4.04	104.89	106.71
19	B	841	CLA	C4D-CHA-C1A	4.03	126.16	121.25
19	A	807	CLA	CHD-C1D-ND	-4.03	120.75	124.45
19	B	805	CLA	C2C-C1C-NC	4.03	113.75	109.97
19	3	307	CLA	CHD-C1D-ND	-4.03	120.75	124.45
19	B	802	CLA	C4A-NA-C1A	-4.03	104.89	106.71
19	1	602	CLA	CHB-C1B-NB	-4.03	120.00	124.26
23	1	617	LHG	O6-P-O5	4.03	124.79	109.07
19	B	830	CLA	C1-C2-C3	-4.02	119.08	126.04
19	L	305	CLA	C2C-C1C-NC	4.02	113.74	109.97
19	B	831	CLA	C1D-ND-C4D	-4.02	103.48	106.33
19	B	842	CLA	C4A-NA-C1A	-4.01	104.90	106.71
19	A	810	CLA	CHD-C1D-ND	-4.01	120.77	124.45
19	A	828	CLA	C3A-C2A-C1A	-4.00	95.35	101.34
19	B	829	CLA	CHD-C1D-ND	-3.99	120.78	124.45
18	4	319	CHL	CHB-C4A-NA	3.98	130.02	124.51
19	B	824	CLA	CHD-C1D-ND	-3.98	120.80	124.45
19	A	805	CLA	C1D-ND-C4D	-3.98	103.51	106.33
19	A	844	CLA	CHD-C1D-ND	-3.98	120.80	124.45
19	A	807	CLA	CHB-C1B-NB	-3.97	120.05	124.26
29	B	817	DGD	O5D-C6D-C5D	-3.92	101.79	109.05
19	1	603	CLA	C1-C2-C3	-3.92	119.27	126.04
19	F	306	CLA	C1D-ND-C4D	-3.91	103.56	106.33
19	K	203	CLA	CHA-C1A-NA	-3.90	117.47	126.40
19	J	101	CLA	CHD-C1D-ND	-3.88	120.89	124.45
19	A	843	CLA	C2C-C1C-NC	3.88	113.61	109.97
19	B	802	CLA	C2C-C1C-NC	3.88	113.61	109.97
19	A	801	CLA	CHD-C1D-ND	-3.88	120.89	124.45
19	B	822	CLA	C4A-NA-C1A	-3.88	104.96	106.71
19	3	302	CLA	CHD-C1D-ND	-3.87	120.90	124.45
19	A	822	CLA	C1-C2-C3	-3.87	119.35	126.04
19	A	810	CLA	C2C-C1C-NC	3.87	113.59	109.97
19	2	301	CLA	CHD-C1D-ND	-3.86	120.91	124.45
19	B	831	CLA	CHB-C1B-NB	-3.86	120.17	124.26
19	A	815	CLA	C1D-ND-C4D	-3.85	103.60	106.33
19	B	821	CLA	CHB-C1B-NB	-3.84	120.20	124.26
19	B	828	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
19	H	201	CLA	C2C-C1C-NC	3.82	113.55	109.97
19	1	607	CLA	CAA-C2A-C3A	-3.82	102.31	112.78
18	2	313	CHL	CHC-C1C-NC	3.81	129.99	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	606	CHL	CHD-C1D-ND	-3.81	120.96	124.45
19	A	818	CLA	CHB-C1B-NB	-3.80	120.24	124.26
18	2	316	CHL	CHB-C4A-NA	3.78	129.74	124.51
19	B	818	CLA	CGD-CBD-CAD	3.78	122.97	110.73
19	L	303	CLA	CHD-C1D-ND	-3.78	120.98	124.45
19	A	829	CLA	C1-C2-C3	-3.77	119.52	126.04
19	A	824	CLA	CHD-C1D-ND	-3.77	120.99	124.45
19	A	802	CLA	C1D-ND-C4D	-3.75	103.67	106.33
19	A	821	CLA	C4A-NA-C1A	-3.74	105.02	106.71
19	A	810	CLA	CHA-C1A-NA	-3.74	117.84	126.40
19	1	605	CLA	CHD-C1D-ND	-3.74	121.02	124.45
19	A	801	CLA	O2A-C1-C2	3.73	118.45	108.64
19	A	832	CLA	CMA-C3A-C4A	-3.73	101.75	111.77
19	4	311	CLA	CHB-C1B-NB	-3.72	120.32	124.26
19	B	825	CLA	C4D-CHA-C1A	3.71	125.77	121.25
19	3	307	CLA	C4A-NA-C1A	-3.71	105.04	106.71
19	A	820	CLA	C4A-NA-C1A	-3.71	105.04	106.71
18	3	303	CHL	CHC-C1C-NC	3.70	129.82	124.20
19	A	846	CLA	C2C-C1C-NC	3.70	113.44	109.97
27	A	830	CL0	O2A-C1-C2	-3.70	98.92	108.64
19	A	843	CLA	CHD-C1D-ND	-3.68	121.07	124.45
19	B	821	CLA	CHA-C1A-NA	-3.67	117.99	126.40
19	A	802	CLA	C1-C2-C3	-3.67	119.70	126.04
19	A	828	CLA	CHD-C1D-ND	-3.66	121.09	124.45
19	B	806	CLA	C2C-C1C-NC	3.66	113.40	109.97
19	B	822	CLA	C2C-C1C-NC	3.65	113.39	109.97
27	A	830	CL0	C1D-ND-C4D	3.65	108.93	106.33
19	1	605	CLA	C4A-NA-C1A	-3.65	105.06	106.71
19	H	201	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	A	828	CLA	CHA-C1A-NA	-3.65	118.04	126.40
19	A	817	CLA	C2C-C1C-NC	3.65	113.39	109.97
19	A	823	CLA	CHA-C1A-NA	-3.65	118.05	126.40
18	4	319	CHL	CHD-C1D-ND	-3.64	121.11	124.45
19	A	828	CLA	C2C-C1C-NC	3.64	113.38	109.97
18	2	316	CHL	CHC-C1C-NC	3.63	129.72	124.20
19	A	806	CLA	C1D-ND-C4D	-3.63	103.75	106.33
19	A	823	CLA	CHB-C1B-NB	-3.63	120.41	124.26
19	4	317	CLA	C1-C2-C3	-3.61	119.80	126.04
19	B	818	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
19	B	841	CLA	CHA-C1A-NA	-3.61	118.13	126.40
19	2	310	CLA	C2C-C1C-NC	3.61	113.35	109.97
19	2	310	CLA	C4A-NA-C1A	-3.60	105.09	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	841	CLA	C1-O2A-CGA	-3.59	107.02	116.44
18	4	319	CHL	CHC-C1C-NC	3.57	129.61	124.20
18	2	313	CHL	C2B-C1B-NB	-3.54	107.86	110.23
19	4	317	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	A	818	CLA	CHA-C1A-NA	-3.53	118.31	126.40
19	A	809	CLA	C4D-CHA-C1A	3.53	125.54	121.25
19	A	807	CLA	C2C-C1C-NC	3.52	113.27	109.97
19	L	305	CLA	CHD-C1D-ND	-3.52	121.22	124.45
19	B	818	CLA	C1-C2-C3	-3.52	119.95	126.04
19	A	833	CLA	CHA-C1A-NA	-3.52	118.33	126.40
18	3	315	CHL	CHC-C1C-NC	3.52	129.54	124.20
19	A	816	CLA	C4A-NA-C1A	-3.52	105.12	106.71
19	B	818	CLA	CED-O2D-CGD	-3.51	107.99	115.94
19	B	846	CLA	C2C-C1C-NC	3.51	113.26	109.97
19	A	829	CLA	C2C-C1C-NC	3.50	113.25	109.97
19	A	834	CLA	C4A-NA-C1A	-3.50	105.13	106.71
19	A	815	CLA	CHA-C1A-NA	-3.50	118.38	126.40
18	1	601	CHL	CHD-C1D-ND	-3.50	121.24	124.45
19	A	846	CLA	CMC-C2C-C1C	3.49	130.36	125.04
19	A	825	CLA	C1D-ND-C4D	-3.48	103.86	106.33
19	B	841	CLA	C1-C2-C3	-3.48	120.02	126.04
19	3	308	CLA	CHB-C1B-NB	-3.48	120.58	124.26
19	B	848	CLA	CHA-C1A-NA	-3.48	118.43	126.40
19	A	829	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
19	B	804	CLA	C4A-NA-C1A	-3.45	105.15	106.71
19	K	202	CLA	CHD-C1D-ND	-3.45	121.28	124.45
19	B	834	CLA	C1-C2-C3	-3.45	120.08	126.04
19	B	829	CLA	CHA-C1A-NA	-3.44	118.52	126.40
19	A	829	CLA	C1D-ND-C4D	-3.43	103.89	106.33
19	A	840	CLA	C4D-CHA-C1A	3.43	125.43	121.25
19	B	830	CLA	CHA-C1A-NA	-3.43	118.54	126.40
19	A	844	CLA	CHB-C1B-NB	-3.43	120.63	124.26
18	2	313	CHL	CAA-C2A-C1A	3.42	120.26	111.81
19	A	819	CLA	CHB-C1B-NB	-3.42	120.64	124.26
19	G	203	CLA	CHA-C1A-NA	-3.41	118.58	126.40
18	2	315	CHL	C4D-CHA-C1A	3.41	125.40	121.25
19	K	203	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	A	851	CLA	CAA-CBA-CGA	-3.40	103.33	113.25
19	B	830	CLA	C1D-ND-C4D	-3.39	103.93	106.33
19	A	808	CLA	CHB-C1B-NB	-3.38	120.68	124.26
19	B	841	CLA	C2C-C1C-NC	3.38	113.13	109.97
19	B	832	CLA	CAA-CBA-CGA	-3.37	103.55	112.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	607	CLA	CHA-C1A-NA	-3.37	118.68	126.40
19	G	203	CLA	C2B-C1B-NB	-3.36	107.98	110.23
19	F	306	CLA	CHC-C4B-NB	-3.36	120.70	124.26
19	A	831	CLA	C1-C2-C3	-3.36	120.23	126.04
19	A	836	CLA	C1D-ND-C4D	-3.36	103.95	106.33
19	A	825	CLA	CHB-C1B-NB	-3.35	120.71	124.26
19	A	837	CLA	C1D-ND-C4D	-3.35	103.95	106.33
19	B	828	CLA	CHB-C1B-NB	-3.34	120.72	124.26
19	J	101	CLA	C2C-C1C-NC	3.34	113.10	109.97
19	B	818	CLA	CHA-C1A-NA	-3.34	118.75	126.40
19	1	605	CLA	CHB-C1B-NB	-3.33	120.73	124.26
18	4	313	CHL	CHC-C1C-NC	3.33	129.25	124.20
19	B	826	CLA	C1D-ND-C4D	-3.33	103.97	106.33
19	A	812	CLA	C4A-NA-C1A	-3.33	105.21	106.71
19	A	818	CLA	C2C-C1C-NC	3.30	113.07	109.97
19	B	840	CLA	C2C-C1C-NC	3.30	113.06	109.97
19	B	818	CLA	CHB-C1B-NB	-3.29	120.77	124.26
19	B	845	CLA	C2C-C1C-NC	3.29	113.05	109.97
19	B	828	CLA	CHA-C1A-NA	-3.28	118.89	126.40
19	B	840	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
19	B	833	CLA	C2C-C1C-NC	3.28	113.04	109.97
19	3	314	CLA	C1D-ND-C4D	-3.28	104.01	106.33
19	A	815	CLA	C2C-C1C-NC	3.27	113.04	109.97
19	F	303	CLA	C2A-C3A-C4A	3.27	107.15	101.87
19	4	314	CLA	C1-C2-C3	-3.27	120.39	126.04
19	3	301	CLA	CAA-C2A-C1A	-3.26	101.28	111.97
19	J	101	CLA	C1-C2-C3	-3.26	120.40	126.04
19	H	201	CLA	CHB-C1B-NB	-3.26	120.80	124.26
19	B	832	CLA	CHA-C1A-NA	-3.26	118.94	126.40
19	B	804	CLA	C1D-ND-C4D	-3.25	104.02	106.33
19	B	807	CLA	CHB-C1B-NB	-3.25	120.81	124.26
19	B	833	CLA	CHB-C1B-NB	-3.25	120.81	124.26
19	4	311	CLA	CHD-C1D-ND	-3.25	121.47	124.45
19	B	824	CLA	C2C-C1C-NC	3.25	113.01	109.97
19	A	831	CLA	C3B-C4B-NB	-3.24	107.51	110.52
19	A	802	CLA	CAA-C2A-C1A	-3.23	101.39	111.97
22	3	310	A1LXP	C30-C31-C32	3.23	115.42	111.74
19	3	306	CLA	C2C-C1C-NC	3.22	112.99	109.97
19	A	812	CLA	C2C-C1C-NC	3.22	112.99	109.97
19	A	842	CLA	CHC-C4B-NB	-3.22	120.85	124.26
19	B	823	CLA	CHA-C1A-NA	-3.21	119.04	126.40
19	1	602	CLA	C3A-C2A-C1A	-3.21	96.52	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	311	CLA	C2C-C1C-NC	3.21	112.98	109.97
19	B	847	CLA	CHD-C1D-ND	-3.21	121.50	124.45
19	B	818	CLA	C1D-ND-C4D	-3.21	104.06	106.33
19	B	819	CLA	CHB-C1B-NB	-3.21	120.86	124.26
19	B	804	CLA	C2B-C1B-NB	3.21	112.38	110.23
22	4	303	A1LXP	C25-C26-C27	-3.21	105.92	110.30
19	B	803	CLA	CHC-C4B-NB	-3.20	120.86	124.26
19	2	312	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	A	823	CLA	C2B-C1B-NB	3.19	112.37	110.23
19	2	310	CLA	CHA-C1A-NA	-3.18	119.11	126.40
19	A	851	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
19	A	846	CLA	C9-C8-C10	3.17	122.79	111.29
19	A	809	CLA	CMC-C2C-C1C	3.17	129.87	125.04
19	1	602	CLA	CHA-C1A-NA	-3.17	119.14	126.40
19	B	839	CLA	CHB-C1B-NB	-3.17	120.90	124.26
19	B	844	CLA	C1-C2-C3	3.17	131.53	126.04
19	A	817	CLA	C1D-ND-C4D	-3.17	104.08	106.33
19	2	310	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
18	3	315	CHL	CHB-C4A-NA	3.16	128.88	124.51
19	3	306	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	B	840	CLA	CBA-CAA-C2A	3.15	123.17	113.86
19	B	819	CLA	C1D-ND-C4D	-3.15	104.10	106.33
18	1	601	CHL	CHB-C4A-NA	3.14	128.86	124.51
28	B	811	PQN	C12-C11-C3	-3.14	103.58	112.05
19	B	828	CLA	CHD-C1D-ND	-3.13	121.57	124.45
19	A	806	CLA	CHA-C1A-NA	-3.13	119.22	126.40
19	L	305	CLA	C1D-ND-C4D	-3.13	104.11	106.33
19	B	821	CLA	CBA-CAA-C2A	3.13	120.43	113.47
19	A	828	CLA	CHC-C4B-NB	-3.12	120.95	124.26
19	3	304	CLA	CHD-C1D-ND	-3.12	121.59	124.45
19	B	824	CLA	CHB-C1B-NB	-3.11	120.96	124.26
18	2	313	CHL	C2A-C1A-CHA	3.11	129.28	123.85
19	A	807	CLA	C1D-ND-C4D	-3.11	104.13	106.33
19	A	824	CLA	C1-C2-C3	-3.10	120.67	126.04
19	A	813	CLA	O2A-C1-C2	3.10	116.78	108.64
19	B	802	CLA	C1D-ND-C4D	-3.09	104.14	106.33
18	1	601	CHL	CAA-C2A-C1A	3.09	122.11	111.97
19	A	843	CLA	C2B-C1B-NB	3.09	112.31	110.23
19	4	318	CLA	CHB-C1B-NB	-3.09	120.98	124.26
19	3	308	CLA	CHD-C1D-ND	-3.09	121.61	124.45
19	A	820	CLA	C1D-ND-C4D	-3.09	104.14	106.33
18	1	601	CHL	CHC-C1C-NC	3.09	128.89	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	811	CLA	CHA-C1A-NA	-3.09	119.33	126.40
19	A	840	CLA	CHA-C1A-NA	-3.09	119.33	126.40
18	1	606	CHL	CHB-C4A-NA	3.08	128.78	124.51
19	B	840	CLA	CHA-C1A-NA	-3.08	119.35	126.40
19	J	101	CLA	C4A-NA-C1A	-3.07	105.32	106.71
18	4	319	CHL	C2A-C1A-CHA	3.07	129.23	123.86
18	2	316	CHL	C3A-C2A-C1A	3.07	105.94	101.34
19	F	303	CLA	C3B-C4B-NB	-3.07	107.67	110.52
19	B	802	CLA	CMC-C2C-C1C	3.07	129.71	125.04
19	B	808	CLA	CHA-C1A-NA	-3.06	119.39	126.40
18	3	303	CHL	C3C-C4C-NC	-3.06	107.14	110.57
19	A	840	CLA	C1D-ND-C4D	-3.05	104.17	106.33
19	4	314	CLA	C1D-ND-C4D	-3.05	104.17	106.33
18	2	315	CHL	CHB-C4A-NA	3.05	128.73	124.51
19	B	809	CLA	CAA-C2A-C1A	-3.05	101.97	111.97
19	A	815	CLA	CHB-C1B-NB	-3.05	121.03	124.26
19	B	831	CLA	C1-C2-C3	3.05	131.31	126.04
19	B	805	CLA	CHA-C1A-NA	-3.04	119.43	126.40
19	B	809	CLA	C4A-NA-C1A	-3.04	105.34	106.71
19	F	303	CLA	CHA-C1A-NA	-3.04	119.43	126.40
19	3	304	CLA	C1D-ND-C4D	-3.04	104.17	106.33
19	2	311	CLA	CHC-C4B-NB	-3.04	121.04	124.26
18	4	313	CHL	CHB-C4A-NA	3.04	128.72	124.51
19	2	310	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	1	605	CLA	CHA-C1A-NA	-3.03	119.45	126.40
19	B	834	CLA	C4A-NA-C1A	-3.03	105.34	106.71
19	A	834	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	B	824	CLA	C1D-ND-C4D	-3.03	104.19	106.33
19	A	827	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
19	1	603	CLA	CHA-C1A-NA	-3.02	119.48	126.40
18	4	319	CHL	C2B-C1B-NB	-3.01	108.21	110.23
19	L	304	CLA	C2C-C1C-NC	3.01	112.79	109.97
19	3	308	CLA	C4A-NA-C1A	-3.01	105.35	106.71
19	2	312	CLA	CHB-C1B-NB	-3.01	121.07	124.26
28	A	839	PQN	C11-C3-C4	-3.01	115.28	118.50
19	B	820	CLA	CMC-C2C-C1C	3.01	129.62	125.04
19	B	809	CLA	CGD-CBD-CAD	-3.00	101.00	110.73
19	A	805	CLA	C4A-NA-C1A	-3.00	105.36	106.71
18	2	316	CHL	CHD-C1D-ND	-3.00	121.70	124.45
19	A	809	CLA	CHA-C1A-NA	-3.00	119.53	126.40
19	L	305	CLA	CHB-C1B-NB	-3.00	121.08	124.26
19	2	312	CLA	C1-C2-C3	-3.00	120.86	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	C4D-CHA-C1A	3.00	124.89	121.25
19	A	848	CLA	CHC-C4B-NB	-2.99	121.09	124.26
19	B	801	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
19	4	311	CLA	CHA-C1A-NA	-2.99	119.56	126.40
19	A	828	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
25	N	201	LMG	O1-C7-C8	2.98	114.46	108.76
19	B	820	CLA	CHB-C1B-NB	-2.97	121.11	124.26
19	A	827	CLA	C1D-ND-C4D	-2.97	104.22	106.33
19	B	846	CLA	CHA-C1A-NA	-2.97	119.60	126.40
19	A	811	CLA	CHC-C4B-NB	-2.97	121.11	124.26
19	B	821	CLA	C1D-ND-C4D	-2.97	104.23	106.33
18	2	315	CHL	C2A-C1A-CHA	2.96	129.04	123.86
19	B	837	CLA	C2D-C1D-ND	-2.96	107.92	110.10
19	A	827	CLA	CHA-C1A-NA	-2.95	119.63	126.40
19	B	832	CLA	CBA-CAA-C2A	2.95	122.58	113.86
19	B	833	CLA	C2A-C3A-C4A	2.95	106.64	101.87
19	B	825	CLA	C2D-C1D-ND	2.95	112.28	110.10
19	1	602	CLA	C2C-C1C-NC	2.95	112.74	109.97
19	3	302	CLA	CHA-C1A-NA	-2.95	119.64	126.40
18	3	315	CHL	C2A-C1A-CHA	2.95	129.02	123.86
19	B	801	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
19	B	806	CLA	C1D-ND-C4D	-2.95	104.24	106.33
19	A	814	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
19	B	830	CLA	C4D-CHA-C1A	2.94	124.83	121.25
19	A	851	CLA	CHA-C1A-NA	-2.94	119.66	126.40
19	F	303	CLA	C2C-C1C-NC	2.94	112.72	109.97
19	B	837	CLA	CHD-C1D-ND	-2.94	121.75	124.45
18	3	303	CHL	C2A-C1A-CHA	2.94	128.99	123.86
19	A	820	CLA	CHC-C1C-NC	2.93	128.64	124.20
19	H	201	CLA	CHA-C1A-NA	-2.92	119.71	126.40
19	A	801	CLA	C3B-C4B-NB	-2.92	107.81	110.52
19	A	808	CLA	CHA-C1A-NA	-2.92	119.71	126.40
19	B	826	CLA	CHA-C1A-NA	-2.92	119.71	126.40
19	B	823	CLA	C2A-C3A-C4A	2.92	106.58	101.87
19	J	101	CLA	C1D-ND-C4D	-2.92	104.26	106.33
19	B	841	CLA	CAA-CBA-CGA	2.91	121.77	113.25
19	A	836	CLA	CHB-C1B-NB	-2.91	121.17	124.26
24	B	815	BCR	C16-C15-C14	2.91	129.44	123.47
19	4	317	CLA	C2B-C1B-NB	2.91	112.18	110.23
19	A	821	CLA	CAA-C2A-C3A	2.91	120.75	112.78
19	B	838	CLA	C2C-C1C-NC	2.90	112.69	109.97
19	B	834	CLA	CHD-C1D-C2D	2.90	131.57	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	316	CHL	C2A-C1A-CHA	2.90	128.94	123.86
19	2	310	CLA	CHC-C1C-NC	2.90	128.61	124.20
19	2	312	CLA	C3B-C4B-NB	-2.90	107.82	110.52
19	A	840	CLA	CHD-C1D-C2D	2.89	131.55	125.48
19	A	809	CLA	C2A-C3A-C4A	2.89	106.54	101.87
19	B	804	CLA	CHB-C1B-NB	-2.89	121.19	124.26
19	A	807	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
19	B	832	CLA	C1D-ND-C4D	-2.89	104.28	106.33
19	1	602	CLA	CHC-C1C-C2C	-2.89	118.72	126.73
19	A	846	CLA	CHA-C1A-NA	-2.88	119.80	126.40
19	B	844	CLA	C1D-ND-C4D	-2.88	104.29	106.33
19	A	842	CLA	CHC-C1C-NC	2.88	128.57	124.20
19	2	311	CLA	CHA-C1A-NA	-2.87	119.83	126.40
19	3	302	CLA	C2C-C1C-NC	2.87	112.66	109.97
19	B	828	CLA	C3A-C2A-C1A	-2.86	97.05	101.34
19	B	825	CLA	C2B-C1B-NB	2.86	112.15	110.23
19	A	829	CLA	CHB-C1B-NB	-2.86	121.23	124.26
19	B	834	CLA	CHC-C4B-NB	-2.86	121.23	124.26
25	F	305	LMG	O1-C7-C8	2.86	117.80	110.90
19	A	813	CLA	CHA-C1A-NA	-2.86	119.85	126.40
19	A	817	CLA	CHA-C1A-NA	-2.86	119.86	126.40
19	4	307	CLA	CHC-C1C-NC	2.86	128.54	124.20
19	B	840	CLA	CAA-C2A-C3A	-2.86	104.96	112.78
19	A	817	CLA	CHB-C1B-NB	-2.86	121.23	124.26
19	B	806	CLA	O2A-C1-C2	2.85	116.14	108.64
19	B	823	CLA	CHD-C1D-ND	-2.85	121.83	124.45
19	A	848	CLA	CAA-CBA-CGA	-2.85	104.92	113.25
19	A	842	CLA	C1-C2-C3	2.85	130.97	126.04
19	B	841	CLA	CHB-C1B-NB	-2.85	121.24	124.26
19	A	813	CLA	CHD-C1D-ND	-2.84	121.84	124.45
19	A	826	CLA	C2D-C1D-ND	2.84	112.20	110.10
18	1	606	CHL	C2A-C1A-CHA	2.84	128.83	123.86
19	A	821	CLA	CHA-C1A-NA	-2.84	119.89	126.40
19	B	809	CLA	C2C-C1C-NC	2.84	112.63	109.97
19	3	312	CLA	C1D-ND-C4D	-2.84	104.32	106.33
19	A	837	CLA	C7-C6-C5	-2.84	105.65	113.36
19	A	837	CLA	C1-C2-C3	-2.84	121.14	126.04
19	2	310	CLA	CHB-C1B-NB	-2.84	121.25	124.26
19	3	308	CLA	CHA-C1A-NA	-2.83	119.91	126.40
19	A	843	CLA	CHA-C1A-NA	-2.83	119.92	126.40
19	1	602	CLA	CAA-C2A-C3A	2.83	120.52	112.78
19	B	838	CLA	CHB-C1B-NB	-2.83	121.27	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	304	CLA	CHC-C1C-NC	2.82	128.49	124.20
29	B	817	DGD	C6D-O5D-C1E	2.82	119.24	113.74
19	B	833	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
19	A	829	CLA	CMC-C2C-C1C	2.81	129.32	125.04
19	B	804	CLA	CHA-C1A-NA	-2.81	119.96	126.40
19	A	832	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	B	848	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
19	1	602	CLA	CHC-C1C-NC	2.81	128.47	124.20
19	A	826	CLA	CGD-CBD-CAD	-2.81	101.65	110.73
19	G	203	CLA	CHD-C1D-ND	-2.81	121.88	124.45
19	1	612	CLA	C1D-ND-C4D	-2.80	104.34	106.33
19	B	844	CLA	CHA-C1A-NA	-2.80	119.98	126.40
19	B	818	CLA	CMC-C2C-C1C	2.80	129.31	125.04
19	B	810	CLA	CHA-C1A-NA	-2.80	119.98	126.40
19	A	832	CLA	CHC-C4B-NB	-2.80	121.30	124.26
19	H	201	CLA	C1D-ND-C4D	-2.80	104.35	106.33
18	4	313	CHL	CAA-C2A-C1A	2.80	121.14	111.97
19	A	836	CLA	C3D-C4D-ND	2.79	114.75	110.24
18	2	313	CHL	CHA-C1A-NA	-2.79	120.00	126.40
19	B	810	CLA	CMC-C2C-C1C	2.79	129.29	125.04
19	A	822	CLA	C3A-C2A-C1A	2.79	105.52	101.34
19	B	807	CLA	C1D-ND-C4D	-2.79	104.36	106.33
19	A	810	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
19	A	834	CLA	CHA-C1A-NA	-2.78	120.02	126.40
19	A	842	CLA	CMC-C2C-C1C	2.78	129.27	125.04
19	B	832	CLA	CMC-C2C-C1C	2.78	129.27	125.04
24	A	847	BCR	C15-C16-C17	-2.78	117.78	123.47
19	2	312	CLA	CHA-C1A-NA	-2.78	120.03	126.40
19	B	834	CLA	CHD-C4C-C3C	2.78	128.93	124.84
21	1	615	XAT	C18-C5-C4	2.78	117.41	114.28
19	A	850	CLA	C9-C8-C7	2.78	121.35	111.29
19	A	834	CLA	CMC-C2C-C1C	2.77	129.26	125.04
19	3	308	CLA	C1D-ND-C4D	-2.77	104.37	106.33
18	4	319	CHL	C3B-C4B-NB	-2.77	107.94	110.52
21	2	306	XAT	C7-C8-C9	2.77	129.83	125.53
19	A	829	CLA	CHD-C1D-C2D	2.77	131.29	125.48
19	3	307	CLA	CHB-C1B-NB	-2.77	121.33	124.26
19	B	809	CLA	C1D-ND-C4D	-2.76	104.37	106.33
18	1	601	CHL	C3B-C4B-NB	-2.76	107.95	110.52
19	A	814	CLA	CHD-C1D-C2D	2.76	131.27	125.48
19	B	840	CLA	C1D-ND-C4D	-2.76	104.38	106.33
19	A	801	CLA	C3D-C4D-ND	2.76	114.70	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	806	CLA	C4D-CHA-C1A	2.75	124.59	121.25
19	A	848	CLA	C3B-C4B-NB	-2.75	107.97	110.52
19	A	846	CLA	C4C-C3C-C2C	2.75	110.90	106.90
19	B	827	CLA	O2A-C1-C2	-2.75	101.42	108.64
19	1	605	CLA	C2C-C1C-NC	2.74	112.54	109.97
19	A	822	CLA	CHC-C4B-NB	-2.74	121.36	124.26
19	B	839	CLA	CED-O2D-CGD	-2.74	109.75	115.94
19	L	303	CLA	CHC-C4B-NB	-2.73	121.36	124.26
19	A	843	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
19	B	837	CLA	CHA-C1A-NA	-2.73	120.14	126.40
19	A	814	CLA	C9-C8-C7	2.73	121.17	111.29
22	J	102	A1LXP	O41-C31-C32	2.73	116.69	110.53
19	A	821	CLA	CHB-C1B-NB	-2.73	121.37	124.26
19	B	828	CLA	CAA-C2A-C1A	-2.72	103.05	111.97
19	A	827	CLA	CHD-C1D-C2D	2.72	131.19	125.48
18	2	315	CHL	CHC-C1C-NC	2.71	128.32	124.20
19	A	831	CLA	C2C-C1C-NC	2.71	112.51	109.97
19	A	842	CLA	CHD-C1D-C2D	2.71	131.16	125.48
19	A	823	CLA	C2C-C1C-NC	2.71	112.51	109.97
19	A	802	CLA	C3D-C4D-ND	2.71	114.62	110.24
19	B	835	CLA	CMC-C2C-C1C	2.71	129.16	125.04
19	L	303	CLA	CHB-C1B-NB	-2.71	121.39	124.26
19	A	812	CLA	C1-O2A-CGA	2.70	123.54	116.44
19	A	837	CLA	C9-C8-C7	2.70	121.08	111.29
19	B	844	CLA	C2C-C1C-NC	2.70	112.50	109.97
19	A	817	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
19	B	821	CLA	CMC-C2C-C1C	2.70	129.15	125.04
19	A	848	CLA	CHC-C1C-NC	2.70	128.29	124.20
19	B	827	CLA	CAA-C2A-C1A	-2.70	103.14	111.97
19	A	846	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
19	B	818	CLA	O2D-CGD-CBD	2.69	116.05	111.27
19	A	831	CLA	C4D-CHA-C1A	2.69	124.53	121.25
28	B	811	PQN	C11-C3-C4	-2.69	115.62	118.50
19	K	203	CLA	CMC-C2C-C1C	2.69	129.13	125.04
19	A	814	CLA	CHA-C1A-NA	-2.69	120.25	126.40
19	A	837	CLA	CHA-C1A-NA	-2.69	120.25	126.40
19	2	310	CLA	C1-C2-C3	-2.68	121.41	126.04
19	A	848	CLA	C1-C2-C3	-2.68	122.42	126.75
19	B	847	CLA	C2C-C1C-NC	2.68	112.48	109.97
19	K	203	CLA	CHB-C1B-NB	-2.68	121.42	124.26
19	A	829	CLA	C4D-CHA-C1A	2.68	124.51	121.25
24	B	812	BCR	C7-C8-C9	-2.68	122.19	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	849	CLA	CHA-C1A-NA	-2.67	120.27	126.40
18	2	316	CHL	C3B-C4B-NB	-2.67	108.04	110.52
19	A	848	CLA	C1D-ND-C4D	-2.67	104.44	106.33
19	3	304	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
19	3	306	CLA	CHA-C1A-NA	-2.66	120.30	126.40
18	1	606	CHL	CHC-C1C-NC	2.66	128.24	124.20
19	A	809	CLA	C2C-C1C-NC	2.66	112.46	109.97
27	A	830	CL0	C2D-C1D-ND	-2.65	108.15	110.10
19	B	835	CLA	C2B-C1B-NB	-2.65	108.45	110.23
19	K	202	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
19	B	844	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	B	834	CLA	CHB-C1B-NB	-2.65	121.45	124.26
19	A	833	CLA	C2C-C1C-NC	2.65	112.45	109.97
19	G	202	CLA	C3D-C4D-ND	2.65	114.52	110.24
19	B	806	CLA	CHA-C1A-NA	-2.65	120.33	126.40
19	B	807	CLA	C2C-C1C-NC	2.65	112.45	109.97
19	A	832	CLA	CHC-C1C-NC	2.65	128.22	124.20
19	B	828	CLA	C2C-C1C-NC	2.65	112.45	109.97
22	3	305	A1LXP	C42-C2-C3	2.65	130.23	126.23
19	3	306	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
19	B	829	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	B	834	CLA	O2A-C1-C2	2.64	115.58	108.64
19	B	824	CLA	C6-C5-C3	2.64	118.94	114.62
19	B	841	CLA	CAC-C3C-C4C	2.64	128.23	124.81
19	B	844	CLA	CBA-CAA-C2A	2.64	121.64	113.86
19	B	829	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
19	B	808	CLA	CMC-C2C-C1C	2.63	129.05	125.04
19	H	201	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	B	810	CLA	C7-C6-C5	-2.63	106.21	113.36
19	B	834	CLA	C10-C8-C7	2.62	125.93	112.13
19	A	826	CLA	C1-C2-C3	-2.62	121.51	126.04
19	A	851	CLA	CHB-C1B-NB	-2.62	121.48	124.26
19	B	806	CLA	CHB-C1B-NB	-2.61	121.49	124.26
19	B	835	CLA	C4C-C3C-C2C	2.61	110.70	106.90
19	2	310	CLA	CBA-CAA-C2A	2.61	121.57	113.86
19	1	612	CLA	O2A-C1-C2	2.61	115.49	108.64
19	A	818	CLA	CHC-C4B-NB	-2.61	121.50	124.26
19	B	835	CLA	C2A-C3A-C4A	2.61	106.08	101.87
19	A	814	CLA	C1D-ND-C4D	-2.61	104.48	106.33
19	B	828	CLA	O2A-C1-C2	2.60	115.48	108.64
19	B	827	CLA	CHA-C1A-NA	-2.60	120.44	126.40
19	B	824	CLA	CMA-C3A-C4A	-2.60	104.78	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	C2D-C1D-ND	2.60	112.02	110.10
19	B	810	CLA	CHD-C1D-ND	-2.60	122.07	124.45
19	4	318	CLA	CHA-C1A-NA	-2.60	120.45	126.40
19	A	819	CLA	C2A-C3A-C4A	2.59	106.06	101.87
19	B	836	CLA	CHD-C1D-C2D	2.59	130.92	125.48
19	F	306	CLA	CHA-C1A-NA	-2.59	120.46	126.40
19	A	819	CLA	CHA-C1A-NA	-2.59	120.47	126.40
19	A	814	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
19	A	822	CLA	CAA-CBA-CGA	-2.59	105.69	113.25
19	B	834	CLA	CMC-C2C-C1C	2.59	128.98	125.04
19	A	840	CLA	C7-C6-C5	-2.58	106.34	113.36
19	2	311	CLA	CHD-C1D-C2D	2.58	130.88	125.48
19	L	304	CLA	CHB-C1B-NB	-2.58	121.53	124.26
18	4	313	CHL	C2A-C1A-CHA	2.57	128.35	123.86
19	B	803	CLA	CMC-C2C-C1C	2.57	128.95	125.04
19	B	843	CLA	CHA-C1A-NA	-2.57	120.52	126.40
19	B	845	CLA	C9-C8-C7	2.57	120.59	111.29
19	1	603	CLA	CBA-CAA-C2A	2.57	121.44	113.86
19	2	301	CLA	CHB-C1B-NB	-2.56	121.54	124.26
19	B	822	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
19	B	801	CLA	CAA-CBA-CGA	-2.56	105.77	113.25
19	A	851	CLA	C2D-C1D-ND	-2.56	108.22	110.10
19	1	602	CLA	CHC-C4B-NB	-2.56	121.55	124.26
19	3	314	CLA	CHA-C1A-NA	-2.56	120.54	126.40
19	B	801	CLA	CHB-C1B-NB	-2.56	121.55	124.26
19	B	829	CLA	CBA-CAA-C2A	2.56	119.41	114.02
19	A	846	CLA	C1D-ND-C4D	-2.55	104.52	106.33
19	B	804	CLA	CHC-C4B-NB	-2.55	121.56	124.26
19	3	301	CLA	CHC-C1C-NC	2.55	128.07	124.20
19	A	826	CLA	O2A-C1-C2	-2.55	101.94	108.64
19	A	818	CLA	C1-C2-C3	-2.55	121.64	126.04
19	A	811	CLA	C2C-C1C-NC	2.55	112.36	109.97
19	3	301	CLA	CHC-C1C-C2C	-2.55	119.65	126.73
19	A	805	CLA	C2C-C1C-NC	2.55	112.36	109.97
19	B	843	CLA	C16-C15-C13	2.55	124.15	115.92
19	B	828	CLA	CBA-CAA-C2A	2.54	121.37	113.86
19	A	832	CLA	C3A-C2A-C1A	-2.54	97.53	101.34
19	1	612	CLA	CHC-C1C-NC	2.54	128.06	124.20
19	B	809	CLA	C6-C5-C3	2.54	120.12	113.45
19	A	832	CLA	C2D-C1D-ND	2.54	111.97	110.10
18	3	303	CHL	CHD-C1D-C2D	2.54	130.80	125.48
19	B	802	CLA	C1C-C2C-C3C	-2.54	104.29	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	823	CLA	C4D-CHA-C1A	2.53	124.33	121.25
19	A	815	CLA	C4D-CHA-C1A	2.53	124.33	121.25
19	B	842	CLA	C1-C2-C3	2.53	130.84	126.75
19	B	846	CLA	CHD-C1D-C2D	2.53	130.78	125.48
19	B	844	CLA	CAA-C2A-C3A	2.52	119.69	112.78
19	4	311	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
19	A	801	CLA	C7-C6-C5	2.52	120.20	113.36
19	1	602	CLA	C1D-ND-C4D	-2.52	104.55	106.33
19	A	824	CLA	CHA-C1A-NA	-2.52	120.63	126.40
19	3	304	CLA	C2A-C3A-C4A	2.52	105.93	101.87
19	A	809	CLA	CMA-C3A-C4A	-2.52	105.01	111.77
19	A	814	CLA	CAA-C2A-C1A	-2.52	103.73	111.97
19	B	803	CLA	C3C-C4C-NC	-2.52	107.75	110.57
19	B	840	CLA	CHB-C1B-NB	-2.51	121.59	124.26
18	2	313	CHL	CMB-C2B-C1B	-2.51	121.54	125.37
19	A	844	CLA	C1D-ND-C4D	-2.51	104.55	106.33
19	G	202	CLA	CHD-C1D-C2D	2.51	130.75	125.48
19	B	803	CLA	C2D-C1D-ND	2.51	111.95	110.10
19	B	825	CLA	CHC-C4B-NB	-2.51	121.60	124.26
19	B	833	CLA	CHC-C1C-NC	2.51	128.01	124.20
19	B	825	CLA	CHA-C1A-NA	-2.51	120.66	126.40
19	B	808	CLA	C1D-ND-C4D	-2.51	104.56	106.33
19	3	314	CLA	CHC-C1C-NC	2.51	128.00	124.20
19	A	812	CLA	CHD-C1D-C2D	2.50	130.73	125.48
19	3	304	CLA	C2B-C1B-NB	2.50	111.91	110.23
19	A	828	CLA	CBA-CAA-C2A	2.49	121.23	113.86
19	3	312	CLA	CHA-C1A-NA	-2.49	120.69	126.40
19	B	807	CLA	CHA-C1A-NA	-2.49	120.69	126.40
19	B	820	CLA	C2C-C1C-NC	2.49	112.31	109.97
19	A	851	CLA	CMA-C3A-C2A	-2.49	103.78	113.83
19	L	305	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
19	A	808	CLA	C2B-C1B-NB	2.49	111.90	110.23
19	A	850	CLA	C1D-ND-C4D	-2.49	104.57	106.33
19	A	820	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
19	B	819	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
19	A	822	CLA	C1D-ND-C4D	-2.48	104.57	106.33
19	1	602	CLA	C4D-CHA-C1A	2.48	124.27	121.25
18	2	315	CHL	CHA-C1A-NA	-2.48	120.71	126.40
19	B	824	CLA	CHA-C1A-NA	-2.48	120.71	126.40
19	B	805	CLA	C1D-ND-C4D	-2.48	104.57	106.33
19	B	835	CLA	CHD-C1D-C2D	2.48	130.68	125.48
19	A	821	CLA	CMC-C2C-C1C	2.47	128.81	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	103	LMG	C7-O1-C1	2.47	118.57	113.74
19	L	304	CLA	CHA-C1A-NA	-2.47	120.73	126.40
24	A	804	BCR	C2-C1-C6	2.47	114.29	110.48
19	A	827	CLA	C4A-NA-C1A	-2.47	105.59	106.71
19	A	844	CLA	CHC-C4B-NB	-2.47	121.64	124.26
19	K	202	CLA	C2A-C1A-CHA	2.47	128.18	123.86
19	A	813	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
19	A	848	CLA	C3B-C2B-C1B	2.47	110.14	107.16
19	2	301	CLA	CHC-C1C-NC	2.47	127.95	124.20
19	B	846	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
19	A	816	CLA	CHA-C1A-NA	-2.47	120.75	126.40
19	A	829	CLA	CHA-C1A-NA	-2.47	120.75	126.40
19	4	317	CLA	C3D-C4D-ND	2.47	114.23	110.24
19	3	306	CLA	CHB-C1B-NB	-2.47	121.65	124.26
19	A	809	CLA	CHC-C4B-NB	-2.47	121.65	124.26
19	B	845	CLA	CHB-C1B-NB	-2.47	121.65	124.26
19	3	307	CLA	CHC-C1C-C2C	-2.46	119.88	126.73
19	2	301	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
19	B	803	CLA	CGD-CBD-CAD	-2.46	102.76	110.73
19	A	811	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
19	B	837	CLA	CAC-C3C-C4C	-2.46	121.62	124.81
19	A	809	CLA	C2D-C1D-ND	2.46	111.92	110.10
19	A	816	CLA	CHC-C4B-NB	-2.46	121.65	124.26
19	B	830	CLA	CHB-C4A-NA	-2.46	121.11	124.51
19	4	311	CLA	C2D-C1D-ND	-2.46	108.29	110.10
19	B	843	CLA	C10-C8-C7	2.46	125.04	112.13
18	4	313	CHL	CHA-C1A-NA	-2.45	120.78	126.40
19	B	830	CLA	CHD-C1D-C2D	2.45	130.63	125.48
19	B	834	CLA	CAA-C2A-C1A	-2.45	103.94	111.97
19	3	307	CLA	CHC-C1C-NC	2.45	127.92	124.20
19	1	612	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
19	3	301	CLA	C2C-C1C-NC	2.45	112.27	109.97
19	4	314	CLA	C3B-C2B-C1B	2.45	110.12	107.16
19	B	809	CLA	CHD-C1D-C2D	2.45	130.62	125.48
19	A	826	CLA	C1D-ND-C4D	-2.45	104.59	106.33
19	3	308	CLA	C2C-C1C-NC	2.45	112.26	109.97
19	3	301	CLA	C1D-ND-C4D	-2.45	104.60	106.33
19	A	832	CLA	CHC-C1C-C2C	-2.45	119.94	126.73
19	B	842	CLA	CHA-C1A-NA	-2.44	120.81	126.40
19	B	832	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
19	B	845	CLA	CHA-C1A-NA	-2.44	120.81	126.40
19	F	303	CLA	CHD-C1D-C2D	2.44	130.60	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	802	CLA	CHC-C4B-NB	-2.44	121.67	124.26
23	A	835	LHG	O4-P-O5	2.44	124.30	112.24
19	A	805	CLA	CHD-C1D-C2D	2.44	130.59	125.48
19	A	812	CLA	C2A-C3A-C4A	2.43	105.80	101.87
19	B	835	CLA	CHD-C4C-NC	2.43	128.04	124.20
19	B	835	CLA	CAC-C3C-C4C	-2.43	121.65	124.81
19	L	303	CLA	CHA-C1A-NA	-2.43	120.83	126.40
18	4	313	CHL	C4D-CHA-C1A	2.43	124.21	121.25
19	A	813	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
19	A	827	CLA	C2C-C1C-NC	2.43	112.25	109.97
19	A	849	CLA	C1D-ND-C4D	-2.43	104.61	106.33
19	B	837	CLA	CHC-C1C-C2C	-2.43	119.99	126.73
18	3	303	CHL	C2C-C3C-C4C	2.42	108.22	106.49
19	2	310	CLA	CGD-CBD-CAD	-2.42	102.89	110.73
18	3	315	CHL	CHA-C1A-NA	-2.42	120.86	126.40
18	1	606	CHL	CAA-C2A-C1A	2.42	117.49	112.14
19	A	833	CLA	C1D-ND-C4D	-2.41	104.62	106.33
19	B	828	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	B	826	CLA	CGD-CBD-CAD	-2.41	102.92	110.73
25	N	201	LMG	C7-O1-C1	2.41	118.45	113.74
19	A	842	CLA	C3C-C4C-NC	-2.41	107.86	110.57
19	A	817	CLA	C2B-C1B-NB	2.41	111.85	110.23
19	A	844	CLA	CHA-C1A-NA	-2.41	120.88	126.40
19	A	831	CLA	CHD-C1D-C2D	2.41	130.53	125.48
19	B	810	CLA	CGD-CBD-CAD	2.40	118.52	110.73
19	B	820	CLA	C3B-C4B-NB	-2.40	108.29	110.52
19	B	835	CLA	C3B-C4B-NB	-2.40	108.29	110.52
19	A	818	CLA	C2A-C1A-CHA	2.40	128.05	123.86
19	1	608	CLA	CHA-C1A-NA	-2.39	120.92	126.40
19	1	608	CLA	CHB-C1B-NB	-2.39	121.72	124.26
19	A	817	CLA	C2D-C1D-ND	2.39	111.87	110.10
19	A	813	CLA	C1D-CHD-C4C	-2.39	120.90	126.06
19	A	810	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
19	A	807	CLA	C3D-C4D-ND	2.38	114.09	110.24
18	2	313	CHL	CHB-C4A-NA	2.38	127.81	124.51
19	G	202	CLA	CMC-C2C-C1C	2.38	128.67	125.04
19	1	605	CLA	C2A-C3A-C4A	2.38	105.72	101.87
19	4	307	CLA	CHC-C1C-C2C	-2.38	120.12	126.73
19	B	835	CLA	CMA-C3A-C4A	-2.38	105.38	111.77
19	3	306	CLA	C1D-ND-C4D	-2.38	104.64	106.33
18	2	315	CHL	CHD-C4C-C3C	2.38	128.33	124.84
19	2	301	CLA	CHD-C1D-C2D	2.38	130.46	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	318	CLA	CHD-C1D-C2D	2.38	130.46	125.48
19	A	831	CLA	CHA-C1A-NA	-2.37	120.96	126.40
19	A	823	CLA	CHC-C1C-C2C	-2.37	120.13	126.73
19	B	823	CLA	C1D-ND-C4D	-2.37	104.65	106.33
19	A	807	CLA	CHC-C1C-NC	2.37	127.80	124.20
19	A	825	CLA	CHC-C1C-NC	2.37	127.80	124.20
19	A	828	CLA	CHB-C1B-NB	-2.37	121.75	124.26
19	A	826	CLA	CHA-C1A-NA	-2.36	120.99	126.40
19	B	835	CLA	CHA-C1A-NA	-2.36	120.99	126.40
19	B	803	CLA	CHC-C1C-NC	2.36	127.78	124.20
19	A	802	CLA	CAC-C3C-C4C	2.36	127.87	124.81
19	3	304	CLA	C2C-C1C-NC	2.36	112.18	109.97
19	B	831	CLA	C2A-C3A-C4A	2.36	105.68	101.87
19	B	823	CLA	CHB-C1B-NB	-2.36	121.76	124.26
19	B	808	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
19	B	847	CLA	CHA-C1A-NA	-2.35	121.01	126.40
19	B	841	CLA	C3C-C4C-NC	2.35	113.21	110.57
19	3	314	CLA	CHB-C1B-NB	-2.35	121.77	124.26
19	B	836	CLA	CHA-C1A-NA	-2.35	121.01	126.40
19	1	608	CLA	C1D-ND-C4D	-2.35	104.66	106.33
19	B	838	CLA	CHA-C1A-NA	-2.35	121.02	126.40
19	B	840	CLA	CHC-C1C-C2C	-2.35	120.20	126.73
19	A	851	CLA	CMC-C2C-C1C	2.35	128.61	125.04
18	2	316	CHL	CAA-C2A-C1A	2.35	119.67	111.97
19	B	835	CLA	O2A-C1-C2	-2.35	102.47	108.64
19	A	825	CLA	CAA-C2A-C1A	-2.35	106.95	112.14
18	4	313	CHL	CHD-C1D-C2D	2.34	130.40	125.48
19	2	311	CLA	C1D-ND-C4D	-2.34	104.67	106.33
18	2	315	CHL	CAA-C2A-C1A	2.34	119.65	111.97
19	4	314	CLA	CHD-C1D-C2D	2.34	130.39	125.48
19	1	607	CLA	CBA-CAA-C2A	2.34	120.76	113.86
19	A	826	CLA	CHC-C4B-NB	-2.34	121.78	124.26
19	A	815	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
19	A	819	CLA	CAC-C3C-C4C	2.34	127.84	124.81
19	B	839	CLA	C2A-C3A-C4A	2.34	105.64	101.87
19	B	841	CLA	C1D-ND-C4D	-2.33	104.68	106.33
19	2	301	CLA	C2C-C1C-NC	2.33	112.16	109.97
19	B	828	CLA	CMA-C3A-C2A	2.33	123.24	113.83
19	A	837	CLA	CHB-C1B-NB	-2.33	121.79	124.26
19	A	814	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
19	A	811	CLA	CHC-C1C-NC	2.33	127.74	124.20
19	2	311	CLA	CMC-C2C-C1C	2.33	128.58	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	802	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
19	A	816	CLA	CHC-C1C-C2C	-2.32	120.29	126.73
19	B	808	CLA	C1-C2-C3	2.32	130.05	126.04
19	B	808	CLA	O2A-C1-C2	-2.31	102.55	108.64
19	B	834	CLA	C6-C7-C8	-2.31	108.44	115.92
18	2	313	CHL	CHB-C1B-NB	2.31	126.71	124.26
19	3	307	CLA	C2C-C1C-NC	2.31	112.14	109.97
23	A	835	LHG	C32-C31-C30	2.31	126.16	114.42
19	A	823	CLA	CHD-C1D-C2D	2.31	130.32	125.48
18	3	303	CHL	CHA-C1A-NA	-2.31	121.11	126.40
19	B	837	CLA	CHD-C1D-C2D	2.31	130.32	125.48
21	1	615	XAT	C27-C28-C29	2.30	129.10	125.53
19	A	851	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
19	B	803	CLA	C3D-C4D-ND	2.30	113.95	110.24
19	4	317	CLA	C4A-NA-C1A	-2.30	105.67	106.71
19	B	836	CLA	CHC-C1C-NC	2.30	127.69	124.20
19	B	838	CLA	C1D-ND-C4D	-2.29	104.71	106.33
19	A	846	CLA	C2B-C1B-NB	2.29	111.77	110.23
19	B	819	CLA	C9-C8-C10	2.29	119.59	111.29
19	A	846	CLA	CHD-C1D-C2D	2.29	130.28	125.48
19	3	308	CLA	CHC-C1C-C2C	-2.29	120.38	126.73
19	A	809	CLA	CHD-C1D-C2D	2.29	130.28	125.48
19	A	813	CLA	CMC-C2C-C1C	2.28	128.52	125.04
19	B	843	CLA	C2D-C1D-ND	-2.28	108.42	110.10
19	B	846	CLA	O2A-C1-C2	-2.28	102.64	108.64
18	2	316	CHL	CHC-C1C-C2C	-2.28	117.84	126.11
18	1	606	CHL	C4D-CHA-C1A	2.28	124.02	121.25
19	A	842	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
19	A	825	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
19	B	842	CLA	C2C-C1C-NC	2.28	112.11	109.97
19	L	304	CLA	CMA-C3A-C4A	-2.28	105.66	111.77
19	3	307	CLA	CHD-C1D-C2D	2.28	130.25	125.48
19	A	849	CLA	C3C-C4C-NC	2.28	113.12	110.57
18	3	315	CHL	C2B-C1B-NB	-2.27	108.71	110.23
19	A	846	CLA	C3D-C4D-ND	2.27	113.92	110.24
19	A	851	CLA	CHD-C1D-ND	-2.27	122.36	124.45
19	3	314	CLA	C1-C2-C3	-2.27	122.11	126.04
19	A	817	CLA	CHC-C4B-NB	-2.27	121.85	124.26
19	A	814	CLA	CHC-C4B-NB	-2.27	121.85	124.26
19	4	311	CLA	CHD-C1D-C2D	2.27	130.24	125.48
19	B	809	CLA	C3B-C2B-C1B	2.27	109.90	107.16
19	A	848	CLA	CHC-C1C-C2C	-2.27	120.43	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	829	CLA	CHA-C4D-ND	2.27	137.24	132.50
19	A	810	CLA	C1-C2-C3	-2.26	123.09	126.75
19	B	841	CLA	CMA-C3A-C4A	2.26	117.85	111.77
19	A	813	CLA	CAC-C3C-C4C	-2.26	121.88	124.81
19	A	827	CLA	C4C-C3C-C2C	2.26	110.19	106.90
19	A	820	CLA	CHB-C1B-NB	-2.26	121.86	124.26
19	A	816	CLA	C2C-C1C-NC	2.26	112.09	109.97
19	A	819	CLA	CHC-C4B-NB	-2.26	121.87	124.26
19	A	811	CLA	CHA-C4D-ND	2.26	137.22	132.50
19	2	301	CLA	CHA-C1A-NA	-2.26	121.23	126.40
19	A	848	CLA	CMA-C3A-C2A	-2.25	104.73	113.83
19	A	810	CLA	CHD-C1D-C2D	2.25	130.21	125.48
19	A	848	CLA	C3A-C2A-C1A	2.25	104.71	101.34
19	L	303	CLA	C2A-C3A-C4A	2.25	105.50	101.87
25	4	304	LMG	O8-C9-C8	2.25	114.98	108.43
19	A	843	CLA	CHD-C1D-C2D	2.25	130.19	125.48
19	A	828	CLA	CAA-C2A-C1A	-2.25	104.61	111.97
19	A	822	CLA	CHD-C1D-C2D	2.25	130.19	125.48
19	4	307	CLA	CHC-C4B-NB	-2.24	121.89	124.26
19	B	808	CLA	C3A-C2A-C1A	2.24	104.69	101.34
22	3	310	A1LXP	C37-C29-C30	-2.24	105.19	109.44
19	A	807	CLA	CAA-CBA-CGA	-2.24	106.56	112.51
18	2	315	CHL	CHD-C1D-C2D	2.24	130.17	125.48
19	B	835	CLA	C2C-C1C-NC	2.24	112.07	109.97
19	A	837	CLA	O2A-C1-C2	-2.24	102.75	108.64
19	A	828	CLA	C1-C2-C3	-2.24	122.18	126.04
19	1	602	CLA	CHD-C1D-C2D	2.24	130.17	125.48
19	A	819	CLA	C3D-C4D-ND	2.24	113.85	110.24
19	B	827	CLA	CHD-C1D-C2D	2.23	130.17	125.48
19	B	837	CLA	C4C-C3C-C2C	2.23	110.15	106.90
19	B	826	CLA	CAC-C3C-C4C	2.23	127.71	124.81
27	A	830	CL0	C2B-C1B-NB	-2.23	108.73	110.23
19	G	202	CLA	CHB-C1B-NB	-2.23	121.89	124.26
19	4	318	CLA	C2C-C1C-NC	2.23	112.06	109.97
19	A	836	CLA	C3C-C4C-NC	-2.23	108.07	110.57
19	B	827	CLA	C3B-C4B-NB	-2.23	108.44	110.52
19	A	846	CLA	CAC-C3C-C4C	-2.23	121.92	124.81
19	A	807	CLA	C4A-NA-C1A	-2.23	105.70	106.71
19	F	303	CLA	CHA-C4D-ND	2.23	137.16	132.50
19	B	822	CLA	CMC-C2C-C1C	2.23	128.43	125.04
19	F	306	CLA	C3D-C4D-ND	2.22	113.83	110.24
19	1	612	CLA	CHA-C1A-NA	-2.22	121.31	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	C2C-C1C-NC	2.22	112.06	109.97
19	A	808	CLA	C3D-C4D-ND	2.22	113.83	110.24
19	A	840	CLA	C3A-C2A-C1A	-2.22	98.01	101.34
19	A	812	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
19	3	306	CLA	CHC-C1C-NC	2.22	127.57	124.20
19	3	301	CLA	CHA-C1A-NA	-2.22	121.31	126.40
19	3	314	CLA	CHC-C4B-NB	-2.22	121.91	124.26
19	B	835	CLA	C3B-C2B-C1B	2.22	109.84	107.16
19	A	816	CLA	CHC-C1C-NC	2.22	127.57	124.20
27	A	830	CL0	CHA-C1A-NA	-2.22	121.32	126.40
19	4	307	CLA	CHA-C1A-NA	-2.22	121.32	126.40
19	B	808	CLA	C3B-C4B-NB	-2.22	108.46	110.52
19	B	804	CLA	CHC-C1C-NC	2.22	127.57	124.20
19	A	848	CLA	CHD-C1D-C2D	2.22	130.13	125.48
18	4	319	CHL	C4D-CHA-C1A	2.22	123.94	121.25
19	A	846	CLA	C1-C2-C3	-2.21	122.21	126.04
19	A	843	CLA	C2D-C1D-ND	-2.21	108.47	110.10
19	A	814	CLA	CHB-C4A-NA	-2.21	121.45	124.51
19	A	814	CLA	C4D-CHA-C1A	2.21	123.94	121.25
19	G	203	CLA	C2A-C1A-CHA	2.21	127.73	123.86
19	B	820	CLA	C12-C11-C10	-2.21	103.08	113.24
19	B	832	CLA	CHB-C4A-NA	-2.21	121.46	124.51
19	B	818	CLA	CHC-C4B-NB	-2.21	121.92	124.26
19	A	805	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
19	B	832	CLA	CHD-C1D-C2D	2.21	130.11	125.48
19	A	808	CLA	C2D-C1D-ND	2.21	111.73	110.10
19	4	318	CLA	CMC-C2C-C1C	2.21	128.40	125.04
19	B	806	CLA	CMC-C2C-C1C	2.20	128.40	125.04
18	2	313	CHL	CHD-C1D-C2D	2.20	130.10	125.48
19	A	802	CLA	CHB-C1B-NB	-2.20	121.93	124.26
19	B	837	CLA	CMC-C2C-C1C	2.20	128.39	125.04
19	B	844	CLA	CHD-C1D-C2D	2.20	130.10	125.48
19	B	845	CLA	CHD-C1D-C2D	2.20	130.10	125.48
19	3	314	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
19	A	827	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
19	A	815	CLA	C2D-C1D-ND	2.20	111.72	110.10
19	B	848	CLA	CHD-C1D-C2D	2.20	130.09	125.48
19	F	306	CLA	CHD-C1D-C2D	2.20	130.09	125.48
19	B	835	CLA	C3C-C4C-NC	-2.20	108.11	110.57
19	1	603	CLA	CHD-C1D-C2D	2.20	130.09	125.48
19	3	307	CLA	CHA-C1A-NA	-2.20	121.37	126.40
19	B	833	CLA	CHA-C4D-ND	2.19	137.09	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	CHB-C1B-NB	-2.19	121.94	124.26
19	A	831	CLA	C1D-ND-C4D	-2.19	104.78	106.33
19	B	803	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	B	804	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
19	A	828	CLA	C3C-C4C-NC	2.19	113.03	110.57
19	A	842	CLA	O2A-C1-C2	2.18	114.37	108.64
19	1	612	CLA	C2C-C1C-NC	2.18	112.02	109.97
19	L	304	CLA	CMC-C2C-C1C	2.18	128.36	125.04
19	A	831	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
19	B	804	CLA	CHD-C1D-C2D	2.18	130.05	125.48
19	B	823	CLA	CAA-C2A-C1A	-2.18	104.84	111.97
19	A	836	CLA	CMC-C2C-C1C	2.18	128.35	125.04
19	A	834	CLA	C1D-ND-C4D	-2.17	104.79	106.33
19	B	836	CLA	CMC-C2C-C1C	2.17	128.35	125.04
19	A	823	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
18	4	319	CHL	CHA-C1A-NA	-2.17	121.42	126.40
19	A	828	CLA	CAA-CBA-CGA	-2.17	106.90	113.25
19	B	821	CLA	C4D-CHA-C1A	2.17	123.89	121.25
19	4	314	CLA	C2B-C1B-NB	-2.17	108.78	110.23
19	A	842	CLA	C2B-C1B-NB	2.17	111.69	110.23
19	A	842	CLA	CHB-C1B-NB	-2.17	121.96	124.26
19	A	849	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
19	B	842	CLA	CGD-CBD-CAD	-2.17	103.70	110.73
19	4	314	CLA	CHA-C1A-NA	-2.17	121.43	126.40
19	A	820	CLA	CHD-C1D-C2D	2.17	130.03	125.48
19	B	830	CLA	C17-C16-C15	-2.17	103.28	113.24
19	A	843	CLA	CAA-CBA-CGA	2.17	119.58	113.25
19	A	851	CLA	CMA-C3A-C4A	2.16	117.58	111.77
19	B	801	CLA	CHA-C1A-NA	-2.16	121.45	126.40
19	B	835	CLA	C3D-C4D-ND	2.16	113.73	110.24
19	B	809	CLA	C1-O2A-CGA	-2.16	110.78	116.44
19	A	828	CLA	CAC-C3C-C4C	2.16	127.61	124.81
19	4	314	CLA	CHC-C1C-NC	2.16	127.48	124.20
19	1	605	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
23	A	835	LHG	O7-C5-C4	-2.15	100.61	108.40
19	B	846	CLA	C1D-ND-C4D	-2.15	104.81	106.33
19	1	608	CLA	C2C-C1C-NC	2.15	111.99	109.97
19	H	201	CLA	CHC-C1C-C2C	-2.15	120.76	126.73
18	2	313	CHL	CHC-C1C-C2C	-2.15	118.32	126.11
19	L	304	CLA	CHD-C1D-C2D	2.15	129.99	125.48
19	1	603	CLA	CHC-C1C-NC	2.15	127.46	124.20
19	A	825	CLA	CHB-C4A-NA	2.15	127.48	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	852	BCR	C23-C24-C25	2.15	133.23	127.20
19	4	317	CLA	CHA-C1A-NA	-2.15	121.48	126.40
19	A	820	CLA	CHA-C1A-NA	-2.15	121.48	126.40
19	3	304	CLA	CMC-C2C-C1C	2.15	128.31	125.04
19	2	301	CLA	C2D-C1D-ND	-2.15	108.52	110.10
19	2	311	CLA	CHB-C1B-NB	-2.15	121.99	124.26
24	L	302	BCR	C23-C24-C25	2.14	133.22	127.20
19	2	312	CLA	C1D-ND-C4D	-2.14	104.81	106.33
19	A	812	CLA	C3B-C4B-NB	-2.14	108.53	110.52
19	L	305	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	B	834	CLA	C7-C6-C5	2.14	119.17	113.36
19	B	819	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	B	843	CLA	C1-C2-C3	-2.14	122.34	126.04
19	A	806	CLA	CBA-CAA-C2A	2.14	118.23	113.47
19	A	801	CLA	CMC-C2C-C1C	2.14	128.29	125.04
18	3	303	CHL	C1D-ND-C4D	-2.14	104.82	106.33
19	F	303	CLA	CMC-C2C-C1C	2.14	128.29	125.04
19	3	302	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
24	B	816	BCR	C39-C30-C29	2.13	117.44	108.91
19	4	314	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
19	A	812	CLA	CHA-C1A-NA	-2.13	121.51	126.40
19	B	845	CLA	C6-C5-C3	2.13	119.05	113.45
19	A	812	CLA	C9-C8-C10	2.13	119.01	111.29
19	B	818	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
19	B	821	CLA	C3A-C2A-C1A	-2.13	98.15	101.34
19	A	844	CLA	CHD-C1D-C2D	2.12	129.93	125.48
19	B	803	CLA	CHD-C1D-C2D	2.12	129.93	125.48
19	A	818	CLA	C1D-ND-C4D	-2.12	104.83	106.33
19	4	311	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
19	B	809	CLA	C2B-C1B-NB	-2.12	108.81	110.23
18	1	601	CHL	CMB-C2B-C1B	-2.12	122.14	125.37
19	B	846	CLA	CHC-C1C-C2C	-2.12	120.84	126.73
19	4	307	CLA	CHB-C1B-NB	-2.12	122.02	124.26
19	A	842	CLA	C3D-C4D-ND	2.12	113.66	110.24
19	B	842	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
19	A	810	CLA	CHC-C1C-NC	2.11	127.41	124.20
19	B	822	CLA	CHD-C1D-C2D	2.11	129.91	125.48
19	B	837	CLA	CHB-C1B-NB	-2.11	122.02	124.26
19	A	818	CLA	C3A-C2A-C1A	2.11	104.50	101.34
19	1	605	CLA	C1D-ND-C4D	-2.11	104.83	106.33
19	3	312	CLA	CHD-C1D-C2D	2.11	129.91	125.48
19	K	203	CLA	CHC-C1C-NC	2.11	127.41	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	814	CLA	C3A-C2A-C1A	-2.11	98.18	101.34
19	B	839	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	A	842	CLA	C4C-C3C-C2C	2.11	109.97	106.90
24	A	804	BCR	C2-C3-C4	2.11	116.08	111.38
19	A	836	CLA	CHC-C1C-NC	2.11	127.40	124.20
23	A	835	LHG	C10-C9-C8	-2.10	105.62	113.19
19	1	612	CLA	C1-C2-C3	-2.10	122.40	126.04
19	A	814	CLA	CMC-C2C-C1C	2.10	128.24	125.04
19	A	810	CLA	CHA-C4D-ND	2.10	136.90	132.50
19	L	303	CLA	CHD-C1D-C2D	2.10	129.89	125.48
19	A	802	CLA	C2C-C1C-NC	2.10	111.94	109.97
19	1	612	CLA	CHD-C1D-C2D	2.10	129.88	125.48
19	A	811	CLA	CHB-C1B-NB	-2.10	122.03	124.26
19	B	801	CLA	C1D-ND-C4D	-2.10	104.84	106.33
27	A	830	CL0	CGD-CBD-CAD	-2.10	103.94	110.73
19	A	836	CLA	CHA-C1A-NA	-2.10	121.60	126.40
19	B	843	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
19	A	821	CLA	CBA-CAA-C2A	2.09	120.04	113.86
19	1	603	CLA	CHC-C1C-C2C	-2.09	120.92	126.73
19	B	831	CLA	CHC-C4B-NB	-2.09	122.04	124.26
19	B	832	CLA	CMA-C3A-C4A	2.09	117.39	111.77
19	A	828	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
19	A	801	CLA	CHD-C1D-C2D	2.09	129.85	125.48
19	A	817	CLA	CHC-C1C-NC	2.08	127.36	124.20
19	B	842	CLA	CHB-C1B-NB	-2.08	122.05	124.26
18	3	315	CHL	CHD-C1D-C2D	2.08	129.84	125.48
19	F	306	CLA	CHC-C1C-NC	2.08	127.36	124.20
19	B	839	CLA	C2C-C1C-NC	2.08	111.92	109.97
19	B	826	CLA	C3B-C4B-NB	-2.08	108.59	110.52
19	B	827	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
19	A	806	CLA	C2D-C1D-ND	2.07	111.63	110.10
19	A	825	CLA	CHD-C1D-C2D	2.07	129.83	125.48
19	A	808	CLA	C1-C2-C3	-2.07	122.46	126.04
19	2	310	CLA	C1D-CHD-C4C	-2.07	121.58	126.06
19	B	827	CLA	C3B-C2B-C1B	2.07	109.67	107.16
23	A	835	LHG	C25-C24-C23	-2.07	106.08	113.62
19	B	833	CLA	C1-C2-C3	-2.07	122.46	126.04
19	A	829	CLA	O2A-C1-C2	-2.07	103.19	108.64
19	A	823	CLA	CHC-C1C-NC	2.07	127.34	124.20
19	B	843	CLA	C17-C16-C15	2.07	122.74	113.24
19	A	802	CLA	CHD-C1D-C2D	2.07	129.82	125.48
19	A	846	CLA	CHB-C1B-NB	-2.07	122.07	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	101	CLA	C4D-CHA-C1A	-2.06	118.74	121.25
19	3	301	CLA	CHD-C1D-C2D	2.06	129.81	125.48
19	B	832	CLA	C4D-CHA-C1A	2.06	123.76	121.25
19	G	203	CLA	CMC-C2C-C1C	2.06	128.18	125.04
19	B	845	CLA	CHC-C4B-NB	-2.06	122.08	124.26
19	A	801	CLA	CBA-CAA-C2A	-2.06	107.78	113.86
19	3	308	CLA	CHC-C1C-NC	2.06	127.33	124.20
19	A	807	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	G	203	CLA	CHA-C4D-ND	2.06	136.80	132.50
19	B	839	CLA	CGD-CBD-CAD	-2.05	104.08	110.73
19	B	820	CLA	CHC-C1C-C2C	-2.05	121.03	126.73
19	B	826	CLA	C2D-C1D-ND	2.05	111.62	110.10
19	A	837	CLA	CHA-C4D-ND	2.05	136.79	132.50
19	1	603	CLA	CAA-CBA-CGA	2.05	119.23	113.25
19	2	310	CLA	C2A-C1A-CHA	2.05	127.44	123.86
19	K	202	CLA	CAA-CBA-CGA	2.05	117.94	112.51
19	B	836	CLA	C1-C2-C3	-2.04	122.51	126.04
19	B	835	CLA	CHB-C1B-NB	-2.04	122.09	124.26
19	B	823	CLA	CHC-C1C-NC	2.04	127.30	124.20
24	B	813	BCR	C39-C30-C25	-2.04	106.98	110.30
18	3	315	CHL	C4D-CHA-C1A	2.04	123.74	121.25
19	B	824	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
19	B	847	CLA	C3A-C2A-C1A	2.04	104.40	101.34
18	1	606	CHL	CHA-C1A-NA	-2.04	121.73	126.40
19	A	843	CLA	C1-O2A-CGA	2.04	121.80	116.44
19	4	311	CLA	CHC-C1C-NC	2.04	127.30	124.20
19	A	815	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	2	312	CLA	C2A-C3A-C4A	2.04	105.16	101.87
19	G	203	CLA	C3B-C4B-NB	-2.04	108.62	110.52
19	A	844	CLA	CAA-C2A-C1A	-2.04	107.63	112.14
29	B	817	DGD	O6D-C5D-C6D	2.04	110.78	106.67
23	1	617	LHG	C6-C5-C4	2.04	116.60	111.79
19	A	840	CLA	C1-C2-C3	2.04	129.56	126.04
19	4	311	CLA	CHC-C4B-NB	-2.03	122.10	124.26
19	J	101	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
19	A	816	CLA	CHD-C1D-C2D	2.03	129.75	125.48
19	B	833	CLA	CHD-C1D-C2D	2.03	129.75	125.48
19	G	203	CLA	CAA-CBA-CGA	2.03	117.90	112.51
19	A	825	CLA	CAC-C3C-C4C	2.03	127.44	124.81
19	A	809	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
19	B	831	CLA	C7-C6-C5	-2.03	107.85	113.36
19	A	801	CLA	CHC-C1C-NC	2.03	127.28	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	306	CLA	CHC-C1C-C2C	-2.03	121.10	126.73
19	A	823	CLA	C11-C10-C8	2.03	122.47	115.92
19	A	815	CLA	C4C-C3C-C2C	2.03	109.85	106.90
19	2	312	CLA	CHC-C1C-NC	2.03	127.28	124.20
19	B	826	CLA	C4D-CHA-C1A	2.03	123.71	121.25
19	G	203	CLA	C3B-C2B-C1B	2.03	109.61	107.16
19	A	819	CLA	O2A-C1-C2	-2.02	103.31	108.64
19	A	844	CLA	CHC-C1C-NC	2.02	127.27	124.20
19	B	827	CLA	CHC-C4B-NB	-2.02	122.12	124.26
19	4	317	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	A	810	CLA	CHB-C1B-NB	-2.02	122.12	124.26
19	B	845	CLA	C1-O2A-CGA	2.02	121.74	116.44
19	B	829	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	4	318	CLA	CHC-C1C-C2C	-2.02	121.12	126.73
19	A	827	CLA	C3B-C4B-NB	-2.02	108.64	110.52
19	B	836	CLA	C3B-C4B-NB	-2.02	108.64	110.52
19	A	801	CLA	CHC-C1C-C2C	-2.02	121.13	126.73
19	B	822	CLA	C1D-ND-C4D	-2.02	104.90	106.33
19	3	306	CLA	C3B-C4B-NB	-2.02	108.64	110.52
22	3	310	A1LXP	C17-C16-C15	-2.02	115.85	118.94
19	A	819	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
19	A	822	CLA	C3B-C4B-NB	-2.01	108.65	110.52
19	A	818	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
19	B	843	CLA	C12-C11-C10	2.01	122.49	113.24
19	B	820	CLA	CHA-C1A-NA	-2.01	121.79	126.40
19	B	840	CLA	C3B-C4B-NB	-2.01	108.65	110.52
19	A	801	CLA	C1D-CHD-C4C	-2.01	121.72	126.06
19	1	608	CLA	C3B-C4B-NB	-2.01	108.65	110.52
18	3	303	CHL	CMA-C3A-C4A	-2.01	106.38	111.77
19	2	310	CLA	CAA-CBA-CGA	2.01	119.11	113.25
19	A	828	CLA	C10-C8-C7	-2.01	101.58	112.13
19	A	827	CLA	C1-C2-C3	-2.00	122.58	126.04
19	A	840	CLA	C2C-C1C-NC	2.00	111.85	109.97
19	A	814	CLA	CMA-C3A-C4A	2.00	117.15	111.77
19	A	824	CLA	CBB-CAB-C3B	2.00	137.57	127.62

All (65) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	1	601	CHL	C8
18	2	316	CHL	C8
18	3	303	CHL	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
19	1	602	CLA	C8
19	1	603	CLA	C8
19	1	608	CLA	C8
19	1	612	CLA	C8
19	2	310	CLA	C8
19	2	312	CLA	C8
19	3	301	CLA	C8
19	3	304	CLA	C8
19	3	314	CLA	C8
19	4	317	CLA	C8
19	A	801	CLA	C8
19	A	802	CLA	C8
19	A	808	CLA	C8
19	A	809	CLA	C8
19	A	811	CLA	C8
19	A	812	CLA	C8
19	A	813	CLA	C8
19	A	814	CLA	C8
19	A	818	CLA	C8
19	A	819	CLA	C8
19	A	824	CLA	C8
19	A	826	CLA	C8
19	A	827	CLA	C8
19	A	828	CLA	C8
19	A	829	CLA	C8
19	A	831	CLA	C8
19	A	833	CLA	C8
19	A	834	CLA	C8
19	A	837	CLA	C8
19	A	840	CLA	C8
19	A	842	CLA	C8
19	A	846	CLA	C8
19	A	850	CLA	C8
19	A	851	CLA	C8
19	B	801	CLA	C8
19	B	802	CLA	C8
19	B	806	CLA	C8
19	B	808	CLA	C8
19	B	809	CLA	C8
19	B	810	CLA	C8
19	B	818	CLA	C8
19	B	819	CLA	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
19	B	820	CLA	C8
19	B	822	CLA	C8
19	B	823	CLA	C8
19	B	825	CLA	C8
19	B	826	CLA	C8
19	B	827	CLA	C8
19	B	830	CLA	C8
19	B	831	CLA	C8
19	B	833	CLA	C8
19	B	834	CLA	C8
19	B	835	CLA	C8
19	B	836	CLA	C8
19	B	841	CLA	C8
19	B	843	CLA	C8
19	B	844	CLA	C8
19	B	845	CLA	C8
19	B	846	CLA	C8
19	H	201	CLA	C8
19	J	101	CLA	C8
19	L	304	CLA	C8

All (1026) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	601	CHL	C1C-C2C-CMC-OMC
18	1	601	CHL	C3C-C2C-CMC-OMC
18	1	606	CHL	C1C-C2C-CMC-OMC
18	1	606	CHL	C3C-C2C-CMC-OMC
18	2	313	CHL	C1C-C2C-CMC-OMC
18	2	315	CHL	C1C-C2C-CMC-OMC
18	2	315	CHL	C3C-C2C-CMC-OMC
18	2	315	CHL	CBD-CGD-O2D-CED
18	2	316	CHL	C1C-C2C-CMC-OMC
18	2	316	CHL	C3C-C2C-CMC-OMC
18	3	303	CHL	C1C-C2C-CMC-OMC
18	3	303	CHL	C3C-C2C-CMC-OMC
18	3	315	CHL	C3C-C2C-CMC-OMC
18	4	313	CHL	C1C-C2C-CMC-OMC
18	4	313	CHL	C3C-C2C-CMC-OMC
18	4	319	CHL	C1C-C2C-CMC-OMC
19	1	602	CLA	C3A-C2A-CAA-CBA
19	1	603	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	603	CLA	C3A-C2A-CAA-CBA
19	1	603	CLA	C11-C10-C8-C9
19	1	605	CLA	C2B-C3B-CAB-CBB
19	1	605	CLA	C4B-C3B-CAB-CBB
19	1	607	CLA	O2A-C1-C2-C3
19	1	607	CLA	C2-C3-C5-C6
19	1	607	CLA	C4-C3-C5-C6
19	1	608	CLA	C6-C7-C8-C9
19	2	301	CLA	C2B-C3B-CAB-CBB
19	2	301	CLA	C4B-C3B-CAB-CBB
19	2	310	CLA	CBD-CGD-O2D-CED
19	3	302	CLA	C2B-C3B-CAB-CBB
19	3	302	CLA	C4B-C3B-CAB-CBB
19	3	312	CLA	C1A-C2A-CAA-CBA
19	3	312	CLA	C3A-C2A-CAA-CBA
19	4	318	CLA	C2B-C3B-CAB-CBB
19	4	318	CLA	C4B-C3B-CAB-CBB
19	A	819	CLA	C6-C7-C8-C9
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	C2B-C3B-CAB-CBB
19	A	824	CLA	C4B-C3B-CAB-CBB
19	A	825	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C2B-C3B-CAB-CBB
19	A	825	CLA	C4B-C3B-CAB-CBB
19	A	825	CLA	CHA-CBD-CGD-O1D
19	A	825	CLA	CHA-CBD-CGD-O2D
19	A	827	CLA	CHA-CBD-CGD-O1D
19	A	827	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	C11-C12-C13-C14
19	A	833	CLA	C6-C7-C8-C9
19	A	836	CLA	C1A-C2A-CAA-CBA
19	A	837	CLA	CHA-CBD-CGD-O1D
19	A	837	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	C6-C7-C8-C9
19	A	844	CLA	CHA-CBD-CGD-O1D
19	A	844	CLA	CHA-CBD-CGD-O2D
19	A	846	CLA	CHA-CBD-CGD-O1D
19	A	846	CLA	CHA-CBD-CGD-O2D
19	A	848	CLA	CHA-CBD-CGD-O2D
19	A	850	CLA	C6-C7-C8-C9
19	A	851	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	851	CLA	C4-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	B	809	CLA	C2-C3-C5-C6
19	B	809	CLA	C4-C3-C5-C6
19	B	809	CLA	C11-C10-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	B	818	CLA	C2-C1-O2A-CGA
19	B	818	CLA	CHA-CBD-CGD-O2D
19	B	819	CLA	C11-C10-C8-C9
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C3A-C2A-CAA-CBA
19	B	823	CLA	C6-C7-C8-C10
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	826	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C4-C3-C5-C6
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C2-C3-C5-C6
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C12-C13-C15-C16
19	B	831	CLA	C2-C3-C5-C6
19	B	831	CLA	C14-C13-C15-C16
19	B	840	CLA	CHA-CBD-CGD-O1D
19	B	840	CLA	CHA-CBD-CGD-O2D
19	B	842	CLA	CHA-CBD-CGD-O1D
19	B	842	CLA	CHA-CBD-CGD-O2D
19	B	844	CLA	C1A-C2A-CAA-CBA
19	B	844	CLA	C3A-C2A-CAA-CBA
19	B	846	CLA	C6-C7-C8-C9
19	G	203	CLA	C2B-C3B-CAB-CBB
19	G	203	CLA	C4B-C3B-CAB-CBB
19	K	203	CLA	C1A-C2A-CAA-CBA
19	K	203	CLA	C2B-C3B-CAB-CBB
19	K	203	CLA	C4B-C3B-CAB-CBB
21	2	306	XAT	O4-C6-C7-C8
22	3	305	A1LXP	C24-C1-C42-C2
22	J	102	A1LXP	C17-C18-C19-C29
22	J	102	A1LXP	C17-C18-C19-C33
23	1	617	LHG	C3-O3-P-O4
23	1	617	LHG	C3-O3-P-O5
23	1	617	LHG	C4-O6-P-O4
23	1	617	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	302	LHG	C4-O6-P-O4
23	2	302	LHG	C4-O6-P-O5
23	A	835	LHG	C3-O3-P-O5
24	3	316	BCR	C1-C6-C7-C8
24	3	316	BCR	C5-C6-C7-C8
24	3	316	BCR	C23-C24-C25-C30
24	4	308	BCR	C23-C24-C25-C26
24	4	308	BCR	C23-C24-C25-C30
24	A	804	BCR	C22-C23-C24-C25
24	A	841	BCR	C23-C24-C25-C26
24	A	841	BCR	C23-C24-C25-C30
24	B	812	BCR	C7-C8-C9-C10
24	G	205	BCR	C37-C22-C23-C24
24	J	105	BCR	C23-C24-C25-C26
24	K	201	BCR	C1-C6-C7-C8
19	3	302	CLA	O1D-CGD-O2D-CED
19	F	303	CLA	O1D-CGD-O2D-CED
19	H	201	CLA	O1D-CGD-O2D-CED
19	B	843	CLA	C13-C15-C16-C17
19	3	302	CLA	CBD-CGD-O2D-CED
19	4	307	CLA	CBD-CGD-O2D-CED
19	4	314	CLA	CBD-CGD-O2D-CED
19	B	828	CLA	CBD-CGD-O2D-CED
19	F	303	CLA	CBD-CGD-O2D-CED
19	H	201	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	O1A-CGA-O2A-C1
18	2	315	CHL	O1D-CGD-O2D-CED
18	2	313	CHL	CBD-CGD-O2D-CED
19	A	806	CLA	CBD-CGD-O2D-CED
19	B	808	CLA	CBD-CGD-O2D-CED
19	2	310	CLA	O1D-CGD-O2D-CED
18	2	316	CHL	C3-C5-C6-C7
19	1	602	CLA	C3-C5-C6-C7
19	2	310	CLA	C3-C5-C6-C7
19	A	831	CLA	C3-C5-C6-C7
19	A	851	CLA	C3-C5-C6-C7
19	B	802	CLA	C3-C5-C6-C7
19	B	806	CLA	C3-C5-C6-C7
19	B	827	CLA	C3-C5-C6-C7
19	B	830	CLA	C3-C5-C6-C7
19	A	822	CLA	CBA-CGA-O2A-C1
23	1	620	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	823	CLA	C8-C10-C11-C12
19	2	301	CLA	CBD-CGD-O2D-CED
19	B	838	CLA	CBD-CGD-O2D-CED
19	1	603	CLA	C2A-CAA-CBA-CGA
19	A	822	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	B	826	CLA	C2A-CAA-CBA-CGA
19	L	304	CLA	C3-C5-C6-C7
18	1	601	CHL	CBD-CGD-O2D-CED
18	1	606	CHL	CBD-CGD-O2D-CED
19	B	846	CLA	CBD-CGD-O2D-CED
19	B	828	CLA	O1D-CGD-O2D-CED
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	842	CLA	C3-C5-C6-C7
29	B	817	DGD	O6E-C5E-C6E-O5E
19	4	307	CLA	O1D-CGD-O2D-CED
19	4	314	CLA	O1D-CGD-O2D-CED
25	4	304	LMG	C10-C11-C12-C13
19	A	813	CLA	CBD-CGD-O2D-CED
25	N	201	LMG	C32-C33-C34-C35
19	B	822	CLA	C3-C5-C6-C7
19	B	844	CLA	C3-C5-C6-C7
19	A	827	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	O1A-CGA-O2A-C1
19	A	842	CLA	C4-C3-C5-C6
19	B	818	CLA	C4-C3-C5-C6
29	B	817	DGD	C4E-C5E-C6E-O5E
19	A	842	CLA	C2-C3-C5-C6
19	B	818	CLA	C2-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
19	1	603	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBD-CGD-O2D-CED
19	A	806	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
23	1	617	LHG	C1-C2-C3-O3
25	J	103	LMG	C4-C5-C6-O5
19	1	607	CLA	O1A-CGA-O2A-C1
19	A	818	CLA	C3-C5-C6-C7
19	B	831	CLA	C3-C5-C6-C7
19	1	607	CLA	CBA-CGA-O2A-C1
19	3	306	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	847	CLA	CBA-CGA-O2A-C1
19	B	818	CLA	CBD-CGD-O2D-CED
19	G	202	CLA	CBD-CGD-O2D-CED
19	B	826	CLA	C10-C11-C12-C13
19	B	847	CLA	O1A-CGA-O2A-C1
18	3	303	CHL	C10-C11-C12-C13
19	2	312	CLA	C10-C11-C12-C13
19	A	826	CLA	C8-C10-C11-C12
19	A	840	CLA	C8-C10-C11-C12
23	1	617	LHG	O2-C2-C3-O3
23	1	620	LHG	O10-C23-O8-C6
19	1	602	CLA	C2-C3-C5-C6
19	2	312	CLA	C11-C12-C13-C14
19	3	301	CLA	C11-C10-C8-C9
19	A	808	CLA	C11-C10-C8-C9
19	A	809	CLA	C6-C7-C8-C9
19	A	812	CLA	C11-C10-C8-C9
19	A	813	CLA	C6-C7-C8-C9
19	A	823	CLA	C11-C12-C13-C14
19	A	828	CLA	C6-C7-C8-C9
19	A	837	CLA	C6-C7-C8-C9
19	A	846	CLA	C11-C10-C8-C9
19	B	810	CLA	C14-C13-C15-C16
19	B	818	CLA	C11-C10-C8-C9
19	B	820	CLA	C6-C7-C8-C9
19	B	820	CLA	C14-C13-C15-C16
19	B	822	CLA	C11-C10-C8-C9
19	B	825	CLA	C6-C7-C8-C9
19	B	831	CLA	C11-C10-C8-C9
19	B	845	CLA	C6-C7-C8-C9
18	2	313	CHL	O1D-CGD-O2D-CED
19	1	605	CLA	CBD-CGD-O2D-CED
18	2	315	CHL	C2A-CAA-CBA-CGA
19	1	607	CLA	C2A-CAA-CBA-CGA
19	A	851	CLA	C2A-CAA-CBA-CGA
24	4	308	BCR	C37-C22-C23-C24
24	B	812	BCR	C7-C8-C9-C34
24	B	813	BCR	C7-C8-C9-C34
19	B	826	CLA	C15-C16-C17-C18
19	A	837	CLA	CBD-CGD-O2D-CED
19	A	802	CLA	CBA-CGA-O2A-C1
19	A	819	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	828	CLA	C10-C11-C12-C13
19	B	802	CLA	C10-C11-C12-C13
19	B	806	CLA	C8-C10-C11-C12
19	B	808	CLA	C5-C6-C7-C8
19	B	825	CLA	C15-C16-C17-C18
19	B	830	CLA	C8-C10-C11-C12
19	3	301	CLA	C8-C10-C11-C12
19	A	813	CLA	C5-C6-C7-C8
19	B	809	CLA	C5-C6-C7-C8
19	B	825	CLA	C10-C11-C12-C13
19	L	304	CLA	C10-C11-C12-C13
19	A	818	CLA	C10-C11-C12-C13
18	3	303	CHL	C5-C6-C7-C8
19	B	801	CLA	C13-C15-C16-C17
19	B	831	CLA	C5-C6-C7-C8
19	1	608	CLA	C5-C6-C7-C8
19	A	812	CLA	C15-C16-C17-C18
19	B	846	CLA	C8-C10-C11-C12
19	B	838	CLA	O1D-CGD-O2D-CED
19	A	819	CLA	C11-C10-C8-C7
19	A	824	CLA	C11-C10-C8-C7
19	A	834	CLA	C6-C7-C8-C10
19	A	850	CLA	C11-C10-C8-C7
19	A	851	CLA	C11-C10-C8-C7
19	B	806	CLA	C6-C7-C8-C10
19	B	819	CLA	C6-C7-C8-C10
19	B	834	CLA	C11-C10-C8-C7
19	B	835	CLA	C6-C7-C8-C10
19	B	843	CLA	C6-C7-C8-C10
19	B	845	CLA	C11-C10-C8-C7
19	B	818	CLA	O1A-CGA-O2A-C1
19	B	808	CLA	O1D-CGD-O2D-CED
19	L	304	CLA	C5-C6-C7-C8
25	J	103	LMG	O6-C5-C6-O5
19	3	306	CLA	O1A-CGA-O2A-C1
19	B	827	CLA	C5-C6-C7-C8
19	A	806	CLA	C2C-C3C-CAC-CBC
19	A	819	CLA	C8-C10-C11-C12
19	B	822	CLA	C5-C6-C7-C8
23	2	302	LHG	C23-C24-C25-C26
18	1	601	CHL	C5-C6-C7-C8
19	A	809	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	824	CLA	C8-C10-C11-C12
19	B	810	CLA	C8-C10-C11-C12
19	B	825	CLA	C8-C10-C11-C12
19	B	834	CLA	C13-C15-C16-C17
19	B	845	CLA	C5-C6-C7-C8
19	A	808	CLA	C5-C6-C7-C8
19	A	834	CLA	C13-C15-C16-C17
19	A	840	CLA	C10-C11-C12-C13
23	1	617	LHG	C3-O3-P-O6
23	1	617	LHG	C4-O6-P-O3
23	2	302	LHG	C4-O6-P-O3
23	A	835	LHG	C3-O3-P-O6
19	B	831	CLA	CBA-CGA-O2A-C1
19	B	846	CLA	O1D-CGD-O2D-CED
19	4	317	CLA	CBD-CGD-O2D-CED
18	1	601	CHL	O1D-CGD-O2D-CED
18	1	606	CHL	O1D-CGD-O2D-CED
19	1	602	CLA	C4-C3-C5-C6
19	A	828	CLA	C8-C10-C11-C12
19	A	833	CLA	C8-C10-C11-C12
19	2	301	CLA	O1D-CGD-O2D-CED
19	A	812	CLA	O1D-CGD-O2D-CED
19	B	822	CLA	C2A-CAA-CBA-CGA
19	B	841	CLA	C3-C5-C6-C7
19	A	846	CLA	C10-C11-C12-C13
19	G	203	CLA	CBD-CGD-O2D-CED
19	H	201	CLA	C5-C6-C7-C8
23	2	302	LHG	C27-C28-C29-C30
19	B	802	CLA	C11-C12-C13-C15
19	B	818	CLA	C16-C17-C18-C19
23	2	302	LHG	C25-C26-C27-C28
19	B	807	CLA	CBD-CGD-O2D-CED
23	1	617	LHG	C27-C28-C29-C30
23	2	302	LHG	C33-C34-C35-C36
19	A	811	CLA	C3-C5-C6-C7
19	B	826	CLA	C3-C5-C6-C7
19	B	823	CLA	CBD-CGD-O2D-CED
25	F	301	LMG	C10-C11-C12-C13
19	A	828	CLA	CBA-CGA-O2A-C1
19	H	201	CLA	CBA-CGA-O2A-C1
25	J	103	LMG	C34-C35-C36-C37
19	B	810	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	827	CLA	C16-C17-C18-C20
19	A	837	CLA	C4-C3-C5-C6
19	A	840	CLA	C11-C10-C8-C9
19	A	840	CLA	C14-C13-C15-C16
19	B	826	CLA	C6-C7-C8-C9
19	B	830	CLA	C14-C13-C15-C16
23	1	617	LHG	C30-C31-C32-C33
19	A	821	CLA	C2A-CAA-CBA-CGA
19	B	831	CLA	O1A-CGA-O2A-C1
23	A	835	LHG	C24-C25-C26-C27
23	A	835	LHG	C32-C33-C34-C35
29	B	817	DGD	C7A-C8A-C9A-CAA
18	3	315	CHL	C4B-C3B-CAB-CBB
18	4	319	CHL	C4B-C3B-CAB-CBB
19	1	608	CLA	C4B-C3B-CAB-CBB
18	3	303	CHL	C16-C17-C18-C20
19	2	310	CLA	C6-C7-C8-C9
19	2	310	CLA	C6-C7-C8-C10
19	B	833	CLA	C11-C12-C13-C14
23	A	835	LHG	C28-C29-C30-C31
25	J	103	LMG	C37-C38-C39-C40
19	A	802	CLA	CBD-CGD-O2D-CED
23	A	835	LHG	C29-C30-C31-C32
19	B	846	CLA	C3-C5-C6-C7
19	A	813	CLA	O1D-CGD-O2D-CED
19	1	605	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	K	202	CLA	C3A-C2A-CAA-CBA
19	1	602	CLA	C10-C11-C12-C13
19	B	819	CLA	C5-C6-C7-C8
19	B	819	CLA	C8-C10-C11-C12
25	F	301	LMG	C11-C12-C13-C14
19	A	837	CLA	O1D-CGD-O2D-CED
19	A	842	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	C11-C12-C13-C15
19	B	807	CLA	O1D-CGD-O2D-CED
25	F	305	LMG	C10-C11-C12-C13
23	2	302	LHG	C11-C12-C13-C14
19	A	802	CLA	O1A-CGA-O2A-C1
18	2	316	CHL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	603	CLA	C4-C3-C5-C6
19	A	824	CLA	C4-C3-C5-C6
19	A	834	CLA	C4-C3-C5-C6
19	1	603	CLA	C2-C3-C5-C6
19	A	824	CLA	C2-C3-C5-C6
19	A	834	CLA	C2-C3-C5-C6
19	A	837	CLA	C2-C3-C5-C6
23	1	617	LHG	C8-C7-O7-C5
25	J	103	LMG	C10-C11-C12-C13
18	3	303	CHL	C16-C17-C18-C19
19	B	810	CLA	C16-C17-C18-C19
18	4	319	CHL	C2B-C3B-CAB-CBB
29	B	817	DGD	CAA-CBA-CCA-CDA
23	A	835	LHG	C33-C34-C35-C36
23	2	302	LHG	O9-C7-O7-C5
25	G	206	LMG	C15-C16-C17-C18
22	1	619	A1LXP	C24-C1-C42-C2
22	1	619	A1LXP	C28-C1-C42-C2
22	2	309	A1LXP	C28-C1-C42-C2
22	3	305	A1LXP	C28-C1-C42-C2
22	4	306	A1LXP	C24-C1-C42-C2
22	4	306	A1LXP	C28-C1-C42-C2
24	3	316	BCR	C23-C24-C25-C26
24	4	308	BCR	C1-C6-C7-C8
24	4	308	BCR	C5-C6-C7-C8
24	A	838	BCR	C1-C6-C7-C8
24	A	838	BCR	C5-C6-C7-C8
24	A	847	BCR	C23-C24-C25-C26
24	A	847	BCR	C23-C24-C25-C30
24	A	852	BCR	C23-C24-C25-C26
24	B	815	BCR	C1-C6-C7-C8
24	B	815	BCR	C5-C6-C7-C8
24	B	815	BCR	C23-C24-C25-C30
24	J	105	BCR	C23-C24-C25-C30
24	K	201	BCR	C5-C6-C7-C8
24	K	201	BCR	C23-C24-C25-C26
24	K	201	BCR	C23-C24-C25-C30
29	B	817	DGD	C4A-C5A-C6A-C7A
19	A	842	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	C5-C6-C7-C8
19	A	829	CLA	C5-C6-C7-C8
19	B	801	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	809	CLA	C6-C7-C8-C10
19	A	824	CLA	C6-C7-C8-C10
19	A	840	CLA	C6-C7-C8-C10
19	A	840	CLA	C12-C13-C15-C16
19	B	801	CLA	C6-C7-C8-C10
19	B	818	CLA	C11-C10-C8-C7
19	B	818	CLA	C11-C12-C13-C15
19	B	820	CLA	C6-C7-C8-C10
19	B	825	CLA	C11-C10-C8-C7
19	B	826	CLA	C6-C7-C8-C10
19	B	830	CLA	C11-C10-C8-C7
19	B	831	CLA	C11-C10-C8-C7
19	B	806	CLA	O1A-CGA-O2A-C1
19	H	201	CLA	O1A-CGA-O2A-C1
19	L	304	CLA	O1A-CGA-O2A-C1
19	A	837	CLA	C5-C6-C7-C8
19	4	311	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	C16-C17-C18-C20
28	A	839	PQN	C26-C27-C28-C29
25	4	304	LMG	O6-C5-C6-O5
19	1	608	CLA	CBA-CGA-O2A-C1
19	L	304	CLA	CBA-CGA-O2A-C1
19	3	301	CLA	C10-C11-C12-C13
19	A	851	CLA	C8-C10-C11-C12
25	J	103	LMG	C33-C34-C35-C36
25	G	206	LMG	C28-C29-C30-C31
23	2	302	LHG	C8-C7-O7-C5
19	A	851	CLA	C5-C6-C7-C8
23	1	617	LHG	O9-C7-O7-C5
19	L	304	CLA	C13-C15-C16-C17
19	B	831	CLA	C4-C3-C5-C6
29	B	817	DGD	C1A-C2A-C3A-C4A
19	A	822	CLA	C2-C3-C5-C6
19	A	819	CLA	C11-C10-C8-C9
19	A	834	CLA	C6-C7-C8-C9
19	B	825	CLA	C11-C10-C8-C9
19	3	304	CLA	C5-C6-C7-C8
19	A	802	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	C8-C10-C11-C12
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
18	2	315	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	3	315	CHL	C1A-C2A-CAA-CBA
19	1	602	CLA	C1A-C2A-CAA-CBA
19	1	605	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	K	202	CLA	C1A-C2A-CAA-CBA
25	F	305	LMG	C11-C12-C13-C14
23	A	835	LHG	O6-C4-C5-C6
19	A	840	CLA	C15-C16-C17-C18
19	B	802	CLA	C11-C12-C13-C14
19	B	806	CLA	C16-C17-C18-C19
19	B	827	CLA	C16-C17-C18-C19
25	J	103	LMG	C32-C33-C34-C35
19	B	834	CLA	C15-C16-C17-C18
19	A	806	CLA	C4C-C3C-CAC-CBC
19	B	833	CLA	C4-C3-C5-C6
19	A	825	CLA	C3A-C2A-CAA-CBA
29	B	817	DGD	CDA-CEA-CFA-CGA
23	2	302	LHG	C31-C32-C33-C34
23	A	835	LHG	C15-C16-C17-C18
25	J	103	LMG	C36-C37-C38-C39
19	B	834	CLA	C2A-CAA-CBA-CGA
25	F	305	LMG	O1-C7-C8-C9
19	F	306	CLA	CBA-CGA-O2A-C1
19	A	818	CLA	C13-C15-C16-C17
19	1	608	CLA	O1A-CGA-O2A-C1
18	3	303	CHL	C15-C16-C17-C18
19	3	302	CLA	C4-C3-C5-C6
19	B	801	CLA	C4-C3-C5-C6
19	1	605	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	A	826	CLA	C10-C11-C12-C13
19	B	844	CLA	C5-C6-C7-C8
29	B	817	DGD	C9B-CAB-CBB-CCB
19	A	834	CLA	C2A-CAA-CBA-CGA
19	B	830	CLA	C10-C11-C12-C13
19	1	608	CLA	C2-C1-O2A-CGA
19	A	816	CLA	C1-C2-C3-C5
19	B	826	CLA	C2-C1-O2A-CGA
19	A	802	CLA	C5-C6-C7-C8
23	A	835	LHG	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	J	103	LMG	C40-C41-C42-C43
18	1	601	CHL	CBA-CGA-O2A-C1
23	2	302	LHG	C24-C23-O8-C6
19	G	203	CLA	O1D-CGD-O2D-CED
23	2	302	LHG	C30-C31-C32-C33
18	2	316	CHL	C10-C11-C12-C13
19	2	310	CLA	C4-C3-C5-C6
19	B	810	CLA	C13-C15-C16-C17
19	1	602	CLA	C11-C10-C8-C7
19	1	608	CLA	C11-C10-C8-C7
19	2	312	CLA	C11-C12-C13-C15
19	2	312	CLA	C12-C13-C15-C16
19	3	301	CLA	C6-C7-C8-C10
19	A	818	CLA	C12-C13-C15-C16
19	A	826	CLA	C11-C12-C13-C15
19	B	818	CLA	C6-C7-C8-C10
19	B	822	CLA	C11-C10-C8-C7
19	B	825	CLA	C6-C7-C8-C10
19	B	846	CLA	C6-C7-C8-C10
19	A	808	CLA	C3-C5-C6-C7
19	A	814	CLA	C6-C7-C8-C9
19	A	814	CLA	C11-C10-C8-C9
19	A	818	CLA	C14-C13-C15-C16
19	A	826	CLA	C11-C10-C8-C9
19	B	808	CLA	C11-C10-C8-C9
19	B	818	CLA	C6-C7-C8-C9
19	B	820	CLA	C11-C10-C8-C9
19	B	843	CLA	C11-C10-C8-C9
18	3	303	CHL	CBD-CGD-O2D-CED
19	2	301	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	C15-C16-C17-C18
19	G	202	CLA	O1D-CGD-O2D-CED
24	4	308	BCR	C21-C22-C23-C24
24	B	813	BCR	C7-C8-C9-C10
23	2	302	LHG	C14-C15-C16-C17
19	1	603	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	O1D-CGD-O2D-CED
29	B	817	DGD	CFA-CGA-CHA-CIA
18	4	313	CHL	C4B-C3B-CAB-CBB
25	J	103	LMG	C39-C40-C41-C42
19	A	822	CLA	C4-C3-C5-C6
19	B	830	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	3	302	CLA	C2-C3-C5-C6
19	B	801	CLA	C2-C3-C5-C6
19	B	833	CLA	C2-C3-C5-C6
19	A	842	CLA	C11-C12-C13-C15
23	A	835	LHG	C31-C32-C33-C34
19	F	306	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	C3A-C2A-CAA-CBA
19	B	825	CLA	C5-C6-C7-C8
23	A	835	LHG	C30-C31-C32-C33
19	A	821	CLA	O1A-CGA-O2A-C1
18	2	316	CHL	CBA-CGA-O2A-C1
19	B	819	CLA	C15-C16-C17-C18
25	J	103	LMG	O1-C7-C8-C9
18	1	601	CHL	O1A-CGA-O2A-C1
19	A	818	CLA	C4-C3-C5-C6
28	A	839	PQN	C26-C27-C28-C30
18	2	313	CHL	C3C-C2C-CMC-OMC
18	4	319	CHL	C3C-C2C-CMC-OMC
19	B	833	CLA	C5-C6-C7-C8
25	N	201	LMG	C29-C30-C31-C32
19	B	808	CLA	C16-C17-C18-C19
28	B	811	PQN	C23-C25-C26-C27
18	4	313	CHL	C2B-C3B-CAB-CBB
23	1	617	LHG	C34-C35-C36-C37
23	2	302	LHG	O10-C23-O8-C6
25	F	305	LMG	O1-C7-C8-O7
19	B	806	CLA	C16-C17-C18-C20
19	J	101	CLA	C16-C17-C18-C19
19	B	806	CLA	C2-C1-O2A-CGA
19	A	824	CLA	C6-C7-C8-C9
19	A	826	CLA	C11-C12-C13-C14
19	A	851	CLA	C11-C10-C8-C9
19	B	801	CLA	C6-C7-C8-C9
19	B	831	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	828	CLA	C4-C3-C5-C6
19	2	301	CLA	O1A-CGA-O2A-C1
19	B	848	CLA	C2C-C3C-CAC-CBC
19	A	826	CLA	C16-C17-C18-C20
19	A	850	CLA	C16-C17-C18-C20
19	B	810	CLA	C16-C17-C18-C20
19	1	608	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	2	309	A1LXP	C24-C1-C42-C2
24	A	852	BCR	C23-C24-C25-C30
24	B	815	BCR	C23-C24-C25-C26
24	G	205	BCR	C23-C24-C25-C26
19	B	841	CLA	CAA-CBA-CGA-O2A
23	2	302	LHG	C11-C10-C9-C8
23	2	302	LHG	O6-C4-C5-C6
19	B	809	CLA	CAA-CBA-CGA-O2A
18	3	303	CHL	C12-C13-C15-C16
19	1	603	CLA	C11-C10-C8-C7
19	2	312	CLA	C11-C10-C8-C7
19	A	823	CLA	C11-C10-C8-C7
19	A	828	CLA	C6-C7-C8-C10
19	A	837	CLA	C12-C13-C15-C16
19	B	801	CLA	C11-C10-C8-C7
19	B	810	CLA	C11-C10-C8-C7
19	B	820	CLA	C11-C10-C8-C7
19	B	822	CLA	C6-C7-C8-C10
19	B	825	CLA	C12-C13-C15-C16
19	B	831	CLA	C6-C7-C8-C10
19	B	831	CLA	C12-C13-C15-C16
19	3	314	CLA	C3-C5-C6-C7
19	3	314	CLA	C5-C6-C7-C8
23	1	617	LHG	C12-C13-C14-C15
19	A	812	CLA	C8-C10-C11-C12
19	A	809	CLA	C2A-CAA-CBA-CGA
23	1	617	LHG	C32-C33-C34-C35
19	K	203	CLA	CBD-CGD-O2D-CED
19	A	846	CLA	C8-C10-C11-C12
19	B	823	CLA	C8-C10-C11-C12
19	3	307	CLA	CBA-CGA-O2A-C1
19	B	842	CLA	CBA-CGA-O2A-C1
29	B	817	DGD	C2A-C3A-C4A-C5A
19	A	825	CLA	CBD-CGD-O2D-CED
25	N	201	LMG	C30-C31-C32-C33
19	3	312	CLA	CAD-CBD-CGD-O2D
19	4	307	CLA	CAD-CBD-CGD-O2D
19	A	817	CLA	CAD-CBD-CGD-O2D
19	B	843	CLA	CAD-CBD-CGD-O2D
19	G	202	CLA	CAD-CBD-CGD-O2D
19	H	201	CLA	CAD-CBD-CGD-O2D
25	4	304	LMG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	837	CLA	C13-C15-C16-C17
19	4	318	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	C16-C17-C18-C19
25	J	103	LMG	C31-C32-C33-C34
19	3	307	CLA	O1A-CGA-O2A-C1
23	2	302	LHG	O6-C4-C5-O7
23	A	835	LHG	O6-C4-C5-O7
28	B	811	PQN	C25-C26-C27-C28
19	B	839	CLA	CBD-CGD-O2D-CED
18	4	319	CHL	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	809	CLA	CHA-CBD-CGD-O1D
19	A	809	CLA	CHA-CBD-CGD-O2D
19	A	814	CLA	CHA-CBD-CGD-O1D
19	A	814	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	CHA-CBD-CGD-O1D
19	A	840	CLA	CHA-CBD-CGD-O2D
19	B	810	CLA	CHA-CBD-CGD-O1D
19	B	810	CLA	CHA-CBD-CGD-O2D
19	B	818	CLA	CHA-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	828	CLA	CHA-CBD-CGD-O1D
19	B	828	CLA	CHA-CBD-CGD-O2D
19	B	841	CLA	CHA-CBD-CGD-O1D
18	2	316	CHL	O1A-CGA-O2A-C1
19	3	302	CLA	O1A-CGA-O2A-C1
19	2	312	CLA	C6-C7-C8-C9
19	A	837	CLA	C11-C10-C8-C9
19	4	317	CLA	O1D-CGD-O2D-CED
19	A	850	CLA	C2A-CAA-CBA-CGA
19	B	826	CLA	O1D-CGD-O2D-CED
19	A	822	CLA	C1A-C2A-CAA-CBA
19	B	839	CLA	C1A-C2A-CAA-CBA
19	3	304	CLA	C6-C7-C8-C10
19	A	811	CLA	C6-C7-C8-C9
19	A	818	CLA	C16-C17-C18-C20
19	3	302	CLA	CBA-CGA-O2A-C1
19	K	203	CLA	O1D-CGD-O2D-CED
25	G	206	LMG	C4-C5-C6-O5
19	2	310	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	830	CLA	C2-C3-C5-C6
19	1	612	CLA	C4B-C3B-CAB-CBB
19	B	831	CLA	C16-C17-C18-C20
19	A	820	CLA	O1D-CGD-O2D-CED
19	B	808	CLA	C3-C5-C6-C7
19	A	842	CLA	C11-C12-C13-C14
19	B	819	CLA	C16-C17-C18-C19
18	2	313	CHL	CAD-CBD-CGD-O1D
18	4	319	CHL	CAD-CBD-CGD-O1D
19	A	806	CLA	CAD-CBD-CGD-O1D
19	A	814	CLA	CAD-CBD-CGD-O1D
19	A	820	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CAD-CBD-CGD-O1D
19	B	830	CLA	CAD-CBD-CGD-O1D
19	A	831	CLA	C5-C6-C7-C8
19	B	806	CLA	C10-C11-C12-C13
19	B	835	CLA	C5-C6-C7-C8
23	1	617	LHG	C18-C19-C20-C21
19	A	821	CLA	CBA-CGA-O2A-C1
19	B	828	CLA	CBA-CGA-O2A-C1
19	2	312	CLA	C6-C7-C8-C10
19	A	826	CLA	C6-C7-C8-C10
19	A	828	CLA	C11-C12-C13-C15
19	A	829	CLA	C11-C10-C8-C7
19	A	829	CLA	C11-C12-C13-C15
19	A	833	CLA	C6-C7-C8-C10
19	B	801	CLA	C11-C12-C13-C15
19	B	809	CLA	C11-C10-C8-C7
19	J	101	CLA	C11-C12-C13-C15
19	4	318	CLA	CBD-CGD-O2D-CED
23	1	617	LHG	C29-C30-C31-C32
25	J	103	LMG	C38-C39-C40-C41
18	3	315	CHL	CBD-CGD-O2D-CED
19	K	202	CLA	C2A-CAA-CBA-CGA
23	1	617	LHG	C23-C24-C25-C26
18	3	315	CHL	C1C-C2C-CMC-OMC
25	J	103	LMG	O1-C7-C8-O7
25	N	201	LMG	C8-C7-O1-C1
18	1	601	CHL	C4-C3-C5-C6
19	2	312	CLA	C8-C10-C11-C12
18	3	303	CHL	C11-C12-C13-C14
18	3	303	CHL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	818	CLA	C11-C12-C13-C14
19	A	824	CLA	C11-C10-C8-C9
19	B	810	CLA	C11-C10-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B	827	CLA	C11-C12-C13-C14
19	B	834	CLA	C6-C7-C8-C9
24	A	841	BCR	C22-C23-C24-C25
19	1	602	CLA	C11-C12-C13-C14
29	B	817	DGD	CEA-CFA-CGA-CHA
19	B	828	CLA	O1A-CGA-O2A-C1
19	B	842	CLA	O1A-CGA-O2A-C1
19	B	827	CLA	C13-C15-C16-C17
18	3	315	CHL	C2B-C3B-CAB-CBB
19	1	608	CLA	C2B-C3B-CAB-CBB
19	L	304	CLA	C2B-C3B-CAB-CBB
19	A	829	CLA	C15-C16-C17-C18
19	B	837	CLA	C2-C1-O2A-CGA
19	B	843	CLA	C3-C5-C6-C7
19	B	830	CLA	C2C-C3C-CAC-CBC
19	A	812	CLA	C10-C11-C12-C13
19	B	823	CLA	C15-C16-C17-C18
19	A	817	CLA	C1-C2-C3-C4
25	F	305	LMG	C7-C8-O7-C10
19	A	801	CLA	CBA-CGA-O2A-C1
19	B	818	CLA	C13-C15-C16-C17
19	1	602	CLA	C2C-C3C-CAC-CBC
19	3	301	CLA	CAA-CBA-CGA-O2A
19	4	311	CLA	O1D-CGD-O2D-CED
23	1	617	LHG	C5-C4-O6-P
24	B	814	BCR	C23-C24-C25-C26
19	2	312	CLA	C2-C3-C5-C6
19	B	823	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	CAA-CBA-CGA-O2A
19	B	830	CLA	C4C-C3C-CAC-CBC
24	A	841	BCR	C20-C21-C22-C23
29	B	817	DGD	CBA-CCA-CDA-CEA
19	1	602	CLA	C11-C12-C13-C15
28	B	811	PQN	C26-C27-C28-C29
23	1	617	LHG	C4-C5-C6-O8
19	A	818	CLA	C11-C12-C13-C15
19	B	833	CLA	C6-C7-C8-C10
19	B	834	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	811	PQN	C16-C17-C18-C20
19	1	602	CLA	C11-C10-C8-C9
19	3	301	CLA	C6-C7-C8-C9
19	A	837	CLA	C14-C13-C15-C16
19	A	846	CLA	C6-C7-C8-C9
19	B	801	CLA	C11-C12-C13-C14
28	A	839	PQN	C25-C26-C27-C28
19	B	822	CLA	C16-C17-C18-C20
25	4	304	LMG	C29-C30-C31-C32
25	J	103	LMG	C41-C42-C43-C44
19	A	828	CLA	C13-C15-C16-C17
18	1	601	CHL	C10-C11-C12-C13
19	3	307	CLA	O2A-C1-C2-C3
19	A	801	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C19
23	1	617	LHG	C33-C34-C35-C36
19	B	830	CLA	C15-C16-C17-C18
23	1	617	LHG	C28-C29-C30-C31
19	A	831	CLA	C16-C17-C18-C19
19	B	822	CLA	CBA-CGA-O2A-C1
25	F	305	LMG	C14-C15-C16-C17
19	B	831	CLA	C16-C17-C18-C19
19	B	826	CLA	C8-C10-C11-C12
19	A	850	CLA	C16-C17-C18-C19
19	A	823	CLA	C15-C16-C17-C18
19	B	824	CLA	O1A-CGA-O2A-C1
19	1	602	CLA	C5-C6-C7-C8
19	B	846	CLA	C10-C11-C12-C13
19	K	202	CLA	CAA-CBA-CGA-O1A
19	B	819	CLA	C2-C1-O2A-CGA
19	B	846	CLA	C2-C1-O2A-CGA
19	K	202	CLA	CAA-CBA-CGA-O2A
23	1	617	LHG	O7-C5-C6-O8
18	3	315	CHL	C3A-C2A-CAA-CBA
19	B	828	CLA	C3A-C2A-CAA-CBA
19	K	203	CLA	C3A-C2A-CAA-CBA
19	A	826	CLA	C16-C17-C18-C19
19	A	831	CLA	C16-C17-C18-C20
19	A	846	CLA	C2-C3-C5-C6
19	A	834	CLA	C11-C10-C8-C9
24	A	845	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	845	BCR	C16-C17-C18-C36
24	B	812	BCR	C11-C10-C9-C34
24	B	813	BCR	C11-C10-C9-C34
24	B	813	BCR	C20-C21-C22-C37
24	F	304	BCR	C35-C13-C14-C15
24	L	306	BCR	C11-C10-C9-C34
19	G	203	CLA	CAA-CBA-CGA-O2A
19	A	825	CLA	O1D-CGD-O2D-CED
19	3	304	CLA	C6-C7-C8-C9
19	B	830	CLA	C16-C17-C18-C20
19	4	307	CLA	CAA-CBA-CGA-O1A
23	1	617	LHG	C35-C36-C37-C38
18	2	315	CHL	CAA-CBA-CGA-O1A
23	A	835	LHG	C6-C5-O7-C7
19	B	820	CLA	C15-C16-C17-C18
19	B	830	CLA	C1A-C2A-CAA-CBA
19	L	304	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C11-C12-C13-C15
19	A	813	CLA	C6-C7-C8-C10
19	A	819	CLA	C12-C13-C15-C16
19	A	833	CLA	C11-C12-C13-C15
19	B	844	CLA	C11-C10-C8-C7
19	B	845	CLA	C6-C7-C8-C10
27	A	830	CL0	C12-C13-C15-C16
19	B	830	CLA	C5-C6-C7-C8
19	G	203	CLA	CAA-CBA-CGA-O1A
18	3	303	CHL	O1D-CGD-O2D-CED
25	G	206	LMG	C29-C30-C31-C32
19	J	101	CLA	C16-C17-C18-C20
18	2	315	CHL	C2B-C3B-CAB-CBB
18	2	316	CHL	C2B-C3B-CAB-CBB
19	1	612	CLA	C2B-C3B-CAB-CBB
19	A	840	CLA	C2B-C3B-CAB-CBB
19	B	832	CLA	CAA-CBA-CGA-O1A
19	J	101	CLA	C5-C6-C7-C8
19	A	843	CLA	C3-C5-C6-C7
19	F	306	CLA	C2C-C3C-CAC-CBC
24	A	845	BCR	C11-C10-C9-C8
24	A	845	BCR	C16-C17-C18-C19
24	B	812	BCR	C11-C10-C9-C8
24	B	813	BCR	C11-C10-C9-C8
24	B	813	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	F	304	BCR	C12-C13-C14-C15
24	L	306	BCR	C11-C10-C9-C8
19	B	832	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	C5-C6-C7-C8
19	2	312	CLA	C4-C3-C5-C6
19	A	816	CLA	C2-C1-O2A-CGA
19	A	821	CLA	C2-C1-O2A-CGA
18	1	601	CHL	C2-C3-C5-C6
19	A	814	CLA	C2-C3-C5-C6
19	A	831	CLA	C2-C3-C5-C6
19	B	822	CLA	O1A-CGA-O2A-C1
18	2	315	CHL	CAA-CBA-CGA-O2A
19	A	836	CLA	CAA-CBA-CGA-O2A
19	1	603	CLA	C6-C7-C8-C9
19	4	317	CLA	C11-C10-C8-C9
19	A	842	CLA	C6-C7-C8-C9
19	B	823	CLA	C6-C7-C8-C9
19	B	801	CLA	C10-C11-C12-C13
22	J	102	A1LXP	C24-C1-C42-C2
24	B	814	BCR	C23-C24-C25-C30
24	G	205	BCR	C23-C24-C25-C30
24	L	306	BCR	C1-C6-C7-C8
19	A	825	CLA	C4C-C3C-CAC-CBC
27	A	830	CL0	CAA-CBA-CGA-O2A
19	3	304	CLA	C3-C5-C6-C7
19	4	307	CLA	CAA-CBA-CGA-O2A
19	A	808	CLA	O1A-CGA-O2A-C1
19	L	303	CLA	CAA-CBA-CGA-O2A
19	A	836	CLA	CAA-CBA-CGA-O1A
19	2	301	CLA	C2A-CAA-CBA-CGA
19	3	306	CLA	C2A-CAA-CBA-CGA
29	B	817	DGD	C6B-C7B-C8B-C9B
25	N	201	LMG	C28-C29-C30-C31
19	B	823	CLA	C4B-C3B-CAB-CBB
19	A	831	CLA	C4-C3-C5-C6
19	4	317	CLA	C11-C10-C8-C7
19	A	813	CLA	C11-C10-C8-C7
19	A	840	CLA	C11-C10-C8-C7
19	A	846	CLA	C6-C7-C8-C10
19	B	832	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	C3-C5-C6-C7
18	3	303	CHL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	612	CLA	C4-C3-C5-C6
19	3	301	CLA	C4-C3-C5-C6
19	A	808	CLA	C4-C3-C5-C6
19	B	834	CLA	C10-C11-C12-C13
19	1	608	CLA	C11-C10-C8-C9
19	2	312	CLA	C11-C10-C8-C9
19	A	829	CLA	C11-C12-C13-C14
19	J	101	CLA	C11-C12-C13-C14
28	B	811	PQN	C16-C17-C18-C19
19	B	820	CLA	C3-C5-C6-C7
19	B	830	CLA	C3A-C2A-CAA-CBA
23	2	302	LHG	C15-C16-C17-C18
19	A	818	CLA	C8-C10-C11-C12
19	B	826	CLA	CBD-CGD-O2D-CED
19	1	605	CLA	CAA-CBA-CGA-O2A
19	3	304	CLA	CAD-CBD-CGD-O2D
19	A	802	CLA	CAD-CBD-CGD-O2D
19	A	805	CLA	CAD-CBD-CGD-O2D
19	A	812	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	A	831	CLA	CAD-CBD-CGD-O2D
19	A	849	CLA	CAD-CBD-CGD-O2D
19	B	805	CLA	CAD-CBD-CGD-O2D
19	B	822	CLA	CAD-CBD-CGD-O2D
19	B	838	CLA	CAD-CBD-CGD-O2D
19	K	202	CLA	CAD-CBD-CGD-O2D
19	A	817	CLA	C2-C1-O2A-CGA
19	A	822	CLA	CAA-CBA-CGA-O2A
19	A	823	CLA	CAA-CBA-CGA-O2A
19	B	846	CLA	CAA-CBA-CGA-O2A
25	4	304	LMG	O7-C10-C11-C12
29	B	817	DGD	O2G-C1B-C2B-C3B
19	A	825	CLA	C2C-C3C-CAC-CBC
25	J	103	LMG	C42-C43-C44-C45
19	B	836	CLA	C4-C3-C5-C6
24	G	205	BCR	C21-C22-C23-C24
19	L	303	CLA	CAA-CBA-CGA-O1A
19	A	808	CLA	CBA-CGA-O2A-C1
19	1	602	CLA	CAA-CBA-CGA-O2A
19	A	831	CLA	CAA-CBA-CGA-O2A
19	1	605	CLA	CAA-CBA-CGA-O1A
19	B	832	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	826	CLA	O2A-C1-C2-C3
19	B	834	CLA	O2A-C1-C2-C3
19	A	818	CLA	C2A-CAA-CBA-CGA
25	G	206	LMG	C14-C15-C16-C17
18	2	313	CHL	CHA-CBD-CGD-O1D
18	2	315	CHL	CHA-CBD-CGD-O2D
18	3	303	CHL	CHA-CBD-CGD-O1D
18	4	319	CHL	CHA-CBD-CGD-O2D
19	1	603	CLA	CHA-CBD-CGD-O1D
19	1	603	CLA	CHA-CBD-CGD-O2D
19	2	312	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	815	CLA	CHA-CBD-CGD-O2D
19	A	820	CLA	CHA-CBD-CGD-O1D
19	A	822	CLA	CHA-CBD-CGD-O2D
19	A	848	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	819	CLA	CHA-CBD-CGD-O1D
19	B	830	CLA	CHA-CBD-CGD-O1D
19	B	831	CLA	CHA-CBD-CGD-O2D
19	B	841	CLA	CHA-CBD-CGD-O2D
19	G	203	CLA	CHA-CBD-CGD-O1D
19	A	851	CLA	CAA-CBA-CGA-O2A
19	B	823	CLA	CAA-CBA-CGA-O2A
19	B	827	CLA	CAA-CBA-CGA-O2A
19	H	201	CLA	CAA-CBA-CGA-O2A
19	A	814	CLA	C2A-CAA-CBA-CGA
19	3	302	CLA	CAA-CBA-CGA-O2A
19	A	812	CLA	CAA-CBA-CGA-O2A
19	A	850	CLA	C6-C7-C8-C10
19	B	810	CLA	C6-C7-C8-C10
19	J	101	CLA	C6-C7-C8-C10
19	2	312	CLA	C14-C13-C15-C16
19	A	814	CLA	C11-C12-C13-C14
19	A	823	CLA	C11-C10-C8-C9
19	A	826	CLA	C6-C7-C8-C9
19	B	822	CLA	C6-C7-C8-C9
19	A	809	CLA	C2B-C3B-CAB-CBB
19	A	821	CLA	C2B-C3B-CAB-CBB
19	A	834	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	206	LMG	C10-C11-C12-C13
19	A	817	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CAA-CBA-CGA-O2A
19	A	817	CLA	O1A-CGA-O2A-C1
19	B	844	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	CAA-CBA-CGA-O2A
19	1	602	CLA	O1A-CGA-O2A-C1
25	G	206	LMG	C30-C31-C32-C33
19	A	851	CLA	C1A-C2A-CAA-CBA
19	B	822	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	846	CLA	C1A-C2A-CAA-CBA
23	A	835	LHG	C27-C28-C29-C30
19	A	823	CLA	CAA-CBA-CGA-O1A
19	1	607	CLA	CAA-CBA-CGA-O2A
19	B	820	CLA	C2A-CAA-CBA-CGA
29	B	817	DGD	C5A-C6A-C7A-C8A
19	A	814	CLA	C16-C17-C18-C19
19	B	830	CLA	C16-C17-C18-C19
19	B	843	CLA	C16-C17-C18-C20
19	A	851	CLA	CAA-CBA-CGA-O1A
19	B	830	CLA	CAA-CBA-CGA-O1A
25	4	304	LMG	O9-C10-C11-C12
19	K	202	CLA	O1D-CGD-O2D-CED
19	2	312	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
19	B	846	CLA	CAA-CBA-CGA-O1A
19	A	831	CLA	CAA-CBA-CGA-O1A
19	B	841	CLA	CAA-CBA-CGA-O1A
23	A	835	LHG	C17-C18-C19-C20
19	A	808	CLA	C13-C15-C16-C17
19	A	812	CLA	CAA-CBA-CGA-O1A
29	B	817	DGD	O1B-C1B-C2B-C3B
19	B	829	CLA	C2A-CAA-CBA-CGA
19	1	602	CLA	CAA-CBA-CGA-O1A
19	H	201	CLA	CAA-CBA-CGA-O1A
19	A	828	CLA	C4-C3-C5-C6
19	B	802	CLA	C4-C3-C5-C6
18	3	315	CHL	O1D-CGD-O2D-CED
19	B	844	CLA	CBA-CGA-O2A-C1
18	1	601	CHL	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	1	606	CHL	CAD-CBD-CGD-O1D
18	2	316	CHL	CAD-CBD-CGD-O1D
19	A	818	CLA	CAD-CBD-CGD-O1D
19	A	836	CLA	CAD-CBD-CGD-O1D
19	B	819	CLA	CAD-CBD-CGD-O1D
19	B	847	CLA	CAD-CBD-CGD-O1D
19	B	823	CLA	CAA-CBA-CGA-O1A
19	A	833	CLA	CAA-CBA-CGA-O2A
19	L	304	CLA	C15-C16-C17-C18
19	A	818	CLA	C6-C7-C8-C9
19	B	835	CLA	C6-C7-C8-C9
19	J	101	CLA	C6-C7-C8-C9
19	A	822	CLA	CAA-CBA-CGA-O1A
19	B	830	CLA	CAA-CBA-CGA-O2A
23	1	617	LHG	O8-C23-C24-C25
28	A	839	PQN	C18-C20-C21-C22
23	2	302	LHG	C34-C35-C36-C37
18	2	316	CHL	C4-C3-C5-C6
19	A	814	CLA	C4-C3-C5-C6
19	2	310	CLA	C3A-C2A-CAA-CBA
19	A	814	CLA	C11-C10-C8-C7
19	A	814	CLA	C11-C12-C13-C15
19	A	828	CLA	C3A-C2A-CAA-CBA
19	A	831	CLA	C11-C10-C8-C7
19	A	851	CLA	C3A-C2A-CAA-CBA
19	B	818	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C12-C13-C15-C16
19	B	843	CLA	C11-C10-C8-C7
19	B	846	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	CAA-CBA-CGA-O1A
19	1	612	CLA	CAA-CBA-CGA-O2A
24	L	301	BCR	C7-C8-C9-C10
19	2	312	CLA	CAA-CBA-CGA-O1A
19	A	818	CLA	CAA-CBA-CGA-O2A
25	4	304	LMG	C30-C31-C32-C33
19	A	833	CLA	CAA-CBA-CGA-O1A
19	B	827	CLA	CAA-CBA-CGA-O1A
23	A	835	LHG	O10-C23-C24-C25
19	4	318	CLA	CAA-CBA-CGA-O2A
25	F	305	LMG	C15-C16-C17-C18
19	J	101	CLA	O1A-CGA-O2A-C1
19	J	101	CLA	C13-C15-C16-C17

There are no ring outliers.

112 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	807	CLA	1	0
24	F	302	BCR	3	0
19	A	814	CLA	2	0
19	A	805	CLA	2	0
19	B	803	CLA	1	0
19	A	823	CLA	1	0
19	B	832	CLA	2	0
19	B	827	CLA	3	0
19	A	826	CLA	2	0
19	B	825	CLA	2	0
22	3	305	A1LXP	1	0
24	G	205	BCR	3	0
19	B	830	CLA	2	0
19	A	815	CLA	1	0
19	A	840	CLA	5	0
19	4	318	CLA	1	0
24	K	201	BCR	2	0
19	A	828	CLA	1	0
19	F	303	CLA	2	0
18	1	606	CHL	2	0
24	B	816	BCR	2	0
19	B	843	CLA	1	0
19	B	822	CLA	2	0
19	A	821	CLA	4	0
19	B	844	CLA	5	0
19	1	612	CLA	1	0
19	1	608	CLA	1	0
19	1	607	CLA	1	0
19	A	818	CLA	1	0
22	2	309	A1LXP	1	0
19	B	834	CLA	4	0
24	B	813	BCR	5	0
21	2	306	XAT	1	0
19	B	819	CLA	1	0
19	B	833	CLA	4	0
19	3	304	CLA	2	0
19	B	840	CLA	1	0
19	B	801	CLA	2	0
19	1	603	CLA	3	0
24	B	812	BCR	4	0

Continued on next page...

Continued from previous page...

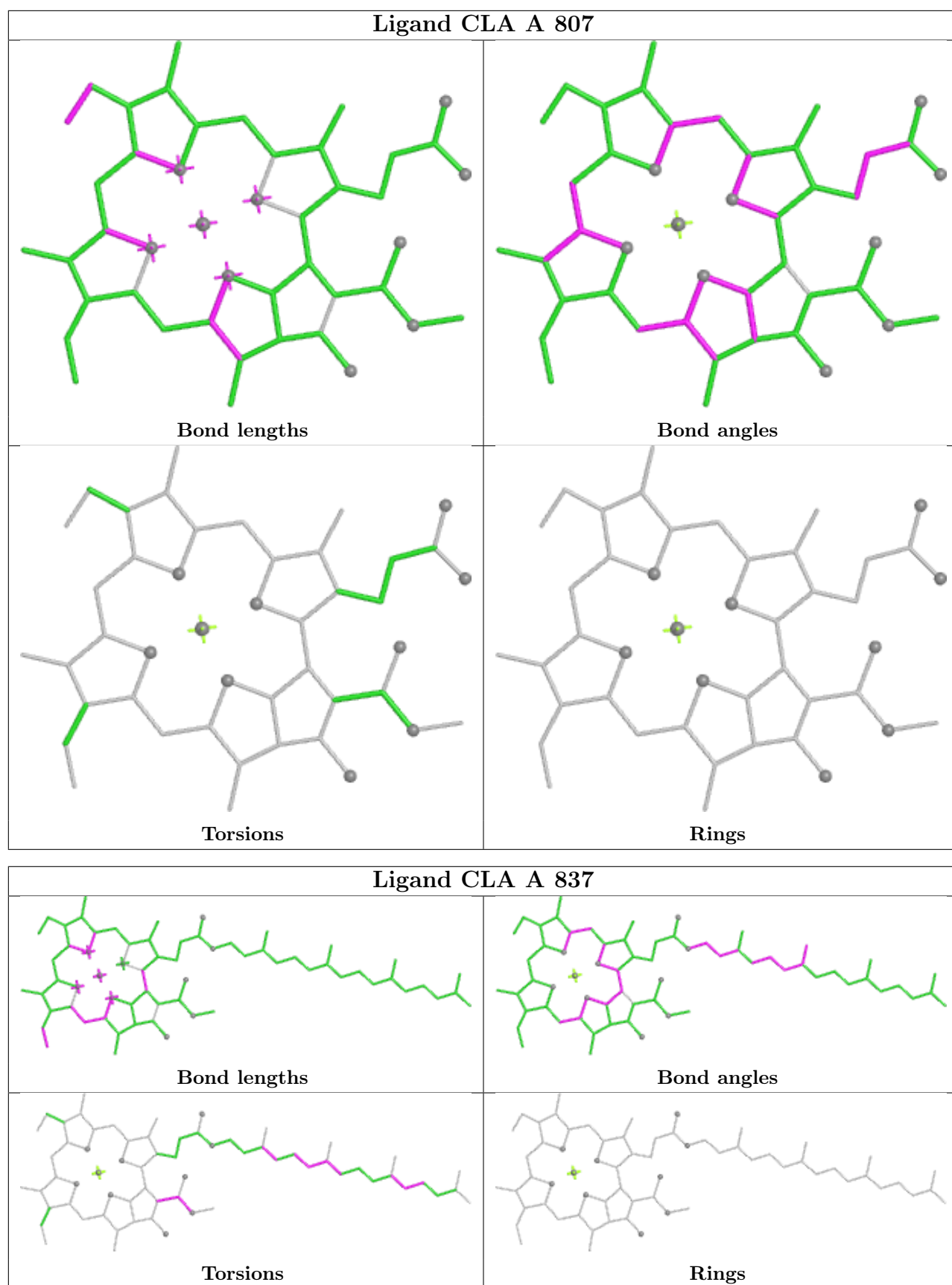
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	818	CLA	5	0
19	A	833	CLA	3	0
24	A	838	BCR	2	0
19	B	802	CLA	1	0
18	4	313	CHL	1	0
24	F	304	BCR	2	0
19	B	842	CLA	1	0
19	B	845	CLA	2	0
19	B	806	CLA	3	0
24	A	845	BCR	7	0
24	A	804	BCR	5	0
18	3	303	CHL	1	0
19	B	846	CLA	1	0
19	A	802	CLA	3	0
24	A	841	BCR	1	0
25	F	305	LMG	2	0
19	4	317	CLA	3	0
19	G	203	CLA	5	0
19	1	602	CLA	3	0
19	A	829	CLA	2	0
19	4	311	CLA	2	0
19	B	810	CLA	2	0
19	B	824	CLA	1	0
25	N	201	LMG	3	0
19	B	808	CLA	3	0
19	B	809	CLA	1	0
22	4	306	A1LXP	1	0
19	L	303	CLA	1	0
19	B	848	CLA	1	0
24	L	301	BCR	2	0
19	A	843	CLA	2	0
19	2	311	CLA	1	0
19	A	827	CLA	1	0
19	A	834	CLA	1	0
19	1	605	CLA	1	0
19	A	813	CLA	4	0
19	A	810	CLA	2	0
19	3	301	CLA	1	0
19	A	831	CLA	5	0
24	4	308	BCR	3	0
19	A	819	CLA	3	0
19	A	849	CLA	2	0

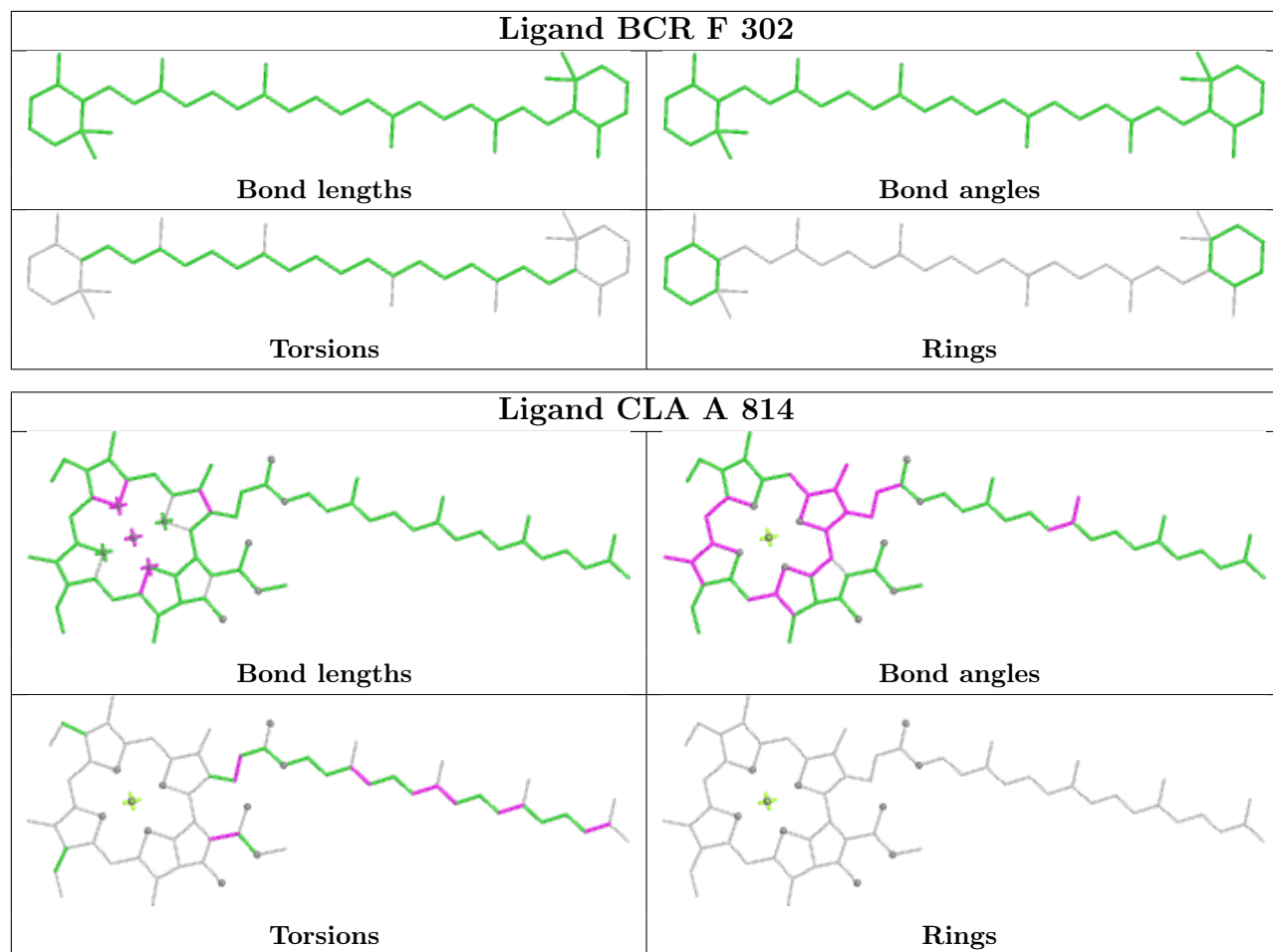
Continued on next page...

Continued from previous page...

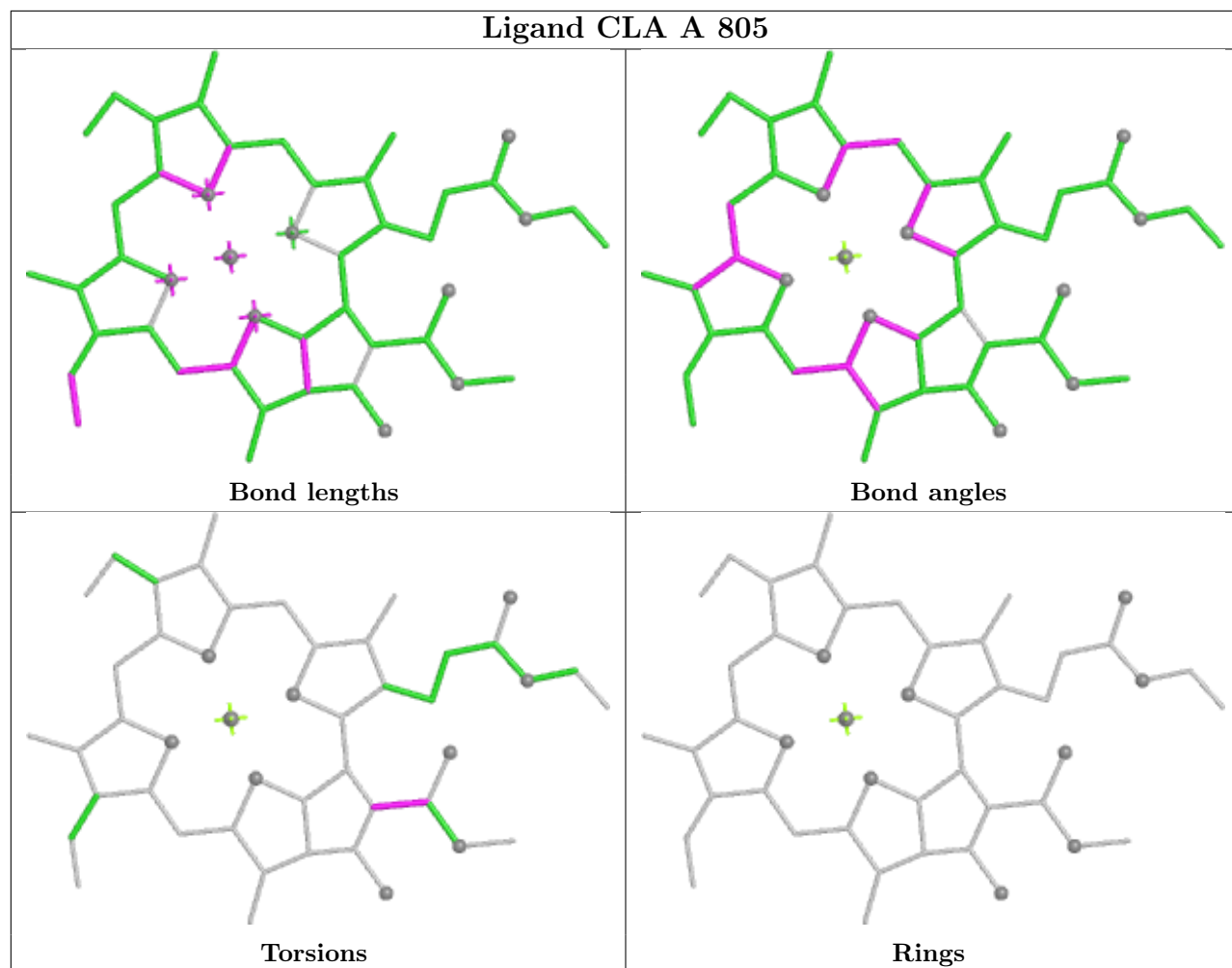
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	I	101	BCR	1	0
24	A	847	BCR	2	0
19	L	304	CLA	1	0
19	A	850	CLA	1	0
19	3	308	CLA	1	0
19	B	841	CLA	1	0
19	J	101	CLA	1	0
19	K	203	CLA	2	0
18	4	319	CHL	1	0
19	2	312	CLA	1	0
24	G	201	BCR	4	0
18	1	601	CHL	2	0
24	A	852	BCR	8	0
24	B	814	BCR	1	0
19	A	851	CLA	5	0
19	B	829	CLA	2	0
19	B	837	CLA	1	0
19	A	812	CLA	1	0
19	B	805	CLA	1	0
19	B	804	CLA	1	0
24	L	302	BCR	2	0
24	B	815	BCR	1	0
19	B	820	CLA	2	0
21	1	615	XAT	3	0
19	A	842	CLA	3	0
29	B	817	DGD	1	0
19	A	806	CLA	2	0
19	A	808	CLA	4	0
21	1	618	XAT	3	0
19	A	809	CLA	3	0

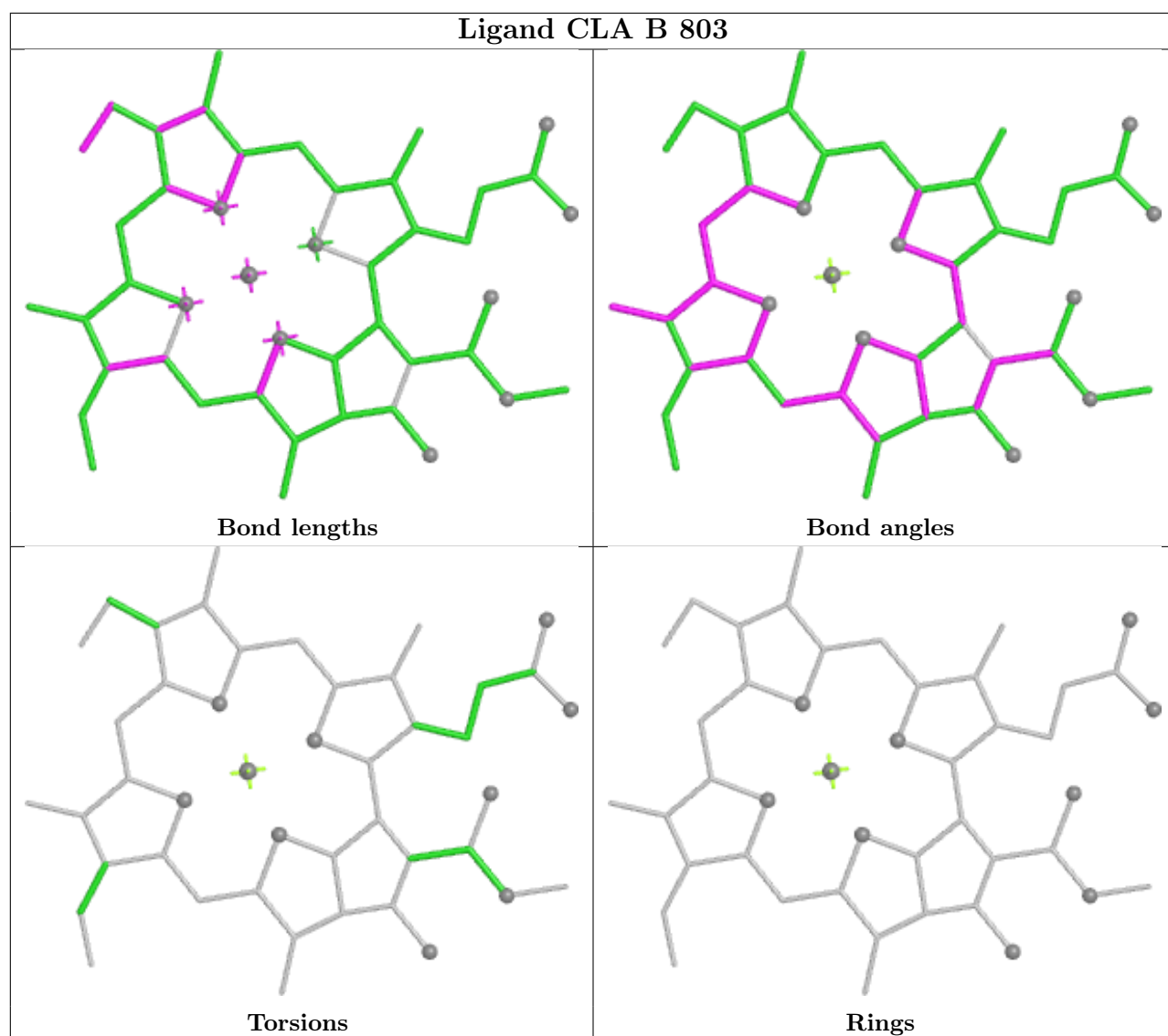
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

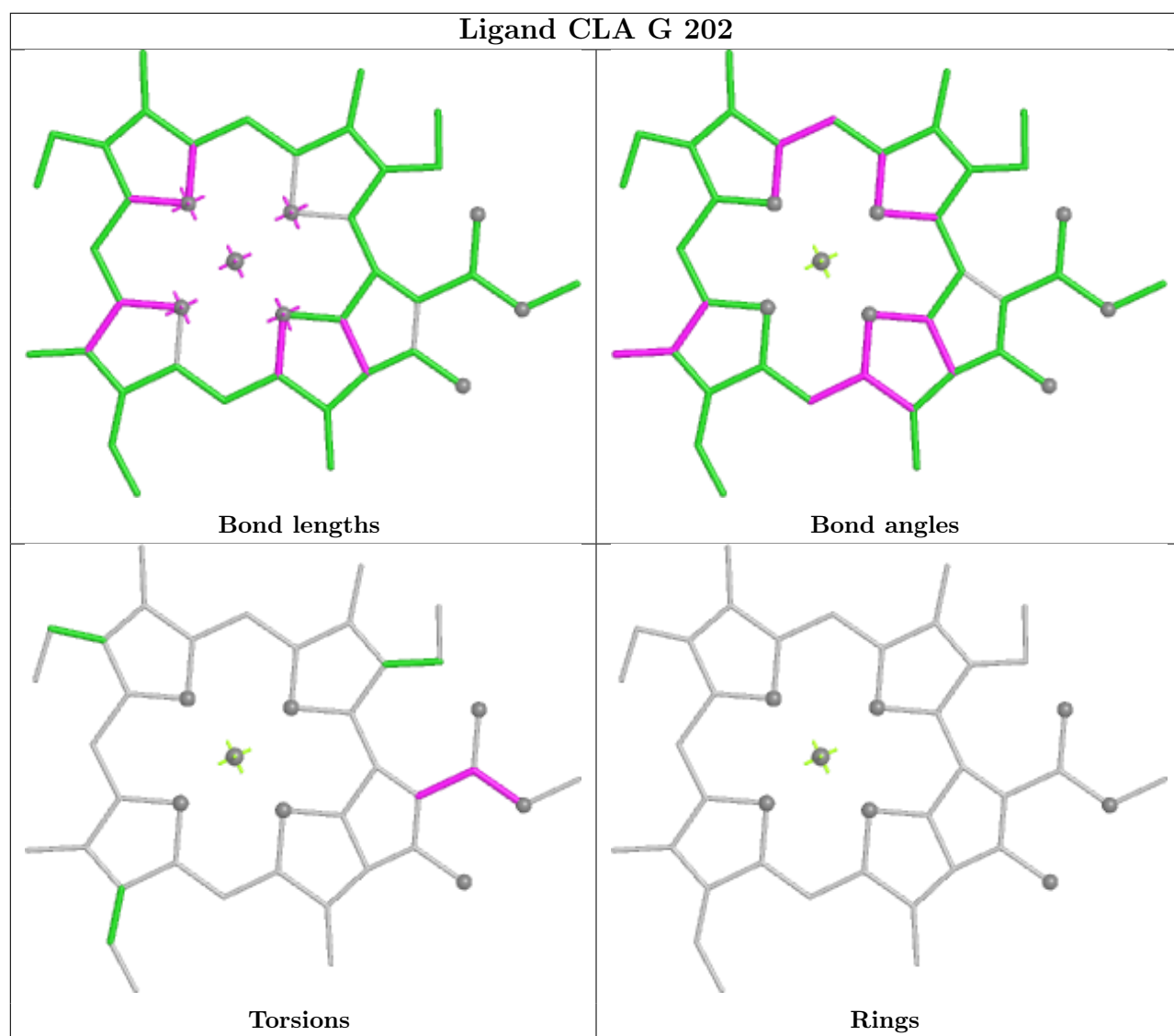




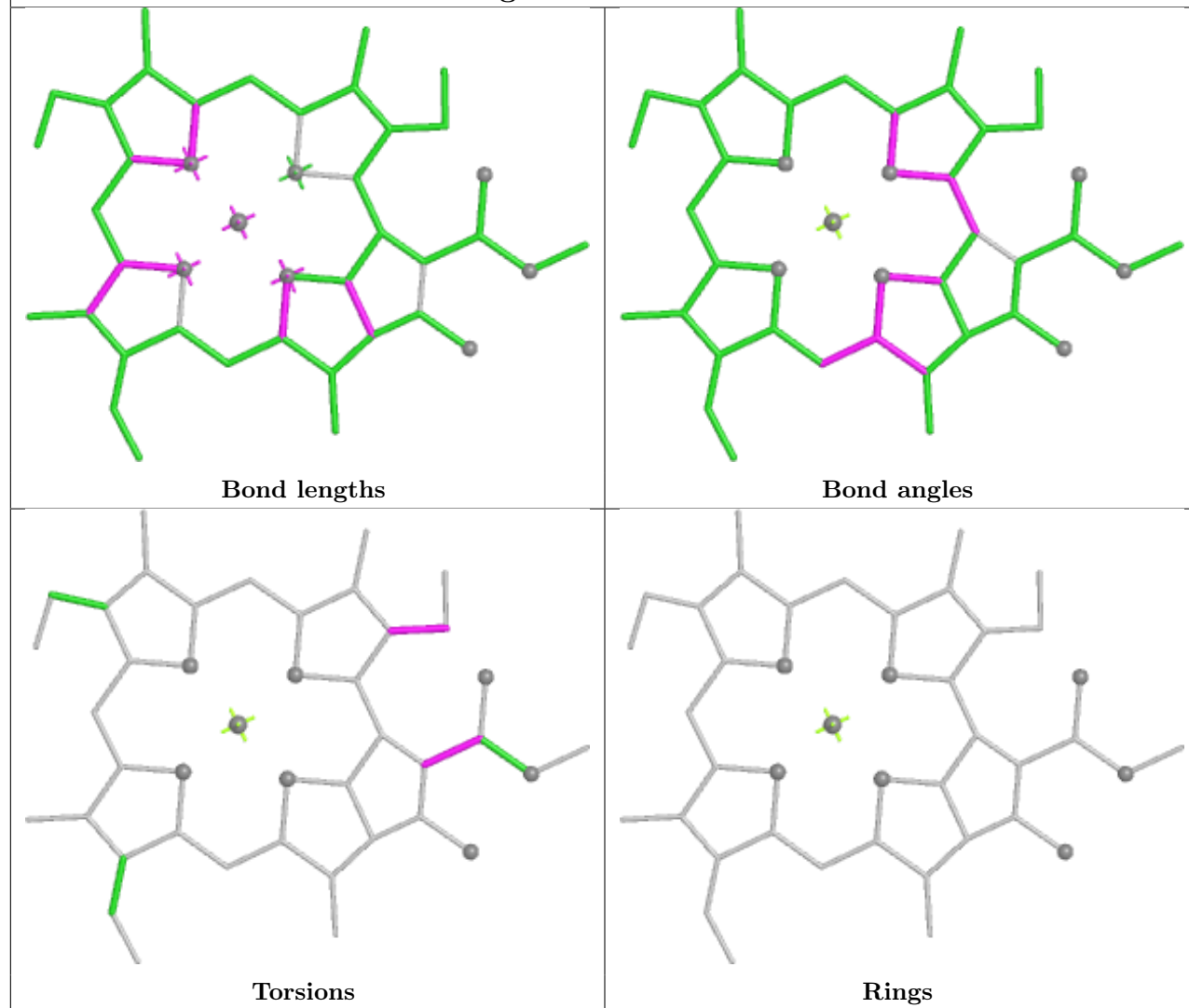
Ligand CLA A 805



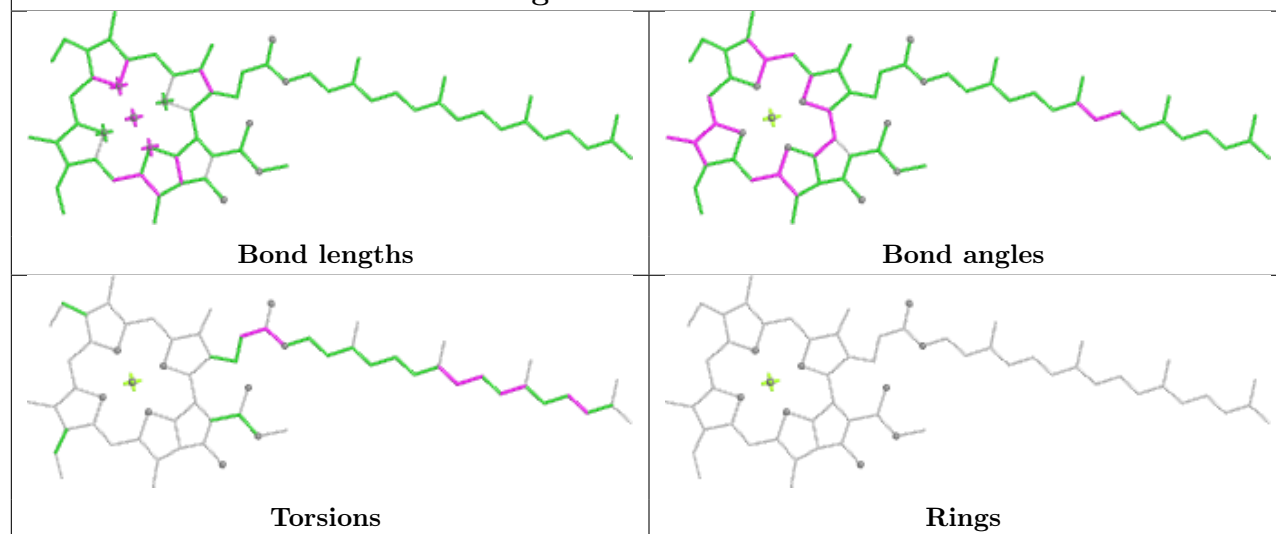




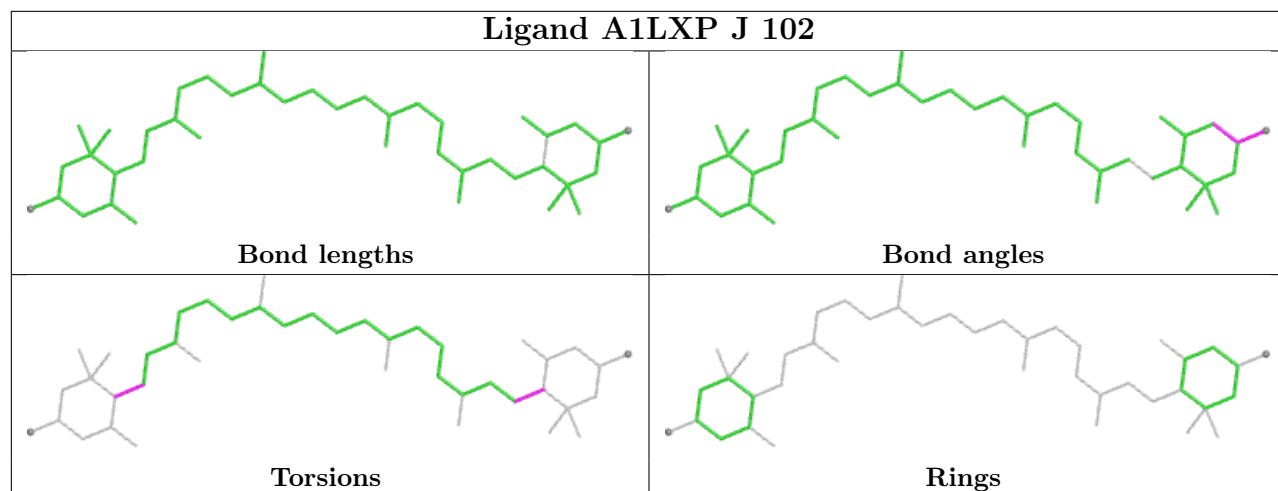
Ligand CLA 3 312



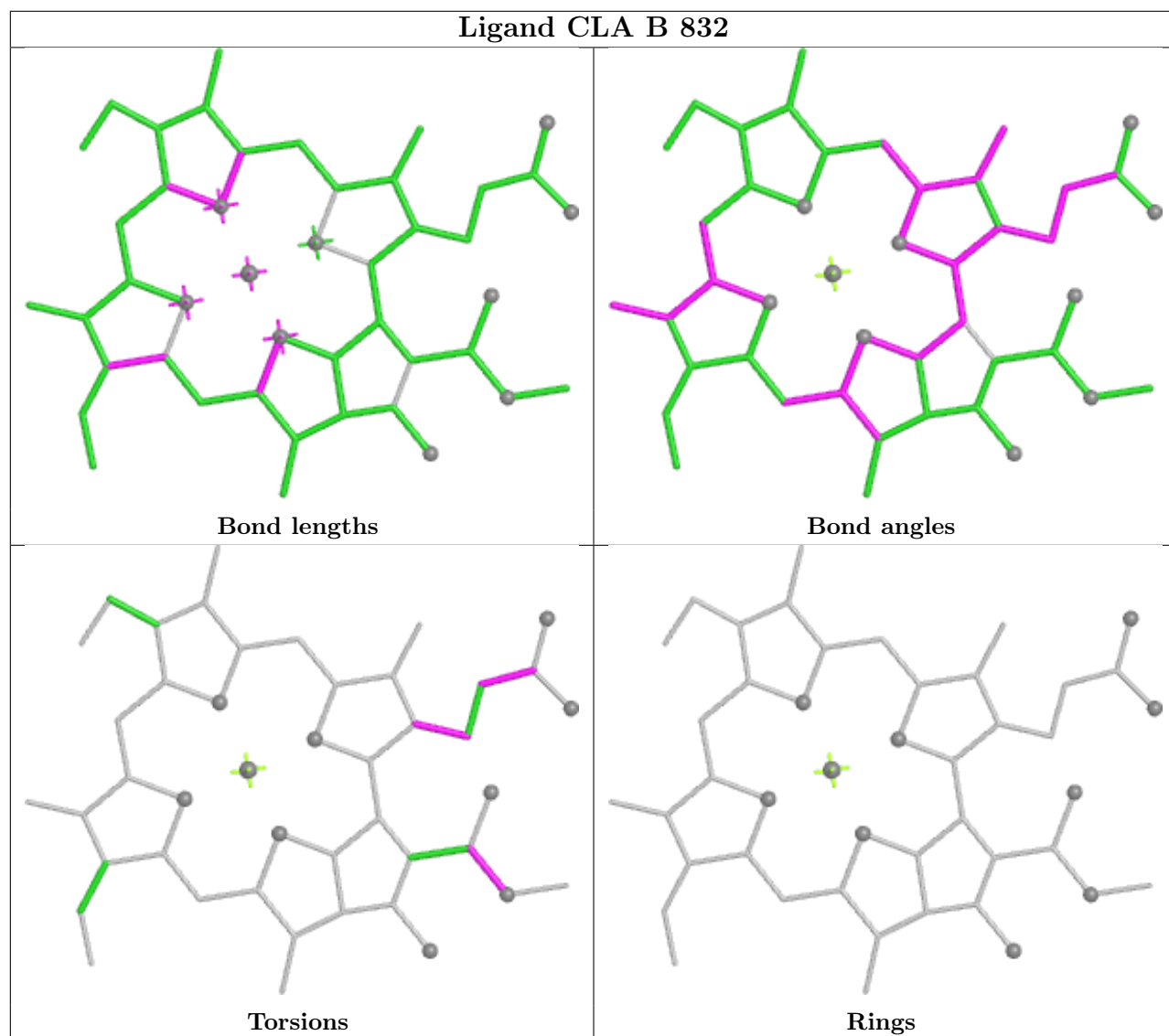
Ligand CLA A 823

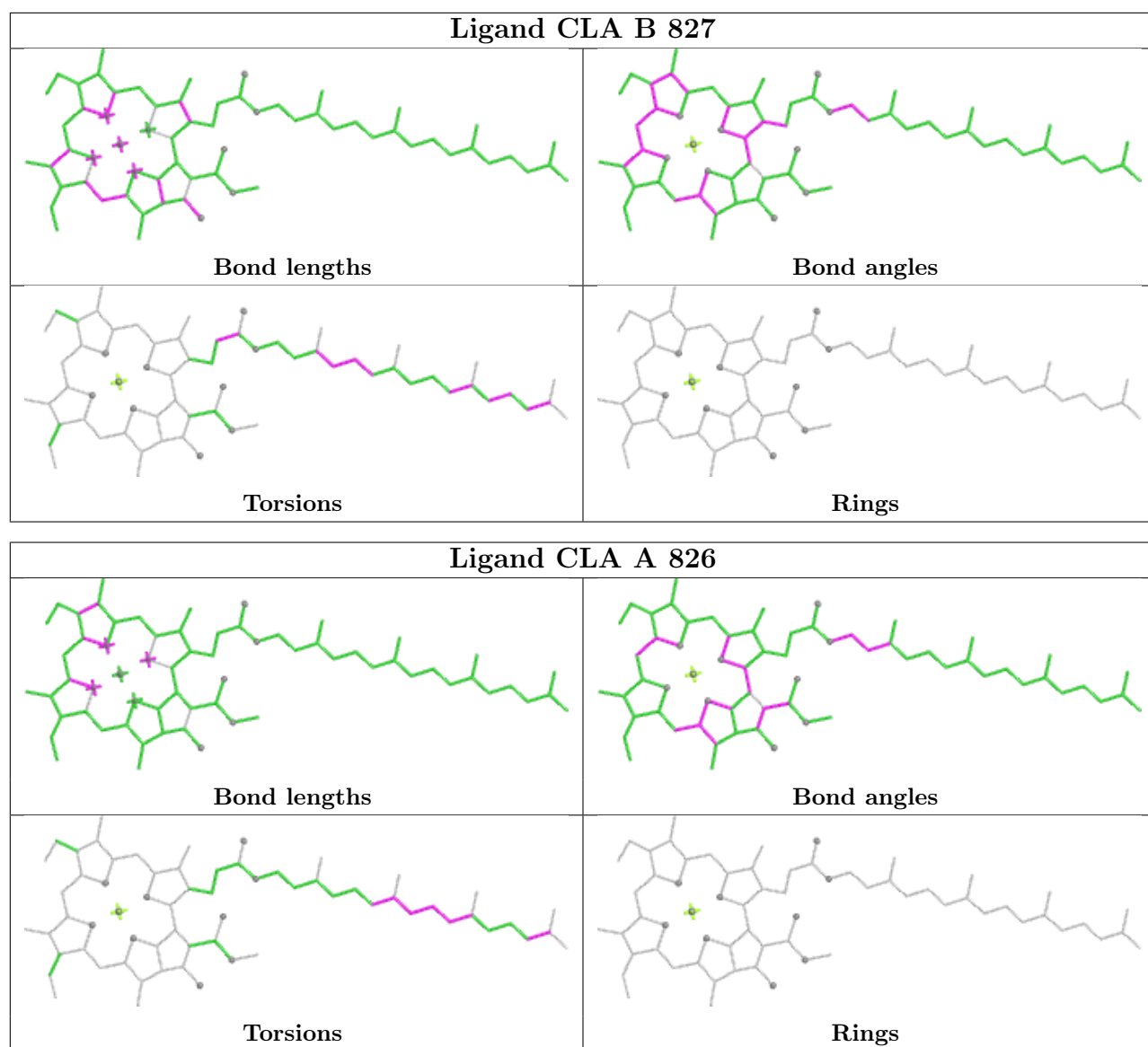


Ligand A1LXP J 102

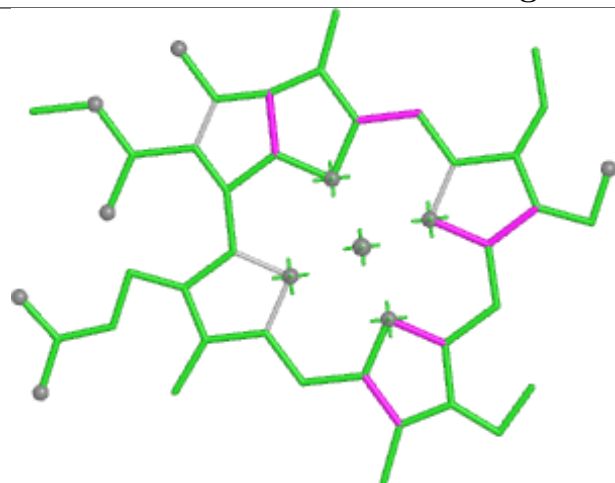


Ligand CLA B 832

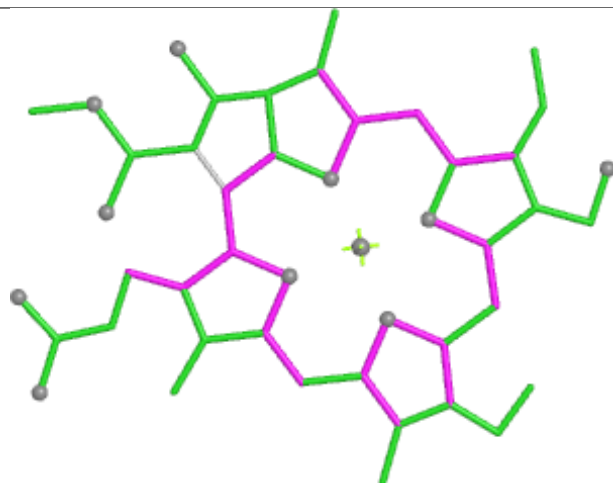




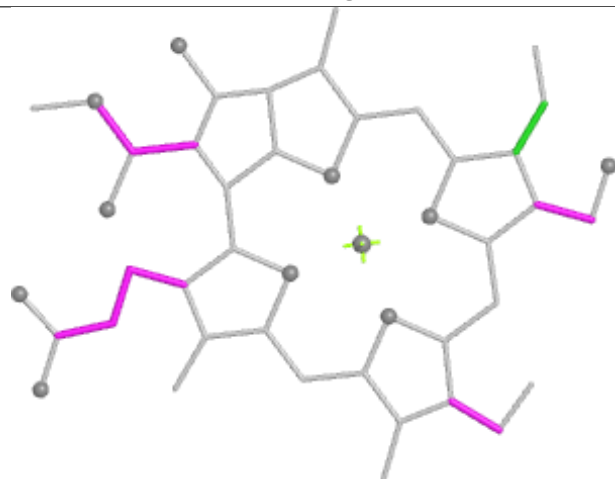
Ligand CHL 2 315



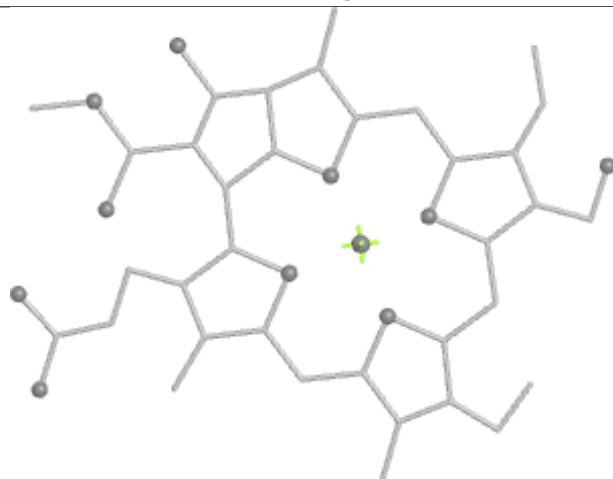
Bond lengths



Bond angles

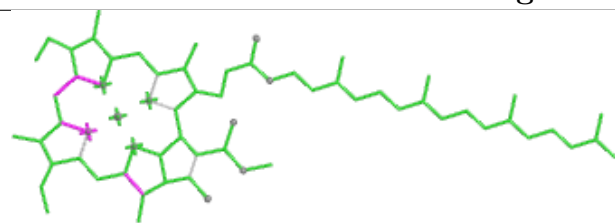


Torsions

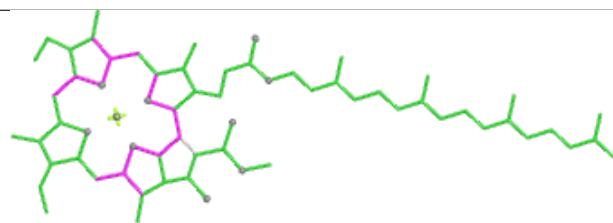


Rings

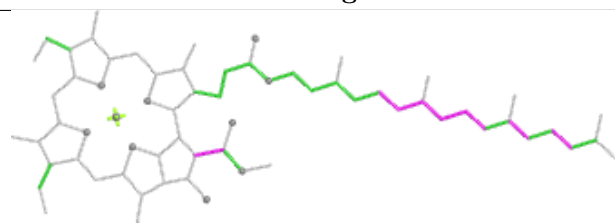
Ligand CLA B 825



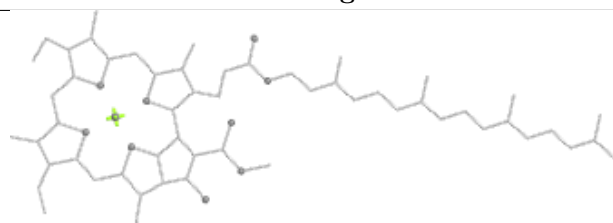
Bond lengths



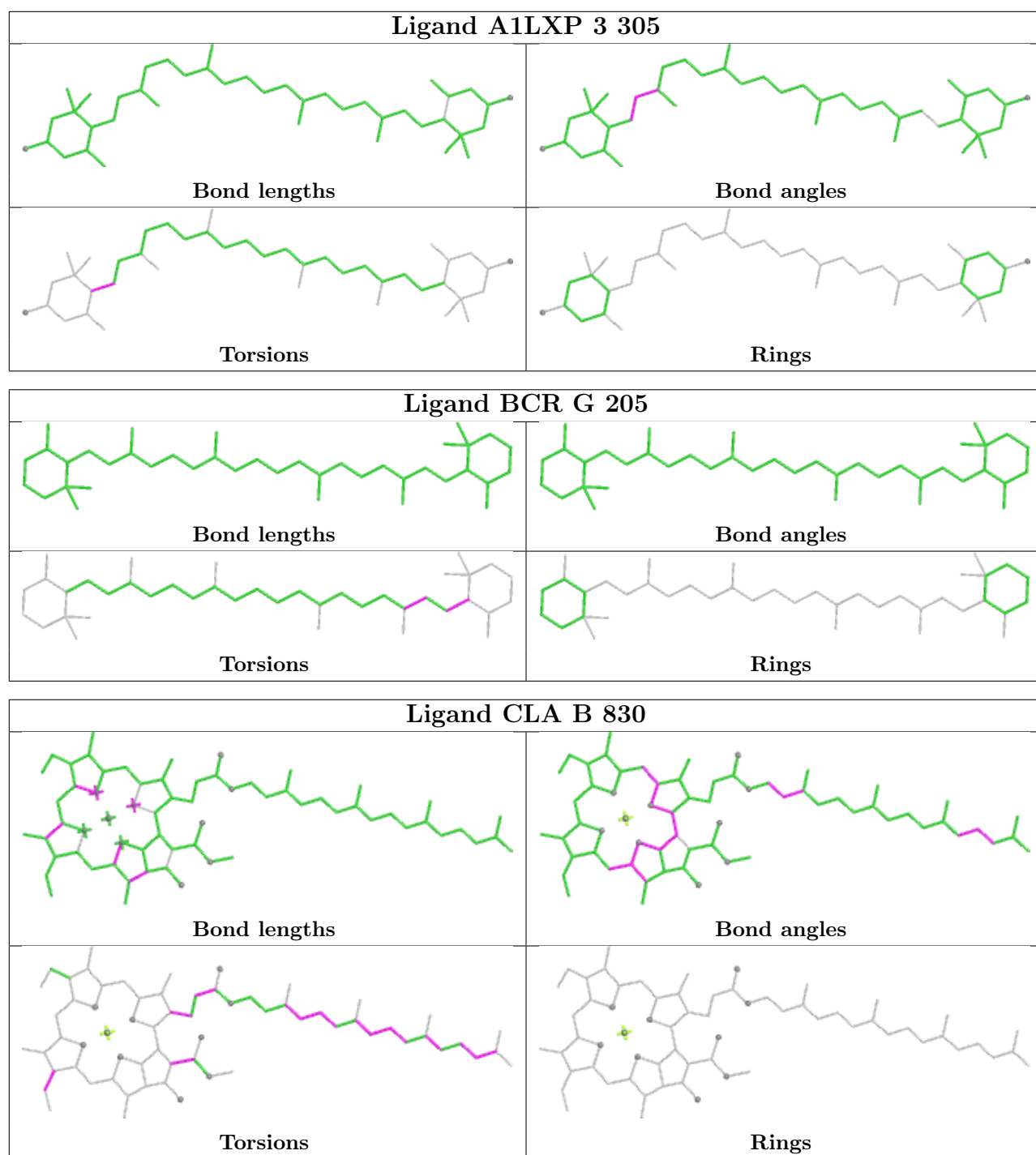
Bond angles



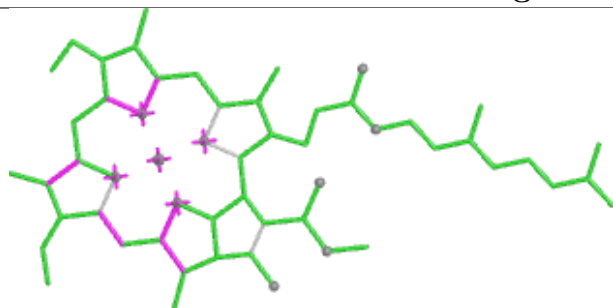
Torsions



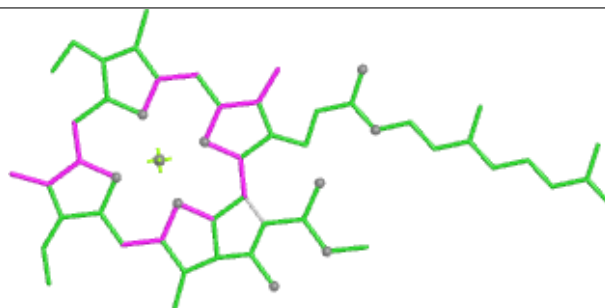
Rings



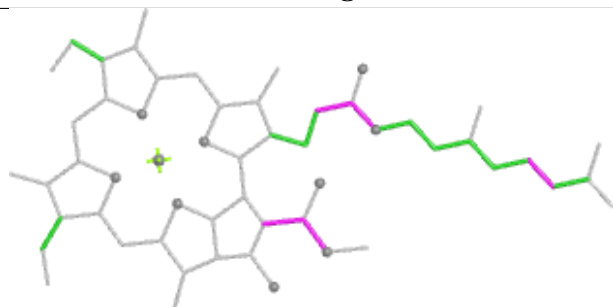
Ligand CLA H 201



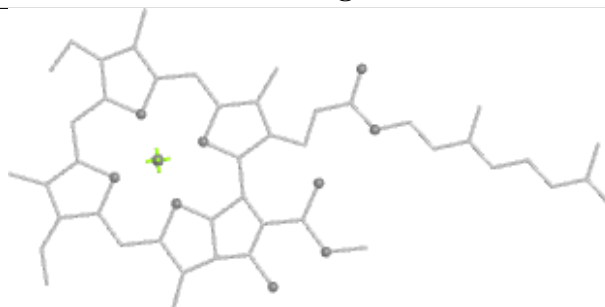
Bond lengths



Bond angles

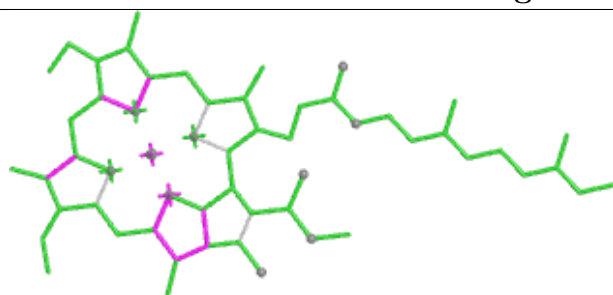


Torsions

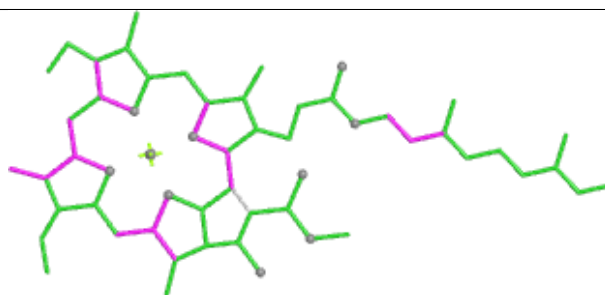


Rings

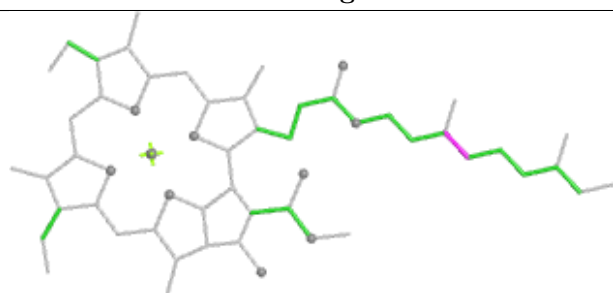
Ligand CLA B 836



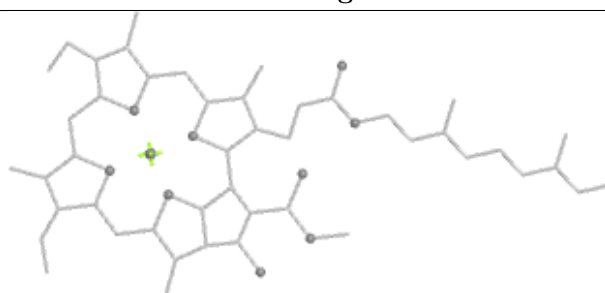
Bond lengths



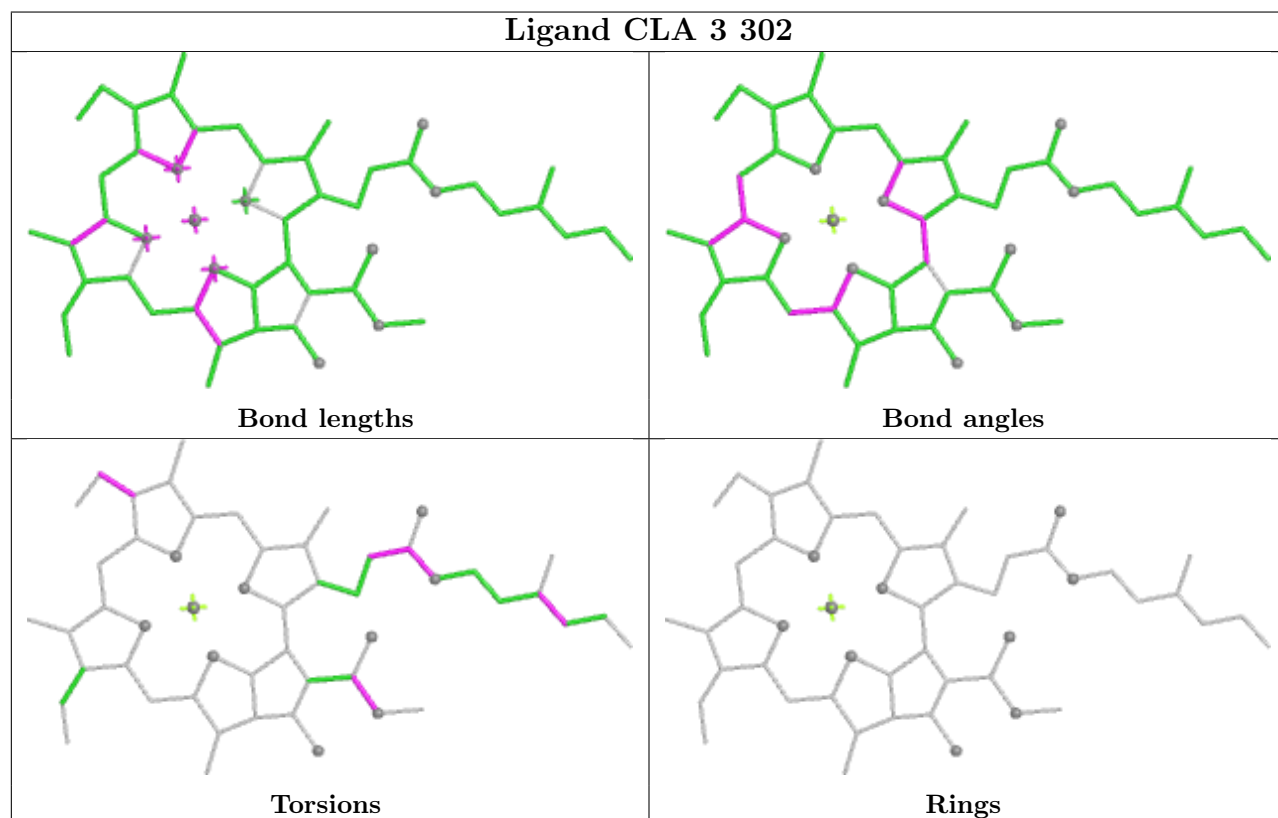
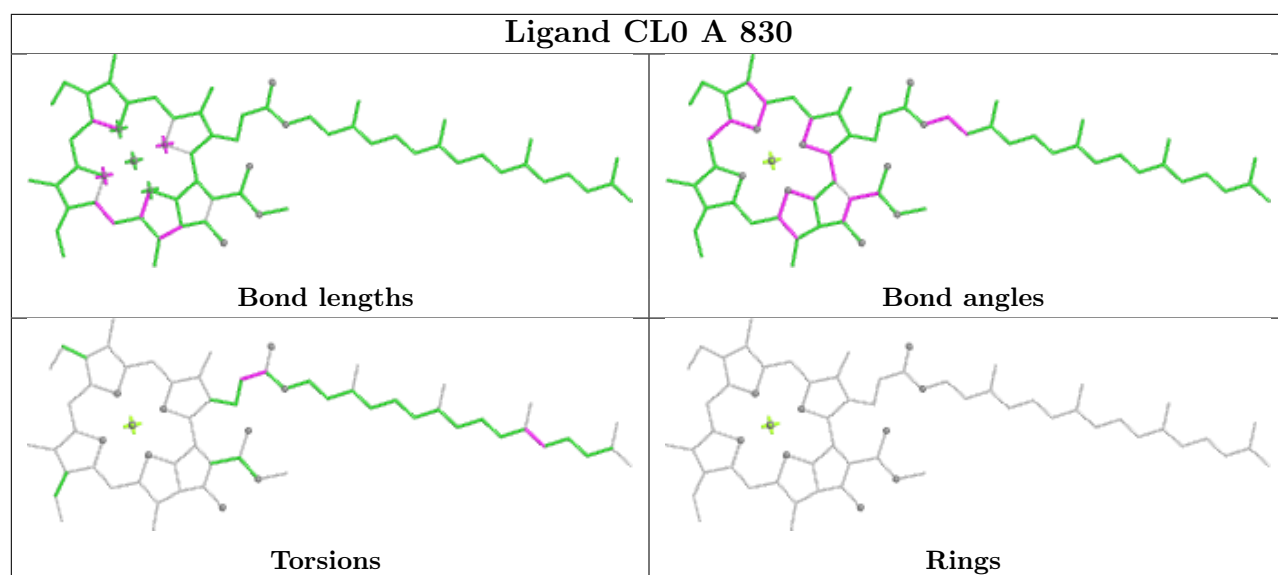
Bond angles

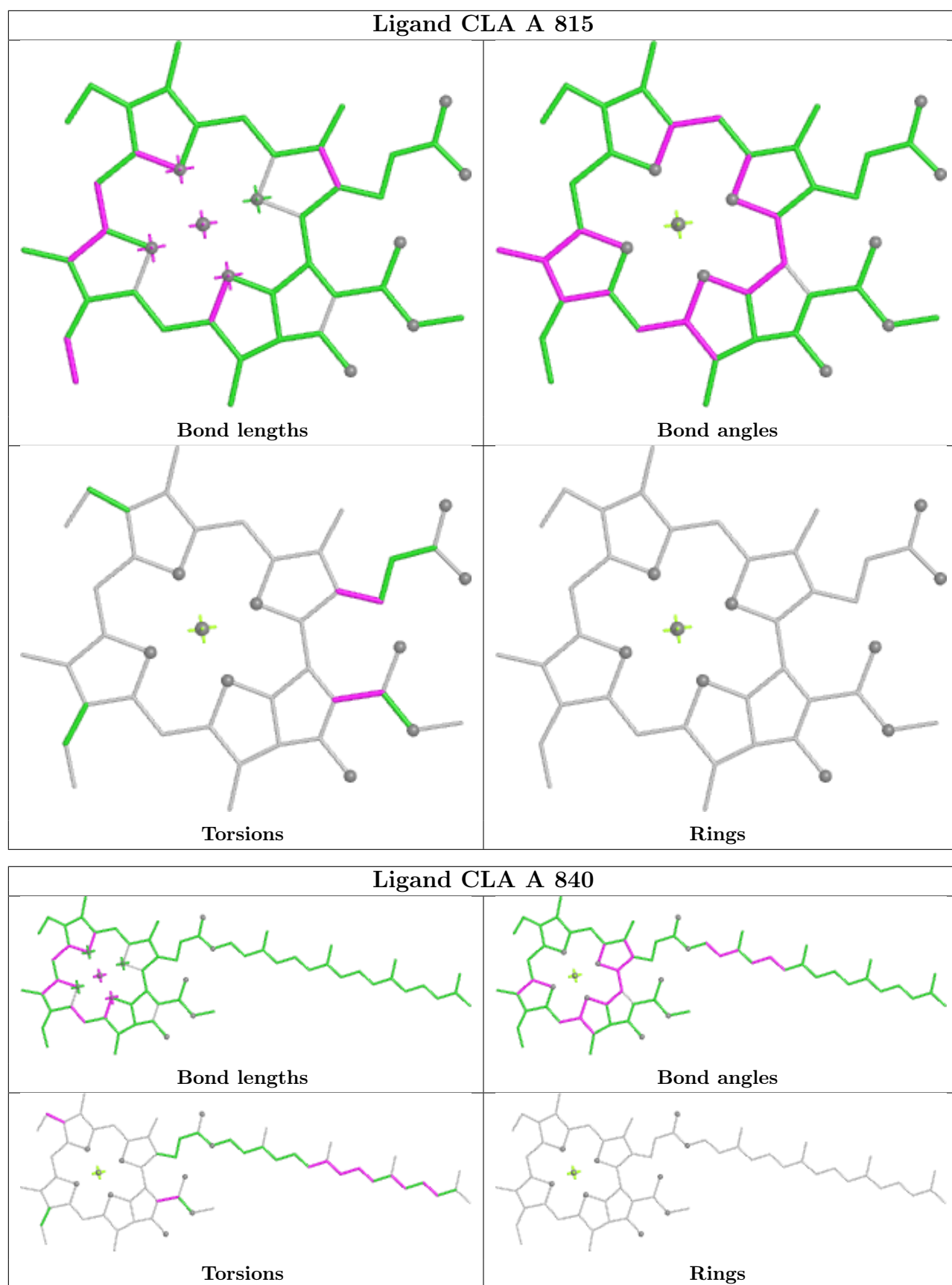


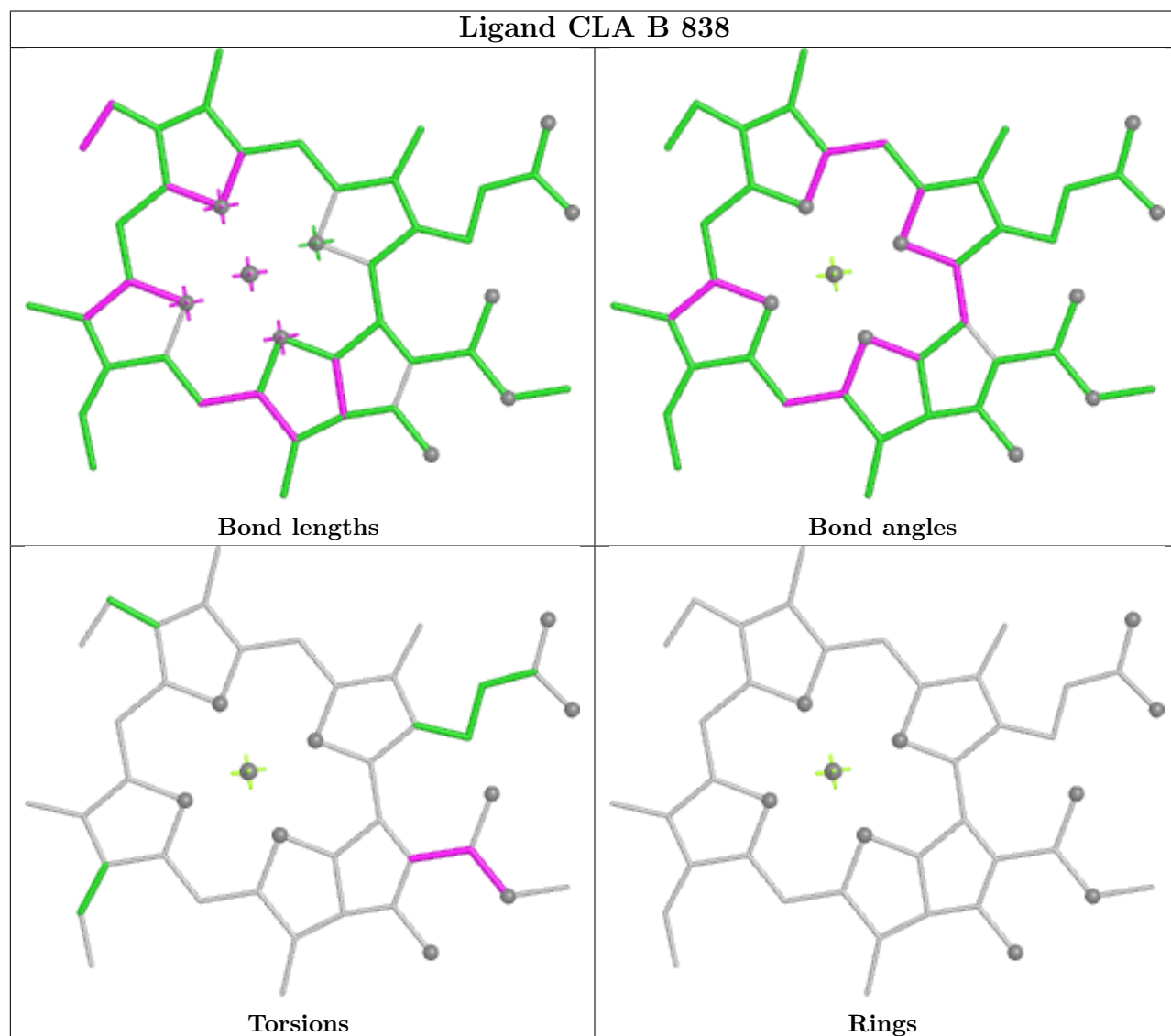
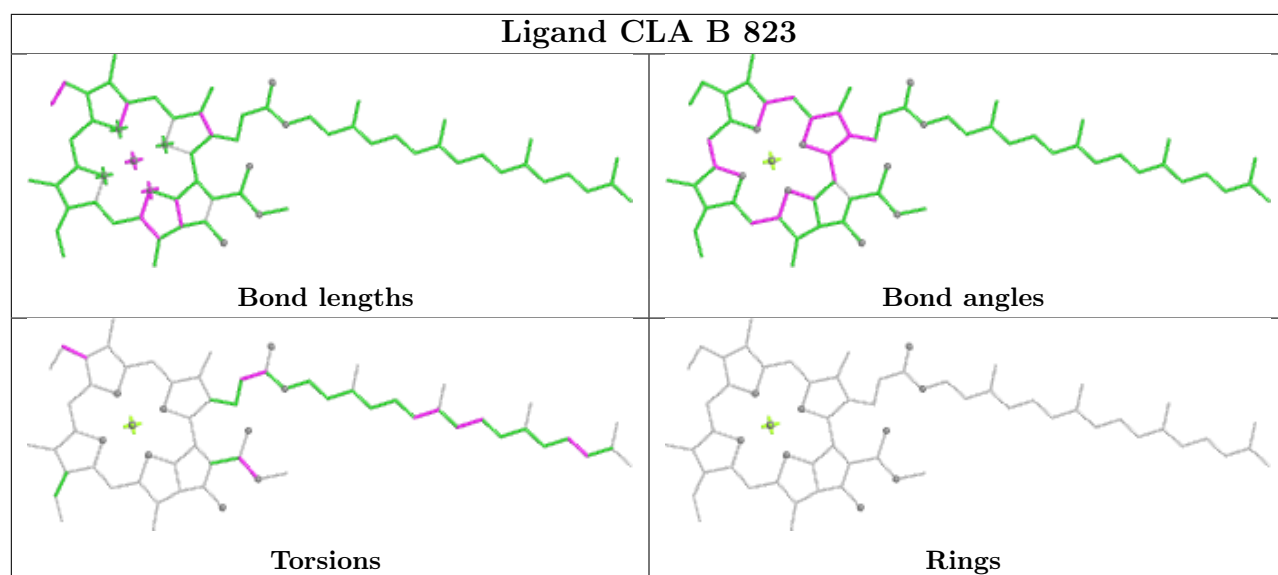
Torsions



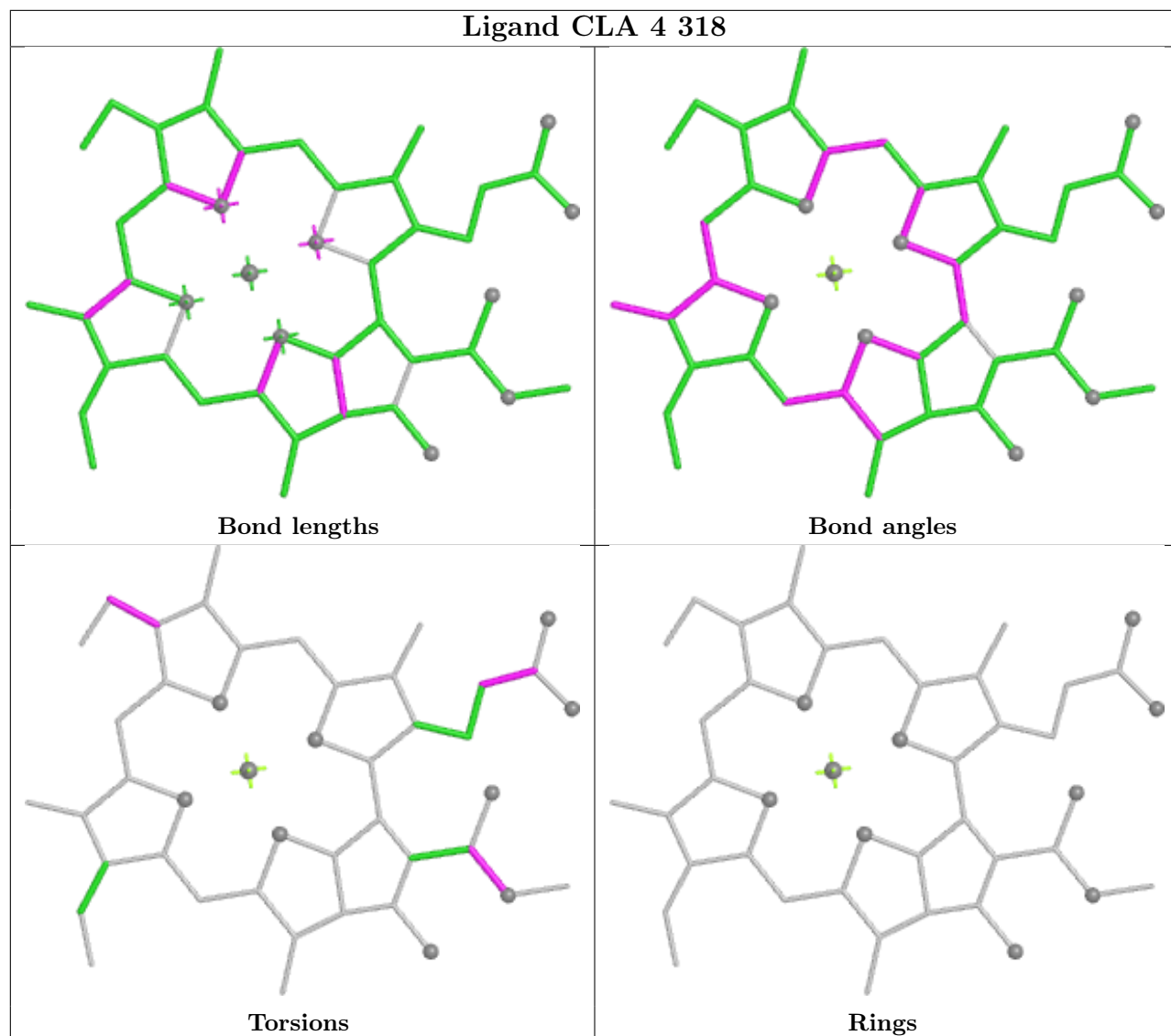
Rings



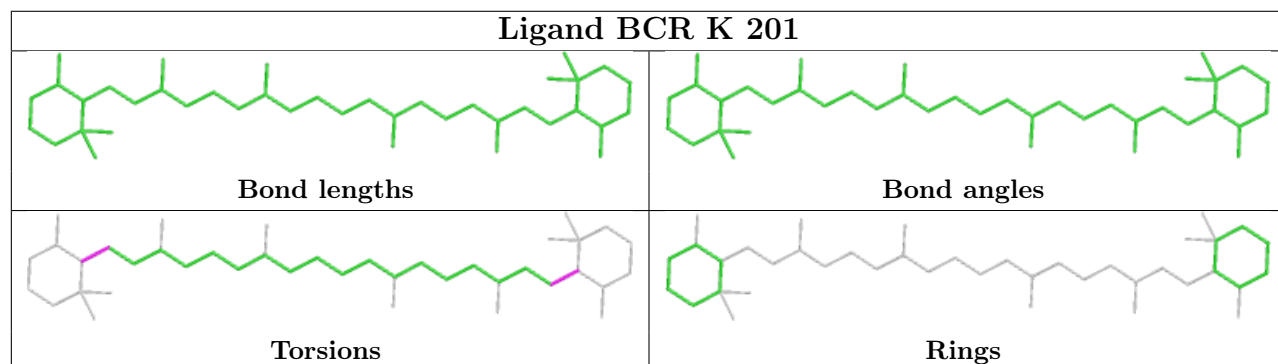


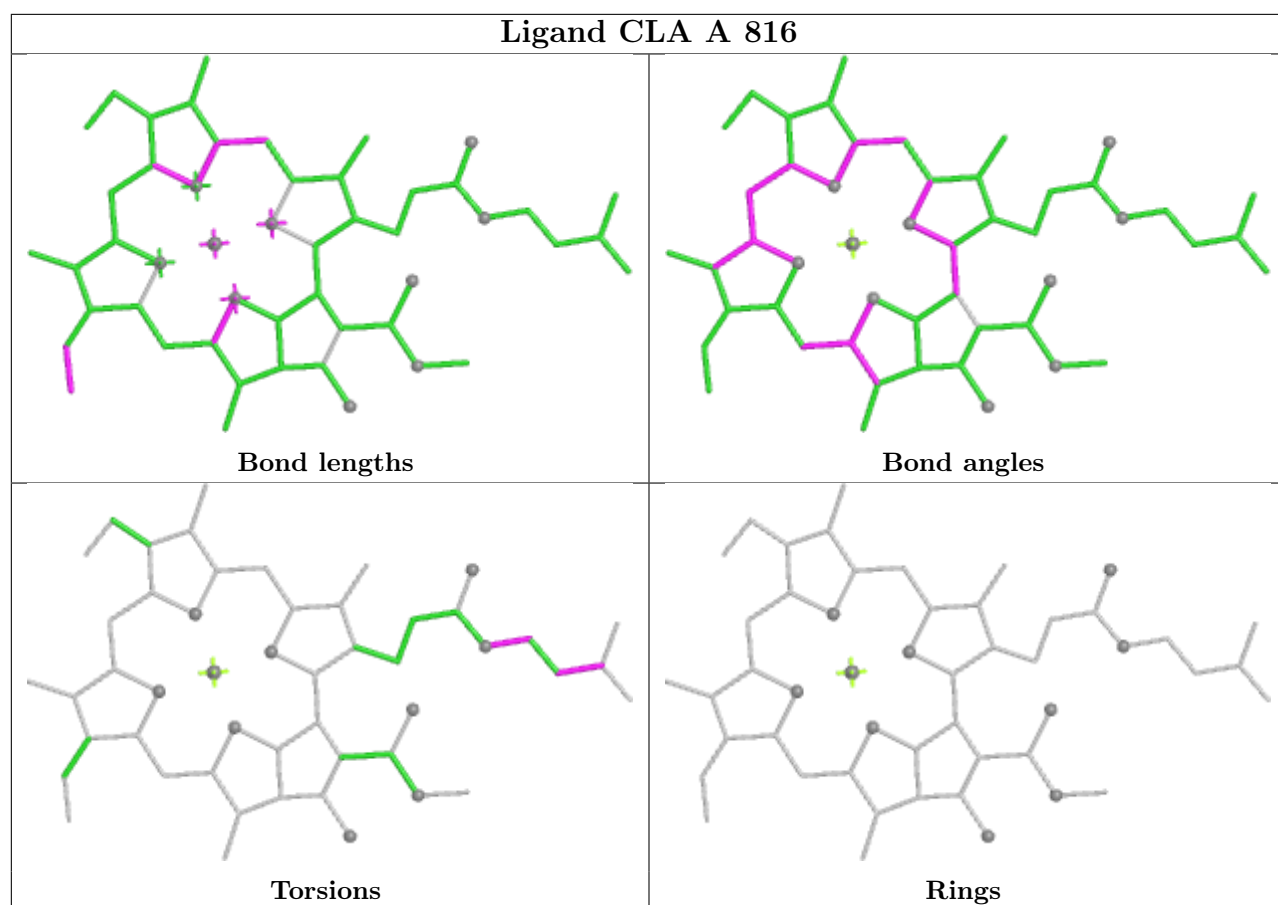


Ligand CLA 4 318

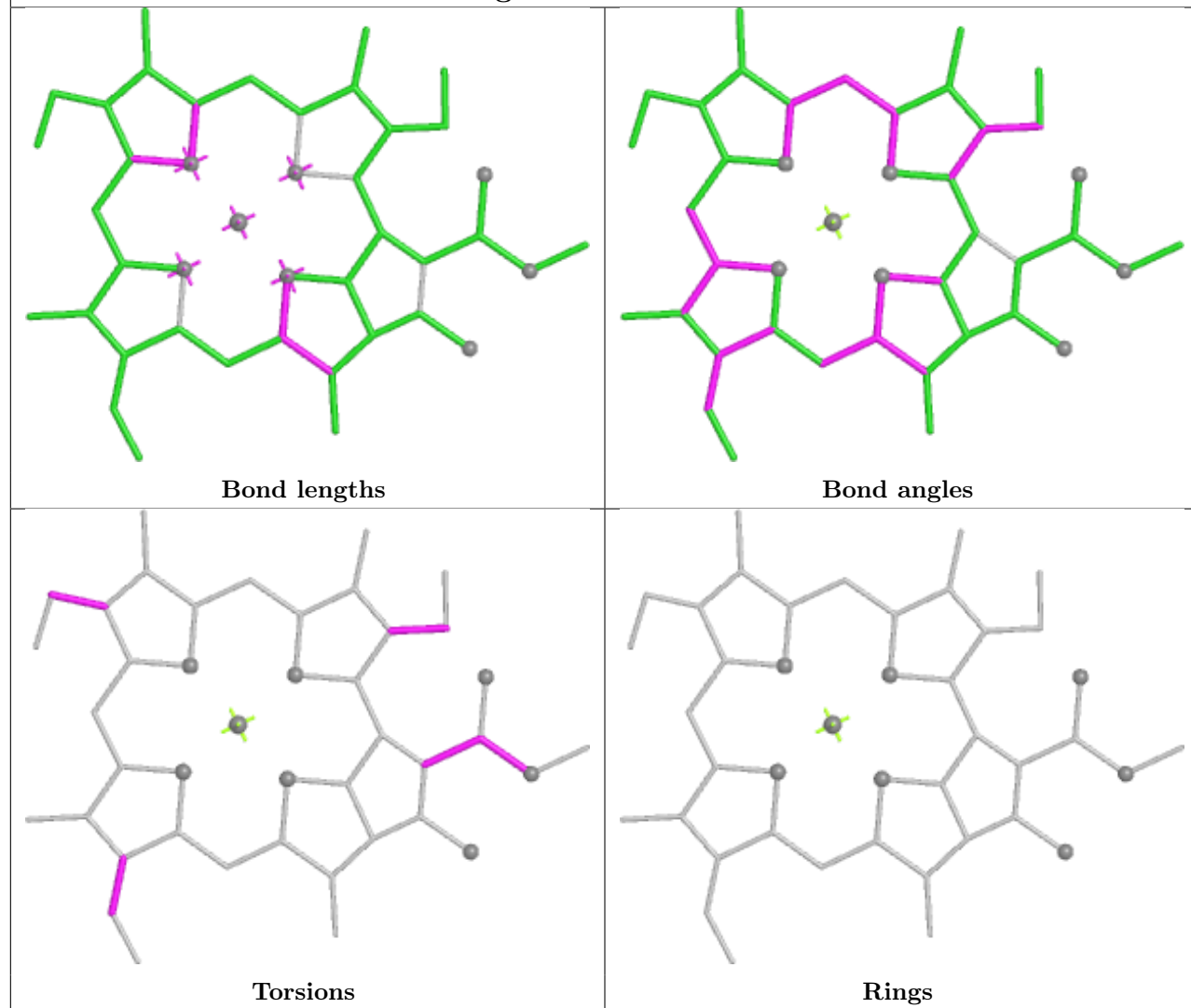


Ligand BCR K 201

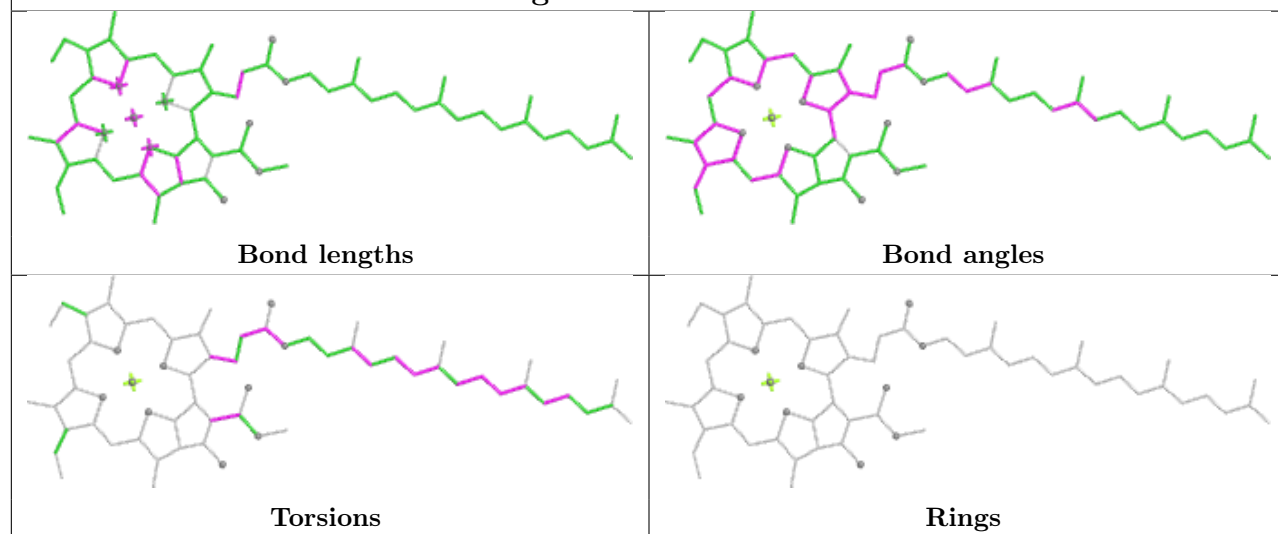


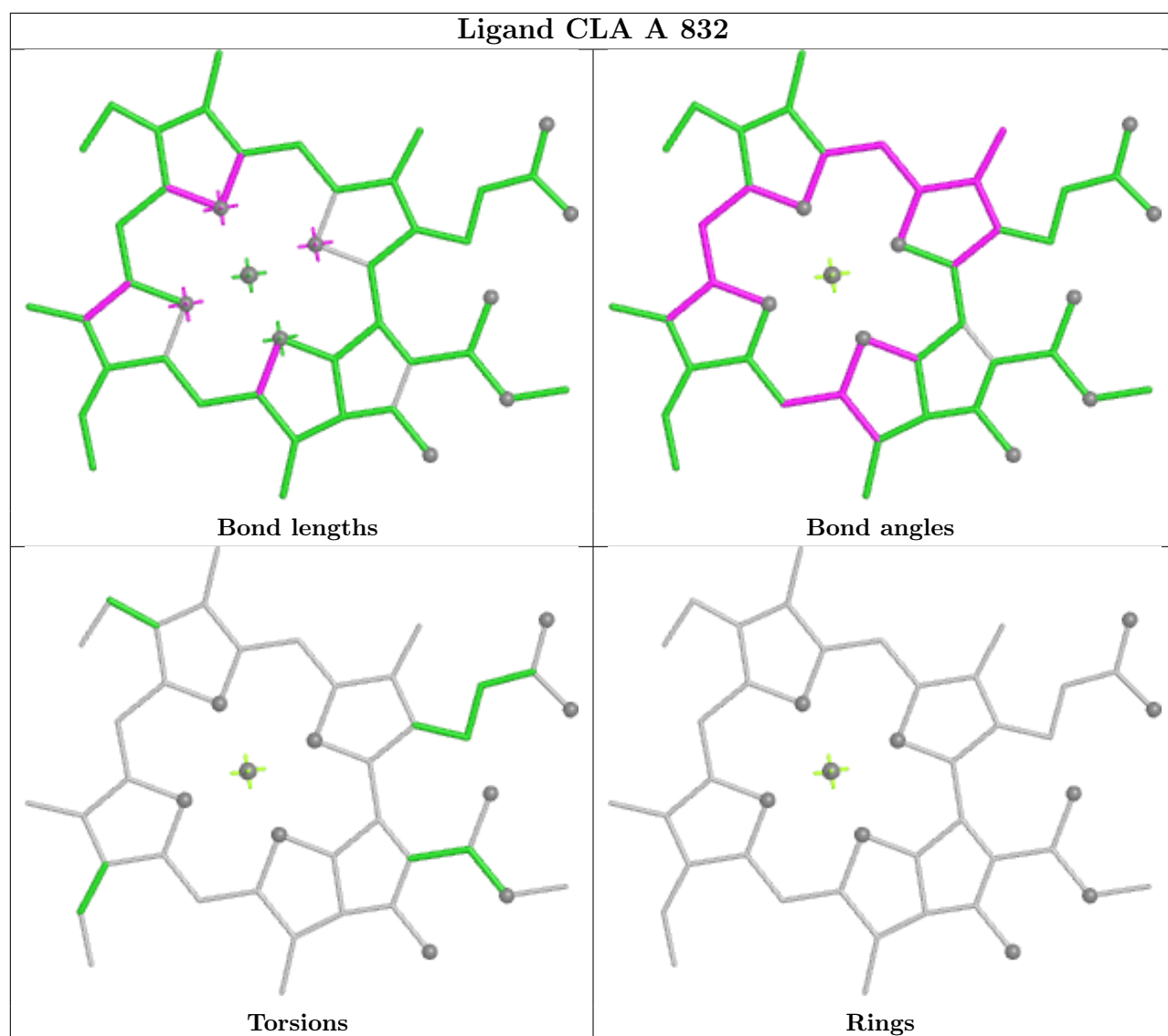


Ligand CLA A 825

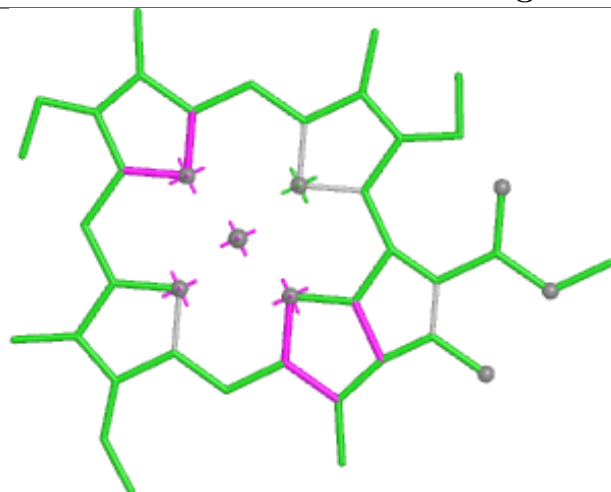


Ligand CLA A 828

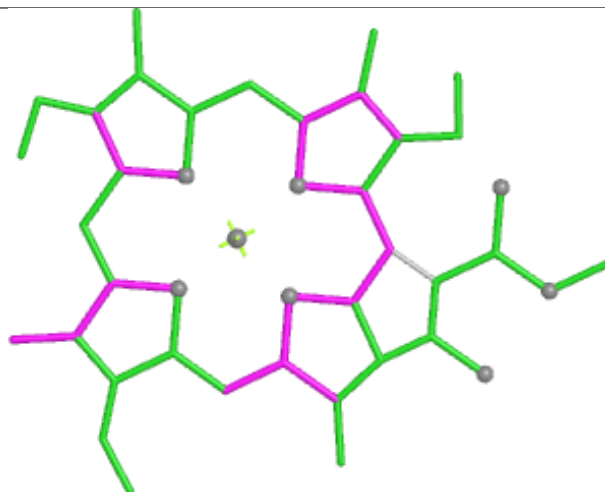




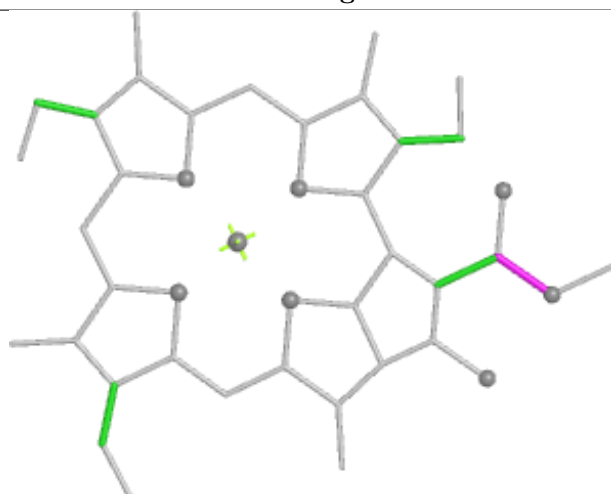
Ligand CLA F 303



Bond lengths



Bond angles

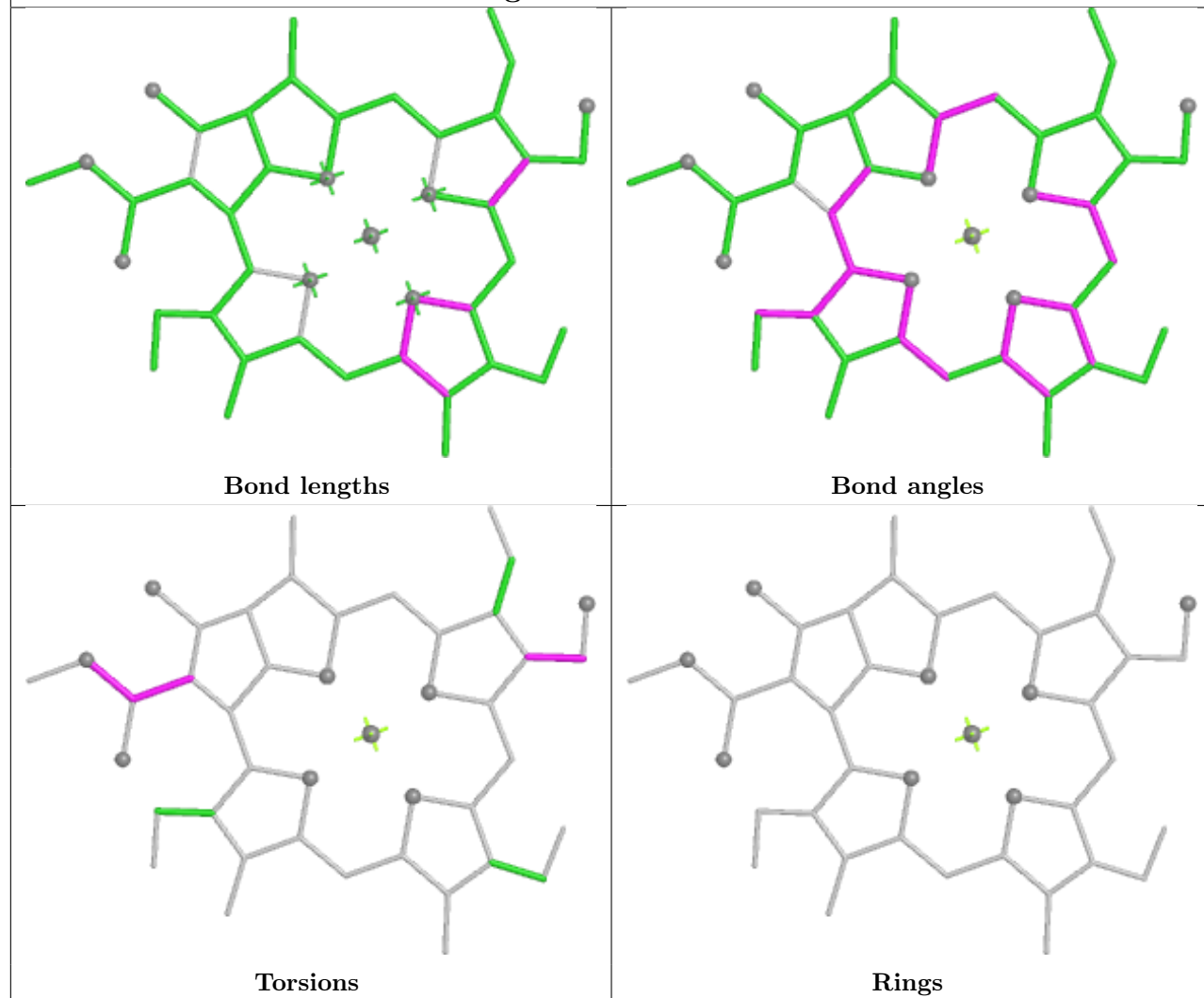


Torsions

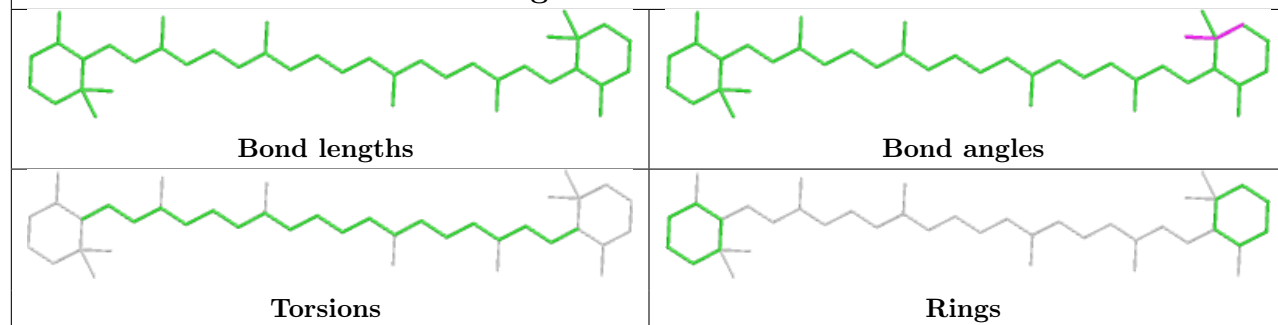


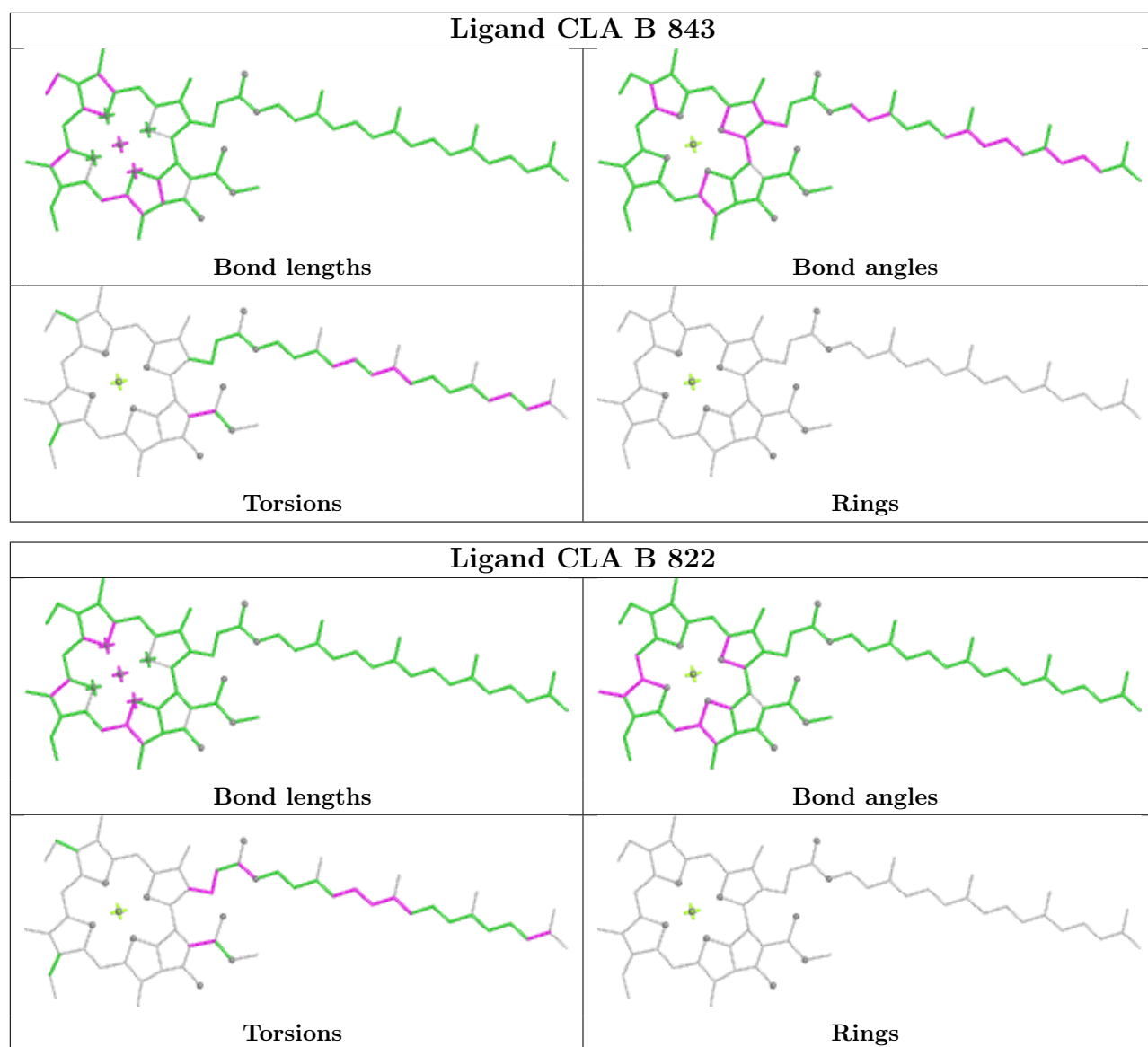
Rings

Ligand CHL 1 606

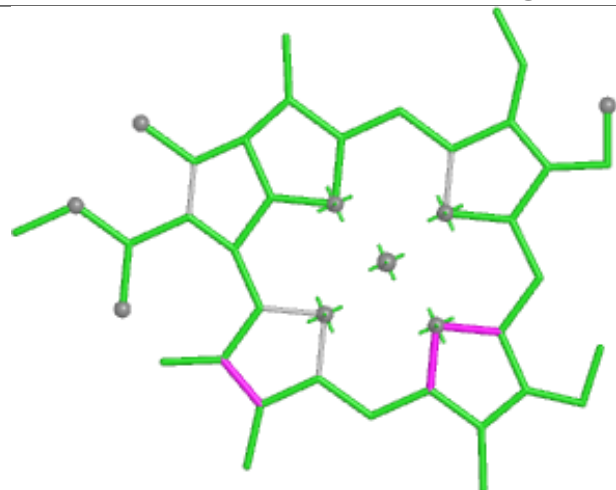


Ligand BCR B 816

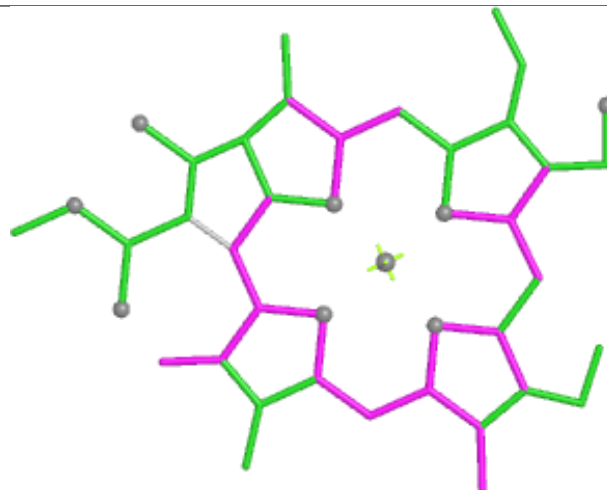




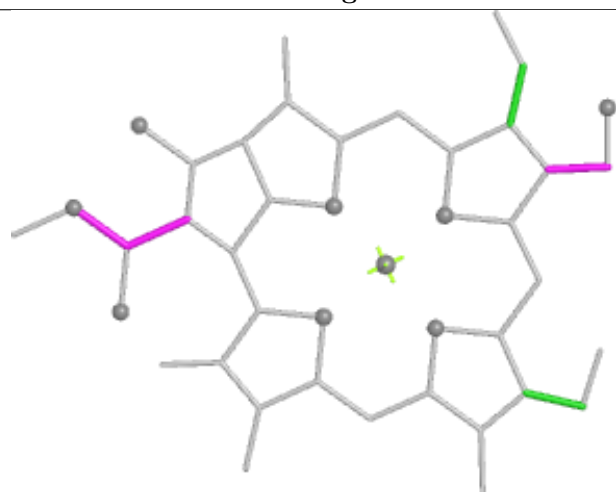
Ligand CHL 2 313



Bond lengths



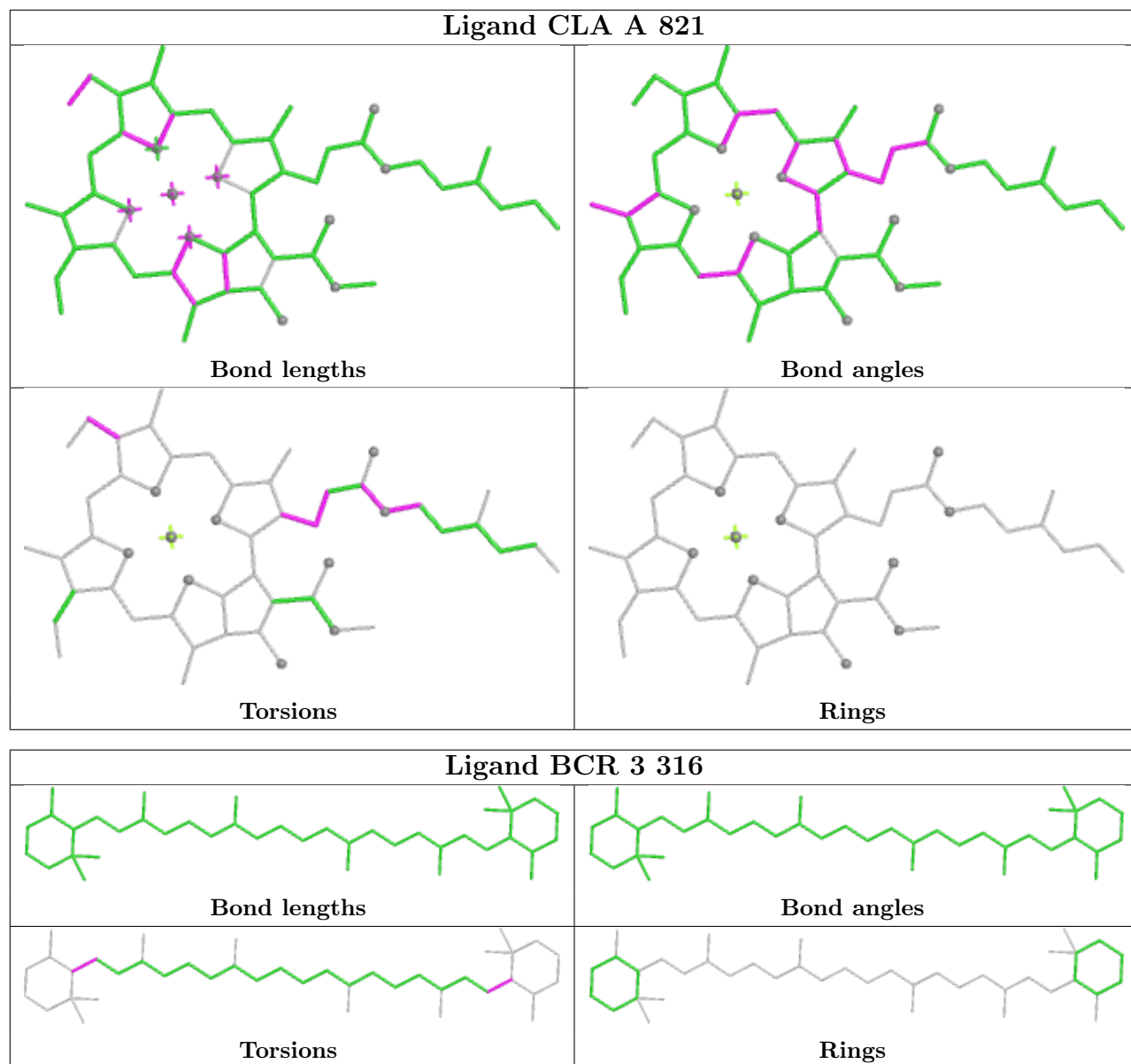
Bond angles



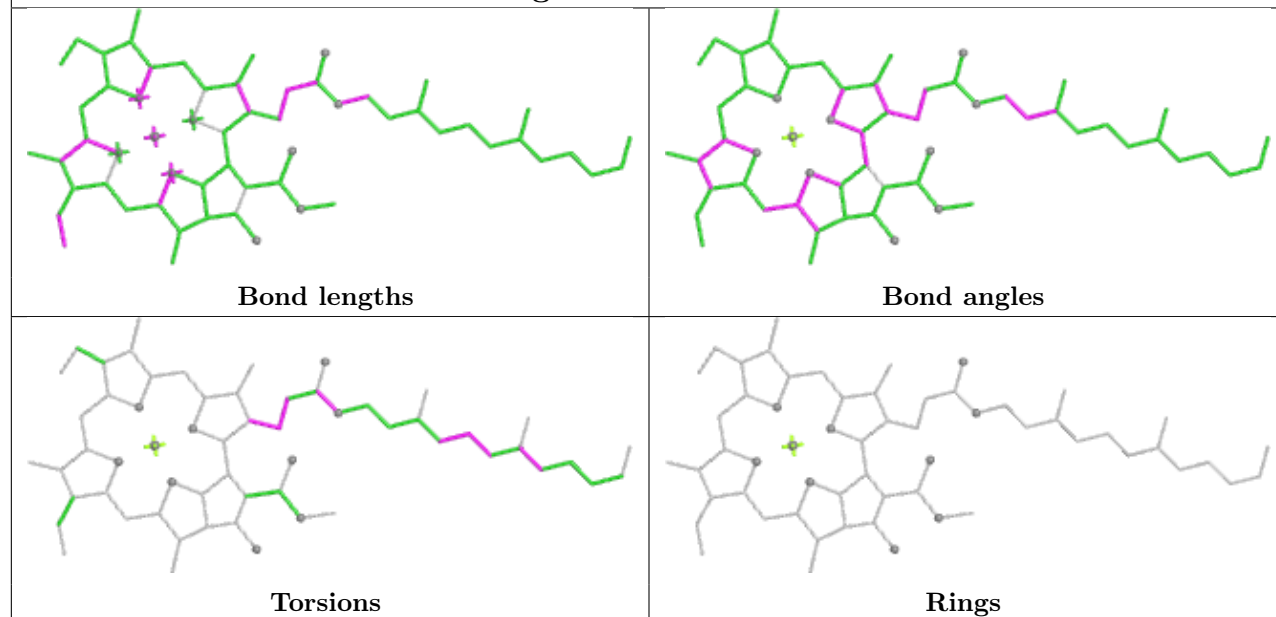
Torsions



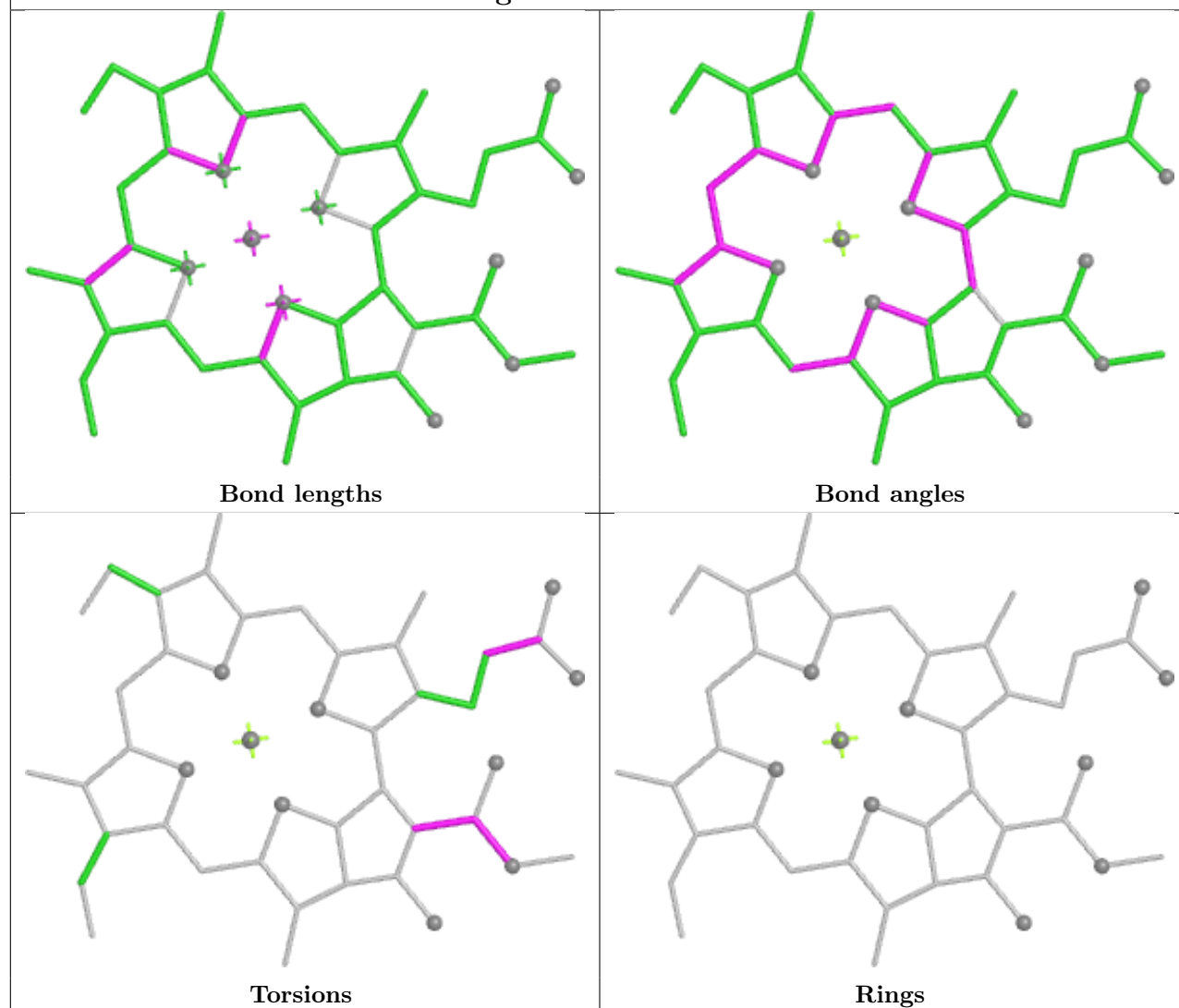
Rings



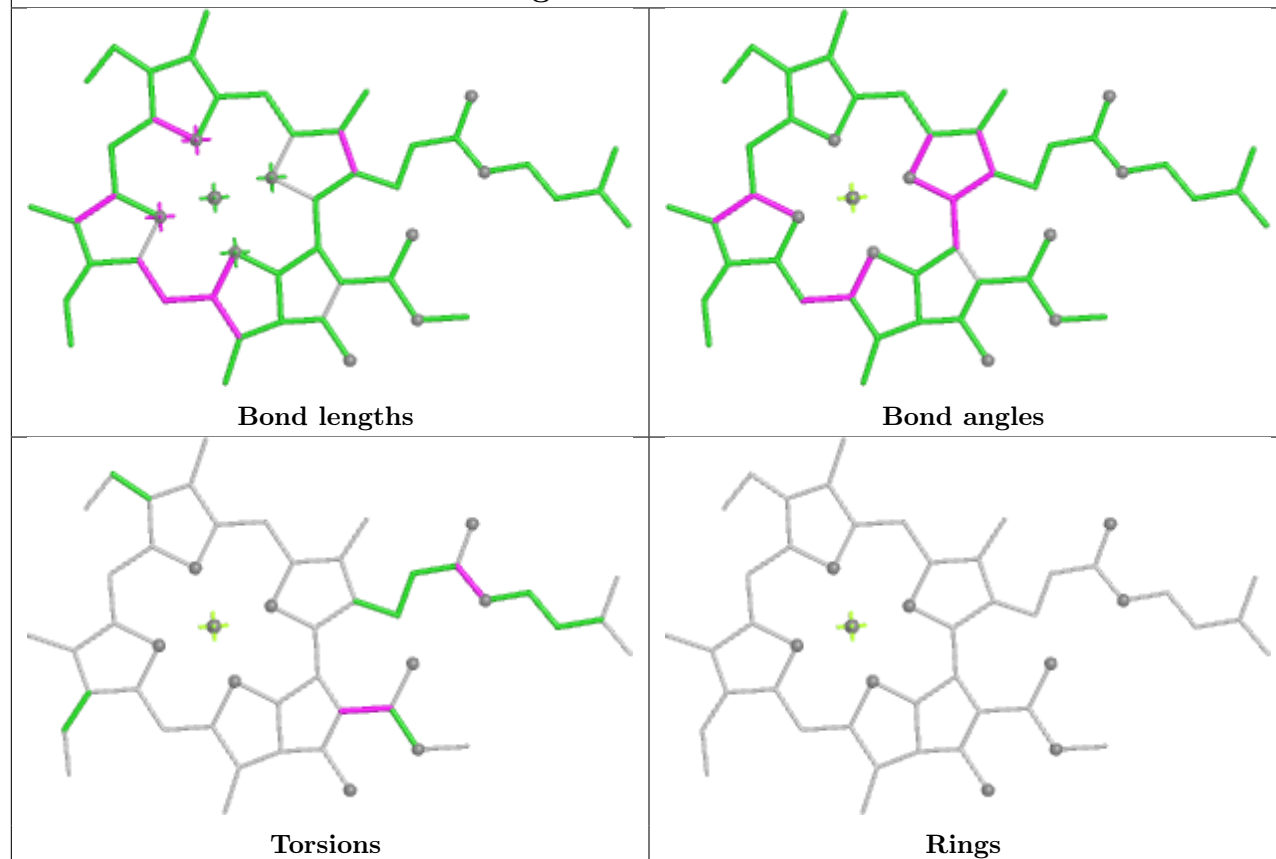
Ligand CLA B 844



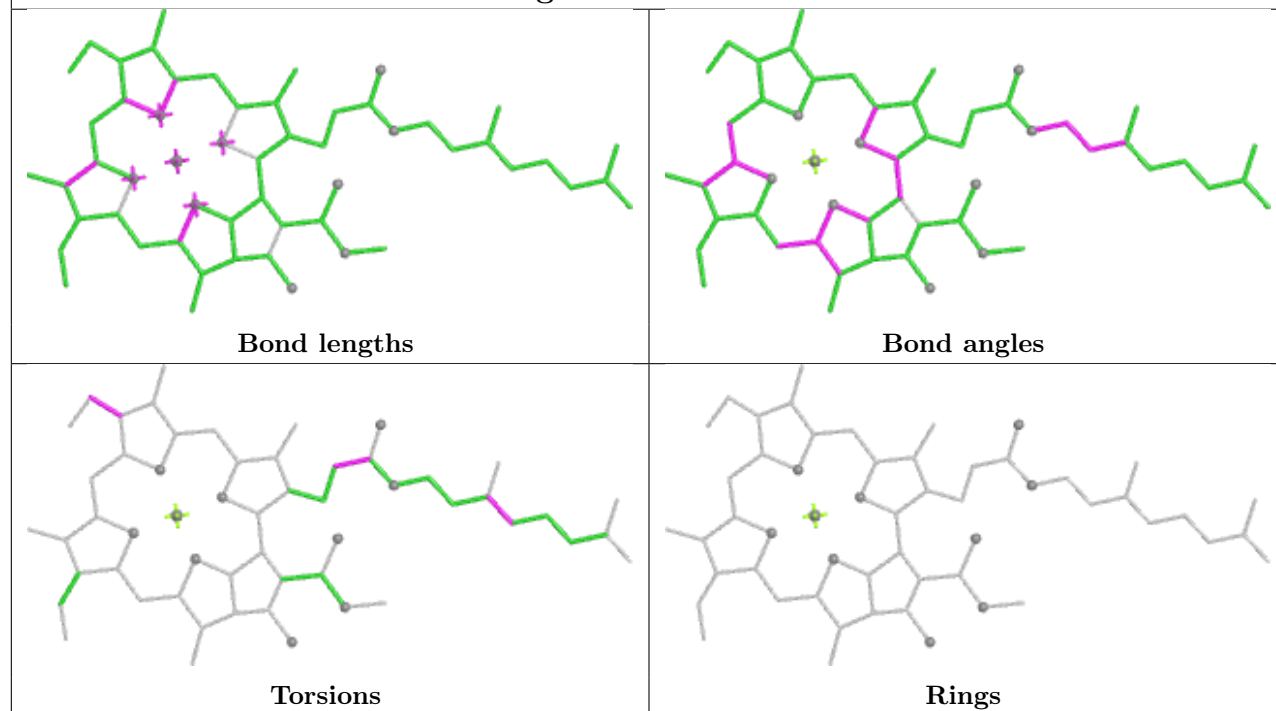
Ligand CLA 4 307

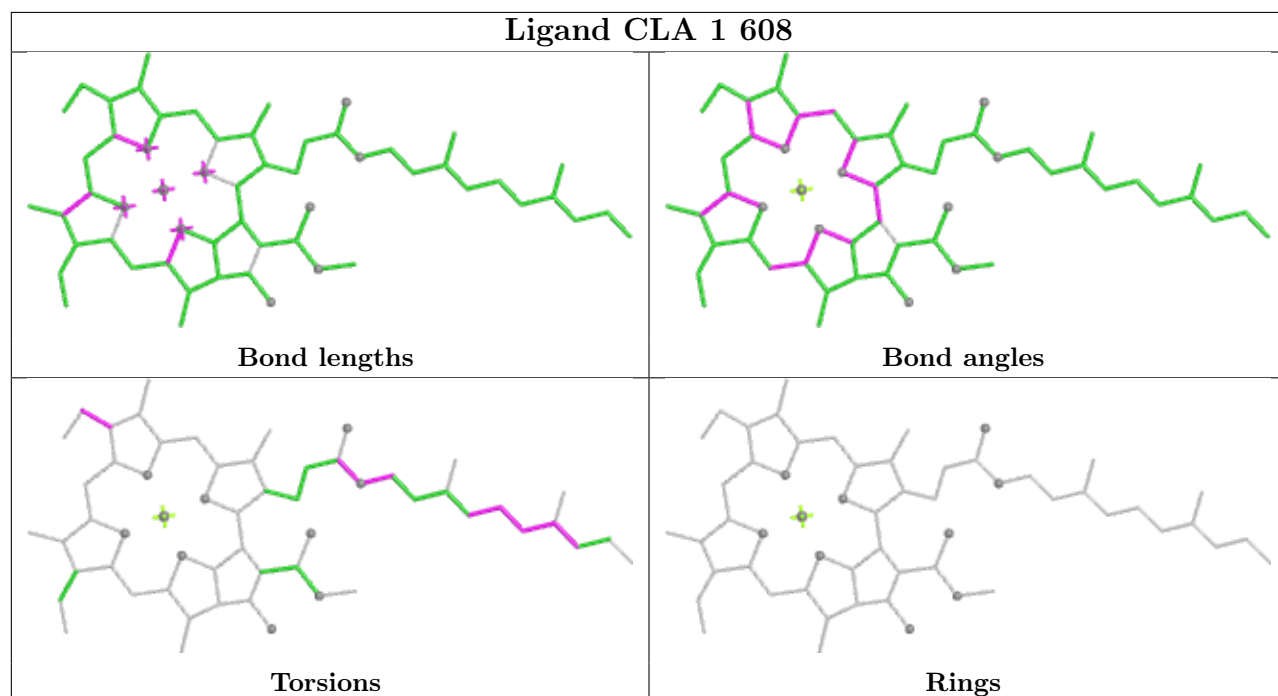
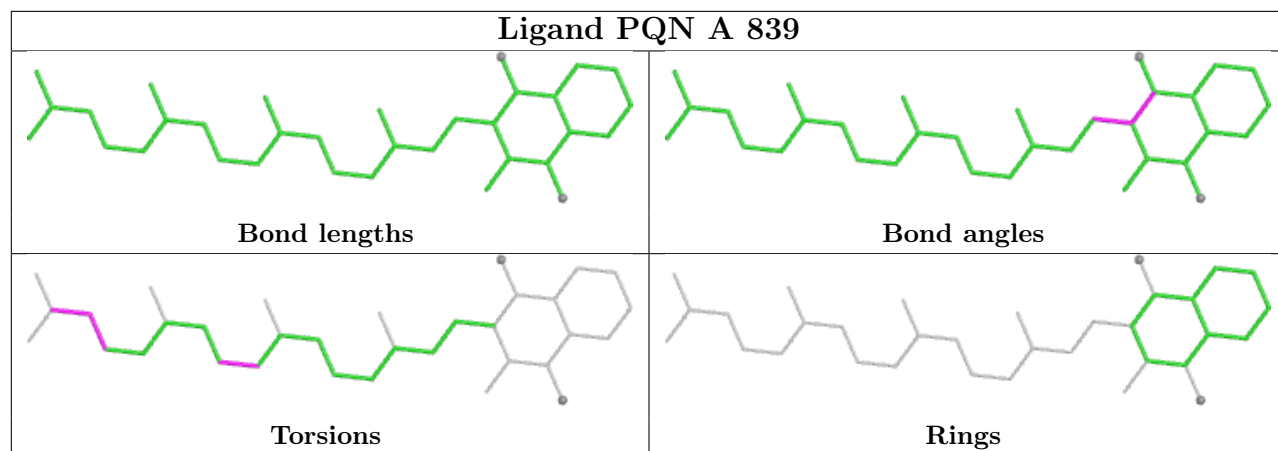


Ligand CLA B 847

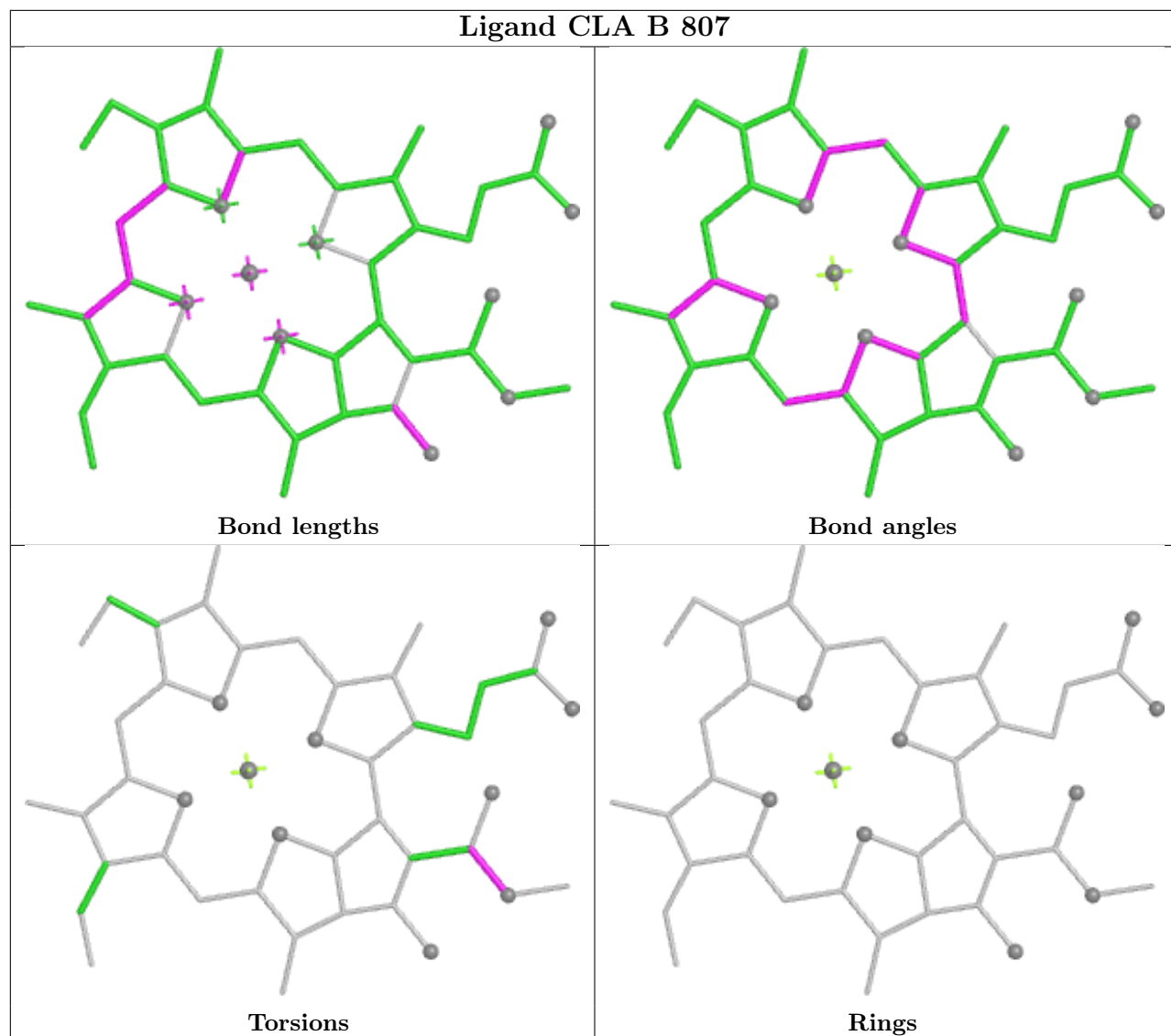


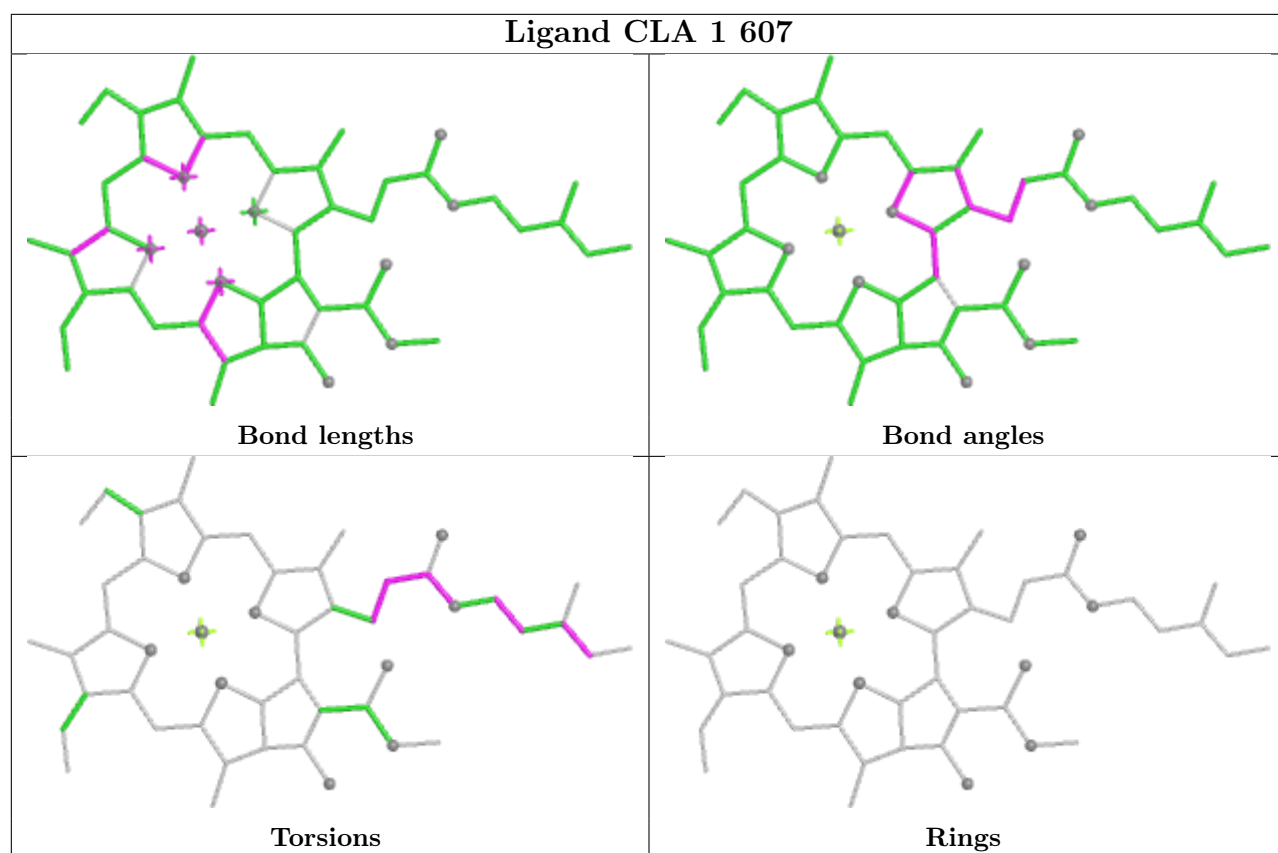
Ligand CLA 1 612



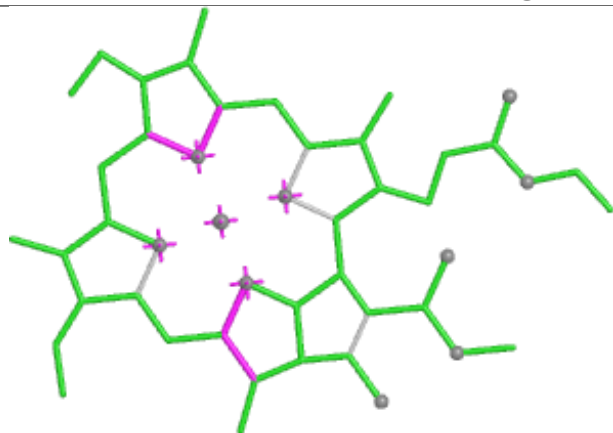


Ligand CLA B 807

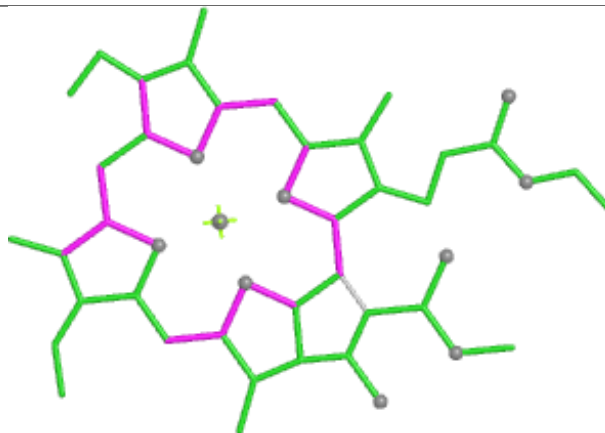




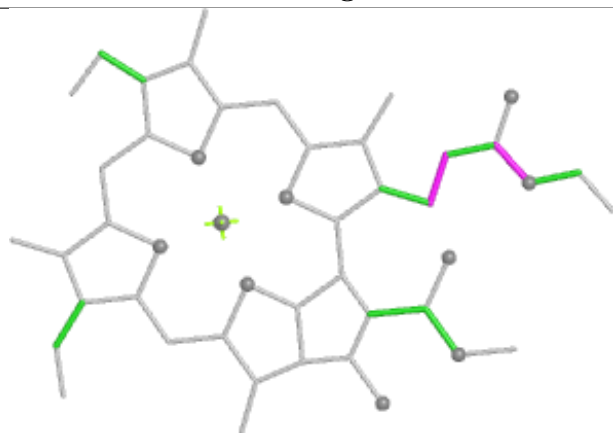
Ligand CLA 3 306



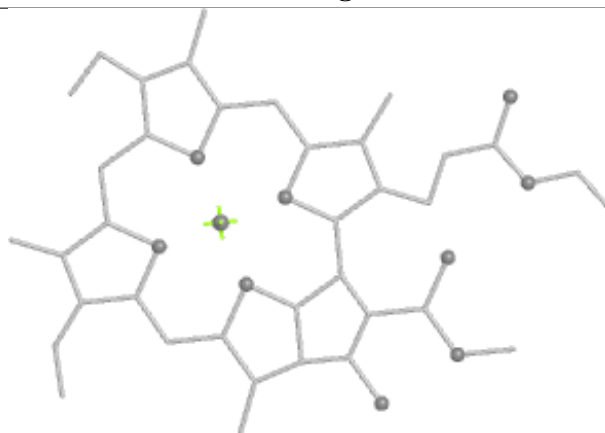
Bond lengths



Bond angles

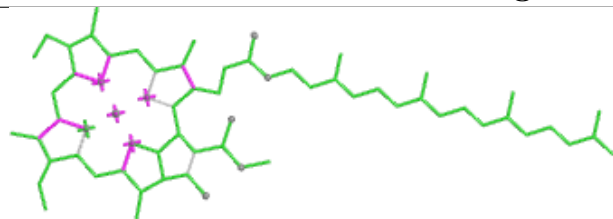


Torsions

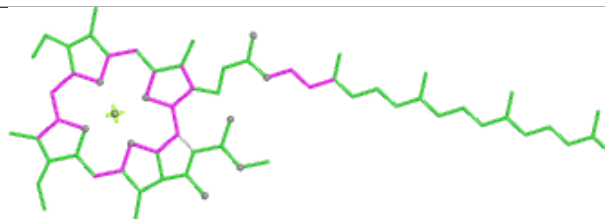


Rings

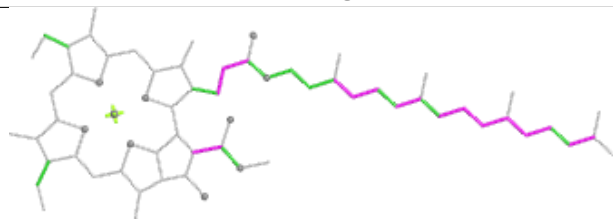
Ligand CLA A 818



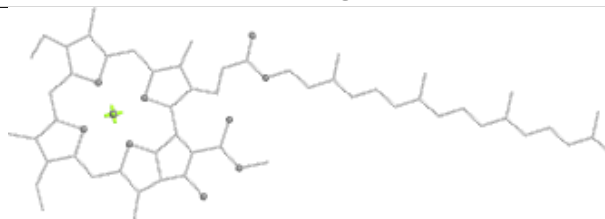
Bond lengths



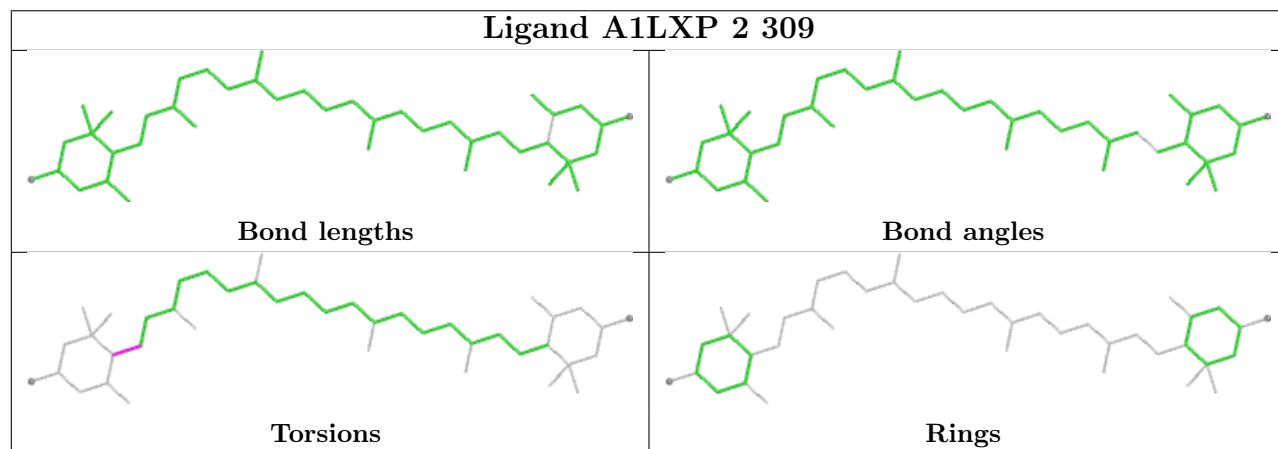
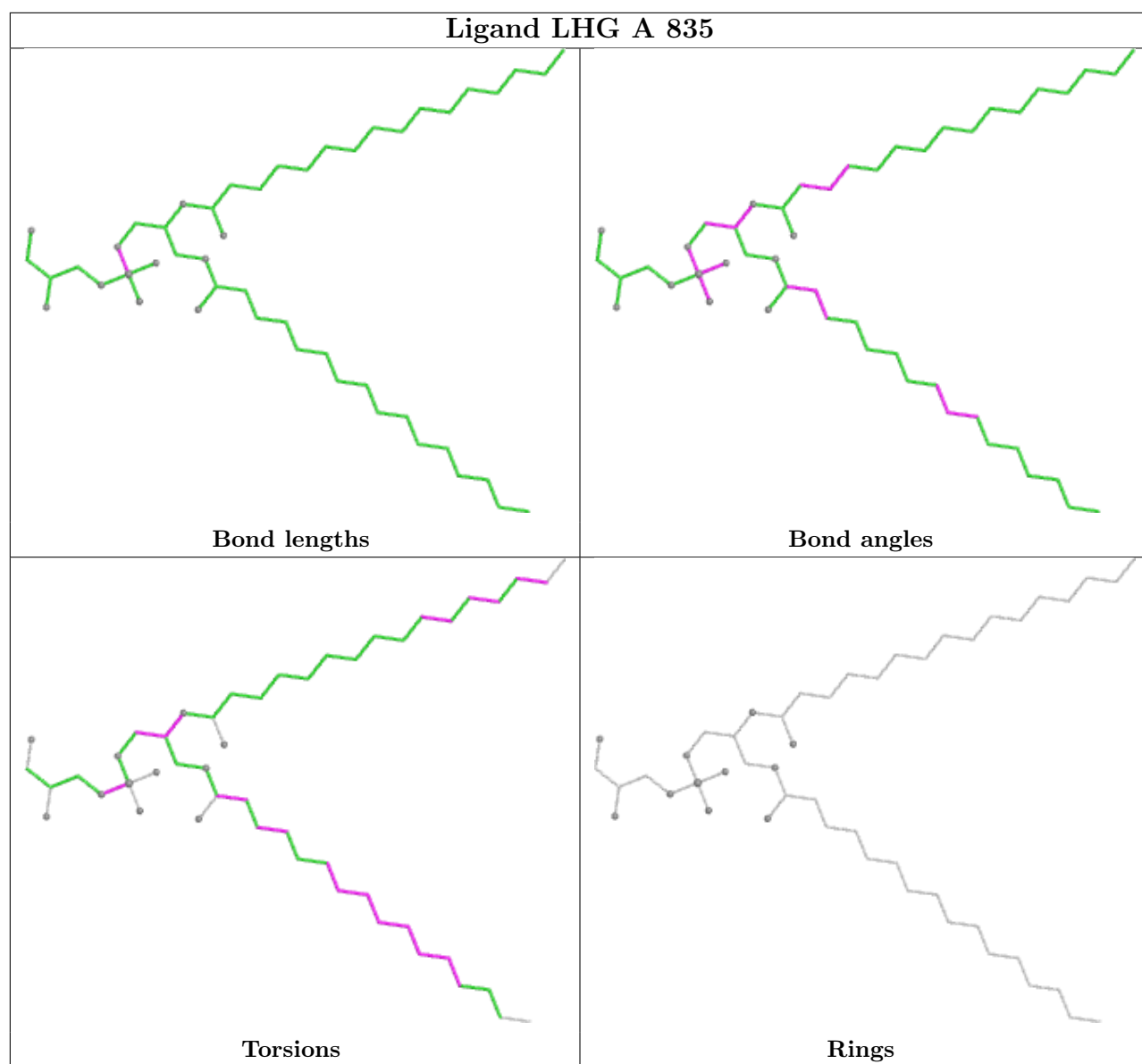
Bond angles

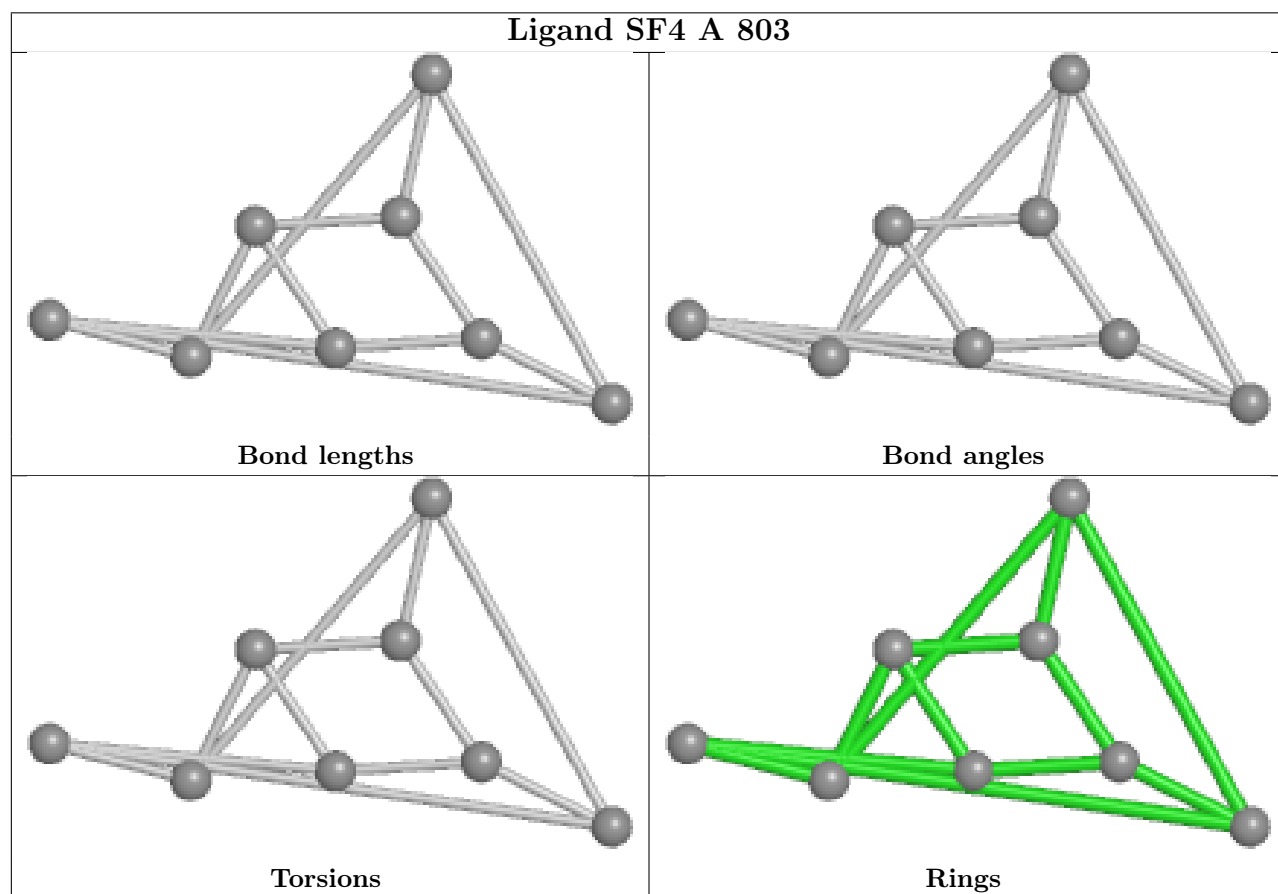
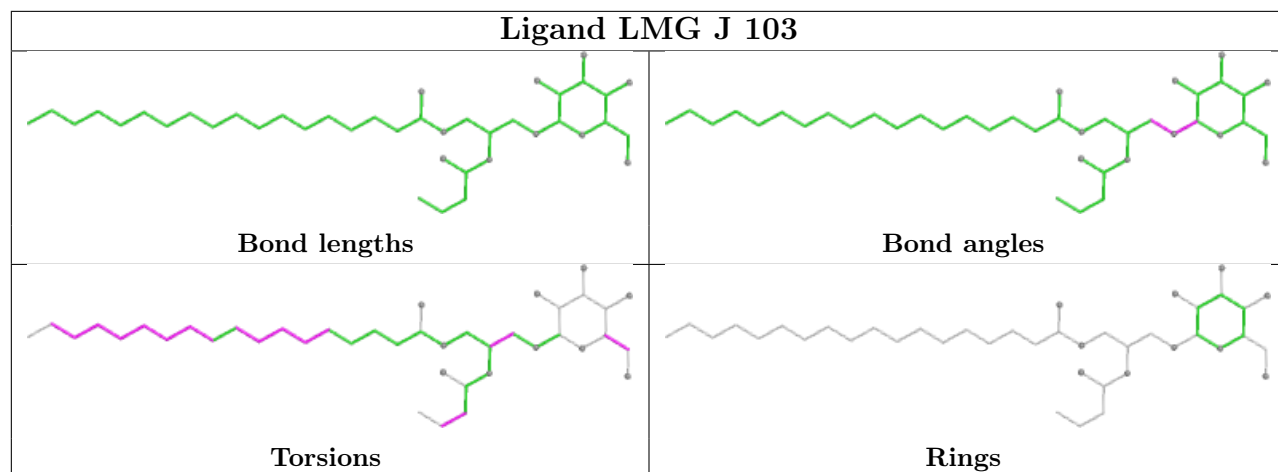


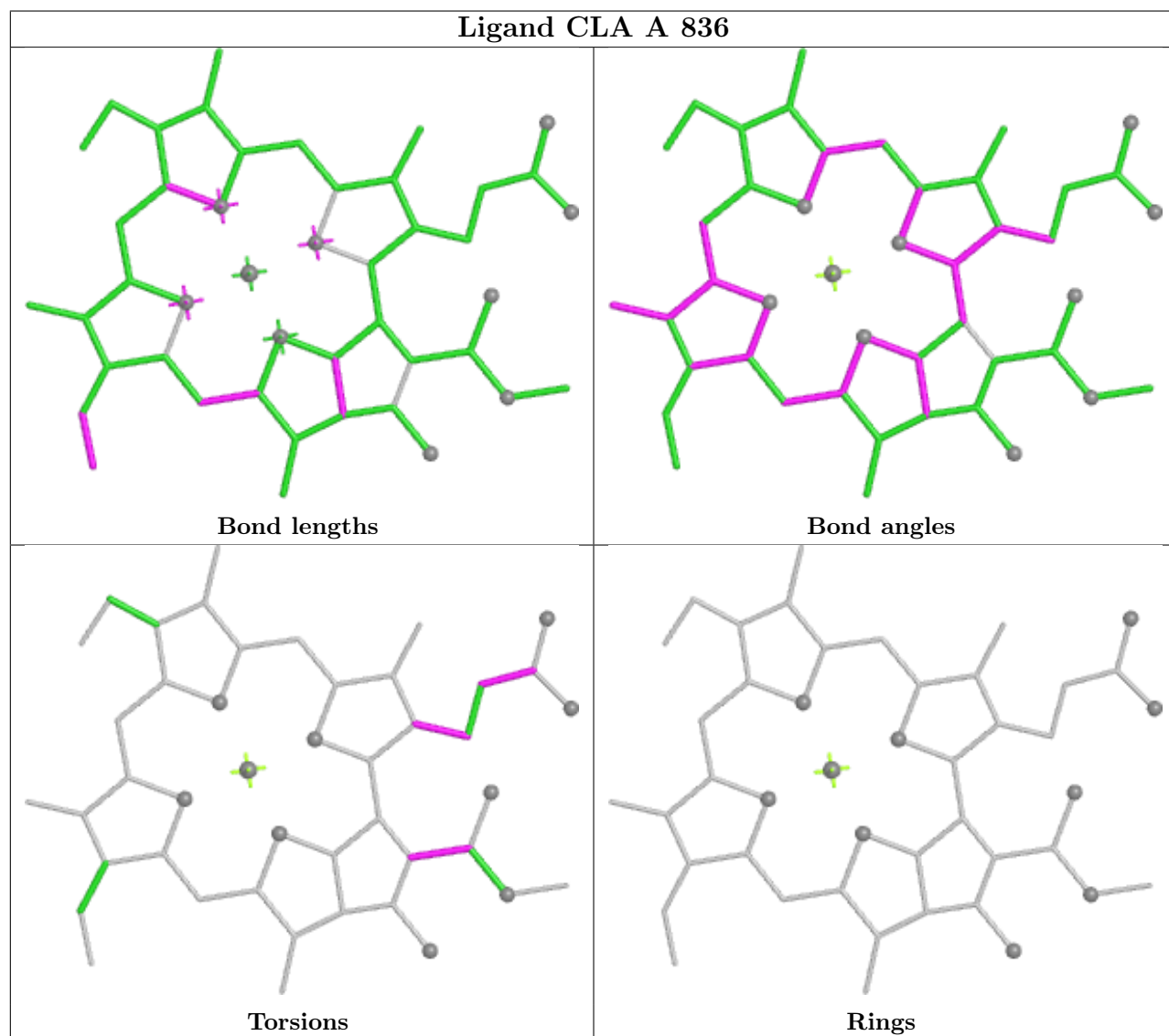
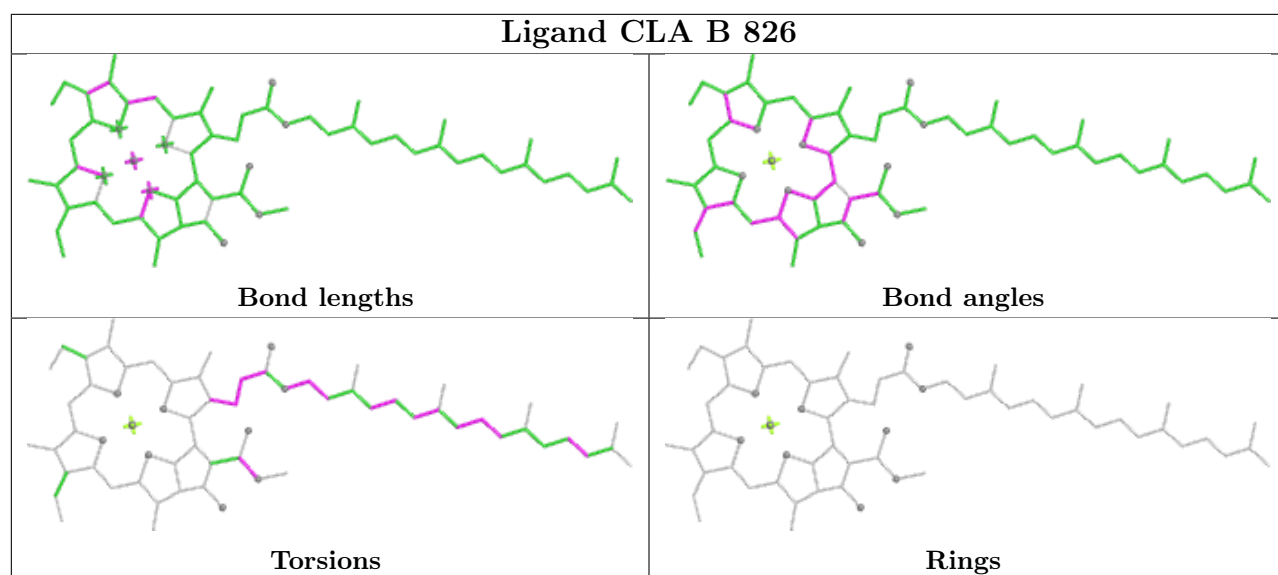
Torsions

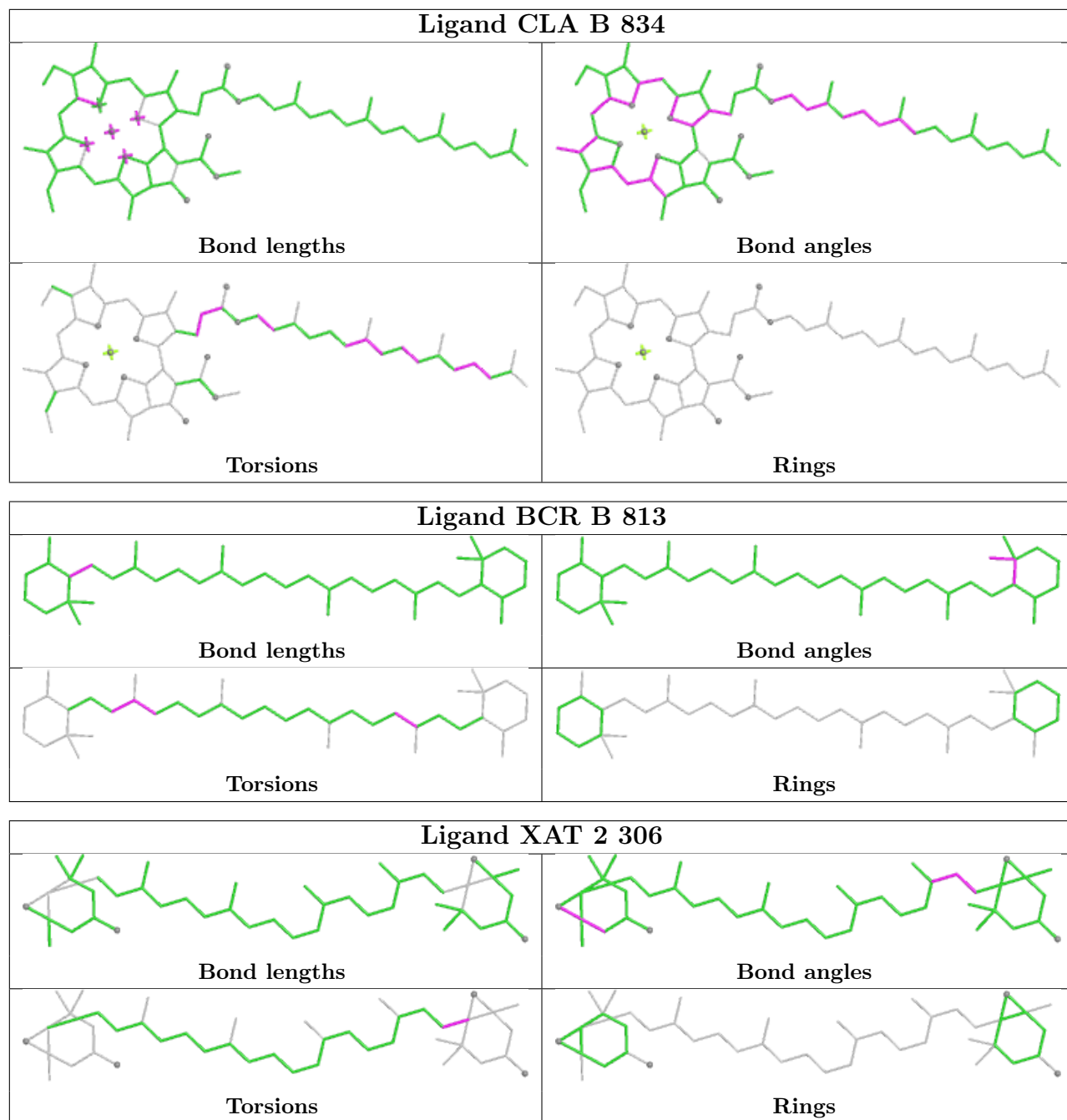


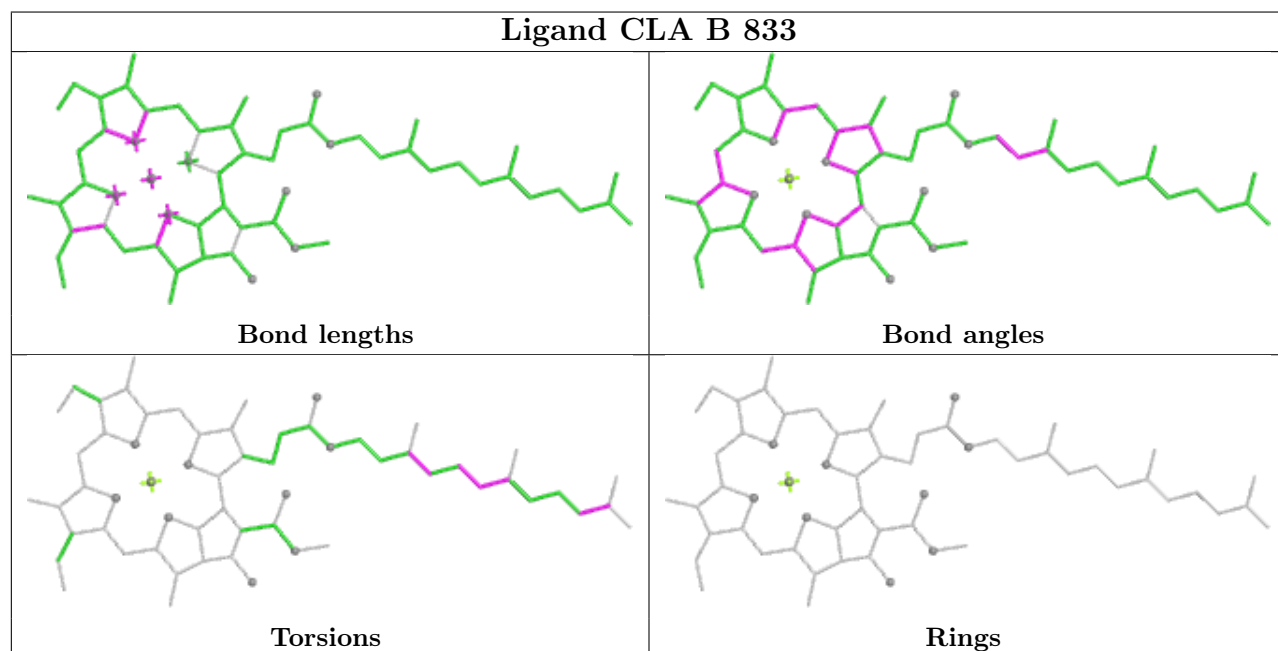
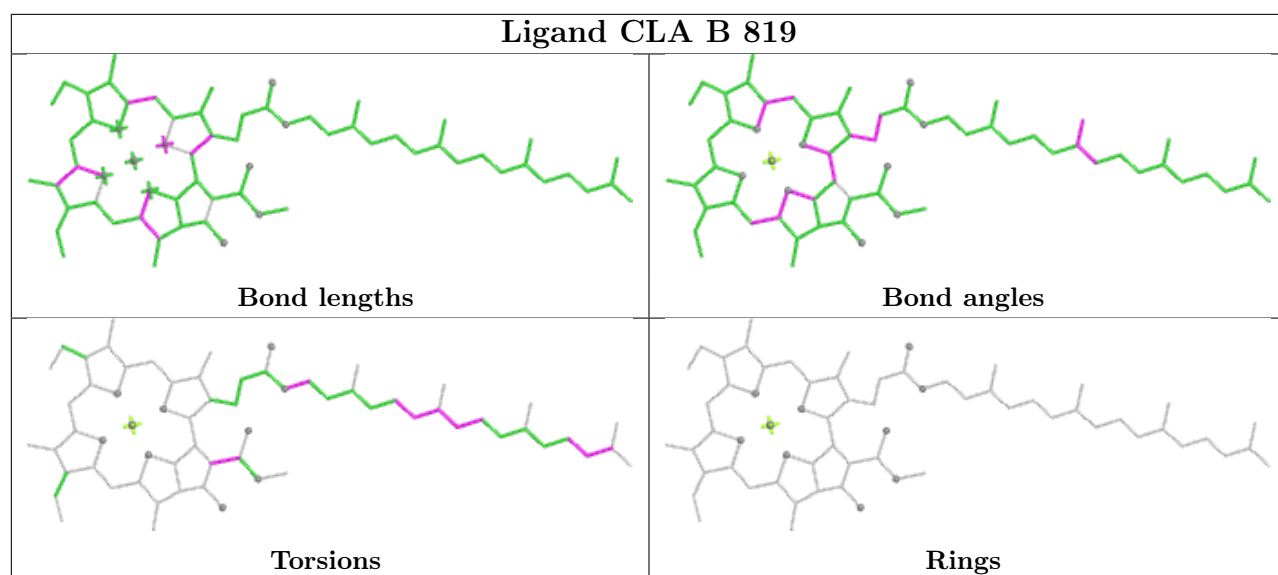
Rings



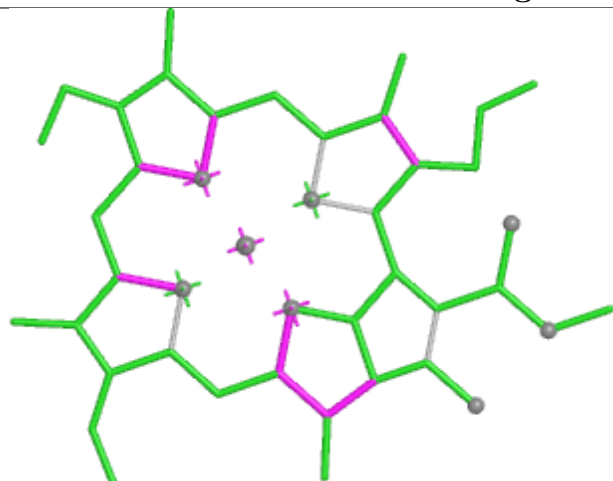




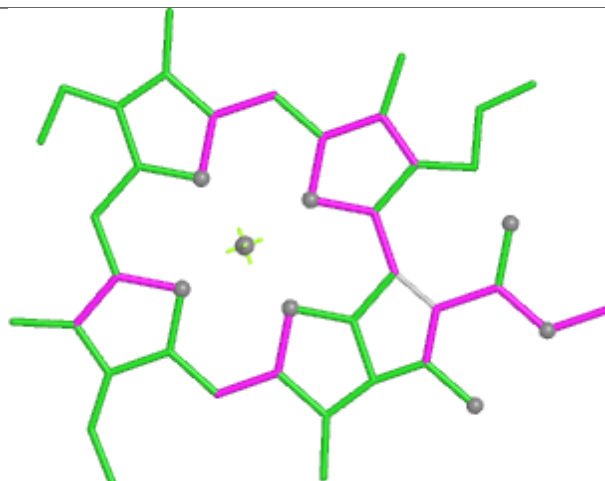




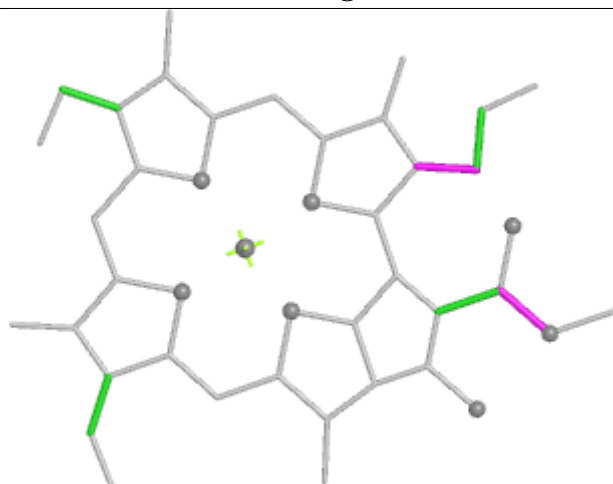
Ligand CLA B 839



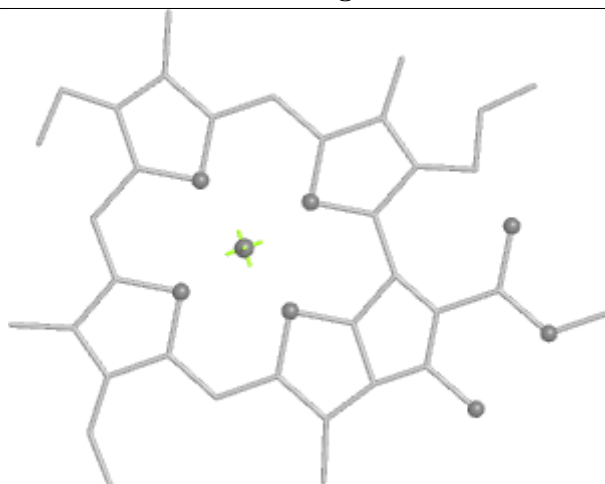
Bond lengths



Bond angles

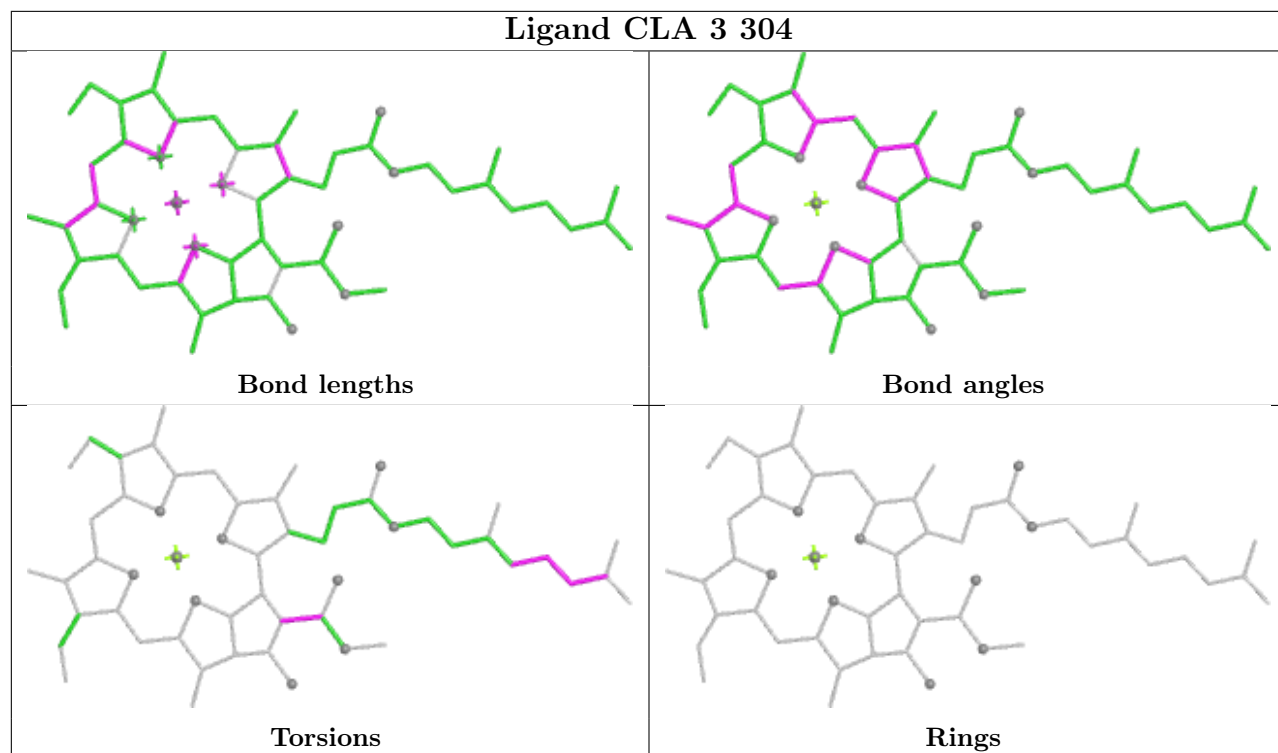


Torsions

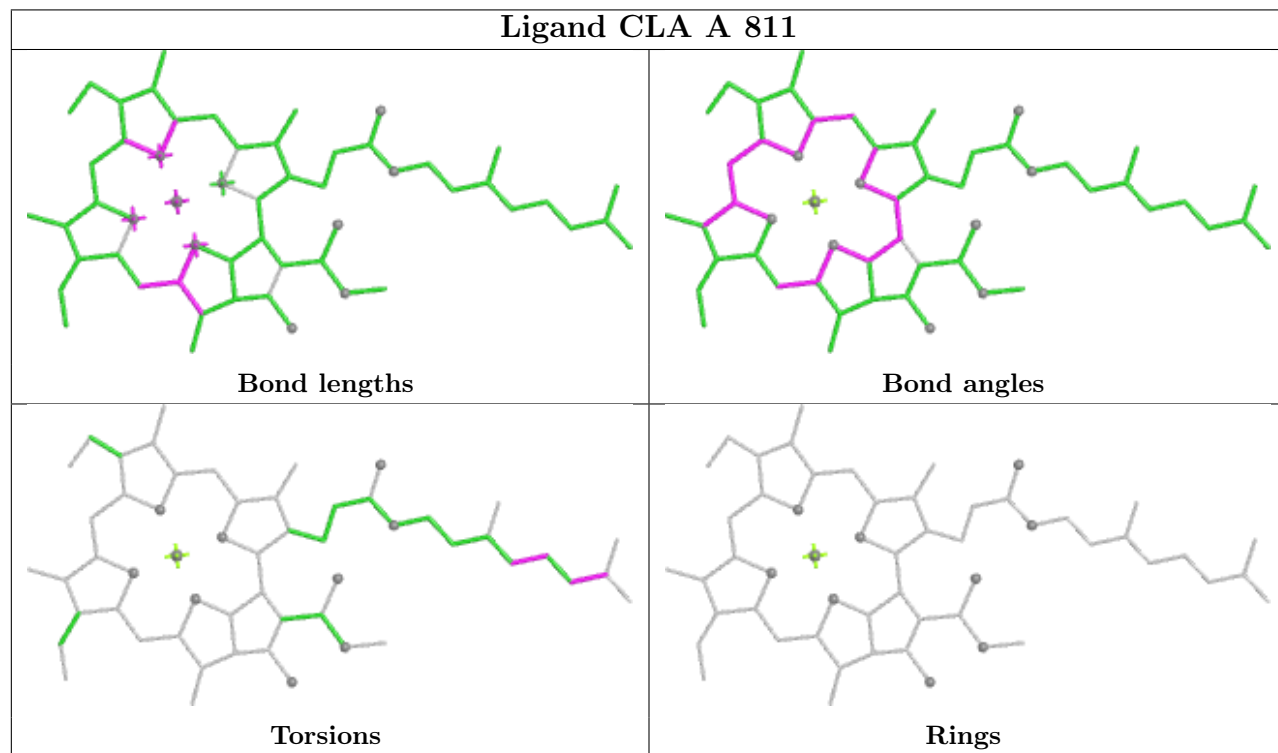


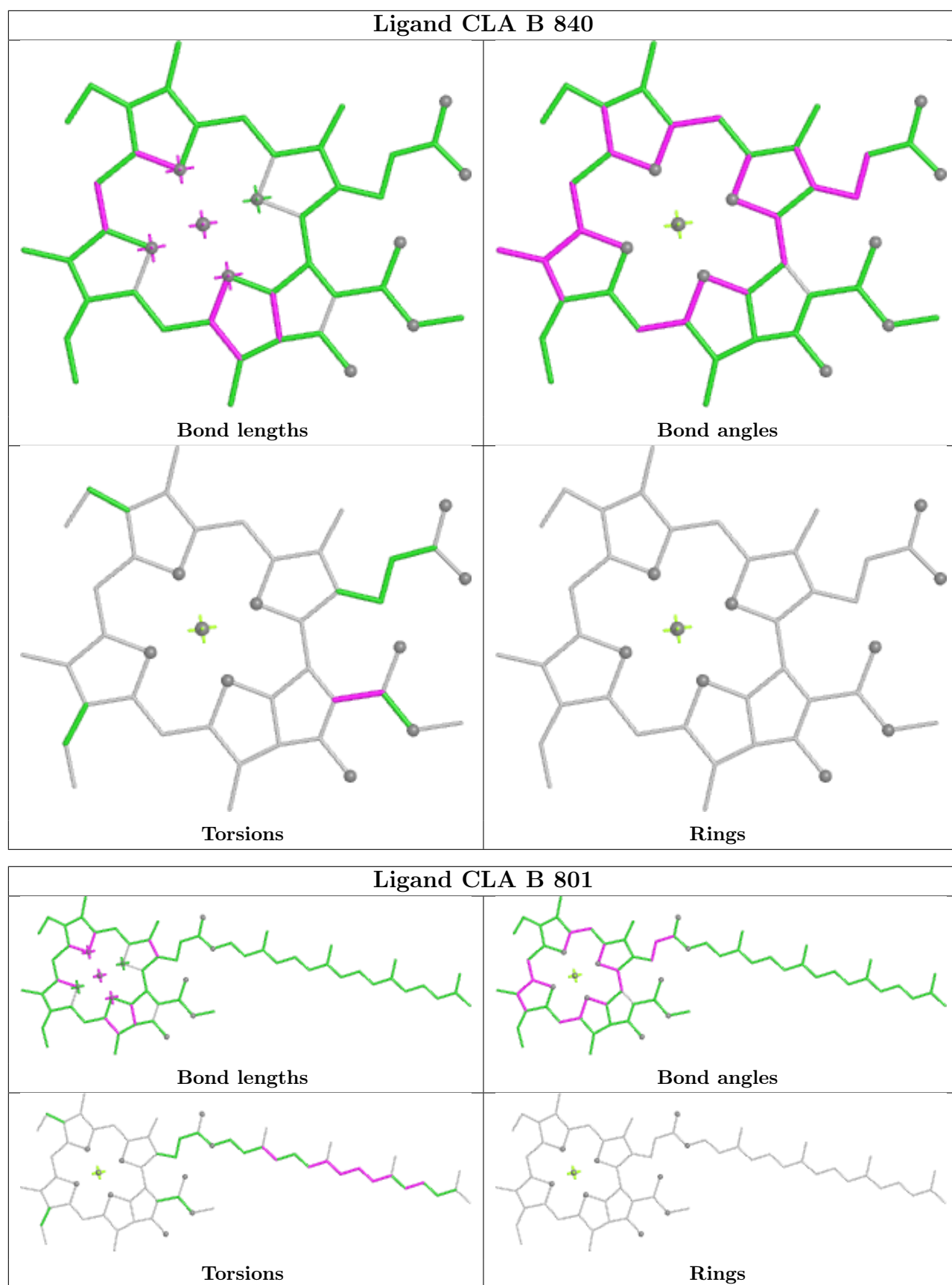
Rings

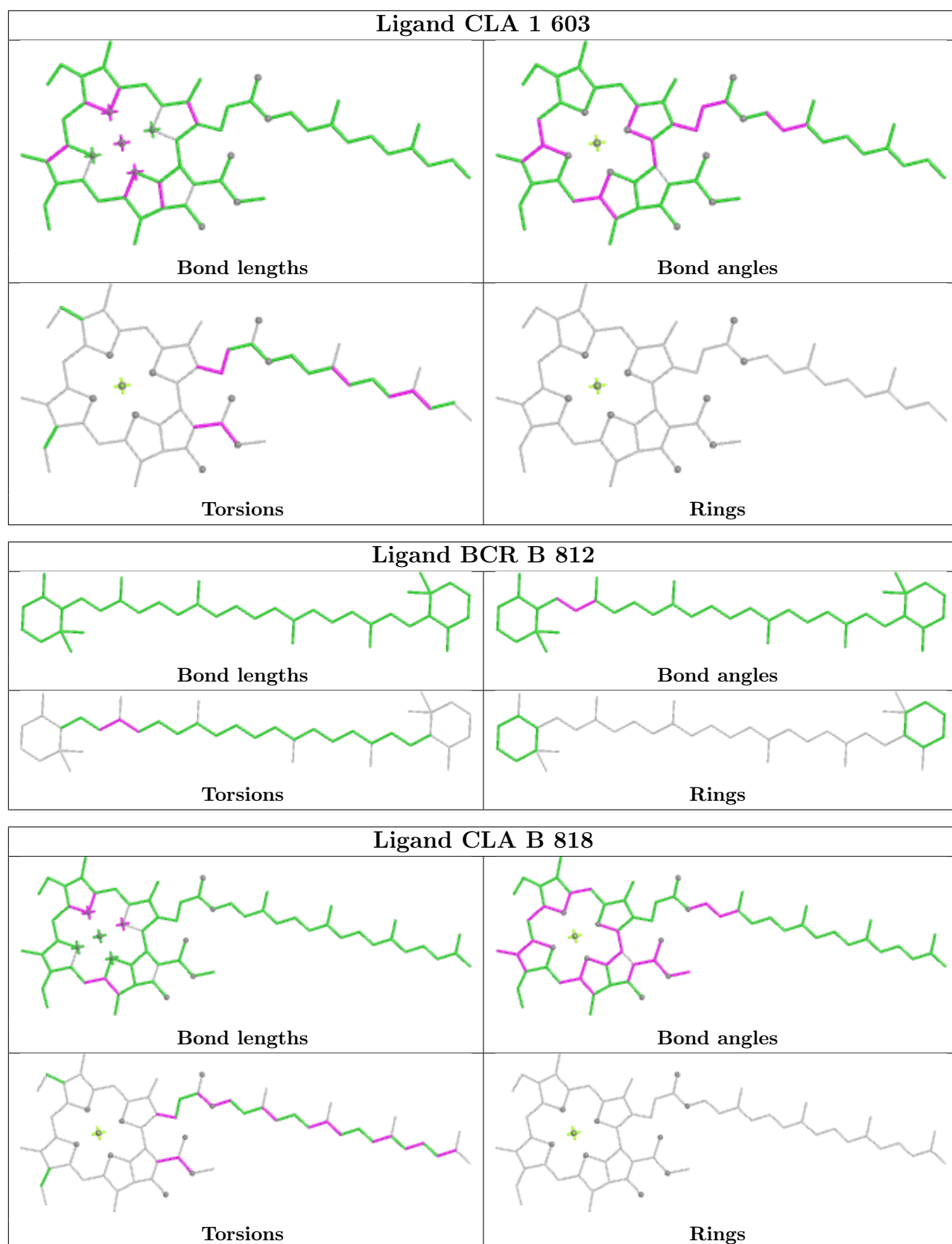
Ligand CLA 3 304



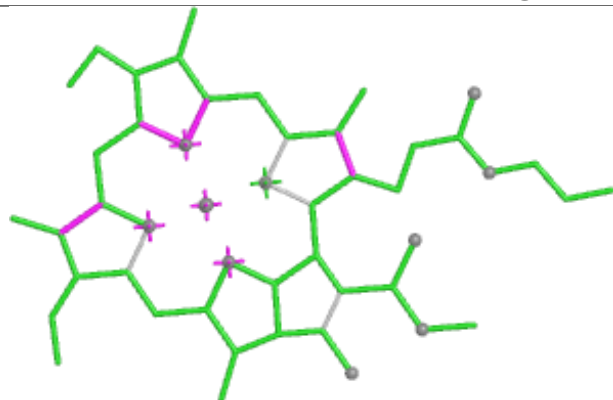
Ligand CLA A 811



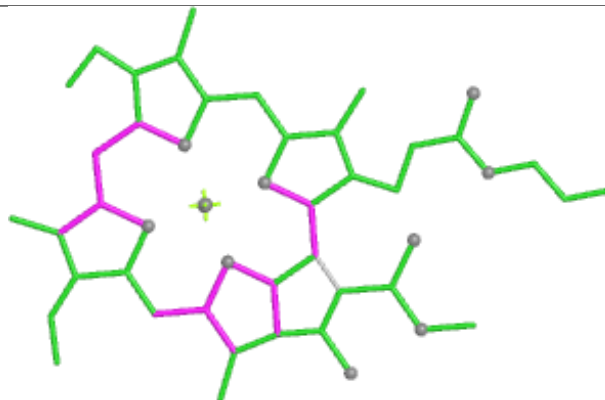




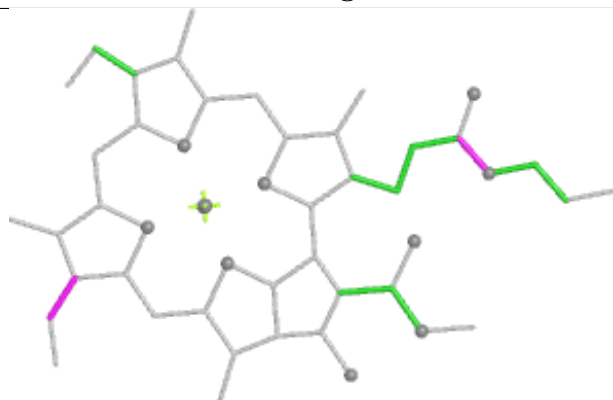
Ligand CLA F 306



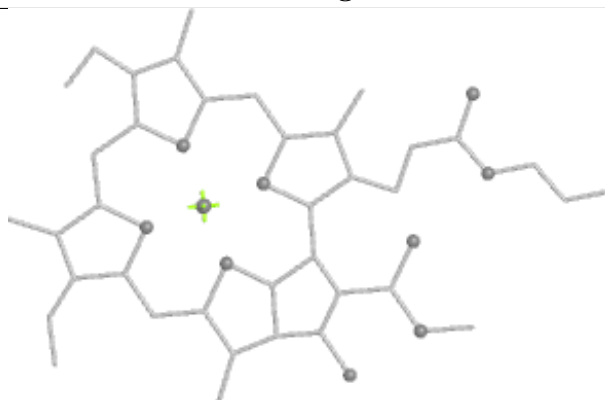
Bond lengths



Bond angles

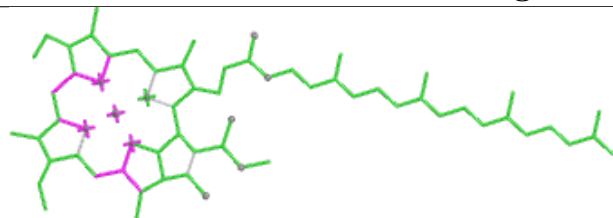


Torsions

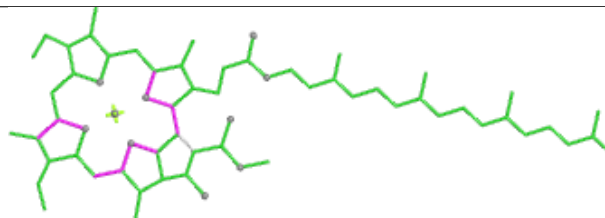


Rings

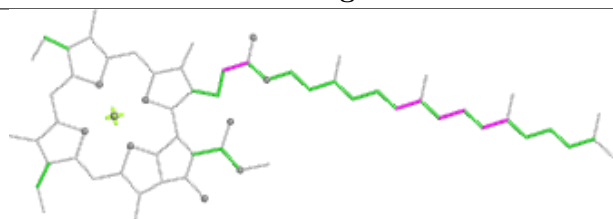
Ligand CLA A 833



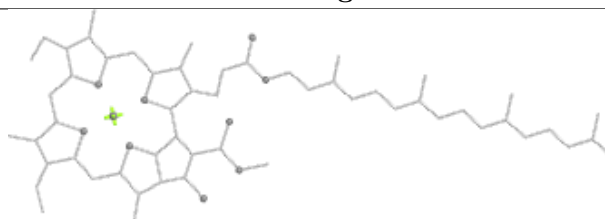
Bond lengths



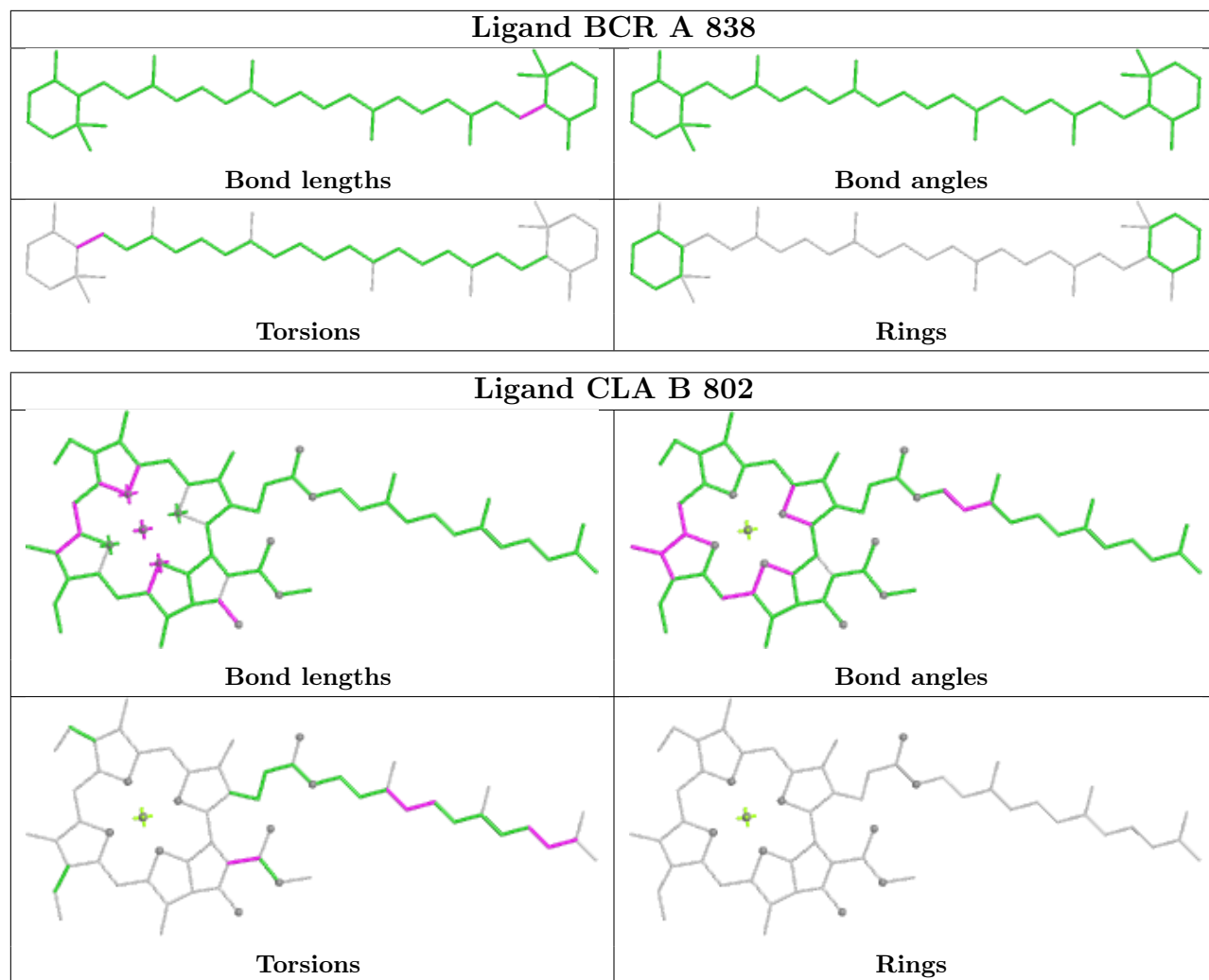
Bond angles



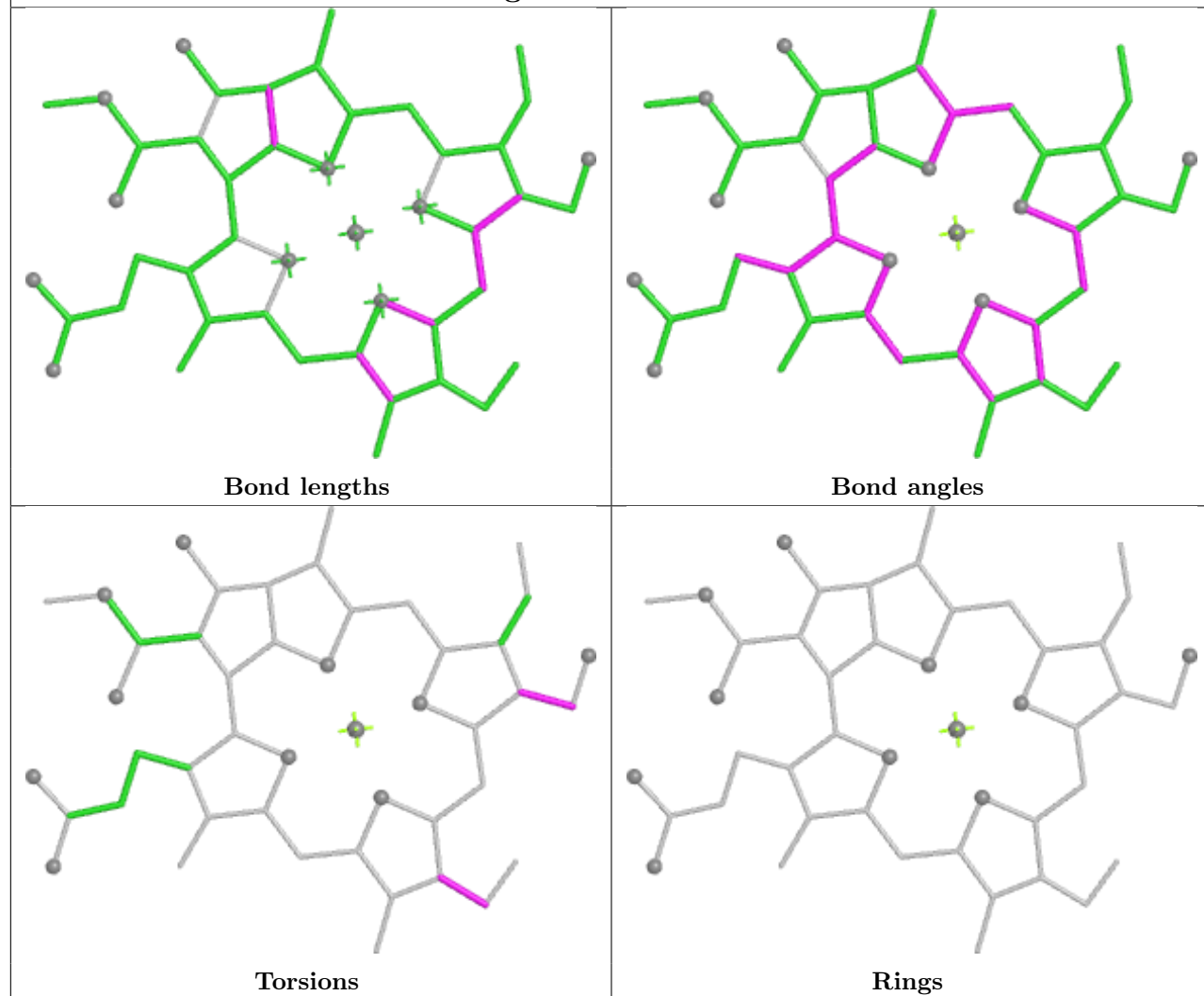
Torsions



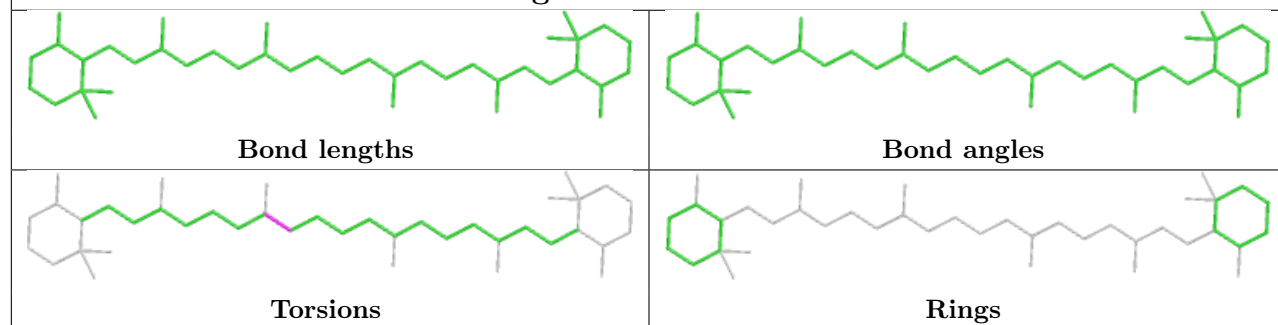
Rings



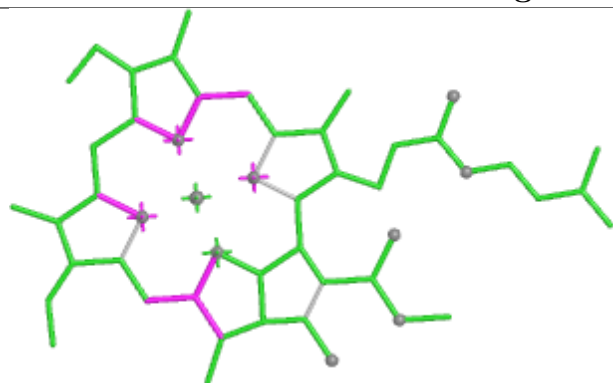
Ligand CHL 4 313



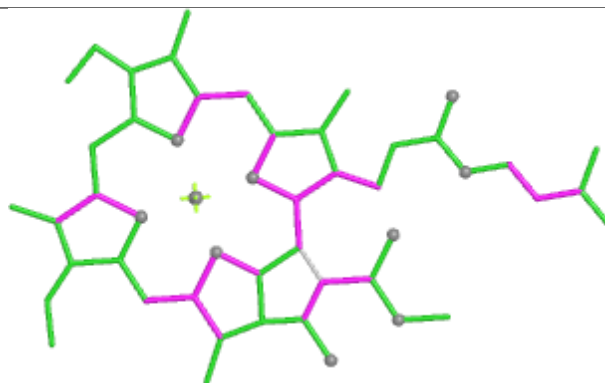
Ligand BCR F 304



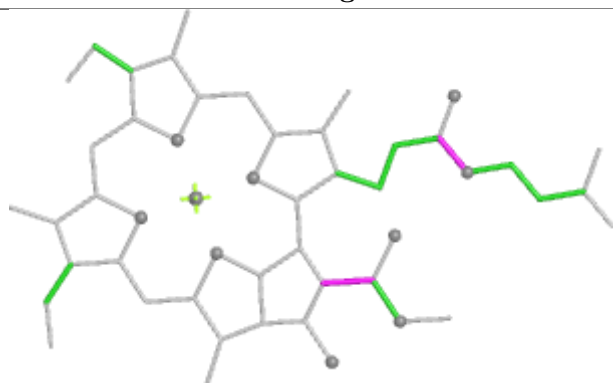
Ligand CLA B 842



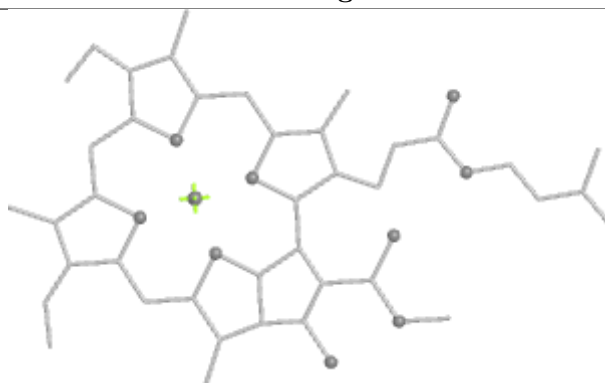
Bond lengths



Bond angles

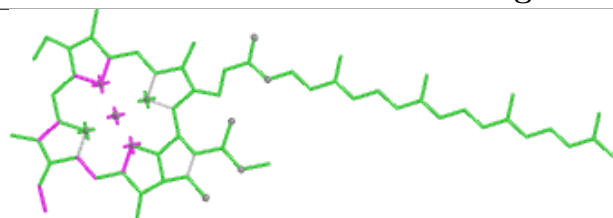


Torsions

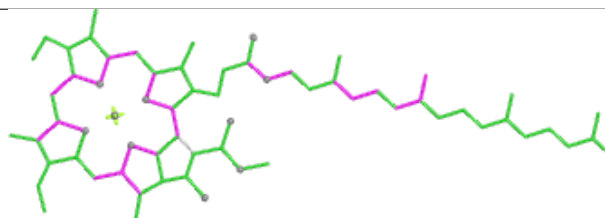


Rings

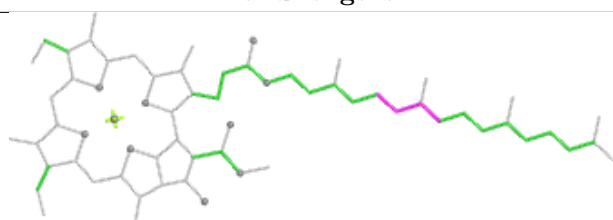
Ligand CLA B 845



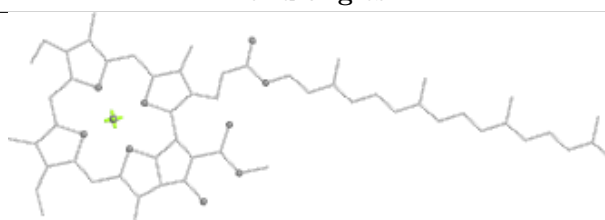
Bond lengths



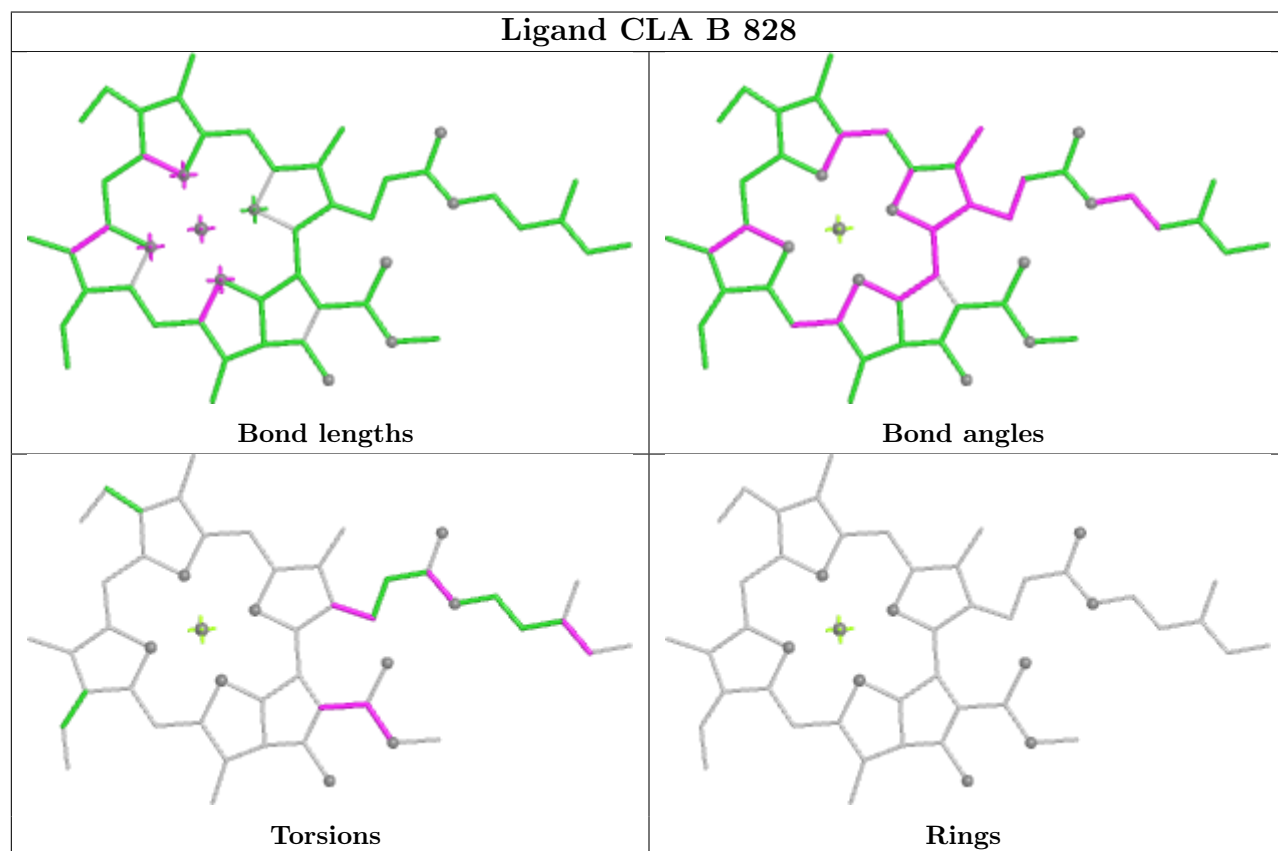
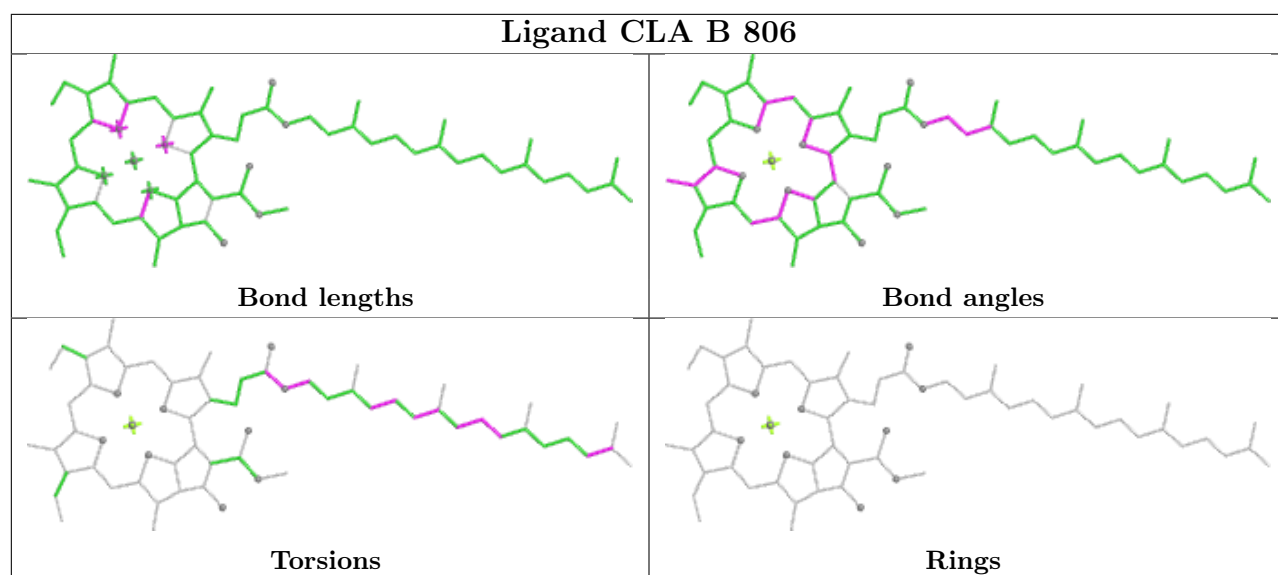
Bond angles

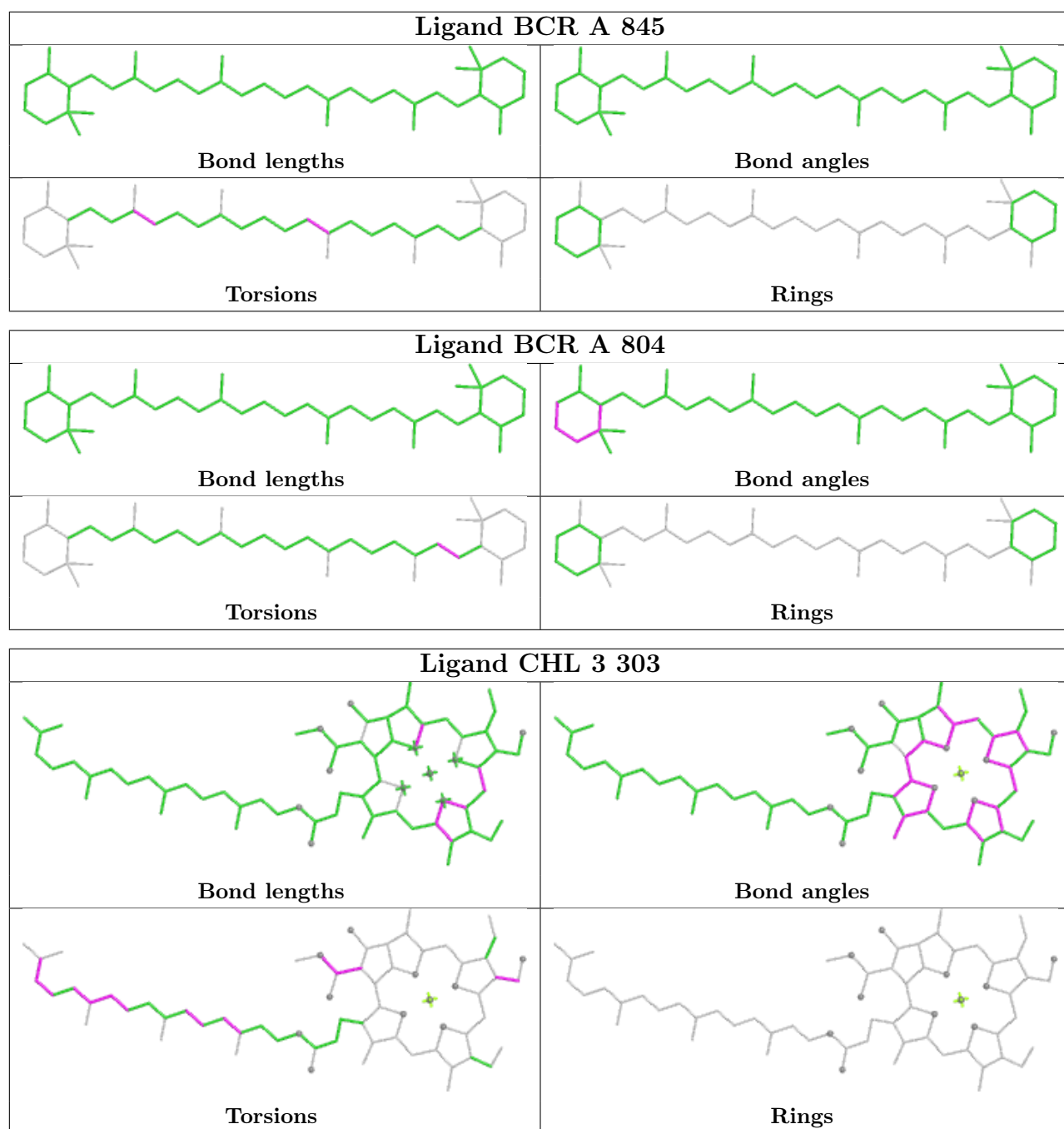


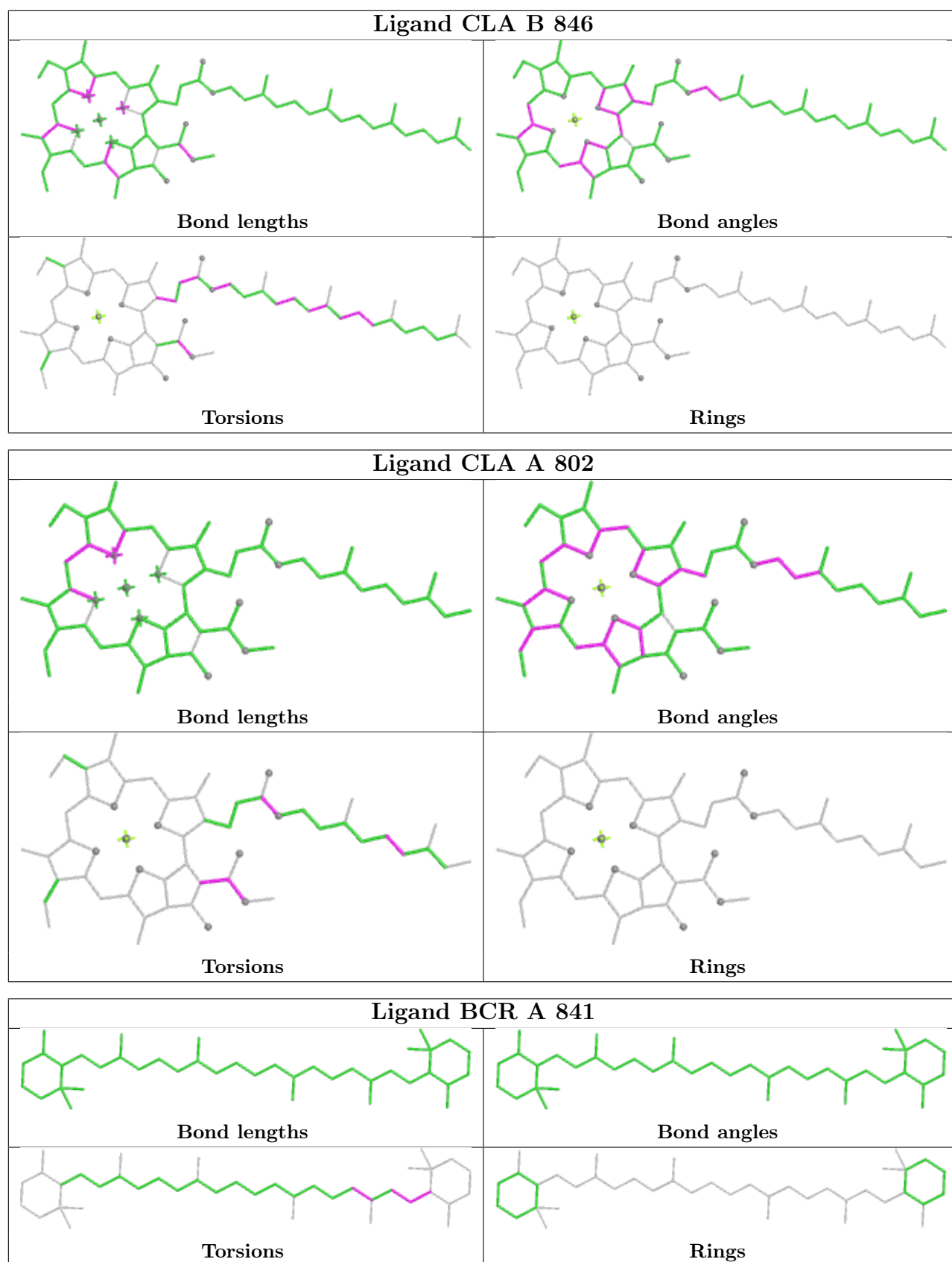
Torsions

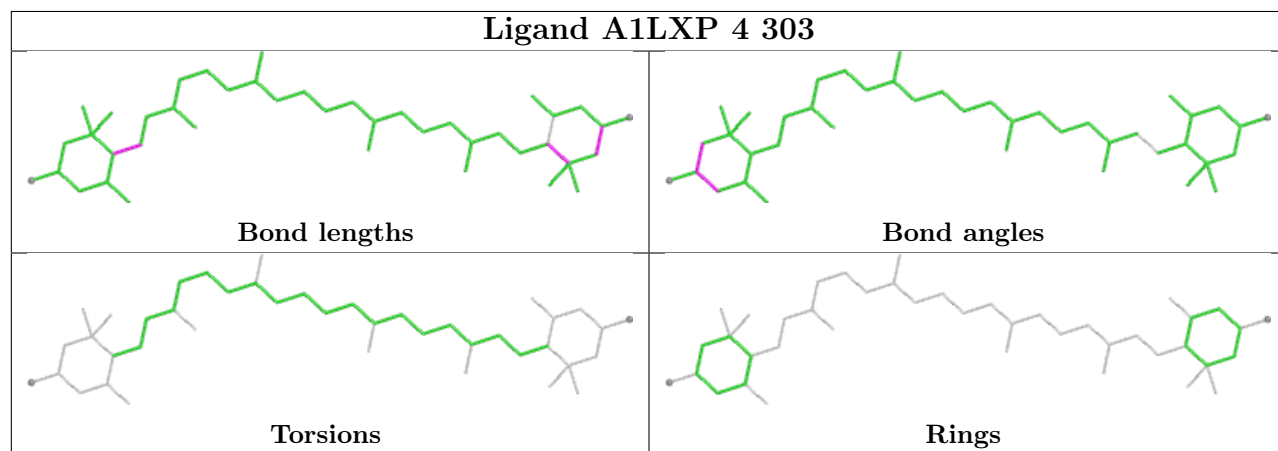
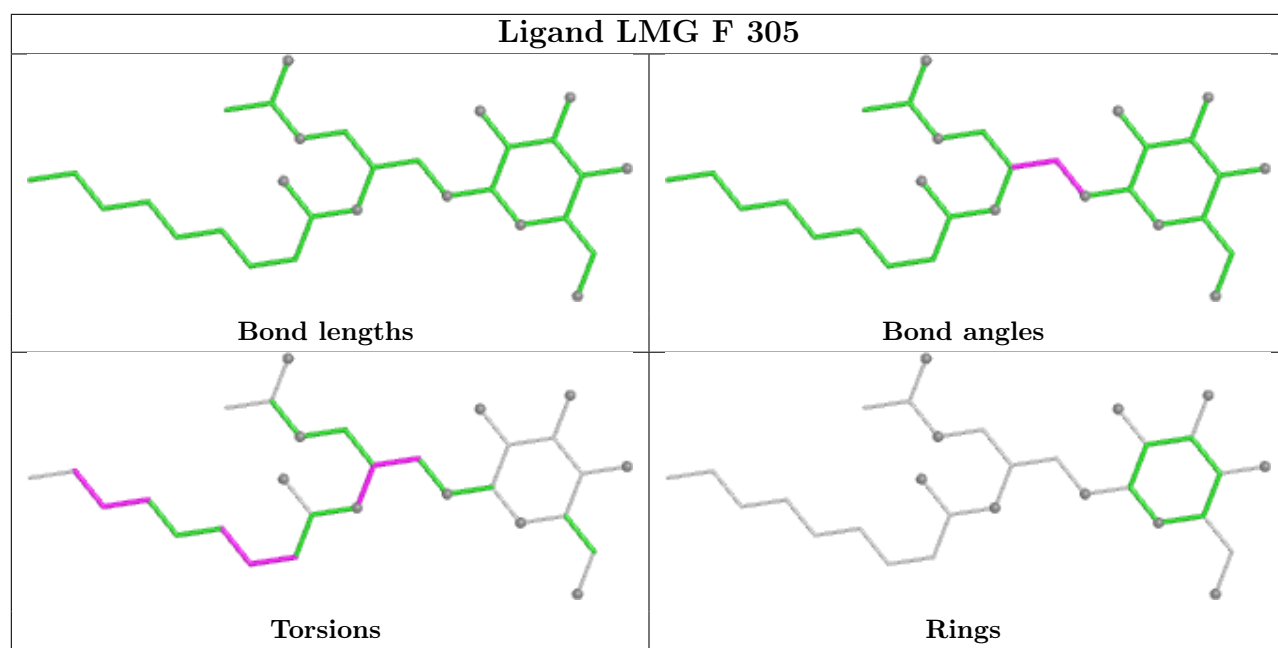


Rings

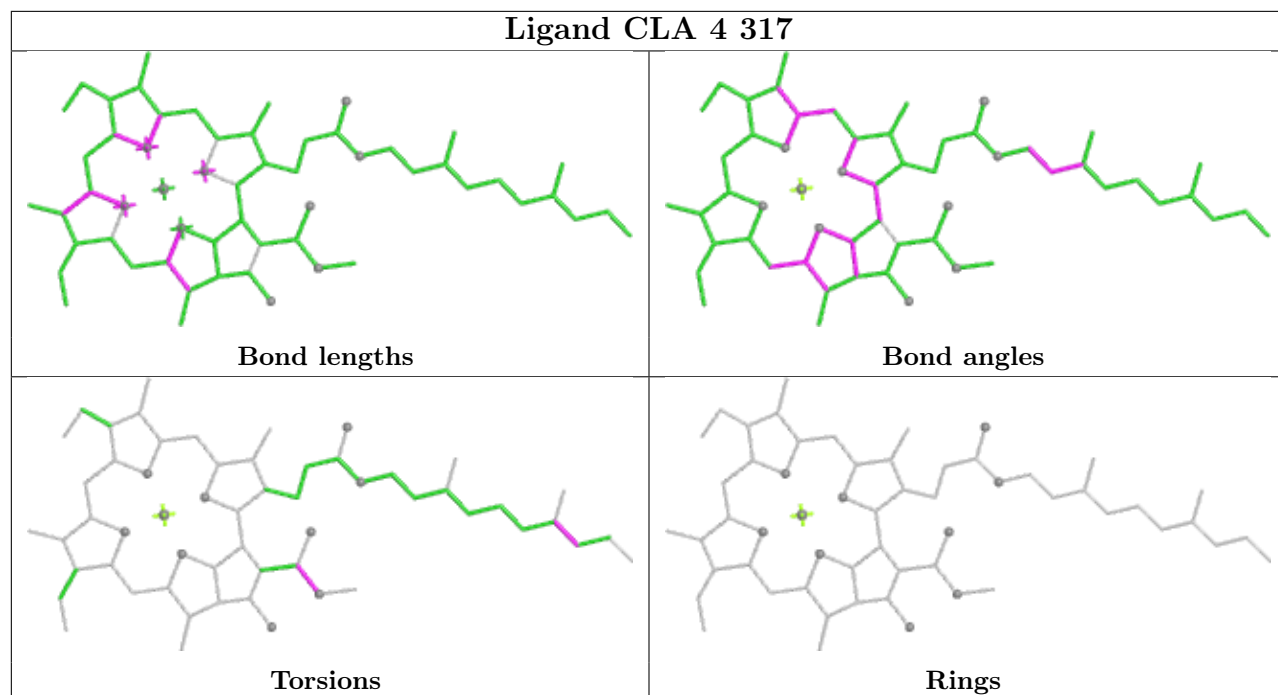




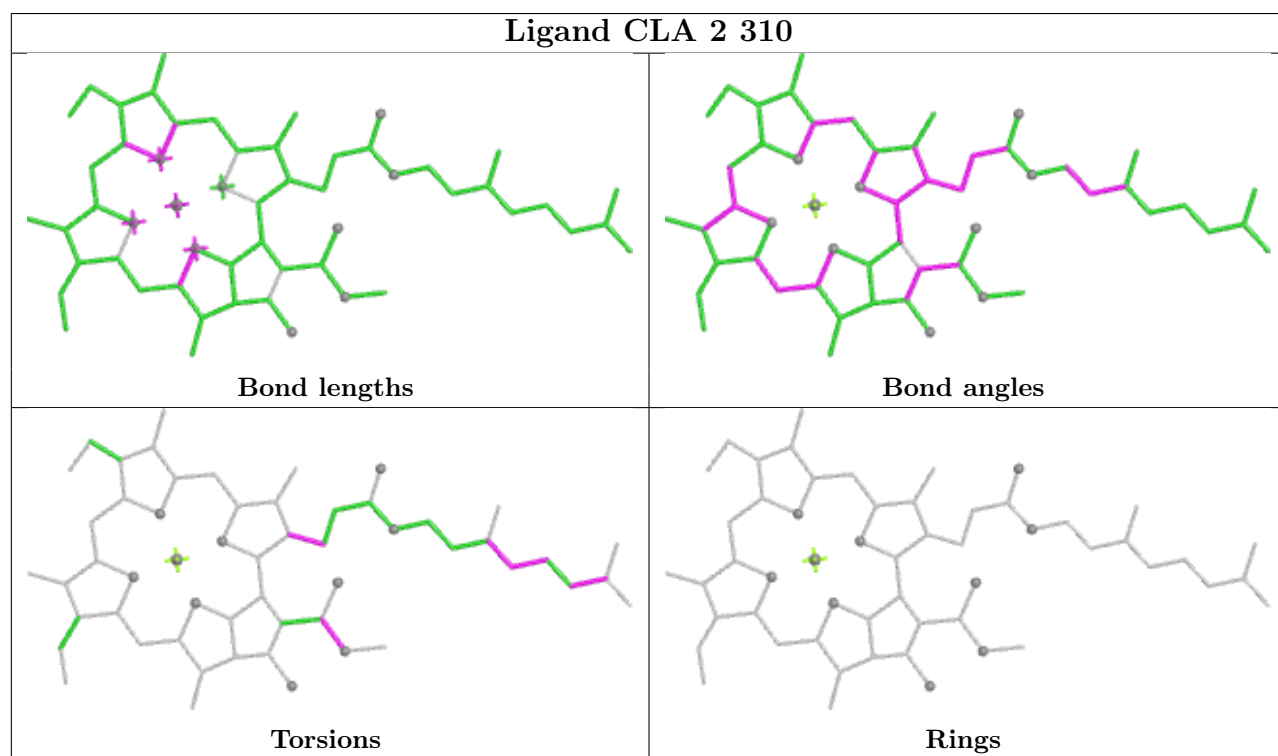




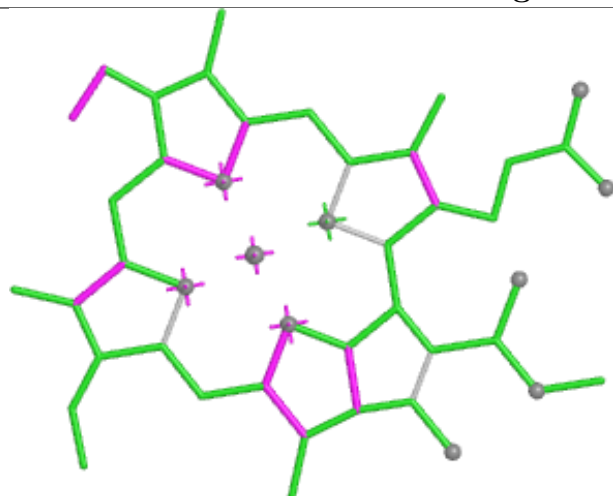
Ligand CLA 4 317



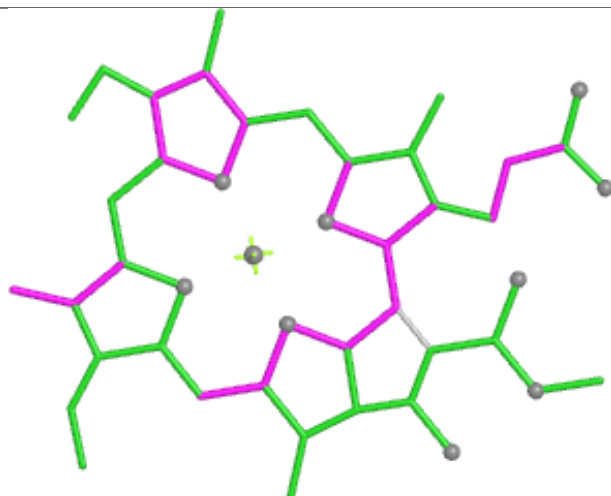
Ligand CLA 2 310



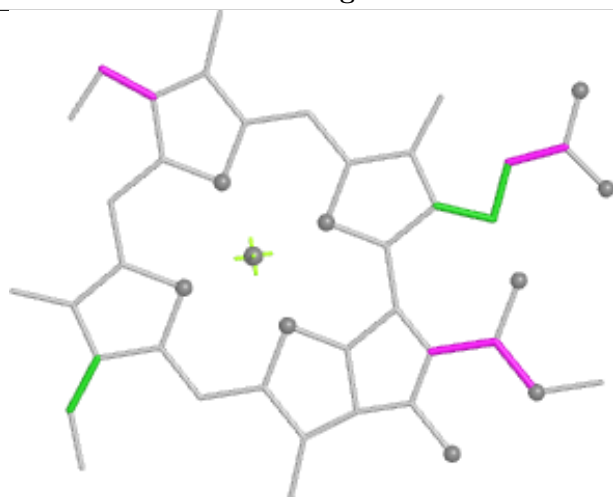
Ligand CLA G 203



Bond lengths



Bond angles

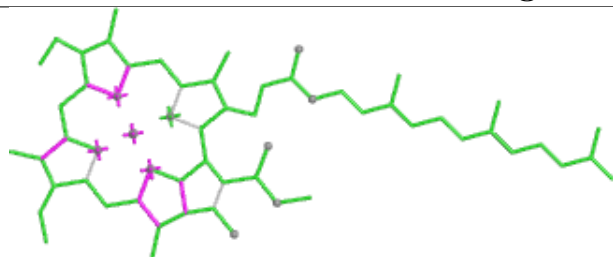


Torsions

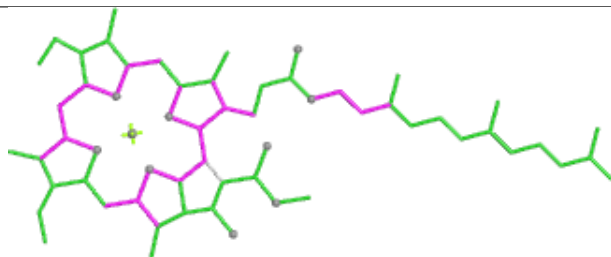


Rings

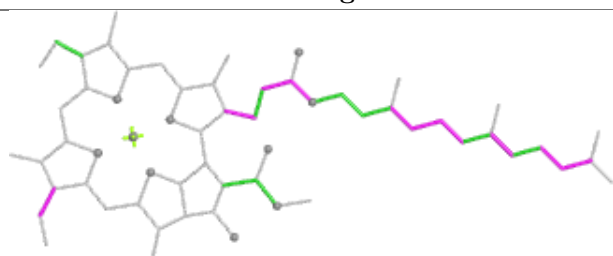
Ligand CLA 1 602



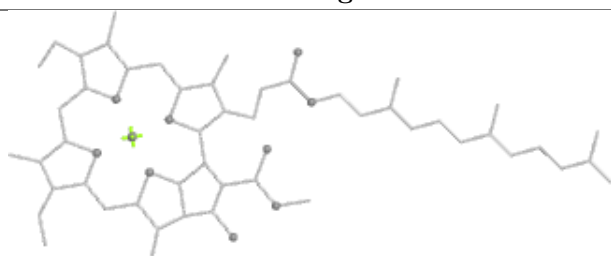
Bond lengths



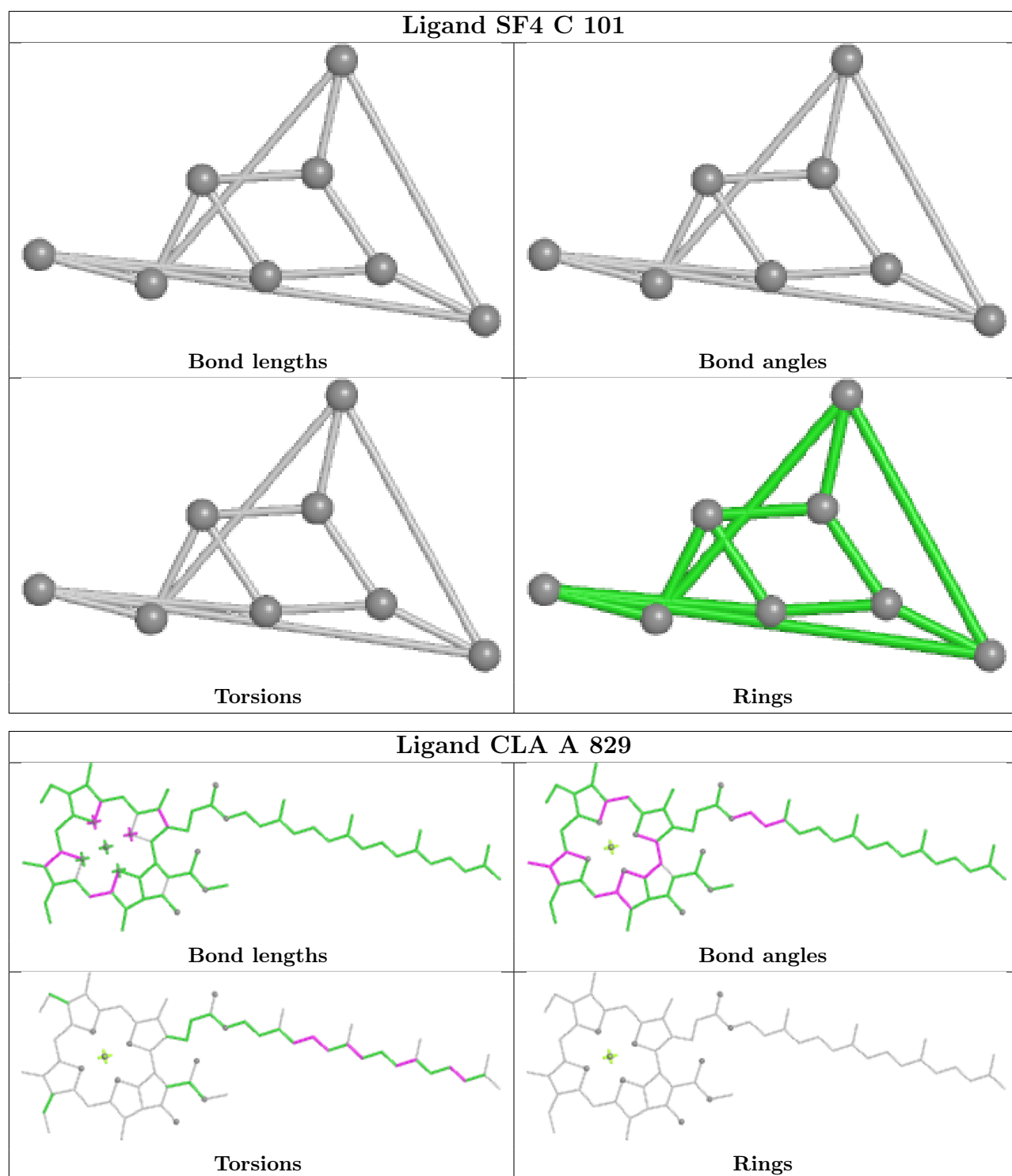
Bond angles

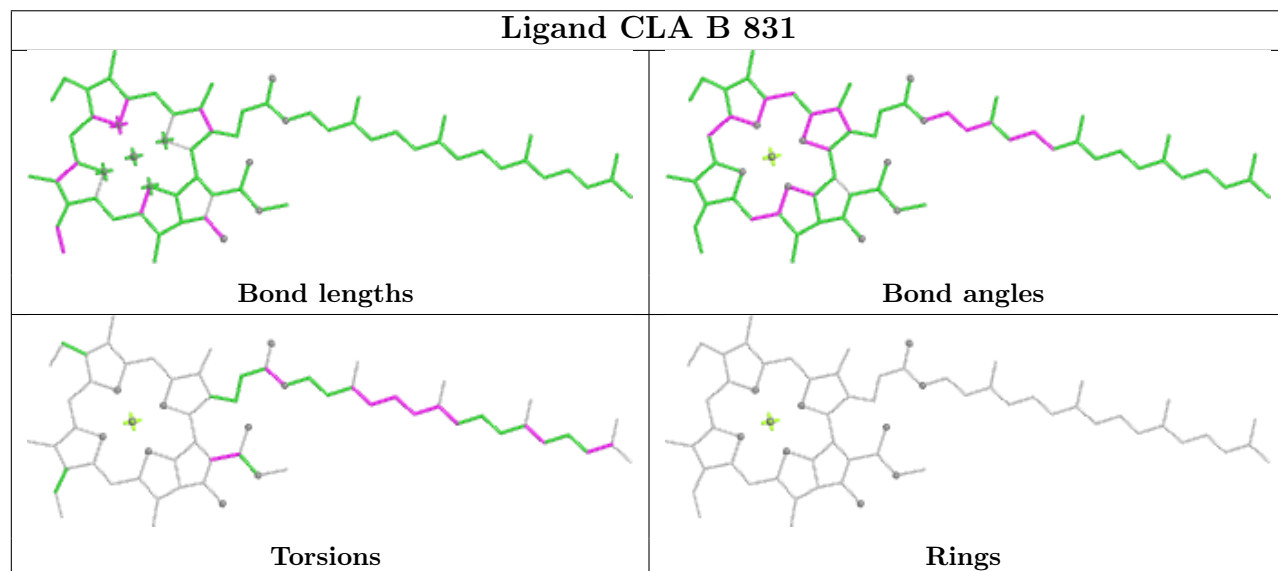
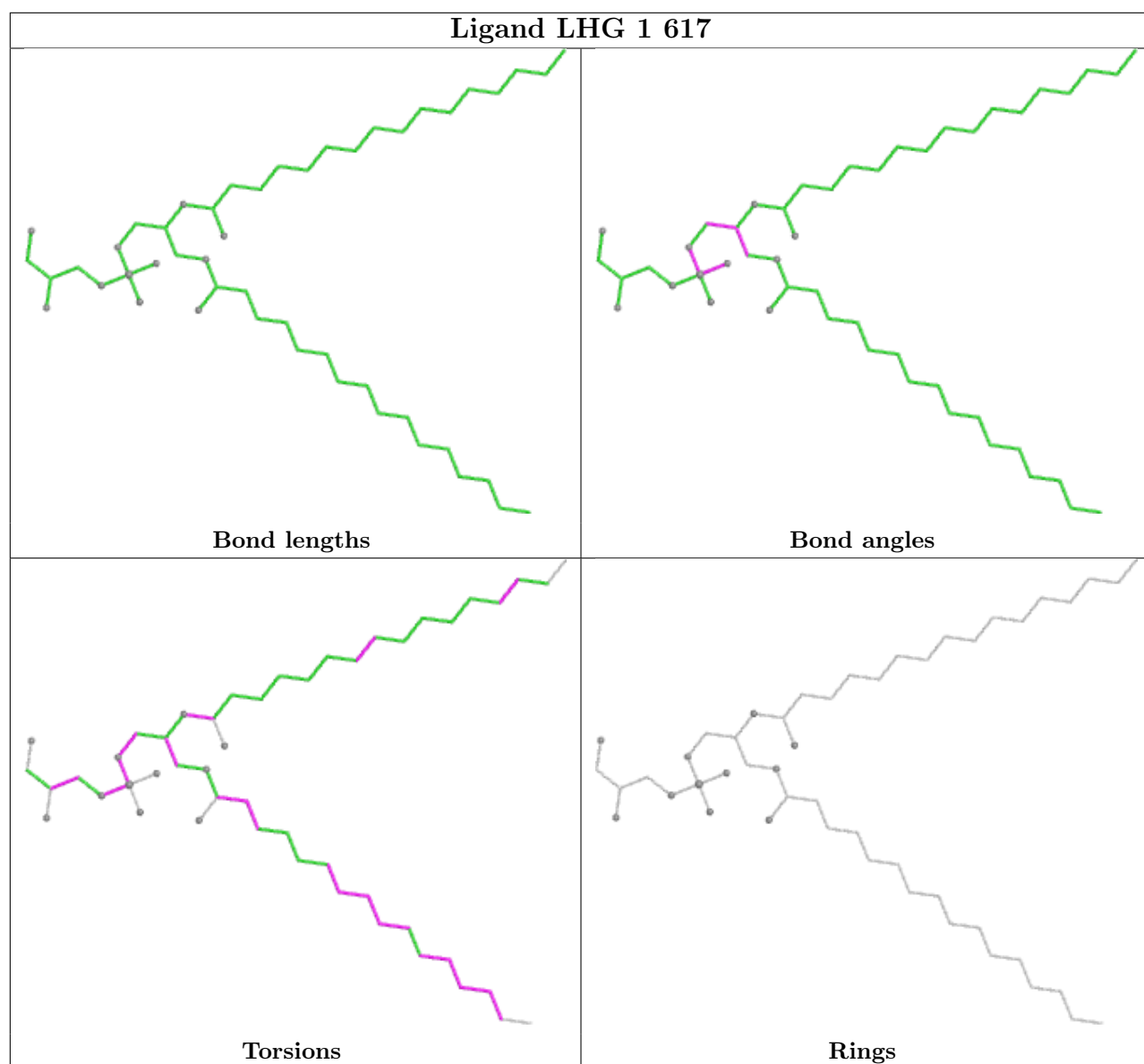


Torsions

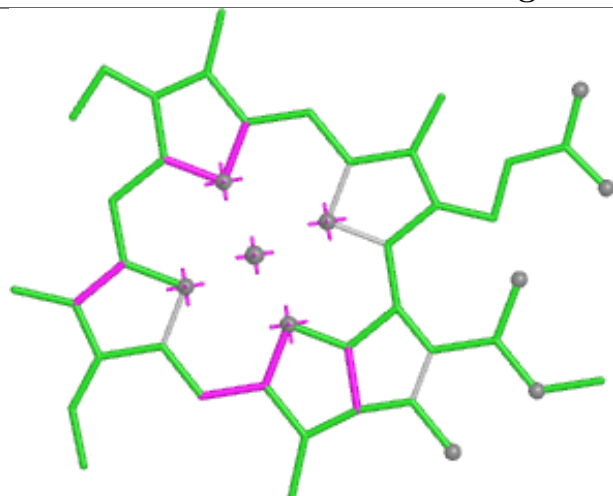


Rings

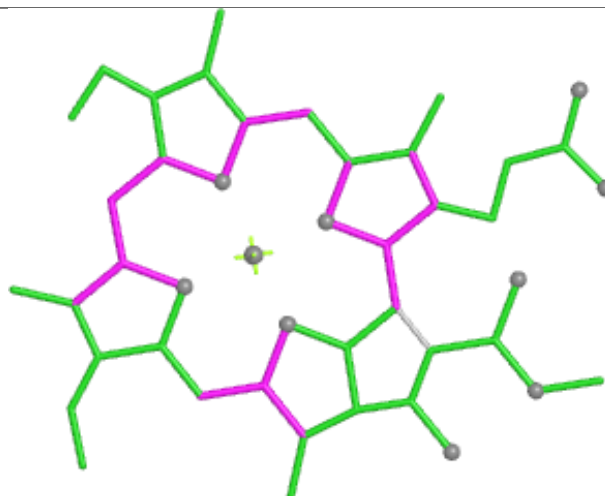




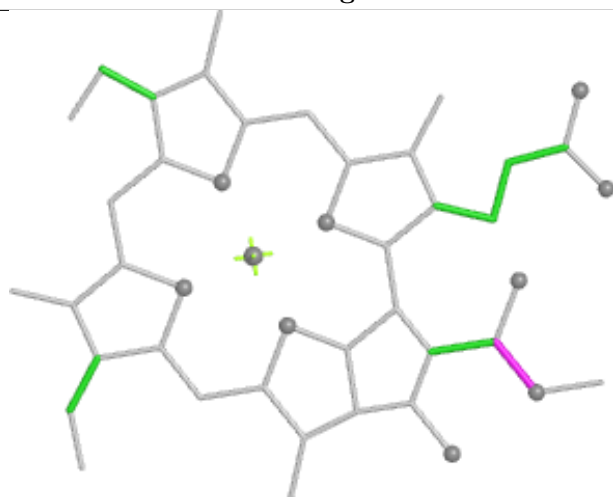
Ligand CLA 4 311



Bond lengths



Bond angles

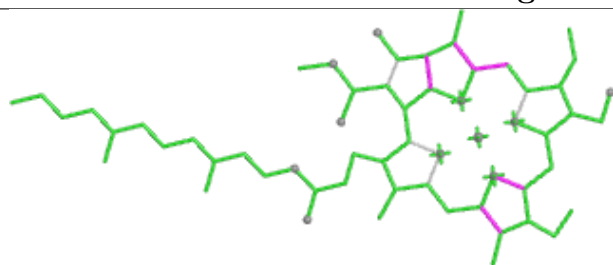


Torsions

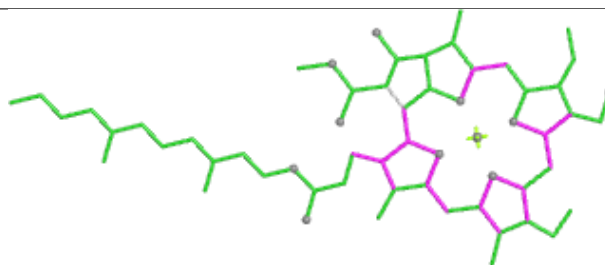


Rings

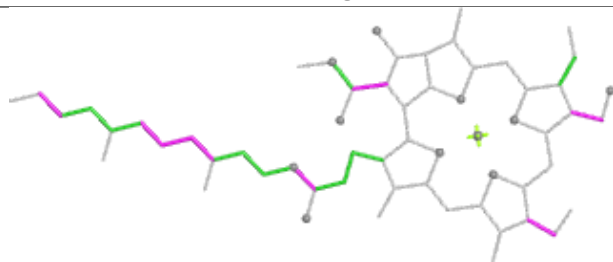
Ligand CHL 2 316



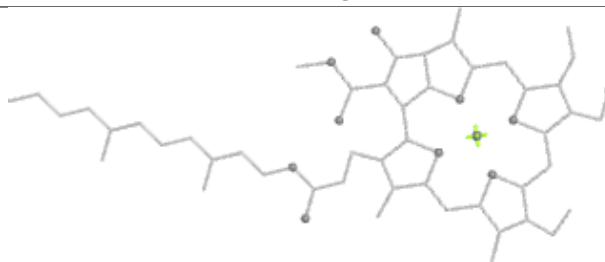
Bond lengths



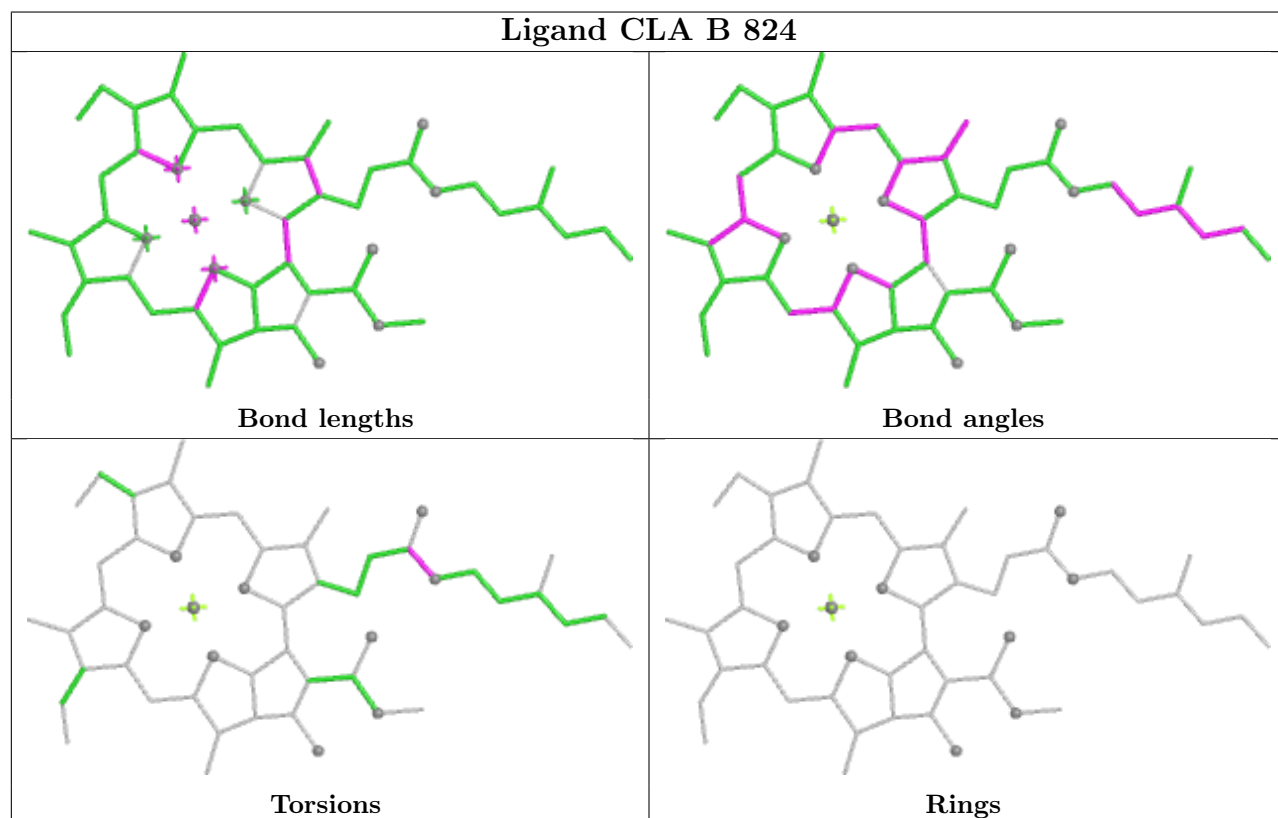
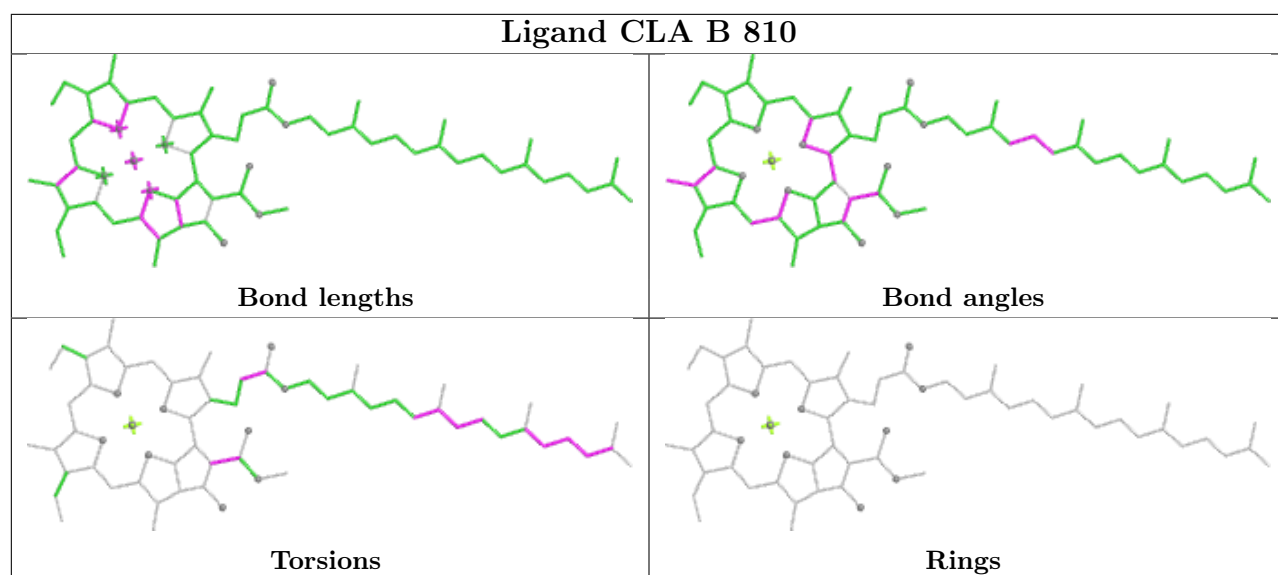
Bond angles



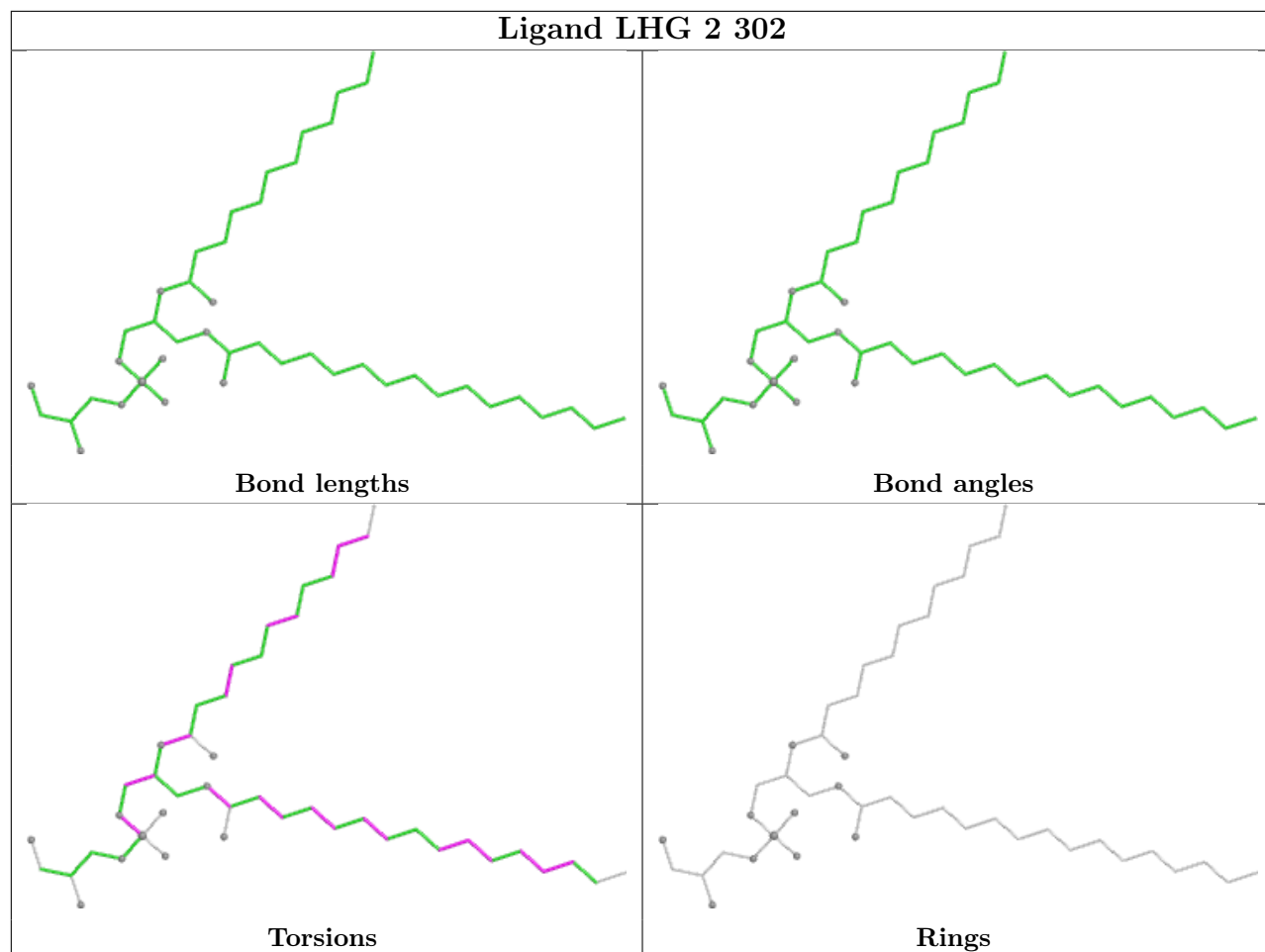
Torsions



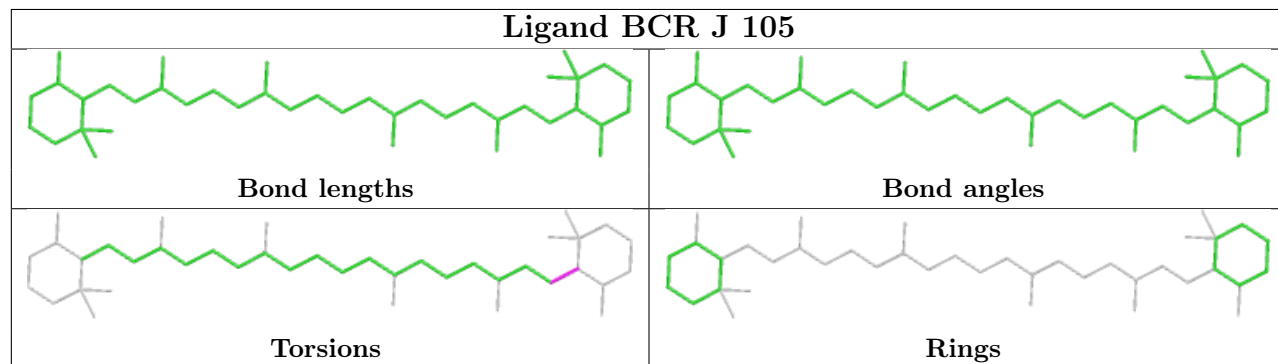
Rings

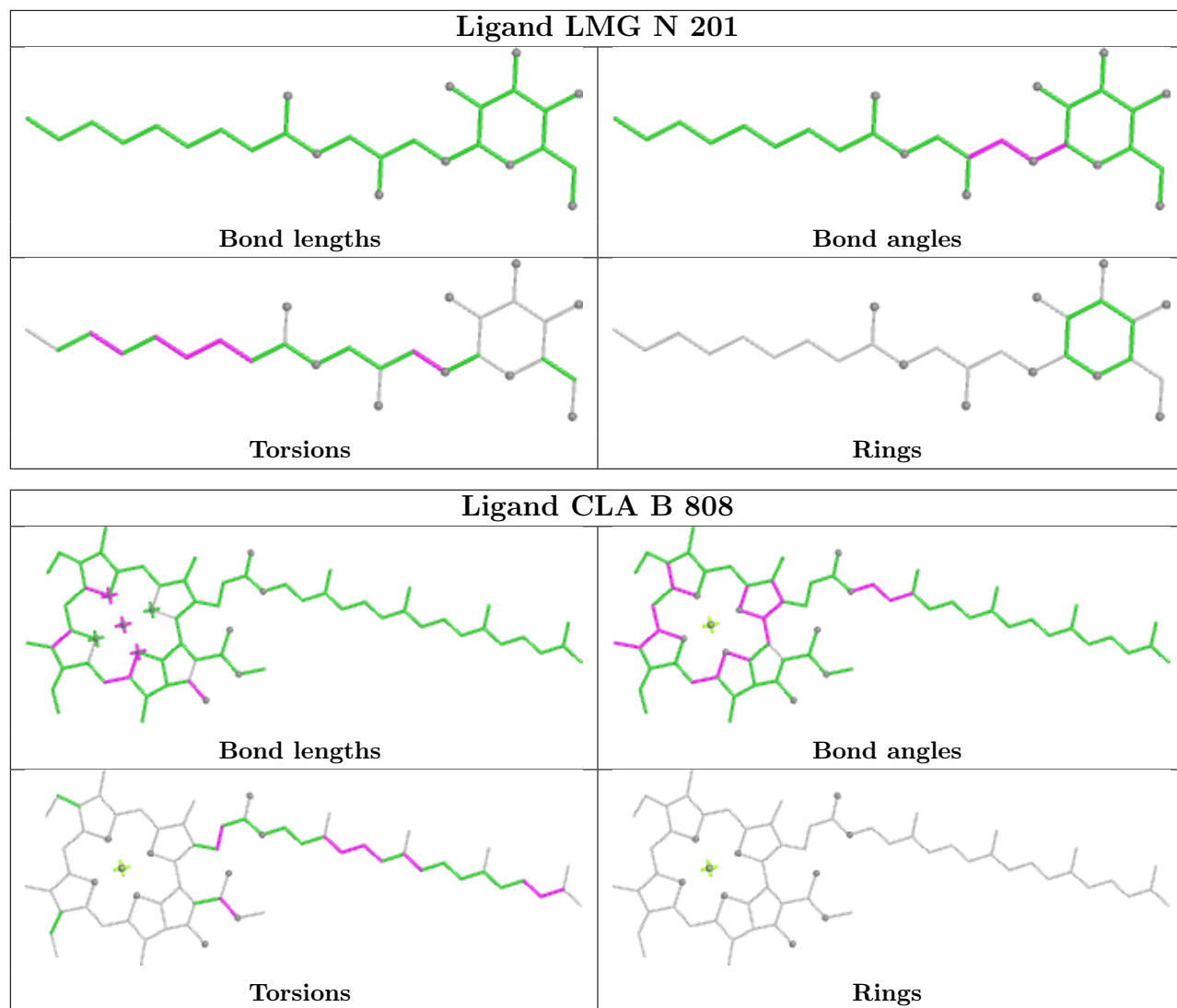


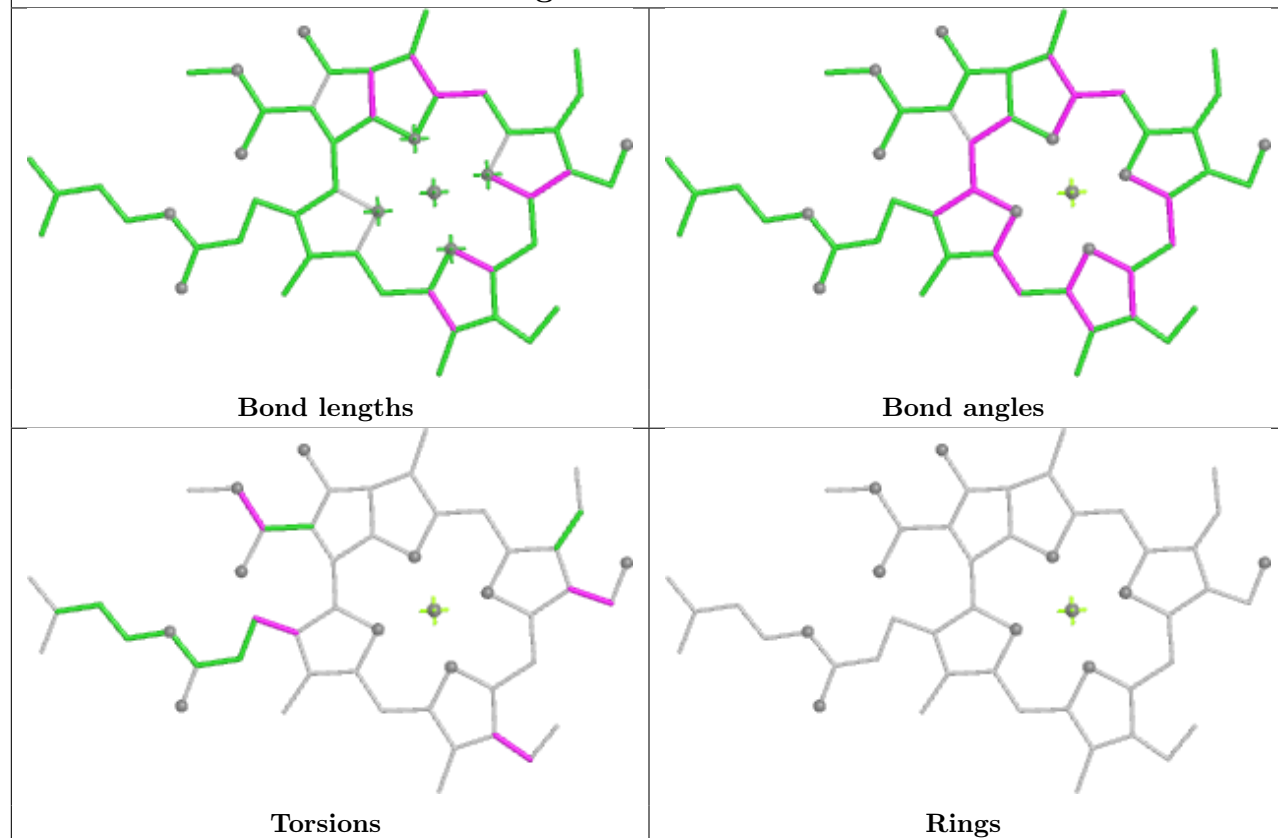
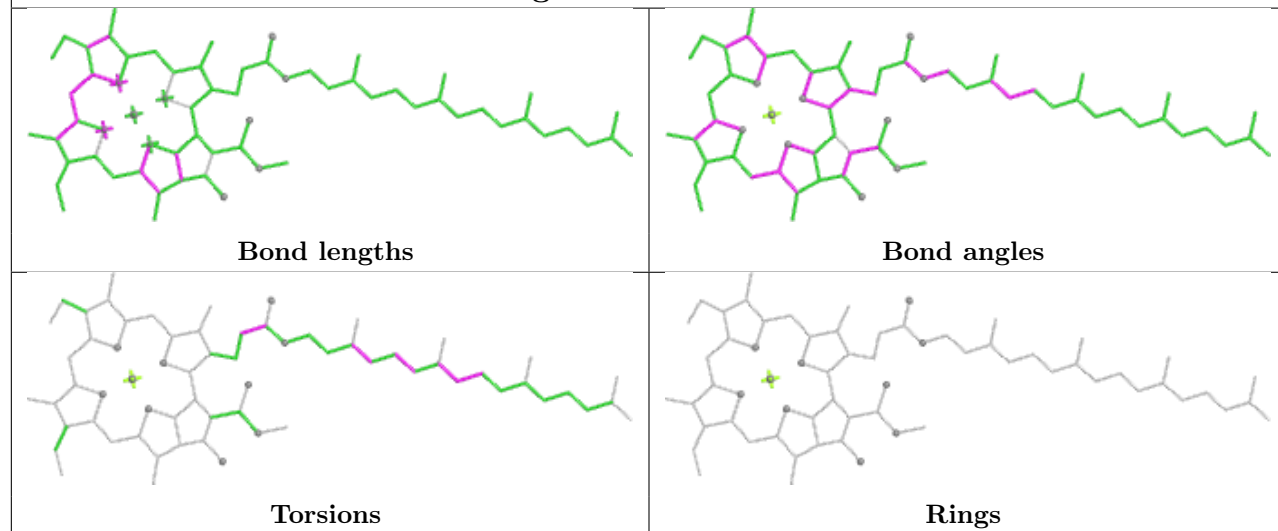
Ligand LHG 2 302

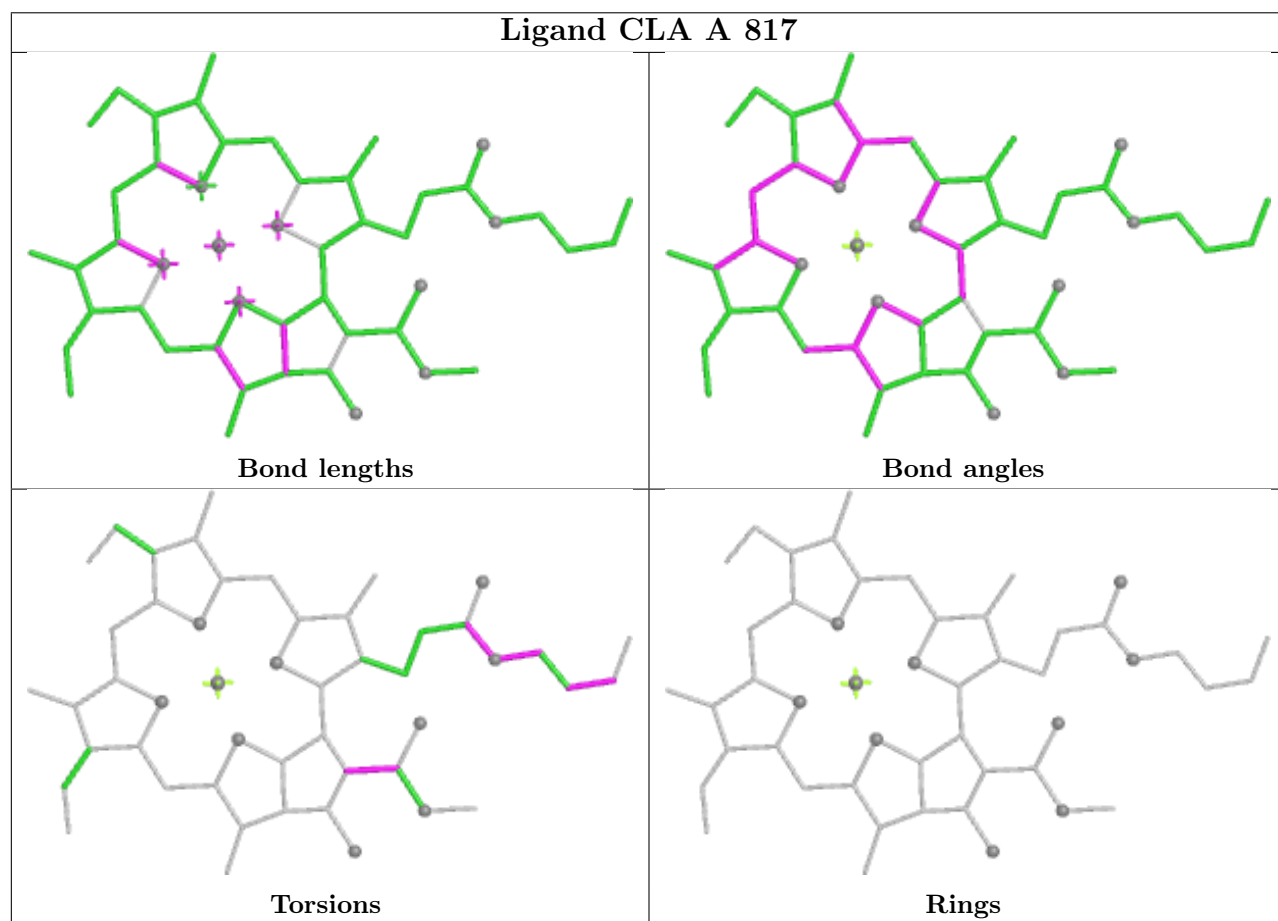
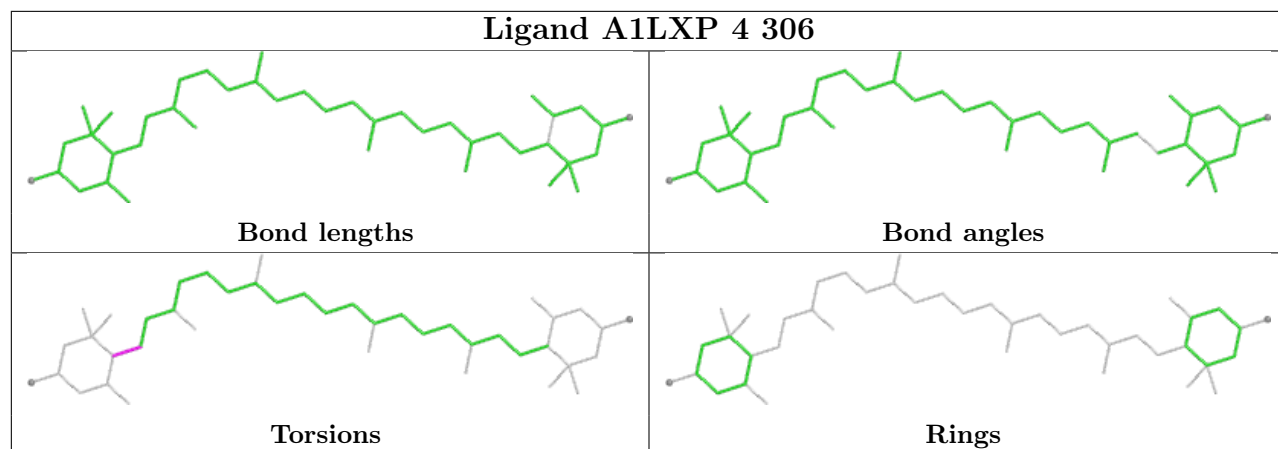


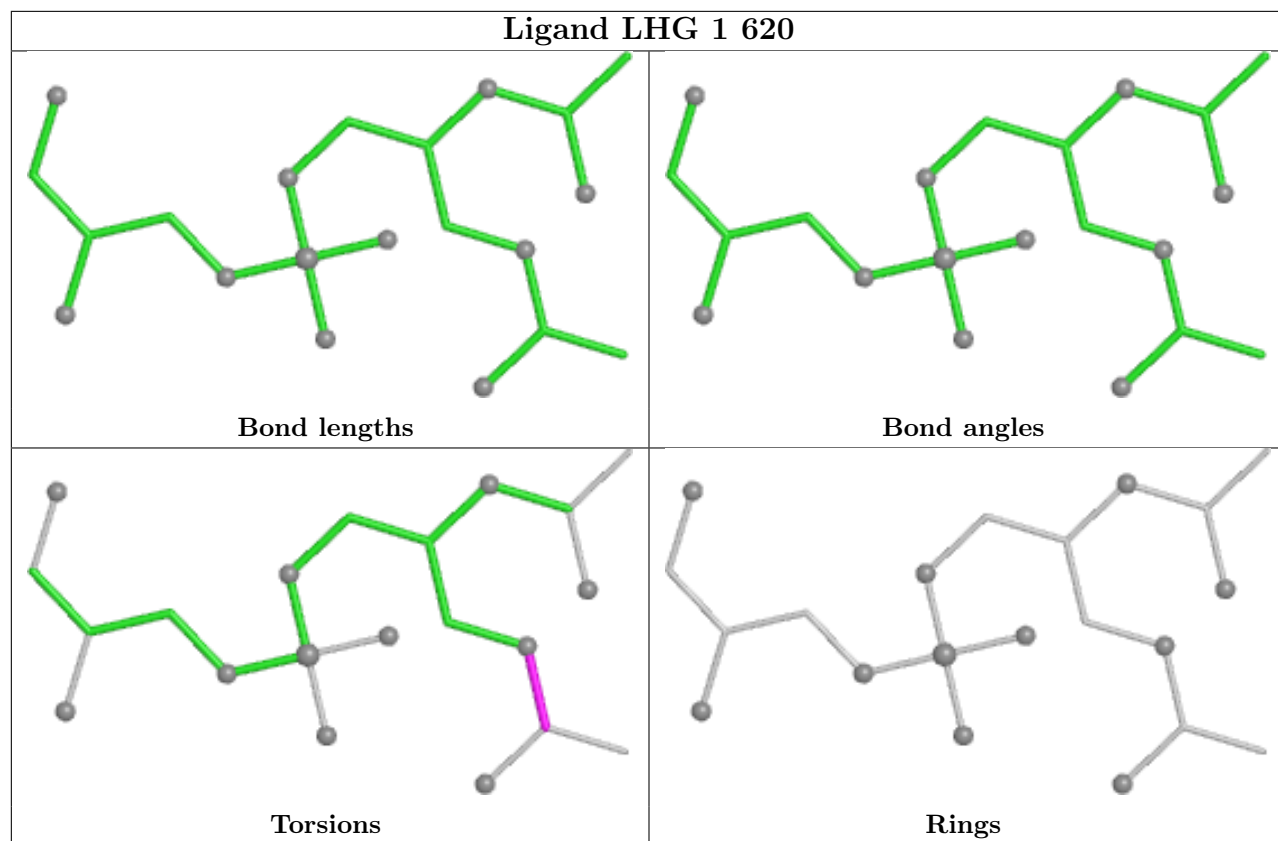
Ligand BCR J 105



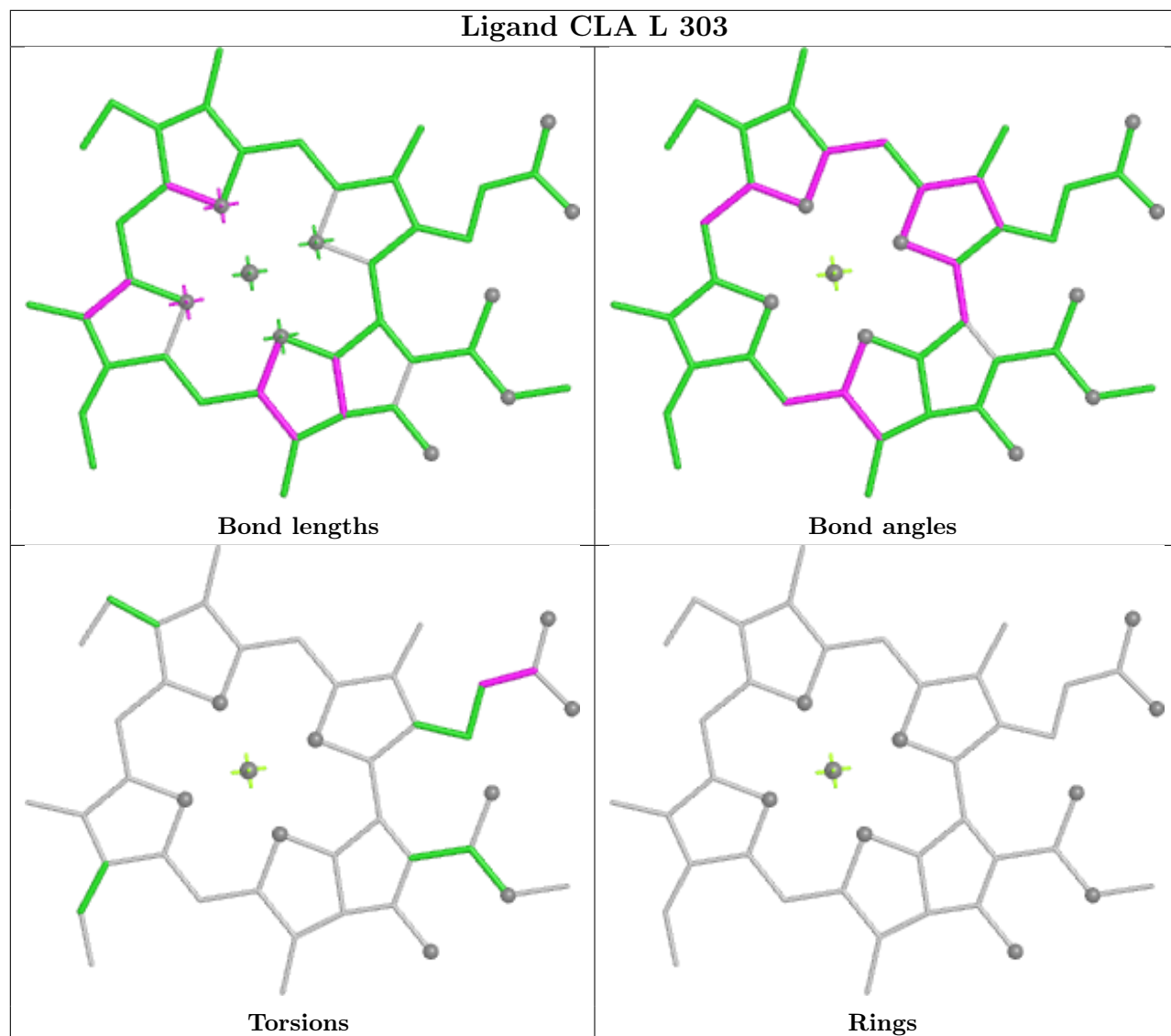


Ligand CHL 3 315**Ligand CLA B 809**

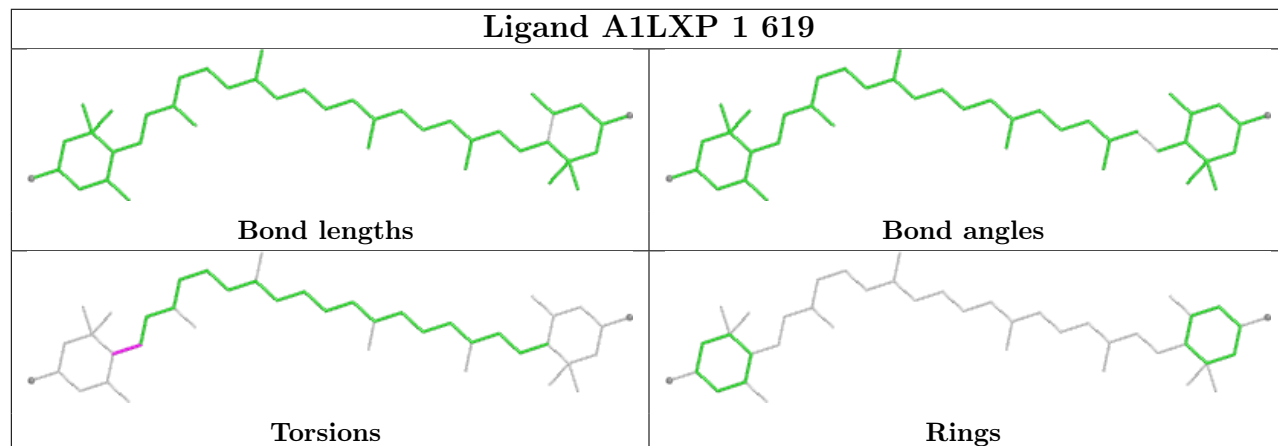


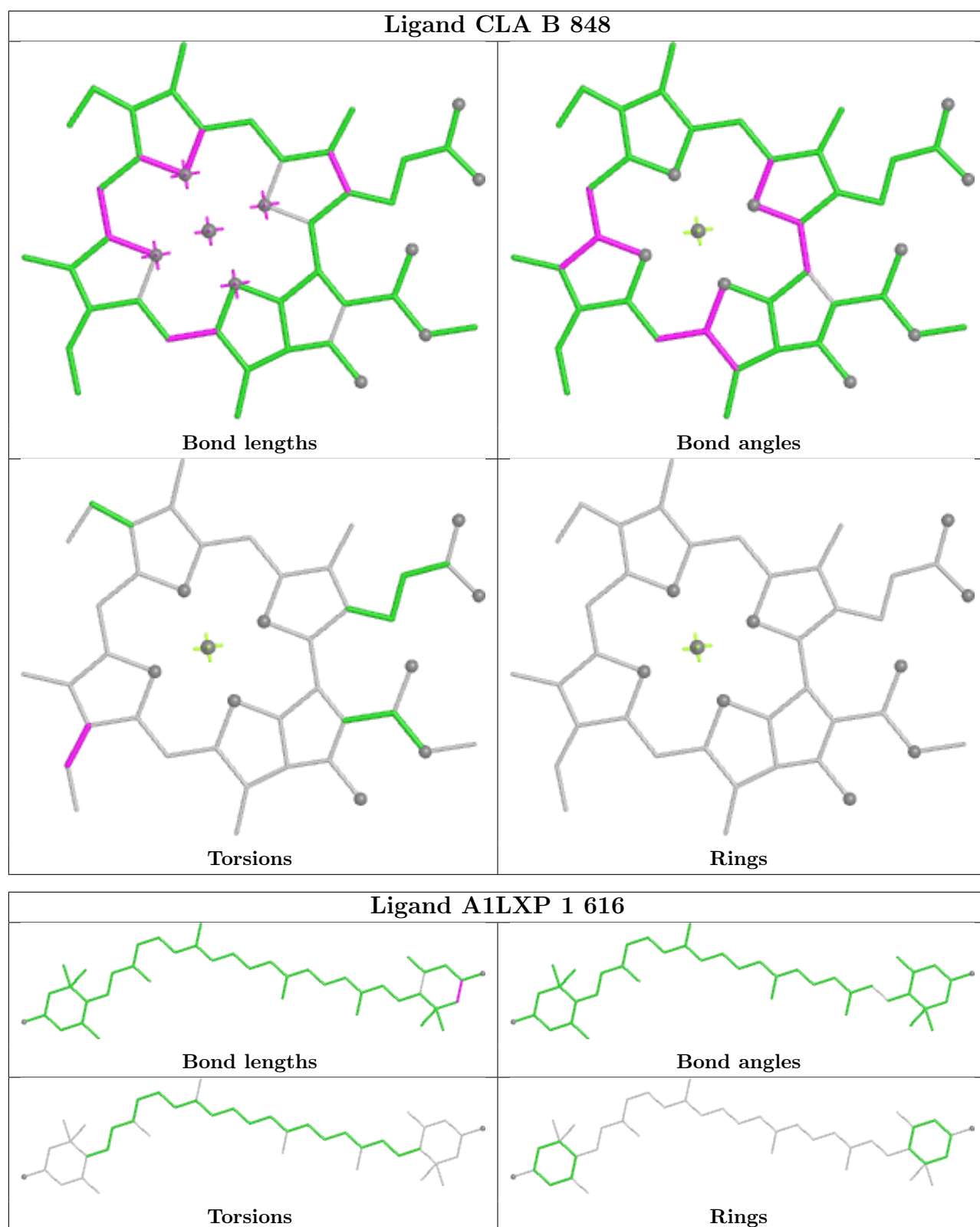


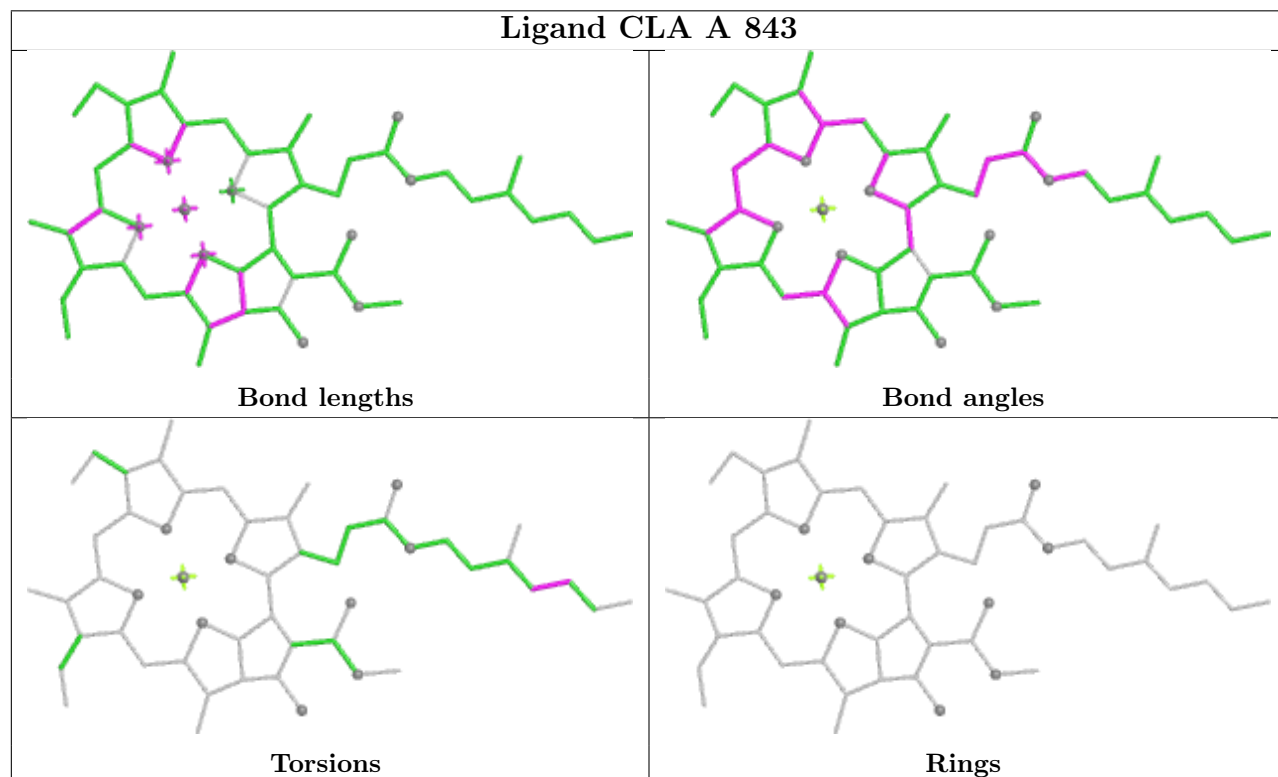
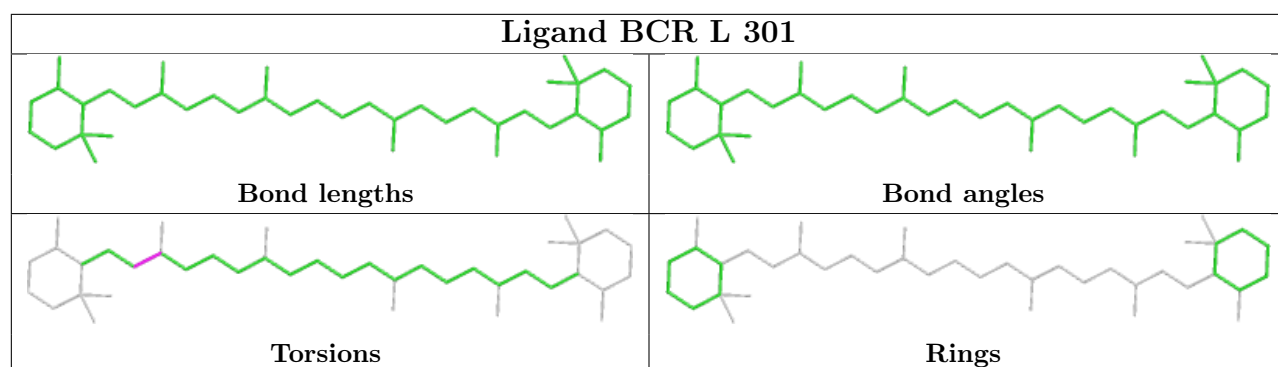
Ligand CLA L 303



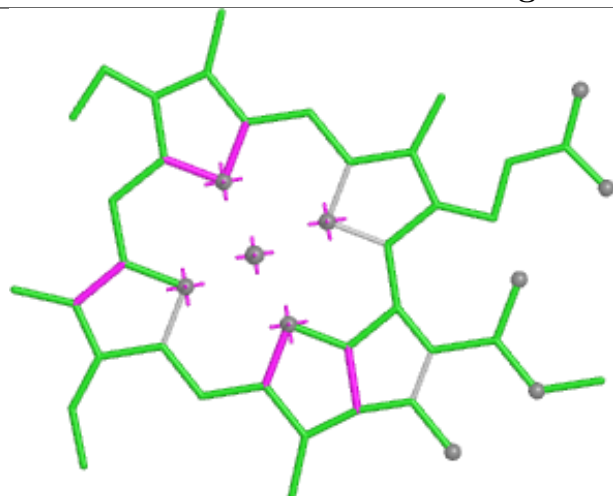
Ligand A1LXP 1 619



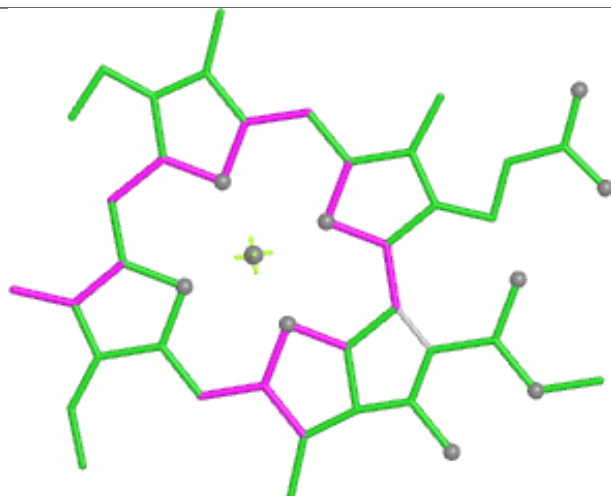




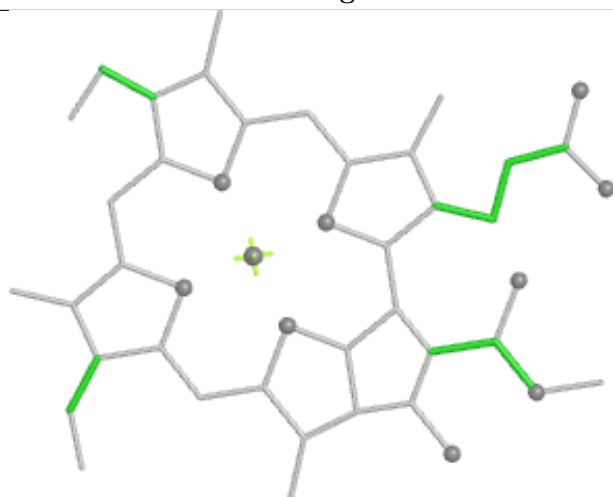
Ligand CLA 2 311



Bond lengths



Bond angles

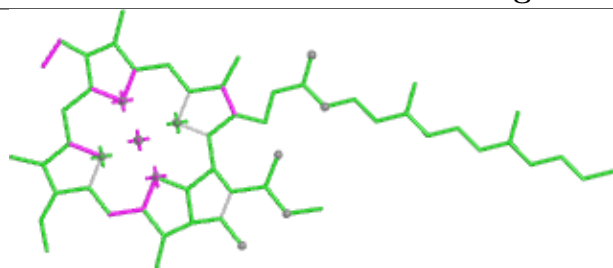


Torsions

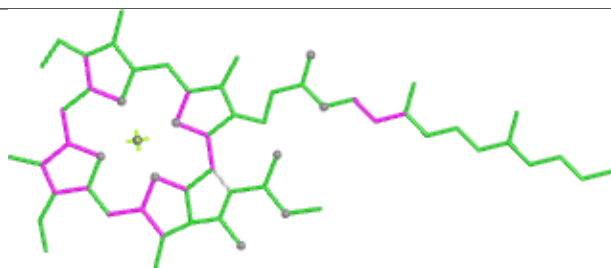


Rings

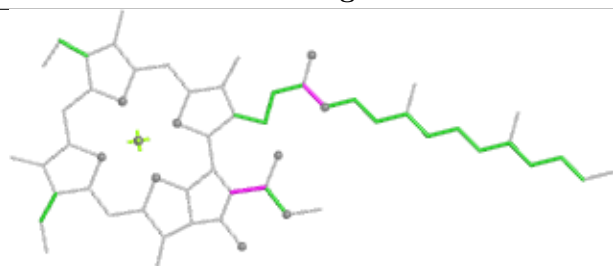
Ligand CLA A 827



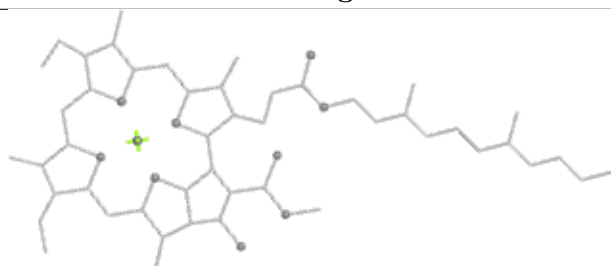
Bond lengths



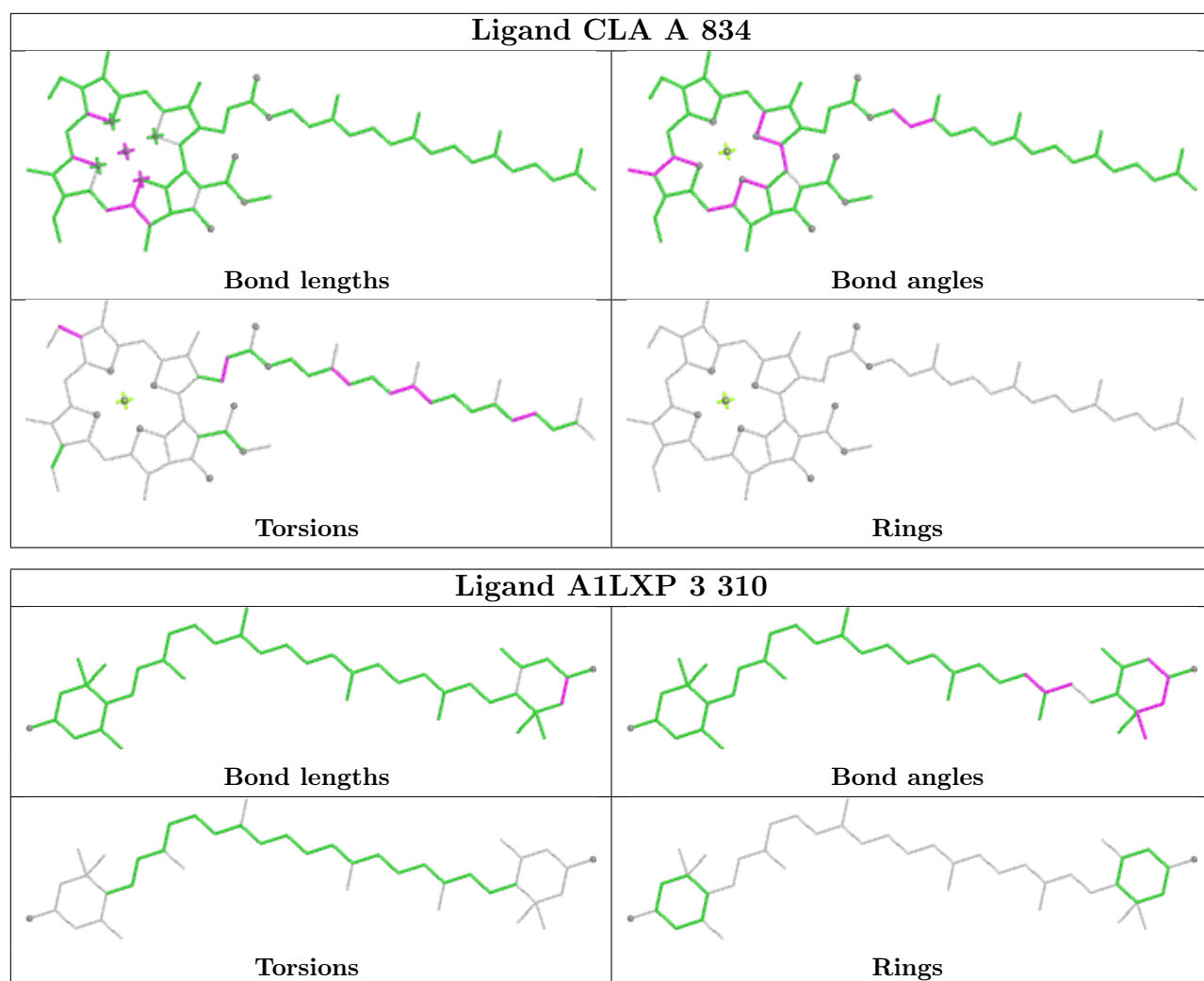
Bond angles



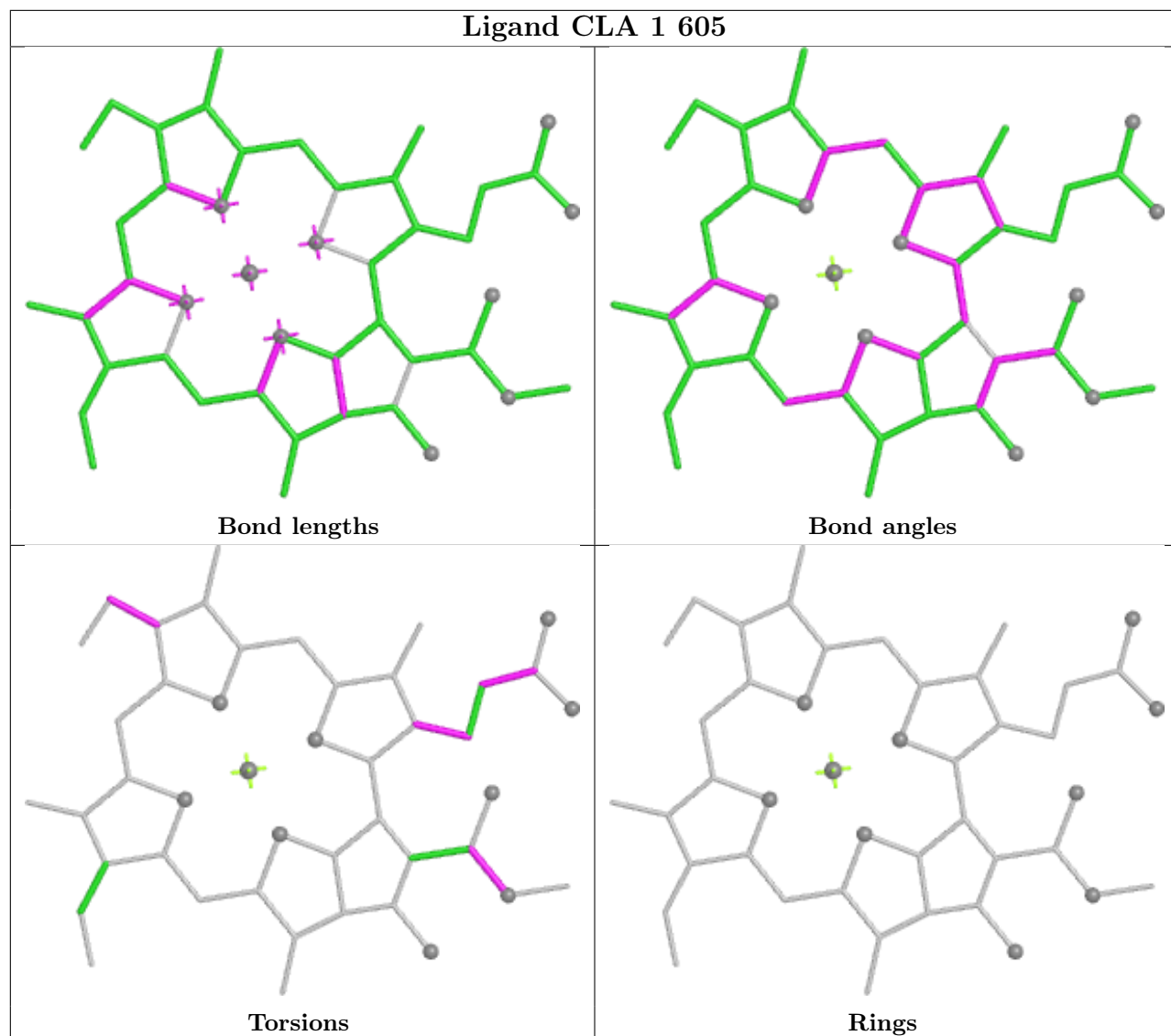
Torsions

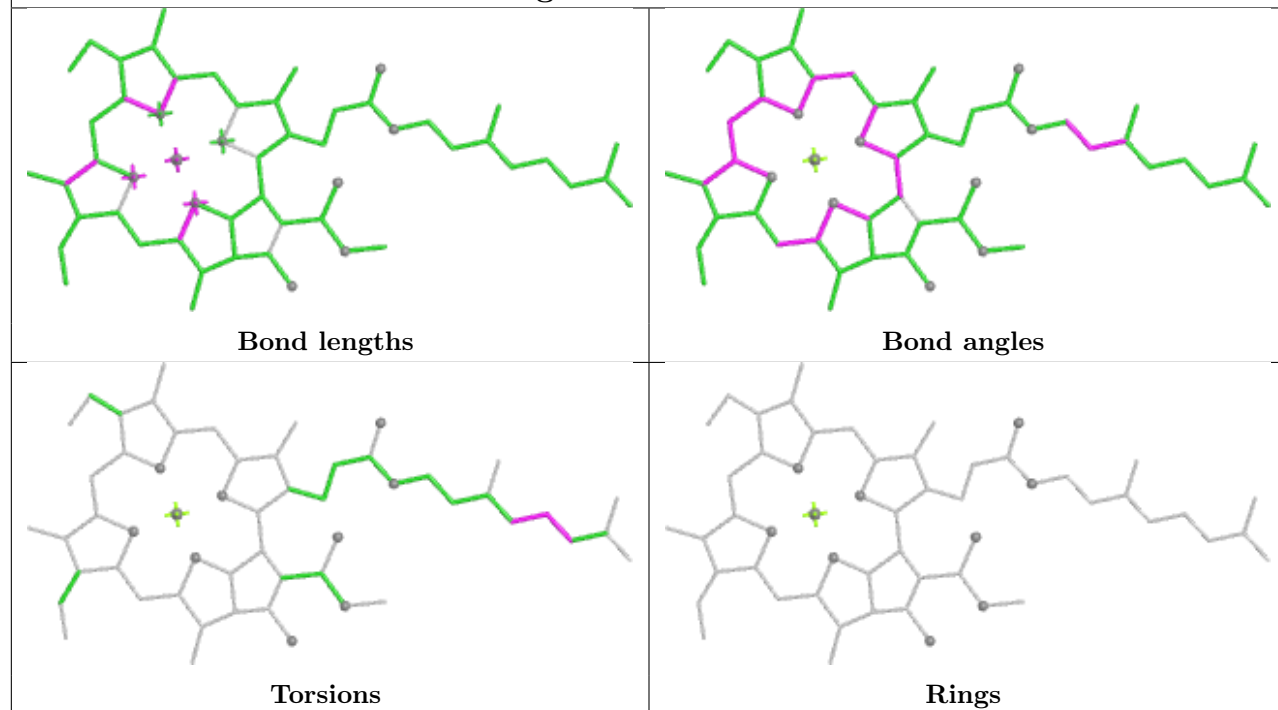
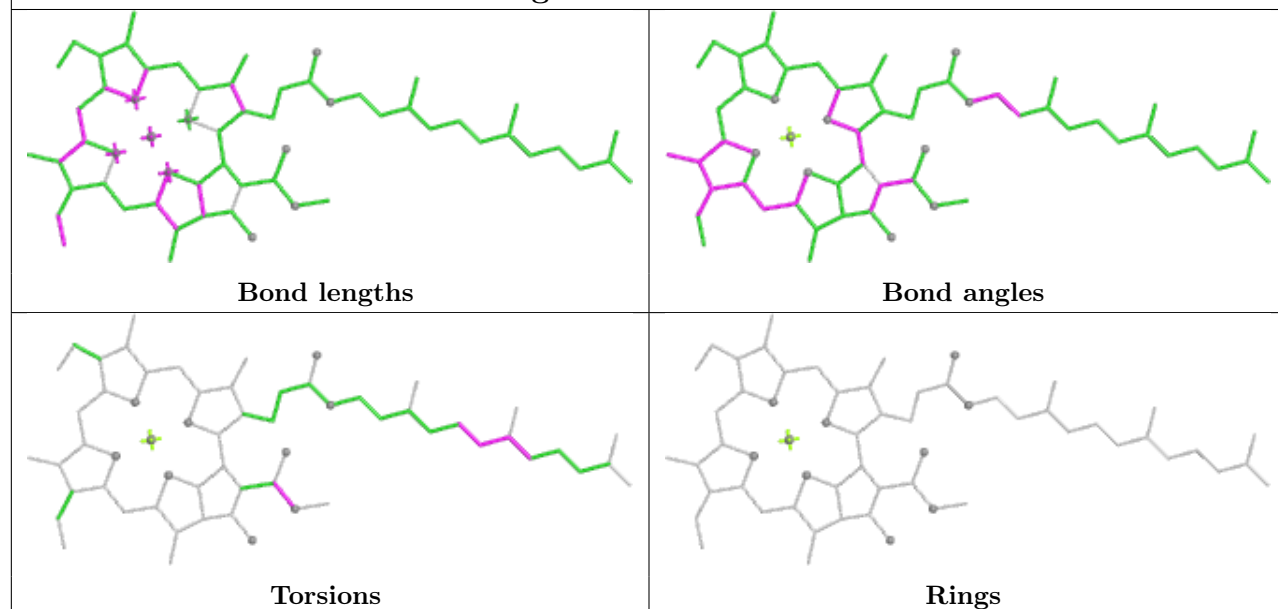


Rings

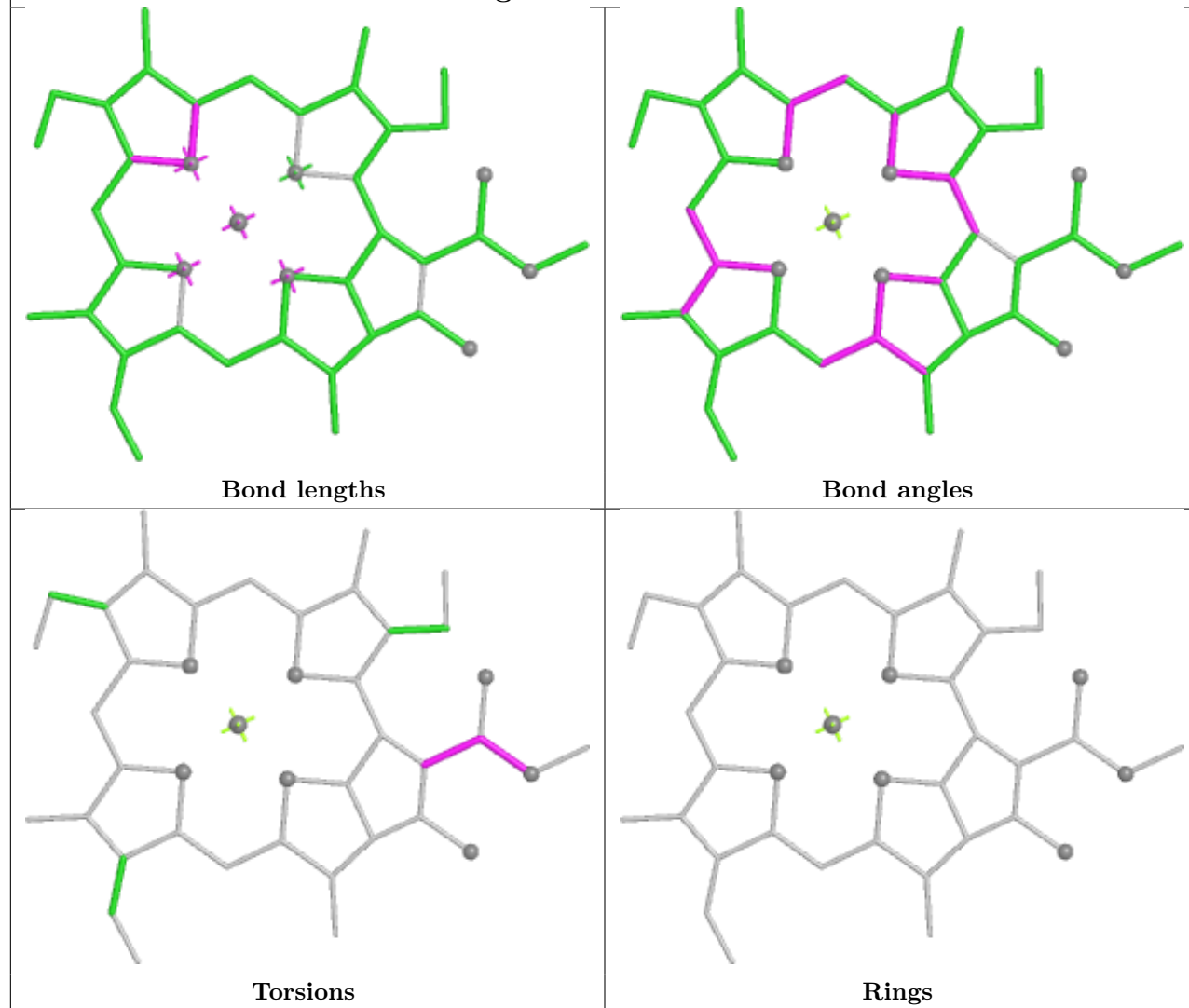


Ligand CLA 1 605

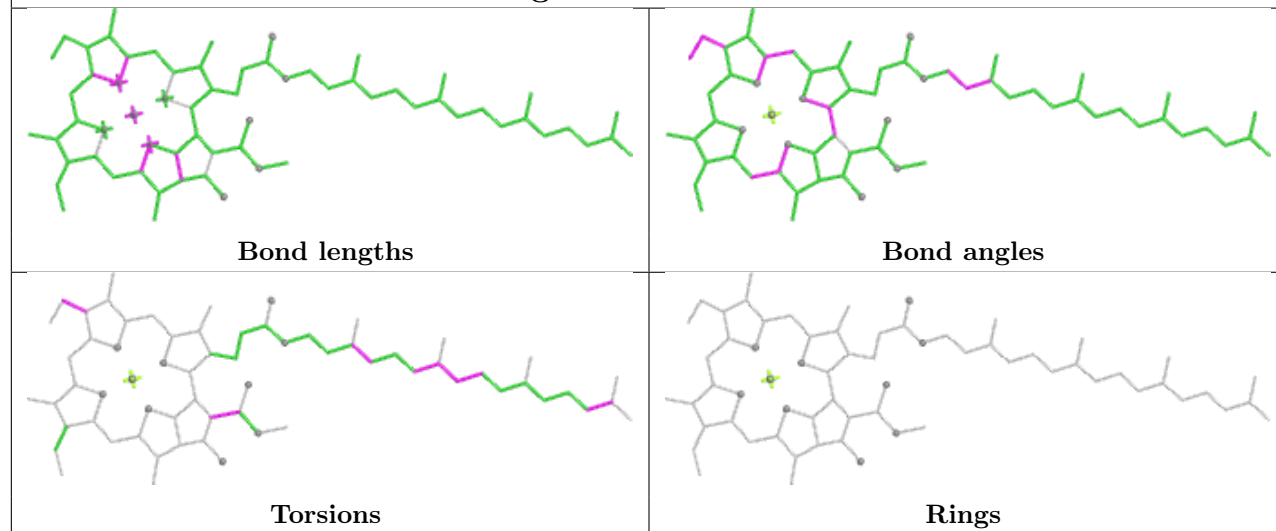


Ligand CLA 3 314**Ligand CLA A 813**

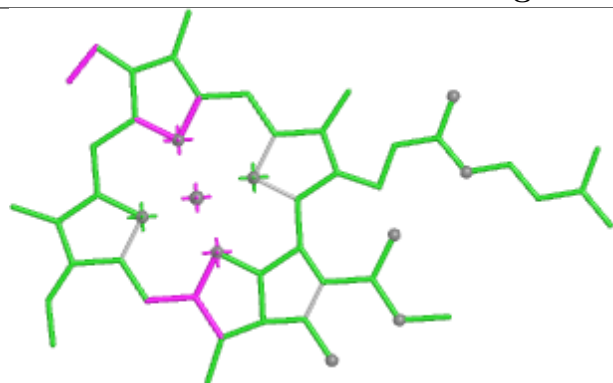
Ligand CLA A 820



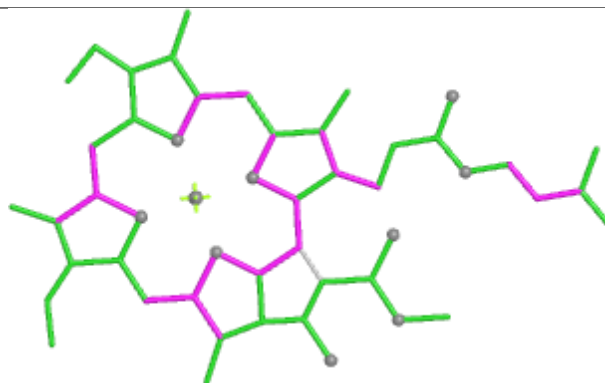
Ligand CLA A 824



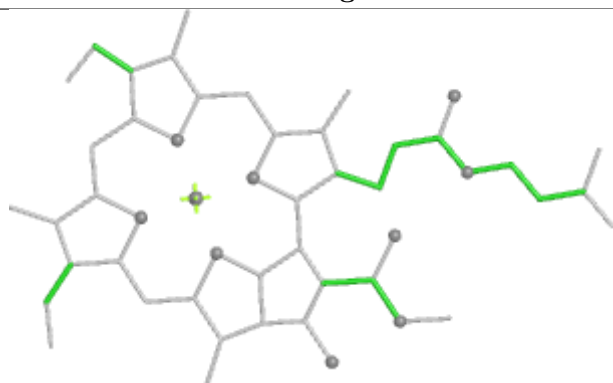
Ligand CLA A 810



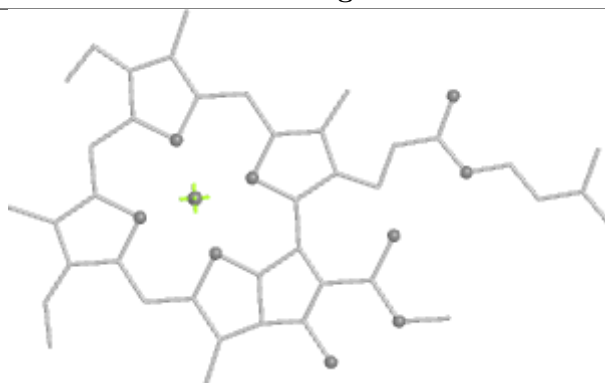
Bond lengths



Bond angles

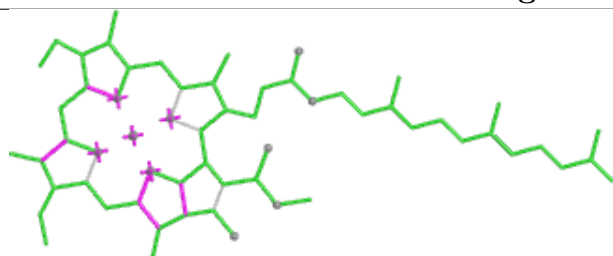


Torsions

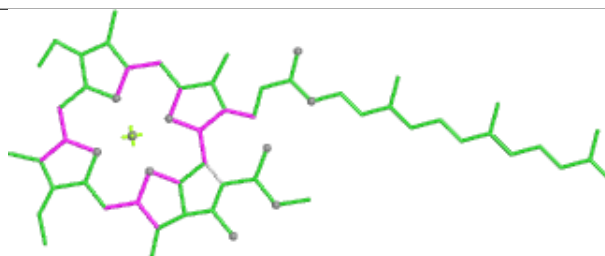


Rings

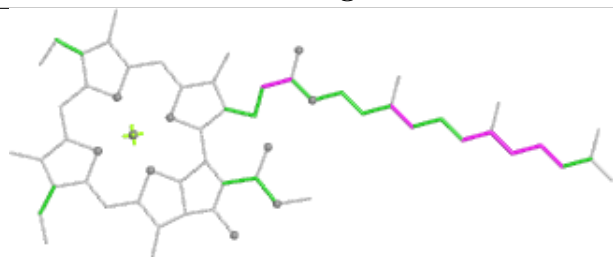
Ligand CLA 3 301



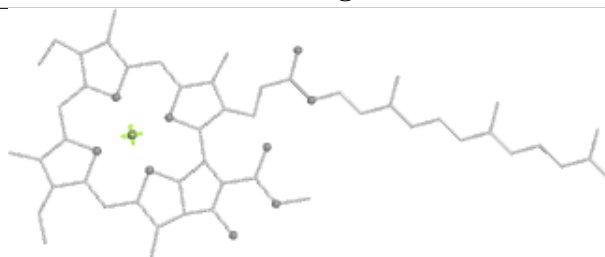
Bond lengths



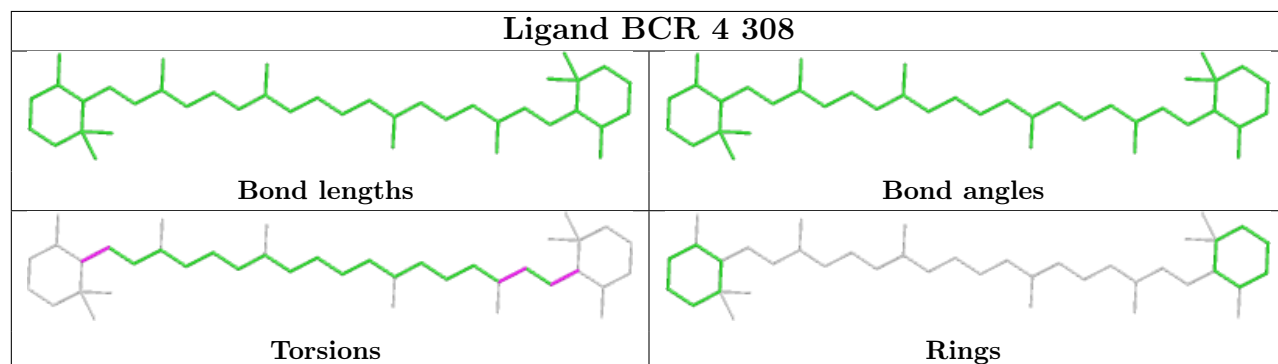
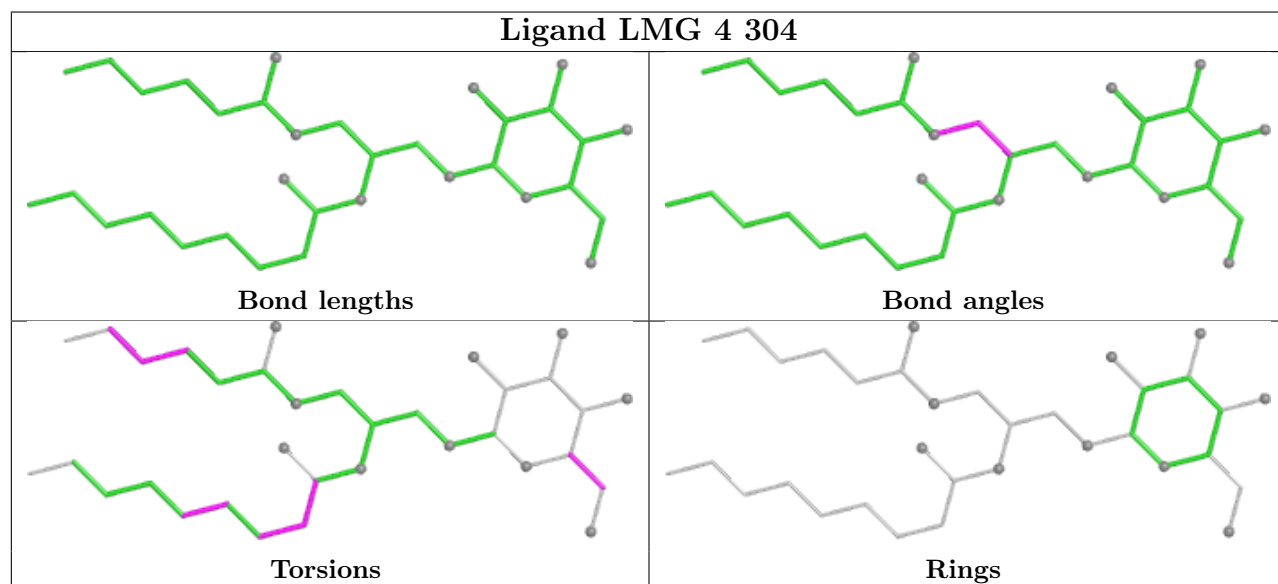
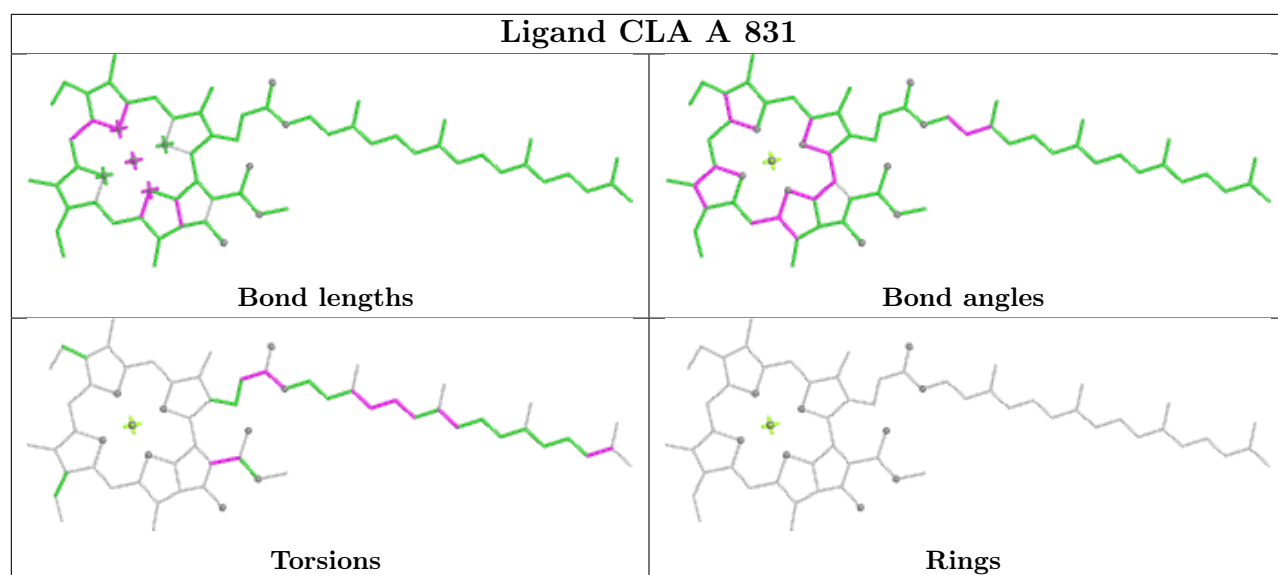
Bond angles

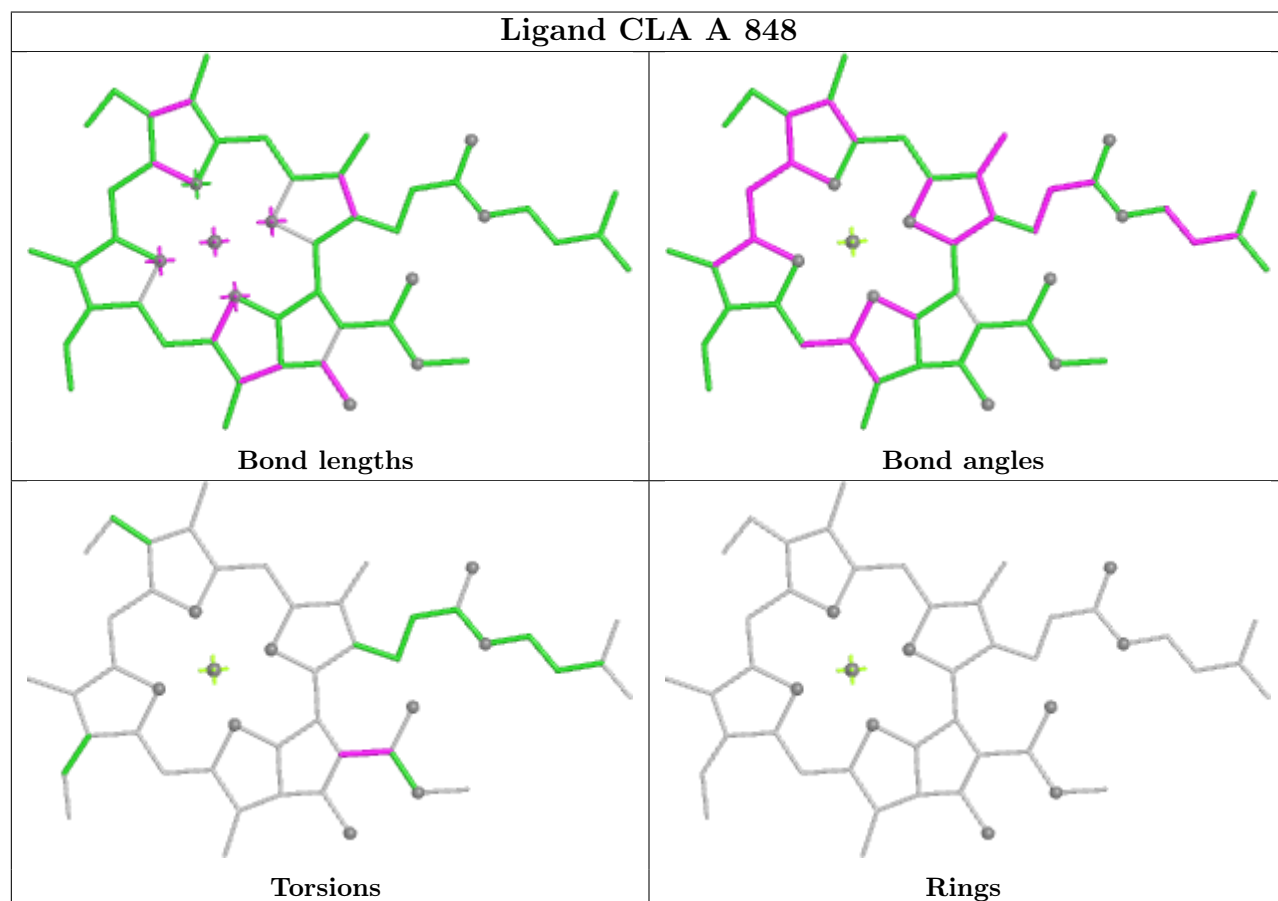
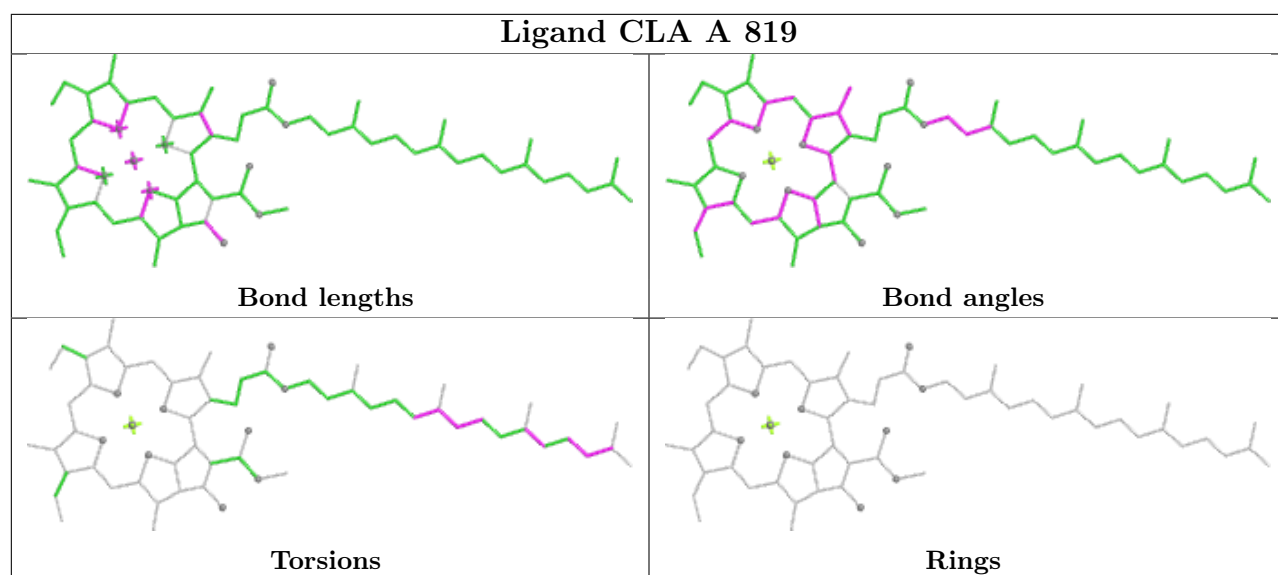


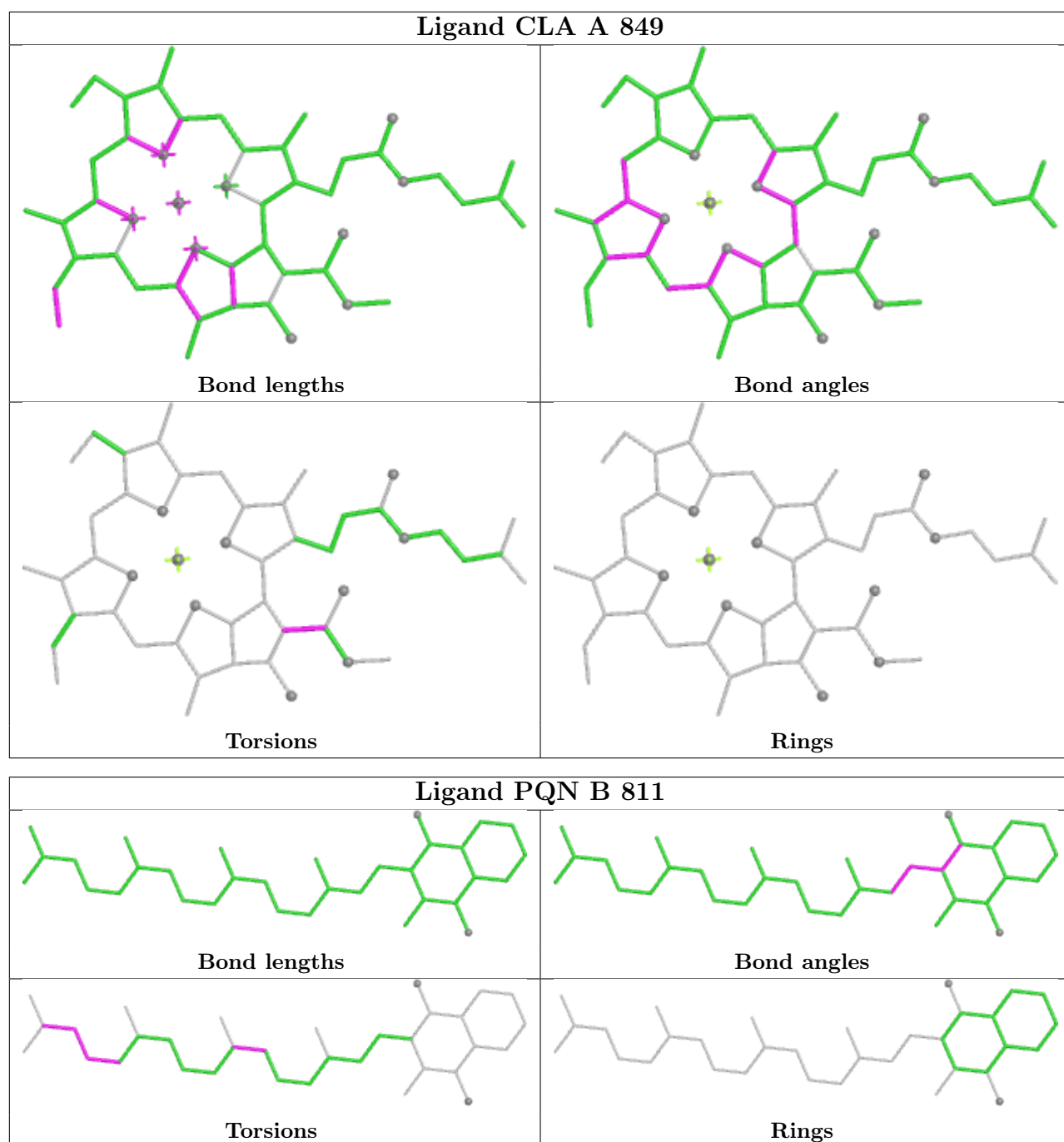
Torsions

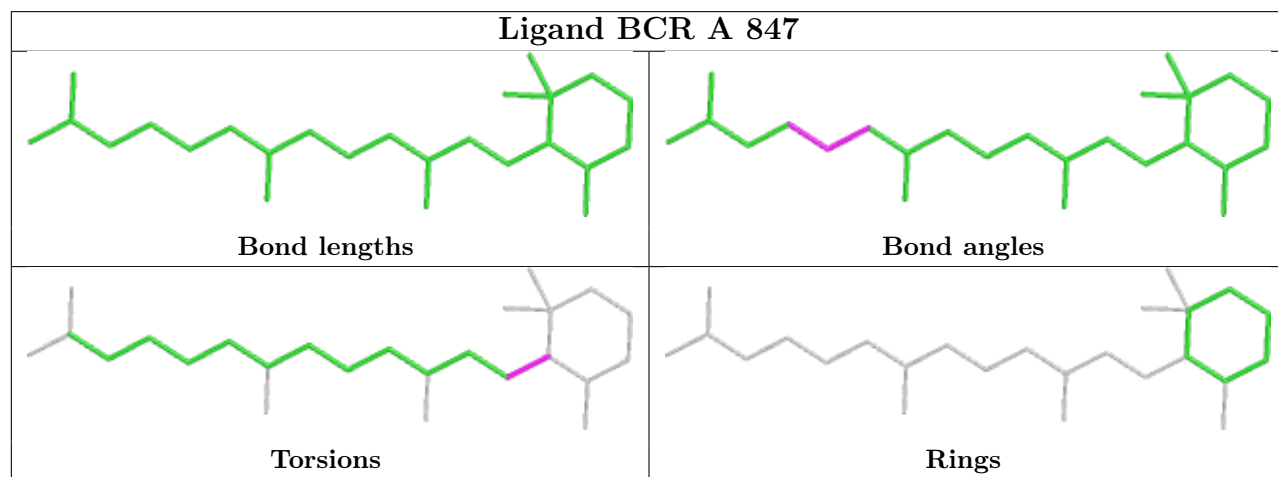
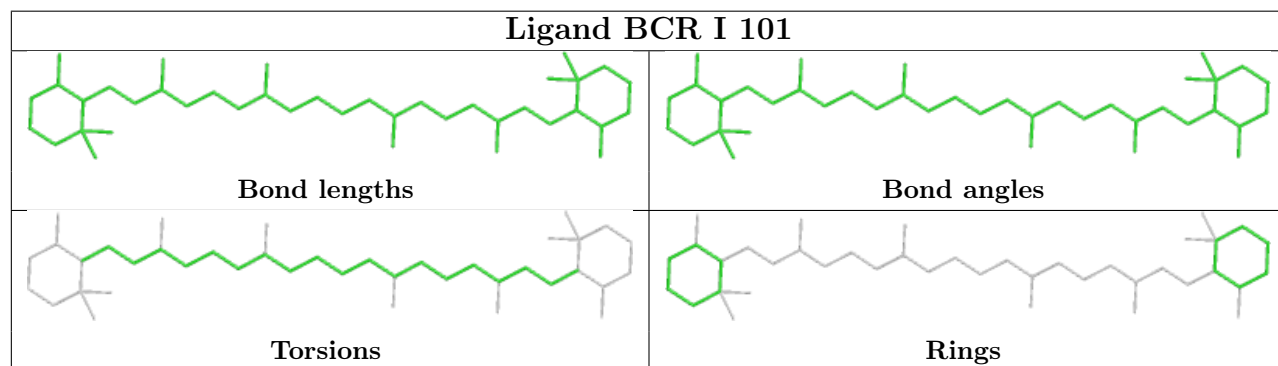
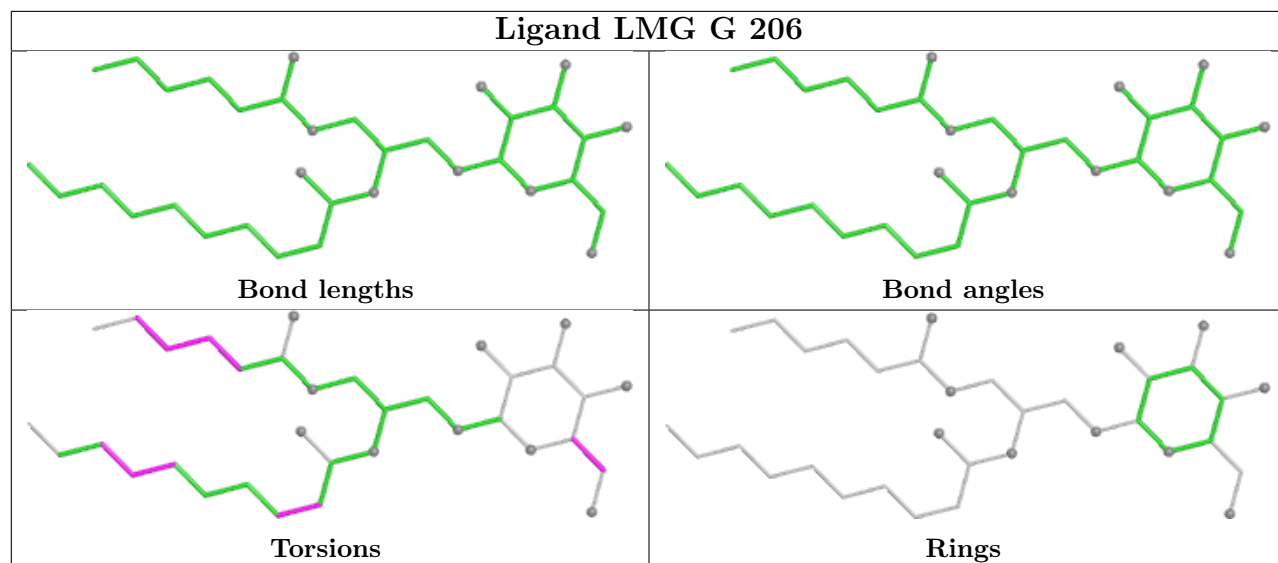


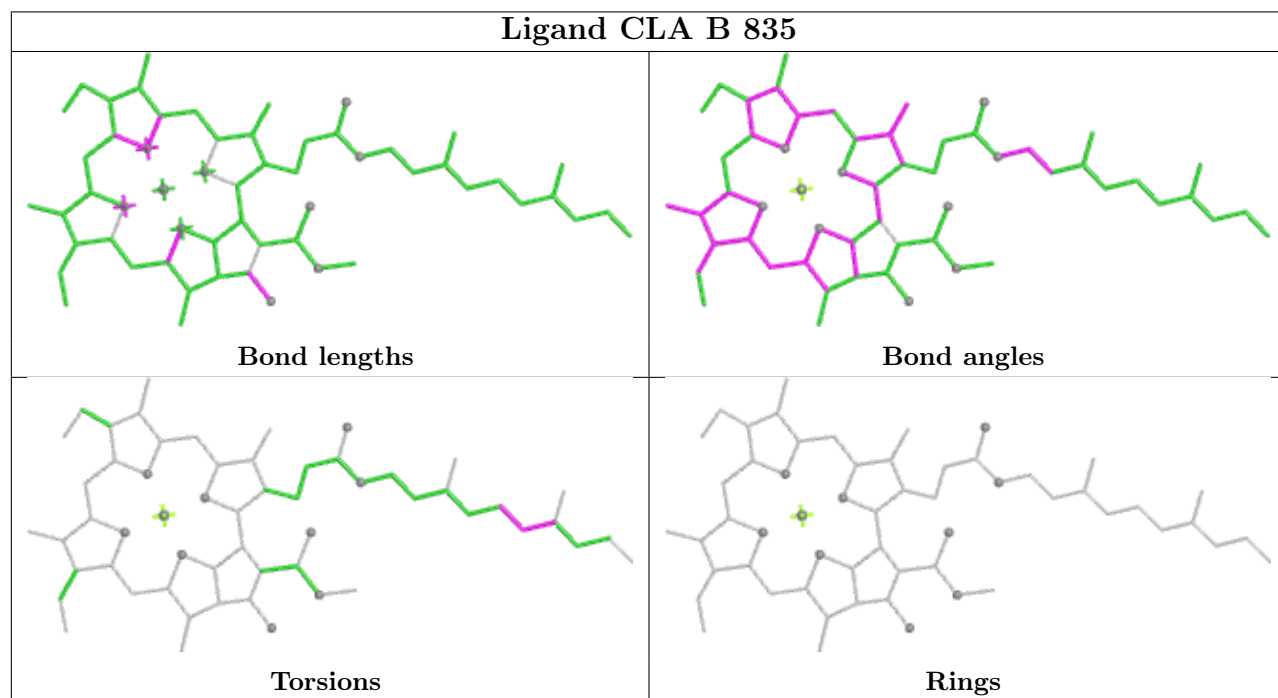
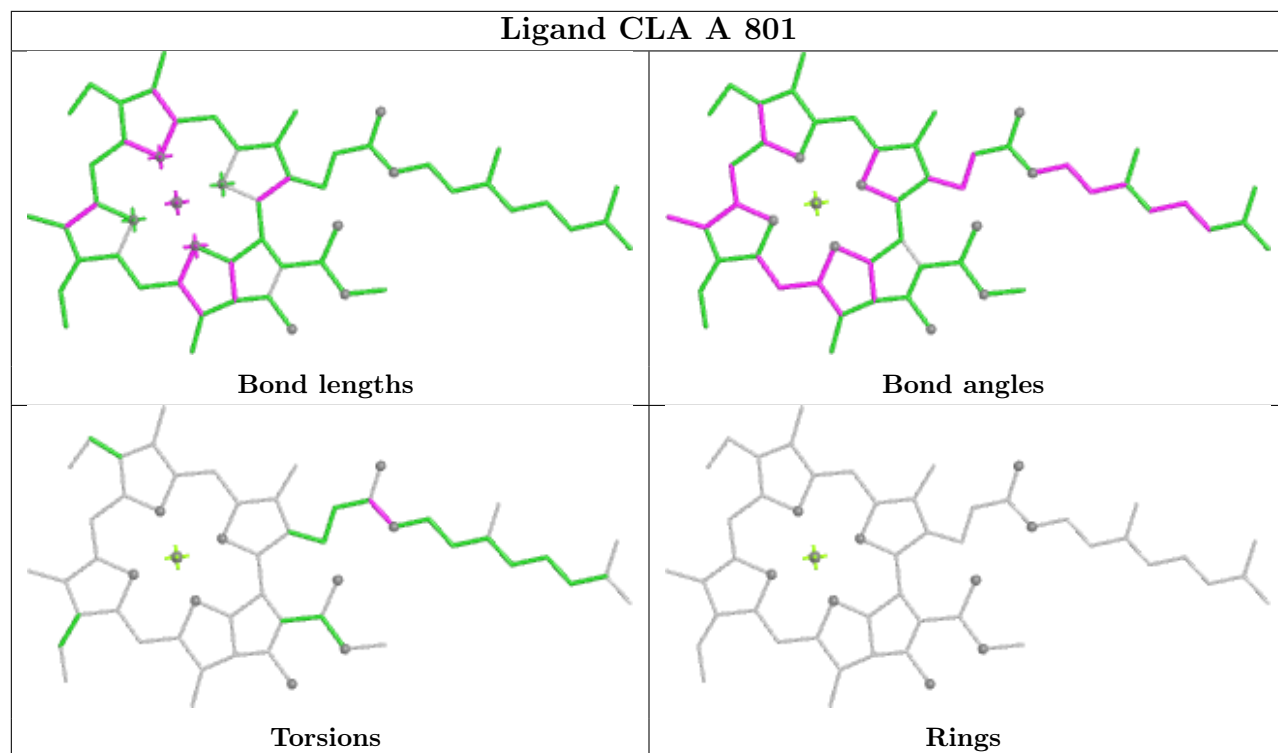
Rings

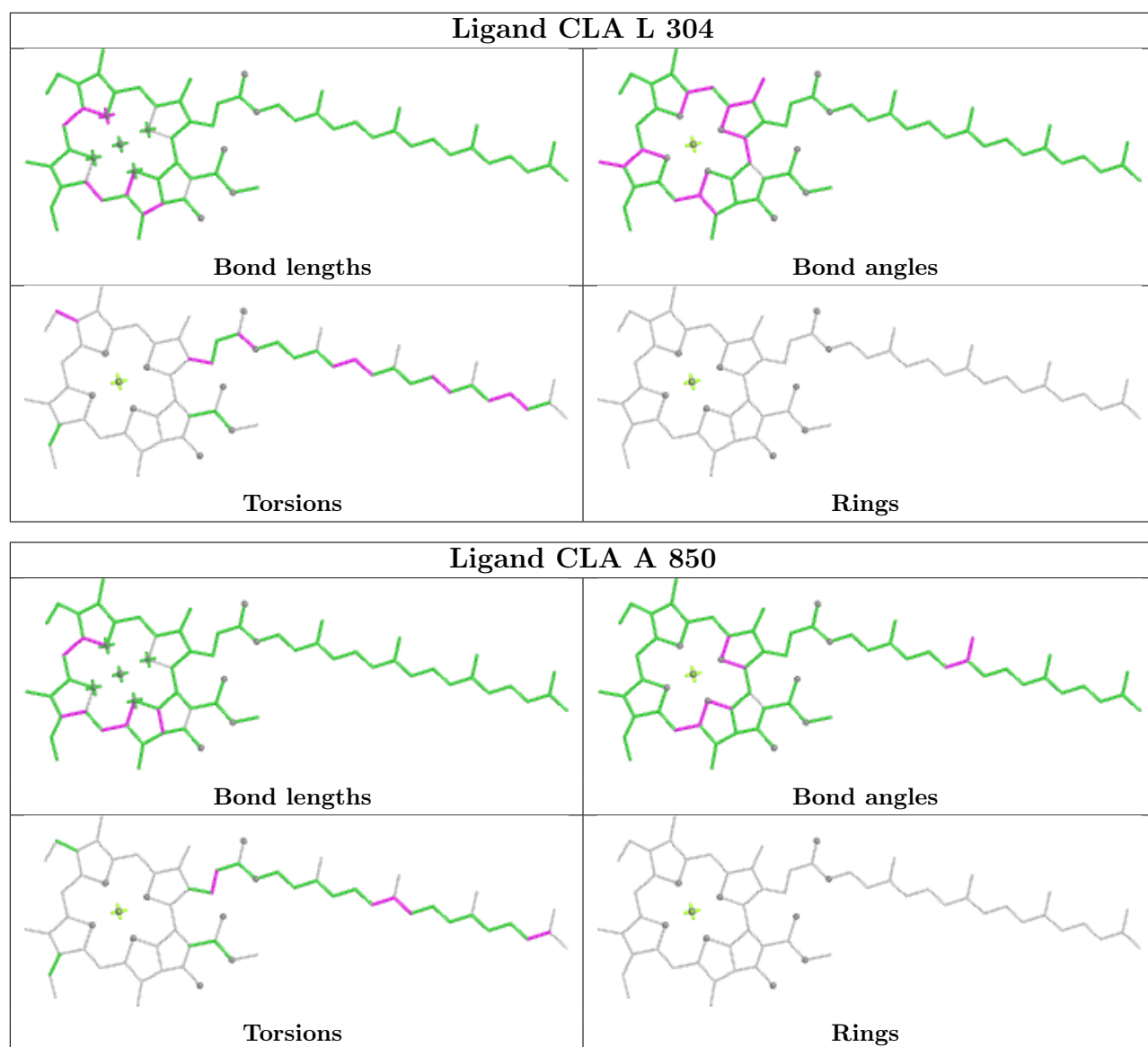




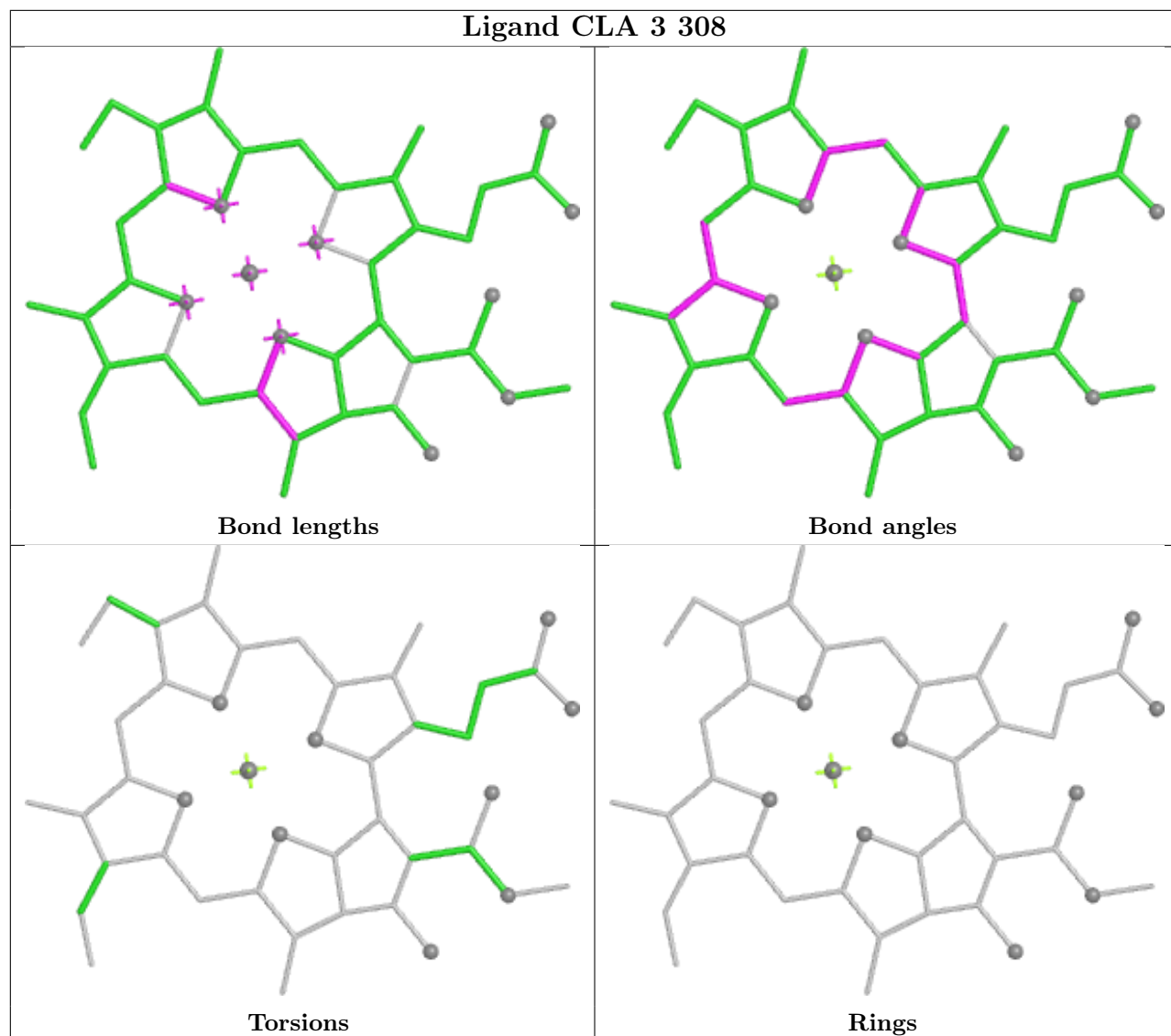


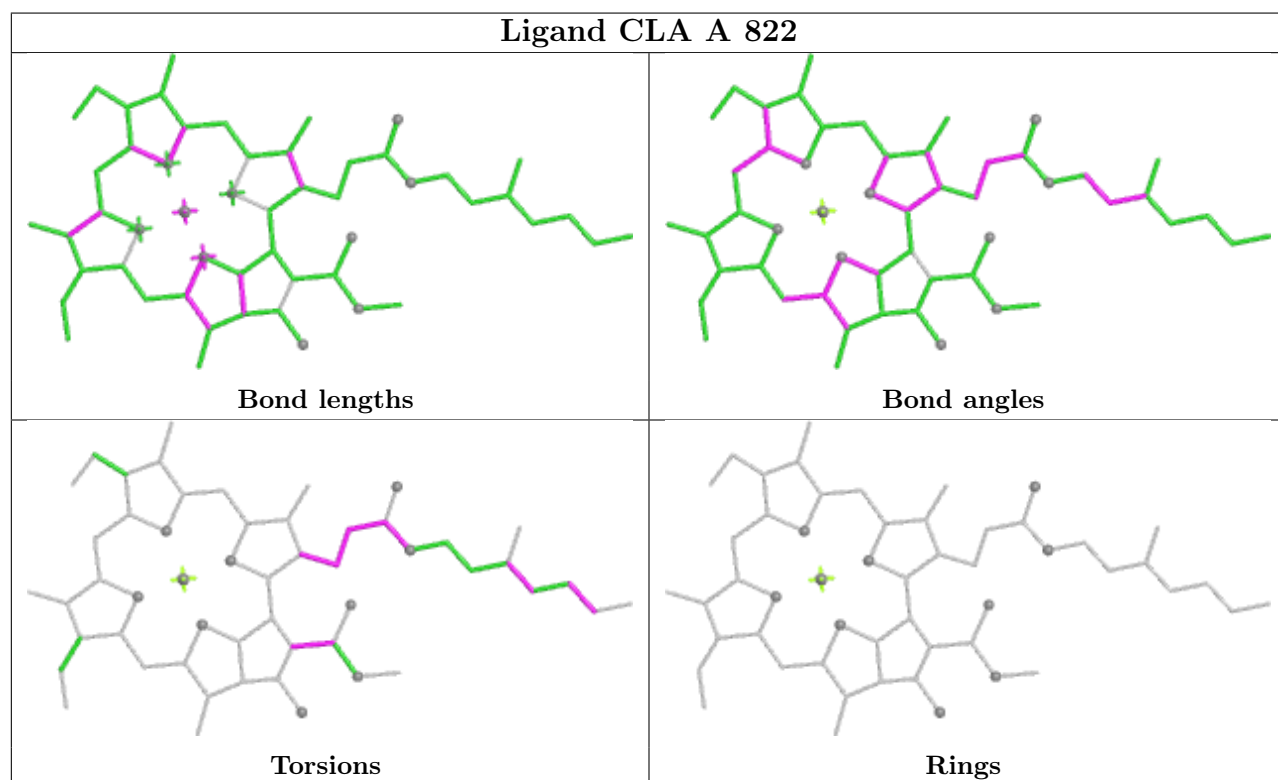
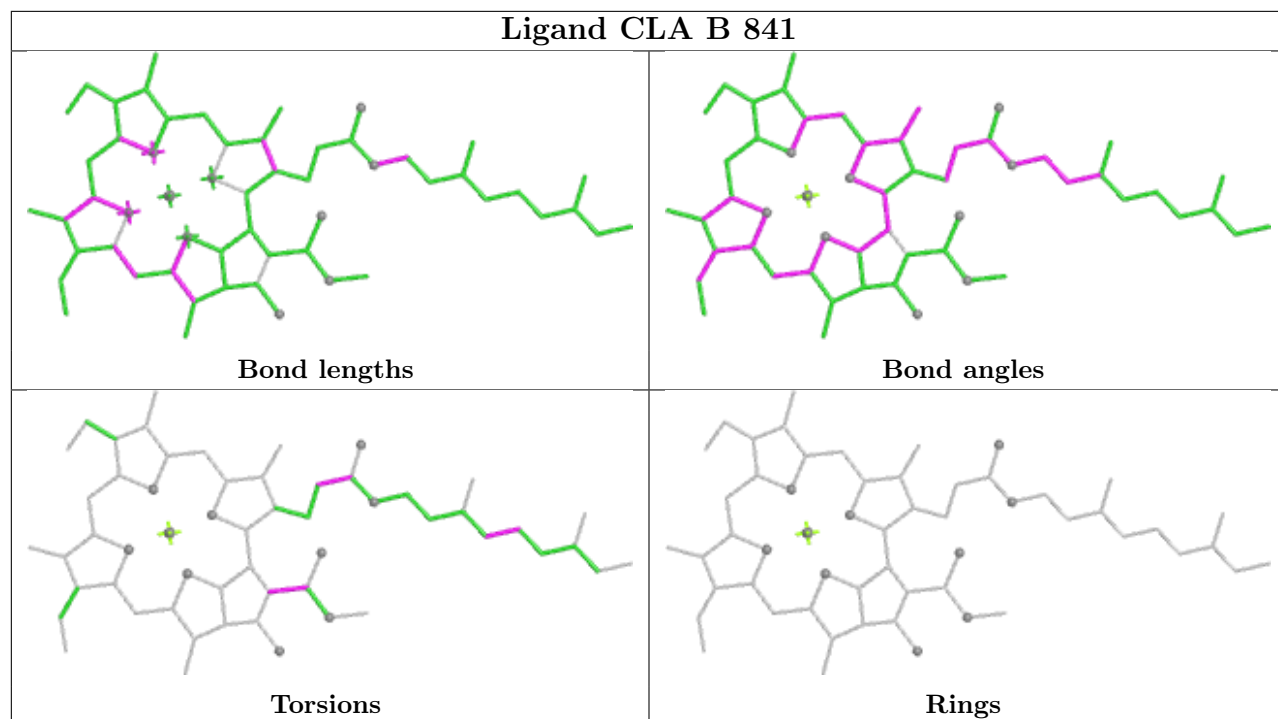




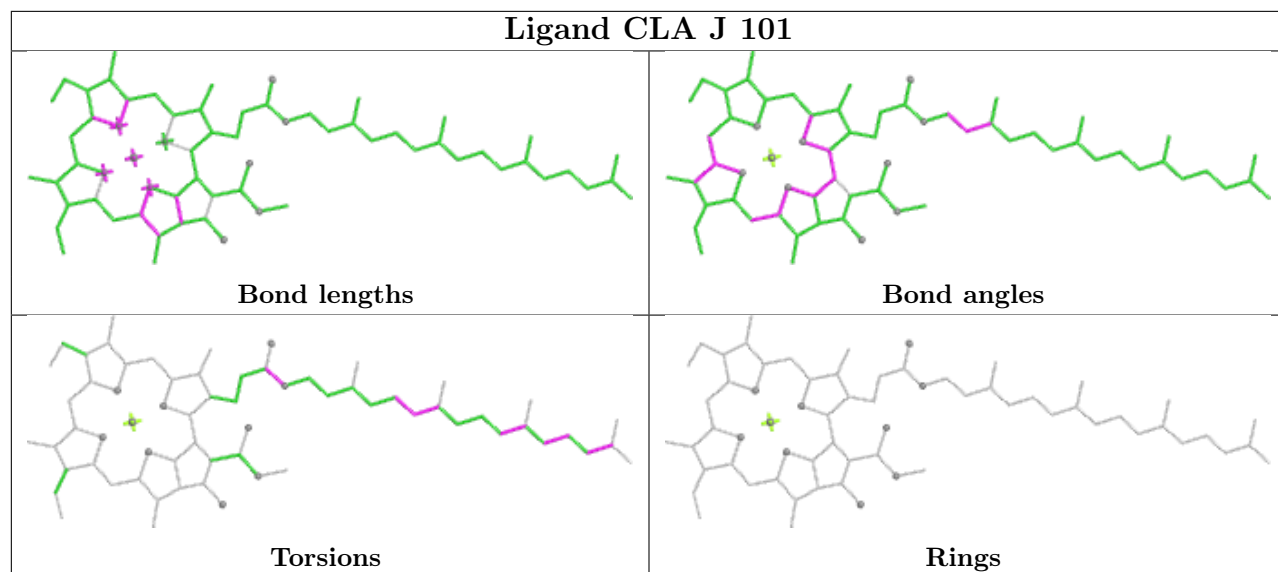


Ligand CLA 3 308

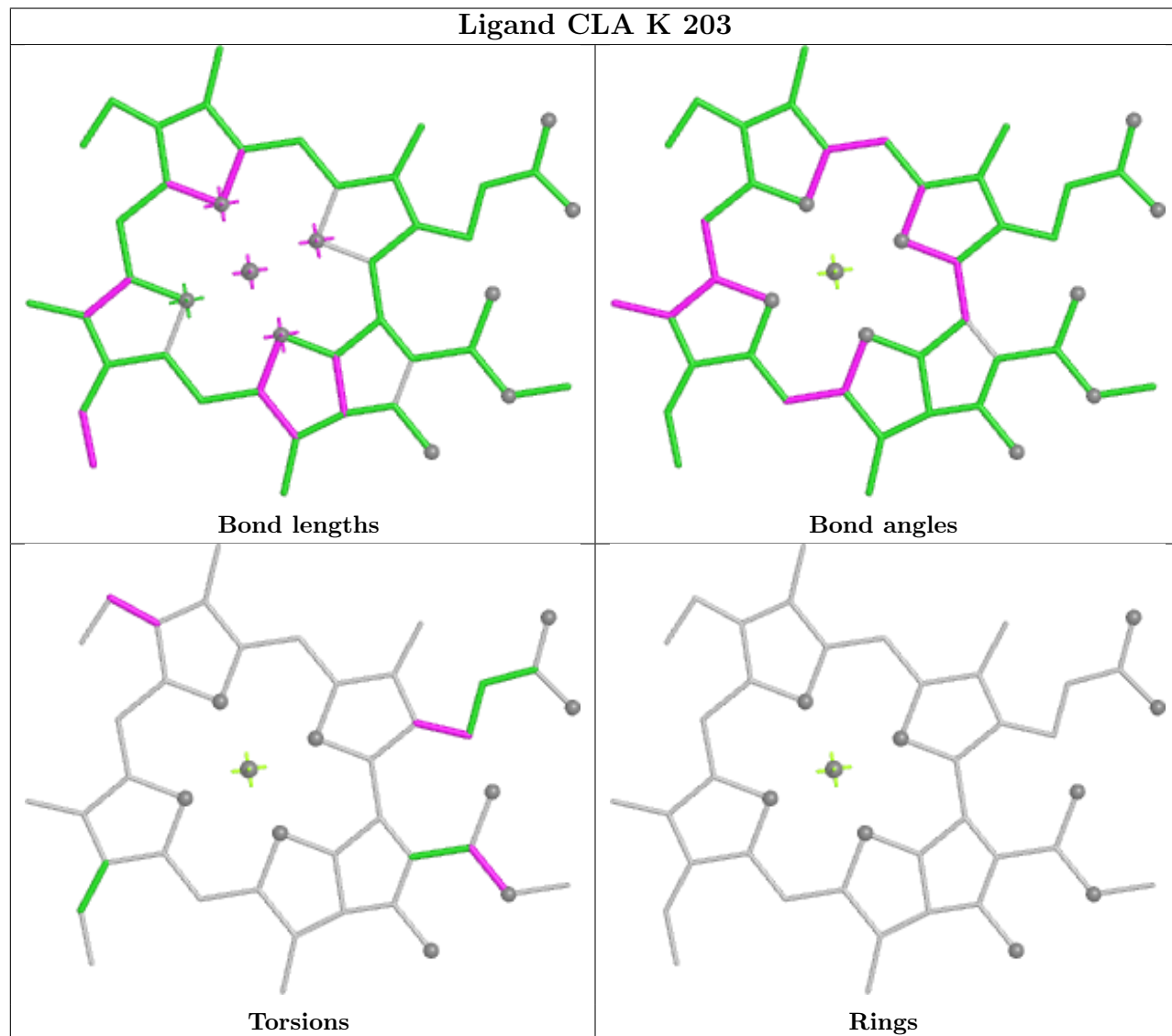


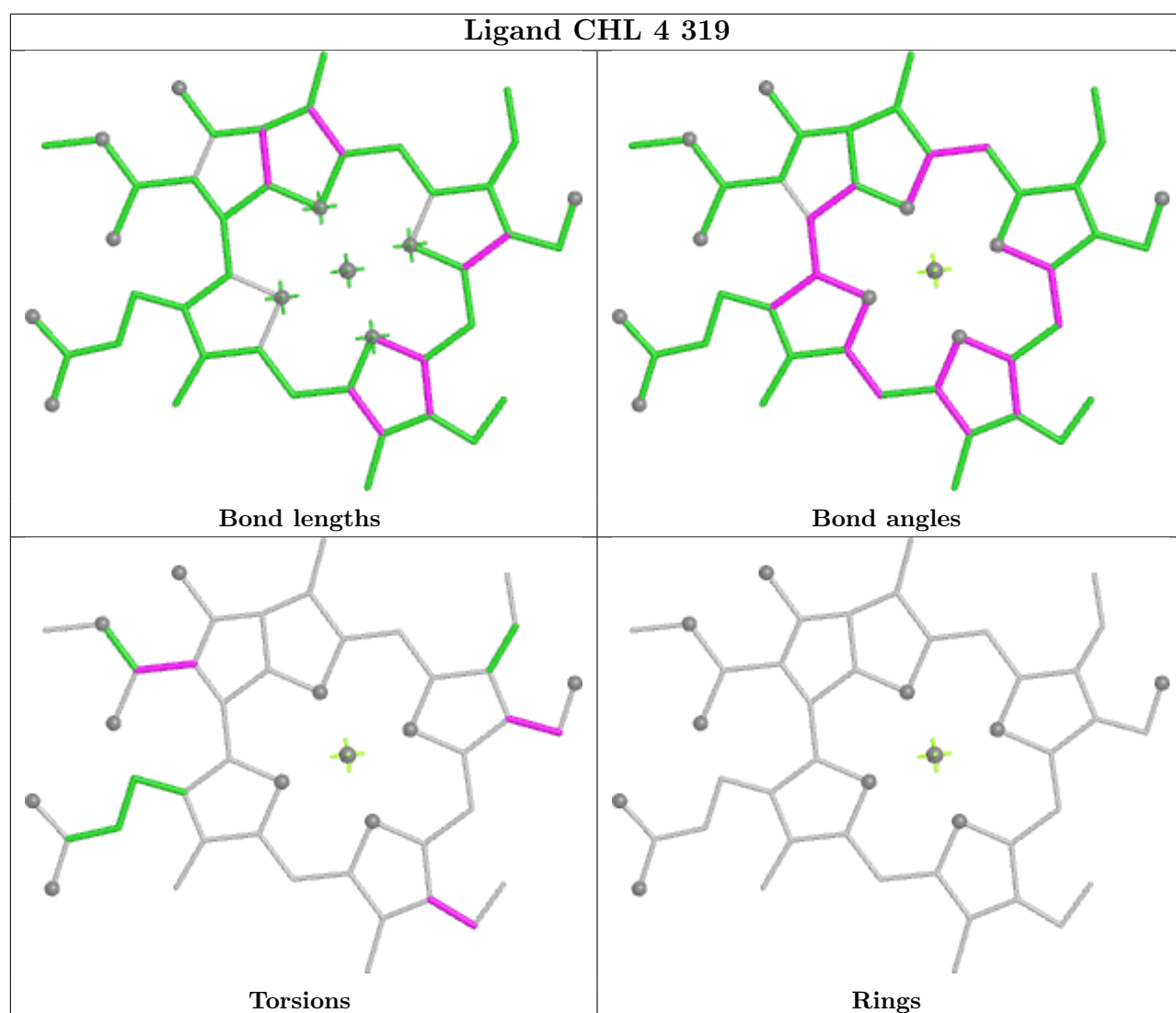
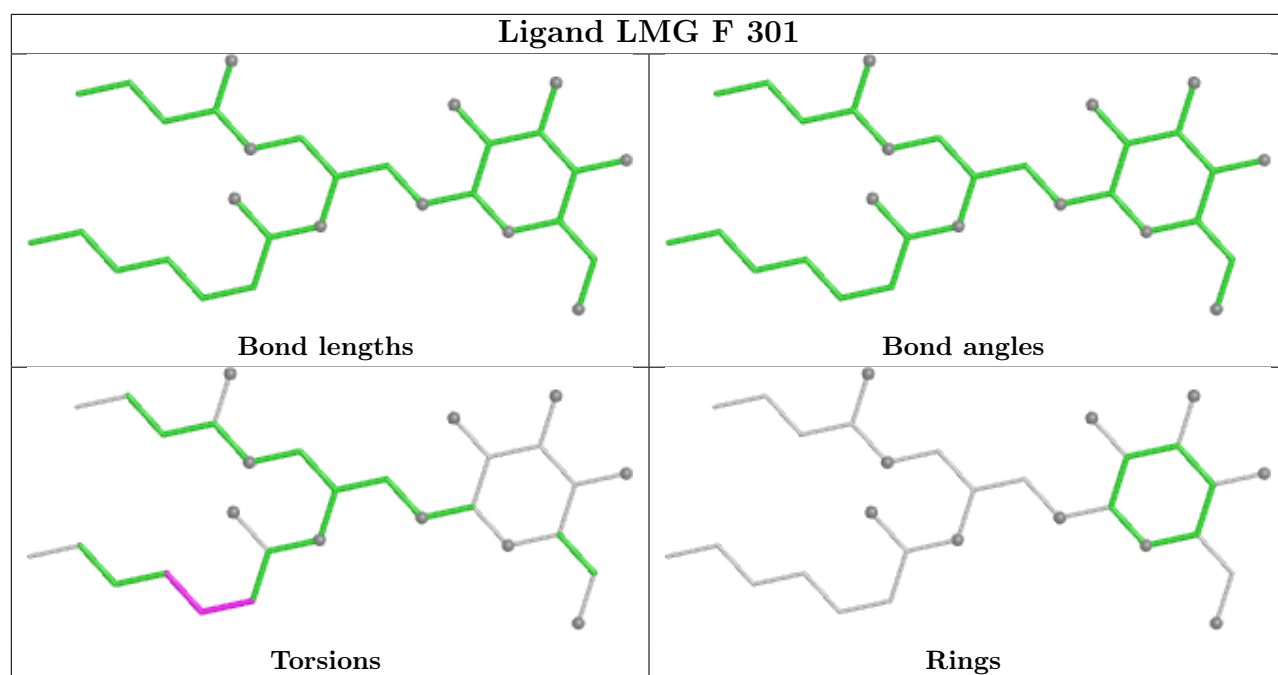


Ligand CLA J 101

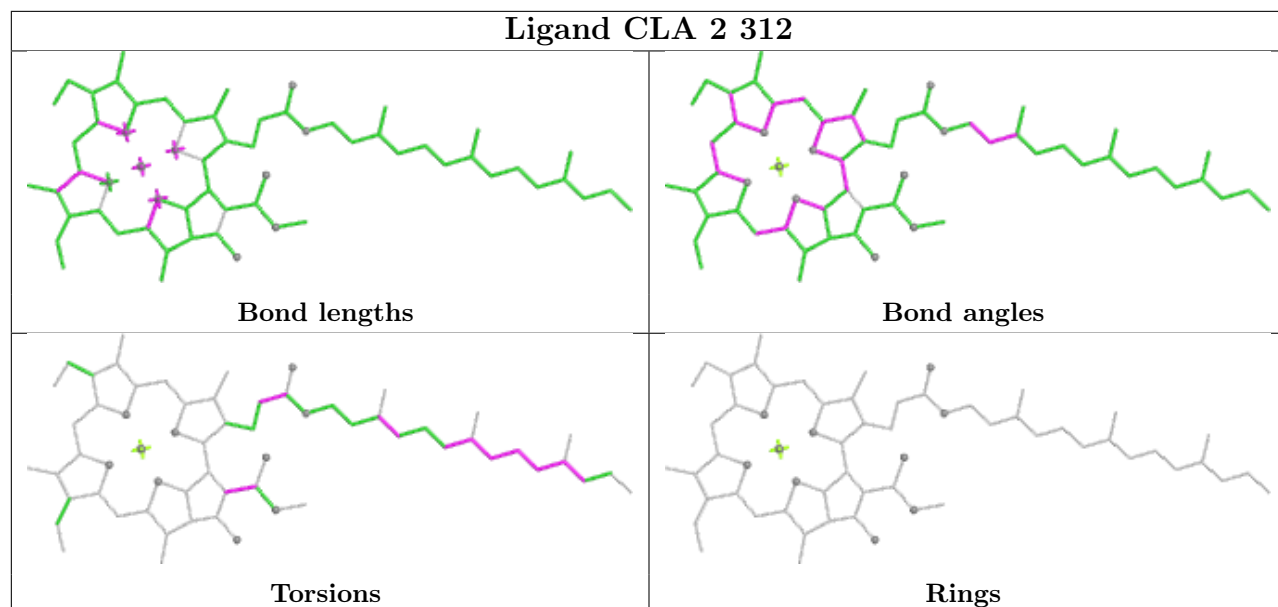


Ligand CLA K 203

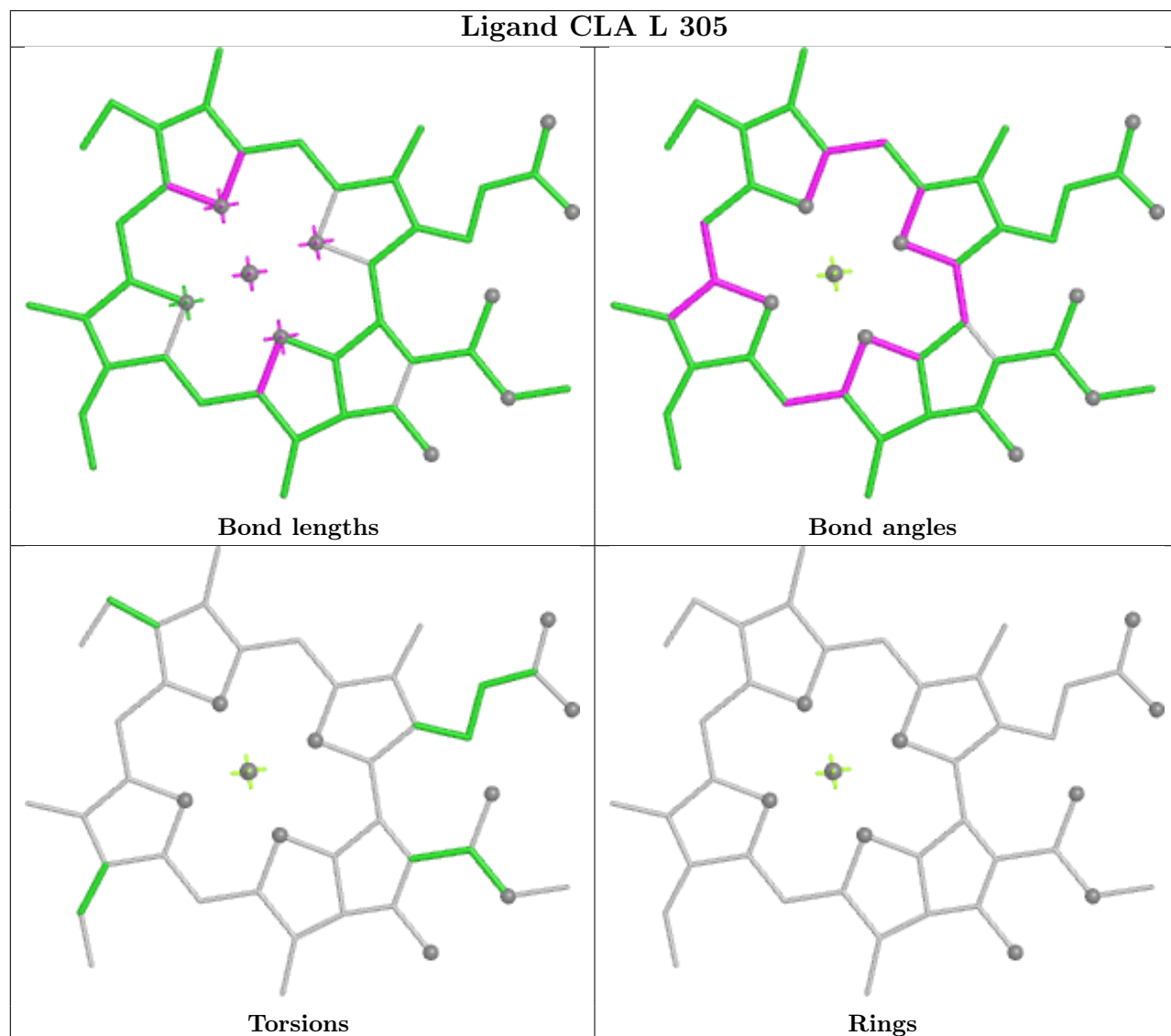


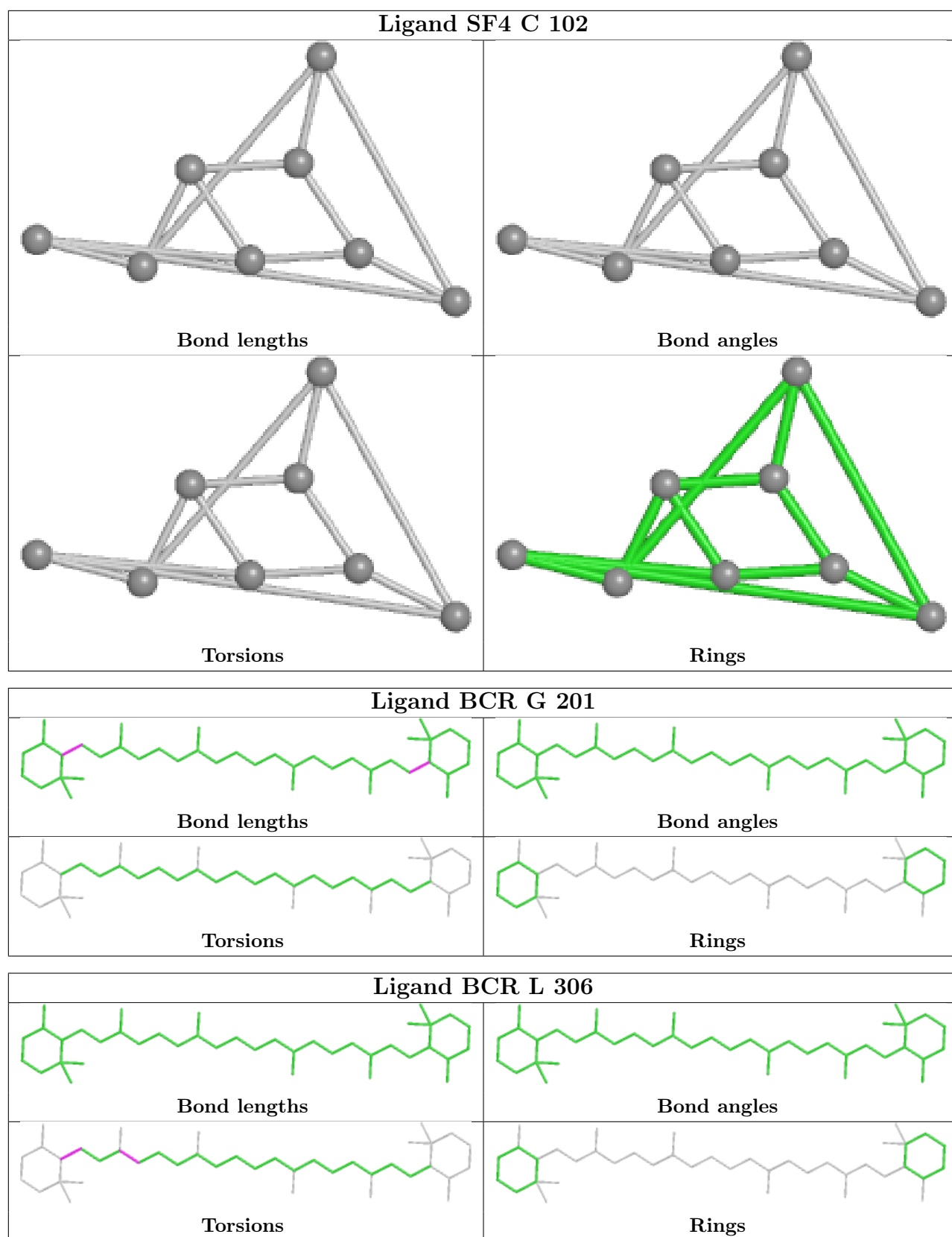


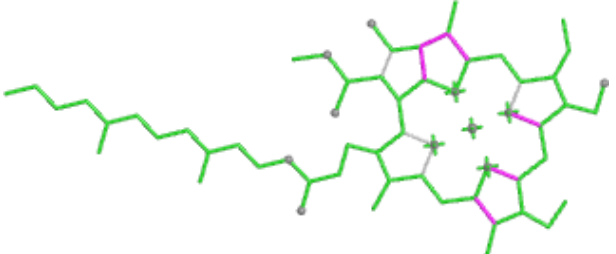
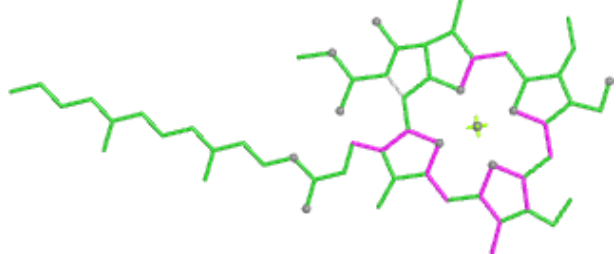
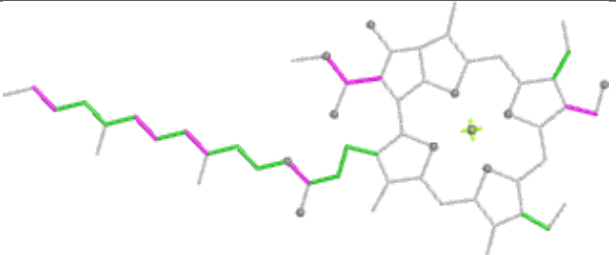
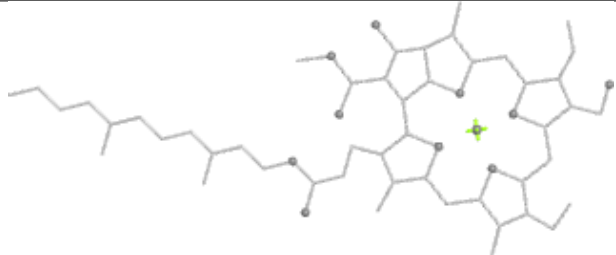
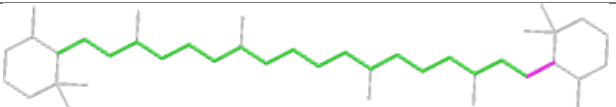
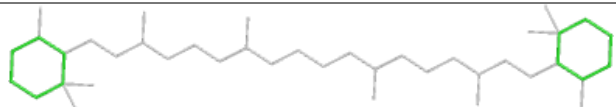
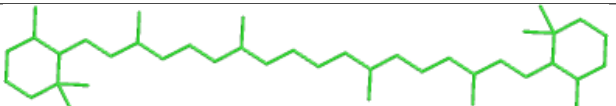
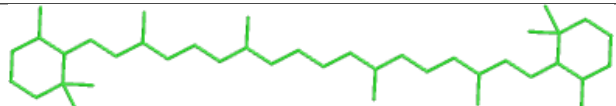
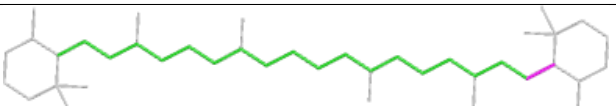
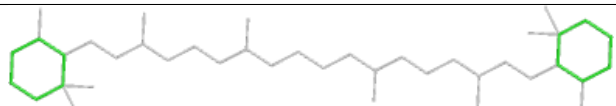
Ligand CLA 2 312

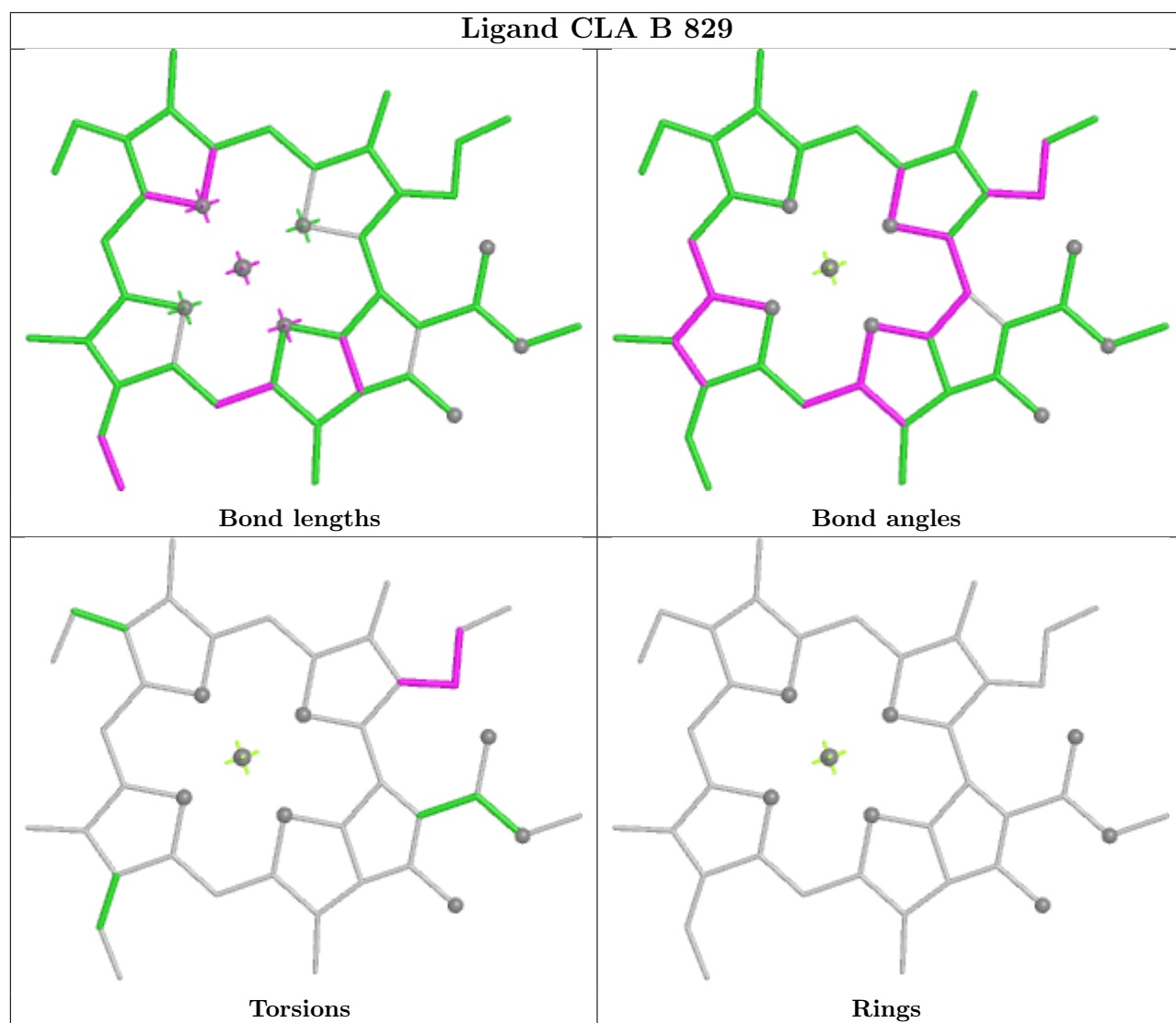
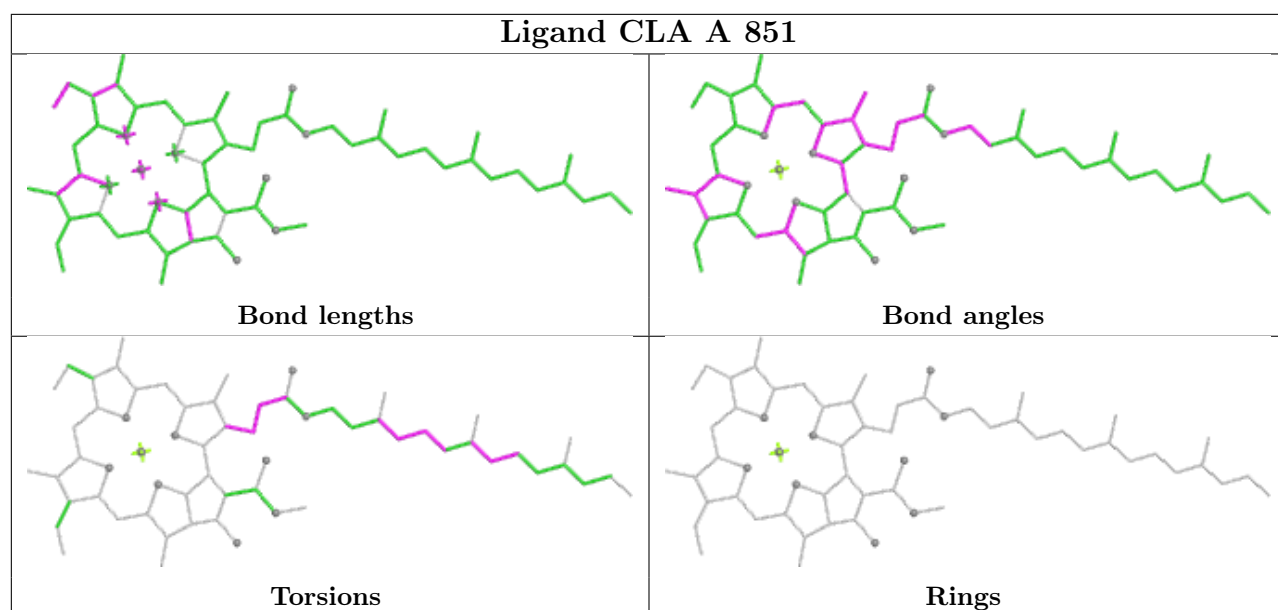


Ligand CLA L 305

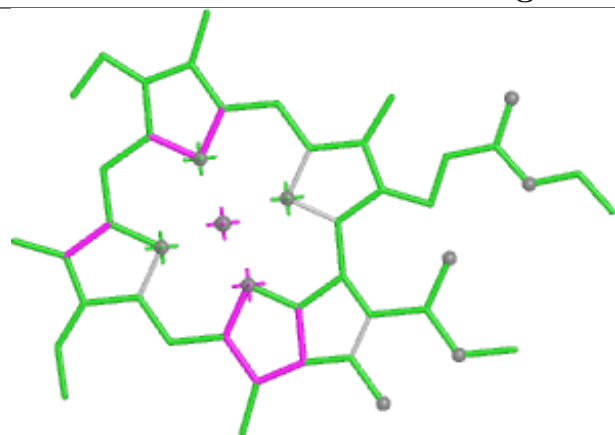




Ligand CHL 1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings



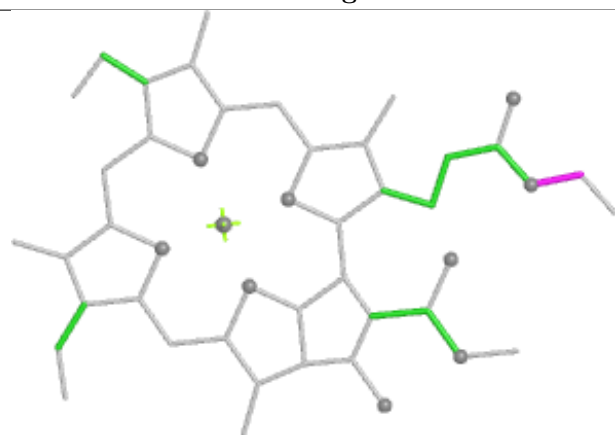
Ligand CLA B 837



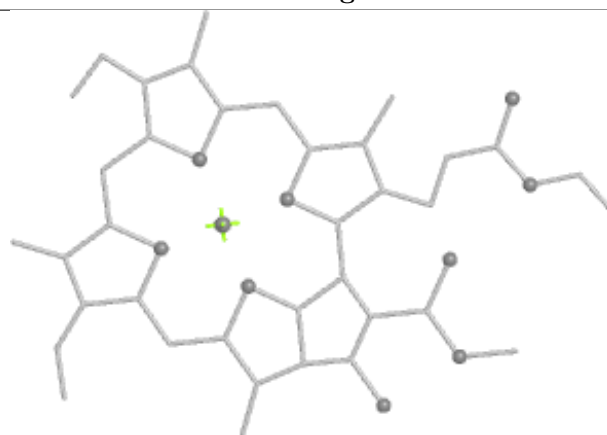
Bond lengths



Bond angles

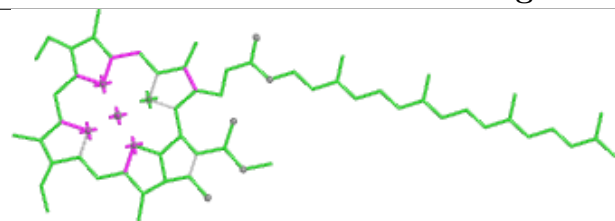


Torsions

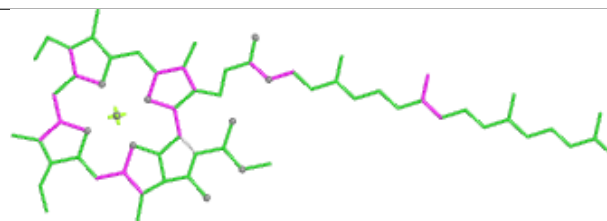


Rings

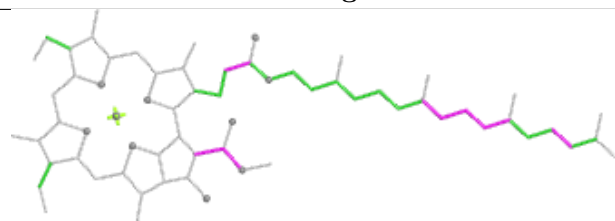
Ligand CLA A 812



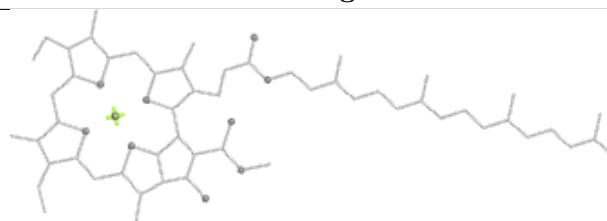
Bond lengths



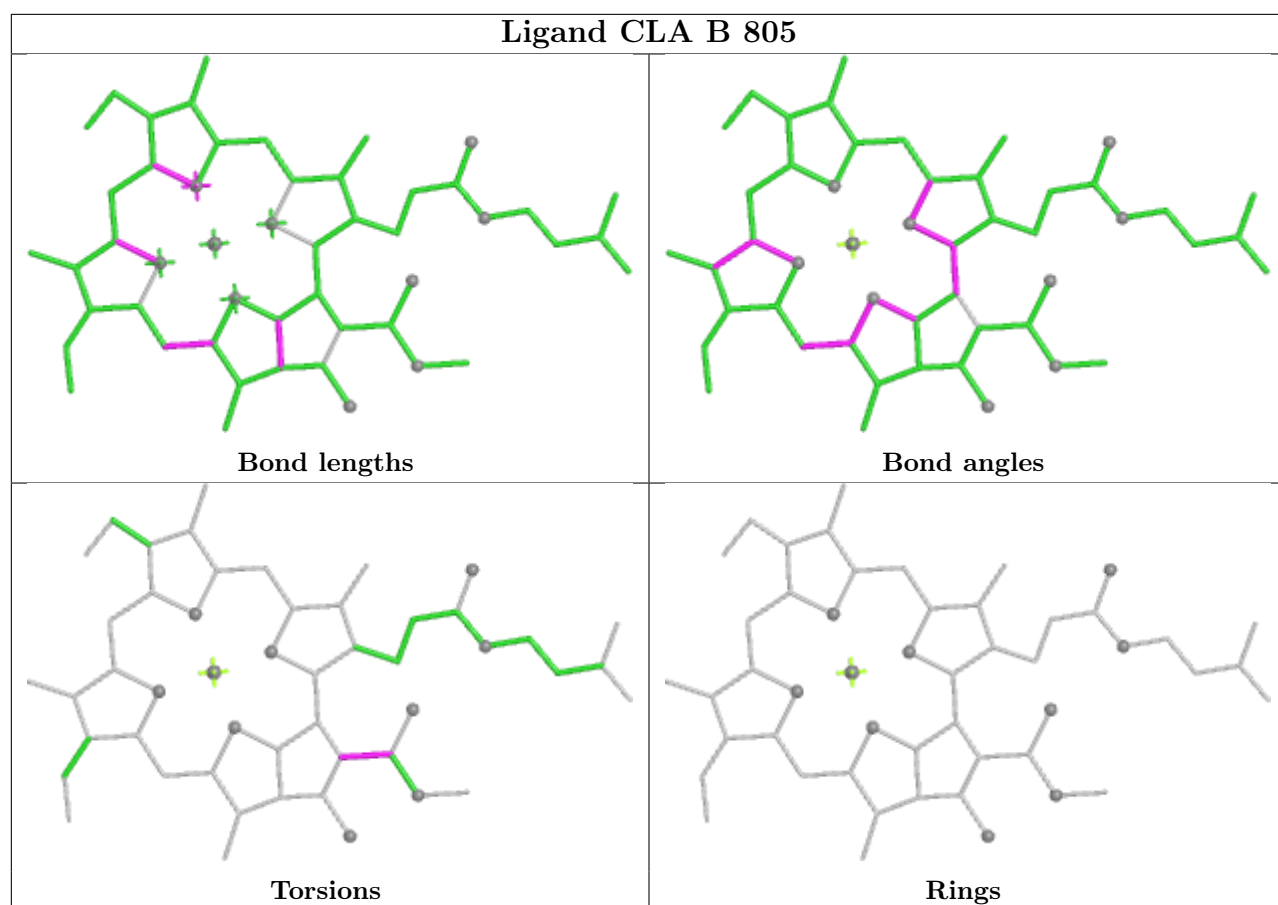
Bond angles

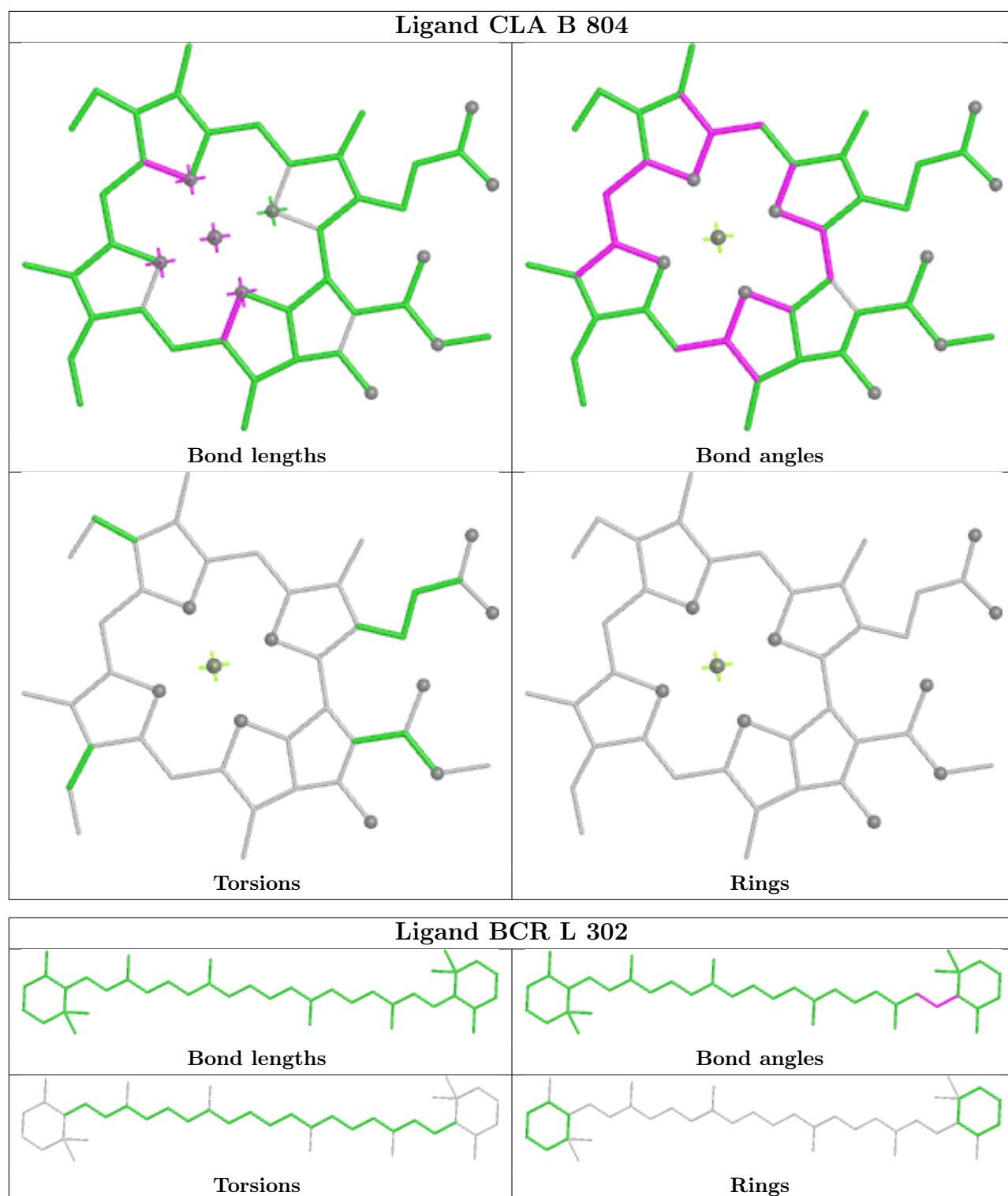


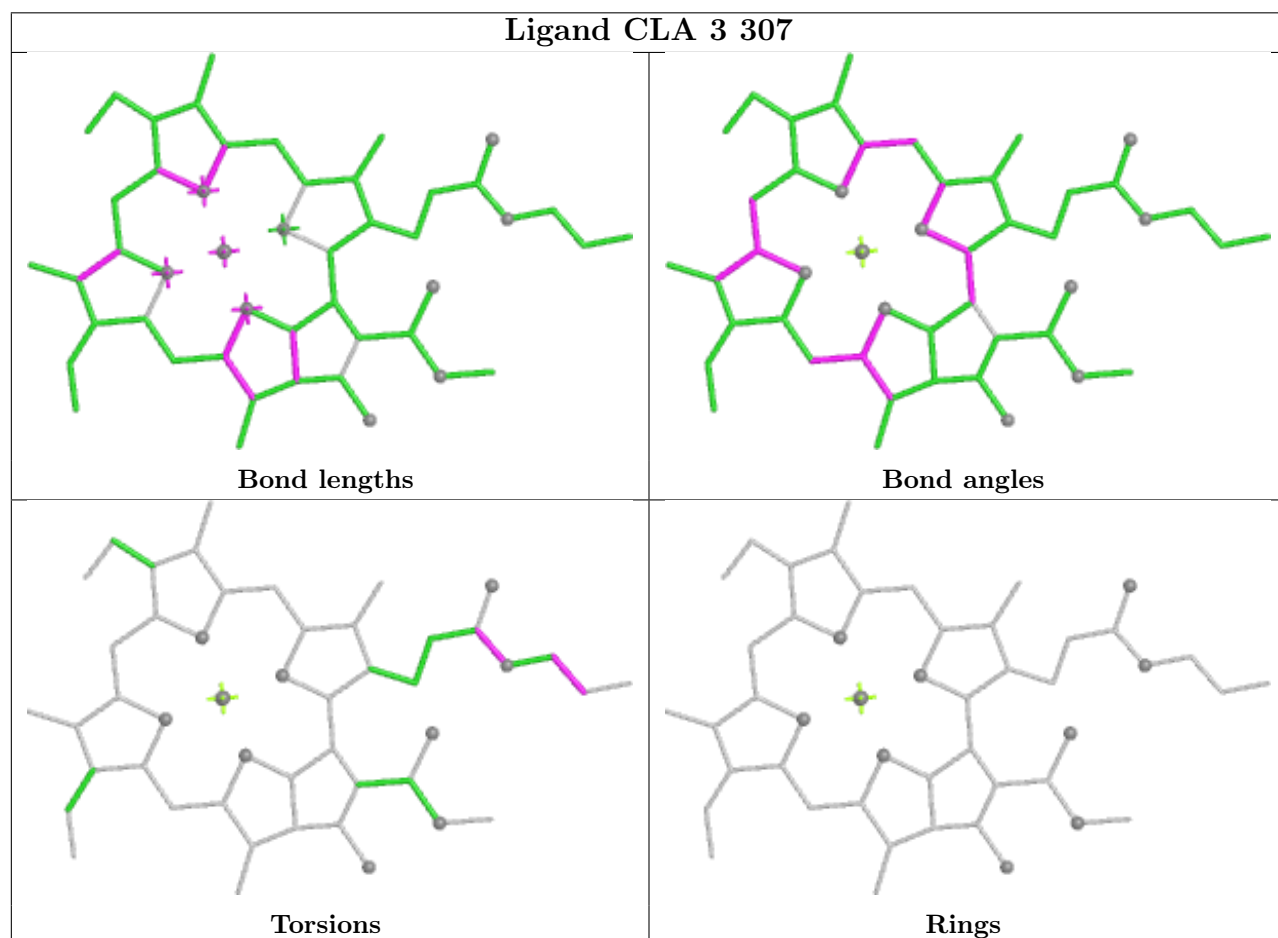
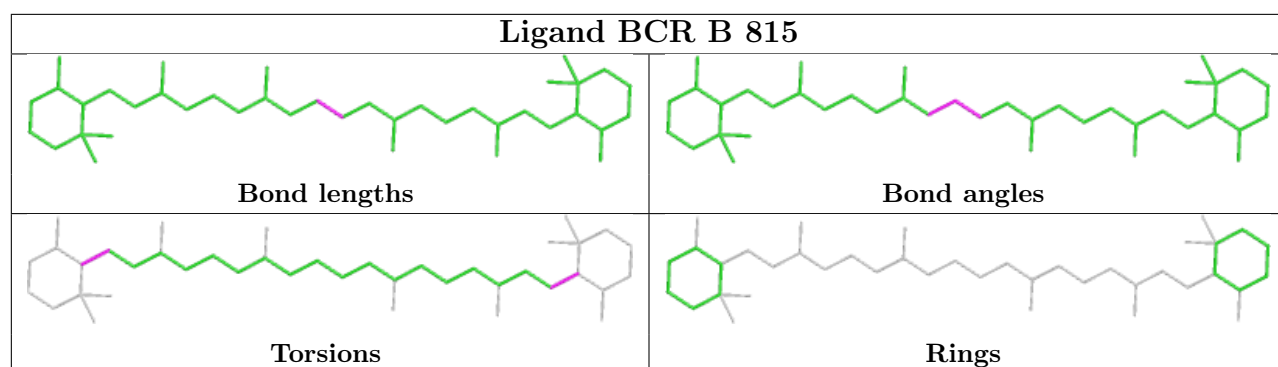
Torsions

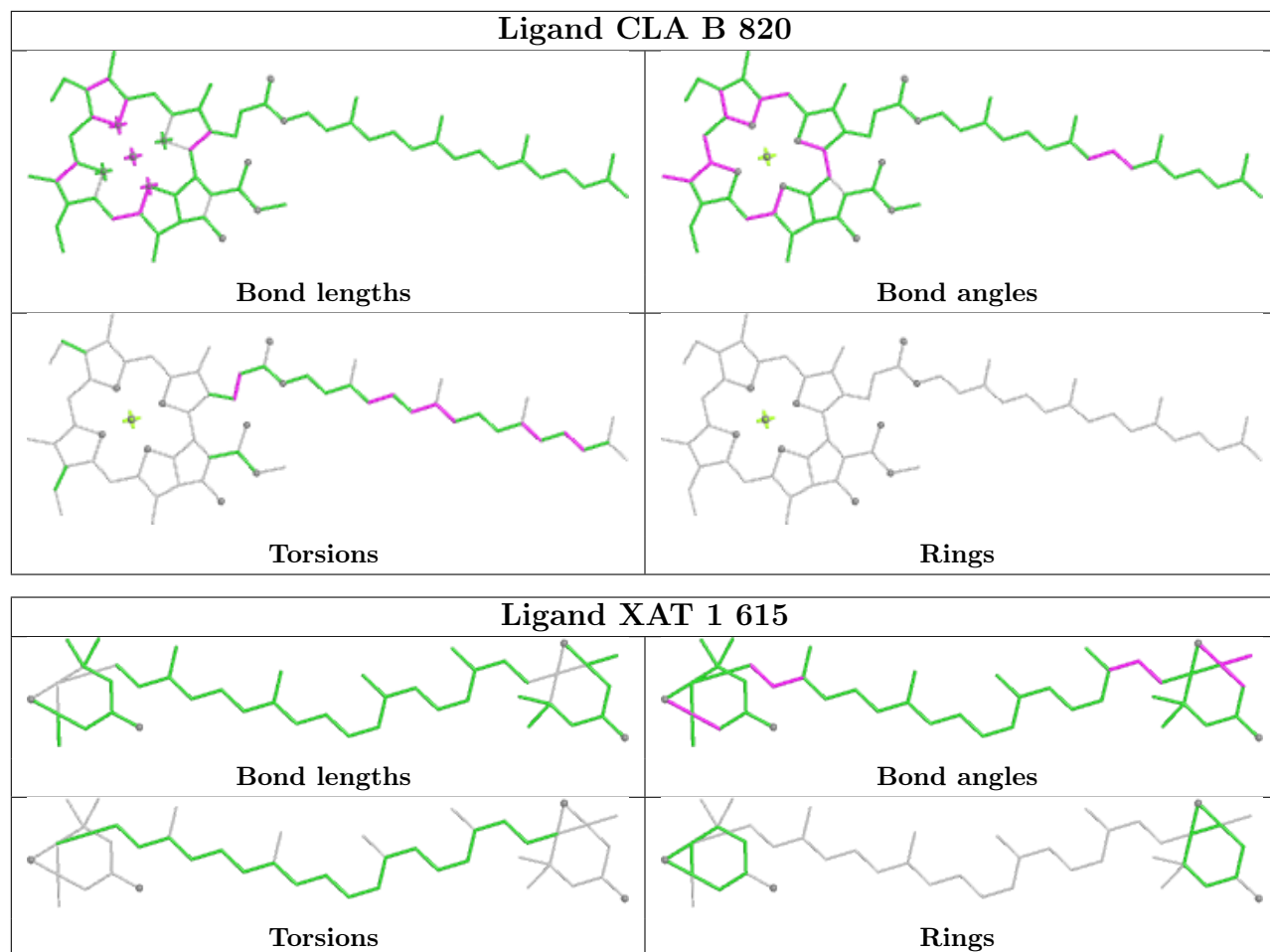


Rings

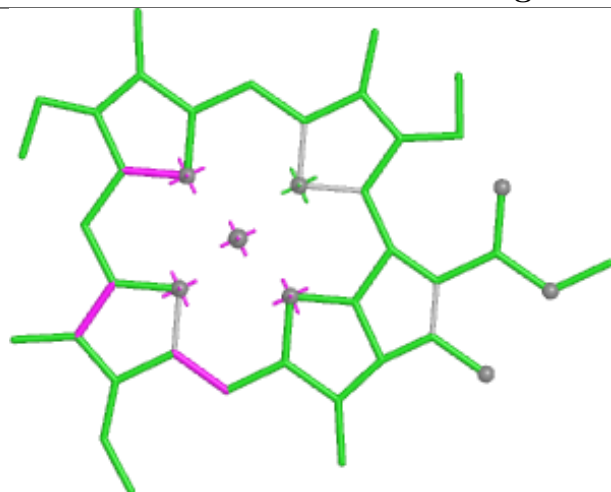




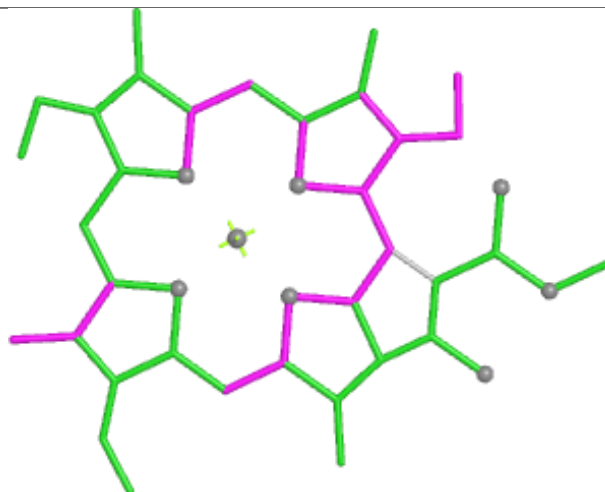




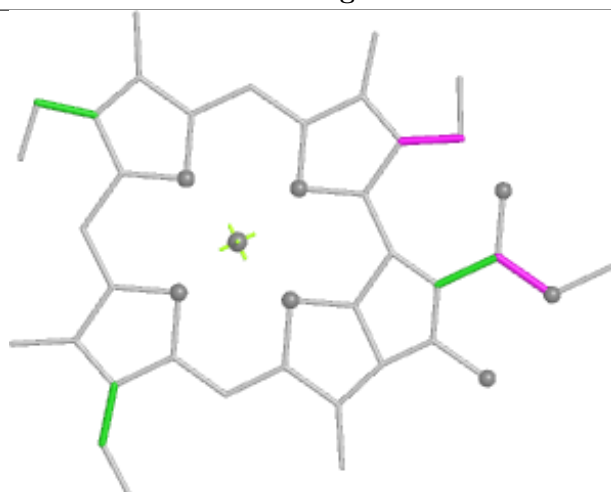
Ligand CLA B 821



Bond lengths



Bond angles

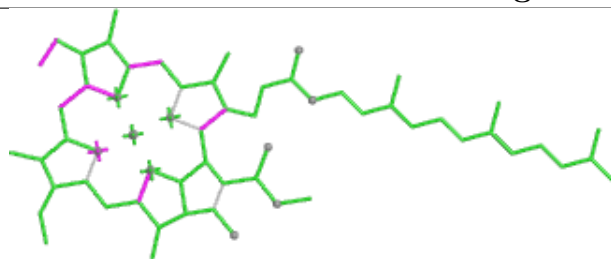


Torsions

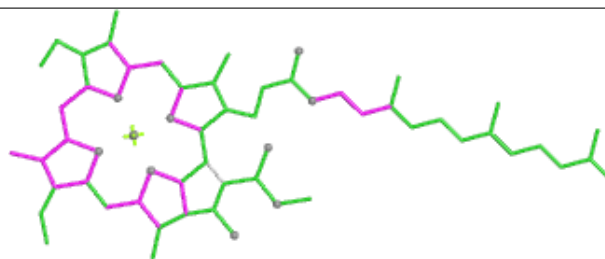


Rings

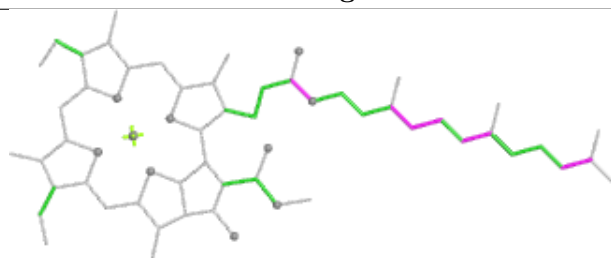
Ligand CLA A 842



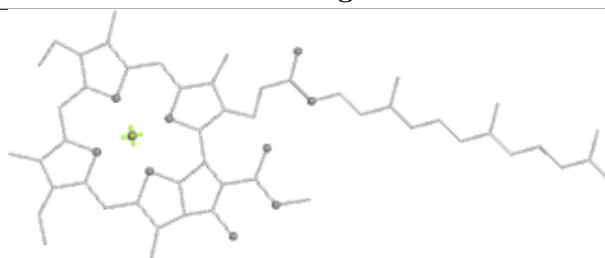
Bond lengths



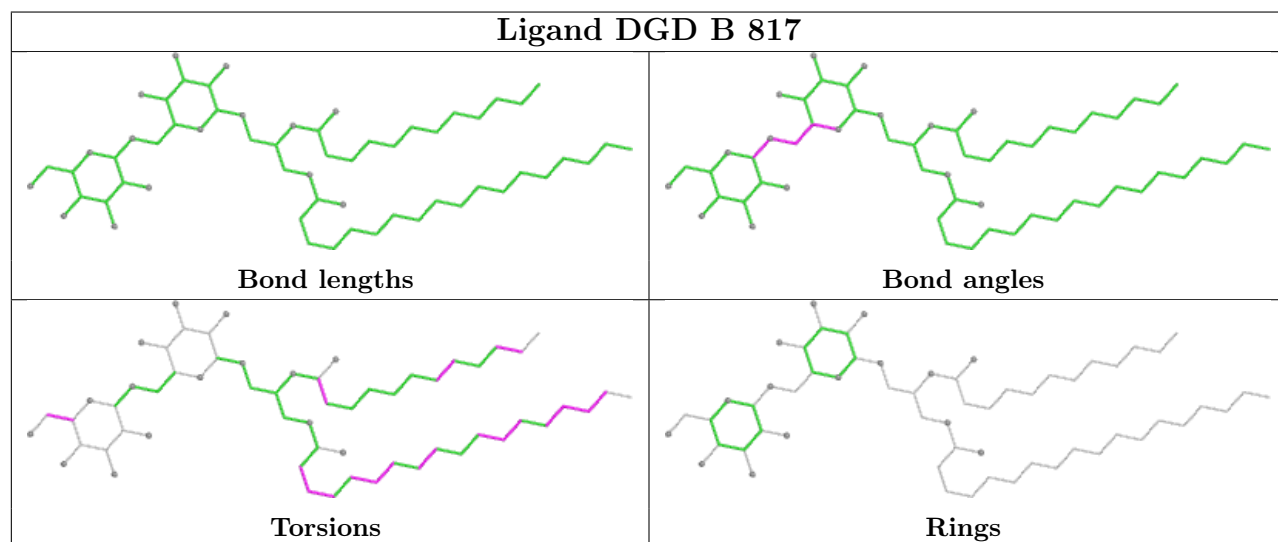
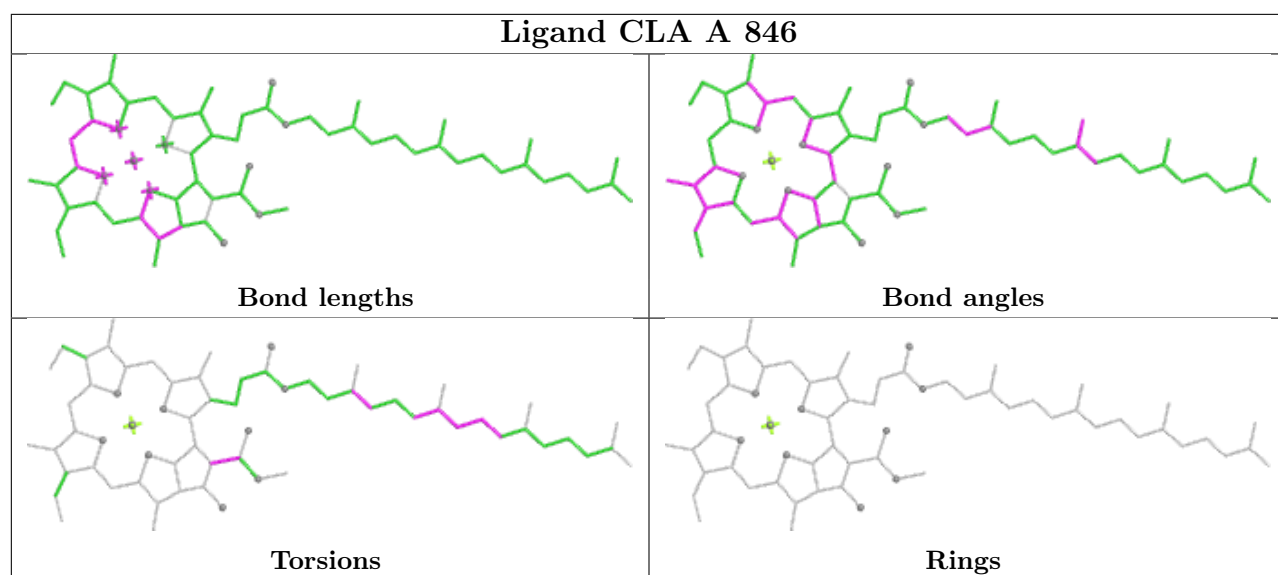
Bond angles

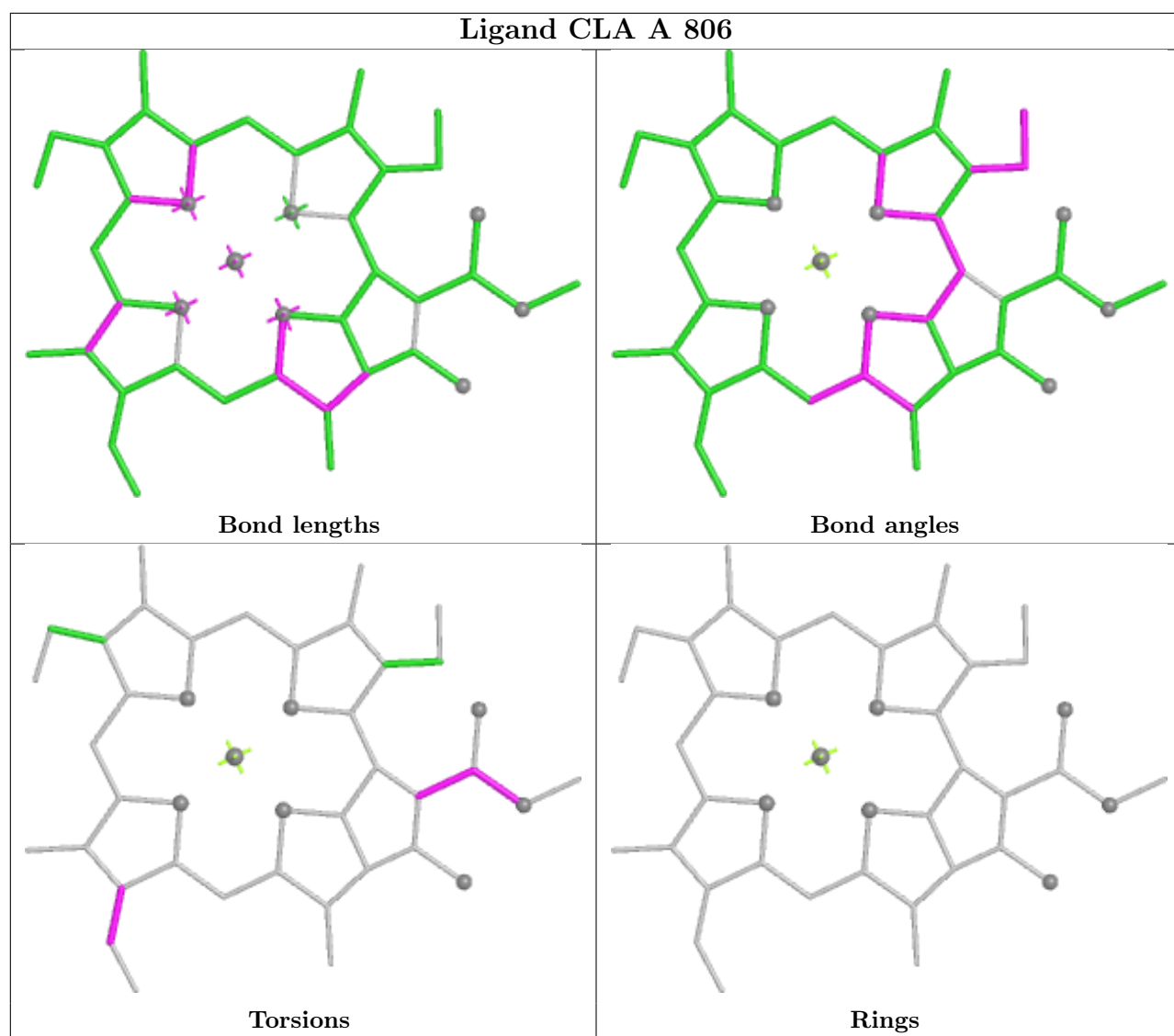


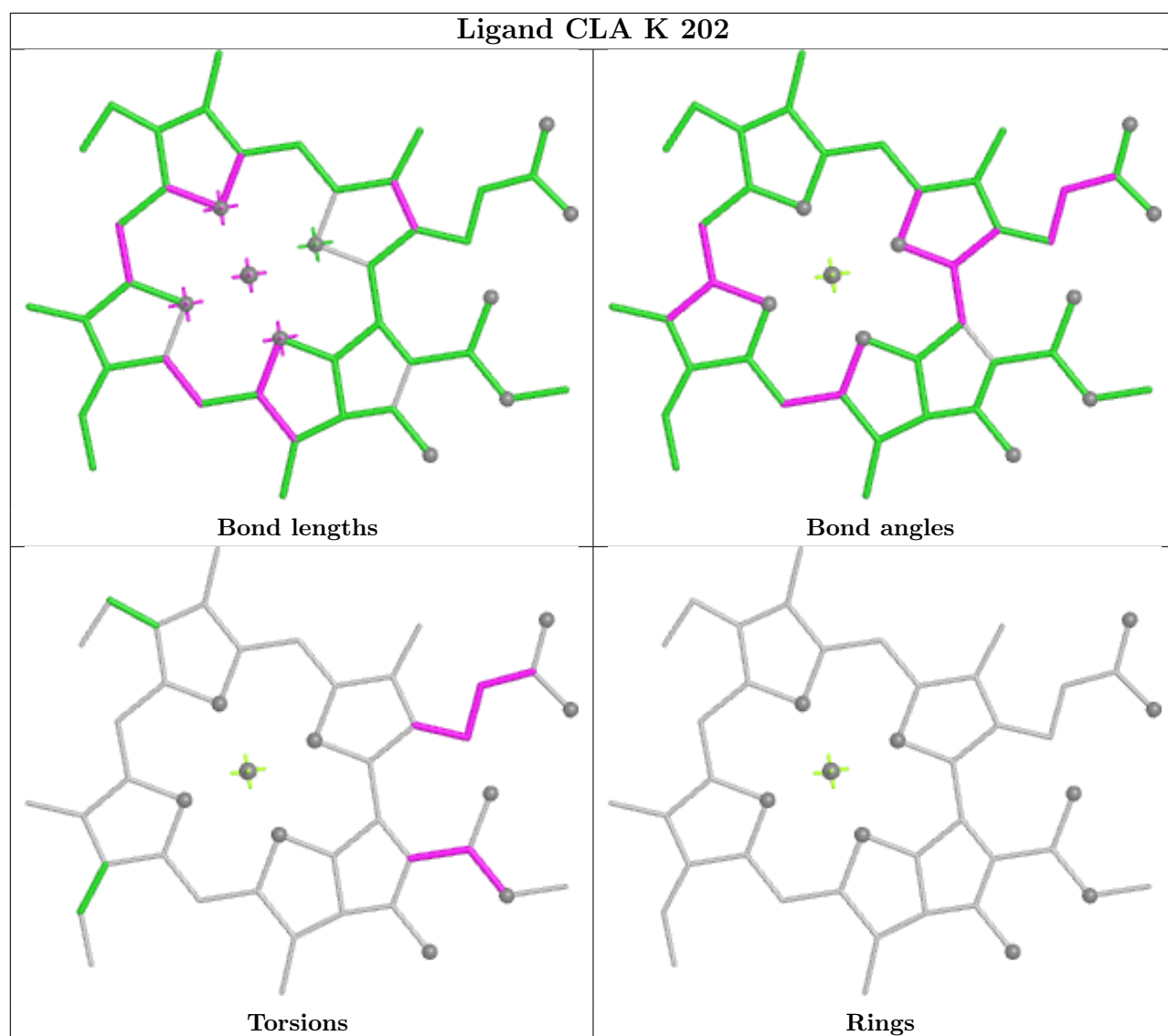
Torsions

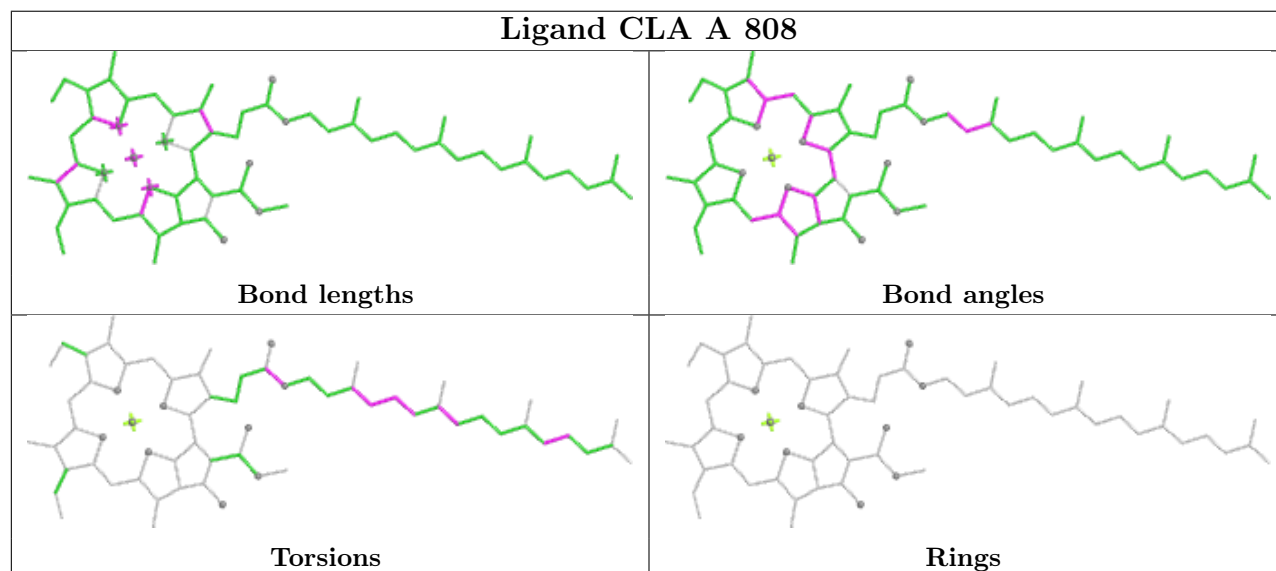
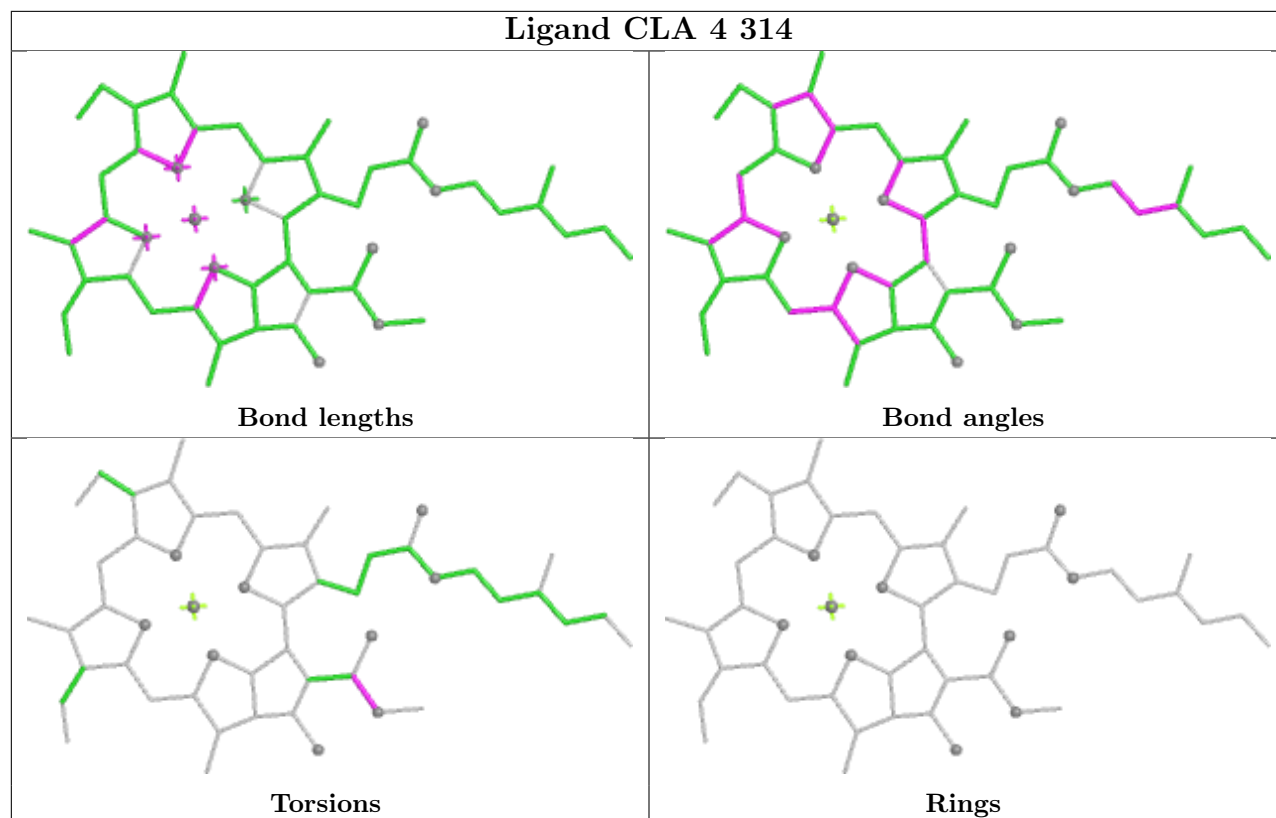


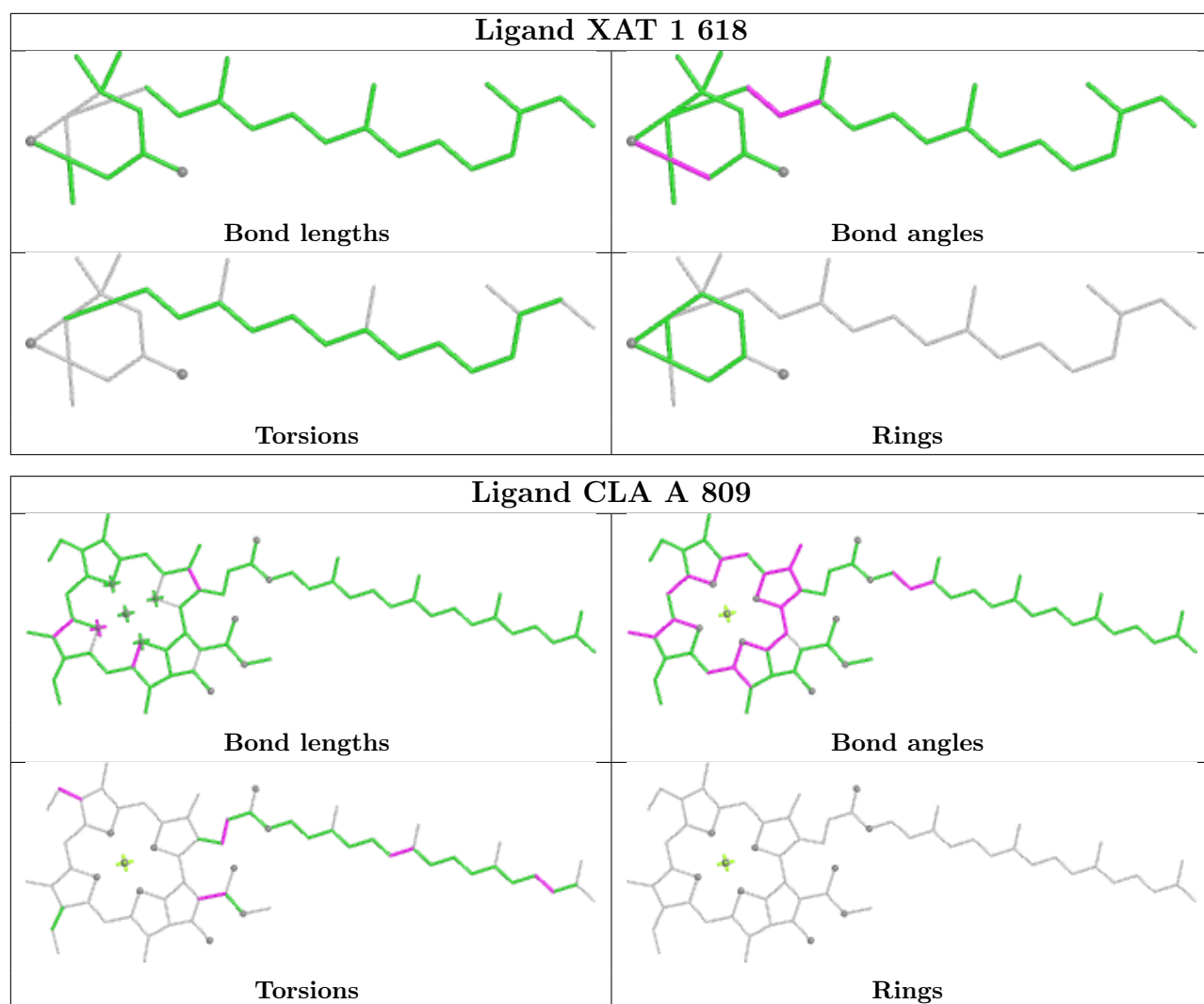
Rings

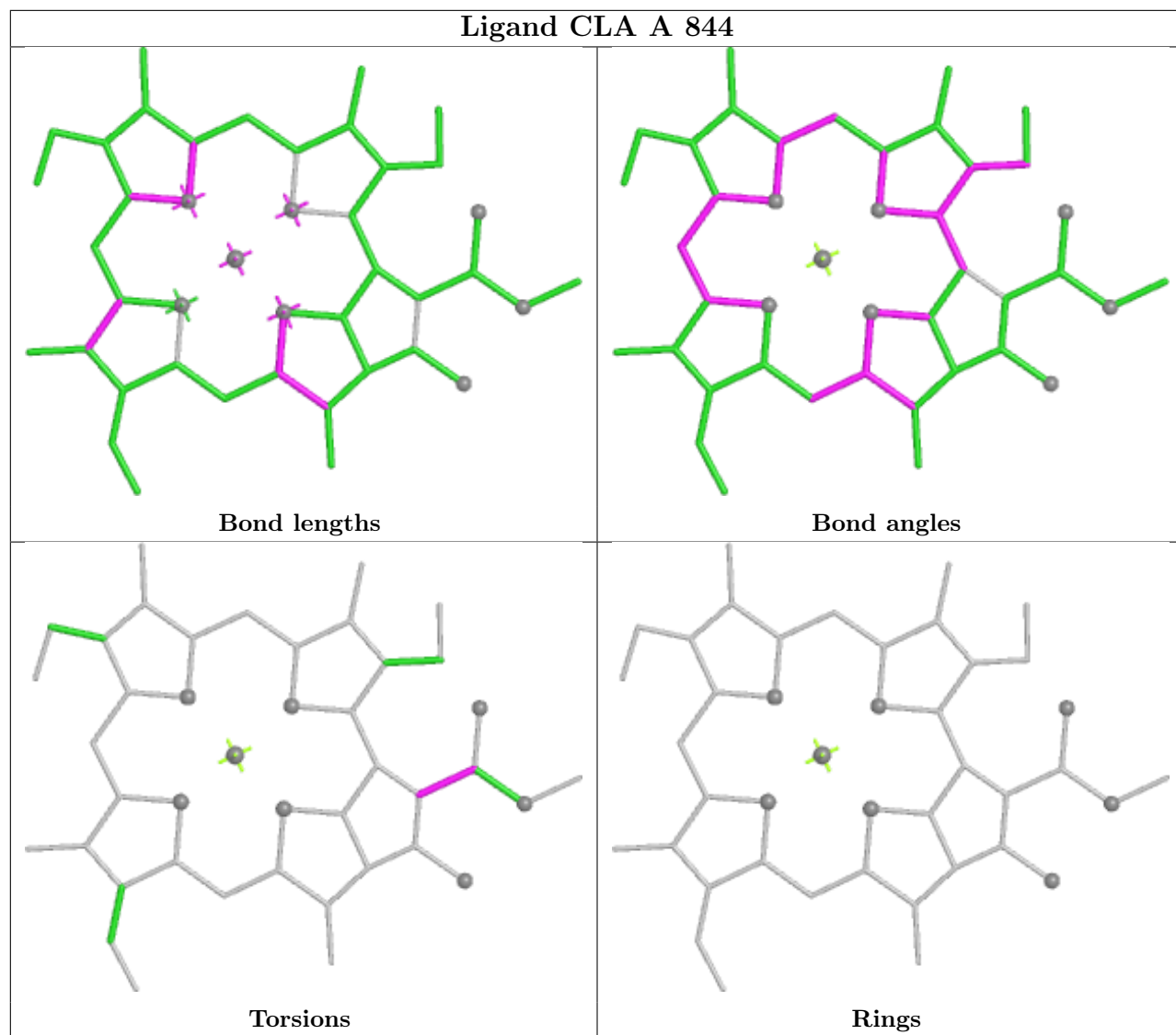


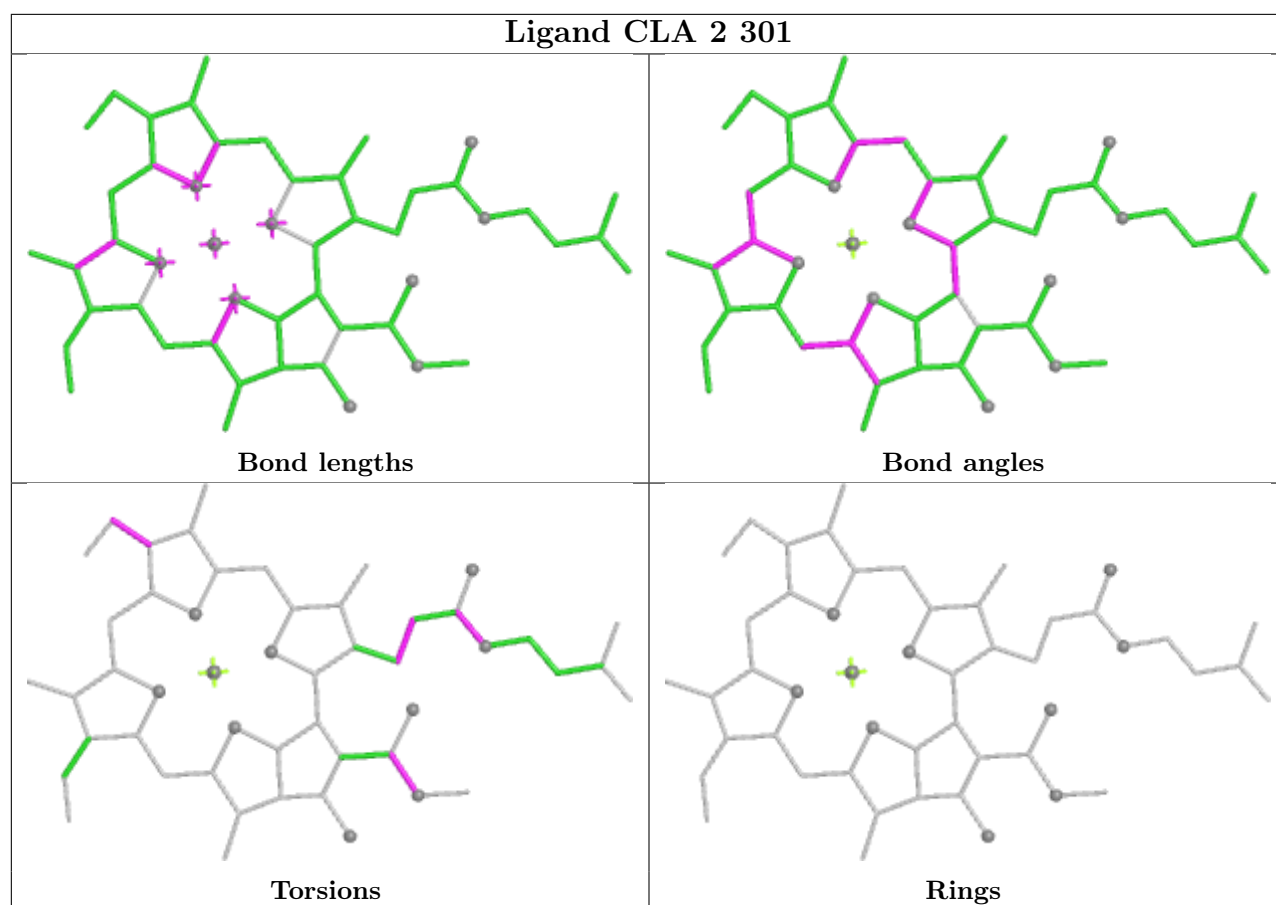












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

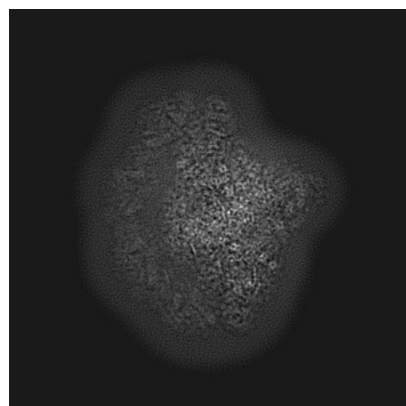
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66073. These allow visual inspection of the internal detail of the map and identification of artifacts.

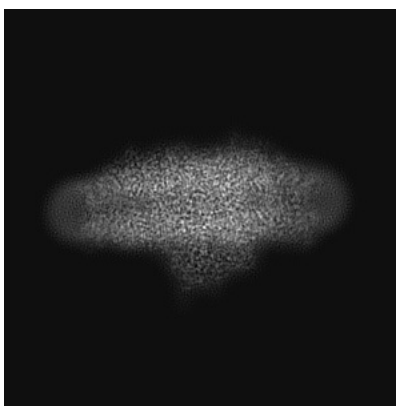
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

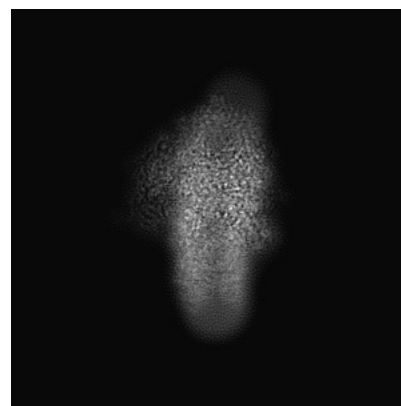
6.1.1 Primary map



X

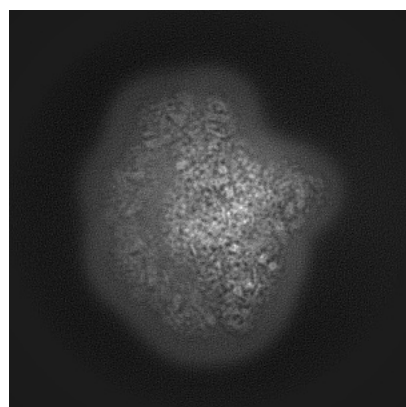


Y

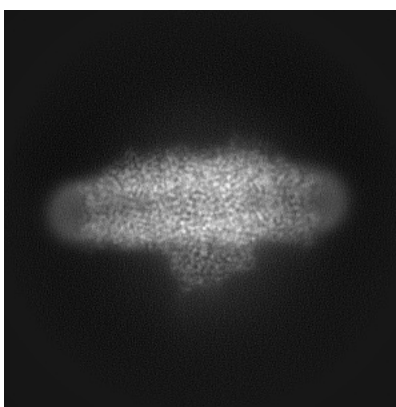


Z

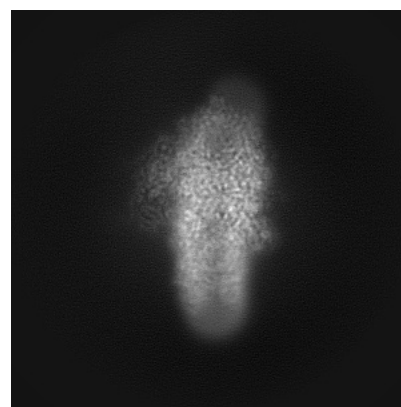
6.1.2 Raw map



X



Y

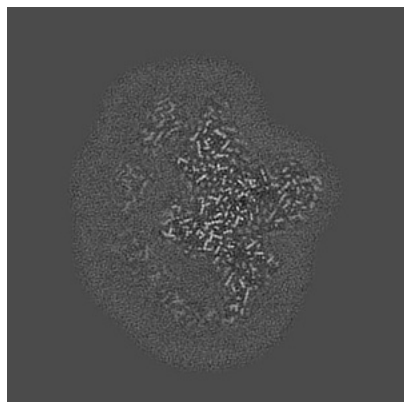


Z

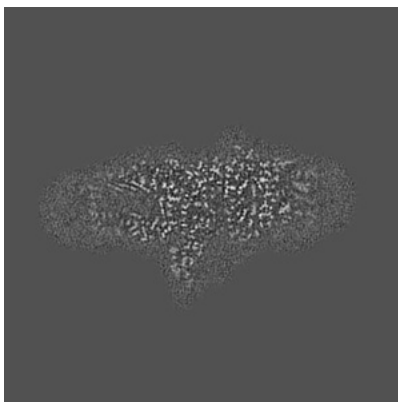
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

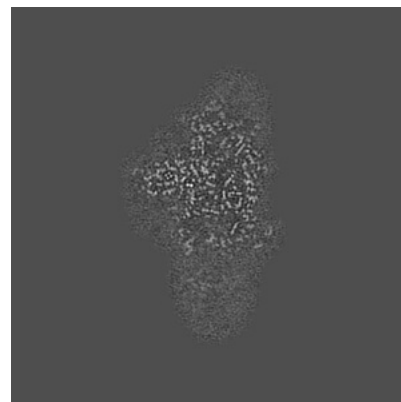
6.2.1 Primary map



X Index: 196

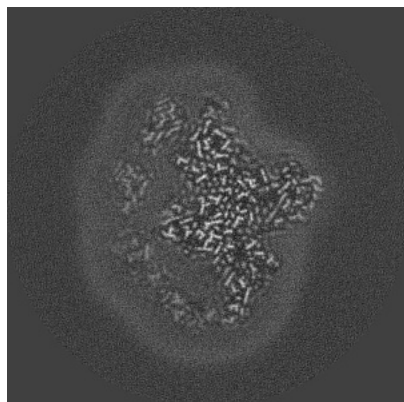


Y Index: 196

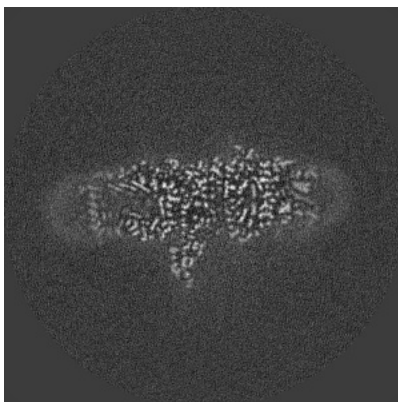


Z Index: 196

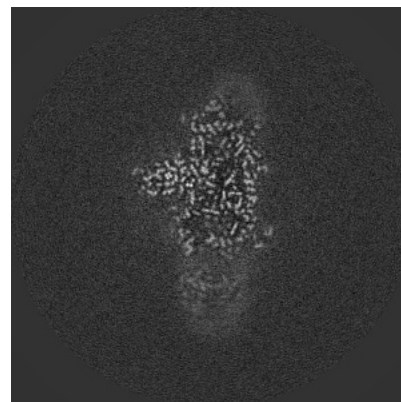
6.2.2 Raw map



X Index: 196



Y Index: 196

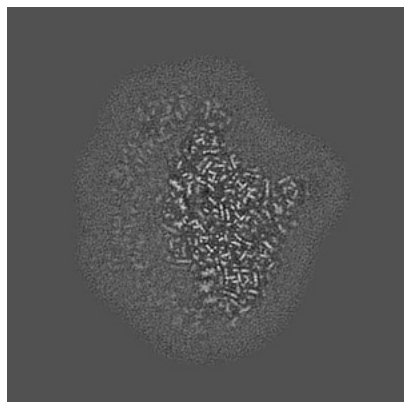


Z Index: 196

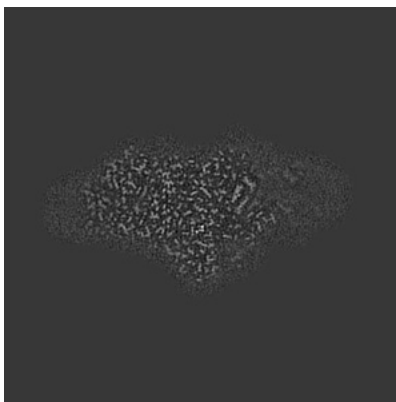
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

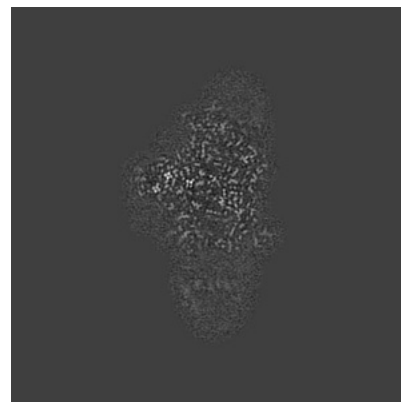
6.3.1 Primary map



X Index: 217

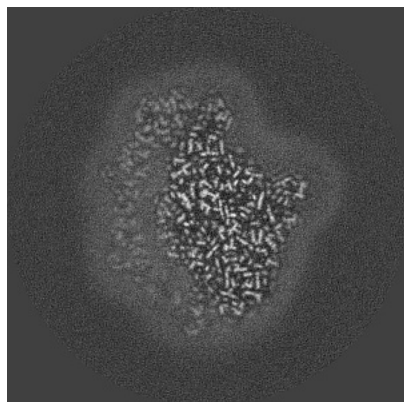


Y Index: 220

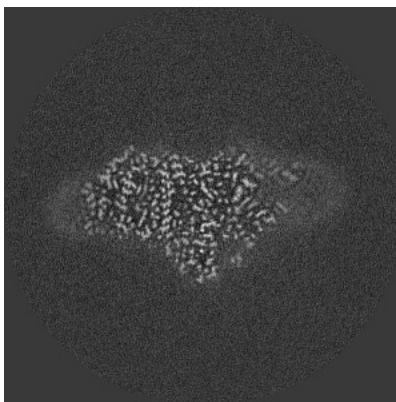


Z Index: 194

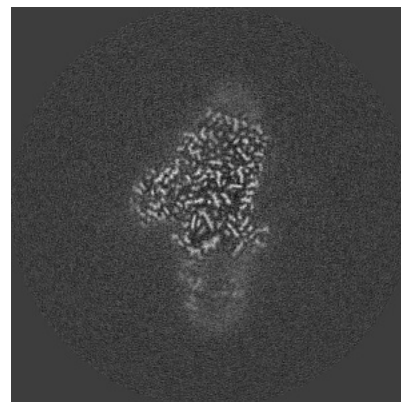
6.3.2 Raw map



X Index: 220



Y Index: 221

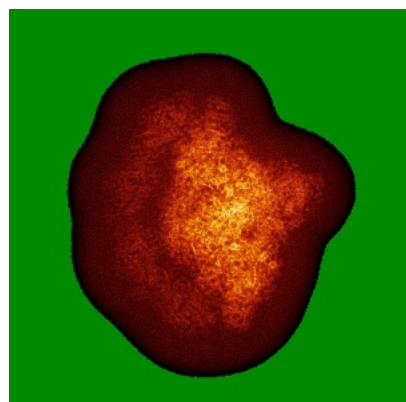


Z Index: 183

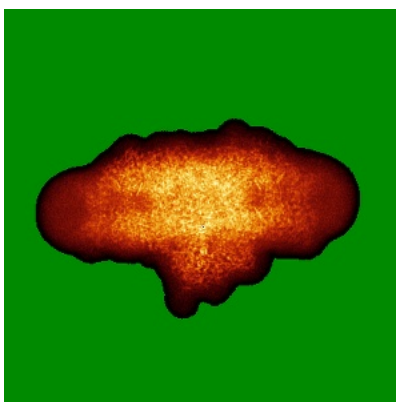
The images above show the largest variance slices of the map in three orthogonal directions.

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

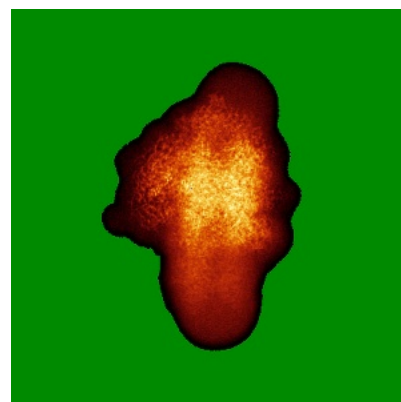
6.4.1 Primary map



X

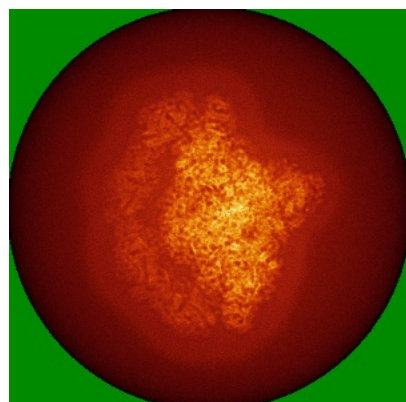


Y

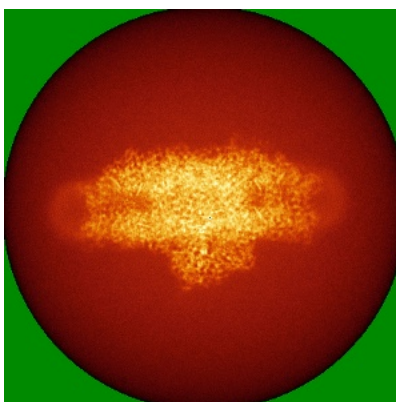


Z

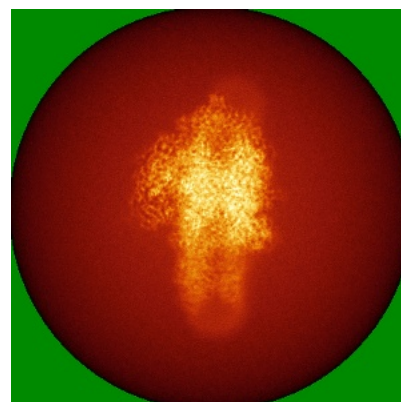
6.4.2 Raw map



X



Y

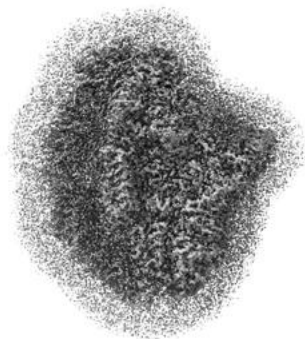


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00994. 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



X



Y



Z

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.

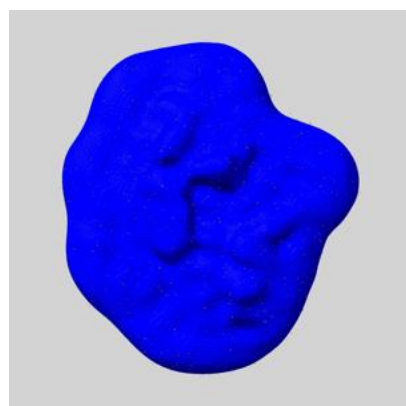
6.6 Mask visualisation [i](#)

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

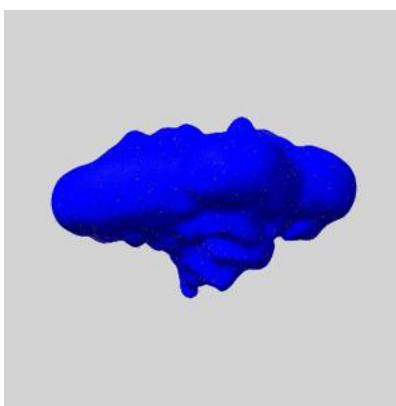
A mask typically either:

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

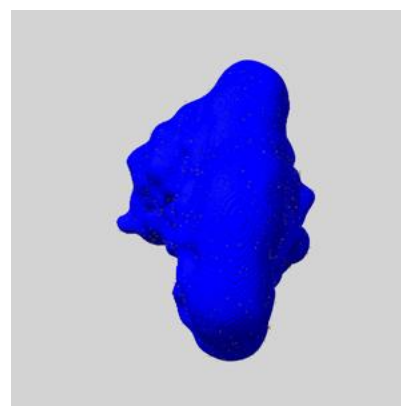
6.6.1 emd_66073_msk_1.map [i](#)



X



Y

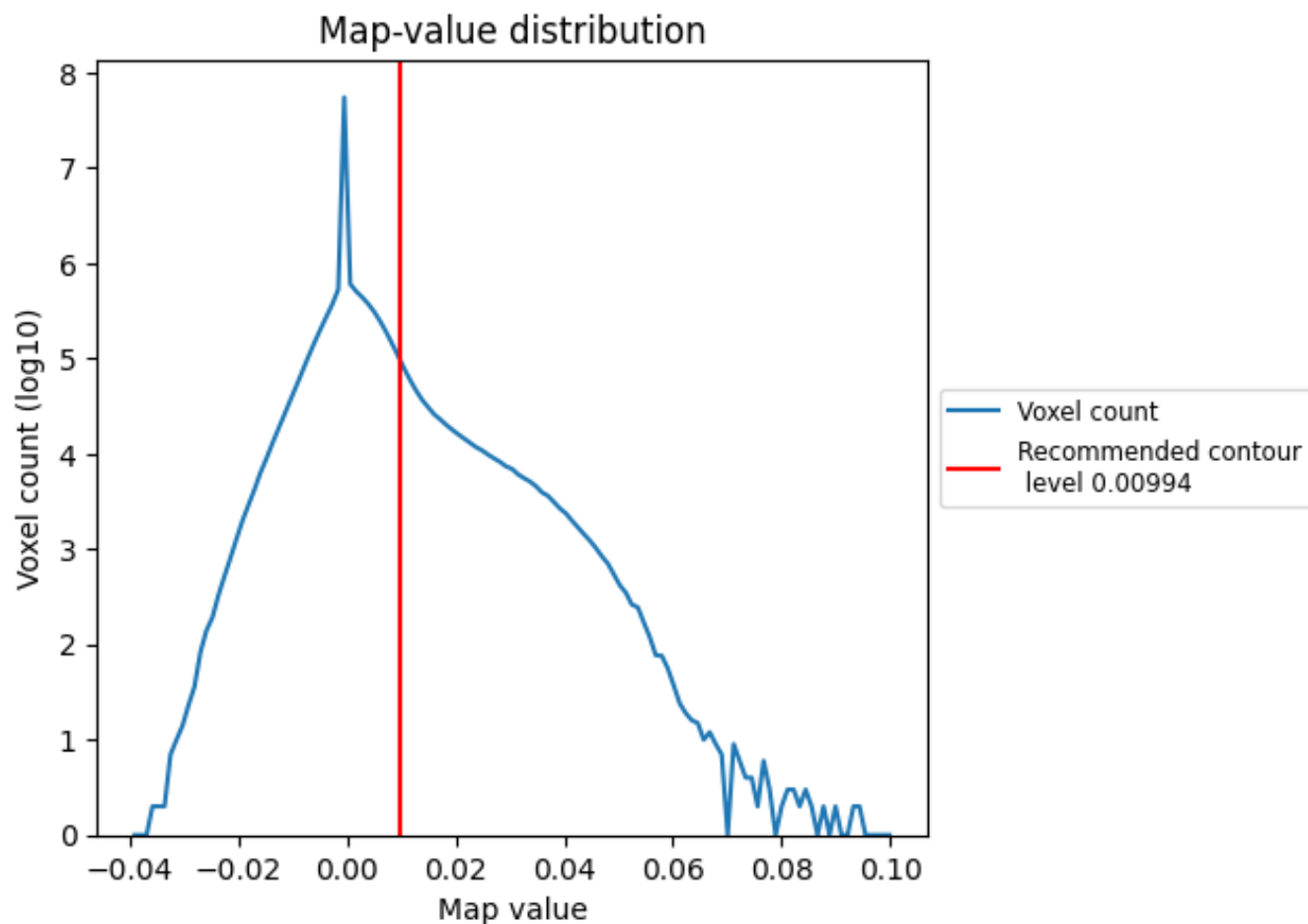


Z

7 Map analysis [i](#)

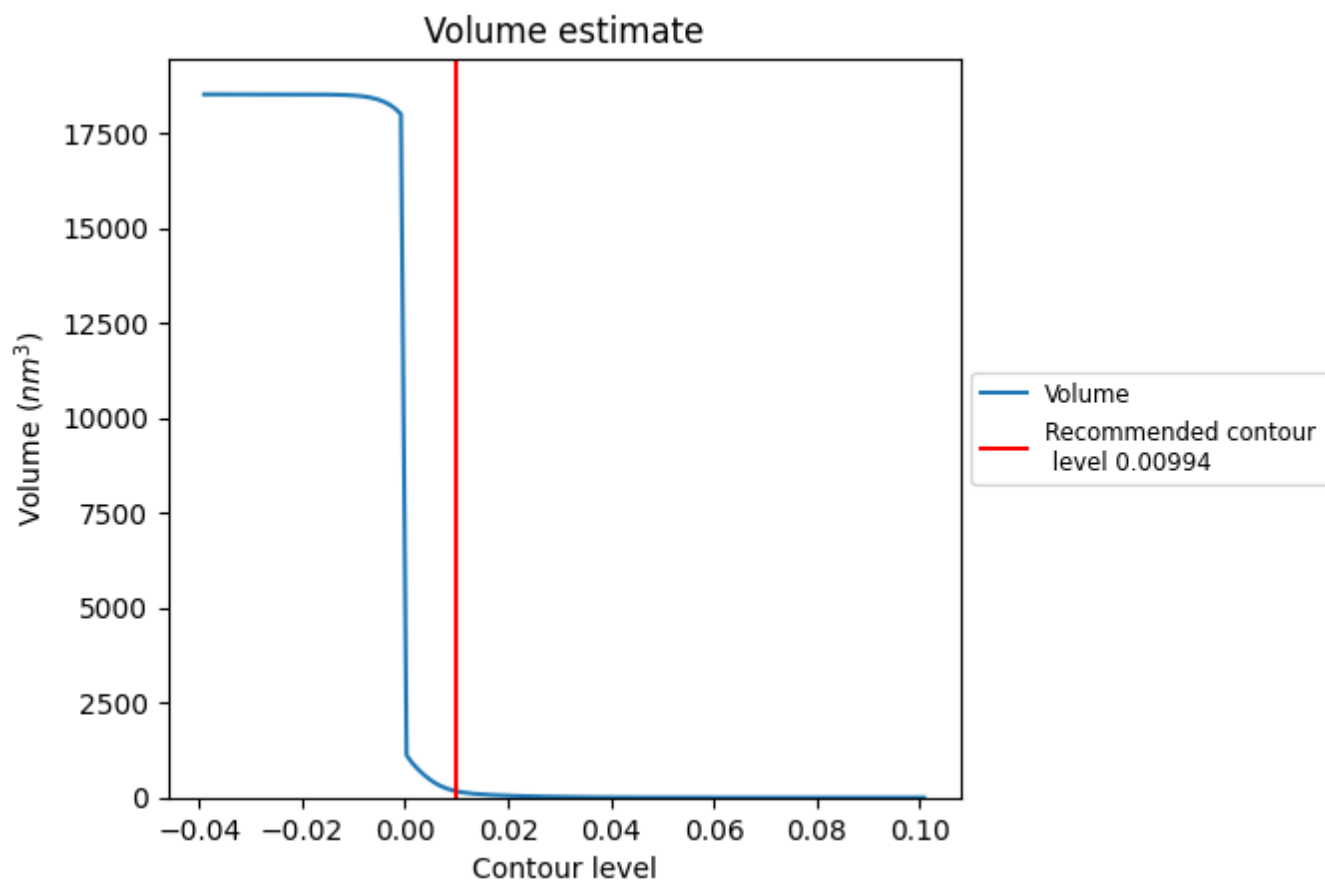
This section contains the results of statistical analysis of the map.

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.

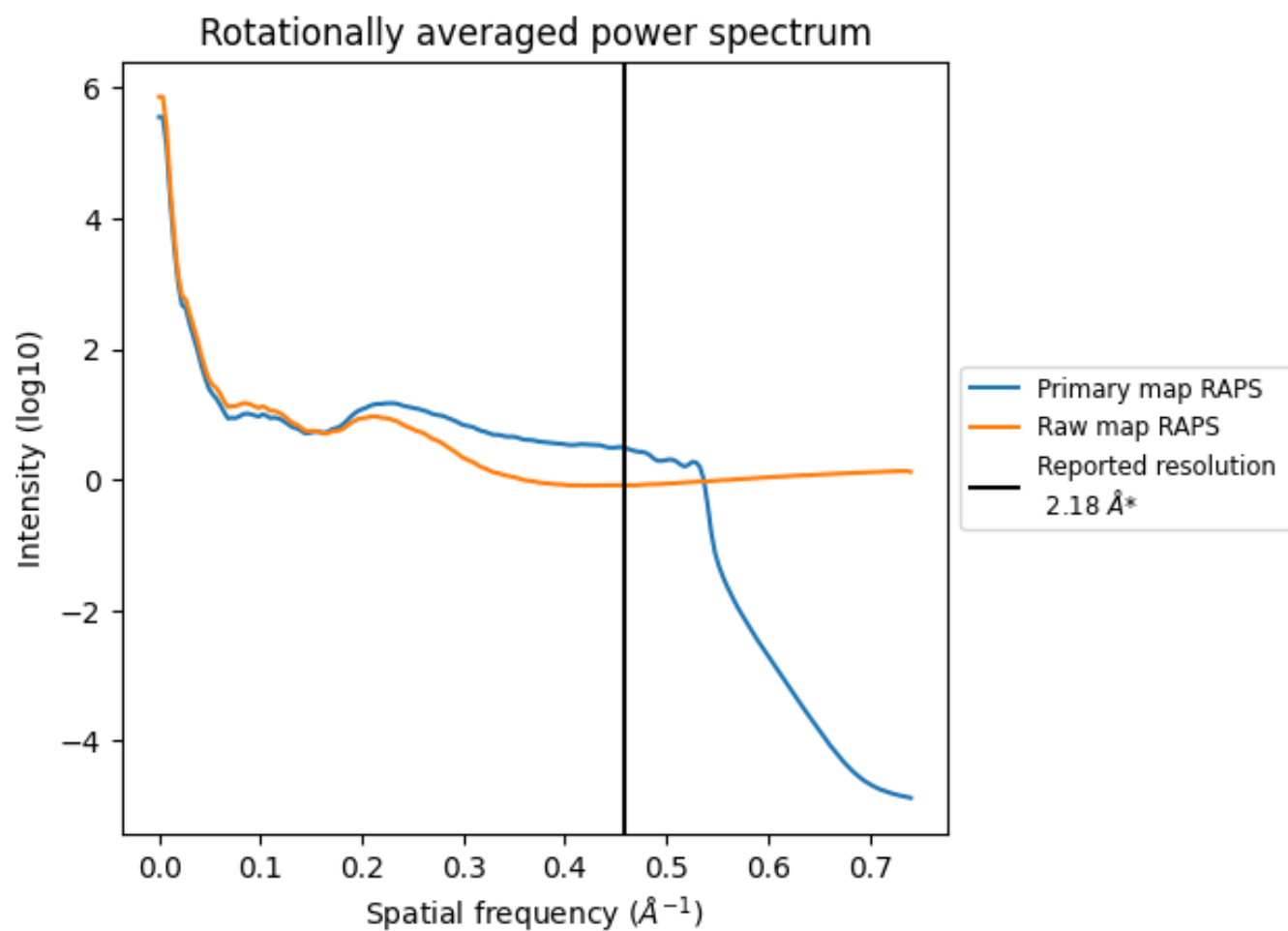
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 153 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 ⓘ

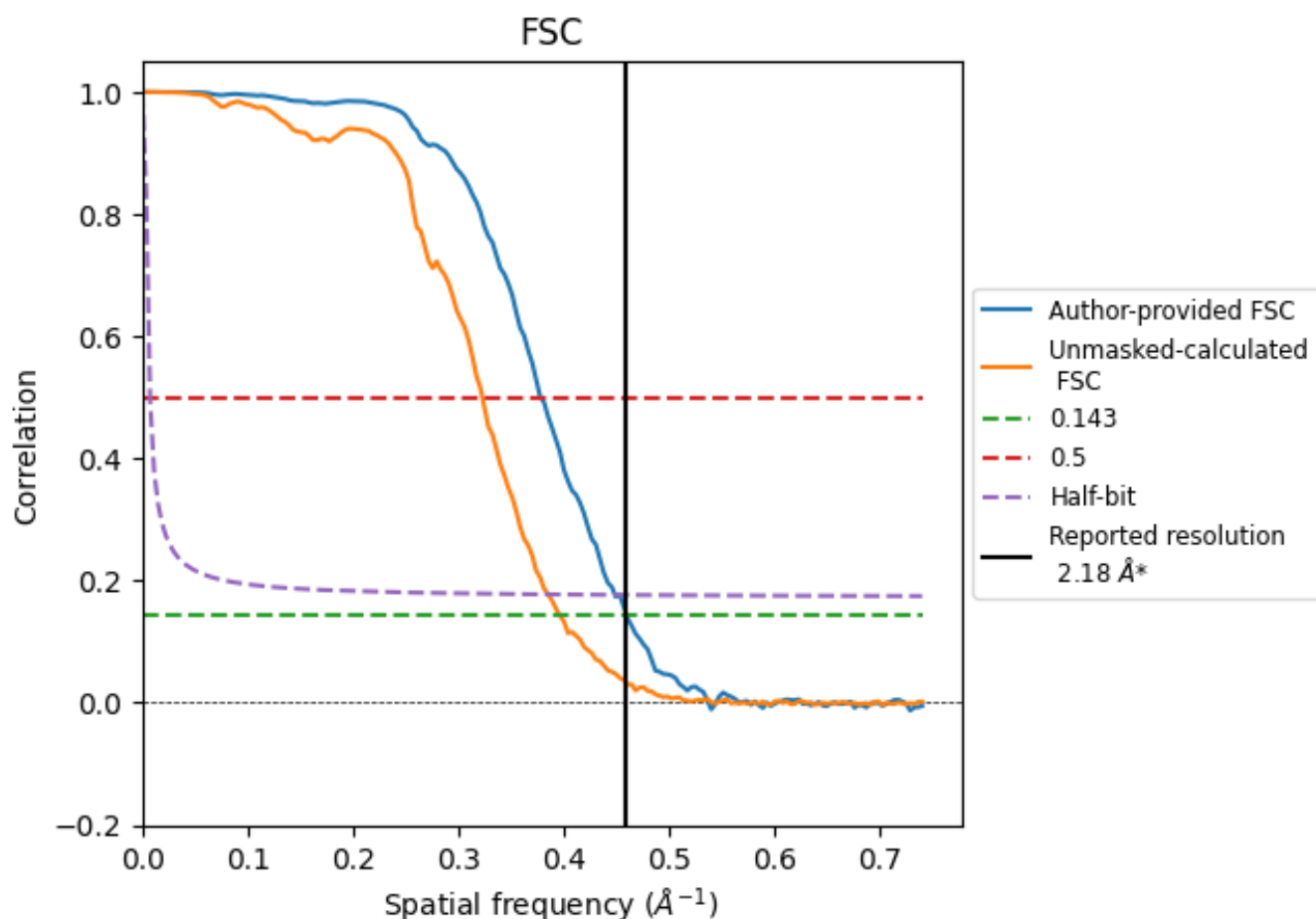


*Reported resolution corresponds to spatial frequency of 0.459 Å⁻¹

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 0.459 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

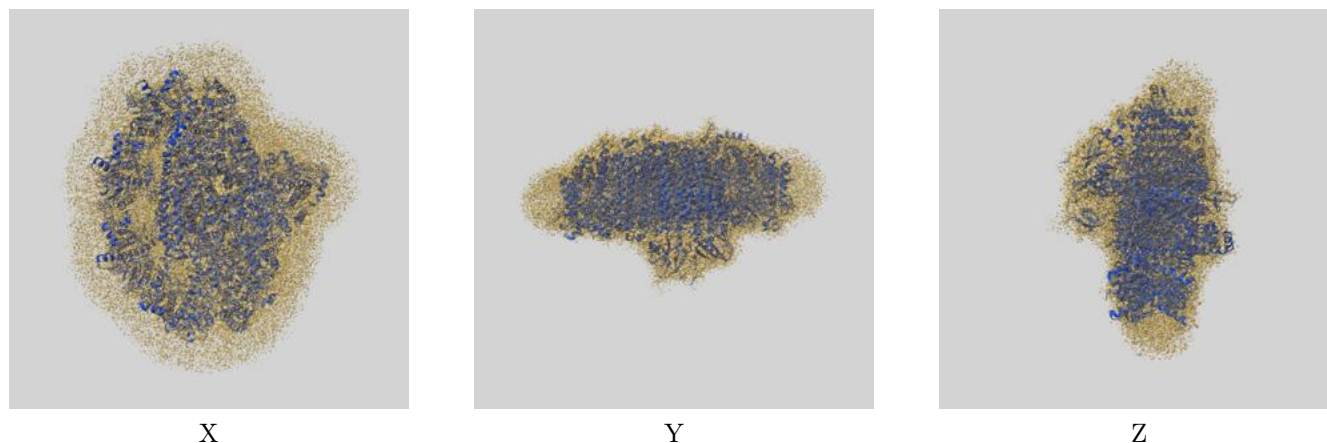
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.17	2.64	2.23
Unmasked-calculated*	2.52	3.10	2.59

*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 2.52 differs from the reported value 2.18 by more than 10 %

9 Map-model fit [i](#)

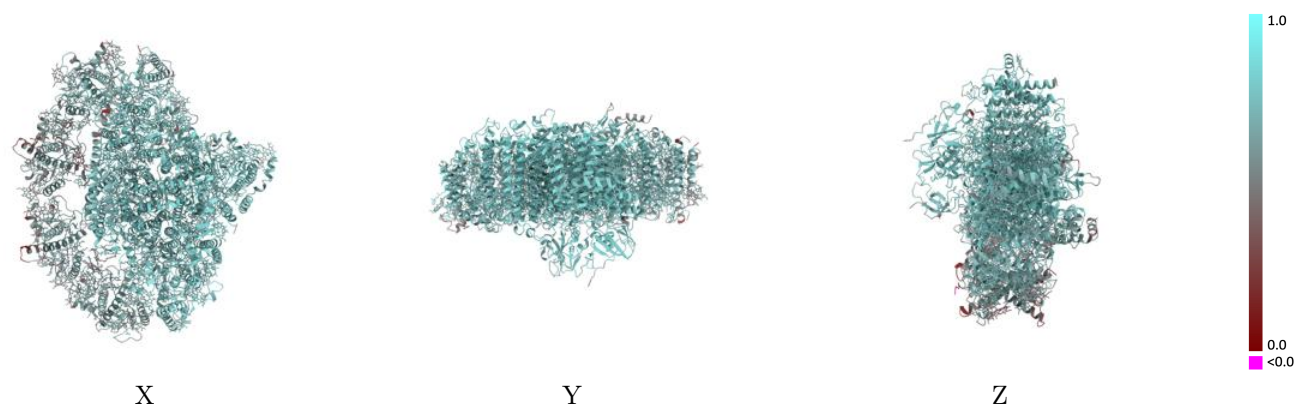
This section contains information regarding the fit between EMDB map EMD-66073 and PDB model 9WLS. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



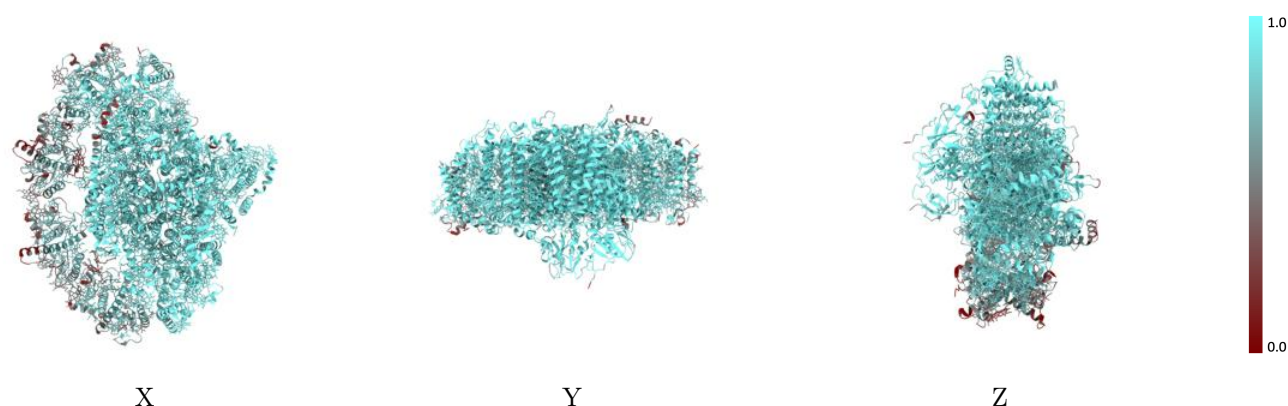
The images above show the 3D surface view of the map at the recommended contour level 0.00994 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



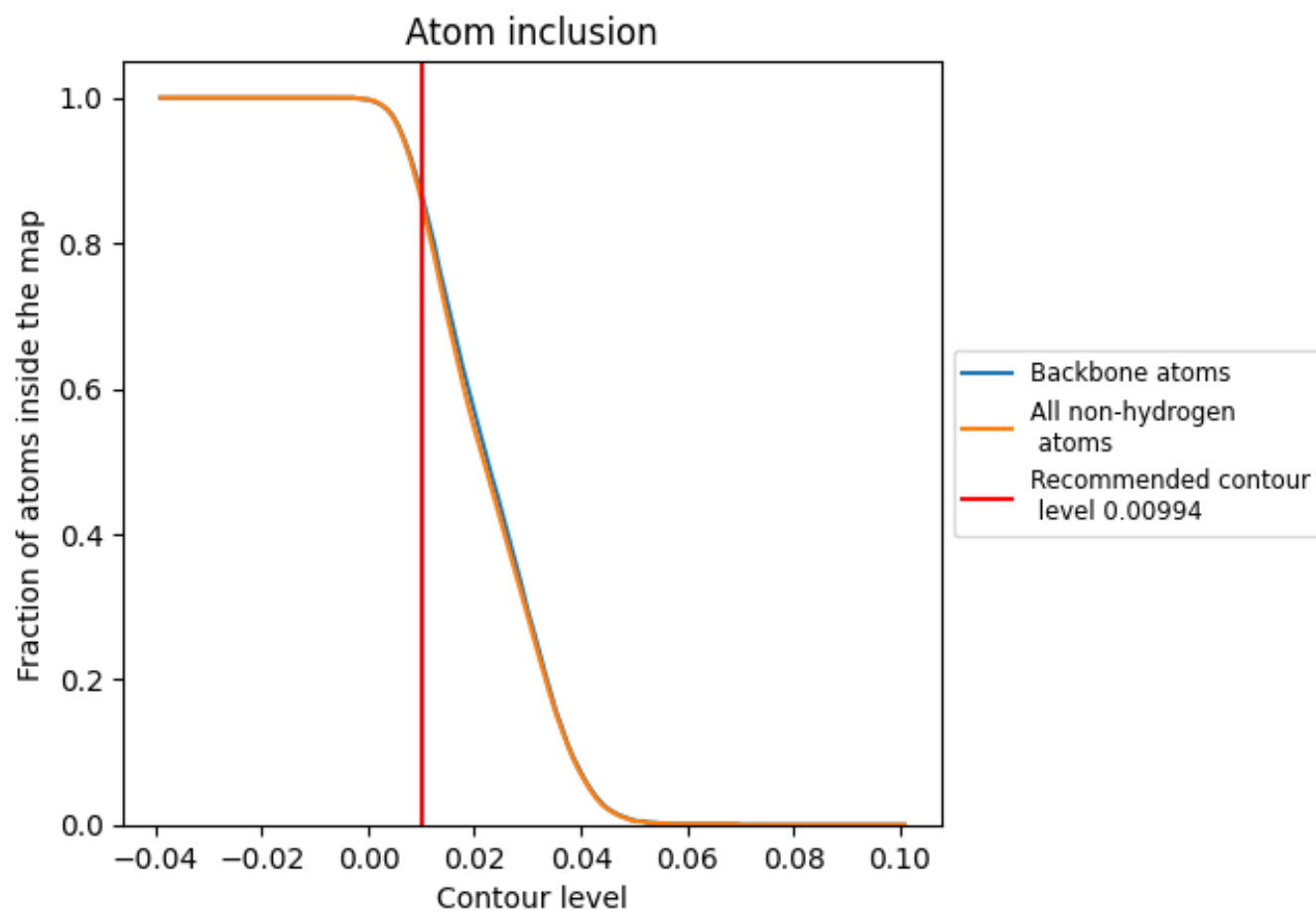
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00994).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.00994) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.7030
1	0.6550	0.5890
2	0.5750	0.5450
3	0.7660	0.6300
4	0.6500	0.5830
A	0.9600	0.7640
B	0.9750	0.7760
C	0.9890	0.7860
D	0.9340	0.7360
E	0.8860	0.7000
F	0.9000	0.7110
G	0.8870	0.6960
H	0.8800	0.6930
I	0.9390	0.7420
J	0.9080	0.7040
K	0.7440	0.6090
L	0.9300	0.7300
N	0.4520	0.5040

1.0

0.0

<0.0