



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 8WGH / pdb_00008wgh
EMDB ID : EMD-37513
Title : Cryo-EM structure of the red-shifted *Fittonia albivenis* PSI-LHCI
Authors : Huang, G.Q.; Li, X.X.; Sui, S.F.; Qin, X.C.
Deposited on : 2023-09-21
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

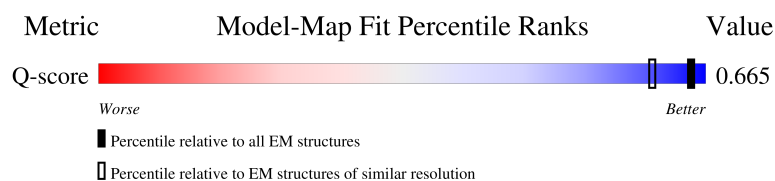
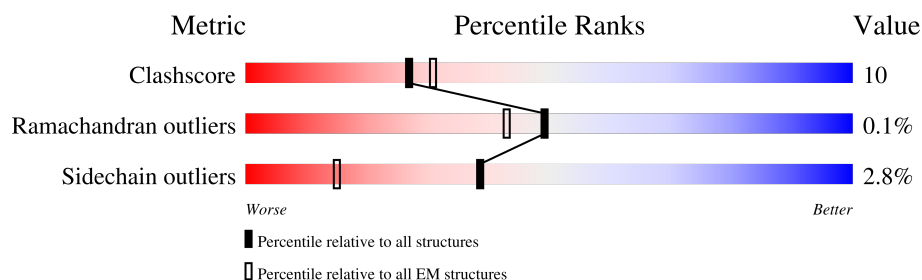
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.



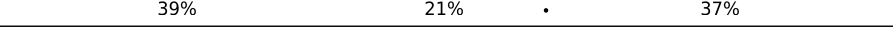
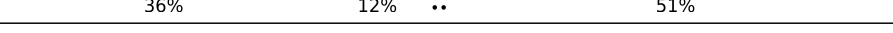
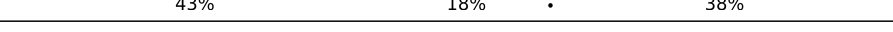
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	246	
2	2	265	
3	3	272	
4	4	248	

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	190	
9	E	151	
10	F	221	
11	G	145	
12	H	145	
13	I	36	
14	J	44	
15	K	132	
16	L	217	
17	N	173	
18	O	144	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CHL	1	301	X	-	-	-
19	CHL	1	306	X	-	-	-
19	CHL	2	301	X	-	-	-
19	CHL	2	305	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	2	307	X	-	-	-
19	CHL	2	314	X	-	-	-
19	CHL	3	306	X	-	-	-
19	CHL	4	305	X	-	-	-
19	CHL	4	306	X	-	-	-
19	CHL	4	307	X	-	-	-
19	CHL	4	315	X	-	-	-
20	CLA	1	302	X	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	841	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	F	802	X	-	-	-
20	CLA	F	804	X	-	-	-
20	CLA	F	805	X	-	-	-
20	CLA	G	603	X	-	-	-
20	CLA	G	604	X	-	-	-
20	CLA	G	605	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	205	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	303	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	307	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	N	203	X	-	-	-
20	CLA	O	201	X	-	-	-
20	CLA	O	202	X	-	-	-
20	CLA	O	203	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 38187 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	199	Total	C	N	O	S	0	0
			1559	1016	261	278	4		

- Molecule 2 is a protein called Chlorophyll a-b binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	209	Total	C	N	O	S	0	0
			1626	1068	264	289	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1727	1139	277	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1568	1027	253	283	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5831	3820	989	1003	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	VAL	conflict	UNP A0A8A0WPY6

- 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
			5854	3843	996	1002	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1116	714	193	206	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			511	324	92	95		

- 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
			1216	793	208	212	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	98	Total	C	N	O	0	0
			768	498	126	144		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	90	Total	C	N	O	0	0
			681	444	109	128		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	29	Total	C	N	O	S	0	0
			221	151	35	34	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O	S	0	0
			318	215	49	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	83	Total	C	N	O	S	0	0
			588	378	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1225	812	195	217	1		

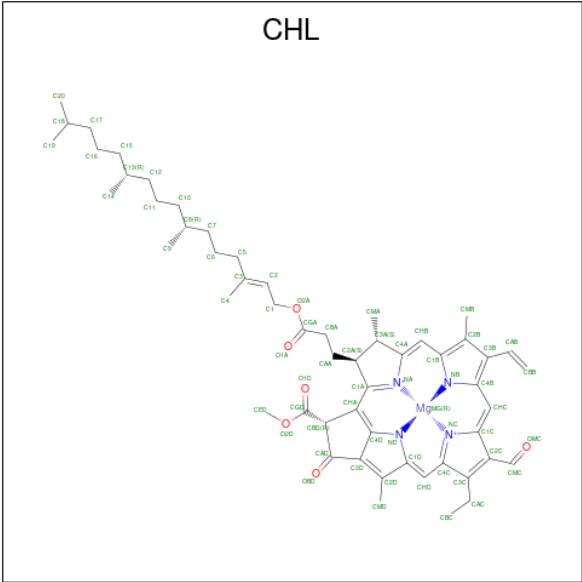
- Molecule 17 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			686	440	111	131	4		

- Molecule 18 is a protein called Photosystem I reaction center subunit O.

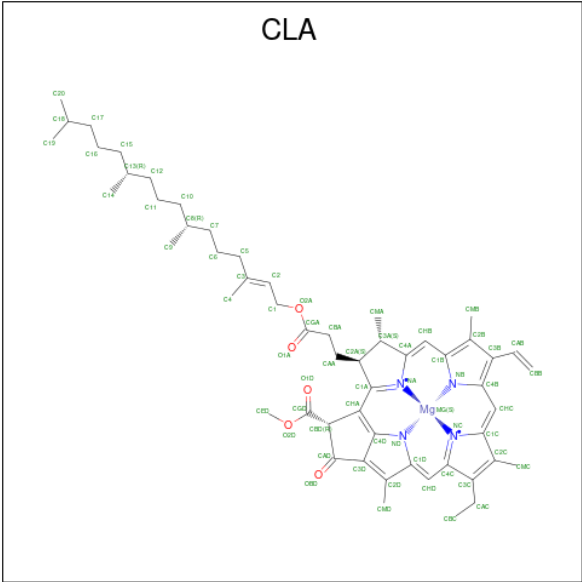
Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	89	Total	C	N	O	S	0	0
			705	475	112	117	1		

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



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
19	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	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
20	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

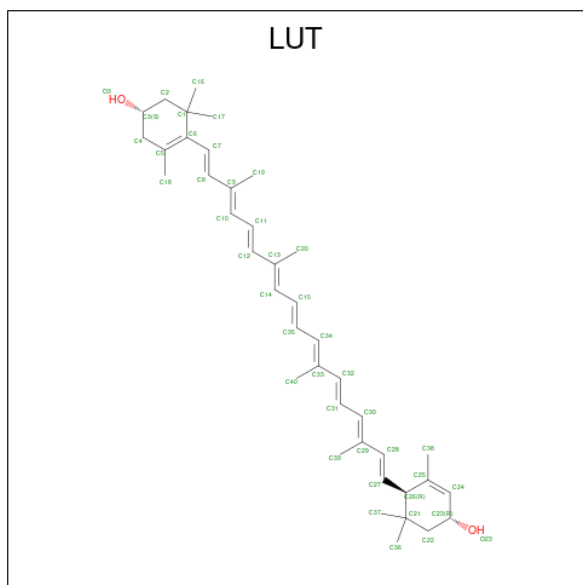
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			65	55	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
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



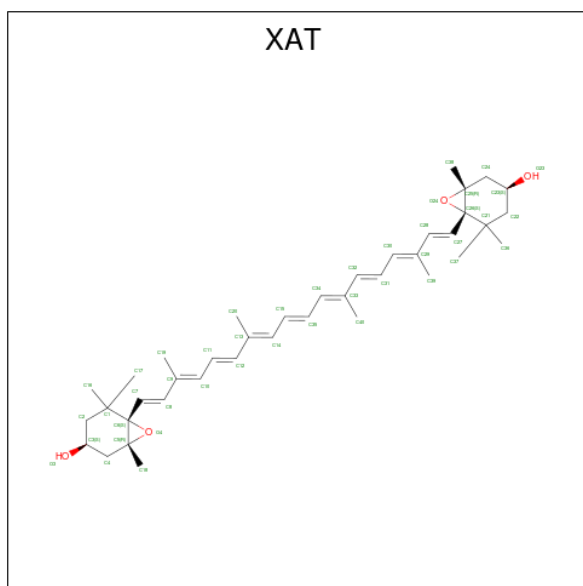
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

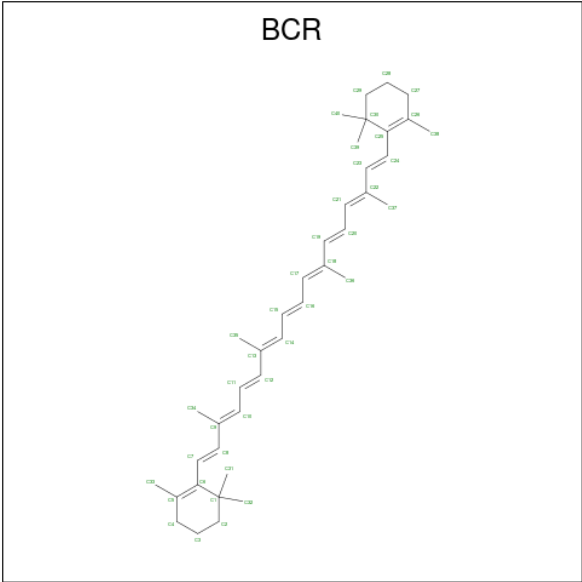
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



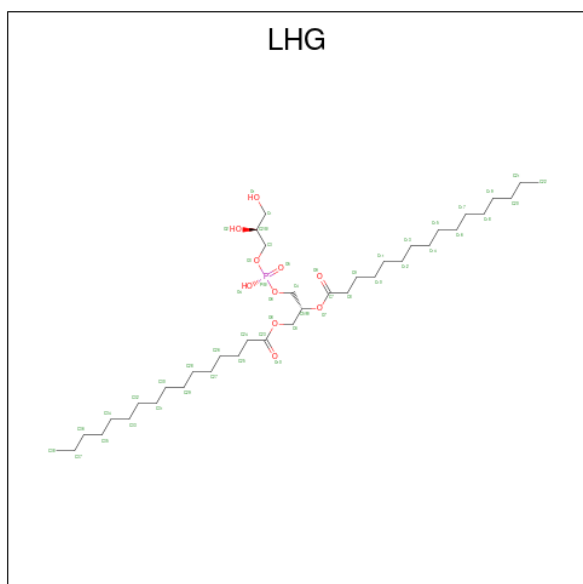
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	2	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

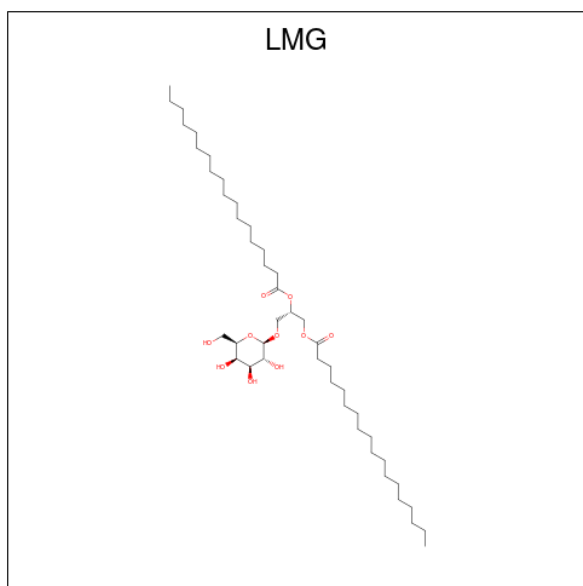
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



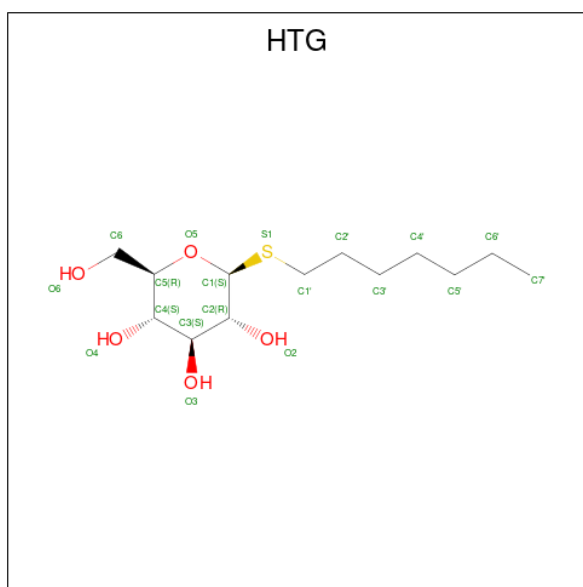
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			37	26	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



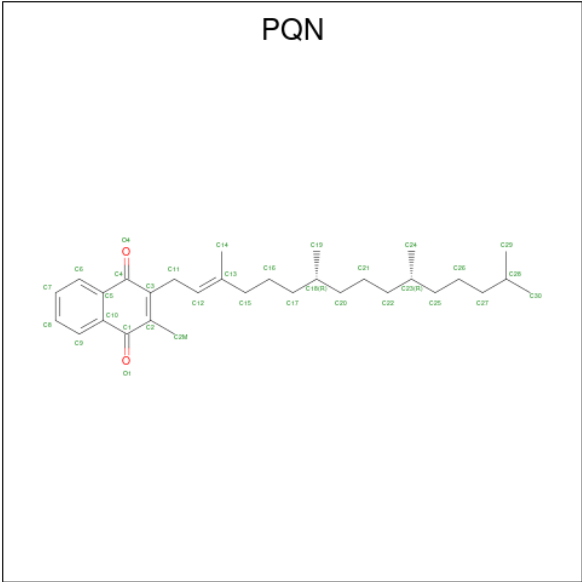
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			49	39	10	
25	1	1	Total	C	O	0
			44	34	10	
25	4	1	Total	C	O	0
			44	34	10	

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



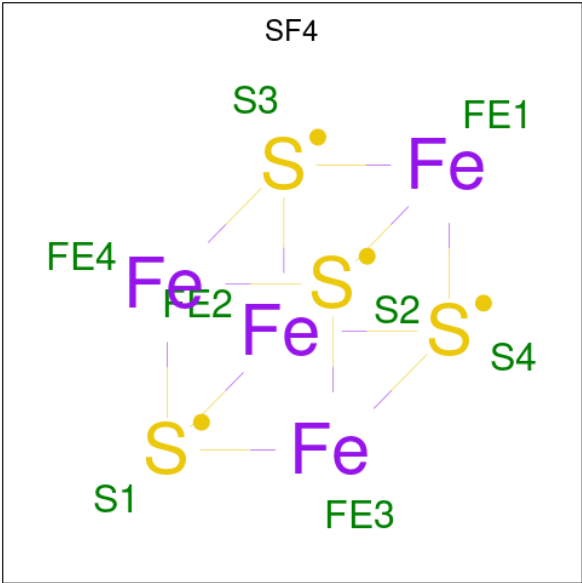
Mol	Chain	Residues	Atoms				AltConf
26	1	1	Total	C	O	S	0
			19	13	5	1	
26	4	1	Total	C	O	S	0
			19	13	5	1	
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	G	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	
26	N	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



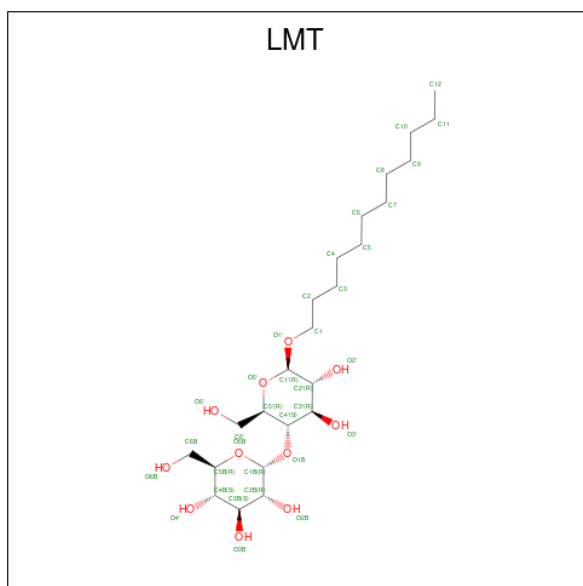
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

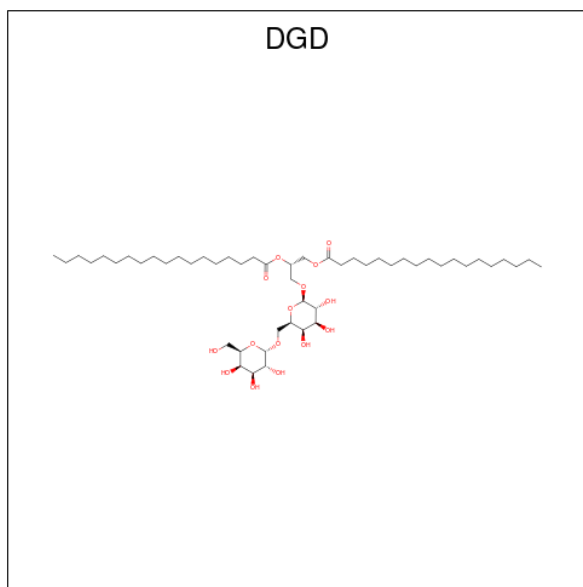
Mol	Chain	Residues	Atoms			AltConf
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			35	24	11	
29	G	1	Total	C	O	0
			35	24	11	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

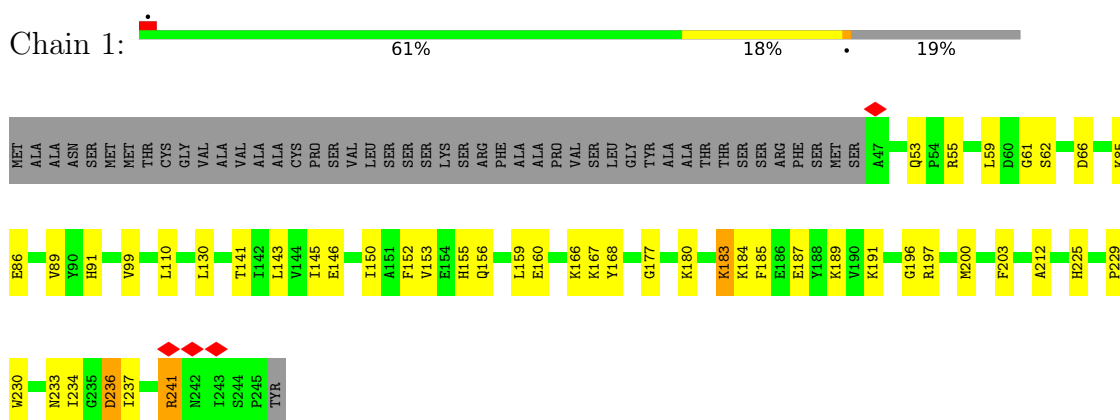


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	66	51	15	0

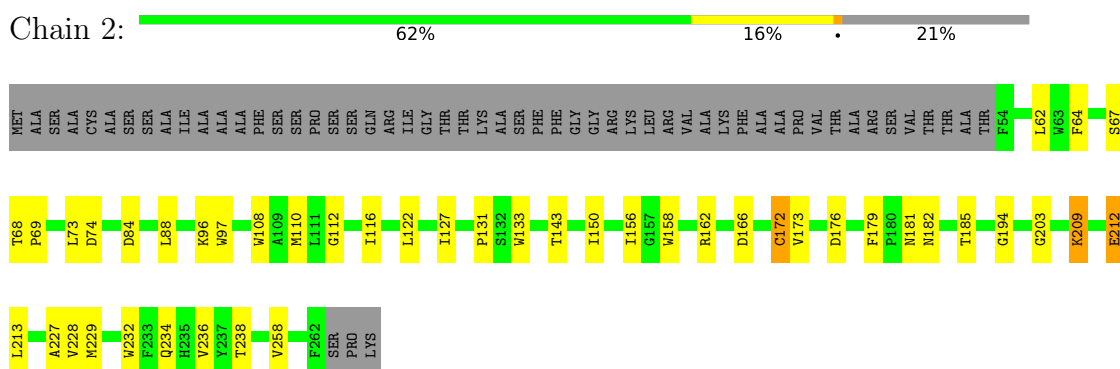
3 Residue-property plots [i](#)

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

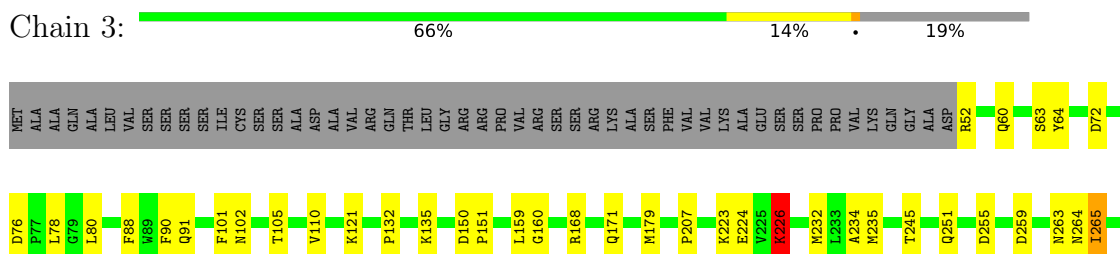
• Molecule 1: Chlorophyll a-b binding protein 1



• Molecule 2: Chlorophyll a-b binding protein 2



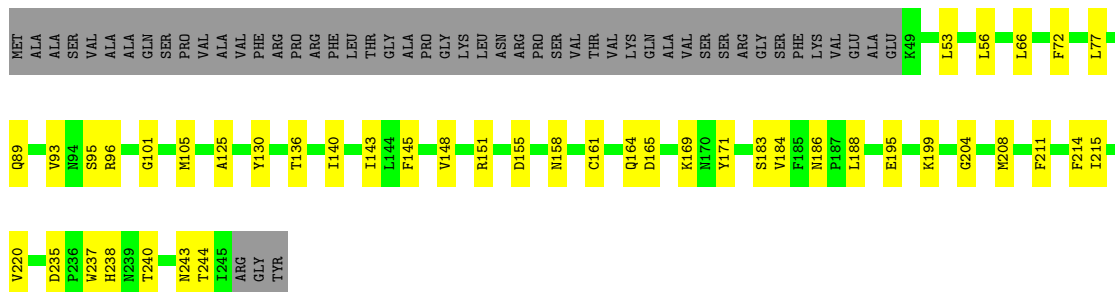
• Molecule 3: Chlorophyll a-b binding protein 3





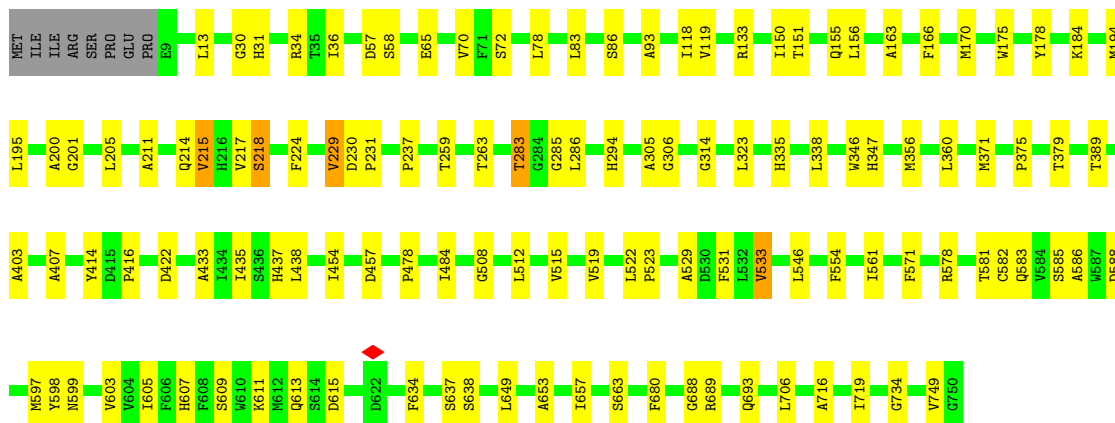
• Molecule 4: Chlorophyll a-b binding protein 4

Chain 4: 62% 18% 21%



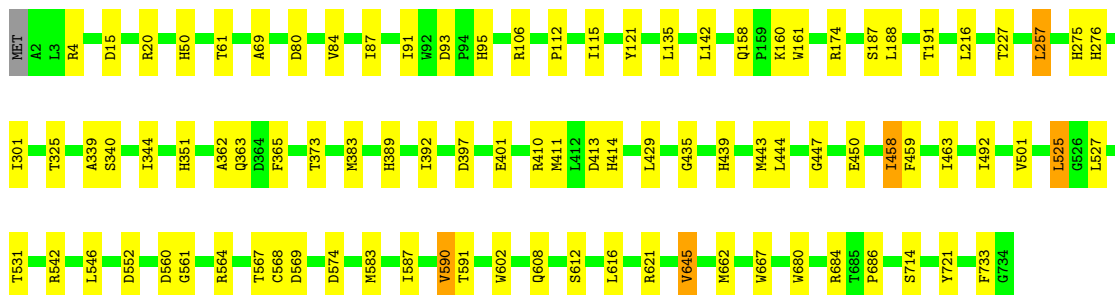
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 83% 15% ..



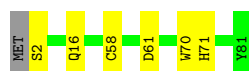
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 87% 12% .



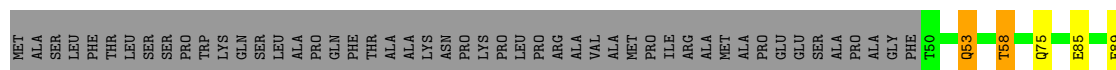
• Molecule 7: Photosystem I iron-sulfur center

Chain C: 91% 7% .



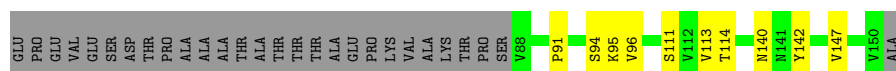
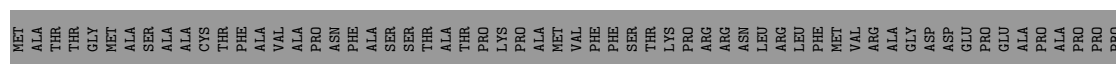
- Molecule 8: Photosystem I reaction center subunit II

Chain D: 63% 9% 26%



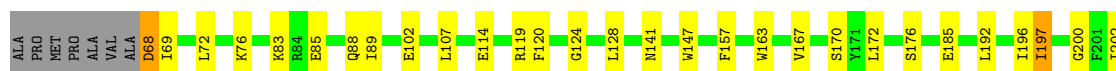
- Molecule 9: Photosystem I reaction center subunit IV

Chain E: 35% 7% 58%



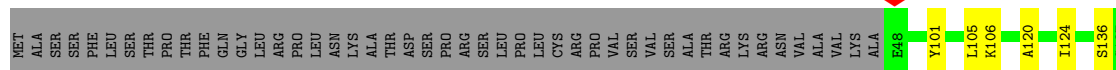
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F: 51% 17% 31%



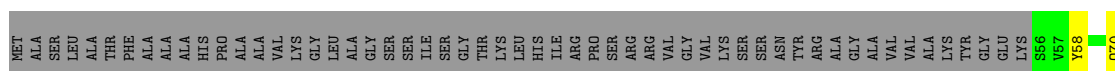
- Molecule 11: Photosystem I reaction center subunit VIII

Chain G: 61% 6% 32%



- Molecule 12: Photosystem I reaction center subunit VI

Chain H: 55% 7% 38%



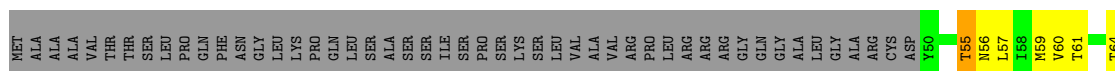
- Molecule 13: Photosystem I reaction center subunit VIII



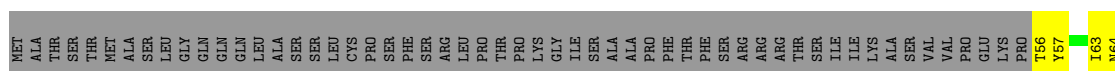
- Molecule 14: Photosystem I reaction center subunit IX



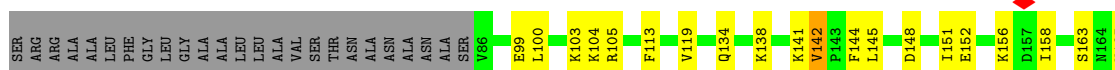
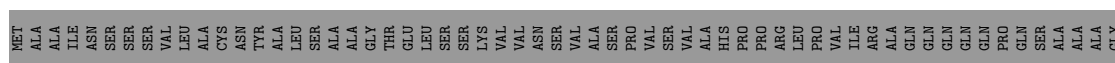
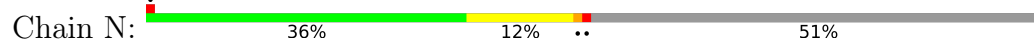
- Molecule 15: Photosystem I reaction center subunit psaK



- Molecule 16: Photosystem I reaction center subunit XI

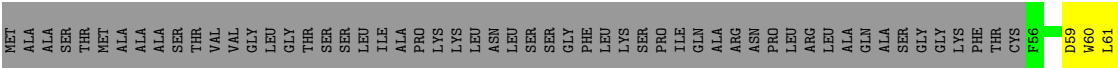


- Molecule 17: Photosystem I reaction center subunit N





• Molecule 18: Photosystem I reaction center subunit O



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.545	Depositor
Minimum map value	-2.048	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.146	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	324.75, 324.75, 324.75	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/1610	0.41	0/2195
2	2	0.34	1/1687 (0.1%)	0.50	2/2313 (0.1%)
3	3	0.27	1/1791 (0.1%)	0.46	0/2435
4	4	0.16	0/1621	0.41	0/2215
5	A	0.15	0/6029	0.37	0/8223
6	B	0.15	0/6066	0.39	0/8285
7	C	0.14	0/628	0.38	0/852
8	D	0.14	0/1143	0.40	0/1546
9	E	0.13	0/522	0.35	0/710
10	F	0.19	0/1246	0.50	0/1681
11	G	0.58	1/788 (0.1%)	0.48	0/1070
12	H	0.13	0/701	0.35	0/955
13	I	0.18	0/227	0.40	0/310
14	J	0.17	0/327	0.39	0/446
15	K	0.18	0/596	0.51	0/809
16	L	0.14	0/1263	0.36	0/1731
17	N	0.32	0/701	0.52	0/942
18	O	0.20	0/733	0.46	0/1001
All	All	0.21	3/27679 (0.0%)	0.42	2/37719 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	173	VAL	C-O	-6.69	1.16	1.24
11	G	141	ASP	C-O	-5.96	1.20	1.25
3	3	226	LYS	C-O	-5.96	1.16	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	172	CYS	N-CA-C	6.04	123.66	110.80
2	2	173	VAL	N-CA-C	5.13	120.02	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1559	0	1536	37	0
2	2	1626	0	1570	38	0
3	3	1727	0	1651	34	0
4	4	1568	0	1517	35	0
5	A	5831	0	5683	91	0
6	B	5854	0	5635	67	0
7	C	615	0	600	4	0
8	D	1116	0	1122	15	0
9	E	511	0	510	6	0
10	F	1216	0	1245	36	0
11	G	768	0	740	7	0
12	H	681	0	671	8	0
13	I	221	0	237	4	0
14	J	318	0	331	9	0
15	K	588	0	619	23	0
16	L	1225	0	1240	15	0
17	N	686	0	664	18	0
18	O	705	0	686	20	0
19	1	100	0	72	4	0
19	2	238	0	169	23	0
19	3	47	0	30	3	0
19	4	198	0	143	12	0
20	1	744	0	720	26	0
20	2	485	0	445	16	0
20	3	633	0	499	22	0
20	4	593	0	524	28	0
20	A	2610	0	2708	118	0
20	B	2361	0	2424	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	156	0	138	7	0
20	G	141	0	105	0	0
20	H	56	0	51	3	0
20	J	107	0	103	2	0
20	K	197	0	158	9	0
20	L	206	0	177	7	0
20	N	95	0	69	2	0
20	O	157	0	135	14	0
21	1	84	0	112	8	0
21	2	42	0	56	2	0
21	3	42	0	56	4	0
21	4	42	0	56	5	0
21	O	84	0	112	8	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	4	0
22	4	44	0	56	7	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	3	0
23	4	40	0	56	5	0
23	A	240	0	336	18	0
23	B	240	0	336	23	0
23	F	80	0	112	7	0
23	G	40	0	56	3	0
23	I	40	0	56	6	0
23	J	80	0	112	10	0
23	K	40	0	56	4	0
23	L	120	0	168	9	0
24	1	49	0	74	7	0
24	2	37	0	44	1	0
24	A	76	0	98	3	0
24	B	23	0	16	2	0
25	1	93	0	132	5	0
25	4	44	0	61	3	0
26	1	19	0	26	2	0
26	4	19	0	26	0	0
26	A	19	0	26	0	0
26	B	38	0	52	1	0
26	F	38	0	52	1	0
26	G	19	0	26	0	0
26	J	19	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	19	0	26	1	0
27	A	33	0	46	3	0
27	B	33	0	46	1	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	B	35	0	46	0	0
29	G	35	0	46	0	0
30	B	66	0	96	2	0
All	All	38187	0	37964	751	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 10.

All (751) 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)
10:F:217:ILE:HG13	20:F:802:CLA:O1A	1.45	1.16
20:1:309:CLA:HAB	21:1:315:LUT:H32	1.42	0.98
3:3:235:MET:HE2	22:3:316:XAT:H10	1.46	0.95
20:3:309:CLA:HBC2	20:3:309:CLA:HHD	1.50	0.93
20:B:831:CLA:HBB1	23:F:801:BCR:HC8	1.53	0.91
20:O:202:CLA:HHC	20:O:202:CLA:HBB1	1.53	0.90
1:1:156:GLN:HA	1:1:159:LEU:HD12	1.53	0.89
19:4:305:CHL:O1A	23:4:318:BCR:H21C	1.75	0.87
20:3:308:CLA:HAB	21:3:315:LUT:H32	1.58	0.86
3:3:105:THR:HG22	19:3:306:CHL:CED	2.10	0.81
10:F:217:ILE:CG1	20:F:802:CLA:O1A	2.27	0.81
20:3:309:CLA:HBC2	20:3:309:CLA:CHD	2.08	0.79
20:B:831:CLA:HAB	20:B:832:CLA:HMB2	1.66	0.77
20:1:303:CLA:HHC	20:1:303:CLA:HBB1	1.67	0.76
20:O:202:CLA:HBC3	20:O:202:CLA:HHD	1.68	0.75
20:4:309:CLA:HAB	21:4:316:LUT:H32	1.68	0.75
23:A:849:BCR:H362	20:A:851:CLA:H42	1.70	0.73
6:B:106:ARG:HH11	6:B:115:ILE:HG12	1.54	0.72
20:B:827:CLA:HHC	20:B:827:CLA:HBB1	1.72	0.72
18:O:94:PHE:HA	18:O:97:ILE:HD12	1.72	0.72
23:2:317:BCR:HC42	25:4:319:LMG:H301	1.71	0.72
19:2:305:CHL:O1D	19:2:305:CHL:H2A	1.90	0.71
4:4:95:SER:HB2	4:4:204:GLY:HA3	1.73	0.71
2:2:64:PHE:CE1	19:2:301:CHL:HED2	2.25	0.71
20:B:825:CLA:HMA1	23:B:845:BCR:H14C	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:306:CHL:H2A	19:2:306:CHL:HED2	1.73	0.71
17:N:134:GLN:O	17:N:138:LYS:NZ	2.24	0.70
19:2:306:CHL:HMB3	19:2:306:CHL:HBB1	1.72	0.70
20:A:806:CLA:H62	20:A:808:CLA:H61	1.72	0.70
20:A:810:CLA:H202	23:J:102:BCR:H24C	1.74	0.69
5:A:706:LEU:HD23	10:F:217:ILE:CD1	2.22	0.69
19:4:305:CHL:CGA	23:4:318:BCR:H21C	2.23	0.69
5:A:214:GLN:HA	5:A:218:SER:HB2	1.72	0.69
20:3:309:CLA:HHC	20:3:309:CLA:HBB1	1.74	0.68
1:1:99:VAL:HG11	21:1:315:LUT:H12	1.76	0.68
20:K:201:CLA:HHC	20:K:201:CLA:HBB1	1.75	0.68
19:2:307:CHL:HBB1	19:2:307:CHL:HMB3	1.75	0.68
2:2:112:GLY:O	2:2:116:ILE:HG13	1.94	0.67
3:3:259:ASP:O	3:3:263:ASN:ND2	2.27	0.67
2:2:112:GLY:HA2	22:2:316:XAT:H181	1.78	0.66
20:A:831:CLA:H43	20:L:303:CLA:H43	1.77	0.66
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.76	0.66
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.79	0.65
14:J:31:ARG:HD3	23:J:102:BCR:H312	1.79	0.65
2:2:122:LEU:HD22	2:2:127:ILE:HD12	1.79	0.65
5:A:230:ASP:OD1	17:N:105:ARG:NH2	2.30	0.65
5:A:706:LEU:CD2	10:F:217:ILE:CD1	2.75	0.64
6:B:411:MET:HE2	23:B:844:BCR:H271	1.78	0.64
6:B:463:ILE:HD11	20:B:835:CLA:H2	1.79	0.64
20:O:203:CLA:H3A	20:O:203:CLA:H11	1.79	0.64
19:2:305:CHL:HAB	19:2:306:CHL:HMC	1.79	0.63
5:A:57:ASP:OD2	5:A:347:HIS:NE2	2.30	0.63
9:E:113:VAL:HG12	9:E:114:THR:HG23	1.80	0.63
20:H:201:CLA:HBB2	23:L:306:BCR:H311	1.80	0.63
16:L:88:ASN:HB3	20:L:302:CLA:HAC1	1.81	0.62
6:B:340:SER:HB3	20:B:824:CLA:H42	1.82	0.62
20:B:828:CLA:HHC	20:B:828:CLA:HBB1	1.82	0.62
5:A:583:GLN:HA	5:A:588:ASP:OD2	1.98	0.62
5:A:403:ALA:HB2	23:A:848:BCR:H323	1.82	0.62
20:B:801:CLA:H122	23:B:846:BCR:H12C	1.82	0.61
6:B:492:ILE:HD11	11:G:140:TYR:CE1	2.35	0.61
23:B:841:BCR:H372	23:G:606:BCR:HC42	1.82	0.61
5:A:166:PHE:O	5:A:170:MET:HG2	2.00	0.61
20:B:805:CLA:H92	20:B:813:CLA:H2	1.83	0.61
20:A:820:CLA:H12	20:A:823:CLA:HBA2	1.81	0.61
8:D:93:GLU:O	8:D:123:ARG:NH1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:109:HIS:HA	16:L:112:LEU:HD23	1.82	0.61
20:B:823:CLA:HAB	20:B:830:CLA:HMD1	1.83	0.60
8:D:89:GLU:HA	8:D:102:MET:O	2.01	0.60
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.82	0.60
3:3:52:ARG:NH1	3:3:72:ASP:OD2	2.34	0.59
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.83	0.59
5:A:283:THR:HG22	5:A:285:GLY:H	1.67	0.59
20:A:853:CLA:H91	10:F:197:ILE:HD11	1.85	0.59
20:B:815:CLA:H93	23:B:841:BCR:H23C	1.85	0.59
20:A:841:CLA:H143	23:L:301:BCR:H17C	1.84	0.59
4:4:165:ASP:HB3	19:4:315:CHL:C4C	2.33	0.59
5:A:706:LEU:HD23	10:F:217:ILE:HD13	1.85	0.59
19:2:306:CHL:HBB1	19:2:306:CHL:CMB	2.32	0.58
20:B:805:CLA:H112	20:B:805:CLA:HBD	1.85	0.58
3:3:226:LYS:HE3	20:3:309:CLA:O1D	2.03	0.58
1:1:212:ALA:HB1	1:1:237:ILE:HD13	1.84	0.58
20:B:806:CLA:H151	20:B:828:CLA:HBB2	1.85	0.58
6:B:301:ILE:HG21	20:B:824:CLA:HAC1	1.85	0.58
12:H:115:LEU:HD21	13:I:16:LEU:HD13	1.85	0.58
2:2:64:PHE:HE1	19:2:301:CHL:HED2	1.67	0.58
5:A:561:ILE:HD11	5:A:581:THR:HG21	1.84	0.58
1:1:196:GLY:O	1:1:200:MET:HG3	2.03	0.58
15:K:100:PRO:HG2	20:K:201:CLA:HBC2	1.85	0.58
20:A:821:CLA:H12	20:K:205:CLA:HMB2	1.85	0.58
20:A:851:CLA:H11	6:B:616:LEU:HD12	1.84	0.58
4:4:101:GLY:O	4:4:105:MET:HG3	2.04	0.57
6:B:389:HIS:HA	6:B:392:ILE:HD12	1.86	0.57
6:B:527:LEU:O	6:B:531:THR:HG23	2.04	0.57
20:B:819:CLA:H203	20:B:824:CLA:H141	1.85	0.57
10:F:76:LYS:NZ	10:F:124:GLY:O	2.36	0.57
24:1:318:LHG:HC81	23:4:318:BCR:HC21	1.86	0.57
19:4:306:CHL:HBB1	22:4:317:XAT:H161	1.85	0.57
3:3:168:ARG:HA	3:3:179:MET:HE2	1.86	0.57
5:A:151:THR:H	5:A:155:GLN:HE22	1.52	0.57
5:A:211:ALA:O	5:A:215:VAL:HG13	2.04	0.57
8:D:137:VAL:HG22	8:D:143:VAL:HG22	1.85	0.57
5:A:438:LEU:HD22	20:A:838:CLA:HBB1	1.85	0.57
6:B:275:HIS:HB3	20:B:817:CLA:HMB2	1.86	0.56
2:2:62:LEU:HD11	2:2:69:PRO:HD3	1.87	0.56
20:4:303:CLA:H12	10:F:205:VAL:HG13	1.87	0.56
5:A:118:ILE:HD13	23:J:102:BCR:H313	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:688:GLY:HA3	6:B:568:CYS:HB2	1.86	0.56
20:B:822:CLA:HBA1	20:B:822:CLA:HBD	1.87	0.56
13:I:26:LEU:O	13:I:30:VAL:HG22	2.05	0.56
19:2:301:CHL:HHD	23:3:317:BCR:HC31	1.86	0.56
20:B:828:CLA:H193	23:B:843:BCR:H17C	1.86	0.56
21:1:319:LUT:H392	20:4:308:CLA:H2	1.88	0.56
5:A:379:THR:HG21	5:A:515:VAL:HB	1.87	0.56
1:1:110:LEU:HD11	1:1:130:LEU:HD23	1.88	0.56
2:2:64:PHE:O	2:2:67:SER:OG	2.21	0.56
20:4:303:CLA:HMD1	20:4:308:CLA:CHD	2.36	0.56
20:A:801:CLA:HAB	20:B:802:CLA:NA	2.21	0.56
6:B:439:HIS:O	6:B:443:MET:HG2	2.05	0.56
18:O:76:LEU:O	18:O:80:SER:OG	2.21	0.56
20:A:825:CLA:H171	18:O:123:LEU:HD22	1.88	0.55
15:K:66:LEU:HD11	20:K:205:CLA:HAB	1.88	0.55
1:1:203:PHE:CD2	22:1:316:XAT:H14	2.41	0.55
3:3:105:THR:HG22	19:3:306:CHL:HED3	1.86	0.55
13:I:19:PRO:HG3	23:I:101:BCR:H12C	1.89	0.55
8:D:118:LEU:O	8:D:122:THR:HG23	2.07	0.55
2:2:229:MET:HE3	2:2:229:MET:HA	1.88	0.55
6:B:410:ARG:O	6:B:414:HIS:ND1	2.37	0.55
4:4:204:GLY:O	4:4:208:MET:HG3	2.07	0.55
1:1:152:PHE:CE2	23:1:317:BCR:H10C	2.42	0.55
1:1:236:ASP:OD1	1:1:236:ASP:N	2.28	0.55
5:A:454:ILE:HG22	20:A:833:CLA:HBC2	1.88	0.55
20:3:307:CLA:CHB	20:3:314:CLA:HBB1	2.36	0.55
20:A:827:CLA:H171	23:J:104:BCR:H17C	1.88	0.55
20:B:812:CLA:H8	20:B:812:CLA:HBB1	1.89	0.55
20:1:313:CLA:HED1	4:4:136:THR:HG23	1.89	0.55
4:4:145:PHE:HA	4:4:148:VAL:HG22	1.89	0.55
20:A:841:CLA:H152	16:L:144:LEU:HD21	1.89	0.55
2:2:96:LYS:NZ	2:2:96:LYS:HB3	2.22	0.54
19:2:305:CHL:HHC	19:2:306:CHL:HMC	1.89	0.54
5:A:30:GLY:HA3	5:A:36:ILE:HG22	1.88	0.54
25:1:320:LMG:H192	25:1:320:LMG:H351	1.89	0.54
20:A:802:CLA:CGA	20:A:802:CLA:H3A	2.37	0.54
1:1:91:HIS:HB3	1:1:200:MET:CE	2.37	0.54
20:2:310:CLA:NC	24:2:318:LHG:HC42	2.22	0.54
20:3:301:CLA:HAB	22:3:316:XAT:H32	1.89	0.54
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.40	0.54
5:A:360:LEU:HD11	20:A:818:CLA:H71	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:542:ARG:NH2	8:D:176:ASN:OD1	2.34	0.54
20:B:822:CLA:HBC2	20:B:823:CLA:HBA2	1.90	0.54
26:B:850:HTG:HI1	26:B:850:HTG:O2	2.04	0.54
1:1:55:ARG:HD3	1:1:59:LEU:O	2.08	0.54
1:1:86:GLU:HB2	1:1:167:LYS:HG2	1.89	0.54
1:1:229:PRO:O	1:1:233:ASN:ND2	2.34	0.54
5:A:598:TYR:OH	20:A:801:CLA:HED2	2.08	0.54
23:2:317:BCR:HC31	20:4:301:CLA:CHD	2.38	0.53
10:F:167:VAL:HG13	10:F:196:ILE:HG22	1.90	0.53
1:1:155:HIS:O	1:1:156:GLN:HG2	2.09	0.53
1:1:225:HIS:CG	20:1:312:CLA:HAA2	2.44	0.53
20:B:832:CLA:H51	23:F:801:BCR:H312	1.90	0.53
24:1:318:LHG:H182	4:4:143:ILE:HG12	1.90	0.53
20:4:311:CLA:HBC1	20:4:312:CLA:H201	1.89	0.53
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.91	0.53
18:O:124:GLY:O	18:O:128:THR:HG23	2.08	0.53
3:3:265:ILE:HG12	20:3:311:CLA:H43	1.91	0.53
4:4:158:ASN:HB2	4:4:161:CYS:SG	2.48	0.52
6:B:276:HIS:HB2	20:B:817:CLA:C1B	2.39	0.52
10:F:206:ALA:O	10:F:210:GLU:HG3	2.08	0.52
4:4:165:ASP:HB3	19:4:315:CHL:NC	2.24	0.52
20:4:312:CLA:HMC1	20:4:312:CLA:H92	1.90	0.52
24:1:318:LHG:H291	24:1:318:LHG:HC91	1.92	0.52
18:O:87:ASN:ND2	18:O:88:SER:H	2.06	0.52
4:4:183:SER:OG	4:4:184:VAL:N	2.40	0.52
20:A:814:CLA:C3B	23:A:854:BCR:H333	2.40	0.52
2:2:232:TRP:O	2:2:236:VAL:HG23	2.09	0.52
3:3:60:GLN:O	3:3:63:SER:OG	2.27	0.52
5:A:529:ALA:O	5:A:533:VAL:HG22	2.10	0.52
4:4:171:TYR:CE1	19:4:315:CHL:HAA2	2.45	0.52
4:4:211:PHE:CD2	22:4:317:XAT:H14	2.45	0.52
14:J:31:ARG:NH2	20:J:103:CLA:O1D	2.42	0.52
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.92	0.52
1:1:141:THR:O	1:1:145:ILE:HG13	2.10	0.52
20:3:310:CLA:HMA3	20:3:310:CLA:H2	1.91	0.52
20:4:303:CLA:H42	10:F:208:TYR:CD1	2.45	0.52
1:1:168:TYR:CZ	1:1:189:LYS:HD3	2.45	0.52
5:A:231:PRO:HD2	17:N:105:ARG:HH21	1.75	0.52
20:A:801:CLA:HAB	20:B:802:CLA:C1A	2.40	0.52
5:A:294:HIS:HB2	20:A:817:CLA:C1B	2.40	0.51
20:H:201:CLA:O1A	20:H:201:CLA:H3A	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:12:PRO:HB2	23:J:102:BCR:H401	1.92	0.51
16:L:90:PRO:O	16:L:101:ARG:HD2	2.11	0.51
1:1:187:GLU:O	1:1:191:LYS:HG3	2.09	0.51
2:2:158:TRP:CH2	23:2:317:BCR:HC8	2.45	0.51
3:3:64:TYR:OH	3:3:76:ASP:OD1	2.22	0.51
20:3:309:CLA:CHD	20:3:309:CLA:CBC	2.86	0.51
6:B:546:LEU:O	6:B:564:ARG:NH1	2.44	0.51
12:H:119:SER:OG	13:I:8:SER:O	2.26	0.51
20:A:853:CLA:H42	14:J:15:SER:HA	1.93	0.51
17:N:142:VAL:HG21	17:N:145:LEU:HD12	1.92	0.51
17:N:148:ASP:O	17:N:152:GLU:HB2	2.10	0.51
2:2:108:TRP:CE2	19:2:307:CHL:HED2	2.46	0.51
19:2:306:CHL:CED	19:2:306:CHL:HAA1	2.40	0.51
19:2:301:CHL:H42	3:3:160:GLY:HA2	1.91	0.51
6:B:561:GLY:O	6:B:567:THR:OG1	2.29	0.51
15:K:66:LEU:CD2	15:K:114:VAL:HG13	2.40	0.51
20:B:834:CLA:HBB1	23:B:845:BCR:HC21	1.93	0.51
1:1:234:ILE:HD13	20:1:312:CLA:H42	1.92	0.51
5:A:283:THR:HG23	5:A:375:PRO:HA	1.93	0.51
16:L:185:TRP:O	16:L:189:THR:HG22	2.11	0.51
6:B:450:GLU:OE1	10:F:119:ARG:NH1	2.44	0.51
1:1:91:HIS:HB3	1:1:200:MET:HE1	1.93	0.50
20:1:321:CLA:HBA1	24:B:849:LHG:HC42	1.93	0.50
4:4:165:ASP:HB3	19:4:315:CHL:C1C	2.42	0.50
20:A:805:CLA:H151	20:A:828:CLA:HBB2	1.94	0.50
20:B:818:CLA:HBB2	20:B:824:CLA:H203	1.93	0.50
5:A:13:LEU:HB3	5:A:184:LYS:HG3	1.93	0.50
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.93	0.50
6:B:80:ASP:HB3	6:B:84:VAL:HG23	1.93	0.50
20:O:202:CLA:HBC3	20:O:202:CLA:CHD	2.39	0.50
1:1:85:LYS:O	1:1:89:VAL:HG23	2.12	0.50
2:2:110:MET:SD	20:2:309:CLA:HAB	2.51	0.50
19:2:305:CHL:CHC	19:2:306:CHL:HMC	2.41	0.50
3:3:251:GLN:NE2	3:3:255:ASP:OD1	2.45	0.50
8:D:75:GLN:HG2	12:H:70:GLN:HG3	1.94	0.50
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.93	0.50
2:2:181:ASN:ND2	2:2:182:ASN:OD1	2.45	0.50
5:A:484:ILE:HD13	20:A:834:CLA:HBB1	1.93	0.50
5:A:86:SER:HB2	5:A:163:ALA:HB3	1.93	0.50
5:A:371:MET:HE1	20:A:826:CLA:CAB	2.42	0.50
5:A:582:CYS:HB3	6:B:667:TRP:HE3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:825:CLA:H193	23:A:848:BCR:H382	1.92	0.50
23:B:841:BCR:H321	11:G:120:ALA:HB1	1.94	0.50
10:F:217:ILE:CD1	20:F:802:CLA:O1A	2.60	0.50
5:A:356:MET:HG3	20:A:824:CLA:HBB	1.94	0.50
14:J:12:PRO:O	14:J:16:THR:HG22	2.12	0.50
19:2:307:CHL:HBB1	19:2:307:CHL:CMB	2.41	0.49
5:A:680:PHE:HZ	20:A:840:CLA:HBC2	1.76	0.49
20:B:803:CLA:H143	23:B:846:BCR:H362	1.94	0.49
20:B:817:CLA:HAC2	20:B:824:CLA:H201	1.93	0.49
7:C:61:ASP:H	9:E:140:ASN:HD21	1.60	0.49
20:1:303:CLA:HBC1	20:1:308:CLA:HAC1	1.94	0.49
6:B:680:TRP:CE2	6:B:684:ARG:HG3	2.47	0.49
15:K:116:HIS:O	15:K:120:VAL:HG23	2.13	0.49
15:K:126:LEU:HB3	15:K:132:ILE:HG13	1.93	0.49
2:2:150:ILE:HG21	20:4:313:CLA:HED1	1.93	0.49
5:A:283:THR:HG22	5:A:285:GLY:N	2.27	0.49
20:A:804:CLA:H152	20:A:812:CLA:H51	1.95	0.49
20:A:816:CLA:CHD	20:A:817:CLA:HBB2	2.43	0.49
20:B:801:CLA:HBB1	20:B:801:CLA:HMB3	1.95	0.49
20:B:816:CLA:O1A	11:G:138:ASN:ND2	2.45	0.49
10:F:208:TYR:O	10:F:212:LEU:HD22	2.13	0.49
19:2:306:CHL:HAA1	19:2:306:CHL:HED3	1.94	0.49
6:B:187:SER:O	6:B:191:THR:HG22	2.12	0.49
23:B:841:BCR:H362	23:G:606:BCR:H312	1.94	0.49
23:A:845:BCR:H402	23:A:854:BCR:HC8	1.94	0.49
20:3:309:CLA:HBB1	20:3:309:CLA:CHC	2.37	0.49
5:A:72:SER:OG	5:A:178:TYR:HB2	2.12	0.49
5:A:217:VAL:HG13	5:A:237:PRO:HB3	1.95	0.49
20:B:808:CLA:O1A	20:B:827:CLA:HBD	2.13	0.49
1:1:150:ILE:HG21	20:1:308:CLA:HMC3	1.95	0.49
6:B:93:ASP:OD1	6:B:95:HIS:ND1	2.33	0.49
15:K:59:MET:HG3	20:K:203:CLA:HMD3	1.95	0.49
25:1:320:LMG:H132	25:1:320:LMG:H301	1.95	0.48
25:1:320:LMG:H312	25:1:320:LMG:H152	1.94	0.48
2:2:97:TRP:CZ2	20:2:308:CLA:HAA2	2.48	0.48
2:2:116:ILE:HG23	2:2:133:TRP:CG	2.49	0.48
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.93	0.48
1:1:146:GLU:OE2	19:1:306:CHL:OMC	2.31	0.48
19:1:301:CHL:HED3	4:4:151:ARG:HD2	1.95	0.48
5:A:231:PRO:HD2	17:N:105:ARG:NH2	2.28	0.48
9:E:95:LYS:NZ	9:E:111:SER:OG	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:59:ASP:O	18:O:59:ASP:OD2	2.32	0.48
4:4:186:ASN:OD1	21:4:316:LUT:O23	2.22	0.48
4:4:238:HIS:O	4:4:243:ASN:ND2	2.46	0.48
6:B:410:ARG:HA	6:B:413:ASP:HB2	1.95	0.48
3:3:223:LYS:HD3	20:3:310:CLA:HBD	1.96	0.48
20:4:303:CLA:HMD3	20:4:308:CLA:ND	2.28	0.48
5:A:57:ASP:OD1	5:A:57:ASP:N	2.44	0.48
1:1:184:LYS:HA	1:1:187:GLU:HG2	1.95	0.48
4:4:89:GLN:O	4:4:93:VAL:HG22	2.14	0.48
5:A:151:THR:H	5:A:155:GLN:NE2	2.12	0.48
20:A:822:CLA:HBB1	18:O:131:PHE:CE2	2.48	0.48
6:B:340:SER:O	6:B:344:ILE:HG23	2.14	0.48
15:K:83:THR:N	15:K:86:LEU:O	2.47	0.48
3:3:101:PHE:O	3:3:105:THR:HG23	2.13	0.48
3:3:269:PHE:O	5:A:259:THR:OG1	2.23	0.48
6:B:174:ARG:HB2	20:B:813:CLA:HBC2	1.96	0.48
6:B:397:ASP:OD1	8:D:181:LYS:NZ	2.44	0.48
23:F:806:BCR:H11C	23:F:806:BCR:H341	1.70	0.48
20:B:814:CLA:HMA2	23:B:843:BCR:H272	1.96	0.48
3:3:105:THR:HG22	19:3:306:CHL:HED1	1.91	0.47
6:B:339:ALA:HB2	23:B:845:BCR:H372	1.95	0.47
6:B:344:ILE:HG21	20:B:824:CLA:H43	1.95	0.47
20:K:202:CLA:HBA1	20:K:202:CLA:HBD	1.96	0.47
16:L:114:VAL:HG21	16:L:203:ALA:HB3	1.95	0.47
20:1:304:CLA:H41	20:1:304:CLA:H61	1.54	0.47
20:4:304:CLA:CHA	20:4:304:CLA:HBA1	2.42	0.47
20:4:312:CLA:HBA1	20:4:312:CLA:HBD	1.95	0.47
20:A:853:CLA:O1D	10:F:185:GLU:HG2	2.14	0.47
20:B:813:CLA:H112	20:B:813:CLA:H143	1.66	0.47
8:D:53:GLN:H	8:D:53:GLN:HG2	1.50	0.47
9:E:91:PRO:O	9:E:94:SER:OG	2.27	0.47
15:K:66:LEU:HD21	15:K:114:VAL:HG13	1.96	0.47
16:L:63:ILE:HA	16:L:73:GLU:HG3	1.96	0.47
20:1:303:CLA:HED2	20:1:303:CLA:H43	1.97	0.47
20:A:810:CLA:H122	20:J:101:CLA:HBB2	1.97	0.47
20:B:801:CLA:H171	20:B:810:CLA:HMC2	1.96	0.47
20:B:812:CLA:H51	20:B:812:CLA:H11	1.74	0.47
21:O:205:LUT:H191	21:O:205:LUT:H11	1.77	0.47
3:3:132:PRO:HD2	3:3:135:LYS:HE3	1.97	0.47
20:A:831:CLA:H111	20:A:831:CLA:H152	1.62	0.47
6:B:458:ILE:HG21	10:F:141:ASN:HD22	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:202:CLA:HBB1	20:O:202:CLA:CHC	2.33	0.47
20:1:307:CLA:H72	20:1:307:CLA:H112	1.75	0.47
19:4:306:CHL:HBA1	19:4:306:CHL:H3A	1.60	0.47
20:B:825:CLA:HBA2	20:B:825:CLA:H3A	1.70	0.47
17:N:167:TRP:HA	17:N:167:TRP:CE3	2.49	0.47
5:A:118:ILE:HG13	5:A:119:VAL:HG13	1.96	0.47
20:B:805:CLA:H141	20:B:805:CLA:H162	1.68	0.47
20:B:810:CLA:H43	20:B:810:CLA:HED2	1.96	0.47
20:B:831:CLA:H202	20:F:802:CLA:HAB	1.96	0.47
16:L:123:LEU:HD12	16:L:132:VAL:HG11	1.96	0.47
5:A:305:ALA:HB2	20:A:820:CLA:HBC2	1.97	0.47
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.49	0.47
6:B:383:MET:HE1	23:B:845:BCR:H361	1.97	0.47
20:1:313:CLA:CED	4:4:136:THR:HG23	2.45	0.47
5:A:133:ARG:HB2	17:N:113:PHE:CE2	2.50	0.47
5:A:693:GLN:NE2	5:A:716:ALA:H	2.12	0.47
23:A:849:BCR:H361	23:A:849:BCR:H20C	1.69	0.47
6:B:188:LEU:HD21	23:B:841:BCR:H383	1.96	0.47
15:K:129:ILE:HG22	15:K:131:VAL:HG23	1.96	0.47
17:N:167:TRP:HA	17:N:167:TRP:HE3	1.79	0.47
20:2:310:CLA:CAB	23:3:317:BCR:H312	2.45	0.46
3:3:80:LEU:HD22	3:3:90:PHE:HE2	1.80	0.46
3:3:102:ASN:ND2	20:3:307:CLA:OBD	2.48	0.46
4:4:235:ASP:OD2	4:4:238:HIS:ND1	2.38	0.46
20:4:303:CLA:CMD	20:4:308:CLA:C1D	2.93	0.46
5:A:224:PHE:O	5:A:229:VAL:HG13	2.15	0.46
20:A:801:CLA:HBB1	20:A:851:CLA:HED1	1.96	0.46
5:A:583:GLN:HB3	5:A:588:ASP:HB3	1.97	0.46
20:A:851:CLA:HMB1	20:A:851:CLA:HBB1	1.96	0.46
20:B:818:CLA:H3A	20:B:818:CLA:HBA2	1.46	0.46
20:B:827:CLA:H3A	20:B:827:CLA:HBA2	1.50	0.46
15:K:104:THR:O	15:K:108:THR:HG23	2.15	0.46
20:A:831:CLA:H92	20:A:831:CLA:H61	1.72	0.46
6:B:733:PHE:HB3	12:H:142:ARG:HE	1.79	0.46
20:B:805:CLA:HBA1	20:B:805:CLA:H3A	1.36	0.46
20:B:806:CLA:H193	20:B:806:CLA:H161	1.67	0.46
20:O:203:CLA:H3A	20:O:203:CLA:HBA2	1.44	0.46
1:1:160:GLU:O	1:1:166:LYS:NZ	2.38	0.46
20:B:825:CLA:HAA2	20:B:826:CLA:OBD	2.16	0.46
9:E:96:VAL:HB	9:E:147:VAL:HG13	1.98	0.46
23:2:317:BCR:H11C	23:2:317:BCR:H341	1.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:118:ILE:HB	23:J:102:BCR:H322	1.96	0.46
20:A:811:CLA:HHC	20:A:811:CLA:HBB1	1.98	0.46
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.98	0.46
10:F:147:TRP:HZ2	20:F:805:CLA:HBA1	1.79	0.46
10:F:192:LEU:O	10:F:196:ILE:HG12	2.16	0.46
2:2:156:ILE:HG21	20:2:308:CLA:HMC3	1.97	0.46
5:A:607:HIS:CE1	20:A:836:CLA:HBC3	2.51	0.46
20:A:803:CLA:HAB	20:A:810:CLA:H142	1.96	0.46
20:B:812:CLA:H3A	20:B:812:CLA:HBA2	1.54	0.46
4:4:243:ASN:OD1	4:4:243:ASN:N	2.49	0.46
5:A:582:CYS:HB2	6:B:667:TRP:HB3	1.96	0.46
1:1:197:ARG:HG2	20:1:302:CLA:C3C	2.45	0.46
19:2:301:CHL:HAB	19:2:301:CHL:HHC	1.82	0.46
3:3:78:LEU:HD23	20:A:811:CLA:H2	1.98	0.46
20:3:313:CLA:HHC	20:3:313:CLA:HBB1	1.97	0.46
20:O:201:CLA:H11	20:O:201:CLA:H52	1.78	0.46
4:4:188:LEU:HD12	21:4:316:LUT:H222	1.97	0.46
6:B:569:ASP:HA	6:B:574:ASP:OD2	2.16	0.46
20:L:303:CLA:H72	20:L:303:CLA:H112	1.59	0.46
18:O:115:TRP:O	18:O:119:VAL:HG23	2.16	0.46
20:O:202:CLA:HHC	20:O:202:CLA:CBB	2.37	0.46
20:A:806:CLA:H202	20:A:806:CLA:H162	1.76	0.46
23:B:845:BCR:H341	23:B:845:BCR:H11C	1.80	0.46
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.51	0.46
5:A:653:ALA:O	5:A:657:ILE:HG12	2.15	0.45
20:4:308:CLA:HHB	20:4:314:CLA:HBC2	1.98	0.45
5:A:435:ILE:HG13	5:A:554:PHE:HE2	1.81	0.45
23:A:849:BCR:H24C	23:A:849:BCR:H371	1.76	0.45
20:B:818:CLA:H112	20:B:818:CLA:H71	1.59	0.45
21:1:315:LUT:H35	21:1:315:LUT:H401	1.76	0.45
3:3:110:VAL:HG11	21:3:315:LUT:H10	1.98	0.45
20:A:823:CLA:HBB2	24:A:844:LHG:H101	1.98	0.45
20:A:827:CLA:HBA1	20:A:827:CLA:HBD	1.97	0.45
6:B:401:GLU:OE1	6:B:401:GLU:N	2.45	0.45
20:B:828:CLA:H3A	20:B:828:CLA:HBA2	1.59	0.45
23:B:841:BCR:HC8	11:G:124:ILE:HD11	1.98	0.45
11:G:106:LYS:O	11:G:106:LYS:HD3	2.16	0.45
4:4:155:ASP:OD1	19:4:307:CHL:HBC1	2.16	0.45
23:A:854:BCR:H351	23:A:854:BCR:H15C	1.69	0.45
20:3:307:CLA:HBB1	20:3:307:CLA:HMB3	1.98	0.45
20:A:811:CLA:H62	20:A:811:CLA:H41	1.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:87:ILE:O	6:B:121:TYR:OH	2.23	0.45
20:B:817:CLA:H202	20:B:817:CLA:H162	1.77	0.45
12:H:73:VAL:HG13	16:L:169:LEU:HD11	1.98	0.45
15:K:56:ASN:ND2	20:K:203:CLA:OBD	2.43	0.45
18:O:118:MET:SD	20:O:202:CLA:O2A	2.75	0.45
23:2:317:BCR:HC42	25:4:319:LMG:H321	1.98	0.45
20:B:834:CLA:HBB1	20:B:834:CLA:HMB3	1.97	0.45
20:A:837:CLA:H202	20:L:303:CLA:H102	1.99	0.45
20:A:839:CLA:H2A	20:A:839:CLA:HED3	1.98	0.45
6:B:160:LYS:HE3	6:B:160:LYS:HB2	1.63	0.45
20:B:832:CLA:H91	20:B:832:CLA:H111	1.72	0.45
15:K:82:ALA:HB2	15:K:88:LEU:HD23	1.97	0.45
21:O:205:LUT:H201	21:O:205:LUT:H15	1.79	0.45
3:3:121:LYS:HB2	3:3:121:LYS:HE2	1.73	0.45
20:3:309:CLA:HHC	20:3:309:CLA:CBB	2.42	0.45
23:4:318:BCR:H11C	23:4:318:BCR:H341	1.82	0.45
5:A:201:GLY:O	5:A:205:LEU:HB2	2.16	0.45
5:A:599:ASN:O	5:A:603:VAL:HG23	2.17	0.45
10:F:85:GLU:HB2	10:F:120:PHE:CD2	2.52	0.45
1:1:241:ARG:HA	1:1:241:ARG:HD2	1.77	0.45
5:A:194:MET:HE2	20:A:812:CLA:HBC2	1.97	0.45
5:A:346:TRP:HB3	20:A:804:CLA:HAC1	1.99	0.45
20:A:826:CLA:H61	20:A:826:CLA:H2	1.72	0.45
20:B:831:CLA:HBB2	23:F:801:BCR:HC41	1.97	0.45
17:N:167:TRP:CE3	17:N:167:TRP:O	2.70	0.45
23:2:317:BCR:H24C	23:2:317:BCR:H371	1.80	0.45
4:4:105:MET:HE2	22:4:317:XAT:H8	1.98	0.45
20:A:853:CLA:H93	20:A:853:CLA:H61	1.77	0.45
20:B:835:CLA:HMB1	20:B:835:CLA:HBB1	1.99	0.45
10:F:83:LYS:NZ	10:F:83:LYS:HB2	2.32	0.45
23:J:102:BCR:H15C	23:J:102:BCR:H351	1.76	0.45
5:A:414:TYR:CE2	5:A:416:PRO:HD3	2.52	0.44
3:3:88:PHE:O	3:3:91:GLN:NE2	2.47	0.44
5:A:314:GLY:HA3	15:K:78:ALA:HA	1.99	0.44
15:K:60:VAL:O	15:K:64:THR:HG23	2.18	0.44
21:O:204:LUT:H15	21:O:204:LUT:H201	1.81	0.44
20:4:301:CLA:H3A	20:4:301:CLA:HBA2	1.76	0.44
20:4:312:CLA:O1A	20:4:313:CLA:C2D	2.65	0.44
20:A:821:CLA:HBA2	20:A:821:CLA:H3A	1.25	0.44
20:A:823:CLA:H12	20:A:838:CLA:H142	1.99	0.44
20:A:825:CLA:HBA2	20:A:825:CLA:H3A	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:205:LUT:H31	21:O:205:LUT:H391	1.70	0.44
21:O:205:LUT:H361	21:O:205:LUT:H28	2.00	0.44
1:1:150:ILE:HA	1:1:153:VAL:HG22	1.99	0.44
3:3:207:PRO:HD2	21:3:315:LUT:H23	1.99	0.44
4:4:72:PHE:HE2	22:4:317:XAT:H383	1.82	0.44
4:4:95:SER:HB3	4:4:208:MET:HE2	1.98	0.44
9:E:140:ASN:HB3	9:E:142:TYR:CE1	2.52	0.44
10:F:209:ARG:O	10:F:213:ASN:ND2	2.50	0.44
15:K:55:THR:O	15:K:59:MET:HG2	2.16	0.44
16:L:64:ASN:O	16:L:64:ASN:ND2	2.51	0.44
17:N:156:LYS:HB2	17:N:156:LYS:HE2	1.70	0.44
21:O:204:LUT:H35	21:O:204:LUT:H401	1.80	0.44
1:1:230:TRP:CE3	20:1:313:CLA:HMA2	2.53	0.44
2:2:209:LYS:O	2:2:212:GLU:HG3	2.17	0.44
2:2:234:GLN:O	2:2:238:THR:OG1	2.22	0.44
20:A:805:CLA:H43	24:A:843:LHG:H261	1.99	0.44
20:A:818:CLA:H141	20:A:826:CLA:H193	2.00	0.44
27:A:842:PQN:H141	27:A:842:PQN:H161	1.59	0.44
23:B:844:BCR:H11C	23:B:844:BCR:H341	1.81	0.44
23:L:301:BCR:H24C	23:L:301:BCR:H371	1.81	0.44
18:O:87:ASN:HD22	18:O:88:SER:H	1.66	0.44
24:1:318:LHG:H321	20:4:314:CLA:HED1	2.00	0.44
5:A:259:THR:O	5:A:263:THR:OG1	2.27	0.44
20:A:808:CLA:H62	20:A:808:CLA:H92	1.84	0.44
20:B:802:CLA:H102	20:B:802:CLA:H62	1.82	0.44
20:B:807:CLA:H62	20:B:807:CLA:H2	1.77	0.44
1:1:152:PHE:CE2	23:1:317:BCR:H12C	2.53	0.44
20:4:302:CLA:H72	22:4:317:XAT:H28	1.99	0.44
20:A:807:CLA:H3A	20:A:807:CLA:HBA2	1.31	0.44
6:B:608:GLN:O	6:B:612:SER:HB2	2.17	0.44
20:1:312:CLA:H91	20:1:312:CLA:H112	1.67	0.44
20:A:803:CLA:HBA1	20:A:803:CLA:H3A	1.57	0.44
20:A:837:CLA:HBB1	20:A:837:CLA:HMB3	1.99	0.44
6:B:351:HIS:ND1	20:B:817:CLA:OBD	2.48	0.44
6:B:458:ILE:HG21	10:F:141:ASN:ND2	2.32	0.44
20:H:201:CLA:HMB2	20:L:302:CLA:HAA1	2.00	0.44
18:O:79:SER:OG	18:O:90:THR:CG2	2.66	0.44
5:A:360:LEU:HB2	20:A:826:CLA:H41	2.00	0.44
5:A:578:ARG:NH2	8:D:115:GLU:OE1	2.47	0.44
20:A:825:CLA:H191	23:A:848:BCR:H393	2.00	0.44
10:F:102:GLU:O	17:N:144:PHE:HZ	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:202:CLA:H93	20:K:202:CLA:H111	1.87	0.44
20:1:321:CLA:HBC1	26:1:322:HTG:H5	2.00	0.43
20:4:302:CLA:HAB	22:4:317:XAT:H32	2.00	0.43
20:A:853:CLA:HED3	10:F:185:GLU:HA	1.99	0.43
20:B:805:CLA:H122	20:B:813:CLA:HBD	1.99	0.43
19:1:301:CHL:HBB1	20:1:302:CLA:HMD2	1.98	0.43
20:1:312:CLA:H152	24:1:318:LHG:H132	1.99	0.43
5:A:335:HIS:HB3	5:A:338:LEU:HD12	2.00	0.43
20:A:806:CLA:H72	20:A:806:CLA:H112	1.73	0.43
7:C:2:SER:N	7:C:71:HIS:O	2.50	0.43
20:3:311:CLA:CHB	21:3:315:LUT:H42	2.49	0.43
20:A:836:CLA:HBB1	20:A:836:CLA:HMB3	2.00	0.43
27:A:842:PQN:H292	27:A:842:PQN:H261	1.83	0.43
20:B:808:CLA:H122	20:B:827:CLA:H13	1.99	0.43
20:N:203:CLA:H2A	20:N:203:CLA:HED2	2.01	0.43
1:1:152:PHE:CZ	23:1:317:BCR:H10C	2.53	0.43
5:A:597:MET:HE3	5:A:597:MET:HB3	1.91	0.43
20:B:803:CLA:CGA	20:B:803:CLA:H3A	2.48	0.43
20:B:833:CLA:H72	20:B:833:CLA:H112	1.93	0.43
20:2:310:CLA:HBD	20:2:311:CLA:OBD	2.18	0.43
5:A:407:ALA:HB1	5:A:586:ALA:HB1	2.01	0.43
20:A:821:CLA:O1A	20:K:205:CLA:HHB	2.18	0.43
20:A:827:CLA:HBA1	20:A:827:CLA:H12	1.67	0.43
23:I:101:BCR:H11C	23:I:101:BCR:H341	1.79	0.43
23:I:101:BCR:H20C	23:I:101:BCR:H361	1.85	0.43
18:O:104:PHE:CG	18:O:105:PRO:HA	2.54	0.43
19:1:306:CHL:H3A	19:1:306:CHL:HBA2	1.56	0.43
2:2:185:THR:HG23	2:2:194:GLY:HA2	2.00	0.43
19:4:305:CHL:CGA	23:4:318:BCR:H19C	2.48	0.43
5:A:286:LEU:HD21	5:A:371:MET:HB3	1.99	0.43
23:A:849:BCR:H15C	23:A:849:BCR:H351	1.85	0.43
6:B:435:GLY:HA3	20:B:832:CLA:HAB	2.00	0.43
6:B:714:SER:HB2	30:B:848:DGD:HBF1	2.00	0.43
14:J:25:LEU:O	14:J:29:ILE:HG13	2.19	0.43
17:N:119:VAL:HG23	26:N:201:HTG:O4	2.19	0.43
1:1:200:MET:HE2	22:1:316:XAT:C34	2.49	0.43
20:A:825:CLA:HAA2	20:A:826:CLA:OBD	2.19	0.43
21:O:205:LUT:H35	21:O:205:LUT:H401	1.71	0.43
24:1:318:LHG:O3	24:1:318:LHG:O1	2.24	0.43
2:2:74:ASP:OD2	2:2:74:ASP:C	2.61	0.43
20:3:307:CLA:HBA2	20:3:307:CLA:H3A	1.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:809:CLA:HAB	20:A:812:CLA:H111	2.01	0.43
2:2:88:LEU:HD13	20:2:302:CLA:H42	2.00	0.43
2:2:227:ALA:HA	20:2:312:CLA:HBB1	2.01	0.43
3:3:159:LEU:HD22	20:3:307:CLA:HBB2	2.01	0.43
21:4:316:LUT:H31	21:4:316:LUT:H391	1.93	0.43
5:A:433:ALA:O	5:A:437:HIS:ND1	2.49	0.43
5:A:719:ILE:HG12	6:B:568:CYS:SG	2.59	0.43
20:A:805:CLA:H61	20:A:805:CLA:H92	1.72	0.43
20:A:817:CLA:H141	20:A:817:CLA:H162	1.76	0.43
20:B:823:CLA:HBD	20:B:823:CLA:HBA1	2.01	0.43
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.43
23:L:306:BCR:H351	23:L:306:BCR:H15C	1.77	0.43
1:1:185:PHE:CZ	20:1:309:CLA:HED3	2.54	0.43
20:1:307:CLA:H2	21:1:315:LUT:H383	2.01	0.43
20:1:313:CLA:HAA1	4:4:140:ILE:HG12	2.00	0.43
4:4:125:ALA:O	4:4:130:TYR:OH	2.29	0.43
5:A:519:VAL:HG11	5:A:522:LEU:HD23	2.00	0.43
5:A:706:LEU:HD21	10:F:217:ILE:CD1	2.49	0.43
20:A:823:CLA:HBB	20:O:201:CLA:CBB	2.48	0.43
20:A:828:CLA:HMB3	20:A:828:CLA:HBB1	2.00	0.43
23:B:841:BCR:H15C	23:B:841:BCR:H351	1.70	0.43
23:B:845:BCR:H351	23:B:845:BCR:H15C	1.67	0.43
15:K:68:PHE:CD1	15:K:68:PHE:C	2.97	0.43
20:L:302:CLA:CHA	20:L:302:CLA:HBA1	2.49	0.43
20:A:833:CLA:H62	20:A:833:CLA:H2	1.79	0.42
23:A:854:BCR:C11	23:K:204:BCR:H333	2.49	0.42
10:F:163:TRP:O	10:F:167:VAL:HG23	2.18	0.42
12:H:72:ASP:OD1	12:H:75:GLY:HA3	2.19	0.42
21:1:319:LUT:H35	21:1:319:LUT:H401	1.85	0.42
20:3:311:CLA:H61	20:3:311:CLA:H2	1.84	0.42
20:A:817:CLA:H3A	20:A:817:CLA:HBA2	1.61	0.42
20:A:831:CLA:H91	20:A:831:CLA:H112	1.72	0.42
6:B:583:MET:O	6:B:587:ILE:HG12	2.20	0.42
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.66	0.42
23:B:846:BCR:H20C	23:B:846:BCR:H361	1.91	0.42
8:D:58:THR:HB	8:D:106:PRO:HB2	2.01	0.42
23:L:305:BCR:H15C	23:L:305:BCR:H351	1.78	0.42
17:N:167:TRP:CE3	17:N:167:TRP:CA	3.02	0.42
19:4:315:CHL:HHC	19:4:315:CHL:HBB1	1.99	0.42
5:A:195:LEU:HG	20:A:824:CLA:HMD2	2.01	0.42
20:A:805:CLA:H161	20:A:805:CLA:H193	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:851:CLA:O1D	20:A:851:CLA:H2A	2.20	0.42
6:B:645:VAL:HG13	20:B:809:CLA:HAC1	2.00	0.42
20:B:803:CLA:H202	20:B:803:CLA:H162	1.81	0.42
20:1:311:CLA:HBB1	20:1:311:CLA:HMB3	2.00	0.42
20:4:303:CLA:HMD1	20:4:308:CLA:C4C	2.50	0.42
19:4:305:CHL:HAB	19:4:306:CHL:OMC	2.20	0.42
6:B:583:MET:HE3	6:B:583:MET:HB3	1.77	0.42
20:B:807:CLA:H2	23:I:101:BCR:HC31	2.01	0.42
20:B:830:CLA:H3A	20:B:830:CLA:HBA2	1.30	0.42
15:K:80:ARG:HG2	15:K:88:LEU:HB3	2.01	0.42
18:O:68:ILE:HD11	21:O:204:LUT:H26	2.01	0.42
20:1:308:CLA:HBA2	20:1:308:CLA:H3A	1.33	0.42
5:A:194:MET:HB2	20:A:812:CLA:HBC2	2.00	0.42
5:A:611:LYS:HE2	5:A:615:ASP:OD2	2.20	0.42
20:A:808:CLA:H111	23:J:102:BCR:H373	2.00	0.42
30:B:848:DGD:HAW1	30:B:848:DGD:HAN2	1.80	0.42
11:G:101:TYR:O	11:G:105:LEU:HG	2.19	0.42
15:K:110:ALA:O	15:K:114:VAL:HG12	2.19	0.42
20:2:311:CLA:H52	20:2:311:CLA:H12	1.75	0.42
4:4:96:ARG:HG2	20:4:309:CLA:C3C	2.49	0.42
5:A:371:MET:HE1	20:A:826:CLA:HAB	2.01	0.42
6:B:587:ILE:HA	6:B:590:VAL:HG13	2.00	0.42
6:B:662:MET:HE3	20:B:839:CLA:HBC2	2.01	0.42
20:B:823:CLA:H51	20:B:824:CLA:H142	2.02	0.42
20:B:838:CLA:HBB2	27:B:840:PQN:H141	2.02	0.42
20:B:838:CLA:H18	23:I:101:BCR:H362	2.02	0.42
20:F:805:CLA:C2D	26:F:807:HTG:H3'2	2.50	0.42
12:H:98:THR:HG22	16:L:187:ARG:HA	2.02	0.42
14:J:1:MET:O	14:J:5:LYS:HG3	2.19	0.42
15:K:103:PHE:CE2	15:K:108:THR:HG22	2.55	0.42
23:K:204:BCR:H20C	23:K:204:BCR:H361	1.81	0.42
16:L:144:LEU:HD22	23:L:305:BCR:H401	2.02	0.42
17:N:100:LEU:HD22	17:N:104:LYS:HE2	2.01	0.42
19:2:301:CHL:HED1	3:3:171:GLN:HG3	2.01	0.42
4:4:164:GLN:NE2	4:4:169:LYS:O	2.53	0.42
20:4:302:CLA:H93	20:4:302:CLA:H112	1.80	0.42
20:A:822:CLA:HBB2	20:A:838:CLA:H172	2.01	0.42
20:A:834:CLA:H11	20:A:834:CLA:H52	1.77	0.42
23:F:806:BCR:H371	23:F:806:BCR:H24C	1.81	0.42
23:K:204:BCR:H15C	23:K:204:BCR:H351	1.84	0.42
17:N:167:TRP:CE3	17:N:167:TRP:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:ARG:HB3	24:1:318:LHG:H252	2.00	0.42
2:2:203:GLY:HA2	20:2:309:CLA:CAA	2.49	0.42
19:2:305:CHL:HAB	19:2:306:CHL:CMC	2.48	0.42
20:4:312:CLA:HAA1	20:4:312:CLA:HED3	2.01	0.42
20:A:801:CLA:H122	20:A:801:CLA:H161	1.58	0.42
20:A:831:CLA:HBA1	6:B:686:PRO:HD3	2.02	0.42
20:A:833:CLA:HAA2	16:L:120:THR:OG1	2.19	0.42
23:A:854:BCR:H24C	23:A:854:BCR:H371	1.80	0.42
20:B:808:CLA:HMB2	20:B:808:CLA:H142	2.01	0.42
8:D:110:LYS:NZ	12:H:58:TYR:O	2.52	0.42
1:1:61:GLY:HA2	1:1:66:ASP:HB3	2.02	0.42
23:A:848:BCR:H15C	23:A:848:BCR:H351	1.79	0.42
23:A:854:BCR:H403	15:K:110:ALA:HB1	2.02	0.42
20:L:303:CLA:H142	20:L:303:CLA:H111	1.73	0.42
21:1:319:LUT:H15	21:1:319:LUT:H201	1.74	0.42
5:A:31:HIS:CE1	20:A:810:CLA:HAA1	2.54	0.42
5:A:634:PHE:O	5:A:638:SER:OG	2.29	0.42
5:A:649:LEU:HD11	20:A:801:CLA:H72	2.02	0.42
20:A:818:CLA:H162	20:A:818:CLA:H122	1.87	0.42
17:N:99:GLU:HG2	17:N:103:LYS:HZ3	1.85	0.42
25:1:323:LMG:HC61	11:G:136:SER:HA	2.02	0.41
20:A:809:CLA:H121	20:A:809:CLA:H162	1.71	0.41
15:K:57:LEU:O	15:K:61:THR:HG22	2.20	0.41
15:K:95:LEU:O	15:K:96:GLN:HB3	2.20	0.41
23:L:306:BCR:H11C	23:L:306:BCR:H341	1.83	0.41
5:A:583:GLN:HA	5:A:588:ASP:CG	2.45	0.41
20:A:802:CLA:H192	20:A:802:CLA:H162	1.72	0.41
20:B:825:CLA:H42	20:B:836:CLA:HBA1	2.01	0.41
23:K:204:BCR:H11C	23:K:204:BCR:H341	1.85	0.41
23:L:305:BCR:H20C	23:L:305:BCR:H361	1.87	0.41
2:2:143:THR:CG2	4:4:237:TRP:HB3	2.50	0.41
2:2:228:VAL:HG11	22:2:316:XAT:H12	2.03	0.41
3:3:224:GLU:HB2	20:3:308:CLA:C1B	2.50	0.41
4:4:240:THR:O	4:4:244:THR:HG23	2.21	0.41
20:4:311:CLA:H12	20:4:311:CLA:H52	1.76	0.41
5:A:689:ARG:HH12	5:A:693:GLN:HE21	1.67	0.41
20:A:834:CLA:H171	20:O:203:CLA:H112	2.01	0.41
6:B:373:THR:HG23	6:B:591:THR:HG21	2.02	0.41
8:D:145:TYR:OH	8:D:148:PRO:O	2.37	0.41
23:1:317:BCR:H15C	23:1:317:BCR:H351	1.76	0.41
2:2:213:LEU:HD12	2:2:213:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:4:319:LMG:H222	25:4:319:LMG:H251	1.89	0.41
5:A:175:TRP:HB2	20:A:810:CLA:CMC	2.51	0.41
20:A:809:CLA:H41	20:A:809:CLA:H62	1.69	0.41
20:A:812:CLA:H61	20:A:812:CLA:H92	1.79	0.41
20:A:812:CLA:H202	20:A:812:CLA:H161	1.84	0.41
20:A:841:CLA:H101	20:A:841:CLA:H13	1.50	0.41
6:B:61:THR:HB	6:B:142:LEU:HD13	2.02	0.41
6:B:662:MET:HB2	20:B:803:CLA:C1C	2.50	0.41
20:2:308:CLA:H3A	20:2:308:CLA:HBA2	1.42	0.41
6:B:721:TYR:HB2	20:B:802:CLA:HED3	2.02	0.41
23:B:844:BCR:H351	23:B:844:BCR:H15C	1.76	0.41
7:C:2:SER:O	7:C:70:TRP:HB3	2.20	0.41
16:L:144:LEU:HB3	23:L:305:BCR:H401	2.02	0.41
20:N:203:CLA:H3A	20:N:203:CLA:HBA2	1.71	0.41
18:O:73:ILE:HD13	18:O:73:ILE:HA	1.69	0.41
21:2:315:LUT:H401	21:2:315:LUT:H35	1.78	0.41
5:A:323:LEU:O	5:A:335:HIS:HB2	2.20	0.41
5:A:571:PHE:CE1	5:A:585:SER:HB3	2.55	0.41
6:B:552:ASP:OD1	8:D:187:VAL:HG21	2.21	0.41
20:B:813:CLA:H43	23:B:842:BCR:H19C	2.03	0.41
10:F:172:LEU:HD23	10:F:172:LEU:HA	1.89	0.41
1:1:183:LYS:HE2	1:1:183:LYS:HB2	1.75	0.41
21:1:319:LUT:H382	20:4:308:CLA:HBA1	2.03	0.41
3:3:80:LEU:HD21	20:A:811:CLA:H2	2.02	0.41
3:3:234:ALA:HA	20:3:311:CLA:HBB1	2.03	0.41
23:J:104:BCR:H351	23:J:104:BCR:H15C	1.78	0.41
17:N:141:LYS:HE3	17:N:141:LYS:HB2	1.71	0.41
18:O:104:PHE:CD1	18:O:105:PRO:HA	2.55	0.41
18:O:131:PHE:HD1	20:O:203:CLA:HBB1	1.84	0.41
20:O:203:CLA:H11	20:O:203:CLA:HBA2	1.66	0.41
1:1:177:GLY:O	1:1:180:LYS:HG3	2.20	0.41
20:1:321:CLA:HBB1	24:B:849:LHG:HC11	2.02	0.41
20:1:321:CLA:HBC2	26:1:322:HTG:H1'1	2.02	0.41
2:2:166:ASP:OD2	19:2:307:CHL:HBC1	2.21	0.41
21:2:315:LUT:H15	21:2:315:LUT:H201	1.88	0.41
4:4:53:LEU:HD23	4:4:56:LEU:HB2	2.03	0.41
20:A:810:CLA:H61	20:A:810:CLA:H41	1.91	0.41
20:A:836:CLA:H11	20:A:837:CLA:O1A	2.21	0.41
6:B:50:HIS:HE1	20:B:805:CLA:H172	1.86	0.41
8:D:178:ILE:H	8:D:178:ILE:HG13	1.36	0.41
15:K:123:VAL:O	15:K:127:LYS:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:130:THR:HG22	18:O:134:ILE:HD12	2.02	0.41
1:1:143:LEU:HD23	1:1:143:LEU:HA	1.87	0.41
2:2:131:PRO:HG2	20:2:304:CLA:HED2	2.03	0.41
19:2:301:CHL:H11	3:3:160:GLY:HA2	2.03	0.41
20:2:304:CLA:H62	20:2:304:CLA:H92	1.79	0.41
23:3:317:BCR:H351	23:3:317:BCR:H15C	1.72	0.41
4:4:77:LEU:HD21	10:F:202:ILE:HD13	2.01	0.41
20:4:304:CLA:C2B	22:4:317:XAT:H183	2.50	0.41
5:A:93:ALA:HB2	5:A:156:LEU:HB2	2.02	0.41
5:A:200:ALA:HB2	5:A:306:GLY:HA3	2.02	0.41
5:A:609:SER:O	5:A:613:GLN:HG3	2.21	0.41
20:A:805:CLA:H201	24:A:843:LHG:H221	2.03	0.41
20:A:807:CLA:CHC	20:A:808:CLA:HMD2	2.50	0.41
20:A:833:CLA:H61	20:A:833:CLA:H92	1.85	0.41
6:B:158:GLN:HB2	6:B:161:TRP:HE3	1.85	0.41
6:B:257:LEU:HD13	20:B:817:CLA:HMB3	2.02	0.41
6:B:447:GLY:O	10:F:88:GLN:NE2	2.37	0.41
20:B:804:CLA:H3A	20:B:804:CLA:HBA2	1.70	0.41
20:B:831:CLA:H142	23:F:806:BCR:HC8	2.03	0.41
10:F:157:PHE:HB2	23:F:801:BCR:H321	2.01	0.41
23:I:101:BCR:H15C	23:I:101:BCR:H351	1.79	0.41
16:L:56:THR:HB	16:L:57:TYR:H	1.66	0.41
2:2:64:PHE:CD1	19:2:301:CHL:HMA3	2.56	0.41
3:3:270:LYS:HB3	3:3:270:LYS:HE2	1.56	0.41
22:3:316:XAT:H35	22:3:316:XAT:H401	1.81	0.41
4:4:195:GLU:OE2	4:4:199:LYS:NZ	2.54	0.41
5:A:78:LEU:HD22	20:A:804:CLA:H92	2.03	0.41
23:A:847:BCR:H15C	23:A:847:BCR:H351	1.81	0.41
6:B:459:PHE:CZ	20:F:805:CLA:HBB1	2.56	0.41
23:J:102:BCR:H361	23:J:102:BCR:H20C	1.87	0.41
18:O:60:TRP:CD1	18:O:60:TRP:H	2.39	0.41
25:1:323:LMG:H152	25:1:323:LMG:H181	1.79	0.40
2:2:162:ARG:NH1	20:4:301:CLA:OBD	2.54	0.40
2:2:162:ARG:NE	19:2:314:CHL:HMC	2.37	0.40
2:2:176:ASP:HB3	2:2:179:PHE:O	2.20	0.40
3:3:78:LEU:HD23	20:A:811:CLA:C2	2.51	0.40
4:4:214:PHE:HE1	21:4:316:LUT:H41	1.87	0.40
5:A:734:GLY:O	20:A:801:CLA:HED1	2.21	0.40
20:A:835:CLA:HBC1	18:O:84:ILE:HG23	2.03	0.40
20:B:829:CLA:H202	20:B:839:CLA:H3A	2.03	0.40
23:G:606:BCR:H24C	23:G:606:BCR:H371	1.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:478:PRO:HG3	5:A:531:PHE:HB2	2.02	0.40
20:A:818:CLA:HAB	20:A:818:CLA:H8	2.02	0.40
20:A:822:CLA:HBA1	20:O:203:CLA:HBA1	2.04	0.40
23:A:847:BCR:H20C	23:A:847:BCR:H361	1.87	0.40
2:2:258:VAL:HG22	20:2:312:CLA:C3D	2.51	0.40
3:3:232:MET:HG2	22:3:316:XAT:C34	2.51	0.40
20:A:804:CLA:H3A	20:A:804:CLA:HBA1	1.48	0.40
20:A:807:CLA:HBB1	20:A:808:CLA:O1A	2.21	0.40
20:A:816:CLA:H61	20:A:816:CLA:H41	1.73	0.40
20:A:824:CLA:H172	20:A:824:CLA:H13	1.95	0.40
20:A:825:CLA:H202	18:O:123:LEU:HD22	2.03	0.40
20:A:838:CLA:H112	20:A:838:CLA:H151	1.79	0.40
27:A:842:PQN:H261	27:A:842:PQN:H222	1.92	0.40
23:A:846:BCR:H351	23:A:846:BCR:H15C	1.76	0.40
7:C:70:TRP:CG	7:C:71:HIS:H	2.39	0.40
10:F:68:ASP:N	10:F:72:LEU:O	2.54	0.40
10:F:163:TRP:CD1	10:F:200:GLY:HA3	2.56	0.40
2:2:73:LEU:HD11	2:2:84:ASP:HB2	2.03	0.40
2:2:97:TRP:CH2	20:2:308:CLA:HAA2	2.57	0.40
2:2:108:TRP:CE2	20:2:308:CLA:HBC3	2.56	0.40
3:3:150:ASP:OD1	3:3:151:PRO:HD2	2.22	0.40
5:A:150:ILE:HG23	5:A:155:GLN:HE21	1.85	0.40
20:A:802:CLA:H41	20:A:802:CLA:H62	1.90	0.40
10:F:68:ASP:HB3	10:F:69:ILE:H	1.50	0.40
20:1:303:CLA:CBC	20:1:308:CLA:HAC1	2.50	0.40
20:4:303:CLA:H41	20:4:303:CLA:H61	1.75	0.40
5:A:578:ARG:HH21	8:D:115:GLU:CD	2.29	0.40
23:A:845:BCR:H361	23:A:845:BCR:H20C	1.84	0.40
20:B:810:CLA:H91	20:B:810:CLA:H111	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	197/246 (80%)	194 (98%)	3 (2%)	0	100	100
2	2	207/265 (78%)	203 (98%)	3 (1%)	1 (0%)	24	37
3	3	218/272 (80%)	206 (94%)	12 (6%)	0	100	100
4	4	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	716 (98%)	14 (2%)	1 (0%)	48	64
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	139/190 (73%)	135 (97%)	4 (3%)	0	100	100
9	E	61/151 (40%)	59 (97%)	2 (3%)	0	100	100
10	F	151/221 (68%)	150 (99%)	1 (1%)	0	100	100
11	G	96/145 (66%)	95 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	87 (99%)	1 (1%)	0	100	100
13	I	27/36 (75%)	27 (100%)	0	0	100	100
14	J	38/44 (86%)	38 (100%)	0	0	100	100
15	K	81/132 (61%)	75 (93%)	5 (6%)	1 (1%)	10	16
16	L	160/217 (74%)	157 (98%)	3 (2%)	0	100	100
17	N	82/173 (47%)	76 (93%)	5 (6%)	1 (1%)	10	16
18	O	87/144 (60%)	85 (98%)	2 (2%)	0	100	100
All	All	3376/4194 (80%)	3289 (97%)	83 (2%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	172	CYS
6	B	362	ALA
17	N	167	TRP
15	K	96	GLN

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	162/198 (82%)	157 (97%)	5 (3%)	35	57
2	2	168/208 (81%)	165 (98%)	3 (2%)	51	73
3	3	175/217 (81%)	170 (97%)	5 (3%)	37	60
4	4	168/207 (81%)	165 (98%)	3 (2%)	51	73
5	A	600/608 (99%)	584 (97%)	16 (3%)	39	62
6	B	598/599 (100%)	586 (98%)	12 (2%)	48	70
7	C	70/71 (99%)	68 (97%)	2 (3%)	37	60
8	D	121/159 (76%)	117 (97%)	4 (3%)	33	55
9	E	57/124 (46%)	57 (100%)	0	100	100
10	F	126/185 (68%)	118 (94%)	8 (6%)	16	29
11	G	84/125 (67%)	84 (100%)	0	100	100
12	H	72/110 (66%)	71 (99%)	1 (1%)	59	79
13	I	25/31 (81%)	23 (92%)	2 (8%)	11	19
14	J	34/38 (90%)	32 (94%)	2 (6%)	18	31
15	K	61/99 (62%)	59 (97%)	2 (3%)	33	55
16	L	129/176 (73%)	127 (98%)	2 (2%)	55	76
17	N	74/139 (53%)	67 (90%)	7 (10%)	8	13
18	O	73/114 (64%)	69 (94%)	4 (6%)	19	34
All	All	2797/3408 (82%)	2719 (97%)	78 (3%)	38	60

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	53	GLN
1	1	62	SER
1	1	183	LYS
1	1	236	ASP
1	1	241	ARG
2	2	68	THR
2	2	209	LYS
2	2	212	GLU
3	3	226	LYS
3	3	245	THR
3	3	264	ASN
3	3	265	ILE
3	3	270	LYS
4	4	66	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	215	ILE
4	4	220	VAL
5	A	34	ARG
5	A	58	SER
5	A	65	GLU
5	A	70	VAL
5	A	83	LEU
5	A	215	VAL
5	A	218	SER
5	A	229	VAL
5	A	283	THR
5	A	422	ASP
5	A	457	ASP
5	A	512	LEU
5	A	533	VAL
5	A	637	SER
5	A	663	SER
5	A	749	VAL
6	B	4	ARG
6	B	216	LEU
6	B	227	THR
6	B	257	LEU
6	B	325	THR
6	B	363	GLN
6	B	444	LEU
6	B	458	ILE
6	B	501	VAL
6	B	525	LEU
6	B	590	VAL
6	B	645	VAL
7	C	16	GLN
7	C	58	CYS
8	D	53	GLN
8	D	58	THR
8	D	85	GLU
8	D	178	ILE
10	F	68	ASP
10	F	89	ILE
10	F	107	LEU
10	F	114	GLU
10	F	170	SER
10	F	176	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	F	197	ILE
10	F	216	LEU
12	H	105	LYS
13	I	8	SER
13	I	13	LEU
14	J	9	SER
14	J	38	THR
15	K	55	THR
15	K	95	LEU
16	L	112	LEU
16	L	118	VAL
17	N	142	VAL
17	N	151	ILE
17	N	158	ILE
17	N	163	SER
17	N	165	VAL
17	N	167	TRP
17	N	168	LYS
18	O	61	LEU
18	O	73	ILE
18	O	125	LEU
18	O	139	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	112	ASN
1	1	117	GLN
1	1	126	GLN
1	1	156	GLN
1	1	195	ASN
1	1	209	GLN
1	1	210	GLN
1	1	221	ASN
1	1	232	ASN
2	2	174	ASN
2	2	181	ASN
2	2	234	GLN
2	2	235	HIS
2	2	245	ASN
3	3	171	GLN
3	3	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	182	GLN
3	3	206	ASN
3	3	241	GLN
3	3	252	ASN
3	3	264	ASN
4	4	164	GLN
4	4	170	ASN
4	4	239	ASN
5	A	155	GLN
5	A	223	GLN
5	A	477	GLN
5	A	482	GLN
5	A	599	ASN
5	A	607	HIS
5	A	623	GLN
5	A	693	GLN
6	B	98	GLN
6	B	114	ASN
6	B	156	HIS
6	B	218	HIS
6	B	236	ASN
6	B	266	GLN
6	B	277	HIS
6	B	327	ASN
6	B	432	HIS
6	B	520	HIS
6	B	627	ASN
6	B	689	ASN
6	B	704	GLN
7	C	16	GLN
7	C	38	GLN
8	D	131	ASN
8	D	167	ASN
9	E	140	ASN
10	F	112	GLN
10	F	213	ASN
11	G	72	ASN
12	H	134	GLN
15	K	79	ASN
16	L	58	GLN
16	L	61	GLN
16	L	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	L	128	ASN
17	N	101	ASN
18	O	85	ASN
18	O	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

225 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	LHG	A	843	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
20	CLA	A	851	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
28	SF4	A	850	-	0,12,12	-	-	-	-	-
20	CLA	3	312	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
20	CLA	2	313	-	47,51,73	1.37	7 (14%)	55,86,113	1.46	5 (9%)
21	LUT	1	319	-	42,43,43	0.67	0	51,60,60	1.83	14 (27%)
20	CLA	2	312	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	A	830	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	1	311	1	56,60,73	1.30	7 (12%)	65,97,113	1.40	7 (10%)
20	CLA	A	809	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
20	CLA	B	817	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
20	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
20	CLA	A	806	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
20	CLA	B	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	6 (7%)
21	LUT	2	315	-	42,43,43	0.71	0	51,60,60	1.84	15 (29%)
20	CLA	B	809	6	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
19	CHL	4	315	-	37,51,74	4.32	23 (62%)	30,86,114	3.95	12 (40%)
20	CLA	A	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
20	CLA	K	201	15	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
20	CLA	A	836	-	55,59,73	1.30	8 (14%)	64,96,113	1.41	8 (12%)
19	CHL	4	305	-	47,61,74	3.97	23 (48%)	41,98,114	3.12	14 (34%)
20	CLA	L	302	16	49,53,73	1.37	8 (16%)	58,89,113	1.49	4 (6%)
20	CLA	3	314	-	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
26	HTG	4	320	-	19,19,19	1.02	2 (10%)	23,24,24	0.56	0
20	CLA	F	805	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)
20	CLA	3	308	3	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	O	203	-	64,68,73	1.22	7 (10%)	76,107,113	1.30	7 (9%)
20	CLA	2	308	2	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	B	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
21	LUT	O	205	-	42,43,43	0.84	2 (4%)	51,60,60	2.06	12 (23%)
19	CHL	2	307	-	45,59,74	3.92	26 (57%)	40,96,114	3.67	19 (47%)
20	CLA	3	311	3	59,63,73	1.27	8 (13%)	70,101,113	1.33	6 (8%)
20	CLA	1	307	-	65,69,73	1.20	7 (10%)	77,108,113	1.29	5 (6%)
23	BCR	B	841	-	41,41,41	0.69	1 (2%)	56,56,56	1.90	14 (25%)
20	CLA	N	203	-	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
20	CLA	L	307	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	5 (8%)
23	BCR	4	318	-	41,41,41	0.63	0	56,56,56	3.43	23 (41%)
23	BCR	K	204	-	41,41,41	0.66	0	56,56,56	2.03	16 (28%)
20	CLA	1	312	1	69,73,73	1.18	6 (8%)	82,113,113	1.24	5 (6%)
20	CLA	A	835	5	49,53,73	1.38	8 (16%)	58,89,113	1.40	4 (6%)
20	CLA	A	833	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	820	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	5 (7%)
26	HTG	N	201	-	19,19,19	0.98	2 (10%)	23,24,24	0.60	0
23	BCR	L	301	-	41,41,41	0.70	0	56,56,56	1.96	12 (21%)
20	CLA	1	302	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	B	832	-	62,66,73	1.23	7 (11%)	73,104,113	1.37	9 (12%)
25	LMG	4	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.02	3 (5%)
22	XAT	2	316	-	41,47,47	0.89	2 (4%)	54,74,74	2.56	21 (38%)
23	BCR	A	848	-	41,41,41	0.70	1 (2%)	56,56,56	1.90	14 (25%)
20	CLA	A	803	20	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
27	PQN	B	840	-	34,34,34	1.63	2 (5%)	43,45,45	1.17	4 (9%)
20	CLA	A	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
19	CHL	4	306	-	45,59,74	4.16	24 (53%)	40,96,114	3.08	18 (45%)
20	CLA	B	833	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
20	CLA	B	813	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
22	XAT	1	316	-	41,47,47	0.89	2 (4%)	54,74,74	2.51	19 (35%)
20	CLA	4	301	4	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
20	CLA	A	853	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
23	BCR	B	844	-	41,41,41	0.68	0	56,56,56	1.87	15 (26%)
23	BCR	A	845	-	41,41,41	0.69	0	56,56,56	1.95	17 (30%)
20	CLA	B	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
20	CLA	A	807	5	69,73,73	1.14	8 (11%)	82,113,113	1.29	8 (9%)
20	CLA	B	834	-	49,53,73	1.37	8 (16%)	58,89,113	1.42	6 (10%)
26	HTG	1	322	-	19,19,19	0.97	2 (10%)	23,24,24	1.03	3 (13%)
20	CLA	A	822	-	55,59,73	1.30	8 (14%)	64,96,113	1.35	7 (10%)
20	CLA	3	302	-	54,58,73	1.33	7 (12%)	64,95,113	1.35	6 (9%)
20	CLA	K	202	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	8 (10%)
20	CLA	F	804	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
20	CLA	A	810	20	69,73,73	1.16	7 (10%)	82,113,113	1.24	4 (4%)
20	CLA	A	821	-	53,57,73	1.31	8 (15%)	61,93,113	1.41	5 (8%)
20	CLA	3	305	3	51,55,73	1.34	8 (15%)	60,91,113	1.38	4 (6%)
20	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
20	CLA	A	801	-	69,73,73	1.17	7 (10%)	82,113,113	1.40	8 (9%)
20	CLA	N	202	17	48,53,73	1.39	7 (14%)	56,89,113	1.40	4 (7%)
20	CLA	A	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	813	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
20	CLA	2	310	24	45,49,73	1.39	8 (17%)	54,84,113	1.48	5 (9%)
20	CLA	A	814	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	6 (9%)
29	LMT	G	601	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
23	BCR	B	842	-	41,41,41	0.70	1 (2%)	56,56,56	2.04	19 (33%)
20	CLA	4	312	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	4 (4%)
23	BCR	A	846	-	41,41,41	0.71	0	56,56,56	1.98	15 (26%)
26	HTG	A	852	-	19,19,19	1.16	2 (10%)	23,24,24	1.41	3 (13%)
20	CLA	1	321	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	811	-	58,62,73	1.28	7 (12%)	68,99,113	1.31	5 (7%)
26	HTG	J	105	-	19,19,19	1.01	2 (10%)	23,24,24	0.55	0
20	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
19	CHL	2	301	2	47,61,74	4.13	30 (63%)	41,98,114	5.07	21 (51%)
20	CLA	4	313	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
23	BCR	A	847	-	41,41,41	0.65	0	56,56,56	2.01	17 (30%)
20	CLA	3	301	3	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
26	HTG	B	850	-	19,19,19	0.97	2 (10%)	23,24,24	0.81	0
23	BCR	J	102	-	41,41,41	0.65	0	56,56,56	1.98	17 (30%)
20	CLA	2	309	2	64,68,73	1.21	9 (14%)	76,107,113	1.28	6 (7%)
25	LMG	1	323	-	44,44,55	0.99	2 (4%)	52,52,63	1.05	3 (5%)
20	CLA	B	830	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
20	CLA	1	313	-	59,63,73	1.25	8 (13%)	70,101,113	1.35	5 (7%)
20	CLA	2	303	-	53,57,73	1.32	8 (15%)	61,93,113	1.39	4 (6%)
20	CLA	4	314	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	6 (9%)
20	CLA	K	203	-	50,54,73	1.35	8 (16%)	59,90,113	1.43	5 (8%)
20	CLA	3	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	5 (8%)
20	CLA	B	815	-	64,68,73	1.19	8 (12%)	76,107,113	1.31	6 (7%)
20	CLA	G	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	6 (9%)
28	SF4	C	101	-	0,12,12	-	-	-	-	-
20	CLA	4	308	4	54,58,73	1.30	7 (12%)	64,95,113	1.39	6 (9%)
20	CLA	A	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
19	CHL	4	307	-	45,59,74	4.04	26 (57%)	40,96,114	3.66	13 (32%)
23	BCR	2	317	-	41,41,41	0.73	0	56,56,56	2.14	16 (28%)
20	CLA	B	811	-	58,62,73	1.35	8 (13%)	71,100,113	1.36	8 (11%)
20	CLA	B	810	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	L	305	-	41,41,41	0.68	0	56,56,56	2.10	14 (25%)
20	CLA	H	201	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	6 (8%)
20	CLA	4	303	-	64,68,73	1.21	8 (12%)	76,107,113	1.31	5 (6%)
23	BCR	I	101	-	41,41,41	0.74	2 (4%)	56,56,56	2.09	17 (30%)
20	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
20	CLA	B	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
23	BCR	B	843	-	41,41,41	0.69	0	56,56,56	2.05	15 (26%)
20	CLA	J	103	14	46,50,73	1.40	8 (17%)	53,85,113	1.42	4 (7%)
20	CLA	1	304	-	56,60,73	1.29	8 (14%)	65,97,113	1.39	6 (9%)
24	LHG	B	849	-	22,22,48	1.20	2 (9%)	25,28,54	1.03	1 (4%)
20	CLA	B	835	-	55,59,73	1.30	8 (14%)	64,96,113	1.37	7 (10%)
22	XAT	4	317	-	41,47,47	0.89	1 (2%)	54,74,74	2.55	20 (37%)
20	CLA	A	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
20	CLA	G	605	11	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
27	PQN	A	842	-	34,34,34	1.66	2 (5%)	43,45,45	1.10	4 (9%)
20	CLA	2	311	2	56,60,73	1.29	7 (12%)	65,97,113	1.41	6 (9%)
26	HTG	G	602	-	19,19,19	0.99	2 (10%)	23,24,24	0.55	0
24	LHG	1	318	20	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
20	CLA	A	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
20	CLA	3	304	-	46,50,73	1.39	8 (17%)	53,85,113	1.45	6 (11%)
22	XAT	3	316	-	41,47,47	0.88	1 (2%)	54,74,74	2.65	21 (38%)
25	LMG	1	320	-	49,49,55	0.94	2 (4%)	57,57,63	1.03	3 (5%)
23	BCR	A	849	-	41,41,41	0.71	0	56,56,56	1.97	14 (25%)
20	CLA	B	816	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
20	CLA	B	823	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	7 (9%)
20	CLA	A	832	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
20	CLA	1	303	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	B	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
26	HTG	B	851	-	19,19,19	0.98	2 (10%)	23,24,24	0.51	0
20	CLA	G	603	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
20	CLA	A	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	F	802	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
20	CLA	A	834	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	L	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	A	802	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	818	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
19	CHL	2	306	-	42,56,74	4.11	22 (52%)	36,92,114	3.65	14 (38%)
20	CLA	3	313	-	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
20	CLA	A	808	5	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	A	827	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	819	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
20	CLA	4	302	4	64,68,73	1.20	8 (12%)	76,107,113	1.31	7 (9%)
23	BCR	1	317	-	41,41,41	0.64	0	56,56,56	1.93	18 (32%)
20	CLA	A	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
20	CLA	K	205	15	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
23	BCR	F	801	-	41,41,41	0.66	0	56,56,56	1.81	14 (25%)
24	LHG	2	318	20	36,36,48	1.07	2 (5%)	39,42,54	1.14	3 (7%)
20	CLA	3	310	-	56,60,73	1.31	8 (14%)	65,97,113	1.37	5 (7%)
26	HTG	F	803	-	19,19,19	1.00	2 (10%)	23,24,24	0.55	0
28	SF4	C	102	-	0,12,12	-	-	-	-	-
20	CLA	4	309	4	64,68,73	1.20	9 (14%)	76,107,113	1.28	8 (10%)
20	CLA	O	201	24	56,60,73	1.29	8 (14%)	65,97,113	1.34	5 (7%)
20	CLA	2	304	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
20	CLA	3	309	-	50,54,73	1.78	12 (24%)	59,90,113	2.30	16 (27%)
19	CHL	2	305	-	37,51,74	4.34	23 (62%)	30,86,114	4.93	13 (43%)
20	CLA	B	827	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
20	CLA	3	307	3	54,58,73	1.30	8 (14%)	64,95,113	1.40	7 (10%)
20	CLA	A	820	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
23	BCR	B	845	-	41,41,41	0.66	0	56,56,56	2.00	17 (30%)
20	CLA	B	819	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
20	CLA	1	310	24	45,49,73	1.40	8 (17%)	54,84,113	1.49	6 (11%)
21	LUT	O	204	-	42,43,43	0.72	0	51,60,60	1.85	14 (27%)
24	LHG	A	844	20	26,26,48	1.26	2 (7%)	29,32,54	1.33	4 (13%)
20	CLA	J	101	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
20	CLA	1	309	1	64,68,73	1.18	7 (10%)	76,107,113	1.28	7 (9%)
20	CLA	1	308	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
20	CLA	A	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	8 (9%)
20	CLA	A	837	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	7 (8%)
20	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
20	CLA	B	804	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	8 (9%)
20	CLA	L	304	-	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)
19	CHL	1	301	1	46,60,74	3.94	18 (39%)	40,97,114	2.40	15 (37%)
20	CLA	2	302	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
20	CLA	B	837	-	51,55,73	1.34	8 (15%)	60,91,113	1.38	5 (8%)
19	CHL	2	314	2	37,51,74	4.23	17 (45%)	30,86,114	2.88	12 (40%)
20	CLA	A	816	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
20	CLA	A	841	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
23	BCR	B	846	-	41,41,41	0.67	0	56,56,56	1.77	15 (26%)
20	CLA	B	806	6	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
23	BCR	J	104	-	41,41,41	0.65	0	56,56,56	1.98	14 (25%)
23	BCR	L	306	-	41,41,41	0.70	0	56,56,56	2.10	12 (21%)
21	LUT	3	315	-	42,43,43	0.71	0	51,60,60	1.71	15 (29%)
20	CLA	B	801	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
23	BCR	F	806	-	41,41,41	0.70	0	56,56,56	2.03	15 (26%)
20	CLA	B	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
19	CHL	3	306	-	41,55,74	4.17	27 (65%)	35,91,114	4.02	18 (51%)
30	DGD	B	848	-	67,67,67	0.84	2 (2%)	81,81,81	0.95	5 (6%)
20	CLA	1	305	-	56,60,73	1.30	8 (14%)	65,97,113	1.34	6 (9%)
23	BCR	A	854	-	41,41,41	0.66	0	56,56,56	1.95	12 (21%)
23	BCR	G	606	-	41,41,41	0.64	0	56,56,56	1.96	17 (30%)
20	CLA	A	829	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	6 (7%)
20	CLA	4	311	4	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
20	CLA	B	821	-	60,64,73	1.25	8 (13%)	71,102,113	1.33	5 (7%)
21	LUT	1	315	-	42,43,43	0.72	0	51,60,60	1.77	14 (27%)
26	HTG	F	807	-	19,19,19	0.96	2 (10%)	23,24,24	0.52	0
29	LMT	B	847	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	A	815	-	49,53,73	1.38	7 (14%)	58,89,113	1.42	4 (6%)
19	CHL	1	306	1	42,56,74	4.17	23 (54%)	36,92,114	3.11	16 (44%)
20	CLA	B	818	-	64,68,73	1.20	7 (10%)	76,107,113	1.28	4 (5%)
20	CLA	A	823	-	59,63,73	1.26	8 (13%)	70,101,113	1.32	6 (8%)
20	CLA	B	812	-	59,63,73	1.26	8 (13%)	70,101,113	1.33	5 (7%)
20	CLA	B	807	-	59,63,73	1.25	8 (13%)	70,101,113	1.33	6 (8%)
20	CLA	4	310	-	59,63,73	1.25	7 (11%)	70,101,113	1.27	5 (7%)
20	CLA	A	840	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	822	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
21	LUT	4	316	-	42,43,43	0.72	0	51,60,60	1.74	14 (27%)
23	BCR	3	317	-	41,41,41	0.63	0	56,56,56	2.01	16 (28%)
20	CLA	O	202	-	49,53,73	1.65	10 (20%)	58,89,113	1.87	8 (13%)
20	CLA	1	314	1	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
20	CLA	A	804	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
20	CLA	4	304	-	54,58,73	1.72	15 (27%)	64,95,113	3.32	20 (31%)

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
24	LHG	A	843	-	-	7/53/53/53	-
20	CLA	A	851	-	1/1/15/20	11/39/115/115	-
28	SF4	A	850	-	-	-	0/6/5/5
20	CLA	3	312	-	1/1/11/20	5/15/91/115	-
20	CLA	2	313	-	1/1/10/20	4/13/89/115	-
21	LUT	1	319	-	-	2/29/67/67	0/2/2/2
20	CLA	2	312	2	1/1/15/20	8/39/115/115	-
20	CLA	A	830	-	1/1/12/20	2/21/97/115	-
20	CLA	B	838	-	1/1/15/20	7/39/115/115	-
20	CLA	1	311	1	1/1/12/20	7/24/100/115	-
20	CLA	A	809	-	1/1/15/20	12/39/115/115	-
20	CLA	B	817	-	1/1/15/20	14/39/115/115	-
20	CLA	B	824	-	1/1/15/20	14/39/115/115	-
20	CLA	A	806	-	1/1/15/20	9/39/115/115	-
20	CLA	B	828	-	1/1/15/20	11/39/115/115	-
21	LUT	2	315	-	-	1/29/67/67	0/2/2/2
20	CLA	B	809	6	1/1/15/20	4/39/115/115	-
19	CHL	4	315	-	3/3/15/26	4/12/110/137	-
20	CLA	A	812	-	1/1/15/20	12/39/115/115	-
20	CLA	B	802	-	1/1/15/20	5/39/115/115	-
20	CLA	K	201	15	1/1/11/20	2/17/93/115	-
20	CLA	A	836	-	1/1/12/20	5/23/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	4	305	-	3/3/17/26	5/24/122/137	-
20	CLA	L	302	16	1/1/11/20	6/15/91/115	-
20	CLA	3	314	-	1/1/11/20	3/17/93/115	-
26	HTG	4	320	-	-	2/10/30/30	0/1/1/1
20	CLA	F	805	-	1/1/11/20	8/17/93/115	-
20	CLA	3	308	3	1/1/12/20	1/21/97/115	-
20	CLA	O	203	-	1/1/14/20	7/33/109/115	-
20	CLA	2	308	2	1/1/12/20	4/21/97/115	-
20	CLA	B	839	-	1/1/15/20	8/39/115/115	-
21	LUT	O	205	-	-	6/29/67/67	0/2/2/2
19	CHL	2	307	-	3/3/17/26	9/21/119/137	-
20	CLA	3	311	3	1/1/13/20	3/27/103/115	-
20	CLA	1	307	-	1/1/14/20	13/35/111/115	-
23	BCR	B	841	-	-	3/29/63/63	0/2/2/2
20	CLA	N	203	-	1/1/12/20	9/21/97/115	-
20	CLA	L	307	-	1/1/11/20	9/15/91/115	-
23	BCR	4	318	-	-	6/29/63/63	0/2/2/2
23	BCR	K	204	-	-	5/29/63/63	0/2/2/2
20	CLA	1	312	1	1/1/15/20	11/39/115/115	-
20	CLA	A	835	5	1/1/11/20	8/15/91/115	-
20	CLA	A	833	-	1/1/15/20	9/39/115/115	-
20	CLA	B	820	-	1/1/12/20	0/21/97/115	-
26	HTG	N	201	-	-	2/10/30/30	0/1/1/1
23	BCR	L	301	-	-	4/29/63/63	0/2/2/2
20	CLA	1	302	1	1/1/15/20	9/39/115/115	-
20	CLA	B	832	-	1/1/13/20	3/31/107/115	-
25	LMG	4	319	-	-	6/39/59/70	0/1/1/1
22	XAT	2	316	-	-	1/31/93/93	0/4/4/4
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	CLA	A	803	20	1/1/13/20	4/27/103/115	-
27	PQN	B	840	-	-	1/23/43/43	0/2/2/2
20	CLA	A	824	-	1/1/15/20	9/39/115/115	-
19	CHL	4	306	-	3/3/17/26	10/21/119/137	-
20	CLA	B	833	-	1/1/15/20	11/39/115/115	-
20	CLA	A	831	-	1/1/15/20	18/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	813	-	1/1/15/20	12/39/115/115	-
22	XAT	1	316	-	-	1/31/93/93	0/4/4/4
20	CLA	4	301	4	1/1/11/20	7/17/93/115	-
20	CLA	A	853	-	1/1/15/20	16/39/115/115	-
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
23	BCR	A	845	-	-	6/29/63/63	0/2/2/2
20	CLA	B	814	-	1/1/15/20	3/39/115/115	-
20	CLA	A	807	5	1/1/15/20	11/39/115/115	-
20	CLA	B	834	-	1/1/11/20	0/15/91/115	-
26	HTG	1	322	-	-	0/10/30/30	0/1/1/1
20	CLA	A	822	-	1/1/12/20	8/23/99/115	-
20	CLA	3	302	-	1/1/12/20	6/21/97/115	-
20	CLA	K	202	-	1/1/14/20	8/33/109/115	-
20	CLA	F	804	-	1/1/11/20	4/15/91/115	-
20	CLA	A	810	20	1/1/15/20	18/39/115/115	-
20	CLA	A	821	-	1/1/11/20	9/20/96/115	-
20	CLA	3	305	3	1/1/11/20	8/18/94/115	-
20	CLA	B	808	-	1/1/15/20	7/39/115/115	-
20	CLA	A	801	-	1/1/15/20	11/39/115/115	-
20	CLA	N	202	17	1/1/11/20	3/15/91/115	-
20	CLA	A	825	-	1/1/15/20	3/39/115/115	-
20	CLA	A	813	-	1/1/11/20	2/15/91/115	-
20	CLA	2	310	24	1/1/10/20	2/10/86/115	-
20	CLA	A	814	-	1/1/12/20	5/21/97/115	-
29	LMT	G	601	-	-	4/21/61/61	0/2/2/2
23	BCR	B	842	-	-	6/29/63/63	0/2/2/2
20	CLA	4	312	-	1/1/15/20	14/39/115/115	-
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
26	HTG	A	852	-	-	2/10/30/30	0/1/1/1
20	CLA	1	321	-	1/1/15/20	6/39/115/115	-
20	CLA	A	811	-	1/1/12/20	5/26/102/115	-
26	HTG	J	105	-	-	0/10/30/30	0/1/1/1
20	CLA	B	831	-	1/1/15/20	13/39/115/115	-
19	CHL	2	301	2	3/3/17/26	7/24/122/137	-
20	CLA	4	313	-	1/1/11/20	1/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	847	-	-	2/29/63/63	0/2/2/2
20	CLA	3	301	3	1/1/14/20	8/33/109/115	-
26	HTG	B	850	-	-	7/10/30/30	0/1/1/1
23	BCR	J	102	-	-	7/29/63/63	0/2/2/2
20	CLA	2	309	2	1/1/14/20	5/33/109/115	-
25	LMG	1	323	-	-	10/39/59/70	0/1/1/1
20	CLA	B	830	-	1/1/12/20	5/21/97/115	-
20	CLA	1	313	-	1/1/13/20	12/27/103/115	-
20	CLA	2	303	-	1/1/11/20	8/20/96/115	-
20	CLA	4	314	-	1/1/12/20	8/21/97/115	-
20	CLA	K	203	-	1/1/11/20	6/17/93/115	-
20	CLA	3	303	-	1/1/11/20	3/15/91/115	-
20	CLA	B	815	-	1/1/14/20	11/33/109/115	-
20	CLA	G	604	-	1/1/12/20	5/21/97/115	-
28	SF4	C	101	-	-	-	0/6/5/5
20	CLA	4	308	4	1/1/12/20	6/21/97/115	-
20	CLA	A	805	-	1/1/15/20	15/39/115/115	-
19	CHL	4	307	-	3/3/17/26	3/21/119/137	-
23	BCR	2	317	-	-	0/29/63/63	0/2/2/2
20	CLA	B	811	-	1/1/13/20	8/25/101/115	-
20	CLA	B	810	-	1/1/15/20	10/39/115/115	-
23	BCR	L	305	-	-	4/29/63/63	0/2/2/2
20	CLA	H	201	-	1/1/13/20	11/29/105/115	-
20	CLA	4	303	-	1/1/14/20	8/33/109/115	-
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
20	CLA	B	805	-	1/1/15/20	14/39/115/115	-
20	CLA	B	826	-	1/1/15/20	2/39/115/115	-
23	BCR	B	843	-	-	4/29/63/63	0/2/2/2
20	CLA	J	103	14	1/1/10/20	4/12/88/115	-
20	CLA	1	304	-	1/1/12/20	5/24/100/115	-
24	LHG	B	849	-	-	7/26/26/53	-
20	CLA	B	835	-	1/1/12/20	2/23/99/115	-
22	XAT	4	317	-	-	0/31/93/93	0/4/4/4
20	CLA	A	826	-	1/1/15/20	5/39/115/115	-
20	CLA	G	605	11	1/1/11/20	5/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PQN	A	842	-	-	7/23/43/43	0/2/2/2
20	CLA	2	311	2	1/1/12/20	7/24/100/115	-
26	HTG	G	602	-	-	0/10/30/30	0/1/1/1
24	LHG	1	318	20	-	12/53/53/53	-
20	CLA	A	817	-	1/1/15/20	16/39/115/115	-
20	CLA	3	304	-	1/1/10/20	1/12/88/115	-
22	XAT	3	316	-	-	0/31/93/93	0/4/4/4
25	LMG	1	320	-	-	9/44/64/70	0/1/1/1
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	6/27/103/115	-
20	CLA	B	823	-	1/1/14/20	11/33/109/115	-
20	CLA	A	832	-	1/1/15/20	8/39/115/115	-
20	CLA	1	303	-	1/1/15/20	10/39/115/115	-
20	CLA	B	829	-	1/1/15/20	4/39/115/115	-
26	HTG	B	851	-	-	2/10/30/30	0/1/1/1
20	CLA	G	603	-	1/1/11/20	4/15/91/115	-
20	CLA	A	838	-	1/1/15/20	10/39/115/115	-
20	CLA	F	802	-	1/1/15/20	7/39/115/115	-
20	CLA	A	834	-	1/1/15/20	9/39/115/115	-
20	CLA	L	303	-	1/1/15/20	10/39/115/115	-
20	CLA	A	802	-	1/1/15/20	13/39/115/115	-
20	CLA	A	818	-	1/1/15/20	7/39/115/115	-
19	CHL	2	306	-	3/3/16/26	11/18/116/137	-
20	CLA	3	313	-	1/1/11/20	2/15/91/115	-
20	CLA	A	808	5	1/1/15/20	17/39/115/115	-
20	CLA	A	827	-	1/1/15/20	11/39/115/115	-
20	CLA	A	819	-	1/1/11/20	2/15/91/115	-
20	CLA	4	302	4	1/1/14/20	9/33/109/115	-
23	BCR	1	317	-	-	2/29/63/63	0/2/2/2
20	CLA	A	839	-	1/1/15/20	14/39/115/115	-
20	CLA	K	205	15	1/1/11/20	2/15/91/115	-
23	BCR	F	801	-	-	3/29/63/63	0/2/2/2
24	LHG	2	318	20	-	11/41/41/53	-
20	CLA	3	310	-	1/1/12/20	2/24/100/115	-
26	HTG	F	803	-	-	2/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	C	102	-	-	-	0/6/5/5
20	CLA	4	309	4	1/1/14/20	7/33/109/115	-
20	CLA	O	201	24	1/1/12/20	10/24/100/115	-
20	CLA	2	304	-	1/1/14/20	12/33/109/115	-
20	CLA	B	827	-	1/1/15/20	12/39/115/115	-
19	CHL	2	305	-	3/3/15/26	6/12/110/137	-
20	CLA	3	309	-	-	4/17/93/115	-
20	CLA	3	307	3	1/1/12/20	5/21/97/115	-
20	CLA	A	820	-	1/1/15/20	9/39/115/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
20	CLA	B	819	-	1/1/15/20	9/39/115/115	-
20	CLA	1	310	24	1/1/10/20	2/10/86/115	-
21	LUT	O	204	-	-	0/29/67/67	0/2/2/2
24	LHG	A	844	20	-	11/31/31/53	-
20	CLA	J	101	-	1/1/15/20	5/39/115/115	-
20	CLA	1	309	1	1/1/14/20	4/33/109/115	-
20	CLA	1	308	1	1/1/15/20	14/39/115/115	-
20	CLA	A	828	-	1/1/15/20	9/39/115/115	-
20	CLA	A	837	-	1/1/15/20	12/39/115/115	-
20	CLA	B	803	-	1/1/15/20	10/39/115/115	-
20	CLA	B	804	-	1/1/11/20	5/15/91/115	-
20	CLA	B	825	-	1/1/15/20	15/39/115/115	-
20	CLA	L	304	-	1/1/12/20	2/21/97/115	-
19	CHL	1	301	1	3/3/17/26	9/23/121/137	-
20	CLA	2	302	2	1/1/15/20	8/39/115/115	-
20	CLA	B	837	-	1/1/11/20	2/18/94/115	-
19	CHL	2	314	2	3/3/15/26	3/12/110/137	-
20	CLA	A	816	-	1/1/15/20	12/39/115/115	-
20	CLA	A	841	-	1/1/15/20	22/39/115/115	-
23	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	B	806	6	1/1/15/20	13/39/115/115	-
23	BCR	J	104	-	-	2/29/63/63	0/2/2/2
23	BCR	L	306	-	-	0/29/63/63	0/2/2/2
21	LUT	3	315	-	-	2/29/67/67	0/2/2/2
20	CLA	B	801	-	1/1/15/20	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	F	806	-	-	2/29/63/63	0/2/2/2
20	CLA	B	836	-	1/1/15/20	6/39/115/115	-
19	CHL	3	306	-	3/3/16/26	5/17/115/137	-
30	DGD	B	848	-	-	10/55/95/95	0/2/2/2
20	CLA	1	305	-	1/1/12/20	3/24/100/115	-
23	BCR	A	854	-	-	0/29/63/63	0/2/2/2
23	BCR	G	606	-	-	0/29/63/63	0/2/2/2
20	CLA	A	829	-	1/1/15/20	9/39/115/115	-
20	CLA	4	311	4	1/1/12/20	5/24/100/115	-
20	CLA	B	821	-	1/1/13/20	11/29/105/115	-
21	LUT	1	315	-	-	2/29/67/67	0/2/2/2
26	HTG	F	807	-	-	2/10/30/30	0/1/1/1
29	LMT	B	847	-	-	6/21/61/61	0/2/2/2
20	CLA	A	815	-	1/1/11/20	2/15/91/115	-
19	CHL	1	306	1	3/3/16/26	10/18/116/137	-
20	CLA	B	818	-	1/1/14/20	10/33/109/115	-
20	CLA	A	823	-	1/1/13/20	4/27/103/115	-
20	CLA	B	812	-	1/1/13/20	8/27/103/115	-
20	CLA	B	807	-	1/1/13/20	7/27/103/115	-
20	CLA	4	310	-	1/1/13/20	7/27/103/115	-
20	CLA	A	840	-	1/1/15/20	7/39/115/115	-
20	CLA	B	822	-	1/1/15/20	12/39/115/115	-
21	LUT	4	316	-	-	1/29/67/67	0/2/2/2
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
20	CLA	O	202	-	1/1/11/20	8/15/91/115	-
20	CLA	1	314	1	1/1/11/20	3/17/93/115	-
20	CLA	A	804	-	1/1/15/20	8/39/115/115	-
20	CLA	4	304	-	1/1/12/20	7/21/97/115	-

All (1534) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	301	CHL	C2C-C3C	11.03	1.47	1.36
19	1	306	CHL	C2C-C3C	10.71	1.46	1.36
19	4	306	CHL	C2C-C3C	10.62	1.46	1.36
19	4	315	CHL	C2C-C3C	10.56	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	301	CHL	C2C-C3C	10.50	1.46	1.36
19	4	305	CHL	C2C-C3C	10.47	1.46	1.36
19	2	314	CHL	C2C-C3C	10.42	1.46	1.36
19	4	306	CHL	C1D-C2D	10.34	1.51	1.39
19	2	306	CHL	C2C-C3C	10.27	1.46	1.36
19	1	301	CHL	C1D-C2D	10.22	1.51	1.39
19	3	306	CHL	C2C-C3C	10.21	1.46	1.36
19	2	305	CHL	C2C-C3C	10.21	1.46	1.36
19	4	307	CHL	C2C-C3C	10.19	1.46	1.36
19	1	306	CHL	C1D-C2D	10.18	1.51	1.39
19	4	315	CHL	C1D-C2D	10.16	1.51	1.39
19	2	307	CHL	C2C-C3C	10.12	1.46	1.36
19	3	306	CHL	C1D-C2D	10.12	1.51	1.39
19	4	305	CHL	C1D-C2D	10.11	1.51	1.39
19	2	305	CHL	C1D-C2D	10.07	1.51	1.39
19	2	301	CHL	C1D-C2D	10.06	1.51	1.39
19	2	314	CHL	C1D-C2D	10.06	1.51	1.39
19	2	306	CHL	C1D-C2D	10.01	1.51	1.39
19	4	307	CHL	C1D-C2D	9.92	1.50	1.39
19	2	307	CHL	C1D-C2D	9.89	1.50	1.39
19	2	306	CHL	C1B-C2B	8.49	1.49	1.39
19	4	315	CHL	C1B-C2B	8.48	1.49	1.39
19	2	314	CHL	C1B-C2B	8.48	1.49	1.39
19	2	301	CHL	C1B-C2B	8.45	1.49	1.39
19	4	307	CHL	C1B-C2B	8.34	1.49	1.39
19	1	306	CHL	C1B-C2B	8.28	1.49	1.39
19	1	301	CHL	C1B-C2B	8.24	1.48	1.39
19	2	305	CHL	C1B-C2B	8.20	1.48	1.39
19	4	306	CHL	C1B-C2B	8.15	1.48	1.39
19	4	305	CHL	C1B-C2B	8.13	1.48	1.39
19	3	306	CHL	C1B-C2B	8.07	1.48	1.39
19	2	305	CHL	C1A-CHA	8.06	1.49	1.40
19	1	306	CHL	C3B-C4B	7.93	1.49	1.41
19	3	306	CHL	C3B-C4B	7.91	1.49	1.41
27	A	842	PQN	C3-C2	7.88	1.49	1.35
19	2	305	CHL	C3B-C4B	7.87	1.49	1.41
19	4	306	CHL	C3B-C4B	7.86	1.49	1.41
19	2	307	CHL	C1B-C2B	7.82	1.48	1.39
27	B	840	PQN	C3-C2	7.76	1.49	1.35
19	1	301	CHL	C3B-C4B	7.73	1.48	1.41
19	2	301	CHL	C3B-C4B	7.67	1.48	1.41
19	2	301	CHL	C1A-CHA	7.55	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	306	CHL	C3B-C4B	7.55	1.48	1.41
19	2	314	CHL	C1A-CHA	7.53	1.48	1.40
19	2	314	CHL	C3B-C4B	7.53	1.48	1.41
19	4	305	CHL	C1A-CHA	7.48	1.48	1.40
19	2	306	CHL	C1A-CHA	7.46	1.48	1.40
19	4	306	CHL	CBD-CGD	-7.43	1.43	1.52
19	4	315	CHL	C1A-CHA	7.41	1.48	1.40
19	4	315	CHL	C3B-C4B	7.40	1.48	1.41
19	4	307	CHL	C1A-CHA	7.34	1.48	1.40
19	4	305	CHL	C3B-C4B	7.32	1.48	1.41
19	2	307	CHL	C1A-CHA	7.32	1.48	1.40
19	3	306	CHL	C1A-CHA	7.26	1.48	1.40
19	1	306	CHL	C1A-CHA	7.21	1.48	1.40
19	2	307	CHL	C3B-C4B	7.15	1.48	1.41
19	4	307	CHL	C3B-C4B	7.08	1.48	1.41
19	1	301	CHL	C1A-CHA	7.08	1.48	1.40
19	4	306	CHL	C1A-CHA	7.06	1.48	1.40
19	4	305	CHL	CBD-CGD	-6.59	1.44	1.52
19	1	306	CHL	CBD-CGD	-5.71	1.45	1.52
19	2	301	CHL	O1D-CGD	-5.69	1.06	1.21
19	4	307	CHL	CBD-CGD	-5.48	1.45	1.52
19	2	301	CHL	OBD-CAD	-5.45	1.15	1.22
19	4	306	CHL	C3D-C4D	-5.33	1.33	1.41
20	3	309	CLA	CAA-C2A	-5.31	1.44	1.54
19	1	306	CHL	C3D-C4D	-5.28	1.33	1.41
19	2	306	CHL	C3D-C4D	-5.24	1.33	1.41
19	3	306	CHL	C3D-C4D	-5.23	1.33	1.41
19	2	307	CHL	C3D-C4D	-5.23	1.33	1.41
19	1	301	CHL	C3D-C4D	-5.22	1.33	1.41
19	4	307	CHL	C3D-C4D	-5.19	1.33	1.41
19	4	305	CHL	C3D-C4D	-5.18	1.33	1.41
19	1	301	CHL	CHC-C4B	5.15	1.48	1.39
19	2	305	CHL	C3D-C4D	-5.10	1.33	1.41
19	2	314	CHL	O2D-CGD	5.08	1.45	1.33
19	4	315	CHL	C3D-C4D	-5.07	1.33	1.41
19	2	314	CHL	C3D-C4D	-5.06	1.33	1.41
19	1	301	CHL	O2D-CGD	5.04	1.45	1.33
19	2	307	CHL	CHB-C4A	-5.03	1.32	1.38
19	2	301	CHL	C3D-C4D	-5.03	1.33	1.41
27	B	840	PQN	C10-C5	5.02	1.48	1.40
27	A	842	PQN	C10-C5	5.01	1.48	1.40
19	1	306	CHL	C3B-C2B	5.00	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	306	CHL	CHC-C4B	5.00	1.47	1.39
19	4	305	CHL	CHB-C4A	-4.99	1.32	1.38
19	4	305	CHL	O2A-CGA	4.97	1.47	1.33
19	3	306	CHL	CHB-C4A	-4.96	1.32	1.38
19	1	306	CHL	CHC-C4B	4.96	1.47	1.39
19	2	314	CHL	OBD-CAD	4.95	1.28	1.22
19	1	301	CHL	OBD-CAD	4.94	1.28	1.22
19	3	306	CHL	CHC-C4B	4.86	1.47	1.39
19	1	301	CHL	CHD-C4C	4.86	1.48	1.39
19	2	306	CHL	CBD-CGD	-4.84	1.46	1.52
19	4	305	CHL	C3A-C2A	-4.83	1.50	1.54
19	4	307	CHL	CHB-C4A	-4.82	1.32	1.38
19	4	307	CHL	C3B-C2B	4.82	1.46	1.40
19	4	306	CHL	OMC-CMC	-4.81	1.11	1.22
19	4	306	CHL	CHB-C4A	-4.79	1.32	1.38
19	2	305	CHL	CHC-C4B	4.79	1.47	1.39
19	1	301	CHL	C3B-C2B	4.78	1.46	1.40
19	2	305	CHL	C3A-C2A	-4.78	1.50	1.54
19	4	315	CHL	C3B-C2B	4.78	1.46	1.40
19	4	306	CHL	CHD-C4C	4.76	1.48	1.39
19	1	301	CHL	CHC-C1C	4.76	1.48	1.39
19	1	301	CHL	CHD-C1D	4.75	1.47	1.39
19	2	301	CHL	CHB-C4A	-4.75	1.32	1.38
20	O	202	CLA	O2D-CGD	4.74	1.44	1.33
19	2	301	CHL	C3B-C2B	4.73	1.46	1.40
19	2	301	CHL	CHC-C4B	4.73	1.47	1.39
19	2	305	CHL	CHB-C4A	-4.72	1.32	1.38
19	2	305	CHL	C3B-C2B	4.72	1.46	1.40
19	2	306	CHL	CHB-C4A	-4.71	1.32	1.38
19	2	314	CHL	C3B-C2B	4.71	1.46	1.40
19	2	306	CHL	C3B-C2B	4.71	1.46	1.40
19	3	306	CHL	C3B-C2B	4.71	1.46	1.40
19	4	305	CHL	CHC-C4B	4.70	1.47	1.39
19	1	306	CHL	CHD-C4C	4.70	1.48	1.39
19	4	307	CHL	CHC-C4B	4.68	1.47	1.39
19	4	315	CHL	CHC-C4B	4.68	1.47	1.39
19	2	314	CHL	C3A-C2A	-4.68	1.50	1.54
19	4	305	CHL	CHD-C4C	4.68	1.48	1.39
19	2	307	CHL	C3A-C2A	-4.67	1.50	1.54
19	1	306	CHL	CHB-C1B	4.67	1.47	1.39
19	2	306	CHL	C3A-C2A	-4.66	1.50	1.54
19	4	306	CHL	CHD-C1D	4.66	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	306	CHL	CHC-C1C	4.66	1.48	1.39
19	2	314	CHL	CHC-C4B	4.66	1.47	1.39
19	4	315	CHL	CHD-C4C	4.65	1.48	1.39
19	4	315	CHL	CHB-C4A	-4.65	1.33	1.38
19	4	306	CHL	C3B-C2B	4.65	1.46	1.40
19	1	306	CHL	CHD-C1D	4.65	1.47	1.39
19	4	315	CHL	C3A-C2A	-4.64	1.50	1.54
19	1	301	CHL	C3D-C2D	4.63	1.47	1.39
19	2	301	CHL	OMC-CMC	-4.63	1.11	1.22
19	3	306	CHL	CHD-C4C	4.62	1.48	1.39
19	1	301	CHL	CHB-C1B	4.61	1.47	1.39
19	2	314	CHL	CHB-C4A	-4.60	1.33	1.38
19	2	306	CHL	CHD-C4C	4.60	1.48	1.39
19	2	306	CHL	CHC-C4B	4.59	1.47	1.39
19	2	307	CHL	CHC-C4B	4.59	1.47	1.39
19	4	306	CHL	C3A-C2A	-4.58	1.50	1.54
19	1	306	CHL	CHB-C4A	-4.55	1.33	1.38
19	2	305	CHL	CHD-C4C	4.54	1.48	1.39
19	4	307	CHL	CHD-C4C	4.53	1.48	1.39
19	1	301	CHL	CHB-C4A	-4.52	1.33	1.38
19	3	306	CHL	CHD-C1D	4.52	1.46	1.39
19	2	301	CHL	CHD-C4C	4.51	1.48	1.39
19	2	314	CHL	CHD-C4C	4.50	1.48	1.39
19	4	307	CHL	CHD-C1D	4.48	1.46	1.39
19	2	306	CHL	CHD-C1D	4.48	1.46	1.39
20	4	304	CLA	O1D-CGD	-4.47	1.10	1.21
20	O	202	CLA	O2A-CGA	4.45	1.45	1.30
19	2	307	CHL	CHD-C4C	4.45	1.47	1.39
19	4	315	CHL	CHB-C1B	4.44	1.46	1.39
19	1	306	CHL	C3D-C2D	4.42	1.47	1.39
19	4	315	CHL	C3D-C2D	4.42	1.47	1.39
19	1	306	CHL	CHC-C1C	4.41	1.47	1.39
19	3	306	CHL	C3A-C2A	-4.41	1.50	1.54
19	2	307	CHL	CHD-C1D	4.39	1.46	1.39
19	4	315	CHL	CHD-C1D	4.39	1.46	1.39
19	2	305	CHL	CBD-CGD	-4.38	1.47	1.52
19	2	301	CHL	C3A-C2A	-4.38	1.50	1.54
19	4	305	CHL	CHD-C1D	4.38	1.46	1.39
19	4	305	CHL	C3D-C2D	4.37	1.47	1.39
19	4	307	CHL	C3A-C2A	-4.36	1.50	1.54
19	4	305	CHL	CHC-C1C	4.36	1.47	1.39
19	4	306	CHL	CHB-C1B	4.36	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	301	CHL	CHB-C1B	4.36	1.46	1.39
19	4	307	CHL	C3D-C2D	4.36	1.47	1.39
19	4	307	CHL	CHB-C1B	4.35	1.46	1.39
19	2	301	CHL	CHD-C1D	4.34	1.46	1.39
24	B	849	LHG	O7-C7	4.32	1.46	1.34
19	4	306	CHL	C3D-C2D	4.32	1.47	1.39
19	2	306	CHL	C3D-C2D	4.32	1.47	1.39
19	2	314	CHL	C3D-C2D	4.31	1.47	1.39
19	2	305	CHL	CHB-C1B	4.31	1.46	1.39
19	2	314	CHL	CHD-C1D	4.30	1.46	1.39
19	2	305	CHL	CHD-C1D	4.30	1.46	1.39
19	3	306	CHL	CHB-C1B	4.30	1.46	1.39
19	4	305	CHL	C3B-C2B	4.29	1.46	1.40
19	3	306	CHL	CHC-C1C	4.29	1.47	1.39
19	4	307	CHL	CHC-C1C	4.29	1.47	1.39
19	3	306	CHL	C3D-C2D	4.29	1.47	1.39
19	2	305	CHL	C3D-C2D	4.29	1.47	1.39
19	2	305	CHL	CHC-C1C	4.27	1.47	1.39
19	4	307	CHL	OBD-CAD	-4.26	1.16	1.22
19	2	307	CHL	C3B-C2B	4.25	1.46	1.40
19	2	307	CHL	C3D-C2D	4.25	1.46	1.39
19	2	301	CHL	C3D-C2D	4.25	1.46	1.39
19	1	301	CHL	O2A-CGA	4.24	1.45	1.33
19	2	301	CHL	CHC-C1C	4.24	1.47	1.39
19	2	306	CHL	CHB-C1B	4.24	1.46	1.39
19	2	314	CHL	CHB-C1B	4.24	1.46	1.39
25	4	319	LMG	O8-C28	4.24	1.45	1.33
25	1	323	LMG	O8-C28	4.22	1.45	1.33
24	A	844	LHG	O8-C23	4.19	1.45	1.33
19	4	306	CHL	CAA-C2A	-4.19	1.45	1.54
19	2	307	CHL	CHC-C1C	4.19	1.47	1.39
25	1	320	LMG	O8-C28	4.18	1.45	1.33
24	2	318	LHG	O8-C23	4.17	1.45	1.33
19	4	315	CHL	CHC-C1C	4.17	1.47	1.39
24	A	843	LHG	O8-C23	4.16	1.45	1.33
19	2	314	CHL	CHC-C1C	4.16	1.47	1.39
19	4	305	CHL	CHB-C1B	4.16	1.46	1.39
24	1	318	LHG	O8-C23	4.15	1.45	1.33
30	B	848	DGD	O1G-C1A	4.15	1.45	1.33
19	3	306	CHL	OMC-CMC	-4.12	1.13	1.22
19	2	306	CHL	CHC-C1C	4.11	1.47	1.39
19	1	306	CHL	C3A-C2A	-4.11	1.51	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	320	LMG	O7-C10	4.09	1.45	1.34
24	1	318	LHG	O7-C7	4.09	1.45	1.34
26	A	852	HTG	C1'-S1	-4.09	1.75	1.81
24	A	844	LHG	O7-C7	4.08	1.45	1.34
19	2	307	CHL	CHB-C1B	4.07	1.46	1.39
19	2	307	CHL	OMC-CMC	-4.07	1.13	1.22
19	2	305	CHL	O1D-CGD	-4.06	1.11	1.21
30	B	848	DGD	O2G-C1B	4.06	1.45	1.34
25	1	323	LMG	O7-C10	4.06	1.45	1.34
24	2	318	LHG	O7-C7	4.05	1.45	1.34
25	4	319	LMG	O7-C10	4.03	1.45	1.34
24	A	843	LHG	O7-C7	4.00	1.45	1.34
19	1	301	CHL	C3A-C2A	-3.97	1.51	1.54
19	4	306	CHL	CMD-C2D	-3.93	1.43	1.51
20	3	309	CLA	C1D-ND	3.91	1.43	1.37
19	1	306	CHL	O2D-CGD	3.88	1.42	1.33
20	A	801	CLA	C1D-ND	3.88	1.43	1.37
19	2	301	CHL	CBD-CGD	-3.80	1.47	1.52
20	4	304	CLA	O2A-C1	-3.75	1.36	1.46
19	3	306	CHL	O2D-CGD	3.73	1.42	1.33
19	2	301	CHL	CAA-C2A	-3.73	1.46	1.54
19	2	306	CHL	OMC-CMC	-3.71	1.13	1.22
19	2	307	CHL	CAA-C2A	-3.65	1.46	1.54
19	4	307	CHL	O2A-CGA	3.64	1.44	1.33
20	O	202	CLA	C1D-ND	3.62	1.42	1.37
20	G	603	CLA	C1D-ND	3.61	1.42	1.37
20	N	203	CLA	C1D-ND	3.60	1.42	1.37
19	1	306	CHL	O2A-CGA	3.60	1.43	1.33
19	4	305	CHL	CMB-C2B	-3.60	1.44	1.51
26	4	320	HTG	C1'-S1	-3.59	1.76	1.81
26	J	105	HTG	C1'-S1	-3.58	1.76	1.81
20	1	308	CLA	C1D-ND	3.58	1.42	1.37
20	4	313	CLA	C1D-ND	3.58	1.42	1.37
19	2	306	CHL	O2D-CED	-3.56	1.37	1.45
20	1	312	CLA	C1D-ND	3.56	1.42	1.37
20	3	313	CLA	C1D-ND	3.56	1.42	1.37
20	1	302	CLA	C1D-ND	3.55	1.42	1.37
19	4	307	CHL	CAC-C3C	-3.55	1.45	1.51
20	2	309	CLA	C1D-ND	3.55	1.42	1.37
20	B	804	CLA	C1D-ND	3.54	1.42	1.37
26	F	803	HTG	C1'-S1	-3.54	1.76	1.81
20	3	304	CLA	C1D-ND	3.54	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	203	CLA	C1D-ND	3.54	1.42	1.37
19	4	315	CHL	CBD-CGD	-3.54	1.48	1.52
20	3	310	CLA	C1D-ND	3.53	1.42	1.37
20	2	311	CLA	C1D-ND	3.53	1.42	1.37
20	4	314	CLA	C1D-ND	3.53	1.42	1.37
20	2	312	CLA	C1D-ND	3.53	1.42	1.37
20	A	834	CLA	C1D-ND	3.53	1.42	1.37
20	4	303	CLA	C1D-ND	3.53	1.42	1.37
20	G	605	CLA	C1D-ND	3.53	1.42	1.37
20	A	820	CLA	C1D-ND	3.52	1.42	1.37
20	A	814	CLA	C1D-ND	3.52	1.42	1.37
20	A	824	CLA	C1D-ND	3.52	1.42	1.37
20	B	824	CLA	C1D-ND	3.52	1.42	1.37
20	1	304	CLA	C1D-ND	3.52	1.42	1.37
20	A	840	CLA	C1D-ND	3.52	1.42	1.37
19	2	306	CHL	O2A-CGA	3.52	1.43	1.33
20	B	837	CLA	C1D-ND	3.52	1.42	1.37
20	B	801	CLA	C1D-ND	3.51	1.42	1.37
20	B	813	CLA	C1D-ND	3.51	1.42	1.37
20	B	820	CLA	C1D-ND	3.51	1.42	1.37
20	L	307	CLA	C1D-ND	3.51	1.42	1.37
20	A	835	CLA	C1D-ND	3.51	1.42	1.37
20	3	308	CLA	C1D-ND	3.51	1.42	1.37
20	A	829	CLA	C1D-ND	3.51	1.42	1.37
20	A	805	CLA	C1D-ND	3.51	1.42	1.37
20	A	810	CLA	C1D-ND	3.51	1.42	1.37
20	J	101	CLA	C1D-ND	3.50	1.42	1.37
26	B	851	HTG	C1'-S1	-3.50	1.76	1.81
19	1	306	CHL	O2D-CED	-3.50	1.37	1.45
20	B	819	CLA	C1D-ND	3.50	1.42	1.37
26	N	201	HTG	C1'-S1	-3.50	1.76	1.81
19	4	307	CHL	OMC-CMC	-3.50	1.14	1.22
20	3	311	CLA	C1D-ND	3.50	1.42	1.37
20	N	202	CLA	C1D-ND	3.50	1.42	1.37
20	H	201	CLA	C1D-ND	3.49	1.42	1.37
20	K	201	CLA	C1D-ND	3.49	1.42	1.37
20	L	302	CLA	C1D-ND	3.49	1.42	1.37
20	3	302	CLA	C1D-ND	3.49	1.42	1.37
20	A	838	CLA	C1D-ND	3.49	1.42	1.37
20	F	802	CLA	C1D-ND	3.49	1.42	1.37
20	4	311	CLA	C1D-ND	3.49	1.42	1.37
20	1	313	CLA	C1D-ND	3.49	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	303	CLA	C1D-ND	3.49	1.42	1.37
20	A	819	CLA	C1D-ND	3.49	1.42	1.37
20	3	305	CLA	C1D-ND	3.49	1.42	1.37
20	2	302	CLA	C1D-ND	3.48	1.42	1.37
20	1	307	CLA	C1D-ND	3.48	1.42	1.37
20	B	822	CLA	C1D-ND	3.48	1.42	1.37
20	G	604	CLA	C1D-ND	3.48	1.42	1.37
20	B	826	CLA	C1D-ND	3.48	1.42	1.37
20	A	808	CLA	C1D-ND	3.48	1.42	1.37
19	2	301	CHL	O2D-CED	-3.48	1.37	1.45
20	4	308	CLA	C1D-ND	3.47	1.42	1.37
20	J	103	CLA	C1D-ND	3.47	1.42	1.37
20	B	829	CLA	C1D-ND	3.47	1.42	1.37
26	G	602	HTG	C1'-S1	-3.47	1.76	1.81
20	3	314	CLA	C1D-ND	3.47	1.42	1.37
20	K	205	CLA	C1D-ND	3.47	1.42	1.37
20	1	311	CLA	C1D-ND	3.46	1.42	1.37
20	B	836	CLA	C1D-ND	3.46	1.42	1.37
20	A	803	CLA	C1D-ND	3.46	1.42	1.37
19	4	315	CHL	O2D-CGD	3.46	1.41	1.33
20	B	812	CLA	C1D-ND	3.46	1.42	1.37
20	A	839	CLA	C1D-ND	3.46	1.42	1.37
20	B	805	CLA	C1D-ND	3.46	1.42	1.37
20	A	806	CLA	C1D-ND	3.46	1.42	1.37
20	B	823	CLA	C1D-ND	3.46	1.42	1.37
20	3	312	CLA	C1D-ND	3.46	1.42	1.37
20	A	841	CLA	C1D-ND	3.45	1.42	1.37
20	A	812	CLA	C1D-ND	3.45	1.42	1.37
20	B	838	CLA	C1D-ND	3.45	1.42	1.37
20	2	310	CLA	C1D-ND	3.45	1.42	1.37
20	A	802	CLA	C1D-ND	3.45	1.42	1.37
20	A	818	CLA	C1D-ND	3.45	1.42	1.37
20	A	809	CLA	C1D-ND	3.45	1.42	1.37
20	A	828	CLA	C1D-ND	3.45	1.42	1.37
20	B	821	CLA	C1D-ND	3.45	1.42	1.37
20	B	814	CLA	C1D-ND	3.45	1.42	1.37
20	O	201	CLA	C1D-ND	3.44	1.42	1.37
20	4	301	CLA	C1D-ND	3.44	1.42	1.37
20	B	834	CLA	C1D-ND	3.44	1.42	1.37
20	3	301	CLA	C1D-ND	3.44	1.42	1.37
20	B	832	CLA	C1D-ND	3.44	1.42	1.37
20	K	203	CLA	C1D-ND	3.44	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	805	CLA	C1D-ND	3.44	1.42	1.37
26	F	807	HTG	C1'-S1	-3.44	1.76	1.81
19	2	307	CHL	CBA-CGA	-3.43	1.40	1.50
20	A	823	CLA	C1D-ND	3.43	1.42	1.37
20	1	314	CLA	C1D-ND	3.43	1.42	1.37
20	B	835	CLA	C1D-ND	3.43	1.42	1.37
20	A	825	CLA	C1D-ND	3.43	1.42	1.37
20	A	833	CLA	C1D-ND	3.43	1.42	1.37
20	A	832	CLA	C1D-ND	3.43	1.42	1.37
20	A	813	CLA	C1D-ND	3.43	1.42	1.37
20	B	811	CLA	C1D-ND	3.43	1.42	1.37
20	B	816	CLA	C1D-ND	3.43	1.42	1.37
20	A	830	CLA	C1D-ND	3.43	1.42	1.37
20	K	202	CLA	C1D-ND	3.43	1.42	1.37
20	A	837	CLA	C1D-ND	3.43	1.42	1.37
20	A	851	CLA	C1D-ND	3.43	1.42	1.37
20	B	806	CLA	C1D-ND	3.42	1.42	1.37
20	B	808	CLA	C1D-ND	3.42	1.42	1.37
20	1	309	CLA	C1D-ND	3.42	1.42	1.37
20	2	308	CLA	C1D-ND	3.42	1.42	1.37
20	A	853	CLA	C1D-ND	3.42	1.42	1.37
20	B	827	CLA	C4B-NB	3.42	1.42	1.37
20	4	302	CLA	C1D-ND	3.42	1.42	1.37
20	B	825	CLA	C1D-ND	3.42	1.42	1.37
20	B	839	CLA	C1D-ND	3.42	1.42	1.37
20	F	804	CLA	C1D-ND	3.42	1.42	1.37
20	A	836	CLA	C1D-ND	3.41	1.42	1.37
20	B	827	CLA	C1D-ND	3.41	1.42	1.37
26	B	850	HTG	C1'-S1	-3.41	1.76	1.81
20	2	313	CLA	C1D-ND	3.41	1.42	1.37
20	4	304	CLA	C1D-ND	3.41	1.42	1.37
20	A	807	CLA	C1D-ND	3.41	1.42	1.37
20	B	815	CLA	C1D-ND	3.41	1.42	1.37
20	L	303	CLA	C1D-ND	3.41	1.42	1.37
20	A	826	CLA	C1D-ND	3.41	1.42	1.37
20	A	827	CLA	C1D-ND	3.41	1.42	1.37
20	A	811	CLA	C1D-ND	3.40	1.42	1.37
20	A	831	CLA	C1D-ND	3.40	1.42	1.37
20	A	815	CLA	C1D-ND	3.40	1.42	1.37
20	B	807	CLA	C1D-ND	3.40	1.42	1.37
20	B	833	CLA	C1D-ND	3.40	1.42	1.37
20	2	303	CLA	C1D-ND	3.40	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	830	CLA	C1D-ND	3.40	1.42	1.37
20	A	804	CLA	C1D-ND	3.39	1.42	1.37
20	A	822	CLA	C1D-ND	3.39	1.42	1.37
20	B	810	CLA	C1D-ND	3.39	1.42	1.37
20	B	802	CLA	C1D-ND	3.39	1.42	1.37
20	L	304	CLA	C1D-ND	3.39	1.42	1.37
20	A	817	CLA	C1D-ND	3.39	1.42	1.37
20	B	828	CLA	C1D-ND	3.39	1.42	1.37
20	1	321	CLA	C1D-ND	3.39	1.42	1.37
20	3	303	CLA	C1D-ND	3.38	1.42	1.37
20	2	304	CLA	C1D-ND	3.38	1.42	1.37
20	B	818	CLA	C1D-ND	3.38	1.42	1.37
20	3	307	CLA	C1D-ND	3.38	1.42	1.37
20	B	817	CLA	C1D-ND	3.36	1.42	1.37
20	O	202	CLA	C1C-NC	3.36	1.43	1.37
26	1	322	HTG	C1'-S1	-3.36	1.76	1.81
20	1	310	CLA	C1D-ND	3.36	1.42	1.37
20	1	305	CLA	C1D-ND	3.36	1.42	1.37
19	4	315	CHL	OMC-CMC	-3.35	1.14	1.22
20	4	310	CLA	C1D-ND	3.34	1.42	1.37
19	2	301	CHL	CMA-C3A	-3.34	1.47	1.53
20	4	312	CLA	C1D-ND	3.34	1.42	1.37
20	B	803	CLA	C1D-ND	3.34	1.42	1.37
20	4	309	CLA	C1D-ND	3.33	1.42	1.37
20	A	821	CLA	C1D-ND	3.31	1.42	1.37
20	B	831	CLA	C1D-ND	3.30	1.42	1.37
19	2	307	CHL	O2D-CGD	3.30	1.41	1.33
20	1	303	CLA	C4B-NB	3.28	1.42	1.37
20	B	809	CLA	C1D-ND	3.28	1.42	1.37
20	3	314	CLA	C4B-NB	3.26	1.42	1.37
19	2	306	CHL	CMD-C2D	-3.25	1.45	1.51
19	2	301	CHL	CMB-C2B	-3.25	1.45	1.51
20	A	816	CLA	C1D-ND	3.24	1.42	1.37
20	3	309	CLA	C4B-NB	3.24	1.42	1.37
20	B	828	CLA	C4B-NB	3.23	1.42	1.37
20	A	811	CLA	C4B-NB	3.21	1.42	1.37
20	3	302	CLA	C4B-NB	3.20	1.42	1.37
20	K	201	CLA	C4B-NB	3.19	1.42	1.37
19	4	305	CHL	CAC-C3C	-3.19	1.46	1.51
20	4	310	CLA	C4B-NB	3.17	1.42	1.37
20	B	811	CLA	CAB-C3B	-3.16	1.44	1.50
20	L	307	CLA	C4B-NB	3.15	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CAA-C2A	-3.14	1.48	1.54
20	3	313	CLA	C4B-NB	3.12	1.42	1.37
20	A	835	CLA	C4B-NB	3.12	1.42	1.37
19	2	305	CHL	OMC-CMC	-3.11	1.15	1.22
20	1	312	CLA	C4B-NB	3.10	1.41	1.37
20	4	301	CLA	C4B-NB	3.10	1.41	1.37
20	J	103	CLA	C4B-NB	3.10	1.41	1.37
20	F	805	CLA	C4B-NB	3.09	1.41	1.37
20	3	311	CLA	C4B-NB	3.09	1.41	1.37
20	A	838	CLA	C4B-NB	3.09	1.41	1.37
20	G	604	CLA	C4B-NB	3.09	1.41	1.37
20	1	321	CLA	C4B-NB	3.09	1.41	1.37
20	B	821	CLA	C4B-NB	3.09	1.41	1.37
20	3	310	CLA	C4B-NB	3.09	1.41	1.37
20	A	803	CLA	C4B-NB	3.08	1.41	1.37
20	A	853	CLA	C4B-NB	3.07	1.41	1.37
20	A	834	CLA	C4B-NB	3.07	1.41	1.37
20	N	203	CLA	C4B-NB	3.07	1.41	1.37
20	A	840	CLA	C4B-NB	3.07	1.41	1.37
20	G	605	CLA	C4B-NB	3.06	1.41	1.37
19	3	306	CHL	O1D-CGD	-3.06	1.13	1.21
19	2	307	CHL	CBD-CGD	-3.05	1.48	1.52
20	B	837	CLA	C4B-NB	3.05	1.41	1.37
20	3	305	CLA	C4B-NB	3.04	1.41	1.37
19	4	307	CHL	CMA-C3A	-3.04	1.48	1.53
20	1	308	CLA	C4B-NB	3.04	1.41	1.37
20	A	832	CLA	C4B-NB	3.04	1.41	1.37
20	O	202	CLA	C4B-NB	3.04	1.41	1.37
20	4	314	CLA	C4B-NB	3.04	1.41	1.37
20	4	312	CLA	C4B-NB	3.04	1.41	1.37
20	B	801	CLA	C4B-NB	3.04	1.41	1.37
20	1	307	CLA	C4B-NB	3.03	1.41	1.37
19	4	307	CHL	O2D-CED	-3.02	1.38	1.45
20	2	304	CLA	C4B-NB	3.02	1.41	1.37
19	4	315	CHL	CAC-C3C	-3.02	1.46	1.51
20	B	811	CLA	C4B-NB	3.02	1.41	1.37
20	B	833	CLA	C4B-NB	3.02	1.41	1.37
20	B	836	CLA	C4B-NB	3.01	1.41	1.37
20	A	817	CLA	C4B-NB	3.01	1.41	1.37
20	4	313	CLA	C4B-NB	3.01	1.41	1.37
20	A	815	CLA	C4B-NB	3.01	1.41	1.37
20	K	202	CLA	C4B-NB	3.01	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	305	CLA	C4B-NB	3.00	1.41	1.37
20	A	826	CLA	C4B-NB	3.00	1.41	1.37
20	G	603	CLA	C4B-NB	3.00	1.41	1.37
20	A	808	CLA	C4B-NB	3.00	1.41	1.37
20	O	201	CLA	C4B-NB	3.00	1.41	1.37
20	L	303	CLA	C4B-NB	3.00	1.41	1.37
20	A	810	CLA	C4B-NB	3.00	1.41	1.37
20	H	201	CLA	C4B-NB	3.00	1.41	1.37
20	B	822	CLA	C4B-NB	2.99	1.41	1.37
20	A	823	CLA	C4B-NB	2.99	1.41	1.37
20	2	312	CLA	C4B-NB	2.99	1.41	1.37
20	3	312	CLA	C4B-NB	2.98	1.41	1.37
20	B	812	CLA	C4B-NB	2.98	1.41	1.37
20	B	838	CLA	C4B-NB	2.98	1.41	1.37
20	B	820	CLA	C4B-NB	2.98	1.41	1.37
20	F	804	CLA	C4B-NB	2.98	1.41	1.37
20	4	304	CLA	C4B-NB	2.98	1.41	1.37
20	A	816	CLA	C4B-NB	2.98	1.41	1.37
20	2	303	CLA	C4B-NB	2.97	1.41	1.37
19	3	306	CHL	CAA-C2A	-2.97	1.48	1.54
20	B	825	CLA	C4B-NB	2.97	1.41	1.37
20	2	313	CLA	C4B-NB	2.97	1.41	1.37
20	B	802	CLA	C4B-NB	2.97	1.41	1.37
20	A	819	CLA	C4B-NB	2.97	1.41	1.37
20	A	813	CLA	C4B-NB	2.97	1.41	1.37
20	B	817	CLA	C4B-NB	2.97	1.41	1.37
20	B	818	CLA	C4B-NB	2.96	1.41	1.37
20	A	841	CLA	C4B-NB	2.96	1.41	1.37
20	B	830	CLA	C4B-NB	2.96	1.41	1.37
20	A	818	CLA	C4B-NB	2.95	1.41	1.37
20	K	205	CLA	C4B-NB	2.95	1.41	1.37
20	3	301	CLA	C4B-NB	2.95	1.41	1.37
20	A	831	CLA	C4B-NB	2.95	1.41	1.37
20	B	810	CLA	C4B-NB	2.95	1.41	1.37
20	A	812	CLA	C4B-NB	2.95	1.41	1.37
20	B	839	CLA	C4B-NB	2.95	1.41	1.37
20	B	805	CLA	C4B-NB	2.95	1.41	1.37
20	1	313	CLA	C4B-NB	2.94	1.41	1.37
20	1	310	CLA	C4B-NB	2.94	1.41	1.37
20	1	314	CLA	C4B-NB	2.94	1.41	1.37
20	L	304	CLA	C4B-NB	2.94	1.41	1.37
20	A	824	CLA	C4B-NB	2.94	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	830	CLA	C4B-NB	2.94	1.41	1.37
20	A	804	CLA	C4B-NB	2.94	1.41	1.37
20	B	829	CLA	C4B-NB	2.93	1.41	1.37
20	N	202	CLA	C4B-NB	2.93	1.41	1.37
20	A	839	CLA	C4B-NB	2.93	1.41	1.37
20	A	825	CLA	C4B-NB	2.93	1.41	1.37
20	B	831	CLA	C4B-NB	2.93	1.41	1.37
20	A	820	CLA	C4B-NB	2.93	1.41	1.37
20	F	802	CLA	C4B-NB	2.92	1.41	1.37
20	1	311	CLA	C4B-NB	2.92	1.41	1.37
20	A	809	CLA	C4B-NB	2.92	1.41	1.37
20	B	813	CLA	C4B-NB	2.92	1.41	1.37
19	4	315	CHL	CAA-C2A	-2.91	1.47	1.53
20	3	303	CLA	C4B-NB	2.91	1.41	1.37
20	A	851	CLA	C4B-NB	2.91	1.41	1.37
20	L	302	CLA	C4B-NB	2.91	1.41	1.37
20	B	824	CLA	C4B-NB	2.91	1.41	1.37
20	B	826	CLA	C4B-NB	2.91	1.41	1.37
20	A	814	CLA	C4B-NB	2.90	1.41	1.37
20	A	822	CLA	C4B-NB	2.90	1.41	1.37
20	B	816	CLA	C4B-NB	2.90	1.41	1.37
20	3	304	CLA	C4B-NB	2.90	1.41	1.37
19	3	306	CHL	O2A-CGA	2.90	1.42	1.33
20	3	309	CLA	O2D-CGD	2.90	1.40	1.33
20	A	802	CLA	C4B-NB	2.90	1.41	1.37
20	A	805	CLA	C4B-NB	2.90	1.41	1.37
20	B	823	CLA	C4B-NB	2.90	1.41	1.37
20	O	203	CLA	C4B-NB	2.90	1.41	1.37
20	1	304	CLA	C4B-NB	2.90	1.41	1.37
20	A	827	CLA	C4B-NB	2.90	1.41	1.37
20	B	814	CLA	C4B-NB	2.89	1.41	1.37
20	1	302	CLA	C4B-NB	2.89	1.41	1.37
20	B	832	CLA	C4B-NB	2.89	1.41	1.37
20	B	804	CLA	C4B-NB	2.89	1.41	1.37
20	4	309	CLA	C4B-NB	2.89	1.41	1.37
20	B	834	CLA	C4B-NB	2.89	1.41	1.37
20	B	819	CLA	C4B-NB	2.89	1.41	1.37
20	4	304	CLA	CMA-C3A	-2.89	1.47	1.53
19	4	315	CHL	CMD-C2D	-2.89	1.45	1.51
20	4	311	CLA	C4B-NB	2.89	1.41	1.37
20	J	101	CLA	C4B-NB	2.89	1.41	1.37
19	2	307	CHL	O2D-CED	-2.88	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	803	CLA	C4B-NB	2.88	1.41	1.37
20	A	833	CLA	C4B-NB	2.88	1.41	1.37
20	A	829	CLA	C4B-NB	2.87	1.41	1.37
20	3	307	CLA	C4B-NB	2.87	1.41	1.37
20	B	807	CLA	C4B-NB	2.87	1.41	1.37
20	4	308	CLA	C4B-NB	2.87	1.41	1.37
20	A	837	CLA	C4B-NB	2.87	1.41	1.37
19	3	306	CHL	CAC-C3C	-2.87	1.46	1.51
20	B	808	CLA	C4B-NB	2.86	1.41	1.37
20	B	815	CLA	C4B-NB	2.86	1.41	1.37
20	A	821	CLA	C4B-NB	2.86	1.41	1.37
20	2	311	CLA	C4B-NB	2.86	1.41	1.37
20	A	828	CLA	C4B-NB	2.85	1.41	1.37
20	A	801	CLA	C4B-NB	2.85	1.41	1.37
20	A	836	CLA	C4B-NB	2.85	1.41	1.37
20	4	302	CLA	C4B-NB	2.85	1.41	1.37
19	2	301	CHL	O1A-CGA	-2.85	1.14	1.22
20	4	303	CLA	C4B-NB	2.85	1.41	1.37
20	B	809	CLA	C4B-NB	2.85	1.41	1.37
20	3	308	CLA	C4B-NB	2.84	1.41	1.37
20	B	835	CLA	C4B-NB	2.83	1.41	1.37
20	2	308	CLA	C4B-NB	2.82	1.41	1.37
20	B	806	CLA	C4B-NB	2.82	1.41	1.37
20	2	310	CLA	C4B-NB	2.82	1.41	1.37
20	K	203	CLA	C4B-NB	2.81	1.41	1.37
20	O	202	CLA	OBD-CAD	2.81	1.27	1.22
19	4	307	CHL	CMD-C2D	-2.80	1.46	1.51
20	A	807	CLA	C4B-NB	2.80	1.41	1.37
19	2	307	CHL	O2A-CGA	2.79	1.41	1.33
20	B	810	CLA	C1B-C2B	2.79	1.49	1.43
20	N	203	CLA	C1B-C2B	2.78	1.49	1.43
20	2	309	CLA	C4B-NB	2.78	1.41	1.37
19	3	306	CHL	O1A-CGA	-2.78	1.14	1.22
19	3	306	CHL	CMA-C3A	-2.78	1.48	1.53
20	B	802	CLA	C1B-C2B	2.78	1.49	1.43
19	2	307	CHL	CMD-C2D	-2.78	1.46	1.51
20	A	801	CLA	C1B-C2B	2.77	1.49	1.43
20	B	816	CLA	C1B-C2B	2.77	1.49	1.43
19	2	305	CHL	CMD-C2D	-2.76	1.46	1.51
19	3	306	CHL	CMD-C2D	-2.76	1.46	1.51
20	1	308	CLA	C1B-C2B	2.75	1.49	1.43
20	B	831	CLA	C1B-C2B	2.75	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	305	CLA	C1B-C2B	2.74	1.49	1.43
20	3	311	CLA	C1B-C2B	2.74	1.49	1.43
20	B	834	CLA	C1B-C2B	2.73	1.49	1.43
20	1	309	CLA	C4B-NB	2.73	1.41	1.37
20	1	312	CLA	C1B-C2B	2.73	1.49	1.43
20	A	806	CLA	C4B-NB	2.73	1.41	1.37
20	A	819	CLA	C1B-C2B	2.73	1.49	1.43
20	O	202	CLA	C1B-C2B	2.72	1.49	1.43
20	2	302	CLA	C4B-NB	2.72	1.41	1.37
20	1	313	CLA	C1B-C2B	2.72	1.49	1.43
20	B	824	CLA	C1B-C2B	2.72	1.49	1.43
20	O	203	CLA	C1B-C2B	2.72	1.49	1.43
26	A	852	HTG	C1-S1	-2.72	1.76	1.80
20	N	202	CLA	C1B-C2B	2.72	1.49	1.43
19	2	301	CHL	CMD-C2D	-2.72	1.46	1.51
20	A	830	CLA	C1B-C2B	2.72	1.49	1.43
20	A	816	CLA	C1B-C2B	2.71	1.49	1.43
20	A	838	CLA	C1B-C2B	2.71	1.49	1.43
20	K	205	CLA	C1B-C2B	2.71	1.49	1.43
20	K	203	CLA	C1B-C2B	2.71	1.49	1.43
20	A	813	CLA	C1B-C2B	2.71	1.49	1.43
20	A	815	CLA	C1B-C2B	2.71	1.49	1.43
20	B	820	CLA	C1B-C2B	2.71	1.49	1.43
20	3	309	CLA	O2A-CGA	2.71	1.41	1.33
20	1	311	CLA	C1B-C2B	2.71	1.49	1.43
20	B	827	CLA	C3B-C4B	2.71	1.50	1.42
20	4	304	CLA	C1B-C2B	2.71	1.49	1.43
20	3	312	CLA	C1B-C2B	2.71	1.49	1.43
20	A	804	CLA	C1B-C2B	2.71	1.49	1.43
20	4	313	CLA	C1B-C2B	2.70	1.49	1.43
20	J	103	CLA	C1B-C2B	2.70	1.49	1.43
20	3	310	CLA	C1B-C2B	2.70	1.49	1.43
20	3	303	CLA	C1B-C2B	2.70	1.49	1.43
20	B	811	CLA	C1B-C2B	2.70	1.49	1.43
20	A	805	CLA	C1B-C2B	2.70	1.49	1.43
20	B	806	CLA	C1B-C2B	2.70	1.49	1.43
19	4	306	CHL	O2A-CGA	2.70	1.41	1.33
20	L	303	CLA	C1B-C2B	2.70	1.49	1.43
20	A	822	CLA	C1B-C2B	2.70	1.49	1.43
20	L	307	CLA	C1B-C2B	2.69	1.49	1.43
20	B	837	CLA	C1B-C2B	2.69	1.49	1.43
20	A	823	CLA	C1B-C2B	2.69	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	812	CLA	C1B-C2B	2.69	1.49	1.43
20	B	838	CLA	C1B-C2B	2.69	1.49	1.43
20	B	813	CLA	C1B-C2B	2.69	1.49	1.43
20	4	303	CLA	C1B-C2B	2.69	1.49	1.43
20	B	832	CLA	C1B-C2B	2.69	1.49	1.43
20	A	832	CLA	C1B-C2B	2.69	1.49	1.43
20	G	603	CLA	C1B-C2B	2.69	1.49	1.43
20	B	804	CLA	C1B-C2B	2.69	1.49	1.43
20	B	811	CLA	C4B-C3B	2.69	1.49	1.43
20	B	808	CLA	C1B-C2B	2.69	1.49	1.43
20	A	853	CLA	C1B-C2B	2.69	1.49	1.43
20	A	829	CLA	C1B-C2B	2.69	1.49	1.43
20	L	304	CLA	C1B-C2B	2.69	1.49	1.43
19	2	307	CHL	O2A-C1	-2.68	1.38	1.46
20	B	807	CLA	C1B-C2B	2.68	1.49	1.43
19	4	305	CHL	O1D-CGD	-2.68	1.14	1.21
20	B	830	CLA	C1B-C2B	2.68	1.49	1.43
20	2	311	CLA	C1B-C2B	2.68	1.49	1.43
20	F	805	CLA	C1B-C2B	2.68	1.49	1.43
20	3	304	CLA	C1B-C2B	2.68	1.49	1.43
20	A	840	CLA	C1B-C2B	2.68	1.49	1.43
20	4	301	CLA	C1B-C2B	2.68	1.49	1.43
20	4	308	CLA	C1B-C2B	2.68	1.49	1.43
20	1	310	CLA	C1B-C2B	2.68	1.49	1.43
20	A	808	CLA	C1B-C2B	2.68	1.49	1.43
20	H	201	CLA	C1B-C2B	2.67	1.49	1.43
20	F	802	CLA	C1B-C2B	2.67	1.49	1.43
20	A	837	CLA	C1B-C2B	2.67	1.49	1.43
20	B	818	CLA	C1B-C2B	2.67	1.49	1.43
20	B	835	CLA	C1B-C2B	2.67	1.49	1.43
20	2	302	CLA	C1B-C2B	2.66	1.49	1.43
19	4	306	CHL	O2D-CGD	2.66	1.39	1.33
20	1	304	CLA	C1B-C2B	2.66	1.49	1.43
20	1	314	CLA	C1B-C2B	2.66	1.49	1.43
19	2	306	CHL	CMB-C2B	-2.66	1.46	1.51
20	4	311	CLA	C1B-C2B	2.66	1.49	1.43
20	4	312	CLA	C1B-C2B	2.66	1.49	1.43
20	B	826	CLA	C1B-C2B	2.66	1.49	1.43
19	2	305	CHL	O2D-CGD	2.66	1.39	1.33
20	1	307	CLA	C1B-C2B	2.65	1.49	1.43
20	B	815	CLA	C1B-C2B	2.65	1.49	1.43
20	G	605	CLA	C1B-C2B	2.65	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	809	CLA	C1B-C2B	2.65	1.49	1.43
20	B	814	CLA	C1B-C2B	2.65	1.49	1.43
20	3	305	CLA	C1B-C2B	2.65	1.49	1.43
20	B	809	CLA	C1B-C2B	2.65	1.49	1.43
20	G	604	CLA	C1B-C2B	2.65	1.49	1.43
20	2	303	CLA	C1B-C2B	2.65	1.49	1.43
20	4	314	CLA	C1B-C2B	2.65	1.49	1.43
20	K	202	CLA	C1B-C2B	2.65	1.49	1.43
20	B	836	CLA	C1B-C2B	2.64	1.49	1.43
20	2	304	CLA	C1B-C2B	2.64	1.49	1.43
20	B	821	CLA	C1B-C2B	2.64	1.49	1.43
20	3	308	CLA	C1B-C2B	2.64	1.49	1.43
20	A	827	CLA	C1B-C2B	2.64	1.49	1.43
20	A	839	CLA	C1B-C2B	2.64	1.49	1.43
20	A	814	CLA	C1B-C2B	2.64	1.49	1.43
20	J	101	CLA	C1B-C2B	2.63	1.49	1.43
20	A	821	CLA	C1B-C2B	2.63	1.49	1.43
20	B	805	CLA	C1B-C2B	2.63	1.49	1.43
20	F	804	CLA	C1B-C2B	2.63	1.49	1.43
20	A	841	CLA	C1B-C2B	2.63	1.49	1.43
19	2	306	CHL	CAA-C2A	-2.63	1.48	1.54
19	2	301	CHL	CAC-C3C	-2.63	1.47	1.51
20	L	302	CLA	C1B-C2B	2.63	1.49	1.43
20	A	833	CLA	C1B-C2B	2.62	1.49	1.43
20	3	302	CLA	C1B-C2B	2.62	1.49	1.43
20	A	834	CLA	C1B-C2B	2.62	1.49	1.43
20	B	812	CLA	C1B-C2B	2.62	1.49	1.43
20	2	308	CLA	C1B-C2B	2.62	1.49	1.43
20	2	313	CLA	C1B-C2B	2.62	1.49	1.43
20	A	806	CLA	C1B-C2B	2.62	1.49	1.43
20	1	321	CLA	C1B-C2B	2.62	1.49	1.43
20	A	831	CLA	C1B-C2B	2.62	1.49	1.43
20	A	807	CLA	C1B-C2B	2.62	1.49	1.43
20	A	836	CLA	C1B-C2B	2.62	1.49	1.43
20	B	839	CLA	C1B-C2B	2.62	1.49	1.43
20	A	851	CLA	C1B-C2B	2.62	1.49	1.43
20	2	310	CLA	C1B-C2B	2.61	1.49	1.43
20	A	828	CLA	C1B-C2B	2.61	1.49	1.43
20	1	303	CLA	C3B-C4B	2.61	1.50	1.42
20	B	803	CLA	C1B-C2B	2.61	1.49	1.43
20	A	803	CLA	C1B-C2B	2.61	1.49	1.43
20	1	302	CLA	C1B-C2B	2.61	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	201	CLA	C1B-C2B	2.61	1.49	1.43
20	A	817	CLA	C1B-C2B	2.61	1.49	1.43
20	A	810	CLA	C1B-C2B	2.61	1.49	1.43
20	1	303	CLA	C1B-C2B	2.60	1.49	1.43
20	K	201	CLA	C3B-C4B	2.60	1.50	1.42
20	A	820	CLA	C1B-C2B	2.60	1.49	1.43
20	4	302	CLA	C1B-C2B	2.60	1.49	1.43
20	B	823	CLA	C1B-C2B	2.59	1.49	1.43
20	3	307	CLA	C1B-C2B	2.59	1.49	1.43
19	2	307	CHL	CAC-C3C	-2.59	1.47	1.51
20	A	824	CLA	C1B-C2B	2.59	1.49	1.43
20	4	310	CLA	C1B-C2B	2.59	1.49	1.43
20	A	835	CLA	C1B-C2B	2.59	1.49	1.43
20	3	301	CLA	C1B-C2B	2.59	1.49	1.43
20	3	313	CLA	C1B-C2B	2.59	1.49	1.43
20	B	822	CLA	C1B-C2B	2.58	1.49	1.43
20	A	825	CLA	C1B-C2B	2.58	1.49	1.43
20	B	829	CLA	C1B-C2B	2.58	1.49	1.43
20	B	828	CLA	C3B-C4B	2.58	1.50	1.42
20	B	819	CLA	C1B-C2B	2.57	1.49	1.43
20	B	833	CLA	C1B-C2B	2.57	1.49	1.43
20	A	811	CLA	C3B-C4B	2.57	1.50	1.42
19	4	315	CHL	CMB-C2B	-2.57	1.46	1.51
20	B	828	CLA	C1B-C2B	2.56	1.49	1.43
20	A	802	CLA	C1B-C2B	2.56	1.49	1.43
20	3	314	CLA	C1B-C2B	2.56	1.49	1.43
20	K	201	CLA	C1B-C2B	2.56	1.49	1.43
19	2	305	CHL	CAC-C3C	-2.56	1.47	1.51
24	B	849	LHG	O8-C23	2.55	1.45	1.33
20	2	312	CLA	C1B-C2B	2.55	1.49	1.43
20	3	309	CLA	C1C-NC	2.55	1.42	1.37
20	B	825	CLA	C1B-C2B	2.55	1.49	1.43
20	A	818	CLA	C1B-C2B	2.55	1.49	1.43
20	3	314	CLA	C3B-C4B	2.55	1.50	1.42
20	B	817	CLA	C1B-C2B	2.55	1.49	1.43
19	4	305	CHL	CAA-C2A	-2.54	1.48	1.54
20	B	801	CLA	C1B-C2B	2.54	1.49	1.43
19	4	307	CHL	O1A-CGA	-2.54	1.14	1.22
20	A	826	CLA	C1B-C2B	2.54	1.49	1.43
20	A	811	CLA	C1B-C2B	2.53	1.49	1.43
20	3	313	CLA	C3B-C4B	2.53	1.50	1.42
20	4	309	CLA	C1B-C2B	2.53	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	306	CHL	CMD-C2D	-2.53	1.46	1.51
19	1	306	CHL	CMB-C2B	-2.53	1.46	1.51
19	3	306	CHL	O2D-CED	-2.53	1.39	1.45
20	B	827	CLA	C1B-C2B	2.52	1.49	1.43
19	4	305	CHL	CMD-C2D	-2.51	1.46	1.51
19	2	305	CHL	CMB-C2B	-2.51	1.46	1.51
20	3	309	CLA	C1B-C2B	2.50	1.49	1.43
20	4	304	CLA	CAA-CBA	-2.50	1.45	1.52
20	2	309	CLA	C3B-C4B	2.48	1.50	1.42
19	4	307	CHL	C4-C3	-2.48	1.43	1.50
19	2	307	CHL	O1A-CGA	-2.47	1.15	1.22
20	2	309	CLA	C1B-C2B	2.47	1.48	1.43
20	1	309	CLA	C1B-C2B	2.45	1.48	1.43
20	4	309	CLA	C3B-C4B	2.45	1.49	1.42
20	2	309	CLA	CHC-C1C	2.44	1.43	1.38
20	F	805	CLA	C3B-C4B	2.43	1.49	1.42
20	1	321	CLA	C3B-C4B	2.43	1.49	1.42
20	4	309	CLA	CHC-C1C	2.43	1.43	1.38
20	1	309	CLA	C3B-C4B	2.42	1.49	1.42
26	4	320	HTG	C1-S1	-2.42	1.76	1.80
20	A	826	CLA	CHC-C1C	2.42	1.43	1.38
20	A	853	CLA	C3B-C4B	2.42	1.49	1.42
20	B	833	CLA	C3B-C4B	2.42	1.49	1.42
20	2	312	CLA	C3B-C4B	2.41	1.49	1.42
20	B	825	CLA	CHC-C1C	2.41	1.43	1.38
20	A	817	CLA	C3B-C4B	2.41	1.49	1.42
20	4	304	CLA	O2D-CGD	2.40	1.39	1.33
26	J	105	HTG	C1-S1	-2.39	1.76	1.80
20	1	307	CLA	C3B-C4B	2.39	1.49	1.42
20	B	825	CLA	C3B-C4B	2.39	1.49	1.42
20	B	812	CLA	C3B-C4B	2.39	1.49	1.42
20	K	202	CLA	C3B-C4B	2.38	1.49	1.42
20	4	302	CLA	C3B-C4B	2.38	1.49	1.42
20	3	308	CLA	C3B-C4B	2.38	1.49	1.42
20	4	314	CLA	C3B-C4B	2.38	1.49	1.42
20	G	605	CLA	C3B-C4B	2.38	1.49	1.42
20	A	810	CLA	C3B-C4B	2.37	1.49	1.42
20	2	311	CLA	C3B-C4B	2.37	1.49	1.42
20	G	604	CLA	C3B-C4B	2.37	1.49	1.42
20	B	821	CLA	C3B-C4B	2.36	1.49	1.42
20	3	301	CLA	C3B-C4B	2.36	1.49	1.42
20	O	202	CLA	C3B-C4B	2.36	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	310	CLA	C3B-C4B	2.36	1.49	1.42
20	A	826	CLA	C3B-C4B	2.36	1.49	1.42
20	4	310	CLA	C3B-C4B	2.36	1.49	1.42
20	3	311	CLA	C3B-C4B	2.36	1.49	1.42
20	A	815	CLA	C3B-C4B	2.36	1.49	1.42
19	4	307	CHL	O1D-CGD	-2.35	1.15	1.21
20	B	814	CLA	C3B-C4B	2.35	1.49	1.42
20	1	311	CLA	C3B-C4B	2.35	1.49	1.42
20	F	802	CLA	C3B-C4B	2.35	1.49	1.42
20	B	823	CLA	CHC-C1C	2.35	1.43	1.38
20	A	840	CLA	C3B-C4B	2.35	1.49	1.42
20	1	312	CLA	C3B-C4B	2.34	1.49	1.42
20	B	823	CLA	C3B-C4B	2.34	1.49	1.42
20	3	302	CLA	C3B-C4B	2.34	1.49	1.42
20	B	827	CLA	CHC-C1C	2.34	1.43	1.38
20	1	305	CLA	CMD-C2D	-2.34	1.46	1.50
20	1	304	CLA	C3B-C4B	2.34	1.49	1.42
20	A	812	CLA	C3B-C4B	2.34	1.49	1.42
20	N	202	CLA	C3B-C4B	2.34	1.49	1.42
20	A	817	CLA	CHC-C1C	2.34	1.43	1.38
20	4	311	CLA	C3B-C4B	2.34	1.49	1.42
20	A	825	CLA	CHC-C1C	2.34	1.43	1.38
26	G	602	HTG	C1-S1	-2.34	1.76	1.80
20	4	301	CLA	C3B-C4B	2.34	1.49	1.42
20	L	303	CLA	C3B-C4B	2.34	1.49	1.42
20	4	312	CLA	C3B-C4B	2.34	1.49	1.42
20	A	825	CLA	C3B-C4B	2.34	1.49	1.42
20	A	831	CLA	CHC-C1C	2.33	1.43	1.38
20	J	103	CLA	C3B-C4B	2.33	1.49	1.42
20	L	304	CLA	C3B-C4B	2.33	1.49	1.42
20	4	302	CLA	CHC-C1C	2.33	1.43	1.38
20	1	302	CLA	C3B-C4B	2.33	1.49	1.42
20	1	321	CLA	CHC-C1C	2.33	1.43	1.38
20	L	304	CLA	CHC-C1C	2.33	1.43	1.38
20	A	839	CLA	C3B-C4B	2.33	1.49	1.42
20	A	851	CLA	CHC-C1C	2.33	1.43	1.38
20	A	832	CLA	C3B-C4B	2.33	1.49	1.42
20	1	310	CLA	C3B-C4B	2.33	1.49	1.42
20	A	802	CLA	C3B-C4B	2.33	1.49	1.42
20	N	203	CLA	C3B-C4B	2.33	1.49	1.42
20	B	815	CLA	C3B-C4B	2.33	1.49	1.42
20	A	835	CLA	C3B-C4B	2.33	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CMD-C2D	-2.33	1.46	1.50
20	A	818	CLA	C3B-C4B	2.33	1.49	1.42
20	B	805	CLA	C3B-C4B	2.33	1.49	1.42
20	4	313	CLA	C3B-C4B	2.32	1.49	1.42
20	L	307	CLA	C3B-C4B	2.32	1.49	1.42
20	A	809	CLA	C3B-C4B	2.32	1.49	1.42
20	A	814	CLA	C3B-C4B	2.32	1.49	1.42
20	A	807	CLA	C3B-C4B	2.32	1.49	1.42
20	2	308	CLA	CHC-C1C	2.32	1.43	1.38
20	B	811	CLA	CHC-C1C	2.32	1.43	1.38
20	B	838	CLA	C3B-C4B	2.32	1.49	1.42
20	3	304	CLA	C3B-C4B	2.32	1.49	1.42
20	4	308	CLA	C3B-C4B	2.32	1.49	1.42
20	B	805	CLA	CHC-C1C	2.32	1.43	1.38
20	A	823	CLA	C3B-C4B	2.32	1.49	1.42
20	3	309	CLA	CBD-CGD	-2.32	1.45	1.52
20	F	804	CLA	C3B-C4B	2.32	1.49	1.42
20	B	801	CLA	C3B-C4B	2.32	1.49	1.42
20	4	311	CLA	CHC-C1C	2.32	1.43	1.38
20	2	303	CLA	C3B-C4B	2.32	1.49	1.42
20	3	301	CLA	CHC-C1C	2.32	1.43	1.38
20	N	203	CLA	CHC-C1C	2.32	1.43	1.38
20	1	305	CLA	CHC-C1C	2.32	1.43	1.38
20	3	308	CLA	CHC-C1C	2.32	1.43	1.38
20	A	803	CLA	CHC-C1C	2.32	1.43	1.38
20	A	808	CLA	C3B-C4B	2.31	1.49	1.42
20	1	305	CLA	C3B-C4B	2.31	1.49	1.42
26	F	803	HTG	C1-S1	-2.31	1.76	1.80
20	B	837	CLA	C3B-C4B	2.31	1.49	1.42
20	3	305	CLA	C3B-C4B	2.31	1.49	1.42
20	O	203	CLA	C3B-C4B	2.31	1.49	1.42
20	1	308	CLA	C3B-C4B	2.31	1.49	1.42
20	A	839	CLA	CHC-C1C	2.31	1.43	1.38
20	3	307	CLA	C3B-C4B	2.31	1.49	1.42
20	K	203	CLA	C3B-C4B	2.31	1.49	1.42
20	1	302	CLA	CHC-C1C	2.31	1.43	1.38
20	O	201	CLA	CHC-C1C	2.31	1.43	1.38
20	J	101	CLA	C3B-C4B	2.31	1.49	1.42
20	O	201	CLA	C3B-C4B	2.31	1.49	1.42
20	A	804	CLA	CHC-C1C	2.31	1.43	1.38
20	B	819	CLA	C3B-C4B	2.31	1.49	1.42
20	4	304	CLA	C3B-C4B	2.31	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	824	CLA	CHC-C1C	2.31	1.43	1.38
20	F	804	CLA	CHC-C1C	2.31	1.43	1.38
20	2	304	CLA	C3B-C4B	2.31	1.49	1.42
20	G	603	CLA	C3B-C4B	2.30	1.49	1.42
20	B	803	CLA	CMC-C2C	-2.30	1.46	1.50
20	1	313	CLA	C3B-C4B	2.30	1.49	1.42
20	A	803	CLA	C3B-C4B	2.30	1.49	1.42
20	B	836	CLA	CHC-C1C	2.30	1.43	1.38
20	A	820	CLA	C3B-C4B	2.30	1.49	1.42
20	2	308	CLA	C3B-C4B	2.30	1.49	1.42
20	B	813	CLA	C3B-C4B	2.30	1.49	1.42
20	A	816	CLA	C3B-C4B	2.30	1.49	1.42
20	A	830	CLA	C3B-C4B	2.30	1.49	1.42
20	1	309	CLA	CHC-C1C	2.30	1.43	1.38
20	B	804	CLA	C3B-C4B	2.30	1.49	1.42
20	B	836	CLA	C3B-C4B	2.30	1.49	1.42
20	A	828	CLA	C3B-C4B	2.30	1.49	1.42
20	A	816	CLA	CHC-C1C	2.30	1.43	1.38
20	3	305	CLA	CHC-C1C	2.30	1.43	1.38
20	A	807	CLA	CHC-C1C	2.30	1.43	1.38
20	A	802	CLA	CHC-C1C	2.30	1.43	1.38
20	K	203	CLA	CHC-C1C	2.30	1.43	1.38
20	A	824	CLA	C3B-C4B	2.30	1.49	1.42
20	A	831	CLA	C3B-C4B	2.30	1.49	1.42
20	A	851	CLA	C3B-C4B	2.30	1.49	1.42
20	A	806	CLA	C3B-C4B	2.29	1.49	1.42
20	B	803	CLA	C3B-C4B	2.29	1.49	1.42
20	B	817	CLA	C3B-C4B	2.29	1.49	1.42
20	2	312	CLA	CHC-C1C	2.29	1.43	1.38
20	B	839	CLA	C3B-C4B	2.29	1.49	1.42
20	A	804	CLA	C3B-C4B	2.29	1.49	1.42
20	3	309	CLA	C3B-C4B	2.29	1.49	1.42
20	L	303	CLA	CHC-C1C	2.29	1.43	1.38
20	A	821	CLA	C3B-C4B	2.29	1.49	1.42
20	2	302	CLA	C3B-C4B	2.29	1.49	1.42
20	F	802	CLA	CHC-C1C	2.29	1.43	1.38
20	B	801	CLA	CHC-C1C	2.29	1.43	1.38
20	G	605	CLA	CHC-C1C	2.29	1.43	1.38
20	B	806	CLA	C3B-C4B	2.29	1.49	1.42
20	B	834	CLA	C3B-C4B	2.29	1.49	1.42
20	L	302	CLA	C3B-C4B	2.29	1.49	1.42
20	O	202	CLA	CHC-C1C	2.29	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	C3B-C4B	2.29	1.49	1.42
20	A	813	CLA	C3B-C4B	2.29	1.49	1.42
20	3	307	CLA	CHC-C1C	2.29	1.43	1.38
20	A	806	CLA	CHC-C1C	2.29	1.43	1.38
20	B	803	CLA	CHC-C1C	2.29	1.43	1.38
20	K	202	CLA	CHC-C1C	2.29	1.43	1.38
20	B	821	CLA	CHC-C1C	2.28	1.43	1.38
20	B	816	CLA	C3B-C4B	2.28	1.49	1.42
20	B	819	CLA	CHC-C1C	2.28	1.43	1.38
20	2	303	CLA	CHC-C1C	2.28	1.43	1.38
20	3	310	CLA	CHC-C1C	2.28	1.43	1.38
19	4	315	CHL	CMC-C2C	-2.28	1.40	1.44
20	A	818	CLA	CHC-C1C	2.28	1.43	1.38
20	A	828	CLA	CHC-C1C	2.28	1.43	1.38
20	A	809	CLA	CHC-C1C	2.28	1.43	1.38
20	2	313	CLA	C3B-C4B	2.28	1.49	1.42
20	A	833	CLA	C3B-C4B	2.28	1.49	1.42
20	B	820	CLA	C3B-C4B	2.28	1.49	1.42
20	H	201	CLA	C3B-C4B	2.28	1.49	1.42
20	4	308	CLA	CHC-C1C	2.28	1.43	1.38
20	A	810	CLA	CHC-C1C	2.28	1.43	1.38
20	B	835	CLA	C3B-C4B	2.27	1.49	1.42
20	B	833	CLA	CHC-C1C	2.27	1.43	1.38
20	B	835	CLA	CHC-C1C	2.27	1.43	1.38
20	A	822	CLA	C3B-C4B	2.27	1.49	1.42
20	A	837	CLA	C3B-C4B	2.27	1.49	1.42
20	B	807	CLA	C3B-C4B	2.27	1.49	1.42
20	A	805	CLA	C3B-C4B	2.27	1.49	1.42
20	B	802	CLA	C3B-C4B	2.27	1.49	1.42
20	B	837	CLA	CHC-C1C	2.27	1.43	1.38
20	F	805	CLA	CHC-C1C	2.27	1.43	1.38
20	A	813	CLA	CHC-C1C	2.27	1.43	1.38
20	B	826	CLA	C3B-C4B	2.27	1.49	1.42
20	B	822	CLA	C3B-C4B	2.27	1.49	1.42
20	A	801	CLA	C3B-C4B	2.27	1.49	1.42
20	A	827	CLA	C3B-C4B	2.27	1.49	1.42
20	B	834	CLA	CHC-C1C	2.27	1.43	1.38
20	O	203	CLA	CHC-C1C	2.27	1.43	1.38
26	N	201	HTG	C1-S1	-2.27	1.76	1.80
20	B	810	CLA	C3B-C4B	2.27	1.49	1.42
20	B	808	CLA	C3B-C4B	2.27	1.49	1.42
20	B	818	CLA	C3B-C4B	2.27	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	CHC-C1C	2.27	1.43	1.38
20	3	304	CLA	CHC-C1C	2.27	1.43	1.38
20	3	303	CLA	C3B-C4B	2.26	1.49	1.42
20	1	312	CLA	CHC-C1C	2.26	1.43	1.38
20	1	314	CLA	CHC-C1C	2.26	1.43	1.38
20	A	841	CLA	C3B-C4B	2.26	1.49	1.42
20	A	838	CLA	C3B-C4B	2.26	1.49	1.42
20	A	819	CLA	C3B-C4B	2.26	1.49	1.42
20	4	312	CLA	CHC-C1C	2.26	1.43	1.38
20	A	814	CLA	CHC-C1C	2.26	1.43	1.38
20	3	312	CLA	C3B-C4B	2.26	1.49	1.42
20	N	202	CLA	CHC-C1C	2.26	1.43	1.38
20	A	822	CLA	CHC-C1C	2.26	1.43	1.38
20	A	821	CLA	CHC-C1C	2.26	1.43	1.38
26	1	322	HTG	C1-S1	-2.26	1.76	1.80
20	A	836	CLA	C3B-C4B	2.26	1.49	1.42
20	2	304	CLA	CHC-C1C	2.25	1.43	1.38
20	L	307	CLA	CHC-C1C	2.25	1.43	1.38
26	B	850	HTG	C1-S1	-2.25	1.76	1.80
20	1	304	CLA	CHC-C1C	2.25	1.43	1.38
20	A	815	CLA	CHC-C1C	2.25	1.43	1.38
20	A	833	CLA	CHC-C1C	2.25	1.43	1.38
20	B	820	CLA	CHC-C1C	2.25	1.43	1.38
20	A	841	CLA	CHC-C1C	2.25	1.43	1.38
20	2	310	CLA	C3B-C4B	2.25	1.49	1.42
20	A	837	CLA	CHC-C1C	2.25	1.43	1.38
20	J	101	CLA	CHC-C1C	2.25	1.43	1.38
20	2	311	CLA	CHC-C1C	2.25	1.43	1.38
20	B	802	CLA	CHC-C1C	2.25	1.43	1.38
20	B	830	CLA	CHC-C1C	2.25	1.43	1.38
20	J	103	CLA	CHC-C1C	2.25	1.43	1.38
20	1	314	CLA	C3B-C4B	2.25	1.49	1.42
20	B	829	CLA	C3B-C4B	2.25	1.49	1.42
20	A	830	CLA	CHC-C1C	2.25	1.43	1.38
20	B	832	CLA	C3B-C4B	2.25	1.49	1.42
20	A	812	CLA	CHC-C1C	2.24	1.43	1.38
20	A	840	CLA	CHC-C1C	2.24	1.43	1.38
20	B	818	CLA	CHC-C1C	2.24	1.43	1.38
20	A	811	CLA	CHC-C1C	2.24	1.43	1.38
20	3	312	CLA	CHC-C1C	2.24	1.43	1.38
20	B	830	CLA	C3B-C4B	2.24	1.49	1.42
20	1	308	CLA	CHC-C1C	2.24	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	313	CLA	CHC-C1C	2.24	1.43	1.38
20	A	823	CLA	CHC-C1C	2.24	1.43	1.38
20	G	604	CLA	CHC-C1C	2.24	1.43	1.38
20	3	314	CLA	CHC-C1C	2.24	1.43	1.38
20	A	820	CLA	CHC-C1C	2.24	1.43	1.38
20	B	804	CLA	CHC-C1C	2.24	1.43	1.38
20	B	838	CLA	CHC-C1C	2.24	1.43	1.38
20	1	311	CLA	CHC-C1C	2.24	1.43	1.38
20	B	809	CLA	C3B-C4B	2.24	1.49	1.42
20	A	801	CLA	CHC-C1C	2.23	1.43	1.38
20	4	303	CLA	C3B-C4B	2.23	1.49	1.42
19	2	305	CHL	MG-NB	2.23	2.10	2.05
20	B	812	CLA	CHC-C1C	2.23	1.43	1.38
20	2	302	CLA	CHC-C1C	2.23	1.43	1.38
20	A	853	CLA	CHC-C1C	2.23	1.43	1.38
19	1	306	CHL	OMC-CMC	-2.23	1.17	1.22
26	B	851	HTG	C1-S1	-2.23	1.77	1.80
20	B	815	CLA	CHC-C1C	2.23	1.43	1.38
20	K	205	CLA	C3B-C4B	2.23	1.49	1.42
20	A	836	CLA	CHC-C1C	2.23	1.43	1.38
20	B	822	CLA	CHC-C1C	2.23	1.43	1.38
20	G	603	CLA	CHC-C1C	2.23	1.43	1.38
20	H	201	CLA	CHC-C1C	2.23	1.43	1.38
20	4	314	CLA	CHC-C1C	2.23	1.43	1.38
20	B	826	CLA	CHC-C1C	2.23	1.43	1.38
20	1	307	CLA	CHC-C1C	2.23	1.43	1.38
20	K	201	CLA	CHC-C1C	2.23	1.42	1.38
20	K	205	CLA	CHC-C1C	2.23	1.42	1.38
20	B	816	CLA	CHC-C1C	2.23	1.42	1.38
20	B	828	CLA	CHC-C1C	2.22	1.42	1.38
20	B	814	CLA	CHC-C1C	2.22	1.42	1.38
20	B	813	CLA	CHC-C1C	2.22	1.42	1.38
20	A	805	CLA	CHC-C1C	2.22	1.42	1.38
20	A	822	CLA	CMD-C2D	-2.22	1.46	1.50
20	B	824	CLA	C3B-C4B	2.22	1.49	1.42
20	A	829	CLA	C3B-C4B	2.22	1.49	1.42
20	4	310	CLA	CHC-C1C	2.22	1.42	1.38
20	A	819	CLA	CHC-C1C	2.22	1.42	1.38
20	4	301	CLA	CHC-C1C	2.21	1.42	1.38
20	B	829	CLA	CHC-C1C	2.21	1.42	1.38
20	A	835	CLA	CHC-C1C	2.21	1.42	1.38
20	A	808	CLA	CHC-C1C	2.21	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CHC-C1C	2.21	1.42	1.38
20	B	806	CLA	CHC-C1C	2.21	1.42	1.38
20	B	832	CLA	CHC-C1C	2.21	1.42	1.38
20	A	832	CLA	CHC-C1C	2.21	1.42	1.38
20	4	313	CLA	CHC-C1C	2.20	1.42	1.38
20	4	304	CLA	O1A-CGA	-2.20	1.15	1.22
20	B	830	CLA	MG-NB	-2.20	2.01	2.05
20	1	313	CLA	CHC-C1C	2.20	1.42	1.38
20	A	838	CLA	CHC-C1C	2.20	1.42	1.38
20	B	819	CLA	CMB-C2B	-2.20	1.46	1.50
20	A	827	CLA	CHC-C1C	2.20	1.42	1.38
20	3	302	CLA	CHC-C1C	2.20	1.42	1.38
20	B	839	CLA	CHC-C1C	2.20	1.42	1.38
20	3	303	CLA	CHC-C1C	2.20	1.42	1.38
20	2	313	CLA	CHC-C1C	2.20	1.42	1.38
20	B	831	CLA	C3B-C4B	2.20	1.49	1.42
20	L	302	CLA	CHC-C1C	2.19	1.42	1.38
20	B	807	CLA	CHC-C1C	2.19	1.42	1.38
19	4	306	CHL	O2D-CED	-2.19	1.40	1.45
20	B	829	CLA	CMB-C2B	-2.19	1.46	1.50
20	A	835	CLA	CMB-C2B	-2.19	1.46	1.50
20	1	310	CLA	CHC-C1C	2.19	1.42	1.38
20	B	817	CLA	CHC-C1C	2.19	1.42	1.38
22	4	317	XAT	O4-C5	-2.19	1.43	1.46
20	A	829	CLA	CHC-C1C	2.19	1.42	1.38
20	4	304	CLA	CBD-CGD	-2.19	1.45	1.52
20	B	831	CLA	CHC-C1C	2.19	1.42	1.38
20	3	311	CLA	CHC-C1C	2.18	1.42	1.38
20	B	809	CLA	CMB-C2B	-2.18	1.46	1.50
20	3	309	CLA	CHC-C1C	2.18	1.42	1.38
20	A	826	CLA	MG-NB	-2.18	2.01	2.05
20	B	824	CLA	CHC-C1C	2.18	1.42	1.38
20	B	835	CLA	MG-NB	-2.17	2.01	2.05
19	2	301	CHL	O2A-CGA	2.17	1.39	1.33
20	4	303	CLA	CMD-C2D	-2.17	1.46	1.50
20	A	841	CLA	CMB-C2B	-2.17	1.46	1.50
20	B	839	CLA	CMB-C2B	-2.17	1.46	1.50
20	B	817	CLA	CMB-C2B	-2.17	1.46	1.50
20	A	841	CLA	CMD-C2D	-2.17	1.46	1.50
20	B	838	CLA	CMD-C2D	-2.17	1.46	1.50
20	B	810	CLA	CHC-C1C	2.16	1.42	1.38
20	B	802	CLA	CMD-C2D	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	807	HTG	C1-S1	-2.16	1.77	1.80
20	B	808	CLA	CHC-C1C	2.16	1.42	1.38
20	A	808	CLA	CMD-C2D	-2.16	1.46	1.50
23	A	848	BCR	C1-C6	-2.16	1.51	1.53
20	A	822	CLA	MG-NB	-2.16	2.01	2.05
20	2	310	CLA	CHC-C1C	2.16	1.42	1.38
20	K	205	CLA	MG-NB	-2.16	2.01	2.05
20	B	809	CLA	CHC-C1C	2.16	1.42	1.38
20	B	823	CLA	CMD-C2D	-2.15	1.46	1.50
20	A	820	CLA	CMB-C2B	-2.15	1.46	1.50
20	4	303	CLA	CHC-C1C	2.15	1.42	1.38
20	2	304	CLA	CMB-C2B	-2.15	1.46	1.50
20	B	808	CLA	CMD-C2D	-2.15	1.46	1.50
19	3	306	CHL	CBD-CGD	-2.14	1.49	1.52
20	1	310	CLA	MG-NB	-2.14	2.01	2.05
20	1	303	CLA	CMD-C2D	-2.14	1.46	1.50
20	F	804	CLA	CMB-C2B	-2.14	1.46	1.50
20	A	821	CLA	MG-NB	-2.14	2.01	2.05
20	3	302	CLA	CMB-C2B	-2.14	1.46	1.50
20	A	834	CLA	CMB-C2B	-2.14	1.46	1.50
20	H	201	CLA	CMB-C2B	-2.14	1.46	1.50
20	B	817	CLA	MG-NB	-2.14	2.01	2.05
20	B	828	CLA	CMB-C2B	-2.13	1.46	1.50
21	O	205	LUT	C1-C6	-2.13	1.51	1.53
20	A	836	CLA	MG-NB	-2.13	2.01	2.05
22	3	316	XAT	O4-C5	-2.13	1.43	1.46
23	B	841	BCR	C30-C25	-2.13	1.51	1.53
20	A	831	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	830	CLA	MG-NB	-2.13	2.01	2.05
20	B	831	CLA	MG-NB	-2.13	2.01	2.05
20	B	826	CLA	MG-NB	-2.13	2.01	2.05
20	1	302	CLA	CMD-C2D	-2.13	1.46	1.50
20	3	303	CLA	CMB-C2B	-2.13	1.46	1.50
20	B	838	CLA	CMB-C2B	-2.12	1.46	1.50
20	F	805	CLA	CMD-C2D	-2.12	1.46	1.50
20	A	810	CLA	CMD-C2D	-2.12	1.46	1.50
20	2	309	CLA	CMB-C2B	-2.12	1.46	1.50
20	A	818	CLA	CMB-C2B	-2.12	1.46	1.50
22	1	316	XAT	O4-C5	-2.12	1.43	1.46
20	2	313	CLA	MG-NB	-2.12	2.01	2.05
20	A	816	CLA	CMB-C2B	-2.12	1.46	1.50
20	A	806	CLA	MG-NB	-2.12	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	823	CLA	CMB-C2B	-2.12	1.46	1.50
20	B	830	CLA	CMB-C2B	-2.12	1.46	1.50
20	B	822	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	803	CLA	MG-NB	-2.11	2.01	2.05
20	B	814	CLA	CMD-C2D	-2.11	1.46	1.50
20	K	203	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	825	CLA	CMD-C2D	-2.11	1.46	1.50
20	J	101	CLA	MG-NB	-2.11	2.01	2.05
20	B	814	CLA	MG-NB	-2.11	2.01	2.05
20	1	302	CLA	CMC-C2C	-2.11	1.46	1.50
20	3	311	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	825	CLA	MG-NB	-2.11	2.01	2.05
19	2	301	CHL	CMC-C2C	-2.11	1.40	1.44
20	K	205	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	804	CLA	CMD-C2D	-2.11	1.46	1.50
20	1	303	CLA	CHC-C1C	2.11	1.42	1.38
20	A	829	CLA	CMB-C2B	-2.11	1.46	1.50
20	A	830	CLA	CMD-C2D	-2.11	1.46	1.50
20	3	312	CLA	MG-NB	-2.11	2.01	2.05
20	3	301	CLA	CMC-C2C	-2.11	1.46	1.50
20	2	302	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	824	CLA	CMD-C2D	-2.10	1.46	1.50
20	4	308	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	832	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	816	CLA	MG-NB	-2.10	2.01	2.05
20	B	812	CLA	CMB-C2B	-2.10	1.46	1.50
20	B	817	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	835	CLA	CMD-C2D	-2.10	1.46	1.50
23	B	842	BCR	C30-C25	-2.10	1.51	1.53
20	4	310	CLA	CMB-C2B	-2.10	1.46	1.50
20	2	304	CLA	CMD-C2D	-2.10	1.46	1.50
20	B	822	CLA	CMB-C2B	-2.10	1.46	1.50
20	N	202	CLA	CMD-C2D	-2.10	1.46	1.50
19	1	306	CHL	O1D-CGD	-2.10	1.16	1.21
20	A	817	CLA	CMC-C2C	-2.10	1.46	1.50
20	L	302	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	804	CLA	CMC-C2C	-2.10	1.46	1.50
20	B	833	CLA	CMD-C2D	-2.10	1.46	1.50
22	2	316	XAT	O24-C25	-2.10	1.43	1.46
20	A	801	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	819	CLA	CMD-C2D	-2.10	1.46	1.50
20	H	201	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	312	CLA	CMB-C2B	-2.10	1.46	1.50
20	A	816	CLA	CMD-C2D	-2.10	1.46	1.50
20	2	302	CLA	MG-NB	-2.09	2.01	2.05
20	1	321	CLA	MG-NB	-2.09	2.01	2.05
20	B	819	CLA	MG-NB	-2.09	2.01	2.05
22	1	316	XAT	O24-C25	-2.09	1.43	1.46
20	A	804	CLA	MG-NB	-2.09	2.01	2.05
20	H	201	CLA	MG-NB	-2.09	2.01	2.05
20	A	840	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	816	CLA	MG-NB	-2.09	2.01	2.05
20	B	807	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	831	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	806	CLA	MG-NB	-2.09	2.01	2.05
20	B	832	CLA	CMD-C2D	-2.09	1.46	1.50
20	K	203	CLA	CMC-C2C	-2.09	1.46	1.50
20	A	802	CLA	MG-NB	-2.09	2.01	2.05
20	3	310	CLA	CMD-C2D	-2.09	1.46	1.50
20	J	103	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	813	CLA	MG-NB	-2.09	2.01	2.05
20	B	832	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	837	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	841	CLA	MG-NB	-2.09	2.01	2.05
20	B	839	CLA	CMD-C2D	-2.09	1.46	1.50
20	3	307	CLA	MG-NB	-2.09	2.01	2.05
20	1	311	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	817	CLA	CMD-C2D	-2.09	1.46	1.50
20	4	311	CLA	CMD-C2D	-2.09	1.46	1.50
20	B	808	CLA	MG-NB	-2.09	2.01	2.05
20	3	313	CLA	CMB-C2B	-2.09	1.46	1.50
20	B	827	CLA	CMD-C2D	-2.09	1.46	1.50
21	O	205	LUT	C26-C27	2.09	1.53	1.50
20	1	309	CLA	CMB-C2B	-2.09	1.46	1.50
20	1	310	CLA	CMD-C2D	-2.09	1.46	1.50
20	2	303	CLA	CMD-C2D	-2.09	1.46	1.50
20	A	817	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	838	CLA	CMD-C2D	-2.08	1.46	1.50
20	4	303	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	830	CLA	CMD-C2D	-2.08	1.46	1.50
20	L	304	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	823	CLA	MG-NB	-2.08	2.01	2.05
20	A	837	CLA	MG-NB	-2.08	2.01	2.05
20	4	302	CLA	CMD-C2D	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	309	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	821	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	829	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	809	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	818	CLA	MG-NB	-2.08	2.01	2.05
20	A	831	CLA	MG-NB	-2.08	2.01	2.05
20	B	839	CLA	MG-NB	-2.08	2.01	2.05
20	1	312	CLA	CMB-C2B	-2.08	1.46	1.50
20	2	312	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	824	CLA	MG-NB	-2.08	2.01	2.05
20	A	827	CLA	CMD-C2D	-2.08	1.46	1.50
20	2	303	CLA	MG-NB	-2.08	2.01	2.05
20	1	321	CLA	CMD-C2D	-2.08	1.46	1.50
20	2	313	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	815	CLA	CMD-C2D	-2.08	1.46	1.50
20	B	809	CLA	MG-NB	-2.08	2.01	2.05
20	A	826	CLA	CMC-C2C	-2.08	1.46	1.50
20	A	813	CLA	MG-NB	-2.08	2.01	2.05
20	B	808	CLA	CMB-C2B	-2.08	1.46	1.50
20	A	822	CLA	CMB-C2B	-2.08	1.46	1.50
20	3	301	CLA	CMD-C2D	-2.08	1.46	1.50
20	4	308	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	853	CLA	CMD-C2D	-2.08	1.46	1.50
20	G	603	CLA	CMB-C2B	-2.08	1.46	1.50
20	B	819	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	821	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	819	CLA	MG-NB	-2.08	2.01	2.05
20	1	304	CLA	CMD-C2D	-2.08	1.46	1.50
20	F	802	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	828	CLA	MG-NB	-2.08	2.01	2.05
20	3	309	CLA	CBA-CGA	-2.08	1.44	1.50
20	O	201	CLA	MG-NB	-2.08	2.01	2.05
20	A	833	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	836	CLA	CMB-C2B	-2.07	1.46	1.50
20	L	302	CLA	CMB-C2B	-2.07	1.46	1.50
20	2	310	CLA	MG-NB	-2.07	2.01	2.05
20	2	308	CLA	CMD-C2D	-2.07	1.46	1.50
20	F	804	CLA	CMD-C2D	-2.07	1.46	1.50
20	K	205	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	810	CLA	MG-NB	-2.07	2.01	2.05
20	A	831	CLA	CMB-C2B	-2.07	1.46	1.50
20	A	803	CLA	CMD-C2D	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	805	CLA	CMB-C2B	-2.07	1.46	1.50
20	1	314	CLA	MG-NB	-2.07	2.01	2.05
20	4	314	CLA	MG-NB	-2.07	2.01	2.05
20	2	311	CLA	CMD-C2D	-2.07	1.46	1.50
20	1	304	CLA	MG-NB	-2.07	2.01	2.05
20	A	837	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	810	CLA	CMD-C2D	-2.07	1.46	1.50
23	I	101	BCR	C1-C6	-2.07	1.51	1.53
20	B	838	CLA	MG-NB	-2.07	2.01	2.05
20	1	314	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	832	CLA	MG-NB	-2.07	2.01	2.05
20	O	203	CLA	MG-NB	-2.07	2.01	2.05
20	2	309	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	310	CLA	CMB-C2B	-2.07	1.46	1.50
20	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	310	CLA	MG-NB	-2.07	2.01	2.05
20	A	811	CLA	CMB-C2B	-2.07	1.46	1.50
20	A	810	CLA	CMB-C2B	-2.07	1.46	1.50
20	B	811	CLA	CMB-C2B	-2.07	1.46	1.50
20	O	203	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	821	CLA	MG-NB	-2.07	2.01	2.05
20	K	202	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	818	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	853	CLA	CMB-C2B	-2.07	1.46	1.50
20	3	301	CLA	MG-NB	-2.07	2.01	2.05
20	A	803	CLA	MG-NB	-2.07	2.01	2.05
20	A	818	CLA	CMD-C2D	-2.07	1.46	1.50
20	G	604	CLA	CMB-C2B	-2.07	1.46	1.50
20	1	311	CLA	MG-NB	-2.07	2.01	2.05
20	A	840	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	803	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	813	CLA	CMD-C2D	-2.06	1.46	1.50
20	J	103	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	808	CLA	CMB-C2B	-2.06	1.46	1.50
20	K	202	CLA	CMB-C2B	-2.06	1.46	1.50
20	3	307	CLA	CMD-C2D	-2.06	1.46	1.50
20	J	101	CLA	CMD-C2D	-2.06	1.46	1.50
20	3	308	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	824	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	828	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	829	CLA	CMC-C2C	-2.06	1.46	1.50
20	A	805	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	830	CLA	CMB-C2B	-2.06	1.46	1.50
20	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	308	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	838	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	817	CLA	MG-NB	-2.06	2.01	2.05
20	2	303	CLA	CMB-C2B	-2.06	1.46	1.50
20	G	603	CLA	MG-NB	-2.06	2.01	2.05
20	B	819	CLA	CMD-C2D	-2.06	1.46	1.50
20	L	307	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	307	CLA	CMB-C2B	-2.06	1.46	1.50
20	1	305	CLA	MG-NB	-2.06	2.01	2.05
20	B	805	CLA	MG-NB	-2.06	2.01	2.05
20	A	815	CLA	CMB-C2B	-2.06	1.46	1.50
20	2	304	CLA	MG-NB	-2.06	2.01	2.05
20	4	309	CLA	CMB-C2B	-2.06	1.46	1.50
20	A	811	CLA	CMD-C2D	-2.06	1.46	1.50
20	K	201	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	821	CLA	CMB-C2B	-2.06	1.46	1.50
20	O	201	CLA	CMD-C2D	-2.06	1.46	1.50
20	A	820	CLA	MG-NB	-2.06	2.01	2.05
20	B	823	CLA	CMC-C2C	-2.06	1.46	1.50
20	3	311	CLA	CMD-C2D	-2.06	1.46	1.50
20	3	304	CLA	MG-NB	-2.06	2.01	2.05
20	A	838	CLA	MG-NB	-2.06	2.01	2.05
20	A	851	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	816	CLA	CMC-C2C	-2.06	1.46	1.50
20	G	605	CLA	MG-NB	-2.06	2.01	2.05
20	A	805	CLA	MG-NB	-2.05	2.01	2.05
20	B	818	CLA	MG-NB	-2.05	2.01	2.05
20	1	307	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	816	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	804	CLA	MG-NB	-2.05	2.01	2.05
20	A	832	CLA	CMD-C2D	-2.05	1.46	1.50
20	K	201	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	834	CLA	MG-NB	-2.05	2.01	2.05
20	A	839	CLA	MG-NB	-2.05	2.01	2.05
20	K	203	CLA	MG-NB	-2.05	2.01	2.05
20	A	805	CLA	CMB-C2B	-2.05	1.46	1.50
20	A	824	CLA	CMB-C2B	-2.05	1.46	1.50
20	L	307	CLA	CMB-C2B	-2.05	1.46	1.50
20	4	312	CLA	CMB-C2B	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	826	CLA	CMD-C2D	-2.05	1.46	1.50
20	O	201	CLA	CMB-C2B	-2.05	1.46	1.50
20	1	302	CLA	MG-NB	-2.05	2.01	2.05
20	B	801	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	304	CLA	CMD-C2D	-2.05	1.46	1.50
20	1	309	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	834	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	803	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	805	CLA	CMD-C2D	-2.05	1.46	1.50
20	1	308	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	813	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
20	G	605	CLA	CMB-C2B	-2.05	1.46	1.50
20	2	312	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	839	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	820	CLA	CMD-C2D	-2.05	1.46	1.50
20	G	604	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	831	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	303	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	826	CLA	CMB-C2B	-2.05	1.46	1.50
20	4	301	CLA	CMB-C2B	-2.05	1.46	1.50
20	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	814	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	824	CLA	MG-NB	-2.05	2.01	2.05
20	B	807	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	812	CLA	CMD-C2D	-2.04	1.46	1.50
20	L	302	CLA	MG-NB	-2.04	2.01	2.05
20	1	308	CLA	MG-NB	-2.04	2.01	2.05
20	4	304	CLA	MG-NB	-2.04	2.01	2.05
20	A	808	CLA	MG-NB	-2.04	2.01	2.05
20	B	804	CLA	CMD-C2D	-2.04	1.46	1.50
20	4	309	CLA	MG-NB	-2.04	2.01	2.05
20	1	303	CLA	CMB-C2B	-2.04	1.46	1.50
20	3	304	CLA	CMC-C2C	-2.04	1.46	1.50
20	A	823	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	824	CLA	CMB-C2B	-2.04	1.46	1.50
20	4	313	CLA	MG-NB	-2.04	2.01	2.05
20	4	309	CLA	CMC-C2C	-2.04	1.46	1.50
20	A	820	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	834	CLA	CMD-C2D	-2.04	1.46	1.50
20	1	313	CLA	CMB-C2B	-2.04	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	809	CLA	CMD-C2D	-2.04	1.46	1.50
20	L	303	CLA	CMB-C2B	-2.04	1.46	1.50
20	N	203	CLA	CMD-C2D	-2.04	1.46	1.50
20	2	310	CLA	CMD-C2D	-2.04	1.46	1.50
20	3	302	CLA	CMD-C2D	-2.04	1.46	1.50
20	3	308	CLA	MG-NB	-2.04	2.01	2.05
20	4	301	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	807	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	804	CLA	CMB-C2B	-2.04	1.46	1.50
20	4	301	CLA	MG-NB	-2.04	2.01	2.05
19	4	306	CHL	O2A-C1	-2.04	1.40	1.46
20	B	836	CLA	CMD-C2D	-2.04	1.46	1.50
20	4	303	CLA	MG-NB	-2.04	2.01	2.05
20	L	303	CLA	MG-NB	-2.04	2.01	2.05
20	G	603	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	806	CLA	CMD-C2D	-2.04	1.46	1.50
20	3	309	CLA	O2D-CED	-2.04	1.40	1.45
20	2	311	CLA	MG-NB	-2.04	2.01	2.05
20	2	309	CLA	CMC-C2C	-2.04	1.46	1.50
20	A	826	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	802	CLA	CMD-C2D	-2.04	1.46	1.50
20	4	313	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	833	CLA	CMB-C2B	-2.04	1.46	1.50
20	G	605	CLA	CMD-C2D	-2.04	1.46	1.50
20	3	314	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	826	CLA	CMC-C2C	-2.04	1.46	1.50
19	2	301	CHL	O2A-C1	-2.04	1.40	1.46
20	A	853	CLA	MG-NB	-2.04	2.01	2.05
20	2	310	CLA	CMB-C2B	-2.04	1.46	1.50
20	A	812	CLA	MG-NB	-2.04	2.01	2.05
20	B	822	CLA	MG-NB	-2.04	2.01	2.05
20	3	303	CLA	MG-NB	-2.03	2.01	2.05
20	B	820	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	826	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	836	CLA	MG-NB	-2.03	2.01	2.05
20	A	835	CLA	MG-NB	-2.03	2.01	2.05
20	A	806	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	835	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	802	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	813	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	823	CLA	CMB-C2B	-2.03	1.46	1.50
20	O	202	CLA	MG-NB	-2.03	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	305	CLA	CMD-C2D	-2.03	1.46	1.50
19	4	305	CHL	O2D-CED	-2.03	1.40	1.45
20	4	313	CLA	CMC-C2C	-2.03	1.46	1.50
20	1	310	CLA	CMB-C2B	-2.03	1.46	1.50
20	4	314	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	839	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	809	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	836	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	827	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	828	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	833	CLA	MG-NB	-2.03	2.01	2.05
23	I	101	BCR	C30-C25	-2.03	1.51	1.53
20	3	305	CLA	MG-NB	-2.03	2.01	2.05
20	G	604	CLA	MG-NB	-2.03	2.01	2.05
20	B	808	CLA	CMC-C2C	-2.03	1.46	1.50
20	A	814	CLA	CMD-C2D	-2.03	1.46	1.50
20	4	302	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	828	CLA	CMB-C2B	-2.03	1.46	1.50
20	3	305	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	801	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	802	CLA	CMC-C2C	-2.03	1.46	1.50
20	L	304	CLA	MG-NB	-2.03	2.01	2.05
20	B	815	CLA	CMD-C2D	-2.03	1.46	1.50
20	L	303	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	309	CLA	MG-NB	-2.03	2.01	2.05
20	3	313	CLA	CMD-C2D	-2.03	1.46	1.50
20	3	314	CLA	CMB-C2B	-2.03	1.46	1.50
20	4	314	CLA	CMB-C2B	-2.03	1.46	1.50
20	B	815	CLA	CMC-C2C	-2.03	1.46	1.50
19	2	301	CHL	O2D-CGD	2.03	1.38	1.33
20	B	833	CLA	MG-NB	-2.03	2.01	2.05
20	4	311	CLA	CMB-C2B	-2.03	1.46	1.50
20	A	827	CLA	MG-NB	-2.02	2.01	2.05
20	N	202	CLA	MG-NB	-2.02	2.01	2.05
20	3	312	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	316	XAT	O4-C5	-2.02	1.43	1.46
20	B	815	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	801	CLA	MG-NB	-2.02	2.01	2.05
20	B	813	CLA	CMC-C2C	-2.02	1.46	1.50
20	K	205	CLA	CMC-C2C	-2.02	1.46	1.50
19	3	306	CHL	CAA-CBA	-2.02	1.46	1.52
20	4	302	CLA	MG-NB	-2.02	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	820	CLA	MG-NB	-2.02	2.01	2.05
20	F	804	CLA	MG-NB	-2.02	2.01	2.05
20	A	812	CLA	CMD-C2D	-2.02	1.46	1.50
20	2	308	CLA	MG-NB	-2.02	2.01	2.05
20	K	202	CLA	MG-NB	-2.02	2.01	2.05
20	4	311	CLA	MG-NB	-2.02	2.01	2.05
20	B	836	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	829	CLA	MG-NB	-2.02	2.01	2.05
20	B	834	CLA	MG-NB	-2.02	2.01	2.05
20	1	314	CLA	CMC-C2C	-2.02	1.46	1.50
20	3	308	CLA	CMB-C2B	-2.02	1.46	1.50
20	F	802	CLA	CMB-C2B	-2.02	1.46	1.50
20	J	103	CLA	MG-NB	-2.02	2.01	2.05
20	A	833	CLA	CMB-C2B	-2.02	1.46	1.50
20	3	307	CLA	CMB-C2B	-2.02	1.46	1.50
20	A	802	CLA	CMC-C2C	-2.02	1.46	1.50
20	A	814	CLA	CMB-C2B	-2.02	1.46	1.50
20	B	837	CLA	CMB-C2B	-2.02	1.46	1.50
20	L	304	CLA	CMB-C2B	-2.02	1.46	1.50
20	A	840	CLA	MG-NB	-2.02	2.01	2.05
20	F	805	CLA	MG-NB	-2.02	2.01	2.05
20	B	816	CLA	CMB-C2B	-2.02	1.46	1.50
20	3	311	CLA	MG-NB	-2.01	2.01	2.05
20	B	823	CLA	MG-NB	-2.01	2.01	2.05
20	A	804	CLA	CMB-C2B	-2.01	1.46	1.50
20	3	301	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	851	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	803	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	834	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	813	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	821	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	812	CLA	CMC-C2C	-2.01	1.46	1.50
20	K	201	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	814	CLA	MG-NB	-2.01	2.01	2.05
20	B	807	CLA	MG-NB	-2.01	2.01	2.05
20	1	305	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	835	CLA	CMB-C2B	-2.01	1.46	1.50
20	2	308	CLA	CMB-C2B	-2.01	1.46	1.50
20	A	837	CLA	CMC-C2C	-2.01	1.46	1.50
20	K	202	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	837	CLA	MG-NB	-2.01	2.01	2.05
20	1	313	CLA	CMD-C2D	-2.01	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	304	CLA	CMB-C2B	-2.01	1.46	1.50
20	1	321	CLA	CMB-C2B	-2.01	1.46	1.50
20	B	812	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	827	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	825	CLA	MG-NB	-2.01	2.01	2.05
20	A	833	CLA	CMC-C2C	-2.01	1.46	1.50
20	B	828	CLA	CMC-C2C	-2.01	1.46	1.50
20	J	101	CLA	CMB-C2B	-2.01	1.46	1.50
20	1	313	CLA	MG-NB	-2.00	2.01	2.05
20	A	807	CLA	MG-NB	-2.00	2.01	2.05
19	4	306	CHL	CAA-CBA	-2.00	1.46	1.52
20	A	809	CLA	MG-NB	-2.00	2.01	2.05
20	A	825	CLA	CMB-C2B	-2.00	1.46	1.50
20	B	805	CLA	CMB-C2B	-2.00	1.46	1.50
20	B	814	CLA	CMC-C2C	-2.00	1.46	1.50
20	B	825	CLA	CMB-C2B	-2.00	1.46	1.50
20	N	203	CLA	MG-NB	-2.00	2.01	2.05
20	A	807	CLA	CMB-C2B	-2.00	1.46	1.50

All (1683) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	O2D-CGD-CBD	23.29	136.54	110.95
19	2	305	CHL	O2D-CGD-CBD	20.77	133.77	110.95
19	3	306	CHL	O2D-CGD-CBD	15.62	128.11	110.95
23	4	318	BCR	C32-C1-C6	-15.52	85.90	110.24
19	4	307	CHL	O2D-CGD-CBD	15.33	127.79	110.95
20	4	304	CLA	O2D-CGD-CBD	15.15	137.72	111.23
19	2	306	CHL	O2D-CGD-CBD	13.49	125.77	110.95
19	4	305	CHL	O2D-CGD-CBD	12.61	124.80	110.95
19	2	307	CHL	O2D-CGD-CBD	12.57	124.76	110.95
19	4	315	CHL	O2D-CGD-CBD	12.49	124.67	110.95
19	1	306	CHL	O2D-CGD-CBD	11.77	123.88	110.95
19	2	301	CHL	OMC-CMC-C2C	-11.75	104.70	125.12
20	4	304	CLA	O2D-CGD-O1D	-9.93	104.53	123.85
19	2	305	CHL	O2D-CGD-O1D	-9.86	104.66	123.85
23	4	318	BCR	C32-C1-C31	-8.94	83.03	108.63
19	1	301	CHL	O2D-CGD-CBD	8.90	120.72	110.95
19	2	314	CHL	C1B-CHB-C4A	8.80	126.98	121.32
19	2	306	CHL	O2D-CGD-O1D	-8.77	106.78	123.85
19	2	306	CHL	C1B-CHB-C4A	8.60	126.86	121.32
20	4	304	CLA	CAA-C2A-C3A	-8.30	90.58	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	307	CHL	C1B-CHB-C4A	8.28	126.65	121.32
19	2	314	CHL	O2D-CGD-CBD	8.17	119.93	110.95
19	4	315	CHL	OMC-CMC-C2C	-8.09	111.06	125.12
19	4	315	CHL	CAA-C2A-C1A	-7.63	98.23	113.35
19	2	301	CHL	O1D-CGD-CBD	-7.48	113.38	124.72
19	2	307	CHL	O2D-CGD-O1D	-7.44	109.36	123.85
19	2	305	CHL	C1B-CHB-C4A	7.12	125.91	121.32
19	4	307	CHL	O2D-CGD-O1D	-7.12	109.99	123.85
19	2	301	CHL	O2D-CGD-O1D	-7.10	110.02	123.85
20	4	304	CLA	C1-C2-C3	-7.10	115.28	126.76
20	L	302	CLA	C4A-NA-C1A	7.05	109.90	106.68
19	4	306	CHL	O2D-CGD-CBD	6.99	118.63	110.95
20	3	309	CLA	O2D-CGD-CBD	6.98	123.42	111.23
19	4	306	CHL	C1C-C2C-CMC	6.90	139.25	126.80
20	4	312	CLA	C4A-NA-C1A	6.86	109.81	106.68
20	A	830	CLA	C4A-NA-C1A	6.86	109.81	106.68
20	B	836	CLA	C4A-NA-C1A	6.84	109.80	106.68
20	B	803	CLA	C4A-NA-C1A	6.81	109.79	106.68
20	B	808	CLA	C4A-NA-C1A	6.81	109.79	106.68
22	2	316	XAT	C18-C5-C6	-6.81	111.10	122.30
20	B	831	CLA	C4A-NA-C1A	6.77	109.77	106.68
20	B	815	CLA	C4A-NA-C1A	6.76	109.76	106.68
20	A	815	CLA	C4A-NA-C1A	6.75	109.76	106.68
20	B	810	CLA	C4A-NA-C1A	6.74	109.75	106.68
23	4	318	BCR	C31-C1-C6	6.73	120.80	110.24
20	1	308	CLA	C4A-NA-C1A	6.73	109.75	106.68
20	4	304	CLA	C4A-NA-C1A	6.73	109.75	106.68
20	K	203	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	1	316	XAT	C18-C5-C6	-6.73	111.22	122.30
20	B	824	CLA	C4A-NA-C1A	6.72	109.74	106.68
20	B	826	CLA	C4A-NA-C1A	6.71	109.74	106.68
20	B	820	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	3	316	XAT	C38-C25-C26	-6.70	111.27	122.30
20	K	205	CLA	C4A-NA-C1A	6.70	109.73	106.68
20	G	603	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	3	316	XAT	C18-C5-C6	-6.68	111.30	122.30
20	2	311	CLA	C4A-NA-C1A	6.68	109.72	106.68
20	4	303	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	A	829	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	1	313	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	A	804	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	A	813	CLA	C4A-NA-C1A	6.66	109.72	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	311	CLA	C4A-NA-C1A	6.65	109.72	106.68
20	A	805	CLA	C4A-NA-C1A	6.65	109.71	106.68
20	A	839	CLA	C4A-NA-C1A	6.64	109.71	106.68
20	B	818	CLA	C4A-NA-C1A	6.64	109.71	106.68
20	1	311	CLA	C4A-NA-C1A	6.63	109.70	106.68
20	3	309	CLA	CMD-C2D-C1D	6.63	136.40	124.73
20	L	307	CLA	C4A-NA-C1A	6.62	109.70	106.68
20	4	308	CLA	C4A-NA-C1A	6.62	109.70	106.68
20	A	837	CLA	C4A-NA-C1A	6.61	109.70	106.68
20	A	831	CLA	C4A-NA-C1A	6.59	109.69	106.68
20	L	303	CLA	C4A-NA-C1A	6.59	109.68	106.68
20	4	301	CLA	C4A-NA-C1A	6.58	109.68	106.68
20	A	838	CLA	C4A-NA-C1A	6.58	109.68	106.68
20	B	804	CLA	C4A-NA-C1A	6.58	109.68	106.68
20	A	814	CLA	C4A-NA-C1A	6.57	109.68	106.68
20	J	103	CLA	C4A-NA-C1A	6.57	109.68	106.68
20	B	834	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	3	310	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	B	832	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	2	312	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	4	311	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	A	840	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	3	312	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	A	820	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	4	317	XAT	C18-C5-C6	-6.55	111.52	122.30
20	A	833	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	1	314	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	B	821	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	2	303	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	B	812	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	B	807	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	J	101	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	A	853	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	2	307	CHL	C1-C2-C3	-6.53	116.20	126.76
20	2	313	CLA	C4A-NA-C1A	6.53	109.66	106.68
20	A	827	CLA	C4A-NA-C1A	6.53	109.66	106.68
20	B	811	CLA	C4A-NA-C1A	6.53	109.66	106.68
20	2	302	CLA	C4A-NA-C1A	6.52	109.65	106.68
20	B	839	CLA	C4A-NA-C1A	6.52	109.65	106.68
20	B	816	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	B	833	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	N	203	CLA	C4A-NA-C1A	6.51	109.65	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	305	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	B	809	CLA	C4A-NA-C1A	6.50	109.65	106.68
20	B	806	CLA	C4A-NA-C1A	6.50	109.64	106.68
20	A	808	CLA	C4A-NA-C1A	6.49	109.64	106.68
20	A	821	CLA	C4A-NA-C1A	6.49	109.64	106.68
20	N	202	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	4	317	XAT	C38-C25-C26	-6.49	111.63	122.30
20	3	307	CLA	C4A-NA-C1A	6.49	109.64	106.68
20	A	809	CLA	C4A-NA-C1A	6.48	109.63	106.68
20	1	304	CLA	C4A-NA-C1A	6.47	109.63	106.68
20	A	832	CLA	C4A-NA-C1A	6.47	109.63	106.68
20	H	201	CLA	C4A-NA-C1A	6.47	109.63	106.68
20	3	304	CLA	C4A-NA-C1A	6.47	109.63	106.68
20	A	819	CLA	C4A-NA-C1A	6.47	109.63	106.68
20	B	805	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	1	316	XAT	C38-C25-C26	-6.47	111.66	122.30
20	A	816	CLA	C4A-NA-C1A	6.45	109.62	106.68
20	K	201	CLA	C4A-NA-C1A	6.45	109.62	106.68
20	A	807	CLA	C4A-NA-C1A	6.45	109.62	106.68
20	A	825	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	B	835	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	1	307	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	G	604	CLA	C4A-NA-C1A	6.44	109.62	106.68
20	2	304	CLA	C4A-NA-C1A	6.43	109.61	106.68
20	F	805	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	A	812	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	F	802	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	A	803	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	A	810	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	2	316	XAT	C38-C25-C26	-6.41	111.75	122.30
20	3	301	CLA	C4A-NA-C1A	6.41	109.60	106.68
20	3	303	CLA	C4A-NA-C1A	6.40	109.60	106.68
20	B	838	CLA	C4A-NA-C1A	6.40	109.60	106.68
20	B	814	CLA	C4A-NA-C1A	6.39	109.59	106.68
20	4	302	CLA	C4A-NA-C1A	6.38	109.59	106.68
20	A	811	CLA	C4A-NA-C1A	6.38	109.59	106.68
20	3	302	CLA	C4A-NA-C1A	6.37	109.58	106.68
20	A	817	CLA	C4A-NA-C1A	6.37	109.58	106.68
20	3	308	CLA	C4A-NA-C1A	6.37	109.58	106.68
20	A	824	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	A	834	CLA	C4A-NA-C1A	6.36	109.58	106.68
20	A	835	CLA	C4A-NA-C1A	6.36	109.58	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	836	CLA	C4A-NA-C1A	6.35	109.58	106.68
20	1	309	CLA	C4A-NA-C1A	6.35	109.58	106.68
20	B	817	CLA	C4A-NA-C1A	6.35	109.58	106.68
20	B	819	CLA	C4A-NA-C1A	6.35	109.58	106.68
20	A	802	CLA	C4A-NA-C1A	6.34	109.57	106.68
20	1	310	CLA	C4A-NA-C1A	6.33	109.57	106.68
20	O	202	CLA	CMD-C2D-C1D	6.33	135.87	124.73
20	1	305	CLA	C4A-NA-C1A	6.33	109.57	106.68
20	A	818	CLA	C4A-NA-C1A	6.33	109.56	106.68
20	B	837	CLA	C4A-NA-C1A	6.32	109.56	106.68
20	G	605	CLA	C4A-NA-C1A	6.32	109.56	106.68
20	2	310	CLA	C4A-NA-C1A	6.32	109.56	106.68
20	F	804	CLA	C4A-NA-C1A	6.31	109.56	106.68
20	1	312	CLA	C4A-NA-C1A	6.31	109.56	106.68
20	1	321	CLA	C4A-NA-C1A	6.31	109.56	106.68
20	1	303	CLA	C4A-NA-C1A	6.31	109.56	106.68
20	A	823	CLA	C4A-NA-C1A	6.31	109.56	106.68
19	4	306	CHL	C1B-CHB-C4A	6.30	125.37	121.32
20	O	203	CLA	C4A-NA-C1A	6.29	109.55	106.68
20	2	309	CLA	C4A-NA-C1A	6.28	109.55	106.68
20	B	830	CLA	C4A-NA-C1A	6.28	109.55	106.68
20	4	314	CLA	C4A-NA-C1A	6.28	109.54	106.68
20	B	828	CLA	C4A-NA-C1A	6.27	109.54	106.68
20	3	314	CLA	C4A-NA-C1A	6.27	109.54	106.68
20	4	313	CLA	C4A-NA-C1A	6.26	109.53	106.68
19	3	306	CHL	C1B-CHB-C4A	6.25	125.35	121.32
20	L	304	CLA	C4A-NA-C1A	6.25	109.53	106.68
20	A	841	CLA	C4A-NA-C1A	6.24	109.52	106.68
20	4	310	CLA	C4A-NA-C1A	6.23	109.52	106.68
20	B	827	CLA	C4A-NA-C1A	6.22	109.52	106.68
20	A	828	CLA	C4A-NA-C1A	6.22	109.52	106.68
20	A	806	CLA	C4A-NA-C1A	6.21	109.51	106.68
19	4	315	CHL	O2D-CGD-O1D	-6.21	111.75	123.85
20	1	302	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	B	829	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	2	308	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	4	309	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	3	313	CLA	C4A-NA-C1A	6.17	109.50	106.68
20	A	801	CLA	C4A-NA-C1A	6.16	109.49	106.68
20	B	813	CLA	C4A-NA-C1A	6.15	109.48	106.68
20	A	822	CLA	C4A-NA-C1A	6.14	109.48	106.68
20	B	802	CLA	C4A-NA-C1A	6.12	109.47	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	825	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	4	306	CHL	CAA-CBA-CGA	-6.10	95.88	113.21
20	B	823	CLA	C4A-NA-C1A	6.07	109.45	106.68
19	4	305	CHL	C1B-CHB-C4A	6.06	125.22	121.32
20	A	826	CLA	C4A-NA-C1A	6.02	109.43	106.68
22	4	317	XAT	O4-C5-C4	6.01	119.12	113.49
20	B	822	CLA	C4A-NA-C1A	6.01	109.42	106.68
19	2	301	CHL	C1B-CHB-C4A	5.99	125.18	121.32
20	K	202	CLA	C4A-NA-C1A	5.99	109.41	106.68
19	2	307	CHL	CHA-C1A-C2A	-5.98	119.27	133.31
20	O	202	CLA	O2D-CGD-CBD	5.98	121.68	111.23
19	3	306	CHL	O2D-CGD-O1D	-5.98	112.22	123.85
20	O	201	CLA	C4A-NA-C1A	5.95	109.39	106.68
22	2	316	XAT	O24-C25-C24	5.92	119.03	113.49
19	2	301	CHL	CED-O2D-CGD	5.91	129.32	115.92
20	B	801	CLA	C4A-NA-C1A	5.90	109.37	106.68
19	2	314	CHL	CHA-C1A-C2A	-5.90	119.45	133.31
19	2	306	CHL	CHA-C1A-C2A	-5.89	119.49	133.31
19	4	315	CHL	CBC-CAC-C3C	-5.88	104.45	112.87
22	1	316	XAT	O24-C25-C24	5.88	119.00	113.49
23	B	843	BCR	C24-C23-C22	-5.85	117.58	126.23
19	4	306	CHL	CHA-C1A-C2A	-5.84	119.59	133.31
23	B	842	BCR	C7-C8-C9	-5.82	117.62	126.23
23	A	849	BCR	C7-C8-C9	-5.80	117.66	126.23
19	3	306	CHL	CHA-C1A-C2A	-5.77	119.75	133.31
23	B	843	BCR	C7-C8-C9	-5.74	117.75	126.23
23	B	845	BCR	C15-C14-C13	-5.71	119.27	127.28
19	4	315	CHL	C1B-CHB-C4A	5.71	125.00	121.32
20	A	851	CLA	C4A-NA-C1A	5.69	109.28	106.68
20	O	202	CLA	C4A-NA-C1A	5.69	109.28	106.68
19	4	307	CHL	OMC-CMC-C2C	-5.67	115.27	125.12
19	2	305	CHL	CHA-C1A-C2A	-5.64	120.07	133.31
19	2	305	CHL	CBC-CAC-C3C	-5.61	104.85	112.87
19	4	315	CHL	CHA-C1A-C2A	-5.59	120.18	133.31
22	3	316	XAT	O4-C5-C4	5.58	118.72	113.49
19	4	307	CHL	CHA-C1A-C2A	-5.55	120.27	133.31
19	3	306	CHL	CBC-CAC-C3C	-5.55	104.92	112.87
19	1	306	CHL	CHA-C1A-C2A	-5.55	120.27	133.31
19	4	305	CHL	CHA-C1A-C2A	-5.55	120.28	133.31
23	L	305	BCR	C24-C23-C22	-5.54	118.03	126.23
19	2	307	CHL	OMC-CMC-C2C	-5.52	115.53	125.12
19	2	301	CHL	CHA-C1A-C2A	-5.50	120.38	133.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	204	BCR	C16-C17-C18	-5.50	119.56	127.28
23	A	854	BCR	C15-C14-C13	-5.48	119.59	127.28
19	4	307	CHL	C1B-CHB-C4A	5.47	124.84	121.32
20	3	309	CLA	C4A-NA-C1A	5.46	109.17	106.68
19	4	307	CHL	C1C-C2C-CMC	5.43	136.60	126.80
23	A	854	BCR	C16-C17-C18	-5.42	119.68	127.28
23	L	301	BCR	C7-C8-C9	-5.41	118.23	126.23
23	2	317	BCR	C15-C14-C13	-5.41	119.69	127.28
23	4	318	BCR	C32-C1-C2	-5.36	88.36	108.95
22	4	317	XAT	O24-C25-C24	5.36	118.52	113.49
23	B	841	BCR	C15-C14-C13	-5.35	119.77	127.28
19	4	305	CHL	O2A-CGA-CBA	5.34	128.10	111.83
23	F	806	BCR	C11-C10-C9	-5.31	119.83	127.28
23	A	849	BCR	C16-C17-C18	-5.31	119.83	127.28
22	3	316	XAT	C26-C27-C28	-5.30	114.78	125.99
22	1	316	XAT	O4-C5-C18	5.29	120.96	115.05
23	4	318	BCR	C2-C1-C6	5.23	118.03	110.44
19	3	306	CHL	O2A-CGA-CBA	5.23	131.88	112.14
23	L	305	BCR	C3-C4-C5	-5.21	104.76	114.06
22	2	316	XAT	O4-C5-C18	5.19	120.85	115.05
19	1	301	CHL	CHA-C1A-C2A	-5.18	121.14	133.31
19	4	306	CHL	CED-O2D-CGD	5.17	127.63	115.92
23	A	849	BCR	C20-C21-C22	-5.14	120.07	127.28
23	4	318	BCR	C15-C14-C13	-5.13	120.08	127.28
22	1	316	XAT	C6-C7-C8	-5.10	115.20	125.99
21	O	205	LUT	C31-C30-C29	-5.10	120.12	127.28
23	2	317	BCR	C16-C17-C18	-5.09	120.13	127.28
23	L	306	BCR	C28-C27-C26	-5.09	104.98	114.06
23	3	317	BCR	C15-C14-C13	-5.08	120.15	127.28
19	3	306	CHL	CMA-C3A-C4A	5.06	125.52	114.61
23	L	301	BCR	C15-C14-C13	-5.06	120.18	127.28
19	2	301	CHL	O2A-CGA-CBA	5.05	127.24	111.83
19	4	307	CHL	O2A-CGA-CBA	5.04	127.21	111.83
22	3	316	XAT	O24-C25-C38	5.03	120.67	115.05
21	O	205	LUT	C7-C8-C9	-5.02	118.80	126.23
23	F	806	BCR	C15-C14-C13	-5.01	120.25	127.28
21	O	205	LUT	C35-C34-C33	-5.00	120.26	127.28
19	1	306	CHL	O1D-CGD-CBD	-4.99	117.16	124.72
20	3	309	CLA	CAA-CBA-CGA	-4.95	99.16	113.21
21	1	319	LUT	C15-C14-C13	-4.95	120.34	127.28
23	F	801	BCR	C16-C15-C14	-4.92	113.44	123.52
19	2	301	CHL	O2A-CGA-O1A	-4.91	111.35	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	205	LUT	C11-C10-C9	-4.90	120.41	127.28
19	4	306	CHL	OMC-CMC-C2C	-4.88	116.65	125.12
23	A	854	BCR	C11-C10-C9	-4.83	120.50	127.28
23	K	204	BCR	C20-C21-C22	-4.82	120.52	127.28
23	A	847	BCR	C16-C17-C18	-4.82	120.53	127.28
23	I	101	BCR	C24-C23-C22	-4.81	119.12	126.23
23	3	317	BCR	C3-C4-C5	-4.79	105.51	114.06
23	I	101	BCR	C16-C17-C18	-4.76	120.60	127.28
19	4	307	CHL	CBC-CAC-C3C	-4.74	106.09	112.87
22	4	317	XAT	C26-C27-C28	-4.74	115.98	125.99
22	2	316	XAT	C6-C7-C8	-4.72	116.00	125.99
19	3	306	CHL	O2A-CGA-O1A	-4.72	109.11	123.20
22	3	316	XAT	O24-C25-C24	4.71	117.90	113.49
23	J	104	BCR	C16-C17-C18	-4.71	120.68	127.28
23	B	845	BCR	C24-C23-C22	-4.70	119.28	126.23
20	4	304	CLA	CAC-C3C-C4C	4.68	130.88	124.79
23	1	317	BCR	C15-C14-C13	-4.68	120.71	127.28
23	J	102	BCR	C15-C14-C13	-4.68	120.72	127.28
22	2	316	XAT	O4-C5-C4	4.66	117.86	113.49
23	J	102	BCR	C20-C21-C22	-4.65	120.76	127.28
19	3	306	CHL	C1C-C2C-CMC	4.64	135.17	126.80
23	2	317	BCR	C11-C10-C9	-4.62	120.79	127.28
23	F	806	BCR	C7-C8-C9	-4.60	119.43	126.23
23	A	846	BCR	C15-C14-C13	-4.58	120.85	127.28
19	1	306	CHL	O2A-CGA-O1A	-4.58	112.17	123.63
23	2	317	BCR	C38-C26-C25	-4.55	119.51	124.48
23	J	104	BCR	C20-C21-C22	-4.55	120.89	127.28
23	B	844	BCR	C15-C14-C13	-4.55	120.90	127.28
23	B	844	BCR	C28-C27-C26	-4.55	105.95	114.06
23	L	306	BCR	C24-C23-C22	-4.54	119.51	126.23
23	L	306	BCR	C20-C21-C22	-4.53	120.92	127.28
22	1	316	XAT	O24-C25-C38	4.53	120.11	115.05
23	J	102	BCR	C16-C17-C18	-4.52	120.93	127.28
21	2	315	LUT	C26-C27-C28	-4.52	117.55	124.58
22	3	316	XAT	C6-C7-C8	-4.52	116.44	125.99
23	G	606	BCR	C28-C27-C26	-4.50	106.03	114.06
22	4	317	XAT	C6-C7-C8	-4.49	116.49	125.99
23	J	102	BCR	C38-C26-C25	-4.48	119.59	124.48
20	3	309	CLA	CMD-C2D-C3D	-4.47	117.44	127.69
23	B	846	BCR	C16-C17-C18	-4.47	121.02	127.28
21	1	315	LUT	C35-C34-C33	-4.46	121.02	127.28
23	B	842	BCR	C15-C14-C13	-4.46	121.03	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	847	BCR	C28-C27-C26	-4.46	106.11	114.06
20	4	304	CLA	CED-O2D-CGD	4.45	126.02	115.92
19	2	306	CHL	CGD-CBD-CAD	-4.45	96.44	110.85
23	A	848	BCR	C7-C8-C9	-4.45	119.66	126.23
22	2	316	XAT	C26-C27-C28	-4.44	116.60	125.99
23	K	204	BCR	C38-C26-C25	-4.44	119.64	124.48
23	A	845	BCR	C16-C17-C18	-4.44	121.05	127.28
21	2	315	LUT	C35-C34-C33	-4.44	121.06	127.28
22	4	317	XAT	O24-C25-C38	4.42	119.99	115.05
23	A	849	BCR	C24-C23-C22	-4.42	119.70	126.23
23	I	101	BCR	C7-C8-C9	-4.42	119.70	126.23
19	2	307	CHL	CAC-C3C-C4C	4.42	135.38	124.03
23	I	101	BCR	C11-C10-C9	-4.42	121.08	127.28
23	4	318	BCR	C11-C10-C9	-4.42	121.08	127.28
23	G	606	BCR	C16-C17-C18	-4.40	121.11	127.28
23	K	204	BCR	C7-C8-C9	-4.39	119.74	126.23
19	1	306	CHL	C1B-CHB-C4A	4.39	124.14	121.32
23	L	306	BCR	C15-C14-C13	-4.38	121.14	127.28
23	3	317	BCR	C11-C10-C9	-4.37	121.15	127.28
20	A	801	CLA	O2D-CGD-CBD	4.35	118.84	111.23
23	A	848	BCR	C16-C17-C18	-4.35	121.18	127.28
23	J	104	BCR	C15-C14-C13	-4.34	121.19	127.28
22	3	316	XAT	C15-C14-C13	-4.34	121.19	127.28
22	2	316	XAT	O24-C25-C38	4.34	119.90	115.05
23	G	606	BCR	C20-C21-C22	-4.33	121.20	127.28
23	F	801	BCR	C20-C21-C22	-4.31	121.23	127.28
22	4	317	XAT	C35-C34-C33	-4.30	121.25	127.28
23	A	848	BCR	C15-C14-C13	-4.30	121.25	127.28
24	A	844	LHG	O7-C7-C8	4.27	120.73	111.48
19	4	307	CHL	CED-O2D-CGD	4.27	125.60	115.92
22	3	316	XAT	O4-C5-C18	4.27	119.82	115.05
23	B	842	BCR	C3-C4-C5	-4.27	106.45	114.06
21	1	315	LUT	C26-C27-C28	-4.26	117.94	124.58
23	A	846	BCR	C16-C17-C18	-4.26	121.30	127.28
23	B	843	BCR	C15-C14-C13	-4.26	121.31	127.28
23	A	846	BCR	C20-C21-C22	-4.24	121.33	127.28
23	L	306	BCR	C16-C17-C18	-4.22	121.36	127.28
23	L	305	BCR	C15-C14-C13	-4.21	121.37	127.28
19	4	305	CHL	CBC-CAC-C3C	-4.21	106.84	112.87
23	I	101	BCR	C15-C14-C13	-4.19	121.40	127.28
23	B	845	BCR	C33-C5-C6	-4.19	119.91	124.48
23	B	841	BCR	C3-C4-C5	-4.18	106.60	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	301	BCR	C33-C5-C6	-4.18	119.93	124.48
21	O	205	LUT	C15-C14-C13	-4.16	121.45	127.28
23	4	318	BCR	C33-C5-C6	-4.15	119.95	124.48
23	B	845	BCR	C11-C10-C9	-4.15	121.46	127.28
23	2	317	BCR	C33-C5-C6	-4.13	119.98	124.48
23	A	845	BCR	C20-C21-C22	-4.12	121.50	127.28
23	I	101	BCR	C20-C21-C22	-4.11	121.51	127.28
20	O	202	CLA	CMD-C2D-C3D	-4.11	118.26	127.69
23	L	305	BCR	C16-C17-C18	-4.11	121.51	127.28
19	4	305	CHL	C1-O2A-CGA	4.11	126.59	116.65
20	4	304	CLA	C5-C3-C4	4.10	124.03	114.59
20	3	309	CLA	CBC-CAC-C3C	-4.10	101.31	112.42
20	4	304	CLA	CMD-C2D-C1D	4.09	131.93	124.73
19	1	301	CHL	C1-C2-C3	-4.08	119.51	126.20
22	3	316	XAT	C35-C34-C33	-4.08	121.56	127.28
22	1	316	XAT	C26-C27-C28	-4.08	117.37	125.99
20	4	304	CLA	C1-O2A-CGA	-4.08	106.78	116.65
23	A	846	BCR	C24-C23-C22	-4.06	120.23	126.23
25	1	320	LMG	O7-C10-C11	4.05	120.25	111.48
19	4	305	CHL	O2A-C1-C2	4.05	123.69	108.11
23	L	305	BCR	C20-C21-C22	-4.05	121.60	127.28
19	4	305	CHL	O1D-CGD-CBD	-4.04	118.60	124.72
21	O	204	LUT	C35-C34-C33	-4.04	121.61	127.28
23	4	318	BCR	C16-C17-C18	-4.04	121.61	127.28
23	L	305	BCR	C38-C26-C25	-4.03	120.09	124.48
19	2	301	CHL	C1-O2A-CGA	4.02	126.38	116.65
22	4	317	XAT	O4-C5-C18	4.02	119.54	115.05
23	L	301	BCR	C38-C26-C25	-4.02	120.10	124.48
23	G	606	BCR	C24-C23-C22	-4.00	120.32	126.23
19	1	306	CHL	OMC-CMC-C2C	-4.00	118.17	125.12
22	1	316	XAT	O4-C5-C4	4.00	117.24	113.49
19	1	306	CHL	CMA-C3A-C4A	-3.98	106.03	114.61
23	B	846	BCR	C33-C5-C6	-3.98	120.14	124.48
21	O	204	LUT	C15-C14-C13	-3.98	121.70	127.28
23	B	843	BCR	C16-C17-C18	-3.98	121.70	127.28
23	L	306	BCR	C27-C26-C25	-3.96	117.35	122.70
23	B	843	BCR	C33-C5-C6	-3.95	120.17	124.48
24	1	318	LHG	O7-C7-C8	3.94	120.01	111.48
23	A	847	BCR	C15-C14-C13	-3.94	121.75	127.28
23	B	841	BCR	C20-C21-C22	-3.92	121.78	127.28
23	B	844	BCR	C11-C10-C9	-3.91	121.80	127.28
20	A	801	CLA	O2D-CGD-O1D	-3.90	116.25	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	848	DGD	O2G-C1B-C2B	3.90	119.92	111.48
23	A	845	BCR	C24-C23-C22	-3.89	120.48	126.23
23	J	104	BCR	C24-C23-C22	-3.88	120.49	126.23
19	2	305	CHL	CAA-C2A-C1A	3.88	121.04	113.35
23	A	846	BCR	C11-C10-C9	-3.87	121.85	127.28
23	2	317	BCR	C20-C21-C22	-3.86	121.86	127.28
23	A	847	BCR	C33-C5-C6	-3.86	120.27	124.48
19	1	306	CHL	O2A-CGA-CBA	3.85	123.58	111.83
23	2	317	BCR	C24-C23-C22	-3.84	120.55	126.23
23	A	845	BCR	C15-C14-C13	-3.84	121.89	127.28
23	L	306	BCR	C7-C8-C9	-3.82	120.58	126.23
23	3	317	BCR	C7-C8-C9	-3.82	120.58	126.23
21	O	204	LUT	C31-C30-C29	-3.82	121.92	127.28
26	A	852	HTG	C1-O5-C5	3.81	119.39	112.56
24	2	318	LHG	O7-C7-C8	3.80	119.71	111.48
23	1	317	BCR	C28-C27-C26	-3.79	107.30	114.06
23	4	318	BCR	C28-C27-C26	-3.77	107.33	114.06
23	A	846	BCR	C33-C5-C6	-3.77	120.37	124.48
25	4	319	LMG	O7-C10-C11	3.77	119.64	111.48
23	J	102	BCR	C33-C5-C6	-3.77	120.37	124.48
19	2	307	CHL	CED-O2D-CGD	3.76	124.45	115.92
20	O	202	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
21	4	316	LUT	C35-C34-C33	-3.76	122.00	127.28
24	A	843	LHG	O7-C7-C8	3.76	119.61	111.48
19	4	305	CHL	O2A-CGA-O1A	-3.76	114.23	123.63
23	L	301	BCR	C24-C23-C22	-3.76	120.68	126.23
21	4	316	LUT	C26-C27-C28	-3.75	118.74	124.58
21	1	319	LUT	C11-C10-C9	-3.75	122.02	127.28
23	J	104	BCR	C11-C10-C9	-3.75	122.02	127.28
23	B	841	BCR	C16-C17-C18	-3.74	122.03	127.28
23	1	317	BCR	C33-C5-C6	-3.74	120.41	124.48
23	3	317	BCR	C28-C27-C26	-3.73	107.40	114.06
19	4	305	CHL	O2D-CGD-O1D	-3.73	116.59	123.85
23	A	854	BCR	C20-C21-C22	-3.72	122.06	127.28
19	2	306	CHL	O2A-CGA-CBA	3.71	123.16	111.83
19	2	305	CHL	OBD-CAD-CBD	-3.71	120.38	125.82
22	2	316	XAT	C35-C34-C33	-3.70	122.09	127.28
21	3	315	LUT	C26-C27-C28	-3.70	118.82	124.58
23	A	848	BCR	C11-C10-C9	-3.70	122.09	127.28
19	4	306	CHL	C5-C3-C4	3.70	123.09	114.59
23	G	606	BCR	C15-C14-C13	-3.68	122.12	127.28
23	F	806	BCR	C24-C23-C22	-3.68	120.80	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	323	LMG	O7-C10-C11	3.67	119.41	111.48
20	4	304	CLA	O2A-CGA-O1A	-3.66	114.47	123.63
21	3	315	LUT	C35-C34-C33	-3.66	122.15	127.28
23	A	847	BCR	C20-C21-C22	-3.64	122.17	127.28
23	B	846	BCR	C24-C23-C22	-3.64	120.85	126.23
19	2	307	CHL	CBC-CAC-C3C	-3.63	107.67	112.87
19	2	301	CHL	C4-C3-C5	3.63	121.53	115.23
23	B	845	BCR	C16-C17-C18	-3.63	122.19	127.28
21	O	204	LUT	C26-C27-C28	-3.63	118.94	124.58
23	2	317	BCR	C8-C7-C6	-3.62	117.31	127.00
23	B	841	BCR	C38-C26-C25	-3.62	120.53	124.48
21	O	204	LUT	C21-C26-C27	-3.62	108.67	112.83
23	L	301	BCR	C16-C17-C18	-3.61	122.22	127.28
23	1	317	BCR	C16-C17-C18	-3.60	122.23	127.28
23	F	806	BCR	C20-C21-C22	-3.60	122.23	127.28
23	K	204	BCR	C11-C10-C9	-3.58	122.26	127.28
23	F	806	BCR	C33-C5-C6	-3.58	120.58	124.48
19	4	306	CHL	CBA-CAA-C2A	-3.57	103.26	113.78
20	4	304	CLA	O1D-CGD-CBD	-3.56	117.49	124.52
23	J	104	BCR	C28-C27-C26	-3.54	107.74	114.06
23	A	847	BCR	C11-C10-C9	-3.54	122.31	127.28
21	4	316	LUT	C21-C26-C27	-3.54	108.76	112.83
23	A	845	BCR	C33-C5-C6	-3.53	120.63	124.48
23	A	848	BCR	C38-C26-C25	-3.53	120.63	124.48
23	A	847	BCR	C24-C23-C22	-3.53	121.02	126.23
20	4	304	CLA	O2A-CGA-CBA	3.52	122.57	111.83
23	B	844	BCR	C16-C17-C18	-3.52	122.35	127.28
23	K	204	BCR	C15-C14-C13	-3.52	122.35	127.28
19	4	306	CHL	O1D-CGD-CBD	-3.52	119.39	124.72
23	L	305	BCR	C4-C5-C6	-3.51	117.96	122.70
19	2	307	CHL	C5-C3-C4	3.51	122.66	114.59
23	B	841	BCR	C11-C10-C9	-3.50	122.36	127.28
19	4	315	CHL	C1C-C2C-CMC	3.50	133.11	126.80
23	L	306	BCR	C33-C5-C6	-3.49	120.68	124.48
23	L	306	BCR	C11-C10-C9	-3.48	122.39	127.28
23	A	846	BCR	C38-C26-C25	-3.48	120.69	124.48
22	3	316	XAT	C10-C11-C12	-3.47	113.13	123.20
19	2	307	CHL	CBA-CAA-C2A	-3.46	103.58	113.78
24	B	849	LHG	O7-C7-C8	3.46	118.97	111.48
23	3	317	BCR	C16-C17-C18	-3.46	122.43	127.28
23	1	317	BCR	C7-C8-C9	-3.45	121.13	126.23
21	2	315	LUT	C21-C26-C27	-3.45	108.86	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	806	BCR	C38-C26-C25	-3.44	120.73	124.48
23	L	305	BCR	C11-C10-C9	-3.44	122.45	127.28
21	4	316	LUT	C18-C5-C6	-3.44	120.73	124.48
20	3	309	CLA	CBA-CAA-C2A	-3.43	103.58	113.79
21	3	315	LUT	C15-C14-C13	-3.43	122.47	127.28
23	A	845	BCR	C28-C27-C26	-3.42	107.96	114.06
23	A	854	BCR	C15-C16-C17	-3.41	116.54	123.52
23	4	318	BCR	C38-C26-C25	-3.41	120.77	124.48
20	A	829	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
23	A	848	BCR	C23-C24-C25	-3.40	117.91	127.00
20	3	309	CLA	C3B-C4B-NB	-3.40	107.49	110.53
19	2	306	CHL	CBA-CAA-C2A	-3.40	103.76	113.78
23	A	854	BCR	C24-C23-C22	-3.40	121.21	126.23
20	2	313	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
23	F	801	BCR	C3-C4-C5	-3.39	108.01	114.06
21	1	319	LUT	C35-C34-C33	-3.39	122.52	127.28
21	4	316	LUT	C15-C14-C13	-3.38	122.53	127.28
23	F	806	BCR	C28-C27-C26	-3.38	108.03	114.06
23	J	104	BCR	C7-C8-C9	-3.38	121.24	126.23
19	2	301	CHL	C1C-C2C-CMC	3.37	132.88	126.80
23	A	845	BCR	C7-C8-C9	-3.36	121.26	126.23
23	G	606	BCR	C7-C8-C9	-3.36	121.27	126.23
20	B	825	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
20	A	803	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	F	806	BCR	C16-C17-C18	-3.34	122.59	127.28
19	3	306	CHL	O1D-CGD-CBD	-3.34	119.65	124.72
20	B	808	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
23	1	317	BCR	C3-C4-C5	-3.34	108.10	114.06
21	O	205	LUT	C27-C28-C29	-3.33	119.15	126.32
23	A	849	BCR	C15-C14-C13	-3.33	122.60	127.28
23	B	842	BCR	C16-C17-C18	-3.33	122.61	127.28
23	K	204	BCR	C24-C23-C22	-3.33	121.31	126.23
20	B	822	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
21	1	315	LUT	C15-C14-C13	-3.32	122.62	127.28
20	3	309	CLA	CMA-C3A-C4A	-3.32	102.85	111.77
26	A	852	HTG	C1'-S1-C1	3.31	107.61	100.45
23	L	301	BCR	C11-C10-C9	-3.31	122.64	127.28
23	J	104	BCR	C33-C5-C6	-3.31	120.87	124.48
23	G	606	BCR	C33-C5-C6	-3.31	120.88	124.48
19	2	307	CHL	O2A-CGA-CBA	3.30	121.89	111.83
21	O	205	LUT	C36-C21-C26	3.29	114.53	109.55
20	4	313	CLA	O2D-CGD-O1D	-3.29	117.45	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	826	CLA	C3B-C4B-NB	-3.28	107.60	110.53
23	4	318	BCR	C21-C20-C19	-3.28	113.70	123.20
27	A	842	PQN	C14-C13-C15	3.27	120.90	115.23
19	1	301	CHL	O2A-CGA-CBA	3.26	121.77	111.83
23	J	102	BCR	C3-C4-C5	-3.25	108.27	114.06
21	3	315	LUT	C31-C30-C29	-3.24	122.73	127.28
23	K	204	BCR	C33-C5-C6	-3.24	120.95	124.48
20	3	309	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
20	K	202	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
23	B	842	BCR	C30-C25-C26	-3.22	118.23	122.64
21	2	315	LUT	C18-C5-C6	-3.22	120.97	124.48
23	L	305	BCR	C7-C8-C9	-3.22	121.47	126.23
22	1	316	XAT	C18-C5-C4	3.22	117.86	114.24
20	A	851	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
23	B	841	BCR	C2-C1-C6	3.21	115.11	110.44
20	4	304	CLA	CAA-CBA-CGA	-3.21	104.10	113.21
23	B	845	BCR	C15-C16-C17	-3.20	116.97	123.52
19	2	307	CHL	C1C-C2C-CMC	3.20	132.56	126.80
20	J	101	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
20	O	201	CLA	C3B-C4B-NB	-3.19	107.69	110.53
20	A	838	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
19	2	301	CHL	OBD-CAD-C3D	-3.18	122.93	127.89
20	L	307	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
23	4	318	BCR	C3-C4-C5	-3.18	108.39	114.06
23	B	841	BCR	C24-C23-C22	-3.17	121.54	126.23
23	J	104	BCR	C3-C4-C5	-3.17	108.40	114.06
23	2	317	BCR	C33-C5-C4	3.17	120.35	113.60
23	B	845	BCR	C7-C8-C9	-3.17	121.55	126.23
20	A	825	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
20	1	321	CLA	C3B-C4B-NB	-3.16	107.70	110.53
20	A	833	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
22	2	316	XAT	C15-C14-C13	-3.16	122.84	127.28
19	4	306	CHL	C1-C2-C3	-3.16	121.66	126.76
19	2	306	CHL	C1-O2A-CGA	3.15	125.63	116.67
19	4	307	CHL	O2A-CGA-O1A	-3.15	115.74	123.63
19	3	306	CHL	CMB-C2B-C3B	-3.15	118.39	124.68
27	B	840	PQN	C11-C12-C13	-3.15	121.41	126.83
20	O	202	CLA	C3B-C4B-NB	-3.14	107.72	110.53
22	3	316	XAT	C24-C23-C22	-3.14	104.91	110.79
20	1	313	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
20	B	804	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	A	848	BCR	C28-C27-C26	-3.14	108.46	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	606	BCR	C29-C30-C25	3.14	114.99	110.44
20	4	314	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
20	A	801	CLA	C3B-C4B-NB	-3.13	107.74	110.53
21	1	319	LUT	C18-C5-C6	-3.13	121.07	124.48
20	A	816	CLA	C3B-C4B-NB	-3.12	107.74	110.53
21	1	319	LUT	C26-C27-C28	-3.12	119.73	124.58
23	A	854	BCR	C28-C27-C26	-3.12	108.50	114.06
23	K	204	BCR	C3-C4-C5	-3.12	108.50	114.06
20	A	831	CLA	C3B-C4B-NB	-3.11	107.75	110.53
21	3	315	LUT	C21-C26-C27	-3.11	109.25	112.83
23	B	844	BCR	C24-C23-C22	-3.11	121.63	126.23
20	A	811	CLA	C3B-C4B-NB	-3.11	107.76	110.53
23	L	301	BCR	C20-C21-C22	-3.10	122.92	127.28
23	1	317	BCR	C38-C26-C25	-3.10	121.10	124.48
20	B	824	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
20	A	807	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
20	G	603	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
23	B	842	BCR	C28-C27-C26	-3.10	108.53	114.06
19	2	314	CHL	C1C-CHC-C4B	3.09	127.14	116.07
23	A	847	BCR	C7-C8-C9	-3.09	121.66	126.23
23	A	845	BCR	C11-C10-C9	-3.09	122.94	127.28
23	L	305	BCR	C2-C1-C6	3.09	114.93	110.44
21	3	315	LUT	C18-C5-C6	-3.09	121.11	124.48
23	B	845	BCR	C38-C26-C25	-3.09	121.11	124.48
20	1	304	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
21	1	315	LUT	C18-C5-C6	-3.08	121.12	124.48
20	A	853	CLA	C3B-C4B-NB	-3.08	107.78	110.53
20	G	605	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	2	316	XAT	C10-C11-C12	-3.08	114.28	123.20
20	2	310	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
19	2	305	CHL	C1C-CHC-C4B	3.07	127.06	116.07
23	L	306	BCR	C38-C26-C27	3.07	120.14	113.60
20	L	303	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
20	B	832	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	A	847	BCR	C29-C30-C25	3.06	114.89	110.44
20	A	818	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
20	A	817	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	B	843	BCR	C38-C26-C25	-3.06	121.14	124.48
20	K	202	CLA	C3B-C4B-NB	-3.06	107.80	110.53
22	2	316	XAT	C4-C3-C2	-3.06	105.07	110.79
19	3	306	CHL	CAC-C3C-C4C	3.06	131.89	124.03
20	F	805	CLA	O2D-CGD-O1D	-3.06	117.90	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	836	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
23	B	842	BCR	C33-C5-C6	-3.05	121.16	124.48
20	B	807	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
20	A	830	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
20	1	310	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
20	B	823	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
21	2	315	LUT	C15-C14-C13	-3.05	123.00	127.28
23	B	846	BCR	C7-C8-C9	-3.05	121.73	126.23
23	B	846	BCR	C20-C21-C22	-3.05	123.01	127.28
23	G	606	BCR	C11-C10-C9	-3.04	123.01	127.28
20	2	309	CLA	C3B-C4B-NB	-3.04	107.81	110.53
20	A	831	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	A	837	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	B	815	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
21	2	315	LUT	C7-C8-C9	-3.04	121.74	126.23
20	B	838	CLA	C3B-C4B-NB	-3.04	107.82	110.53
21	1	319	LUT	C7-C8-C9	-3.03	121.75	126.23
19	4	315	CHL	C1C-CHC-C4B	3.03	126.92	116.07
20	B	822	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	B	846	BCR	C15-C14-C13	-3.03	123.03	127.28
20	B	812	CLA	C3B-C4B-NB	-3.03	107.83	110.53
20	A	806	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
20	B	830	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
20	O	203	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
23	1	317	BCR	C21-C20-C19	-3.02	114.44	123.20
20	3	304	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
20	A	836	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
20	B	819	CLA	C3B-C4B-NB	-3.02	107.83	110.53
20	B	811	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
19	3	306	CHL	C1C-CHC-C4B	3.02	126.87	116.07
22	4	317	XAT	C10-C11-C12	-3.02	114.46	123.20
19	2	306	CHL	C1C-CHC-C4B	3.02	126.86	116.07
20	B	829	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
20	B	837	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
20	A	802	CLA	C3B-C4B-NB	-3.01	107.84	110.53
23	A	854	BCR	C33-C5-C6	-3.01	121.19	124.48
20	B	820	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
19	4	315	CHL	CMD-C2D-C3D	3.01	130.70	124.68
20	4	308	CLA	C3B-C4B-NB	-3.01	107.84	110.53
20	F	805	CLA	C3B-C4B-NB	-3.01	107.84	110.53
23	B	843	BCR	C28-C27-C26	-3.01	108.69	114.06
20	B	833	CLA	C3B-C4B-NB	-3.01	107.84	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	814	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
20	B	812	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
21	1	319	LUT	C21-C26-C27	-3.01	109.37	112.83
20	3	301	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
20	B	818	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
23	F	801	BCR	C28-C27-C26	-3.00	108.70	114.06
20	B	803	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	2	301	CHL	C1C-CHC-C4B	3.00	126.80	116.07
20	A	804	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	3	316	XAT	C38-C25-C24	3.00	117.61	114.24
20	G	604	CLA	C3B-C4B-NB	-3.00	107.86	110.53
23	A	846	BCR	C8-C7-C6	-3.00	119.00	127.00
20	A	826	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
21	O	204	LUT	C18-C5-C6	-2.99	121.22	124.48
20	A	822	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
20	A	823	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	A	819	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	3	311	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	L	303	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	L	304	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
20	3	305	CLA	C3B-C4B-NB	-2.99	107.86	110.53
20	K	201	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	1	317	BCR	C23-C24-C25	-2.99	119.02	127.00
20	G	604	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
23	B	844	BCR	C29-C30-C25	2.98	114.77	110.44
23	A	849	BCR	C38-C26-C25	-2.98	121.23	124.48
20	2	304	CLA	C3B-C4B-NB	-2.98	107.87	110.53
20	B	839	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
19	1	306	CHL	C1C-CHC-C4B	2.98	126.73	116.07
20	K	203	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	F	804	CLA	C3B-C4B-NB	-2.98	107.87	110.53
20	B	814	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
20	2	308	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	B	810	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	B	828	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	A	835	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	1	311	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	K	205	CLA	C3B-C4B-NB	-2.97	107.88	110.53
27	B	840	PQN	C14-C13-C15	2.97	120.38	115.23
20	4	308	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	3	313	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	B	817	CLA	C3B-C4B-NB	-2.97	107.88	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	302	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
23	3	317	BCR	C38-C26-C25	-2.96	121.25	124.48
20	1	303	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
20	A	822	CLA	C3B-C4B-NB	-2.96	107.89	110.53
20	A	841	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
20	A	823	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
20	F	804	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
20	4	311	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	B	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	1	316	XAT	C4-C3-C2	-2.96	105.26	110.79
23	J	102	BCR	C20-C19-C18	-2.96	118.26	126.36
20	3	310	CLA	C3B-C4B-NB	-2.96	107.89	110.53
20	B	801	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	B	817	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
20	2	312	CLA	C3B-C4B-NB	-2.95	107.89	110.53
23	A	847	BCR	C8-C7-C6	-2.95	119.11	127.00
20	G	603	CLA	C3B-C4B-NB	-2.95	107.90	110.53
20	A	808	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	4	304	CLA	CAC-C3C-C2C	-2.95	122.14	127.56
20	K	201	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
22	1	316	XAT	C10-C11-C12	-2.95	114.66	123.20
20	B	826	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	4	302	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
23	A	845	BCR	C30-C25-C26	-2.94	118.61	122.64
23	J	104	BCR	C38-C26-C25	-2.94	121.27	124.48
20	A	810	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
20	B	831	CLA	C3B-C4B-NB	-2.94	107.90	110.53
20	J	103	CLA	C3B-C4B-NB	-2.94	107.90	110.53
20	B	835	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
23	F	801	BCR	C24-C23-C22	-2.94	121.89	126.23
20	A	812	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	B	802	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
20	3	303	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	1	306	CHL	CMB-C2B-C3B	-2.94	118.81	124.68
20	A	841	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	4	317	XAT	C24-C23-C22	-2.93	105.31	110.79
22	2	316	XAT	C24-C23-C22	-2.93	105.31	110.79
20	1	307	CLA	C3B-C4B-NB	-2.93	107.92	110.53
19	4	306	CHL	C1C-CHC-C4B	2.93	126.54	116.07
20	3	307	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	1	321	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
23	A	847	BCR	C3-C4-C5	-2.92	108.84	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	312	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	4	301	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	A	817	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	B	819	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
20	O	201	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	O	204	LUT	C11-C10-C9	-2.92	123.18	127.28
20	3	308	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	J	101	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	2	302	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	B	823	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
20	A	840	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	B	830	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	B	831	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	A	839	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
20	4	310	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	A	840	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	A	824	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
20	K	202	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
20	3	314	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	B	839	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	1	317	BCR	C11-C10-C9	-2.91	123.20	127.28
20	B	816	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	1	301	CHL	C4-C3-C5	2.91	119.55	116.13
19	4	307	CHL	C5-C3-C4	2.91	121.28	114.59
23	J	102	BCR	C15-C16-C17	-2.91	117.57	123.52
20	A	813	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
20	4	309	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	A	839	CLA	C3B-C4B-NB	-2.91	107.94	110.53
20	A	834	CLA	C3B-C4B-NB	-2.91	107.94	110.53
23	A	849	BCR	C20-C19-C18	-2.90	118.40	126.36
21	O	205	LUT	C1-C6-C5	-2.90	118.67	122.64
19	2	307	CHL	C1C-CHC-C4B	2.90	126.45	116.07
20	F	802	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
20	A	810	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	2	311	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	1	316	XAT	C31-C30-C29	-2.90	123.22	127.28
30	B	848	DGD	C2G-O2G-C1B	-2.89	110.87	117.80
23	L	306	BCR	C29-C30-C25	2.89	114.64	110.44
20	3	301	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	A	801	CLA	CGD-CBD-CAD	2.89	120.20	110.85
20	A	805	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
19	1	301	CHL	O1D-CGD-CBD	-2.89	120.34	124.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	305	CHL	C1C-CHC-C4B	2.89	126.41	116.07
20	B	823	CLA	C3B-C4B-NB	-2.89	107.95	110.53
20	A	811	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	4	301	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	A	844	LHG	O8-C23-C24	2.89	119.91	111.15
20	A	821	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	2	315	LUT	C35-C15-C14	-2.89	117.61	123.52
19	4	307	CHL	C1C-CHC-C4B	2.89	126.39	116.07
23	A	846	BCR	C7-C8-C9	-2.88	121.97	126.23
20	L	307	CLA	C3B-C4B-NB	-2.88	107.96	110.53
20	B	813	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
20	B	806	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
20	4	312	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	4	312	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	4	317	XAT	C38-C25-C24	2.88	117.47	114.24
20	B	834	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	N	203	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
20	A	815	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
20	G	605	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	A	825	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	2	317	BCR	C3-C4-C5	-2.87	108.93	114.06
20	K	205	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
20	A	813	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	A	820	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	J	103	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	I	101	BCR	C1-C6-C5	-2.87	118.72	122.64
20	3	310	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	B	808	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	A	816	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
20	B	805	CLA	C3B-C4B-NB	-2.86	107.97	110.53
20	A	828	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	2	304	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	3	317	BCR	C4-C5-C6	-2.86	118.84	122.70
23	I	101	BCR	C27-C26-C25	-2.86	118.84	122.70
20	H	201	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
20	B	838	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
20	B	825	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	B	844	BCR	C7-C8-C9	-2.85	122.02	126.23
23	A	846	BCR	C3-C4-C5	-2.85	108.97	114.06
23	G	606	BCR	C27-C26-C25	-2.85	118.85	122.70
24	1	318	LHG	O8-C23-C24	2.85	120.52	111.83
19	1	301	CHL	C1B-CHB-C4A	2.85	123.16	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	820	CLA	C3B-C4B-NB	-2.85	107.99	110.53
20	A	814	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	3	305	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
20	4	314	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	B	821	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	1	304	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	3	312	CLA	C3B-C4B-NB	-2.84	107.99	110.53
20	1	302	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	2	303	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
20	B	827	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
20	3	314	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
23	I	101	BCR	C28-C27-C26	-2.84	109.00	114.06
20	B	833	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
22	4	317	XAT	C4-C3-C2	-2.83	105.49	110.79
20	2	308	CLA	C3B-C4B-NB	-2.83	108.00	110.53
20	A	809	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
19	3	306	CHL	CED-O2D-CGD	2.83	122.34	115.92
23	B	845	BCR	C21-C20-C19	-2.83	114.99	123.20
21	2	315	LUT	C11-C10-C9	-2.83	123.31	127.28
20	3	311	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	B	804	CLA	C3B-C4B-NB	-2.83	108.00	110.53
23	F	801	BCR	C33-C5-C6	-2.82	121.40	124.48
20	1	313	CLA	C3B-C4B-NB	-2.82	108.01	110.53
20	A	815	CLA	C3B-C4B-NB	-2.82	108.01	110.53
23	4	318	BCR	C23-C24-C25	-2.82	119.47	127.00
20	A	808	CLA	C3B-C4B-NB	-2.82	108.01	110.53
20	1	312	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	4	302	CLA	C3B-C4B-NB	-2.82	108.02	110.53
23	A	845	BCR	C27-C26-C25	-2.82	118.90	122.70
20	3	313	CLA	C3B-C4B-NB	-2.82	108.02	110.53
20	A	812	CLA	C3B-C4B-NB	-2.82	108.02	110.53
20	B	826	CLA	C3B-C4B-NB	-2.82	108.02	110.53
20	A	819	CLA	C3B-C4B-NB	-2.82	108.02	110.53
20	B	809	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	3	316	XAT	C4-C3-C2	-2.81	105.53	110.79
20	B	821	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
21	1	315	LUT	C10-C11-C12	-2.81	115.05	123.20
25	1	323	LMG	O8-C28-C29	2.81	120.40	111.83
20	1	314	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
23	A	845	BCR	C38-C26-C27	2.81	119.58	113.60
20	1	307	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
20	B	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	311	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	B	813	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	B	842	BCR	C27-C26-C25	-2.80	118.92	122.70
20	A	802	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	4	318	BCR	C8-C7-C6	-2.80	119.52	127.00
20	4	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	A	807	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	3	309	CLA	O1D-CGD-CBD	-2.80	119.00	124.52
20	1	312	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	L	302	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	4	318	BCR	C11-C12-C13	-2.80	118.70	126.36
20	A	827	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	A	834	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
20	B	814	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	H	201	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	2	312	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	B	843	BCR	C20-C21-C22	-2.79	123.37	127.28
23	B	846	BCR	C16-C15-C14	-2.79	117.82	123.52
20	4	303	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	B	836	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	4	306	CHL	CGD-CBD-CAD	-2.78	101.84	110.85
20	A	832	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
20	1	305	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	A	833	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	B	828	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	A	848	BCR	C20-C21-C22	-2.78	123.38	127.28
20	L	304	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	3	316	XAT	C18-C5-C4	2.78	117.36	114.24
20	1	310	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
23	B	844	BCR	C20-C21-C22	-2.78	123.38	127.28
21	2	315	LUT	C30-C31-C32	-2.78	115.15	123.20
23	I	101	BCR	C3-C4-C5	-2.78	109.11	114.06
20	1	302	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	4	317	XAT	C35-C15-C14	-2.77	117.84	123.52
20	1	314	CLA	C3B-C4B-NB	-2.77	108.05	110.53
21	1	315	LUT	C8-C7-C6	-2.77	119.59	127.00
23	F	801	BCR	C21-C20-C19	-2.77	115.17	123.20
20	A	835	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	1	319	LUT	C31-C30-C29	-2.77	123.39	127.28
20	A	809	CLA	C3B-C4B-NB	-2.77	108.06	110.53
20	3	302	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
20	A	821	CLA	C3B-C4B-NB	-2.76	108.06	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	803	CLA	C3B-C4B-NB	-2.76	108.06	110.53
23	B	842	BCR	C2-C1-C6	2.76	114.45	110.44
20	A	818	CLA	C3B-C4B-NB	-2.76	108.07	110.53
21	3	315	LUT	C10-C11-C12	-2.76	115.21	123.20
21	1	315	LUT	C21-C26-C27	-2.76	109.65	112.83
22	2	316	XAT	C18-C5-C4	2.76	117.34	114.24
23	4	318	BCR	C31-C1-C2	2.75	119.52	108.95
22	1	316	XAT	C24-C23-C22	-2.75	105.64	110.79
20	B	816	CLA	C3B-C4B-NB	-2.75	108.08	110.53
20	A	830	CLA	C3B-C4B-NB	-2.75	108.08	110.53
27	B	840	PQN	C11-C3-C2	-2.75	120.18	124.89
20	1	305	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
20	1	310	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	A	820	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	2	302	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	A	805	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	A	804	CLA	C3B-C4B-NB	-2.74	108.08	110.53
20	1	309	CLA	C3B-C4B-NB	-2.74	108.09	110.53
24	A	844	LHG	C5-O7-C7	-2.74	111.25	117.80
23	B	842	BCR	C24-C23-C22	-2.73	122.19	126.23
19	2	306	CHL	CAC-C3C-C4C	2.73	131.05	124.03
20	A	824	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	B	808	CLA	C1-C2-C3	-2.73	121.73	126.20
22	4	317	XAT	C18-C5-C4	2.73	117.30	114.24
23	A	849	BCR	C33-C5-C6	-2.72	121.51	124.48
20	2	311	CLA	CHB-C4A-NA	2.72	128.33	124.40
20	1	308	CLA	C3B-C4B-NB	-2.72	108.10	110.53
23	A	845	BCR	C38-C26-C25	-2.72	121.51	124.48
19	4	306	CHL	C1-O2A-CGA	2.72	123.24	116.65
30	B	848	DGD	O1G-C1A-C2A	2.72	120.13	111.83
20	B	806	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	3	309	CLA	CMA-C3A-C2A	-2.72	103.48	113.98
20	2	303	CLA	C3B-C4B-NB	-2.72	108.11	110.53
21	O	204	LUT	C8-C7-C6	-2.71	119.75	127.00
20	A	832	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	2	313	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	1	303	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	1	320	LMG	O8-C28-C29	2.70	120.07	111.83
23	B	845	BCR	C20-C21-C22	-2.70	123.49	127.28
20	A	853	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
20	B	810	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	N	202	CLA	C3B-C4B-NB	-2.69	108.13	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	308	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
23	I	101	BCR	C30-C25-C26	-2.69	118.96	122.64
19	1	301	CHL	C1C-CHC-C4B	2.69	125.68	116.07
19	4	306	CHL	CMA-C3A-C4A	-2.69	108.83	114.61
20	2	310	CLA	C3B-C4B-NB	-2.69	108.13	110.53
20	B	835	CLA	C3B-C4B-NB	-2.68	108.13	110.53
20	N	203	CLA	C3B-C4B-NB	-2.68	108.13	110.53
20	O	203	CLA	C3B-C4B-NB	-2.68	108.13	110.53
20	B	803	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
23	A	848	BCR	C21-C20-C19	-2.68	115.43	123.20
20	K	203	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	L	305	BCR	C33-C5-C4	2.68	119.30	113.60
20	A	828	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	G	606	BCR	C3-C4-C5	-2.67	109.29	114.06
20	1	308	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
21	4	316	LUT	C8-C7-C6	-2.67	119.88	127.00
23	B	843	BCR	C33-C5-C4	2.66	119.27	113.60
20	4	309	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
20	A	801	CLA	C1D-ND-C4D	-2.66	104.45	106.31
23	B	846	BCR	C10-C11-C12	-2.66	115.50	123.20
23	J	102	BCR	C11-C10-C9	-2.66	123.55	127.28
23	B	845	BCR	C8-C7-C6	-2.65	119.91	127.00
23	B	845	BCR	C3-C4-C5	-2.65	109.32	114.06
20	2	311	CLA	C3B-C4B-NB	-2.65	108.16	110.53
23	B	843	BCR	C3-C4-C5	-2.65	109.33	114.06
21	1	319	LUT	C8-C7-C6	-2.65	119.92	127.00
20	3	307	CLA	C3B-C4B-NB	-2.65	108.17	110.53
20	3	303	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	B	807	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	3	317	BCR	C2-C1-C6	2.64	114.27	110.44
20	4	310	CLA	C3B-C4B-NB	-2.64	108.17	110.53
21	O	204	LUT	C7-C8-C9	-2.64	122.33	126.23
23	3	317	BCR	C23-C24-C25	-2.64	119.96	127.00
20	A	806	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	L	302	CLA	CHB-C4A-NA	2.63	128.20	124.40
20	G	604	CLA	C1-C2-C3	-2.63	122.50	126.76
20	4	304	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	3	315	LUT	C7-C8-C9	-2.63	122.35	126.23
20	B	808	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
21	2	315	LUT	C10-C11-C12	-2.63	115.59	123.20
23	A	848	BCR	C33-C5-C6	-2.62	121.62	124.48
19	2	305	CHL	CBA-CAA-C2A	-2.62	108.62	113.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	319	LUT	C15-C35-C34	-2.62	118.16	123.52
20	4	304	CLA	CHB-C4A-NA	2.62	128.18	124.40
23	K	204	BCR	C16-C15-C14	-2.62	118.16	123.52
23	3	317	BCR	C21-C20-C19	-2.62	115.62	123.20
23	L	301	BCR	C15-C16-C17	-2.62	118.17	123.52
23	4	318	BCR	C33-C5-C4	2.62	119.17	113.60
20	B	818	CLA	C3B-C4B-NB	-2.61	108.20	110.53
23	J	102	BCR	C8-C7-C6	-2.61	120.02	127.00
19	2	314	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
20	B	824	CLA	CHB-C4A-NA	2.61	128.17	124.40
19	2	307	CHL	CMB-C2B-C3B	-2.61	119.46	124.68
20	B	817	CLA	CHB-C4A-NA	2.61	128.17	124.40
21	4	316	LUT	C10-C11-C12	-2.61	115.63	123.20
20	B	824	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	1	323	LMG	C8-O7-C10	-2.61	111.55	117.80
19	1	306	CHL	C1C-C2C-CMC	-2.61	122.10	126.80
20	B	815	CLA	C3B-C4B-NB	-2.60	108.20	110.53
20	J	101	CLA	CHB-C4A-NA	2.60	128.16	124.40
22	3	316	XAT	C19-C9-C8	2.60	122.06	118.09
20	1	309	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
29	B	847	LMT	C1B-O1B-C4'	-2.60	111.81	117.98
23	A	854	BCR	C11-C12-C13	-2.60	119.23	126.36
20	A	802	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	2	310	CLA	CAA-C2A-C3A	-2.60	110.28	116.23
20	A	839	CLA	CHB-C4A-NA	2.60	128.15	124.40
23	A	847	BCR	C33-C5-C4	2.59	119.12	113.60
20	1	311	CLA	CHB-C4A-NA	2.59	128.13	124.40
20	B	824	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
20	A	837	CLA	C3B-C4B-NB	-2.58	108.22	110.53
20	N	202	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
20	B	808	CLA	CHB-C4A-NA	2.58	128.13	124.40
23	2	317	BCR	C11-C12-C13	-2.58	119.28	126.36
20	3	307	CLA	CHB-C4A-NA	2.58	128.13	124.40
26	1	322	HTG	O5-C5-C4	2.58	114.35	109.70
20	A	820	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	A	830	CLA	CHB-C4A-NA	2.58	128.12	124.40
23	B	842	BCR	C34-C9-C10	-2.58	118.64	122.82
20	4	304	CLA	CMD-C2D-C3D	-2.57	121.78	127.69
23	F	801	BCR	C8-C7-C6	-2.57	120.12	127.00
23	I	101	BCR	C38-C26-C27	2.57	119.08	113.60
23	I	101	BCR	C4-C5-C6	-2.57	119.23	122.70
19	2	314	CHL	CMB-C2B-C3B	2.57	129.82	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	849	BCR	C11-C10-C9	-2.57	123.67	127.28
20	1	313	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	A	842	PQN	C11-C3-C2	-2.57	120.49	124.89
20	B	820	CLA	C1-C2-C3	-2.57	122.61	126.76
19	2	305	CHL	OMC-CMC-C2C	-2.57	120.66	125.12
24	2	318	LHG	C5-O7-C7	-2.57	111.66	117.80
20	2	309	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
20	A	814	CLA	CHB-C4A-NA	2.56	128.10	124.40
20	A	831	CLA	CHB-C4A-NA	2.56	128.10	124.40
20	A	836	CLA	C3B-C4B-NB	-2.56	108.24	110.53
21	1	315	LUT	C35-C15-C14	-2.56	118.28	123.52
20	B	823	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	A	852	HTG	C4-C3-C2	-2.55	106.34	110.83
23	F	806	BCR	C15-C16-C17	-2.55	118.29	123.52
19	4	306	CHL	O2A-CGA-CBA	2.55	119.61	111.83
23	F	806	BCR	C3-C4-C5	-2.55	109.51	114.06
20	2	309	CLA	CHB-C4A-NA	2.55	128.08	124.40
23	1	317	BCR	C29-C30-C25	2.55	114.14	110.44
23	A	846	BCR	C33-C5-C4	2.55	119.03	113.60
21	2	315	LUT	C8-C7-C6	-2.55	120.19	127.00
23	F	801	BCR	C36-C18-C19	2.54	121.97	118.09
20	1	307	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	B	823	CLA	C1-C2-C3	-2.54	122.03	126.20
20	B	833	CLA	CHB-C4A-NA	2.54	128.07	124.40
20	B	815	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	B	844	BCR	C33-C5-C6	-2.54	121.71	124.48
21	O	205	LUT	C18-C5-C6	-2.54	121.71	124.48
20	1	308	CLA	CHB-C4A-NA	2.54	128.06	124.40
23	B	842	BCR	C38-C26-C27	2.54	119.00	113.60
20	1	311	CLA	C3B-C4B-NB	-2.54	108.27	110.53
20	2	302	CLA	CHB-C4A-NA	2.54	128.06	124.40
20	B	820	CLA	CHB-C4A-NA	2.53	128.06	124.40
19	2	306	CHL	O2A-CGA-O1A	-2.53	117.29	123.63
21	1	315	LUT	C30-C31-C32	-2.53	115.86	123.20
20	B	822	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	4	302	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	4	308	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	B	844	BCR	C21-C20-C19	-2.53	115.87	123.20
20	1	321	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	G	606	BCR	C10-C11-C12	-2.53	115.88	123.20
20	A	805	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	B	809	CLA	C3B-C4B-NB	-2.53	108.28	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	808	CLA	O2D-CGD-CBD	2.53	115.64	111.23
20	4	311	CLA	CHB-C4A-NA	2.53	128.04	124.40
19	1	301	CHL	O2D-CGD-O1D	-2.52	118.93	123.85
20	B	836	CLA	CHB-C4A-NA	2.52	128.04	124.40
21	4	316	LUT	C31-C30-C29	-2.52	123.74	127.28
23	A	846	BCR	C28-C27-C26	-2.52	109.56	114.06
20	4	312	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	H	201	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	3	303	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	4	319	LMG	O8-C28-C29	2.52	119.52	111.83
20	A	809	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	F	806	BCR	C11-C12-C13	-2.52	119.45	126.36
20	A	810	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	B	806	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	3	308	CLA	C1-C2-C3	-2.52	122.69	126.76
20	K	203	CLA	CHB-C4A-NA	2.52	128.03	124.40
20	3	310	CLA	CHB-C4A-NA	2.52	128.03	124.40
20	2	304	CLA	CHB-C4A-NA	2.51	128.03	124.40
19	1	306	CHL	O2D-CGD-O1D	-2.51	118.96	123.85
20	B	825	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	3	306	CHL	OBD-CAD-C3D	-2.51	123.97	127.89
23	K	204	BCR	C20-C19-C18	-2.51	119.48	126.36
20	N	202	CLA	CHB-C4A-NA	2.51	128.02	124.40
20	4	301	CLA	CHB-C4A-NA	2.51	128.02	124.40
20	A	829	CLA	CHB-C4A-NA	2.51	128.02	124.40
20	B	802	CLA	C3B-C4B-NB	-2.51	108.29	110.53
20	2	308	CLA	C1-C2-C3	-2.51	122.71	126.76
20	G	603	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	I	101	BCR	C33-C5-C4	2.50	118.94	113.60
20	A	804	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	K	205	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	A	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	1	317	BCR	C37-C22-C23	2.50	121.91	118.09
20	2	313	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	A	813	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	B	832	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	B	830	CLA	C1-C2-C3	-2.50	122.72	126.76
20	3	305	CLA	CHB-C4A-NA	2.50	128.00	124.40
21	1	319	LUT	C30-C31-C32	-2.50	115.97	123.20
20	1	304	CLA	CHB-C4A-NA	2.50	128.00	124.40
20	B	819	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	1	301	CHL	CBC-CAC-C3C	-2.49	109.30	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	842	PQN	C2M-C2-C3	-2.49	120.35	124.45
22	2	316	XAT	C38-C25-C24	2.49	117.04	114.24
20	B	826	CLA	CHB-C4A-NA	2.49	127.99	124.40
20	A	821	CLA	CHB-C4A-NA	2.49	127.99	124.40
20	3	309	CLA	CBB-CAB-C3B	-2.49	115.09	127.53
22	3	316	XAT	C35-C15-C14	-2.49	118.43	123.52
20	4	303	CLA	CHB-C4A-NA	2.49	127.99	124.40
27	B	840	PQN	C2M-C2-C3	-2.49	120.36	124.45
23	L	301	BCR	C34-C9-C10	-2.49	118.79	122.82
20	B	804	CLA	CHB-C4A-NA	2.48	127.99	124.40
20	2	312	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	O	204	LUT	C10-C11-C12	-2.48	116.00	123.20
23	K	204	BCR	C2-C1-C6	2.48	114.05	110.44
20	F	802	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	A	836	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	B	832	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	B	837	CLA	C3B-C4B-NB	-2.48	108.31	110.53
20	N	203	CLA	C1-C2-C3	-2.48	122.75	126.76
20	A	817	CLA	CHB-C4A-NA	2.48	127.98	124.40
23	B	844	BCR	C38-C26-C25	-2.48	121.78	124.48
23	I	101	BCR	C33-C5-C6	-2.48	121.78	124.48
20	1	314	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	B	807	CLA	C1-C2-C3	-2.48	122.14	126.20
20	3	312	CLA	CHB-C4A-NA	2.48	127.98	124.40
23	4	318	BCR	C7-C8-C9	-2.48	122.57	126.23
20	B	827	CLA	C1-C2-C3	-2.48	122.14	126.20
20	B	803	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	3	301	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	B	839	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	J	103	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	A	834	CLA	CHB-C4A-NA	2.47	127.97	124.40
20	F	805	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	3	317	BCR	C15-C16-C17	-2.47	118.47	123.52
20	K	202	CLA	CHB-C4A-NA	2.47	127.96	124.40
21	O	205	LUT	C18-C5-C4	2.47	118.95	114.42
23	L	305	BCR	C28-C27-C26	-2.46	109.66	114.06
20	B	805	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	L	303	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	A	819	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	A	812	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	A	840	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	B	845	BCR	C28-C27-C26	-2.46	109.67	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	845	BCR	C29-C30-C25	2.46	114.01	110.44
22	4	317	XAT	C31-C30-C29	-2.46	123.83	127.28
20	B	825	CLA	O2D-CGD-CBD	2.46	115.52	111.23
20	A	837	CLA	CHB-C4A-NA	2.46	127.94	124.40
23	B	842	BCR	C20-C21-C22	-2.46	123.83	127.28
20	3	311	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	A	824	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	B	834	CLA	C3B-C4B-NB	-2.45	108.34	110.53
20	3	304	CLA	C3B-C4B-NB	-2.45	108.34	110.53
20	2	303	CLA	CHB-C4A-NA	2.45	127.94	124.40
20	A	833	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	2	318	LHG	O8-C23-C24	2.45	119.31	111.83
20	1	309	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	2	308	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	N	203	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	A	803	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	A	815	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	2	306	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
23	A	849	BCR	C34-C9-C10	-2.45	118.85	122.82
20	A	808	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	3	317	BCR	C33-C5-C4	2.44	118.81	113.60
20	2	310	CLA	CHB-C4A-NA	2.44	127.93	124.40
23	B	843	BCR	C34-C9-C10	-2.44	118.86	122.82
20	A	803	CLA	O2D-CGD-CBD	2.44	115.50	111.23
20	3	308	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	F	802	CLA	C3B-C4B-NB	-2.44	108.35	110.53
20	B	816	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	B	831	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	B	811	CLA	CAB-C3B-C2B	2.43	130.00	123.53
23	B	846	BCR	C3-C4-C5	-2.43	109.71	114.06
20	A	841	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	K	201	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	A	847	BCR	C27-C26-C25	-2.43	119.42	122.70
20	G	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	L	307	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	J	102	BCR	C24-C23-C22	-2.43	122.64	126.23
20	B	812	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	B	844	BCR	C23-C24-C25	-2.43	120.51	127.00
20	4	302	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
20	A	829	CLA	O2D-CGD-CBD	2.43	115.47	111.23
20	1	303	CLA	CHB-C4A-NA	2.43	127.90	124.40
19	1	301	CHL	CMA-C3A-C4A	-2.42	109.39	114.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	838	CLA	CHB-C4A-NA	2.42	127.90	124.40
20	4	314	CLA	CHB-C4A-NA	2.42	127.90	124.40
20	4	313	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	A	818	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	4	317	XAT	C15-C14-C13	-2.42	123.88	127.28
20	1	302	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	B	822	CLA	C3B-C4B-NB	-2.42	108.37	110.53
23	A	854	BCR	C29-C30-C25	2.42	113.95	110.44
20	A	816	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	3	309	CLA	CHB-C4A-NA	2.42	127.89	124.40
23	B	843	BCR	C11-C10-C9	-2.42	123.89	127.28
20	A	828	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
19	1	306	CHL	CMA-C3A-C2A	-2.41	104.80	114.13
23	B	844	BCR	C38-C26-C27	2.41	118.74	113.60
20	B	814	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	F	804	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	O	203	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	B	813	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	L	304	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	A	825	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	B	841	BCR	C23-C24-C25	-2.41	120.56	127.00
20	A	818	CLA	C1-C2-C3	-2.41	122.25	126.20
20	B	809	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	A	845	BCR	C3-C4-C5	-2.41	109.77	114.06
30	B	848	DGD	O6D-C5D-C6D	2.40	111.46	106.69
20	A	806	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
23	B	844	BCR	C27-C26-C25	-2.40	119.46	122.70
23	4	318	BCR	C16-C15-C14	-2.40	118.61	123.52
20	B	807	CLA	CHB-C4A-NA	2.40	127.86	124.40
20	B	829	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
20	K	202	CLA	C1-C2-C3	-2.40	122.27	126.20
20	G	605	CLA	CHB-C4A-NA	2.39	127.86	124.40
19	2	307	CHL	O1A-CGA-CBA	-2.39	114.42	123.78
20	1	308	CLA	C1-C2-C3	-2.39	122.28	126.20
20	A	830	CLA	C1-C2-C3	-2.39	122.89	126.76
22	4	317	XAT	C19-C9-C8	2.39	121.74	118.09
20	B	829	CLA	C3B-C4B-NB	-2.39	108.40	110.53
20	3	304	CLA	CHB-C4A-NA	2.39	127.84	124.40
20	A	853	CLA	CHB-C4A-NA	2.38	127.84	124.40
20	B	821	CLA	CHB-C4A-NA	2.38	127.84	124.40
20	B	811	CLA	CMB-C2B-C3B	2.38	129.87	123.53
21	O	204	LUT	C18-C5-C4	2.38	118.80	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	806	CLA	CHB-C4A-NA	2.38	127.84	124.40
21	1	319	LUT	C27-C28-C29	-2.38	121.20	126.32
19	4	305	CHL	CAA-C2A-C3A	-2.38	106.57	113.00
25	4	319	LMG	C8-O7-C10	-2.38	112.11	117.80
23	B	841	BCR	C4-C5-C6	-2.38	119.49	122.70
20	B	829	CLA	CHB-C4A-NA	2.37	127.83	124.40
20	1	305	CLA	CHB-C4A-NA	2.37	127.83	124.40
20	B	830	CLA	CHB-C4A-NA	2.37	127.83	124.40
23	A	848	BCR	C16-C15-C14	-2.37	118.67	123.52
20	O	202	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	B	842	BCR	C8-C9-C10	2.37	122.74	119.01
20	A	838	CLA	C3B-C4B-NB	-2.37	108.42	110.53
20	1	310	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	J	102	BCR	C23-C24-C25	-2.37	120.67	127.00
20	B	811	CLA	CHB-C4A-NA	2.37	127.82	124.40
20	A	807	CLA	C1-C2-C3	-2.37	122.32	126.20
29	G	601	LMT	C1B-O1B-C4'	-2.37	112.37	117.98
20	A	811	CLA	CHB-C4A-NA	2.37	127.81	124.40
23	2	317	BCR	C7-C8-C9	-2.37	122.73	126.23
20	B	834	CLA	CHB-C4A-NA	2.37	127.81	124.40
20	B	827	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
23	4	318	BCR	C37-C22-C23	2.36	121.70	118.09
23	B	841	BCR	C20-C19-C18	-2.36	119.88	126.36
20	3	314	CLA	CHB-C4A-NA	2.36	127.81	124.40
20	4	309	CLA	C1-C2-C3	-2.36	122.33	126.20
20	B	835	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	B	843	BCR	C37-C22-C21	-2.36	118.99	122.82
23	B	842	BCR	C21-C20-C19	-2.36	116.36	123.20
20	A	826	CLA	CHB-C4A-NA	2.36	127.81	124.40
20	4	310	CLA	CHB-C4A-NA	2.36	127.80	124.40
20	A	832	CLA	CHB-C4A-NA	2.36	127.80	124.40
21	1	315	LUT	C7-C8-C9	-2.35	122.75	126.23
20	1	321	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
23	B	842	BCR	C11-C10-C9	-2.35	123.99	127.28
20	A	827	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	3	306	CHL	OMC-CMC-C2C	-2.35	121.05	125.12
22	2	316	XAT	C35-C15-C14	-2.35	118.72	123.52
20	4	309	CLA	CHB-C4A-NA	2.35	127.79	124.40
20	A	823	CLA	CHB-C4A-NA	2.34	127.78	124.40
21	4	316	LUT	C35-C15-C14	-2.34	118.72	123.52
23	3	317	BCR	C29-C30-C25	2.34	113.84	110.44
20	A	838	CLA	CHB-C4A-NA	2.34	127.78	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	309	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
23	A	849	BCR	C16-C15-C14	-2.34	118.74	123.52
20	B	828	CLA	C1-C2-C3	-2.34	122.37	126.20
23	F	801	BCR	C2-C1-C6	2.33	113.83	110.44
20	A	814	CLA	C1-C2-C3	-2.33	122.99	126.76
22	1	316	XAT	C19-C9-C8	2.33	121.65	118.09
20	3	313	CLA	CHB-C4A-NA	2.33	127.77	124.40
23	A	846	BCR	C38-C26-C27	2.33	118.57	113.60
21	4	316	LUT	C30-C31-C32	-2.33	116.45	123.20
20	A	836	CLA	C1-C2-C3	-2.33	122.38	126.20
20	B	810	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	2	314	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
23	B	846	BCR	C21-C20-C19	-2.32	116.47	123.20
20	B	818	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	A	845	BCR	C10-C11-C12	-2.32	116.48	123.20
20	1	311	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
20	A	851	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	A	848	BCR	C10-C11-C12	-2.32	116.49	123.20
20	B	837	CLA	CHB-C4A-NA	2.32	127.74	124.40
20	A	837	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
20	A	828	CLA	CHB-C4A-NA	2.31	127.74	124.40
21	1	315	LUT	C31-C30-C29	-2.31	124.03	127.28
20	B	801	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
20	A	835	CLA	CHB-C4A-NA	2.31	127.74	124.40
21	3	315	LUT	C11-C10-C9	-2.31	124.04	127.28
26	1	322	HTG	O5-C1-C2	-2.31	107.13	110.32
23	B	842	BCR	C15-C16-C17	-2.31	118.79	123.52
21	1	319	LUT	C18-C5-C4	2.31	118.67	114.42
24	A	843	LHG	O8-C23-C24	2.31	118.88	111.83
20	A	836	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
20	3	302	CLA	C1-C2-C3	-2.31	123.03	126.76
23	J	104	BCR	C20-C19-C18	-2.31	120.04	126.36
20	B	827	CLA	CHB-C4A-NA	2.30	127.73	124.40
23	B	842	BCR	C33-C5-C4	2.30	118.50	113.60
23	K	204	BCR	C28-C27-C26	-2.30	109.95	114.06
20	3	302	CLA	C3B-C4B-NB	-2.30	108.48	110.53
20	3	302	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	1	306	CHL	CMD-C2D-C3D	-2.30	120.09	124.68
20	A	822	CLA	CHB-C4A-NA	2.30	127.71	124.40
20	O	201	CLA	CHB-C4A-NA	2.29	127.71	124.40
20	2	312	CLA	C1-C2-C3	-2.29	122.44	126.20
23	B	845	BCR	C11-C12-C13	-2.29	120.08	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	204	LUT	C27-C28-C29	-2.29	121.40	126.32
19	1	301	CHL	CMB-C2B-C3B	2.29	129.26	124.68
23	A	847	BCR	C16-C15-C14	-2.29	118.83	123.52
20	1	312	CLA	CHB-C4A-NA	2.29	127.70	124.40
23	F	801	BCR	C15-C14-C13	-2.28	124.07	127.28
19	2	301	CHL	C1-C2-C3	-2.28	122.45	126.20
20	A	823	CLA	C1-C2-C3	-2.28	122.46	126.20
20	B	836	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
20	H	201	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
21	3	315	LUT	C27-C28-C29	-2.28	121.43	126.32
22	3	316	XAT	C39-C29-C28	2.27	121.56	118.09
20	1	309	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
20	B	833	CLA	C1-C2-C3	-2.27	122.48	126.20
20	K	202	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
20	B	835	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
23	F	801	BCR	C29-C30-C25	2.27	113.73	110.44
25	1	320	LMG	C8-O7-C10	-2.27	112.38	117.80
20	A	827	CLA	C1-C2-C3	-2.27	122.49	126.20
23	1	317	BCR	C15-C16-C17	-2.26	118.89	123.52
23	J	102	BCR	C28-C27-C26	-2.26	110.02	114.06
20	L	304	CLA	C1-C2-C3	-2.26	123.10	126.76
23	2	317	BCR	C16-C15-C14	-2.26	118.90	123.52
20	B	811	CLA	C3B-C4B-NB	-2.26	107.98	110.33
22	2	316	XAT	C30-C31-C32	-2.26	116.66	123.20
20	3	304	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
20	4	303	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
20	3	307	CLA	C1-C2-C3	-2.26	123.11	126.76
23	1	317	BCR	C8-C7-C6	-2.26	120.97	127.00
19	2	307	CHL	C1-O2A-CGA	2.25	122.10	116.65
19	2	305	CHL	OBD-CAD-C3D	2.25	131.41	127.89
20	J	101	CLA	C1-C2-C3	-2.25	122.51	126.20
23	I	101	BCR	C16-C15-C14	-2.25	118.91	123.52
23	F	806	BCR	C33-C5-C4	2.25	118.39	113.60
20	B	821	CLA	C1-C2-C3	-2.25	122.51	126.20
20	A	838	CLA	O2D-CGD-CBD	2.25	115.16	111.23
22	3	316	XAT	C31-C30-C29	-2.25	124.13	127.28
20	1	321	CLA	C1-C2-C3	-2.25	122.52	126.20
23	B	842	BCR	C38-C26-C25	-2.25	122.03	124.48
20	B	826	CLA	C1-C2-C3	-2.25	122.52	126.20
23	2	317	BCR	C4-C5-C6	-2.25	119.67	122.70
27	A	842	PQN	C11-C12-C13	-2.24	122.97	126.83
23	B	846	BCR	C11-C10-C9	-2.24	124.13	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	204	BCR	C23-C24-C25	-2.24	121.01	127.00
20	A	851	CLA	C3B-C4B-NB	-2.24	108.53	110.53
22	1	316	XAT	C38-C25-C24	2.24	116.76	114.24
23	I	101	BCR	C38-C26-C25	-2.24	122.04	124.48
22	1	316	XAT	C20-C13-C12	2.24	121.51	118.09
19	2	301	CHL	CAA-CBA-CGA	-2.24	106.85	113.21
23	B	844	BCR	C15-C16-C17	-2.24	118.94	123.52
23	J	104	BCR	C29-C30-C25	2.24	113.69	110.44
20	4	302	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
20	4	308	CLA	C1-C2-C3	-2.23	123.15	126.76
20	B	819	CLA	C1-C2-C3	-2.23	122.54	126.20
19	1	301	CHL	OMC-CMC-C2C	-2.23	121.24	125.12
20	4	309	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
20	B	822	CLA	C1-C2-C3	-2.23	122.54	126.20
20	1	309	CLA	C1-C2-C3	-2.23	122.54	126.20
23	B	841	BCR	C7-C8-C9	-2.23	122.94	126.23
20	1	307	CLA	C1-C2-C3	-2.23	122.55	126.20
20	O	203	CLA	C1-C2-C3	-2.23	122.55	126.20
20	A	829	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
20	2	311	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
20	A	841	CLA	C1-C2-C3	-2.22	122.55	126.20
19	2	301	CHL	OBD-CAD-CBD	2.22	129.09	125.82
20	B	828	CLA	CHB-C4A-NA	2.22	127.60	124.40
20	A	827	CLA	C3B-C4B-NB	-2.22	108.55	110.53
23	1	317	BCR	C39-C30-C25	-2.22	106.76	110.24
20	A	837	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
23	L	301	BCR	C21-C20-C19	-2.22	116.77	123.20
19	3	306	CHL	C4C-CHD-C1D	2.22	124.00	116.07
20	2	309	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
20	B	825	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
20	A	809	CLA	C1-C2-C3	-2.21	122.57	126.20
22	1	316	XAT	C35-C34-C33	-2.21	124.17	127.28
20	A	817	CLA	C1-C2-C3	-2.21	122.58	126.20
21	3	315	LUT	C8-C7-C6	-2.20	121.11	127.00
23	3	317	BCR	C24-C23-C22	-2.20	122.97	126.23
23	L	306	BCR	C3-C4-C5	-2.20	110.13	114.06
20	B	828	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
20	4	303	CLA	C3B-C4B-NB	-2.20	108.56	110.53
20	4	313	CLA	O2D-CGD-CBD	2.20	115.08	111.23
21	O	205	LUT	C31-C32-C33	-2.20	120.33	126.36
20	3	308	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
19	4	307	CHL	C4C-CHD-C1D	2.20	123.94	116.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	C4C-CHD-C1D	2.20	123.93	116.07
20	B	834	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
20	4	314	CLA	C1-C2-C3	-2.20	123.21	126.76
21	2	315	LUT	C31-C30-C29	-2.20	124.20	127.28
20	B	832	CLA	C1-C2-C3	-2.19	122.60	126.20
23	A	845	BCR	C16-C15-C14	-2.19	119.03	123.52
19	4	305	CHL	C4C-CHD-C1D	2.19	123.89	116.07
20	A	838	CLA	C1-C2-C3	-2.19	122.62	126.20
20	B	801	CLA	CMB-C2B-C3B	2.18	131.69	126.55
20	A	829	CLA	C3B-C4B-NB	-2.18	108.58	110.53
23	J	104	BCR	C8-C7-C6	-2.18	121.17	127.00
22	3	316	XAT	C30-C31-C32	-2.18	116.87	123.20
19	2	306	CHL	C4C-CHD-C1D	2.18	123.88	116.07
23	1	317	BCR	C10-C11-C12	-2.18	116.88	123.20
23	A	854	BCR	C8-C7-C6	-2.18	121.17	127.00
22	2	316	XAT	C19-C9-C8	2.18	121.42	118.09
23	1	317	BCR	C33-C5-C4	2.18	118.24	113.60
20	A	808	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
20	A	851	CLA	C1-C2-C3	-2.18	122.63	126.20
20	4	302	CLA	CMB-C2B-C3B	2.18	131.68	126.55
20	A	824	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
20	B	832	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	A	801	CLA	C2A-C1A-CHA	2.17	127.64	123.87
23	K	204	BCR	C10-C11-C12	-2.17	116.91	123.20
23	B	846	BCR	C35-C13-C12	2.17	121.41	118.09
23	A	849	BCR	C28-C27-C26	-2.17	110.18	114.06
20	A	806	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
20	A	816	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
20	B	804	CLA	O2D-CGD-CBD	2.17	115.02	111.23
20	A	826	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
20	A	818	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
23	B	845	BCR	C33-C5-C4	2.17	118.21	113.60
20	A	825	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
20	3	307	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
23	F	801	BCR	C35-C13-C12	2.16	121.39	118.09
20	B	815	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
20	1	304	CLA	C1-C2-C3	-2.16	122.66	126.20
19	4	315	CHL	C4C-CHD-C1D	2.16	123.80	116.07
23	A	848	BCR	C15-C16-C17	-2.16	119.10	123.52
19	2	301	CHL	C4-C3-C2	-2.16	118.08	123.63
20	O	201	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
20	2	312	CLA	O2A-CGA-O1A	-2.16	118.23	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	318	LHG	C5-O7-C7	-2.16	112.64	117.80
20	A	853	CLA	C1-C2-C3	-2.16	122.67	126.20
20	1	304	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
24	A	843	LHG	C5-O7-C7	-2.15	112.64	117.80
20	A	806	CLA	CMB-C2B-C3B	2.15	131.62	126.55
23	L	305	BCR	C38-C26-C27	2.15	118.19	113.60
23	A	849	BCR	C10-C11-C12	-2.15	116.96	123.20
20	A	832	CLA	C1-C2-C3	-2.15	122.67	126.20
22	4	317	XAT	C20-C13-C12	2.15	121.37	118.09
23	B	841	BCR	C11-C12-C13	-2.15	120.47	126.36
20	B	817	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
20	L	307	CLA	O2D-CGD-CBD	2.15	114.99	111.23
20	A	841	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	A	846	BCR	C15-C16-C17	-2.15	119.12	123.52
20	B	802	CLA	CHB-C4A-NA	2.15	127.50	124.40
20	A	839	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
23	2	317	BCR	C23-C24-C25	-2.15	121.26	127.00
20	B	819	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
19	2	305	CHL	C4C-CHD-C1D	2.14	123.74	116.07
20	A	804	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
23	G	606	BCR	C2-C1-C6	2.14	113.55	110.44
23	A	848	BCR	C37-C22-C23	2.14	121.36	118.09
20	A	839	CLA	C1-C2-C3	-2.14	122.69	126.20
22	1	316	XAT	C35-C15-C14	-2.14	119.14	123.52
19	2	314	CHL	C4C-CHD-C1D	2.14	123.72	116.07
21	3	315	LUT	C35-C15-C14	-2.14	119.14	123.52
19	2	314	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
20	B	803	CLA	O1D-CGD-CBD	2.14	128.74	124.52
23	1	317	BCR	C38-C26-C27	2.14	118.15	113.60
20	B	802	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	1	313	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
23	L	301	BCR	C3-C4-C5	-2.13	110.25	114.06
19	3	306	CHL	C4D-ND-C1D	-2.13	103.60	105.22
20	B	809	CLA	C1-C2-C3	-2.13	122.70	126.20
19	2	305	CHL	O1D-CGD-CBD	-2.13	121.49	124.72
20	B	825	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
21	1	315	LUT	C20-C13-C12	2.13	121.34	118.09
21	1	315	LUT	C18-C5-C4	2.13	118.33	114.42
20	4	304	CLA	C5-C3-C2	-2.13	116.27	122.66
23	G	606	BCR	C16-C15-C14	-2.12	119.17	123.52
20	A	833	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
23	B	843	BCR	C8-C9-C10	2.12	122.35	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	205	LUT	C38-C25-C24	-2.12	118.34	123.36
22	2	316	XAT	C20-C13-C12	2.12	121.33	118.09
20	B	813	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
21	4	316	LUT	C7-C8-C9	-2.12	123.10	126.23
20	B	833	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
20	K	202	CLA	O2D-CGD-CBD	2.12	114.94	111.23
20	B	826	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
20	B	805	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
21	1	319	LUT	C40-C33-C32	2.12	121.32	118.09
20	A	828	CLA	CMB-C2B-C3B	2.12	131.53	126.55
20	A	824	CLA	C1-C2-C3	-2.12	122.73	126.20
20	1	311	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
20	A	807	CLA	O2D-CGD-CBD	2.12	114.93	111.23
20	4	308	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
19	1	306	CHL	C4C-CHD-C1D	2.11	123.63	116.07
20	B	823	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
19	4	305	CHL	CED-O2D-CGD	2.11	120.71	115.92
20	B	805	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
20	A	802	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
20	J	101	CLA	O2D-CGD-CBD	2.11	114.92	111.23
23	B	846	BCR	C8-C7-C6	-2.11	121.35	127.00
21	2	315	LUT	C39-C29-C28	2.11	121.31	118.09
20	3	309	CLA	CGD-CBD-CAD	-2.11	104.01	110.85
21	2	315	LUT	C20-C13-C12	2.11	121.31	118.09
19	4	306	CHL	C4C-CHD-C1D	2.11	123.62	116.07
19	2	314	CHL	C4D-ND-C1D	-2.11	103.62	105.22
23	G	606	BCR	C35-C13-C12	2.11	121.31	118.09
20	2	302	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	B	803	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	B	824	CLA	O2D-CGD-CBD	2.11	114.92	111.23
20	B	807	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	2	316	XAT	C39-C29-C28	2.11	121.31	118.09
20	A	805	CLA	C1-C2-C3	-2.11	122.75	126.20
21	3	315	LUT	C30-C31-C32	-2.10	117.10	123.20
23	A	847	BCR	C38-C26-C27	2.10	118.08	113.60
20	K	203	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
19	2	301	CHL	CAC-C3C-C4C	2.10	129.43	124.03
19	2	307	CHL	C4C-CHD-C1D	2.10	123.58	116.07
20	A	853	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
20	2	311	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
20	B	838	CLA	C1-C2-C3	-2.10	122.76	126.20
20	3	301	CLA	O2A-CGA-O1A	-2.10	118.39	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	845	BCR	C23-C24-C25	-2.09	121.41	127.00
20	L	303	CLA	O2D-CGD-CBD	2.09	114.89	111.23
23	B	845	BCR	C36-C18-C19	2.09	121.28	118.09
19	2	314	CHL	OMC-CMC-C2C	-2.09	121.49	125.12
23	B	841	BCR	C15-C16-C17	-2.09	119.24	123.52
20	A	802	CLA	C1-C2-C3	-2.09	122.77	126.20
20	4	304	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
20	B	837	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
23	F	806	BCR	C38-C26-C27	2.09	118.05	113.60
23	G	606	BCR	C8-C7-C6	-2.09	121.42	127.00
20	B	826	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	N	203	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	A	804	CLA	C1-C2-C3	-2.09	122.78	126.20
20	A	814	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	G	604	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
23	A	847	BCR	C39-C30-C25	-2.09	106.97	110.24
19	1	301	CHL	O2A-CGA-O1A	-2.08	118.41	123.63
23	B	846	BCR	C28-C27-C26	-2.08	110.34	114.06
22	3	316	XAT	C8-C9-C10	-2.08	115.73	119.01
20	A	825	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
20	A	812	CLA	C1-C2-C3	-2.08	122.78	126.20
20	A	823	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	1	306	CHL	C1-O2A-CGA	2.08	122.58	116.67
19	1	301	CHL	C4C-CHD-C1D	2.08	123.51	116.07
20	A	824	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	4	306	CHL	CMD-C2D-C3D	-2.08	120.53	124.68
20	B	814	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	A	801	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
20	B	825	CLA	C1-C2-C3	-2.08	122.80	126.20
20	A	840	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
23	A	849	BCR	C8-C9-C10	2.08	122.27	119.01
20	B	832	CLA	O2D-CGD-CBD	2.07	114.86	111.23
20	B	809	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
20	1	305	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
20	A	803	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	B	801	CLA	CHB-C4A-NA	2.07	127.39	124.40
20	2	309	CLA	O1D-CGD-CBD	2.07	128.60	124.52
23	K	204	BCR	C38-C26-C27	2.07	118.00	113.60
20	A	826	CLA	C1-C2-C3	-2.07	122.81	126.20
20	A	828	CLA	C1-C2-C3	-2.07	122.81	126.20
20	L	303	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	B	803	CLA	C1-C2-C3	-2.07	122.81	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	838	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	4	316	LUT	C11-C10-C9	-2.07	124.38	127.28
20	4	309	CLA	CMB-C2B-C3B	2.06	131.41	126.55
20	2	313	CLA	O2D-CGD-CBD	2.06	114.84	111.23
20	A	828	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	B	811	CLA	C1-C2-C3	-2.06	122.82	126.20
20	A	821	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
20	A	822	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	B	835	CLA	CMB-C2B-C3B	2.06	131.40	126.55
20	1	303	CLA	C1-C2-C3	-2.06	122.82	126.20
20	4	310	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	B	816	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	1	311	CLA	CMB-C2B-C3B	2.06	131.40	126.55
20	A	837	CLA	CMB-C2B-C3B	2.06	131.40	126.55
20	L	304	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	A	820	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	B	843	BCR	C21-C20-C19	-2.06	117.23	123.20
20	O	203	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
20	1	303	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
20	3	311	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	J	102	BCR	C7-C8-C9	-2.06	123.19	126.23
20	B	839	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	4	318	BCR	C29-C30-C25	2.06	113.43	110.44
20	B	806	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	3	315	LUT	C19-C9-C8	2.06	121.23	118.09
23	F	806	BCR	C23-C24-C25	-2.06	121.50	127.00
20	A	836	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
20	3	304	CLA	CMB-C2B-C3B	2.06	131.39	126.55
20	A	831	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	2	301	CHL	CBA-CAA-C2A	2.06	119.83	113.78
20	3	310	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
20	3	302	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
20	B	810	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
23	2	317	BCR	C1-C6-C7	2.05	121.22	115.65
20	A	836	CLA	CMB-C2B-C3B	2.05	131.38	126.55
21	2	315	LUT	C18-C5-C4	2.05	118.19	114.42
20	A	817	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	1	309	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
23	J	102	BCR	C11-C12-C13	-2.05	120.74	126.36
23	A	847	BCR	C10-C11-C12	-2.05	117.26	123.20
20	A	807	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
23	F	801	BCR	C34-C9-C8	2.05	121.22	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	314	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	B	832	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
20	B	812	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
20	B	835	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	4	318	BCR	C1-C6-C7	2.05	121.21	115.65
21	1	315	LUT	C11-C10-C9	-2.05	124.41	127.28
20	3	307	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	A	845	BCR	C30-C25-C24	2.05	121.20	115.65
23	A	846	BCR	C23-C24-C25	-2.05	121.53	127.00
20	A	825	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
23	A	854	BCR	C7-C8-C9	-2.04	123.21	126.23
20	B	801	CLA	C3B-C4B-NB	-2.04	108.71	110.53
20	B	834	CLA	CMB-C2B-C3B	2.04	131.35	126.55
20	F	802	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	B	809	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
20	A	805	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
20	A	822	CLA	C1-C2-C3	-2.03	122.86	126.20
20	A	811	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	4	317	XAT	C30-C31-C32	-2.03	117.31	123.20
20	B	815	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
20	A	808	CLA	C1-C2-C3	-2.03	122.87	126.20
20	B	829	CLA	CMB-C2B-C3B	2.03	131.33	126.55
20	B	811	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
20	A	834	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	B	846	BCR	C34-C9-C8	2.03	121.19	118.09
20	2	304	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
19	2	314	CHL	CBC-CAC-C3C	-2.03	109.97	112.87
20	O	203	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	O	204	LUT	C15-C35-C34	-2.03	119.37	123.52
20	2	308	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
20	B	822	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
21	4	316	LUT	C18-C5-C4	2.03	118.14	114.42
21	3	315	LUT	C20-C13-C12	2.02	121.18	118.09
20	A	812	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
20	H	201	CLA	C1-C2-C3	-2.02	122.88	126.20
23	G	606	BCR	C15-C16-C17	-2.02	119.38	123.52
26	1	322	HTG	C3-C4-C5	2.02	113.90	110.23
30	B	848	DGD	O2G-C1B-O1B	-2.02	118.99	123.70
23	L	305	BCR	C8-C7-C6	-2.02	121.61	127.00
20	O	202	CLA	O2A-CGA-CBA	2.02	120.37	114.00
24	A	844	LHG	O7-C7-O9	-2.02	118.99	123.70
20	1	310	CLA	CMB-C2B-C1B	-2.01	122.35	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	832	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
20	B	813	CLA	C1-C2-C3	-2.01	122.90	126.20
20	A	851	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
20	1	305	CLA	C1-C2-C3	-2.01	122.90	126.20
20	A	822	CLA	O2D-CGD-CBD	2.01	114.75	111.23
20	3	311	CLA	C1-C2-C3	-2.01	122.90	126.20
23	J	102	BCR	C33-C5-C4	2.01	117.89	113.60
20	A	827	CLA	C2A-C1A-CHA	2.01	127.36	123.87
20	3	309	CLA	CHB-C1B-NB	2.01	127.07	124.05
21	4	316	LUT	C20-C13-C12	2.01	121.16	118.09
21	O	204	LUT	C30-C31-C32	-2.01	117.37	123.20
20	1	302	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
23	J	104	BCR	C38-C26-C27	2.01	117.87	113.60
20	3	303	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
19	2	306	CHL	C4D-ND-C1D	-2.00	103.70	105.22
19	4	315	CHL	CAC-C3C-C4C	2.00	129.18	124.03
22	2	316	XAT	O4-C5-C6	-2.00	57.34	58.93
20	A	807	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	1	316	XAT	O24-C25-C26	-2.00	57.34	58.93
20	4	311	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
19	2	307	CHL	CGD-CBD-CAD	2.00	117.33	110.85
20	1	312	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	B	832	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
23	J	102	BCR	C34-C9-C8	2.00	121.14	118.09
23	3	317	BCR	C11-C12-C13	-2.00	120.88	126.36

All (185) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	301	CHL	NC
19	1	301	CHL	ND
19	1	301	CHL	NA
19	1	306	CHL	NC
19	1	306	CHL	ND
19	1	306	CHL	NA
19	2	301	CHL	NC
19	2	301	CHL	ND
19	2	301	CHL	NA
19	2	305	CHL	NC
19	2	305	CHL	ND
19	2	305	CHL	NA
19	2	306	CHL	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
19	2	306	CHL	ND
19	2	306	CHL	NA
19	2	307	CHL	NC
19	2	307	CHL	ND
19	2	307	CHL	NA
19	2	314	CHL	NC
19	2	314	CHL	ND
19	2	314	CHL	NA
19	3	306	CHL	NC
19	3	306	CHL	ND
19	3	306	CHL	NA
19	4	305	CHL	NC
19	4	305	CHL	ND
19	4	305	CHL	NA
19	4	306	CHL	NC
19	4	306	CHL	ND
19	4	306	CHL	NA
19	4	307	CHL	NC
19	4	307	CHL	ND
19	4	307	CHL	NA
19	4	315	CHL	NC
19	4	315	CHL	ND
19	4	315	CHL	NA
20	1	302	CLA	ND
20	1	303	CLA	ND
20	1	304	CLA	ND
20	1	305	CLA	ND
20	1	307	CLA	ND
20	1	308	CLA	ND
20	1	309	CLA	ND
20	1	310	CLA	ND
20	1	311	CLA	ND
20	1	312	CLA	ND
20	1	313	CLA	ND
20	1	314	CLA	ND
20	1	321	CLA	ND
20	2	302	CLA	ND
20	2	303	CLA	ND
20	2	304	CLA	ND
20	2	308	CLA	ND
20	2	309	CLA	ND
20	2	310	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	2	311	CLA	ND
20	2	312	CLA	ND
20	2	313	CLA	ND
20	3	301	CLA	ND
20	3	302	CLA	ND
20	3	303	CLA	ND
20	3	304	CLA	ND
20	3	305	CLA	ND
20	3	307	CLA	ND
20	3	308	CLA	ND
20	3	310	CLA	ND
20	3	311	CLA	ND
20	3	312	CLA	ND
20	3	313	CLA	ND
20	3	314	CLA	ND
20	4	301	CLA	ND
20	4	302	CLA	ND
20	4	303	CLA	ND
20	4	304	CLA	ND
20	4	308	CLA	ND
20	4	309	CLA	ND
20	4	310	CLA	ND
20	4	311	CLA	ND
20	4	312	CLA	ND
20	4	313	CLA	ND
20	4	314	CLA	ND
20	A	801	CLA	ND
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	807	CLA	ND
20	A	808	CLA	ND
20	A	809	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	816	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	A	817	CLA	ND
20	A	818	CLA	ND
20	A	819	CLA	ND
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND
20	A	823	CLA	ND
20	A	824	CLA	ND
20	A	825	CLA	ND
20	A	826	CLA	ND
20	A	827	CLA	ND
20	A	828	CLA	ND
20	A	829	CLA	ND
20	A	830	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	836	CLA	ND
20	A	837	CLA	ND
20	A	838	CLA	ND
20	A	839	CLA	ND
20	A	840	CLA	ND
20	A	841	CLA	ND
20	A	851	CLA	ND
20	A	853	CLA	ND
20	B	801	CLA	ND
20	B	802	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND
20	B	806	CLA	ND
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	809	CLA	ND
20	B	810	CLA	ND
20	B	811	CLA	ND
20	B	812	CLA	ND
20	B	813	CLA	ND
20	B	814	CLA	ND
20	B	815	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	B	816	CLA	ND
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	820	CLA	ND
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	824	CLA	ND
20	B	825	CLA	ND
20	B	826	CLA	ND
20	B	827	CLA	ND
20	B	828	CLA	ND
20	B	829	CLA	ND
20	B	830	CLA	ND
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	835	CLA	ND
20	B	836	CLA	ND
20	B	837	CLA	ND
20	B	838	CLA	ND
20	B	839	CLA	ND
20	F	802	CLA	ND
20	F	804	CLA	ND
20	F	805	CLA	ND
20	G	603	CLA	ND
20	G	604	CLA	ND
20	G	605	CLA	ND
20	H	201	CLA	ND
20	J	101	CLA	ND
20	J	103	CLA	ND
20	K	201	CLA	ND
20	K	202	CLA	ND
20	K	203	CLA	ND
20	K	205	CLA	ND
20	L	302	CLA	ND
20	L	303	CLA	ND
20	L	304	CLA	ND
20	L	307	CLA	ND
20	N	202	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
20	N	203	CLA	ND
20	O	201	CLA	ND
20	O	202	CLA	ND
20	O	203	CLA	ND

All (1436) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C2-C3-C5-C6
19	1	301	CHL	C4-C3-C5-C6
19	1	306	CHL	C3A-C2A-CAA-CBA
19	1	306	CHL	C3C-C2C-CMC-OMC
19	1	306	CHL	CBD-CGD-O2D-CED
19	2	301	CHL	C1C-C2C-CMC-OMC
19	2	301	CHL	C3C-C2C-CMC-OMC
19	2	305	CHL	CAD-CBD-CGD-O1D
19	2	305	CHL	CAD-CBD-CGD-O2D
19	2	306	CHL	C1C-C2C-CMC-OMC
19	2	306	CHL	C3C-C2C-CMC-OMC
19	2	306	CHL	CBD-CGD-O2D-CED
19	2	307	CHL	C1A-C2A-CAA-CBA
19	2	307	CHL	C1C-C2C-CMC-OMC
19	2	307	CHL	C3C-C2C-CMC-OMC
19	3	306	CHL	C1C-C2C-CMC-OMC
19	3	306	CHL	C3C-C2C-CMC-OMC
19	4	305	CHL	C1C-C2C-CMC-OMC
19	4	305	CHL	C3C-C2C-CMC-OMC
19	4	306	CHL	C1C-C2C-CMC-OMC
19	4	306	CHL	C3C-C2C-CMC-OMC
20	1	302	CLA	CHA-CBD-CGD-O1D
20	1	302	CLA	CHA-CBD-CGD-O2D
20	1	308	CLA	C1A-C2A-CAA-CBA
20	1	308	CLA	C3A-C2A-CAA-CBA
20	1	311	CLA	CHA-CBD-CGD-O1D
20	1	311	CLA	CHA-CBD-CGD-O2D
20	1	314	CLA	CBA-CGA-O2A-C1
20	1	314	CLA	O1A-CGA-O2A-C1
20	2	308	CLA	C1A-C2A-CAA-CBA
20	2	308	CLA	C3A-C2A-CAA-CBA
20	2	311	CLA	CHA-CBD-CGD-O1D
20	2	311	CLA	CHA-CBD-CGD-O2D
20	2	313	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	2	313	CLA	CAD-CBD-CGD-O2D
20	3	301	CLA	CHA-CBD-CGD-O2D
20	3	305	CLA	C1A-C2A-CAA-CBA
20	3	305	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	C1A-C2A-CAA-CBA
20	3	307	CLA	C3A-C2A-CAA-CBA
20	3	313	CLA	CAD-CBD-CGD-O2D
20	4	301	CLA	CAD-CBD-CGD-O1D
20	4	301	CLA	CAD-CBD-CGD-O2D
20	4	308	CLA	C1A-C2A-CAA-CBA
20	4	308	CLA	C3A-C2A-CAA-CBA
20	4	312	CLA	C1A-C2A-CAA-CBA
20	4	312	CLA	C3A-C2A-CAA-CBA
20	4	312	CLA	CBD-CGD-O2D-CED
20	A	801	CLA	C2B-C3B-CAB-CBB
20	A	801	CLA	C4B-C3B-CAB-CBB
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	803	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	CAD-CBD-CGD-O1D
20	A	804	CLA	CAD-CBD-CGD-O2D
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	807	CLA	CHA-CBD-CGD-O2D
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	C2-C3-C5-C6
20	A	811	CLA	C4-C3-C5-C6
20	A	817	CLA	C3A-C2A-CAA-CBA
20	A	821	CLA	C3A-C2A-CAA-CBA
20	A	822	CLA	C2B-C3B-CAB-CBB
20	A	822	CLA	C4B-C3B-CAB-CBB
20	A	827	CLA	C1A-C2A-CAA-CBA
20	A	827	CLA	CBA-CGA-O2A-C1
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	831	CLA	C2B-C3B-CAB-CBB
20	A	831	CLA	C4B-C3B-CAB-CBB
20	A	833	CLA	CHA-CBD-CGD-O1D
20	A	833	CLA	CHA-CBD-CGD-O2D
20	A	836	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	839	CLA	CBD-CGD-O2D-CED
20	A	841	CLA	C4B-C3B-CAB-CBB
20	A	851	CLA	CAD-CBD-CGD-O1D
20	A	851	CLA	CAD-CBD-CGD-O2D
20	B	802	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	CHA-CBD-CGD-O1D
20	B	808	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	CHA-CBD-CGD-O1D
20	B	810	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	C1A-C2A-CAA-CBA
20	B	812	CLA	C3A-C2A-CAA-CBA
20	B	815	CLA	CHA-CBD-CGD-O2D
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C4B-C3B-CAB-CBB
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	CHA-CBD-CGD-O1D
20	B	824	CLA	CHA-CBD-CGD-O2D
20	B	824	CLA	C2-C3-C5-C6
20	B	824	CLA	C4-C3-C5-C6
20	B	825	CLA	CHA-CBD-CGD-O1D
20	B	825	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	830	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	C3A-C2A-CAA-CBA
20	B	839	CLA	C1A-C2A-CAA-CBA
20	B	839	CLA	C3A-C2A-CAA-CBA
20	F	804	CLA	C2B-C3B-CAB-CBB
20	F	804	CLA	C4B-C3B-CAB-CBB
20	F	805	CLA	CHA-CBD-CGD-O1D
20	F	805	CLA	CHA-CBD-CGD-O2D
20	G	603	CLA	C2B-C3B-CAB-CBB
20	G	603	CLA	C4B-C3B-CAB-CBB
20	H	201	CLA	C6-C7-C8-C9
20	J	103	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	K	202	CLA	C1A-C2A-CAA-CBA
20	K	203	CLA	CHA-CBD-CGD-O1D
20	K	203	CLA	CHA-CBD-CGD-O2D
20	L	302	CLA	C1A-C2A-CAA-CBA
20	L	307	CLA	CHA-CBD-CGD-O1D
20	L	307	CLA	CHA-CBD-CGD-O2D
20	N	202	CLA	CHA-CBD-CGD-O2D
20	O	201	CLA	C1A-C2A-CAA-CBA
20	O	201	CLA	C3A-C2A-CAA-CBA
20	O	201	CLA	C2B-C3B-CAB-CBB
20	O	201	CLA	C4B-C3B-CAB-CBB
20	O	201	CLA	C3-C5-C6-C7
20	O	202	CLA	C1A-C2A-CAA-CBA
20	O	202	CLA	C3A-C2A-CAA-CBA
20	O	203	CLA	C3A-C2A-CAA-CBA
21	O	205	LUT	C21-C26-C27-C28
21	O	205	LUT	C25-C26-C27-C28
23	I	101	BCR	C7-C8-C9-C10
23	I	101	BCR	C21-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
23	J	102	BCR	C21-C22-C23-C24
23	J	102	BCR	C37-C22-C23-C24
23	K	204	BCR	C21-C22-C23-C24
23	K	204	BCR	C37-C22-C23-C24
23	L	305	BCR	C37-C22-C23-C24
24	1	318	LHG	C3-O3-P-O5
24	1	318	LHG	C4-O6-P-O3
24	1	318	LHG	C4-O6-P-O4
24	1	318	LHG	C4-O6-P-O5
24	2	318	LHG	O2-C2-C3-O3
24	2	318	LHG	C4-O6-P-O3
24	2	318	LHG	O6-C4-C5-O7
24	A	844	LHG	C3-O3-P-O5
24	A	844	LHG	C3-O3-P-O6
24	A	844	LHG	C4-O6-P-O3
24	A	844	LHG	C4-O6-P-O4
24	B	849	LHG	C3-O3-P-O4
24	B	849	LHG	C3-O3-P-O6
24	B	849	LHG	C4-O6-P-O3
24	B	849	LHG	C4-O6-P-O4
26	B	850	HTG	C2-C1-S1-C1'
30	B	848	DGD	O6D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	4	307	CHL	O1D-CGD-O2D-CED
19	2	305	CHL	CBD-CGD-O2D-CED
19	4	307	CHL	CBD-CGD-O2D-CED
20	1	312	CLA	CBD-CGD-O2D-CED
20	2	303	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	CBD-CGD-O2D-CED
20	3	312	CLA	CBD-CGD-O2D-CED
20	4	303	CLA	CBD-CGD-O2D-CED
20	4	304	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CBD-CGD-O2D-CED
20	K	203	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	O	203	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	CBA-CGA-O2A-C1
20	F	805	CLA	CBA-CGA-O2A-C1
19	2	306	CHL	O1D-CGD-O2D-CED
20	2	303	CLA	O1D-CGD-O2D-CED
20	B	817	CLA	CBA-CGA-O2A-C1
20	O	203	CLA	CBA-CGA-O2A-C1
19	4	315	CHL	CBD-CGD-O2D-CED
20	1	303	CLA	O1A-CGA-O2A-C1
20	1	305	CLA	O1A-CGA-O2A-C1
20	4	303	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	O1A-CGA-O2A-C1
20	F	802	CLA	O1A-CGA-O2A-C1
19	2	305	CHL	O1D-CGD-O2D-CED
20	4	303	CLA	O1D-CGD-O2D-CED
20	A	827	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	O1D-CGD-O2D-CED
19	1	306	CHL	O1D-CGD-O2D-CED
20	4	312	CLA	O1D-CGD-O2D-CED
26	B	850	HTG	S1-C1'-C2'-C3'
20	A	806	CLA	C3-C5-C6-C7
20	A	809	CLA	C3-C5-C6-C7
20	A	831	CLA	C3-C5-C6-C7
20	A	834	CLA	C3-C5-C6-C7
20	A	837	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	851	CLA	C3-C5-C6-C7
20	B	806	CLA	C3-C5-C6-C7
20	B	818	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	H	201	CLA	C3-C5-C6-C7
20	A	810	CLA	O1D-CGD-O2D-CED
20	B	802	CLA	O1D-CGD-O2D-CED
20	J	103	CLA	O1D-CGD-O2D-CED
20	1	303	CLA	CBA-CGA-O2A-C1
20	1	305	CLA	CBA-CGA-O2A-C1
20	3	305	CLA	CBA-CGA-O2A-C1
20	4	303	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	O	201	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	CBD-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	G	603	CLA	CBD-CGD-O2D-CED
20	N	203	CLA	CBD-CGD-O2D-CED
20	B	810	CLA	O1D-CGD-O2D-CED
20	1	304	CLA	C4-C3-C5-C6
20	A	809	CLA	C4-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	B	822	CLA	C4-C3-C5-C6
27	A	842	PQN	C14-C13-C15-C16
20	1	304	CLA	C2-C3-C5-C6
20	A	809	CLA	C2-C3-C5-C6
20	A	837	CLA	C2-C3-C5-C6
20	B	822	CLA	C2-C3-C5-C6
27	A	842	PQN	C12-C13-C15-C16
20	K	203	CLA	CBA-CGA-O2A-C1
20	1	312	CLA	O1D-CGD-O2D-CED
20	1	311	CLA	C3-C5-C6-C7
20	3	314	CLA	C2A-CAA-CBA-CGA
20	4	314	CLA	C2A-CAA-CBA-CGA
20	B	817	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	O1A-CGA-O2A-C1
20	A	805	CLA	C3-C5-C6-C7
20	A	808	CLA	C3-C5-C6-C7
20	A	832	CLA	C3-C5-C6-C7
19	1	301	CHL	CBA-CGA-O2A-C1
20	4	304	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4	312	CLA	CBA-CGA-O2A-C1
20	A	841	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	F	802	CLA	CBA-CGA-O2A-C1
19	1	306	CHL	C2-C1-O2A-CGA
20	3	305	CLA	O1A-CGA-O2A-C1
20	4	312	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	O	201	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	C10-C11-C12-C13
20	F	805	CLA	O1A-CGA-O2A-C1
20	K	203	CLA	O1A-CGA-O2A-C1
20	2	302	CLA	C3-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	1	307	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBD-CGD-O2D-CED
20	A	833	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	CBD-CGD-O2D-CED
24	A	844	LHG	O2-C2-C3-O3
20	2	303	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	CBA-CGA-O2A-C1
20	L	307	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	O1D-CGD-O2D-CED
20	B	827	CLA	O1D-CGD-O2D-CED
20	B	808	CLA	C3-C5-C6-C7
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	836	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	O1D-CGD-O2D-CED
20	K	203	CLA	O1D-CGD-O2D-CED
19	2	301	CHL	CBA-CGA-O2A-C1
20	A	822	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
19	1	301	CHL	O1A-CGA-O2A-C1
20	2	303	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	3	303	CLA	CBD-CGD-O2D-CED
20	3	312	CLA	O1D-CGD-O2D-CED
20	4	304	CLA	C2A-CAA-CBA-CGA
20	A	835	CLA	C2A-CAA-CBA-CGA
19	4	315	CHL	O1D-CGD-O2D-CED
20	4	304	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	C2C-C3C-CAC-CBC
19	2	307	CHL	CBD-CGD-O2D-CED
20	2	309	CLA	CBD-CGD-O2D-CED
20	2	313	CLA	CBD-CGD-O2D-CED
20	3	302	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	CBD-CGD-O2D-CED
19	3	306	CHL	CBD-CGD-O2D-CED
20	B	811	CLA	CBD-CGD-O2D-CED
20	A	826	CLA	C3-C5-C6-C7
24	2	318	LHG	C1-C2-C3-O3
19	4	306	CHL	CBA-CGA-O2A-C1
20	1	307	CLA	CBA-CGA-O2A-C1
20	4	311	CLA	CBA-CGA-O2A-C1
20	A	803	CLA	CBA-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	CBA-CGA-O2A-C1
20	4	310	CLA	CBD-CGD-O2D-CED
20	N	203	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	O1A-CGA-O2A-C1
20	4	302	CLA	C11-C10-C8-C9
20	A	808	CLA	C14-C13-C15-C16
20	A	810	CLA	C14-C13-C15-C16
20	A	824	CLA	C11-C12-C13-C14
20	A	827	CLA	C11-C10-C8-C9
20	A	837	CLA	C11-C12-C13-C14
20	A	841	CLA	C14-C13-C15-C16
20	A	853	CLA	C6-C7-C8-C9
20	B	803	CLA	C11-C12-C13-C14
20	B	806	CLA	C6-C7-C8-C9
20	B	813	CLA	C11-C12-C13-C14
20	B	822	CLA	C11-C12-C13-C14
20	B	824	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	836	CLA	C14-C13-C15-C16
19	2	301	CHL	O1A-CGA-O2A-C1
19	4	306	CHL	O1A-CGA-O2A-C1
20	4	304	CLA	O1D-CGD-O2D-CED
23	4	318	BCR	C7-C8-C9-C34
23	A	845	BCR	C37-C22-C23-C24
23	I	101	BCR	C7-C8-C9-C34
23	4	318	BCR	C7-C8-C9-C10
23	L	305	BCR	C21-C22-C23-C24
19	4	305	CHL	C3-C5-C6-C7
20	1	304	CLA	C3-C5-C6-C7
20	B	831	CLA	C2A-CAA-CBA-CGA
20	4	311	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	O1A-CGA-O2A-C1
20	A	801	CLA	C3-C5-C6-C7
26	F	803	HTG	O5-C5-C6-O6
20	A	809	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	CBA-CGA-O2A-C1
20	4	314	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	C2-C1-O2A-CGA
20	A	808	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	CBD-CGD-O2D-CED
20	O	202	CLA	C2C-C3C-CAC-CBC
27	A	842	PQN	C18-C20-C21-C22
20	G	603	CLA	O1D-CGD-O2D-CED
20	A	801	CLA	C12-C13-C15-C16
20	A	831	CLA	C11-C12-C13-C15
20	A	841	CLA	C11-C10-C8-C7
20	A	851	CLA	C6-C7-C8-C10
20	B	818	CLA	C11-C10-C8-C7
20	A	820	CLA	C5-C6-C7-C8
20	A	838	CLA	C3-C5-C6-C7
20	B	818	CLA	C8-C10-C11-C12
20	L	303	CLA	C13-C15-C16-C17
20	A	816	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	C8-C10-C11-C12
20	A	838	CLA	C10-C11-C12-C13
20	B	815	CLA	C5-C6-C7-C8
20	F	802	CLA	C8-C10-C11-C12
20	3	305	CLA	C2A-CAA-CBA-CGA
20	B	838	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	802	CLA	C15-C16-C17-C18
20	A	834	CLA	C13-C15-C16-C17
20	B	836	CLA	C5-C6-C7-C8
20	H	201	CLA	C5-C6-C7-C8
20	L	303	CLA	C8-C10-C11-C12
20	L	303	CLA	C10-C11-C12-C13
20	A	803	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	B	830	CLA	O1A-CGA-O2A-C1
20	1	303	CLA	C13-C15-C16-C17
20	1	312	CLA	C10-C11-C12-C13
20	4	302	CLA	C8-C10-C11-C12
20	A	809	CLA	C8-C10-C11-C12
20	A	810	CLA	C8-C10-C11-C12
20	A	812	CLA	C15-C16-C17-C18
20	A	829	CLA	C10-C11-C12-C13
20	A	831	CLA	C8-C10-C11-C12
20	A	834	CLA	C10-C11-C12-C13
20	A	853	CLA	C15-C16-C17-C18
20	B	813	CLA	C13-C15-C16-C17
20	B	833	CLA	C10-C11-C12-C13
20	A	831	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	CBA-CGA-O2A-C1
20	B	816	CLA	CBA-CGA-O2A-C1
20	1	312	CLA	C8-C10-C11-C12
20	A	806	CLA	C10-C11-C12-C13
20	B	803	CLA	O1D-CGD-O2D-CED
29	B	847	LMT	C4'-C5'-C6'-O6'
20	2	311	CLA	O1D-CGD-O2D-CED
20	A	833	CLA	O1D-CGD-O2D-CED
20	4	309	CLA	C5-C6-C7-C8
20	A	801	CLA	C8-C10-C11-C12
20	A	805	CLA	C5-C6-C7-C8
20	B	813	CLA	C10-C11-C12-C13
20	A	817	CLA	CBD-CGD-O2D-CED
20	1	307	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	C13-C15-C16-C17
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	CBA-CGA-O2A-C1
20	3	309	CLA	C4C-C3C-CAC-CBC
19	2	314	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	2	310	CLA	CBD-CGD-O2D-CED
20	B	839	CLA	CBD-CGD-O2D-CED
20	4	310	CLA	O1A-CGA-O2A-C1
20	4	314	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	O1A-CGA-O2A-C1
20	A	832	CLA	C5-C6-C7-C8
20	A	831	CLA	C5-C6-C7-C8
20	1	313	CLA	C2A-CAA-CBA-CGA
20	A	841	CLA	C2A-CAA-CBA-CGA
20	B	804	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	CBA-CGA-O2A-C1
20	B	831	CLA	CBA-CGA-O2A-C1
20	B	807	CLA	C5-C6-C7-C8
20	B	825	CLA	C10-C11-C12-C13
20	J	101	CLA	C13-C15-C16-C17
20	K	202	CLA	C10-C11-C12-C13
27	A	842	PQN	C20-C21-C22-C23
27	A	842	PQN	C25-C26-C27-C28
20	A	818	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	CBD-CGD-O2D-CED
20	A	818	CLA	C15-C16-C17-C18
20	A	831	CLA	C15-C16-C17-C18
27	A	842	PQN	C15-C16-C17-C18
26	B	851	HTG	S1-C1'-C2'-C3'
20	1	303	CLA	C5-C6-C7-C8
20	B	833	CLA	C5-C6-C7-C8
20	B	839	CLA	C15-C16-C17-C18
20	4	303	CLA	C4-C3-C5-C6
20	A	838	CLA	C8-C10-C11-C12
20	A	853	CLA	C5-C6-C7-C8
20	B	813	CLA	C8-C10-C11-C12
20	B	832	CLA	C8-C10-C11-C12
20	H	201	CLA	CBD-CGD-O2D-CED
20	2	309	CLA	C11-C10-C8-C9
20	B	819	CLA	C11-C10-C8-C9
20	L	307	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	C13-C15-C16-C17
20	B	805	CLA	C16-C17-C18-C19
20	2	304	CLA	CBD-CGD-O2D-CED
23	B	845	BCR	C37-C22-C23-C24
26	4	320	HTG	S1-C1'-C2'-C3'
23	A	845	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	H	201	CLA	O1A-CGA-O2A-C1
20	1	314	CLA	C2A-CAA-CBA-CGA
20	2	308	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
20	A	839	CLA	C13-C15-C16-C17
20	A	836	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	C11-C12-C13-C14
20	B	822	CLA	C16-C17-C18-C20
20	B	825	CLA	C16-C17-C18-C19
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	831	CLA	O1A-CGA-O2A-C1
20	A	837	CLA	O1A-CGA-O2A-C1
20	B	816	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	C3-C5-C6-C7
20	2	302	CLA	C13-C15-C16-C17
20	3	303	CLA	O1D-CGD-O2D-CED
19	1	306	CHL	CBA-CGA-O2A-C1
20	A	804	CLA	CBA-CGA-O2A-C1
20	2	304	CLA	C10-C11-C12-C13
20	B	833	CLA	C8-C10-C11-C12
20	L	303	CLA	C15-C16-C17-C18
20	A	814	CLA	O1D-CGD-O2D-CED
19	4	307	CHL	C2-C1-O2A-CGA
20	1	313	CLA	C6-C7-C8-C10
20	2	304	CLA	C11-C12-C13-C15
20	A	839	CLA	C16-C17-C18-C20
20	B	815	CLA	C11-C12-C13-C15
20	B	816	CLA	C6-C7-C8-C9
20	A	806	CLA	O1A-CGA-O2A-C1
20	G	605	CLA	CBA-CGA-O2A-C1
20	1	308	CLA	C4B-C3B-CAB-CBB
20	1	313	CLA	C4B-C3B-CAB-CBB
20	2	304	CLA	C4B-C3B-CAB-CBB
20	4	308	CLA	C4B-C3B-CAB-CBB
20	A	816	CLA	C4B-C3B-CAB-CBB
20	A	820	CLA	C4B-C3B-CAB-CBB
20	B	808	CLA	C4B-C3B-CAB-CBB
20	B	838	CLA	C4B-C3B-CAB-CBB
20	K	205	CLA	C4B-C3B-CAB-CBB
20	B	807	CLA	C6-C7-C8-C9
20	A	807	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	822	CLA	C2A-CAA-CBA-CGA
20	G	604	CLA	C2A-CAA-CBA-CGA
24	1	318	LHG	C9-C10-C11-C12
20	4	309	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	C6-C7-C8-C10
20	A	853	CLA	C6-C7-C8-C10
20	L	303	CLA	C11-C10-C8-C7
24	A	843	LHG	C11-C12-C13-C14
20	A	826	CLA	O1A-CGA-O2A-C1
20	B	828	CLA	O1A-CGA-O2A-C1
20	4	304	CLA	C3A-C2A-CAA-CBA
20	A	827	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	C3A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	F	805	CLA	C3A-C2A-CAA-CBA
20	J	101	CLA	C3A-C2A-CAA-CBA
20	L	302	CLA	C3A-C2A-CAA-CBA
20	2	309	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	C10-C11-C12-C13
20	B	824	CLA	C5-C6-C7-C8
20	B	806	CLA	O1D-CGD-O2D-CED
20	1	313	CLA	C6-C7-C8-C9
20	B	805	CLA	C16-C17-C18-C20
20	B	831	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	CBA-CGA-O2A-C1
25	4	319	LMG	C20-C21-C22-C23
27	A	842	PQN	C13-C15-C16-C17
30	B	848	DGD	CDA-CEA-CFA-CGA
20	A	804	CLA	O1A-CGA-O2A-C1
20	B	831	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	C16-C17-C18-C19
20	A	841	CLA	C16-C17-C18-C20
20	B	816	CLA	C6-C7-C8-C10
25	1	320	LMG	C10-C11-C12-C13
20	1	308	CLA	C2B-C3B-CAB-CBB
20	4	308	CLA	C2B-C3B-CAB-CBB
20	A	834	CLA	C2B-C3B-CAB-CBB
20	A	841	CLA	C2B-C3B-CAB-CBB
20	B	808	CLA	C2B-C3B-CAB-CBB
20	B	819	CLA	C2B-C3B-CAB-CBB
20	B	838	CLA	C2B-C3B-CAB-CBB
21	O	205	LUT	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	O	205	LUT	C5-C6-C7-C8
23	4	318	BCR	C1-C6-C7-C8
23	4	318	BCR	C5-C6-C7-C8
23	B	842	BCR	C23-C24-C25-C26
23	B	842	BCR	C23-C24-C25-C30
23	I	101	BCR	C1-C6-C7-C8
23	I	101	BCR	C5-C6-C7-C8
23	I	101	BCR	C23-C24-C25-C26
23	I	101	BCR	C23-C24-C25-C30
23	J	102	BCR	C1-C6-C7-C8
23	J	102	BCR	C23-C24-C25-C26
23	J	102	BCR	C23-C24-C25-C30
23	K	204	BCR	C23-C24-C25-C26
23	K	204	BCR	C23-C24-C25-C30
23	L	305	BCR	C23-C24-C25-C26
23	L	305	BCR	C23-C24-C25-C30
24	B	849	LHG	C8-C7-O7-C5
25	4	319	LMG	C11-C10-O7-C8
20	1	302	CLA	C15-C16-C17-C18
20	A	841	CLA	C3-C5-C6-C7
25	1	320	LMG	C23-C24-C25-C26
20	3	302	CLA	O1D-CGD-O2D-CED
20	3	312	CLA	C2A-CAA-CBA-CGA
20	A	851	CLA	C2A-CAA-CBA-CGA
20	B	821	CLA	C2A-CAA-CBA-CGA
20	G	605	CLA	C2A-CAA-CBA-CGA
20	1	310	CLA	CBD-CGD-O2D-CED
20	B	805	CLA	C8-C10-C11-C12
20	B	806	CLA	C15-C16-C17-C18
20	4	303	CLA	C2-C3-C5-C6
20	2	304	CLA	C11-C12-C13-C14
20	A	828	CLA	CBA-CGA-O2A-C1
20	1	312	CLA	C6-C7-C8-C9
20	A	811	CLA	C5-C6-C7-C8
26	B	850	HTG	C3'-C4'-C5'-C6'
29	G	601	LMT	C6-C7-C8-C9
20	2	313	CLA	O1D-CGD-O2D-CED
26	A	852	HTG	C3'-C4'-C5'-C6'
20	A	809	CLA	C16-C17-C18-C20
20	B	822	CLA	C16-C17-C18-C19
24	2	318	LHG	C8-C7-O7-C5
25	1	323	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	306	CHL	O1A-CGA-O2A-C1
21	O	205	LUT	C7-C8-C9-C19
23	B	841	BCR	C7-C8-C9-C34
19	2	307	CHL	C2A-CAA-CBA-CGA
20	A	820	CLA	C2A-CAA-CBA-CGA
20	O	202	CLA	C4C-C3C-CAC-CBC
20	A	841	CLA	C16-C17-C18-C19
20	B	825	CLA	C16-C17-C18-C20
20	A	853	CLA	C4-C3-C5-C6
20	B	833	CLA	C4-C3-C5-C6
20	B	838	CLA	C4-C3-C5-C6
24	1	318	LHG	C10-C11-C12-C13
25	4	319	LMG	C21-C22-C23-C24
20	B	811	CLA	O1D-CGD-O2D-CED
29	B	847	LMT	O5'-C5'-C6'-O6'
20	4	301	CLA	CBA-CGA-O2A-C1
20	A	812	CLA	CBD-CGD-O2D-CED
19	2	306	CHL	O1A-CGA-O2A-C1
20	A	809	CLA	C10-C11-C12-C13
20	B	823	CLA	C8-C10-C11-C12
25	4	319	LMG	O9-C10-O7-C8
20	A	808	CLA	C16-C17-C18-C20
20	B	825	CLA	O1A-CGA-O2A-C1
20	4	309	CLA	C10-C11-C12-C13
20	A	812	CLA	C5-C6-C7-C8
20	A	812	CLA	C8-C10-C11-C12
20	4	310	CLA	O1D-CGD-O2D-CED
29	G	601	LMT	C1-C2-C3-C4
20	A	805	CLA	C4-C3-C5-C6
20	A	853	CLA	C2-C3-C5-C6
20	B	833	CLA	C2-C3-C5-C6
20	B	838	CLA	C2-C3-C5-C6
24	A	844	LHG	C1-C2-C3-O3
20	A	801	CLA	C13-C15-C16-C17
24	A	843	LHG	C9-C10-C11-C12
20	B	830	CLA	C2A-CAA-CBA-CGA
20	H	201	CLA	C2A-CAA-CBA-CGA
19	2	307	CHL	O1D-CGD-O2D-CED
25	1	323	LMG	O6-C5-C6-O5
20	1	313	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	817	CLA	C1A-C2A-CAA-CBA
20	A	821	CLA	C1A-C2A-CAA-CBA
20	A	822	CLA	C1A-C2A-CAA-CBA
20	A	823	CLA	C1A-C2A-CAA-CBA
20	A	832	CLA	C1A-C2A-CAA-CBA
20	A	836	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C1A-C2A-CAA-CBA
20	F	805	CLA	C1A-C2A-CAA-CBA
20	J	101	CLA	C1A-C2A-CAA-CBA
20	O	203	CLA	C1A-C2A-CAA-CBA
20	1	312	CLA	C5-C6-C7-C8
20	A	828	CLA	O1A-CGA-O2A-C1
24	B	849	LHG	O9-C7-O7-C5
25	1	323	LMG	O9-C10-O7-C8
20	B	807	CLA	C3-C5-C6-C7
20	2	312	CLA	C6-C7-C8-C10
20	4	302	CLA	C6-C7-C8-C10
20	4	302	CLA	C11-C10-C8-C7
20	A	802	CLA	C11-C10-C8-C7
20	A	805	CLA	C11-C12-C13-C15
20	A	810	CLA	C11-C12-C13-C15
20	A	817	CLA	C11-C12-C13-C15
20	A	829	CLA	C12-C13-C15-C16
20	A	832	CLA	C12-C13-C15-C16
20	A	837	CLA	C6-C7-C8-C10
20	A	837	CLA	C11-C12-C13-C15
20	B	805	CLA	C11-C12-C13-C15
20	B	806	CLA	C6-C7-C8-C10
20	B	806	CLA	C12-C13-C15-C16
20	B	813	CLA	C12-C13-C15-C16
20	B	817	CLA	C12-C13-C15-C16
20	B	824	CLA	C12-C13-C15-C16
20	A	802	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	C13-C15-C16-C17
20	A	828	CLA	C2-C3-C5-C6
20	B	808	CLA	C2-C3-C5-C6
20	1	308	CLA	C2A-CAA-CBA-CGA
20	4	303	CLA	C2A-CAA-CBA-CGA
20	A	828	CLA	C2A-CAA-CBA-CGA
20	B	816	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	1	303	CLA	C11-C12-C13-C14
20	1	309	CLA	C11-C10-C8-C9
20	2	312	CLA	C11-C10-C8-C9
20	A	802	CLA	C11-C10-C8-C9
20	A	805	CLA	C11-C12-C13-C14
20	A	805	CLA	C14-C13-C15-C16
20	A	808	CLA	C11-C12-C13-C14
20	A	812	CLA	C6-C7-C8-C9
20	A	829	CLA	C14-C13-C15-C16
20	A	837	CLA	C6-C7-C8-C9
20	A	839	CLA	C14-C13-C15-C16
20	A	841	CLA	C11-C12-C13-C14
20	B	803	CLA	C6-C7-C8-C9
20	B	824	CLA	C14-C13-C15-C16
20	A	809	CLA	C16-C17-C18-C19
20	A	812	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	CBA-CGA-O2A-C1
25	4	319	LMG	O6-C5-C6-O5
20	A	828	CLA	O1D-CGD-O2D-CED
20	2	304	CLA	C5-C6-C7-C8
20	A	802	CLA	C13-C15-C16-C17
19	3	306	CHL	O1D-CGD-O2D-CED
19	2	306	CHL	CBA-CGA-O2A-C1
20	B	819	CLA	CBA-CGA-O2A-C1
30	B	848	DGD	O6E-C5E-C6E-O5E
19	2	305	CHL	CHA-CBD-CGD-O2D
19	4	306	CHL	CHA-CBD-CGD-O2D
20	B	808	CLA	C4-C3-C5-C6
20	A	805	CLA	C2-C3-C5-C6
30	B	848	DGD	CAB-CBB-CCB-CDB
20	1	312	CLA	C13-C15-C16-C17
24	2	318	LHG	O9-C7-O7-C5
20	A	841	CLA	C15-C16-C17-C18
20	B	822	CLA	C10-C11-C12-C13
25	1	320	LMG	C29-C30-C31-C32
20	B	825	CLA	C15-C16-C17-C18
26	F	807	HTG	C3'-C4'-C5'-C6'
20	2	304	CLA	C3-C5-C6-C7
20	4	312	CLA	C3-C5-C6-C7
20	A	817	CLA	C3-C5-C6-C7
20	A	820	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	848	DGD	C5B-C6B-C7B-C8B
20	1	313	CLA	CBA-CGA-O2A-C1
20	B	807	CLA	C6-C7-C8-C10
20	B	811	CLA	C6-C7-C8-C9
20	1	308	CLA	CBA-CGA-O2A-C1
20	4	308	CLA	CBA-CGA-O2A-C1
26	F	807	HTG	C1'-C2'-C3'-C4'
19	1	306	CHL	C1C-C2C-CMC-OMC
26	B	850	HTG	C2'-C1'-S1-C1
25	1	320	LMG	C30-C31-C32-C33
20	A	837	CLA	C8-C10-C11-C12
20	B	810	CLA	C8-C10-C11-C12
19	2	314	CHL	O1D-CGD-O2D-CED
20	2	310	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	O1D-CGD-O2D-CED
20	B	839	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	C14-C13-C15-C16
20	B	821	CLA	C11-C10-C8-C9
20	2	304	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	2	302	CLA	C11-C12-C13-C14
20	2	312	CLA	C6-C7-C8-C9
20	4	302	CLA	C6-C7-C8-C9
20	A	805	CLA	C6-C7-C8-C9
20	A	810	CLA	C11-C12-C13-C14
20	A	816	CLA	C6-C7-C8-C9
20	A	817	CLA	C11-C12-C13-C14
20	A	832	CLA	C14-C13-C15-C16
20	A	841	CLA	C6-C7-C8-C9
20	B	806	CLA	C14-C13-C15-C16
20	B	810	CLA	C14-C13-C15-C16
20	B	813	CLA	C14-C13-C15-C16
20	B	817	CLA	C14-C13-C15-C16
20	3	305	CLA	C4B-C3B-CAB-CBB
20	3	310	CLA	C4B-C3B-CAB-CBB
20	3	312	CLA	C4B-C3B-CAB-CBB
20	A	808	CLA	C4B-C3B-CAB-CBB
20	A	832	CLA	C4B-C3B-CAB-CBB
20	A	834	CLA	C4B-C3B-CAB-CBB
20	B	817	CLA	C4B-C3B-CAB-CBB
20	B	821	CLA	C4B-C3B-CAB-CBB
20	B	831	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	839	CLA	C4B-C3B-CAB-CBB
20	G	605	CLA	C4B-C3B-CAB-CBB
20	K	202	CLA	C4B-C3B-CAB-CBB
20	A	805	CLA	C10-C11-C12-C13
19	1	306	CHL	C2A-CAA-CBA-CGA
25	1	323	LMG	C16-C17-C18-C19
20	G	605	CLA	O1A-CGA-O2A-C1
20	1	303	CLA	C11-C12-C13-C15
20	1	309	CLA	C11-C10-C8-C7
20	2	302	CLA	C11-C12-C13-C15
20	2	312	CLA	C11-C10-C8-C7
20	4	312	CLA	C11-C12-C13-C15
20	A	805	CLA	C12-C13-C15-C16
20	A	806	CLA	C12-C13-C15-C16
20	A	808	CLA	C11-C12-C13-C15
20	A	824	CLA	C11-C12-C13-C15
20	A	829	CLA	C11-C10-C8-C7
20	A	839	CLA	C12-C13-C15-C16
20	A	841	CLA	C11-C12-C13-C15
20	A	851	CLA	C12-C13-C15-C16
20	A	853	CLA	C12-C13-C15-C16
20	B	803	CLA	C6-C7-C8-C10
20	B	810	CLA	C12-C13-C15-C16
20	B	831	CLA	C12-C13-C15-C16
20	H	201	CLA	C6-C7-C8-C10
24	A	843	LHG	C24-C25-C26-C27
20	4	309	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	O1A-CGA-O2A-C1
20	L	303	CLA	C3-C5-C6-C7
20	A	825	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C4-C3-C5-C6
20	B	827	CLA	C4-C3-C5-C6
20	B	831	CLA	C3A-C2A-CAA-CBA
20	K	202	CLA	C3A-C2A-CAA-CBA
20	L	303	CLA	C3A-C2A-CAA-CBA
20	L	307	CLA	C3A-C2A-CAA-CBA
20	N	203	CLA	C3A-C2A-CAA-CBA
19	4	305	CHL	C2C-C3C-CAC-CBC
29	B	847	LMT	O5'-C1'-O1'-C1
29	G	601	LMT	O5'-C1'-O1'-C1
20	A	834	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	2	307	CHL	CBA-CGA-O2A-C1
23	F	801	BCR	C15-C16-C17-C18
20	A	818	CLA	O1D-CGD-O2D-CED
19	3	306	CHL	CBA-CGA-O2A-C1
24	2	318	LHG	C4-C5-C6-O8
24	A	844	LHG	C4-C5-C6-O8
20	A	838	CLA	C16-C17-C18-C20
20	B	813	CLA	C16-C17-C18-C20
20	1	313	CLA	C5-C6-C7-C8
20	A	838	CLA	C2-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
20	B	819	CLA	O1A-CGA-O2A-C1
20	2	304	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	O1D-CGD-O2D-CED
20	H	201	CLA	O1D-CGD-O2D-CED
20	3	305	CLA	C2B-C3B-CAB-CBB
20	A	808	CLA	C2B-C3B-CAB-CBB
20	B	821	CLA	C2B-C3B-CAB-CBB
20	B	839	CLA	C2B-C3B-CAB-CBB
20	G	605	CLA	C2B-C3B-CAB-CBB
20	K	202	CLA	C2B-C3B-CAB-CBB
21	1	319	LUT	C1-C6-C7-C8
21	3	315	LUT	C1-C6-C7-C8
21	4	316	LUT	C1-C6-C7-C8
23	4	318	BCR	C23-C24-C25-C30
23	A	845	BCR	C23-C24-C25-C30
23	B	842	BCR	C1-C6-C7-C8
23	J	102	BCR	C5-C6-C7-C8
20	A	825	CLA	C15-C16-C17-C18
20	1	321	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	C16-C17-C18-C19
20	A	841	CLA	C8-C10-C11-C12
24	2	318	LHG	O7-C5-C6-O8
24	A	844	LHG	O7-C5-C6-O8
25	1	323	LMG	O1-C7-C8-O7
30	B	848	DGD	O2G-C2G-C3G-O3G
20	A	802	CLA	C16-C17-C18-C20
20	K	202	CLA	C11-C12-C13-C14
20	A	820	CLA	O1A-CGA-O2A-C1
20	A	827	CLA	C6-C7-C8-C9
20	A	839	CLA	C11-C12-C13-C14
20	B	805	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	821	CLA	O2A-C1-C2-C3
19	2	306	CHL	C2A-CAA-CBA-CGA
20	A	808	CLA	C2A-CAA-CBA-CGA
20	A	821	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
20	1	308	CLA	C4-C3-C5-C6
20	A	838	CLA	C16-C17-C18-C19
20	B	811	CLA	C6-C7-C8-C10
20	B	835	CLA	CBD-CGD-O2D-CED
20	1	321	CLA	C13-C15-C16-C17
20	1	313	CLA	O1A-CGA-O2A-C1
20	1	311	CLA	CBA-CGA-O2A-C1
24	2	318	LHG	O6-C4-C5-C6
20	1	302	CLA	C12-C13-C15-C16
20	A	807	CLA	C11-C12-C13-C15
20	A	839	CLA	C11-C10-C8-C7
20	B	819	CLA	C6-C7-C8-C10
20	B	825	CLA	C6-C7-C8-C10
20	B	833	CLA	C11-C12-C13-C15
21	O	205	LUT	C7-C8-C9-C10
23	B	845	BCR	C21-C22-C23-C24
20	1	308	CLA	O1A-CGA-O2A-C1
20	A	804	CLA	C2A-CAA-CBA-CGA
20	2	304	CLA	O1A-CGA-O2A-C1
20	4	308	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	O1A-CGA-O2A-C1
26	B	850	HTG	C2'-C3'-C4'-C5'
20	A	802	CLA	C3-C5-C6-C7
20	A	812	CLA	O1D-CGD-O2D-CED
24	B	849	LHG	C6-C5-O7-C7
20	1	304	CLA	CBA-CGA-O2A-C1
20	1	310	CLA	O1D-CGD-O2D-CED
20	B	813	CLA	C16-C17-C18-C19
20	B	823	CLA	C4-C3-C5-C6
20	B	814	CLA	C2A-CAA-CBA-CGA
20	1	308	CLA	C2-C3-C5-C6
19	2	306	CHL	C2C-C3C-CAC-CBC
20	A	853	CLA	C10-C11-C12-C13
20	4	312	CLA	C11-C10-C8-C9
20	A	807	CLA	C11-C12-C13-C14
20	A	829	CLA	C11-C10-C8-C9
20	A	839	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	839	CLA	C11-C10-C8-C9
20	B	825	CLA	C11-C10-C8-C9
20	A	824	CLA	C16-C17-C18-C19
29	B	847	LMT	O5B-C5B-C6B-O6B
20	1	303	CLA	C15-C16-C17-C18
20	B	803	CLA	C8-C10-C11-C12
20	A	802	CLA	C16-C17-C18-C19
20	B	818	CLA	C4-C3-C5-C6
20	1	311	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C2A-CAA-CBA-CGA
20	B	806	CLA	C16-C17-C18-C19
20	B	809	CLA	C16-C17-C18-C20
20	A	841	CLA	C13-C15-C16-C17
20	A	853	CLA	CBD-CGD-O2D-CED
20	A	818	CLA	C8-C10-C11-C12
20	3	314	CLA	CBA-CGA-O2A-C1
19	2	306	CHL	C4C-C3C-CAC-CBC
19	4	305	CHL	C4C-C3C-CAC-CBC
20	A	802	CLA	O1D-CGD-O2D-CED
29	B	847	LMT	C1-C2-C3-C4
20	2	303	CLA	O2A-C1-C2-C3
20	1	307	CLA	C4B-C3B-CAB-CBB
20	1	312	CLA	C4B-C3B-CAB-CBB
20	1	321	CLA	C4B-C3B-CAB-CBB
20	3	302	CLA	C4B-C3B-CAB-CBB
20	3	311	CLA	C4B-C3B-CAB-CBB
20	4	301	CLA	C4B-C3B-CAB-CBB
20	4	310	CLA	C4B-C3B-CAB-CBB
20	4	312	CLA	C4B-C3B-CAB-CBB
20	4	314	CLA	C4B-C3B-CAB-CBB
20	A	810	CLA	C4B-C3B-CAB-CBB
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	815	CLA	C4B-C3B-CAB-CBB
20	A	817	CLA	C4B-C3B-CAB-CBB
20	A	823	CLA	C4B-C3B-CAB-CBB
20	A	825	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C4B-C3B-CAB-CBB
20	A	840	CLA	C4B-C3B-CAB-CBB
20	B	812	CLA	C4B-C3B-CAB-CBB
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	C4B-C3B-CAB-CBB
20	F	805	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	G	604	CLA	C4B-C3B-CAB-CBB
20	J	103	CLA	C4B-C3B-CAB-CBB
20	L	307	CLA	C1A-C2A-CAA-CBA
20	L	307	CLA	C4B-C3B-CAB-CBB
20	A	840	CLA	C2A-CAA-CBA-CGA
20	B	801	CLA	C2A-CAA-CBA-CGA
24	1	318	LHG	C30-C31-C32-C33
20	1	308	CLA	C11-C10-C8-C7
20	3	301	CLA	C6-C7-C8-C10
20	A	802	CLA	C12-C13-C15-C16
20	A	808	CLA	C12-C13-C15-C16
20	A	831	CLA	C12-C13-C15-C16
20	A	853	CLA	C11-C10-C8-C7
20	B	815	CLA	C6-C7-C8-C10
20	B	822	CLA	C11-C12-C13-C15
20	B	824	CLA	C6-C7-C8-C10
25	1	323	LMG	C18-C19-C20-C21
20	B	801	CLA	CBD-CGD-O2D-CED
20	4	301	CLA	O1A-CGA-O2A-C1
20	N	203	CLA	CBA-CGA-O2A-C1
20	1	304	CLA	O1A-CGA-O2A-C1
19	4	306	CHL	C3A-C2A-CAA-CBA
20	A	839	CLA	C4-C3-C5-C6
20	A	810	CLA	C16-C17-C18-C20
20	K	202	CLA	C11-C12-C13-C15
20	3	301	CLA	C10-C11-C12-C13
20	A	833	CLA	C5-C6-C7-C8
20	B	829	CLA	C5-C6-C7-C8
20	A	801	CLA	C11-C12-C13-C14
20	B	818	CLA	C11-C10-C8-C9
20	B	819	CLA	C6-C7-C8-C9
20	B	825	CLA	C6-C7-C8-C9
20	B	831	CLA	C14-C13-C15-C16
20	B	833	CLA	C11-C12-C13-C14
20	4	312	CLA	C8-C10-C11-C12
20	A	821	CLA	C1-C2-C3-C4
20	A	824	CLA	C16-C17-C18-C20
30	B	848	DGD	C2B-C3B-C4B-C5B
25	1	323	LMG	O1-C7-C8-C9
25	1	323	LMG	C7-C8-C9-O8
30	B	848	DGD	C1G-C2G-C3G-O3G
20	1	321	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	2	307	CHL	O1A-CGA-O2A-C1
19	1	301	CHL	CAD-CBD-CGD-O2D
19	2	301	CHL	CAD-CBD-CGD-O2D
20	B	805	CLA	CAD-CBD-CGD-O2D
20	O	201	CLA	CAD-CBD-CGD-O2D
20	B	829	CLA	C3-C5-C6-C7
20	B	833	CLA	C3-C5-C6-C7
20	A	817	CLA	C2A-CAA-CBA-CGA
26	B	850	HTG	C4'-C5'-C6'-C7'
20	N	203	CLA	O1A-CGA-O2A-C1
20	1	321	CLA	O1D-CGD-O2D-CED
19	1	301	CHL	CAD-CBD-CGD-O1D
19	2	301	CHL	CAD-CBD-CGD-O1D
19	2	305	CHL	CHA-CBD-CGD-O1D
19	2	314	CHL	CHA-CBD-CGD-O2D
19	4	306	CHL	CHA-CBD-CGD-O1D
20	2	302	CLA	CHA-CBD-CGD-O1D
20	2	302	CLA	CHA-CBD-CGD-O2D
20	3	301	CLA	CHA-CBD-CGD-O1D
20	3	313	CLA	CAD-CBD-CGD-O1D
20	4	302	CLA	CHA-CBD-CGD-O1D
20	4	302	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	CHA-CBD-CGD-O1D
20	A	821	CLA	CHA-CBD-CGD-O1D
20	A	821	CLA	CHA-CBD-CGD-O2D
20	A	830	CLA	CHA-CBD-CGD-O1D
20	A	830	CLA	CHA-CBD-CGD-O2D
20	B	805	CLA	CAD-CBD-CGD-O1D
20	B	815	CLA	CHA-CBD-CGD-O1D
20	B	832	CLA	CHA-CBD-CGD-O1D
20	B	832	CLA	CHA-CBD-CGD-O2D
20	N	203	CLA	CHA-CBD-CGD-O1D
20	N	203	CLA	CHA-CBD-CGD-O2D
20	O	201	CLA	CAD-CBD-CGD-O1D
20	O	202	CLA	CHA-CBD-CGD-O1D
20	O	202	CLA	CHA-CBD-CGD-O2D
24	2	318	LHG	C3-O3-P-O5
24	2	318	LHG	C4-O6-P-O5
24	A	844	LHG	C4-O6-P-O5
20	1	313	CLA	C2B-C3B-CAB-CBB
20	2	304	CLA	C2B-C3B-CAB-CBB
20	3	310	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4	310	CLA	C2B-C3B-CAB-CBB
20	A	810	CLA	C2B-C3B-CAB-CBB
20	A	815	CLA	C2B-C3B-CAB-CBB
20	A	816	CLA	C2B-C3B-CAB-CBB
20	A	820	CLA	C2B-C3B-CAB-CBB
20	A	823	CLA	C2B-C3B-CAB-CBB
20	A	832	CLA	C2B-C3B-CAB-CBB
20	A	835	CLA	C2B-C3B-CAB-CBB
20	A	840	CLA	C2B-C3B-CAB-CBB
20	B	817	CLA	C2B-C3B-CAB-CBB
20	K	205	CLA	C2B-C3B-CAB-CBB
20	L	307	CLA	C2B-C3B-CAB-CBB
20	B	823	CLA	C2-C3-C5-C6
20	A	810	CLA	C15-C16-C17-C18
20	B	803	CLA	C13-C15-C16-C17
20	B	805	CLA	C13-C15-C16-C17
25	1	320	LMG	O7-C10-C11-C12
24	1	318	LHG	C23-C24-C25-C26
20	A	806	CLA	C5-C6-C7-C8
20	L	304	CLA	CBA-CGA-O2A-C1
20	1	302	CLA	C14-C13-C15-C16
20	4	312	CLA	C11-C12-C13-C14
20	A	801	CLA	C14-C13-C15-C16
20	A	806	CLA	C14-C13-C15-C16
20	A	851	CLA	C6-C7-C8-C9
20	A	851	CLA	C14-C13-C15-C16
20	A	853	CLA	C14-C13-C15-C16
20	B	827	CLA	C6-C7-C8-C9
30	B	848	DGD	C2A-C3A-C4A-C5A
20	A	801	CLA	C11-C12-C13-C15
20	A	827	CLA	C11-C10-C8-C7
20	B	827	CLA	C6-C7-C8-C10
20	B	827	CLA	C11-C12-C13-C15
25	1	320	LMG	C28-C29-C30-C31
25	1	320	LMG	O6-C1-O1-C7
20	L	303	CLA	C2A-CAA-CBA-CGA
20	B	809	CLA	C16-C17-C18-C19
20	B	817	CLA	C8-C10-C11-C12
20	A	853	CLA	O1D-CGD-O2D-CED
20	A	810	CLA	C16-C17-C18-C19
25	1	323	LMG	C23-C24-C25-C26
20	B	801	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	L	304	CLA	O1A-CGA-O2A-C1
20	4	301	CLA	CAA-CBA-CGA-O2A
26	N	201	HTG	C2'-C3'-C4'-C5'
20	A	817	CLA	C16-C17-C18-C20
20	A	828	CLA	C16-C17-C18-C20
26	B	851	HTG	C1'-C2'-C3'-C4'
26	F	803	HTG	C4-C5-C6-O6
20	B	837	CLA	O1A-CGA-O2A-C1
20	A	820	CLA	C3-C5-C6-C7
20	B	823	CLA	C10-C11-C12-C13
19	1	301	CHL	CAA-CBA-CGA-O2A
20	4	312	CLA	C10-C11-C12-C13
20	A	806	CLA	C16-C17-C18-C20
19	4	315	CHL	C1C-C2C-CMC-OMC
20	B	835	CLA	O1D-CGD-O2D-CED
20	B	811	CLA	O1A-CGA-O2A-C1
20	B	811	CLA	CBA-CGA-O2A-C1
20	B	837	CLA	CBA-CGA-O2A-C1
20	2	312	CLA	C2A-CAA-CBA-CGA
20	3	311	CLA	C2A-CAA-CBA-CGA
20	4	313	CLA	C2A-CAA-CBA-CGA
20	B	805	CLA	C2A-CAA-CBA-CGA
20	1	302	CLA	C16-C17-C18-C20
20	B	824	CLA	C16-C17-C18-C20
20	H	201	CLA	C4-C3-C5-C6
20	A	810	CLA	C10-C11-C12-C13
20	3	301	CLA	C6-C7-C8-C9
20	A	824	CLA	C11-C10-C8-C9
20	A	831	CLA	C14-C13-C15-C16
20	A	838	CLA	C6-C7-C8-C9
20	B	836	CLA	CBA-CGA-O2A-C1
20	B	828	CLA	C5-C6-C7-C8
20	A	853	CLA	C4B-C3B-CAB-CBB
20	3	301	CLA	C11-C12-C13-C14
20	B	823	CLA	C11-C12-C13-C15
20	1	313	CLA	C4-C3-C5-C6
24	A	843	LHG	C13-C14-C15-C16
20	A	817	CLA	CAA-CBA-CGA-O2A
24	A	843	LHG	C26-C27-C28-C29
20	1	307	CLA	C11-C12-C13-C15
20	A	809	CLA	C6-C7-C8-C10
20	B	803	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	838	CLA	C6-C7-C8-C10
20	B	807	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	CAA-CBA-CGA-O2A
20	2	311	CLA	O1A-CGA-O2A-C1
20	B	836	CLA	O1A-CGA-O2A-C1
19	2	307	CHL	C3A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	825	CLA	C3A-C2A-CAA-CBA
20	A	839	CLA	C2-C3-C5-C6
20	K	201	CLA	C2A-CAA-CBA-CGA
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C16-C17-C18-C36
23	B	842	BCR	C11-C10-C9-C34
23	B	843	BCR	C11-C10-C9-C34
23	B	843	BCR	C20-C21-C22-C37
23	F	806	BCR	C35-C13-C14-C15
23	L	301	BCR	C11-C10-C9-C34
20	A	817	CLA	C10-C11-C12-C13
20	A	833	CLA	C13-C15-C16-C17
20	O	203	CLA	C10-C11-C12-C13
20	4	311	CLA	C2-C1-O2A-CGA
22	1	316	XAT	C33-C34-C35-C15
20	B	812	CLA	C5-C6-C7-C8
24	A	843	LHG	C29-C30-C31-C32
20	4	302	CLA	C10-C11-C12-C13
20	3	307	CLA	C2A-CAA-CBA-CGA
20	F	804	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBA-CGA-O2A-C1
20	A	840	CLA	CBA-CGA-O2A-C1
20	1	307	CLA	C11-C12-C13-C14
20	1	312	CLA	C11-C10-C8-C9
20	A	841	CLA	C11-C10-C8-C9
20	B	817	CLA	C11-C12-C13-C14
20	B	819	CLA	C14-C13-C15-C16
20	B	838	CLA	C6-C7-C8-C9
20	F	802	CLA	C11-C10-C8-C9
20	O	203	CLA	C6-C7-C8-C9
19	1	306	CHL	C1A-C2A-CAA-CBA
19	4	306	CHL	C1A-C2A-CAA-CBA
20	A	828	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	852	HTG	S1-C1'-C2'-C3'
20	A	807	CLA	C3-C5-C6-C7
20	A	811	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C2A-CAA-CBA-CGA
20	B	807	CLA	O1A-CGA-O2A-C1
20	2	309	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	B	801	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	L	303	CLA	C1A-C2A-CAA-CBA
20	N	203	CLA	C1A-C2A-CAA-CBA
23	A	849	BCR	C11-C10-C9-C8
23	A	849	BCR	C16-C17-C18-C19
23	B	842	BCR	C11-C10-C9-C8
23	B	843	BCR	C11-C10-C9-C8
23	B	843	BCR	C20-C21-C22-C23
23	F	806	BCR	C12-C13-C14-C15
23	L	301	BCR	C11-C10-C9-C8
20	1	307	CLA	C2B-C3B-CAB-CBB
20	1	312	CLA	C2B-C3B-CAB-CBB
20	1	321	CLA	C2B-C3B-CAB-CBB
20	3	302	CLA	C2B-C3B-CAB-CBB
20	3	311	CLA	C2B-C3B-CAB-CBB
20	3	312	CLA	C2B-C3B-CAB-CBB
20	4	301	CLA	C2B-C3B-CAB-CBB
20	4	312	CLA	C2B-C3B-CAB-CBB
20	4	314	CLA	C2B-C3B-CAB-CBB
20	A	817	CLA	C2B-C3B-CAB-CBB
20	A	853	CLA	C2B-C3B-CAB-CBB
20	B	812	CLA	C2B-C3B-CAB-CBB
20	B	831	CLA	C2B-C3B-CAB-CBB
20	B	833	CLA	C2B-C3B-CAB-CBB
20	F	805	CLA	C2B-C3B-CAB-CBB
20	G	604	CLA	C2B-C3B-CAB-CBB
20	J	103	CLA	C2B-C3B-CAB-CBB
21	1	315	LUT	C1-C6-C7-C8
21	1	319	LUT	C5-C6-C7-C8
21	3	315	LUT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	317	BCR	C23-C24-C25-C30
23	3	317	BCR	C1-C6-C7-C8
23	4	318	BCR	C23-C24-C25-C26
23	A	845	BCR	C1-C6-C7-C8
23	A	845	BCR	C23-C24-C25-C26
23	B	842	BCR	C5-C6-C7-C8
23	B	846	BCR	C1-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C30
20	B	804	CLA	CAA-CBA-CGA-O2A
20	A	840	CLA	O1A-CGA-O2A-C1
24	1	318	LHG	C27-C28-C29-C30
20	F	804	CLA	O1D-CGD-O2D-CED
20	1	313	CLA	C2-C3-C5-C6
20	O	202	CLA	CAA-CBA-CGA-O1A
20	A	805	CLA	C11-C10-C8-C7
20	A	812	CLA	C11-C10-C8-C7
20	A	824	CLA	C11-C10-C8-C7
20	A	824	CLA	C12-C13-C15-C16
20	A	826	CLA	C11-C12-C13-C15
20	A	827	CLA	C11-C12-C13-C15
20	A	840	CLA	C11-C10-C8-C7
20	F	802	CLA	C6-C7-C8-C10
20	A	841	CLA	CBD-CGD-O2D-CED
20	A	817	CLA	C16-C17-C18-C19
20	1	303	CLA	C2A-CAA-CBA-CGA
20	1	312	CLA	C2A-CAA-CBA-CGA
20	2	309	CLA	C2A-CAA-CBA-CGA
20	A	816	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	1	302	CLA	C16-C17-C18-C19
20	A	801	CLA	C16-C17-C18-C20
20	B	824	CLA	C16-C17-C18-C19
20	1	307	CLA	C12-C13-C15-C16
20	B	821	CLA	C11-C10-C8-C7
20	L	302	CLA	CAA-CBA-CGA-O1A
20	A	816	CLA	C4-C3-C5-C6
20	B	816	CLA	C4-C3-C5-C6
20	A	805	CLA	C15-C16-C17-C18
20	A	831	CLA	CBD-CGD-O2D-CED
19	1	301	CHL	O1D-CGD-O2D-CED
20	A	816	CLA	C11-C10-C8-C9
20	A	831	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	802	CLA	C8-C10-C11-C12
20	A	818	CLA	C4-C3-C5-C6
20	B	813	CLA	C4-C3-C5-C6
20	1	307	CLA	C8-C10-C11-C12
20	B	824	CLA	C15-C16-C17-C18
20	B	818	CLA	C2-C3-C5-C6
20	1	303	CLA	C10-C11-C12-C13
20	A	838	CLA	C15-C16-C17-C18
20	B	804	CLA	CAA-CBA-CGA-O1A
20	A	841	CLA	O1D-CGD-O2D-CED
20	1	302	CLA	C2A-CAA-CBA-CGA
20	2	302	CLA	C2A-CAA-CBA-CGA
20	4	302	CLA	C2A-CAA-CBA-CGA
20	A	818	CLA	C2A-CAA-CBA-CGA
20	A	831	CLA	C2A-CAA-CBA-CGA
20	A	839	CLA	C2A-CAA-CBA-CGA
20	N	203	CLA	C2A-CAA-CBA-CGA
20	3	314	CLA	O1A-CGA-O2A-C1
20	A	831	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	CAA-CBA-CGA-O2A
25	1	323	LMG	C22-C23-C24-C25
20	B	802	CLA	C4B-C3B-CAB-CBB
19	2	306	CHL	CHA-CBD-CGD-O1D
19	2	306	CHL	CHA-CBD-CGD-O2D
20	B	809	CLA	C3-C5-C6-C7
20	L	302	CLA	CAA-CBA-CGA-O2A
29	B	847	LMT	C5-C6-C7-C8
20	A	818	CLA	C2-C3-C5-C6
23	B	841	BCR	C7-C8-C9-C10
20	A	808	CLA	C11-C10-C8-C9
20	A	810	CLA	C11-C10-C8-C9
20	A	853	CLA	C11-C10-C8-C9
20	B	802	CLA	C2-C1-O2A-CGA
20	B	828	CLA	C2-C1-O2A-CGA
20	3	301	CLA	C11-C12-C13-C15
20	L	302	CLA	O1D-CGD-O2D-CED
20	3	303	CLA	C3A-C2A-CAA-CBA
20	A	835	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	O	202	CLA	CAA-CBA-CGA-O2A
20	3	307	CLA	CAA-CBA-CGA-O2A
26	B	850	HTG	C1'-C2'-C3'-C4'
20	A	819	CLA	CAA-CBA-CGA-O2A
25	4	319	LMG	C30-C31-C32-C33
20	3	301	CLA	C8-C10-C11-C12
19	4	315	CHL	C3C-C2C-CMC-OMC
20	J	101	CLA	C16-C17-C18-C20
20	A	835	CLA	CAA-CBA-CGA-O2A
20	J	101	CLA	C10-C11-C12-C13
20	2	303	CLA	C2A-CAA-CBA-CGA
20	B	825	CLA	C13-C15-C16-C17
20	B	814	CLA	C8-C10-C11-C12
24	1	318	LHG	C4-C5-C6-O8
20	B	817	CLA	C10-C11-C12-C13
20	1	311	CLA	CAA-CBA-CGA-O2A
20	A	819	CLA	CAA-CBA-CGA-O1A
20	F	802	CLA	C3-C5-C6-C7
20	A	829	CLA	C15-C16-C17-C18
24	1	318	LHG	C29-C30-C31-C32
20	A	835	CLA	CAA-CBA-CGA-O1A
20	1	308	CLA	C11-C10-C8-C9
20	A	820	CLA	C11-C12-C13-C14
20	L	303	CLA	C11-C12-C13-C14
20	1	309	CLA	O1A-CGA-O2A-C1
23	F	801	BCR	C11-C12-C13-C14
23	J	102	BCR	C17-C18-C19-C20
24	A	844	LHG	O7-C7-C8-C9
20	4	303	CLA	C11-C10-C8-C7
20	A	810	CLA	C11-C10-C8-C7
20	A	812	CLA	C12-C13-C15-C16
20	A	816	CLA	C11-C10-C8-C7
20	A	833	CLA	C11-C12-C13-C15
20	A	841	CLA	C12-C13-C15-C16
20	B	819	CLA	C12-C13-C15-C16
25	1	320	LMG	C36-C37-C38-C39
20	3	304	CLA	C2B-C3B-CAB-CBB
21	1	315	LUT	C5-C6-C7-C8
21	2	315	LUT	C1-C6-C7-C8
23	1	317	BCR	C23-C24-C25-C26
23	3	317	BCR	C5-C6-C7-C8
23	3	317	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	3	317	BCR	C23-C24-C25-C30
23	A	845	BCR	C5-C6-C7-C8
23	A	847	BCR	C23-C24-C25-C26
23	A	847	BCR	C23-C24-C25-C30
23	B	844	BCR	C1-C6-C7-C8
23	B	844	BCR	C5-C6-C7-C8
23	B	846	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C26
23	L	301	BCR	C1-C6-C7-C8
23	L	301	BCR	C5-C6-C7-C8
20	B	806	CLA	CAA-CBA-CGA-O2A
19	2	301	CHL	C2-C1-O2A-CGA
20	2	304	CLA	C2-C1-O2A-CGA
20	3	307	CLA	C2-C1-O2A-CGA
20	A	806	CLA	C2-C1-O2A-CGA
20	A	851	CLA	C2-C1-O2A-CGA
20	L	302	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	C2-C3-C5-C6
20	H	201	CLA	C2-C3-C5-C6
20	A	836	CLA	C2A-CAA-CBA-CGA
24	A	843	LHG	C10-C11-C12-C13
20	1	308	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	C4-C3-C5-C6
20	A	805	CLA	CAA-CBA-CGA-O2A
20	B	817	CLA	C13-C15-C16-C17
20	A	821	CLA	O1A-CGA-O2A-C1
20	B	802	CLA	C5-C6-C7-C8
20	A	802	CLA	C14-C13-C15-C16
20	A	812	CLA	C11-C10-C8-C9
20	B	815	CLA	C6-C7-C8-C9
20	F	802	CLA	C6-C7-C8-C9
23	F	801	BCR	C11-C12-C13-C35
20	2	303	CLA	CAA-CBA-CGA-O2A
20	A	834	CLA	CAA-CBA-CGA-O2A
20	1	307	CLA	C1A-C2A-CAA-CBA
20	2	312	CLA	C4B-C3B-CAB-CBB
20	4	309	CLA	C1A-C2A-CAA-CBA
20	4	314	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C1A-C2A-CAA-CBA
20	B	822	CLA	C3-C5-C6-C7
20	3	302	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	808	CLA	CAA-CBA-CGA-O2A
23	B	841	BCR	C17-C18-C19-C20
20	A	816	CLA	C5-C6-C7-C8
24	1	318	LHG	C24-C25-C26-C27
20	A	824	CLA	CAA-CBA-CGA-O2A
20	A	841	CLA	CAA-CBA-CGA-O2A
20	B	821	CLA	CAA-CBA-CGA-O2A
25	1	320	LMG	C34-C35-C36-C37
20	B	803	CLA	C15-C16-C17-C18
20	B	828	CLA	CAA-CBA-CGA-O2A
20	A	822	CLA	C2-C3-C5-C6
19	1	301	CHL	CBD-CGD-O2D-CED
19	4	306	CHL	C2-C1-O2A-CGA
20	A	810	CLA	C2-C1-O2A-CGA
20	A	811	CLA	C2-C1-O2A-CGA
20	B	806	CLA	C2-C1-O2A-CGA
20	B	817	CLA	C2-C1-O2A-CGA
20	B	839	CLA	C2-C1-O2A-CGA
20	O	201	CLA	C2-C1-O2A-CGA
20	4	311	CLA	CAA-CBA-CGA-O2A
20	N	202	CLA	CAA-CBA-CGA-O2A
20	1	303	CLA	C6-C7-C8-C10
20	A	810	CLA	C12-C13-C15-C16
20	A	837	CLA	C11-C10-C8-C7
20	B	813	CLA	C11-C12-C13-C15
20	B	836	CLA	C11-C12-C13-C15
20	B	836	CLA	C12-C13-C15-C16
20	B	823	CLA	C5-C6-C7-C8
20	B	833	CLA	C16-C17-C18-C20
20	1	309	CLA	CBA-CGA-O2A-C1
20	O	203	CLA	C2A-CAA-CBA-CGA
20	1	308	CLA	C8-C10-C11-C12
20	A	820	CLA	C16-C17-C18-C20
20	B	806	CLA	C16-C17-C18-C20
20	G	604	CLA	CBA-CGA-O2A-C1
20	1	313	CLA	C3A-C2A-CAA-CBA
20	4	314	CLA	C3A-C2A-CAA-CBA
20	A	810	CLA	C3A-C2A-CAA-CBA
20	B	801	CLA	C3A-C2A-CAA-CBA
20	B	822	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	N	202	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	B	806	CLA	CAA-CBA-CGA-O1A
20	A	821	CLA	CBA-CGA-O2A-C1
20	A	829	CLA	C5-C6-C7-C8
20	3	308	CLA	C2A-CAA-CBA-CGA
20	4	309	CLA	C2A-CAA-CBA-CGA
20	A	802	CLA	C2A-CAA-CBA-CGA
20	A	807	CLA	C14-C13-C15-C16
20	A	826	CLA	C11-C12-C13-C14
20	A	840	CLA	C11-C10-C8-C9
20	B	827	CLA	C11-C12-C13-C14
20	3	305	CLA	CAA-CBA-CGA-O2A
20	A	805	CLA	CAA-CBA-CGA-O1A
20	A	808	CLA	CAA-CBA-CGA-O1A
22	2	316	XAT	C29-C30-C31-C32
20	G	604	CLA	O1A-CGA-O2A-C1
24	A	844	LHG	O9-C7-C8-C9
20	A	816	CLA	C13-C15-C16-C17
30	B	848	DGD	CAA-CBA-CCA-CDA
20	A	833	CLA	O1A-CGA-O2A-C1
20	B	831	CLA	CAA-CBA-CGA-O2A
20	L	307	CLA	CAA-CBA-CGA-O2A
23	K	204	BCR	C7-C8-C9-C10
29	G	601	LMT	C7-C8-C9-C10
20	1	308	CLA	CAA-CBA-CGA-O1A
20	1	311	CLA	CAA-CBA-CGA-O1A
20	2	303	CLA	CAA-CBA-CGA-O1A
20	A	834	CLA	CAA-CBA-CGA-O1A
20	B	821	CLA	CAA-CBA-CGA-O1A
20	B	815	CLA	C8-C10-C11-C12
26	4	320	HTG	C2'-C3'-C4'-C5'
20	B	821	CLA	CBD-CGD-O2D-CED
20	2	302	CLA	C10-C11-C12-C13
20	2	311	CLA	CAA-CBA-CGA-O2A
20	4	311	CLA	CAA-CBA-CGA-O1A
20	A	824	CLA	CAA-CBA-CGA-O1A
26	N	201	HTG	C1'-C2'-C3'-C4'
20	4	309	CLA	C11-C12-C13-C15
20	1	305	CLA	CAD-CBD-CGD-O2D
20	A	801	CLA	CAD-CBD-CGD-O2D
20	A	817	CLA	CAD-CBD-CGD-O2D
20	B	825	CLA	CAD-CBD-CGD-O2D
20	K	201	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4	310	CLA	C2-C1-O2A-CGA
20	A	805	CLA	C2-C1-O2A-CGA
20	A	853	CLA	C2-C1-O2A-CGA
20	B	812	CLA	C2-C1-O2A-CGA
19	4	306	CHL	CAA-CBA-CGA-O2A
27	B	840	PQN	C13-C15-C16-C17
20	B	831	CLA	CAA-CBA-CGA-O1A
20	A	816	CLA	C15-C16-C17-C18
20	A	831	CLA	C13-C15-C16-C17
20	A	833	CLA	CBA-CGA-O2A-C1
20	1	302	CLA	CAA-CBA-CGA-O2A
20	4	314	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	CAA-CBA-CGA-O1A
20	2	308	CLA	CAA-CBA-CGA-O2A
20	K	202	CLA	CAA-CBA-CGA-O2A
20	3	302	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

186 monomers are involved in 478 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	843	LHG	2	0
20	A	851	CLA	5	0
21	1	319	LUT	4	0
20	2	312	CLA	2	0
20	B	838	CLA	2	0
20	1	311	CLA	1	0
20	A	809	CLA	3	0
20	B	817	CLA	6	0
20	B	824	CLA	7	0
20	A	806	CLA	3	0
20	B	828	CLA	4	0
21	2	315	LUT	2	0
20	B	809	CLA	1	0
19	4	315	CHL	5	0
20	A	812	CLA	6	0
20	B	802	CLA	4	0
20	K	201	CLA	2	0
20	A	836	CLA	3	0
19	4	305	CHL	4	0
20	L	302	CLA	3	0
20	3	314	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	805	CLA	3	0
20	3	308	CLA	2	0
20	O	203	CLA	6	0
20	2	308	CLA	5	0
20	B	839	CLA	2	0
21	O	205	LUT	5	0
19	2	307	CHL	4	0
20	3	311	CLA	4	0
20	1	307	CLA	2	0
23	B	841	BCR	7	0
20	N	203	CLA	2	0
23	4	318	BCR	5	0
23	K	204	BCR	4	0
20	1	312	CLA	4	0
20	A	835	CLA	1	0
20	A	833	CLA	4	0
26	N	201	HTG	1	0
23	L	301	BCR	2	0
20	1	302	CLA	2	0
20	B	832	CLA	4	0
25	4	319	LMG	3	0
22	2	316	XAT	2	0
23	A	848	BCR	4	0
20	A	803	CLA	2	0
27	B	840	PQN	1	0
20	A	824	CLA	3	0
19	4	306	CHL	3	0
20	B	833	CLA	1	0
20	A	831	CLA	5	0
20	B	813	CLA	5	0
22	1	316	XAT	2	0
20	4	301	CLA	3	0
20	A	853	CLA	5	0
23	B	844	BCR	3	0
23	A	845	BCR	2	0
20	B	814	CLA	1	0
20	A	807	CLA	3	0
20	B	834	CLA	2	0
26	1	322	HTG	2	0
20	A	822	CLA	3	0
20	K	202	CLA	2	0
20	A	810	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	821	CLA	3	0
20	B	808	CLA	3	0
20	A	801	CLA	7	0
20	A	825	CLA	6	0
20	2	310	CLA	3	0
20	A	814	CLA	1	0
23	B	842	BCR	1	0
20	4	312	CLA	5	0
23	A	846	BCR	1	0
20	1	321	CLA	4	0
20	A	811	CLA	5	0
20	B	831	CLA	5	0
19	2	301	CHL	8	0
20	4	313	CLA	2	0
23	A	847	BCR	2	0
20	3	301	CLA	1	0
26	B	850	HTG	1	0
23	J	102	BCR	8	0
20	2	309	CLA	2	0
25	1	323	LMG	2	0
20	B	830	CLA	2	0
20	1	313	CLA	4	0
20	4	314	CLA	2	0
20	K	203	CLA	2	0
20	B	815	CLA	1	0
20	4	308	CLA	7	0
20	A	805	CLA	5	0
19	4	307	CHL	1	0
23	2	317	BCR	6	0
20	B	810	CLA	3	0
23	L	305	BCR	4	0
20	H	201	CLA	3	0
20	4	303	CLA	7	0
23	I	101	BCR	6	0
20	B	805	CLA	6	0
20	B	826	CLA	1	0
23	B	843	BCR	3	0
20	J	103	CLA	1	0
20	1	304	CLA	1	0
24	B	849	LHG	2	0
20	B	835	CLA	2	0
22	4	317	XAT	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	826	CLA	6	0
27	A	842	PQN	3	0
20	2	311	CLA	2	0
24	1	318	LHG	7	0
20	A	817	CLA	4	0
22	3	316	XAT	4	0
25	1	320	LMG	3	0
23	A	849	BCR	4	0
20	B	816	CLA	1	0
20	B	823	CLA	4	0
20	1	303	CLA	4	0
20	B	829	CLA	1	0
20	A	838	CLA	4	0
20	F	802	CLA	4	0
20	A	834	CLA	3	0
20	L	303	CLA	4	0
20	A	802	CLA	3	0
20	A	818	CLA	4	0
19	2	306	CHL	9	0
20	3	313	CLA	1	0
20	A	808	CLA	5	0
20	A	827	CLA	3	0
20	4	302	CLA	3	0
23	1	317	BCR	4	0
20	A	839	CLA	1	0
20	K	205	CLA	3	0
23	F	801	BCR	4	0
24	2	318	LHG	1	0
20	3	310	CLA	2	0
20	4	309	CLA	2	0
20	O	201	CLA	2	0
20	2	304	CLA	2	0
20	3	309	CLA	7	0
19	2	305	CHL	5	0
20	B	827	CLA	4	0
20	3	307	CLA	5	0
20	A	820	CLA	2	0
23	B	845	BCR	6	0
20	B	819	CLA	1	0
21	O	204	LUT	3	0
24	A	844	LHG	1	0
20	J	101	CLA	1	0

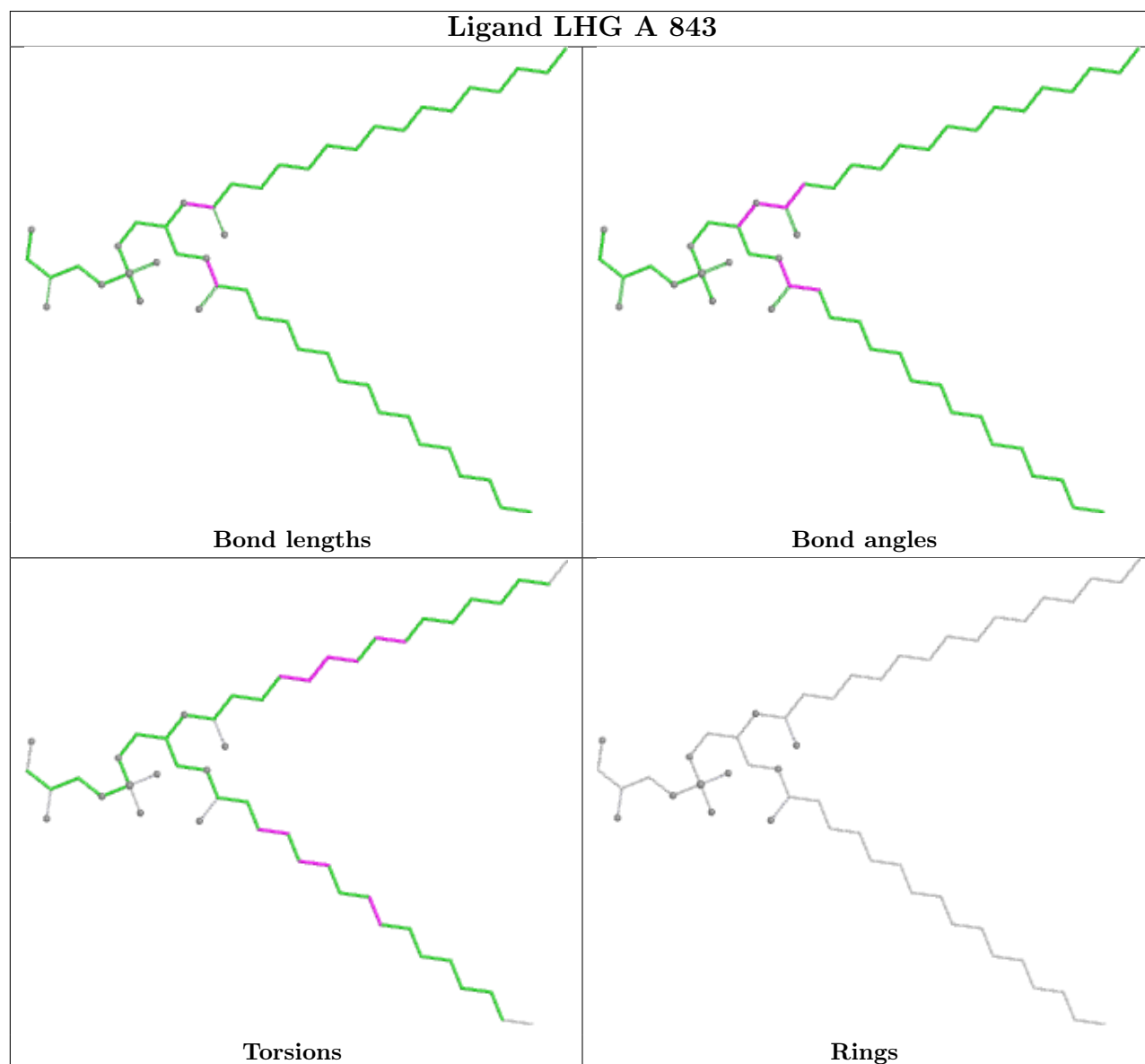
Continued on next page...

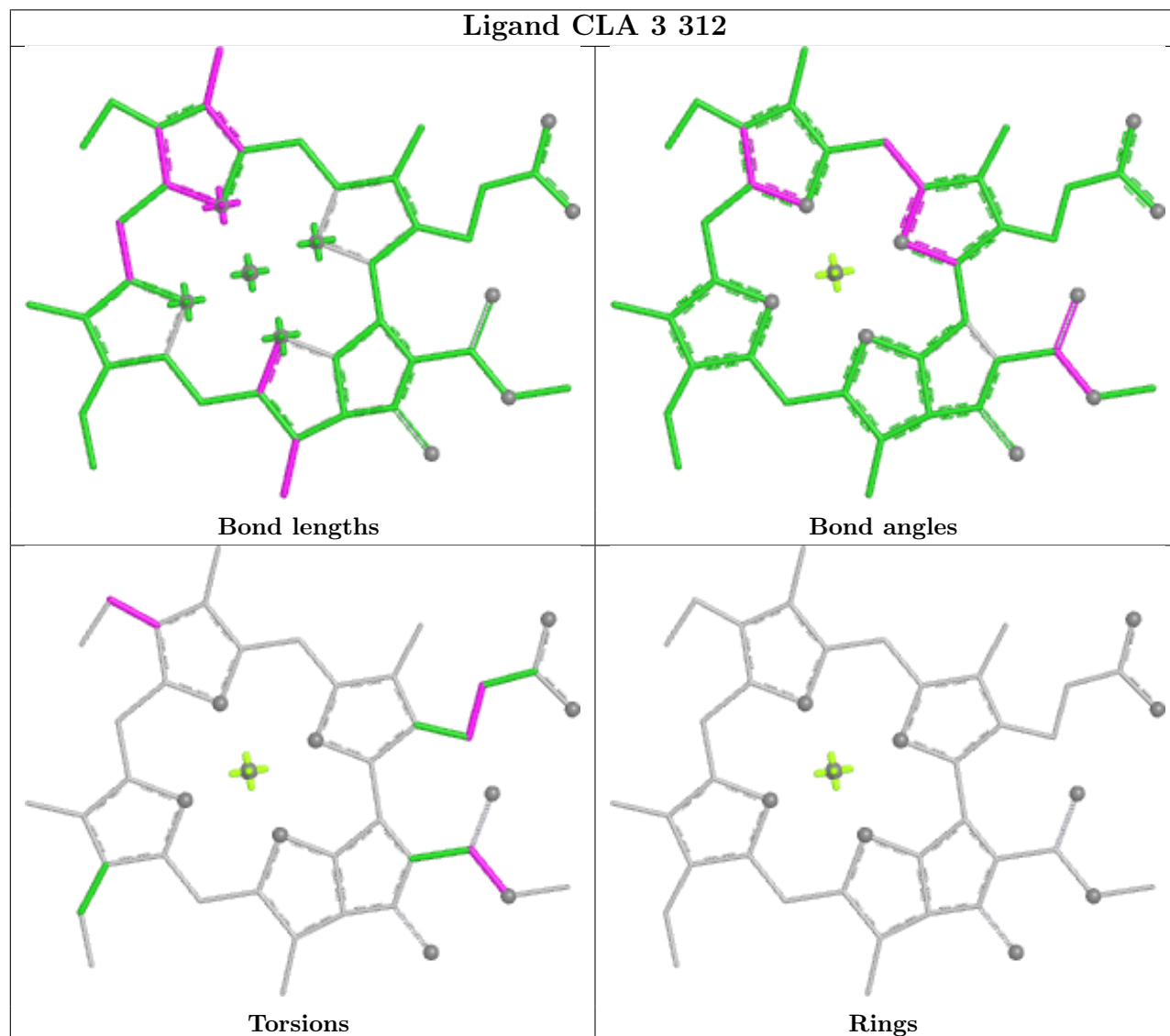
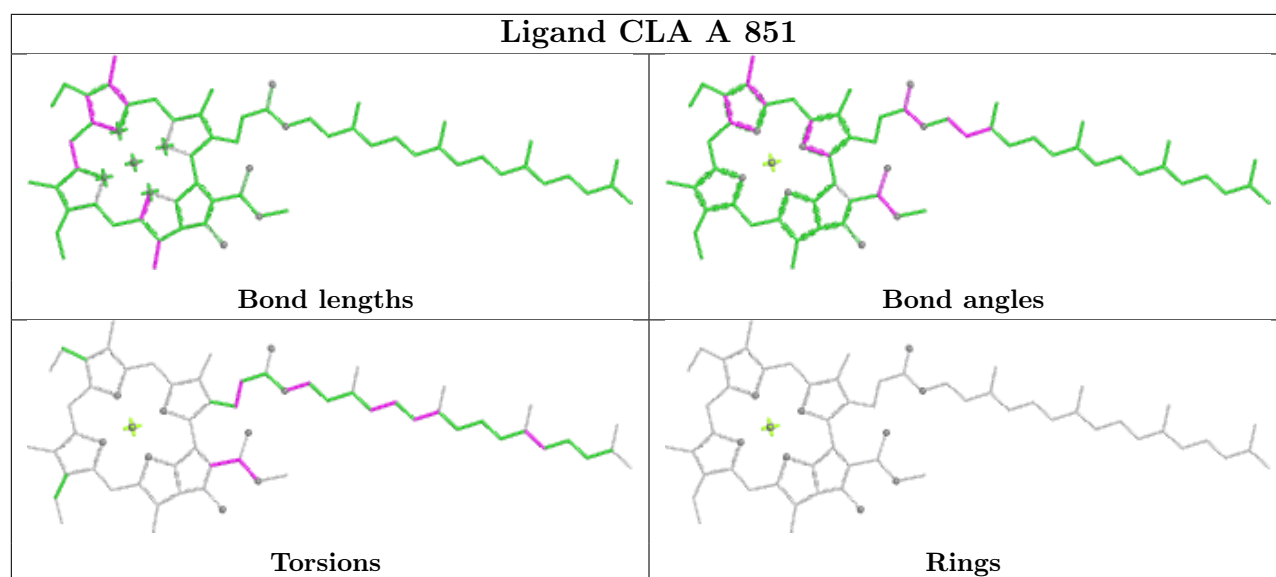
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	309	CLA	2	0
20	1	308	CLA	4	0
20	A	828	CLA	2	0
20	A	837	CLA	3	0
20	B	803	CLA	4	0
20	B	804	CLA	1	0
20	B	825	CLA	4	0
19	1	301	CHL	2	0
20	2	302	CLA	1	0
19	2	314	CHL	1	0
20	A	816	CLA	2	0
20	A	841	CLA	3	0
23	B	846	BCR	3	0
20	B	806	CLA	2	0
23	J	104	BCR	2	0
23	L	306	BCR	3	0
21	3	315	LUT	4	0
20	B	801	CLA	3	0
23	F	806	BCR	3	0
20	B	836	CLA	1	0
19	3	306	CHL	3	0
30	B	848	DGD	2	0
23	A	854	BCR	6	0
23	G	606	BCR	3	0
20	4	311	CLA	2	0
21	1	315	LUT	4	0
26	F	807	HTG	1	0
19	1	306	CHL	2	0
20	B	818	CLA	3	0
20	A	823	CLA	4	0
20	B	812	CLA	3	0
20	B	807	CLA	2	0
20	A	840	CLA	1	0
20	B	822	CLA	2	0
21	4	316	LUT	5	0
23	3	317	BCR	3	0
20	O	202	CLA	6	0
20	A	804	CLA	4	0
20	4	304	CLA	2	0

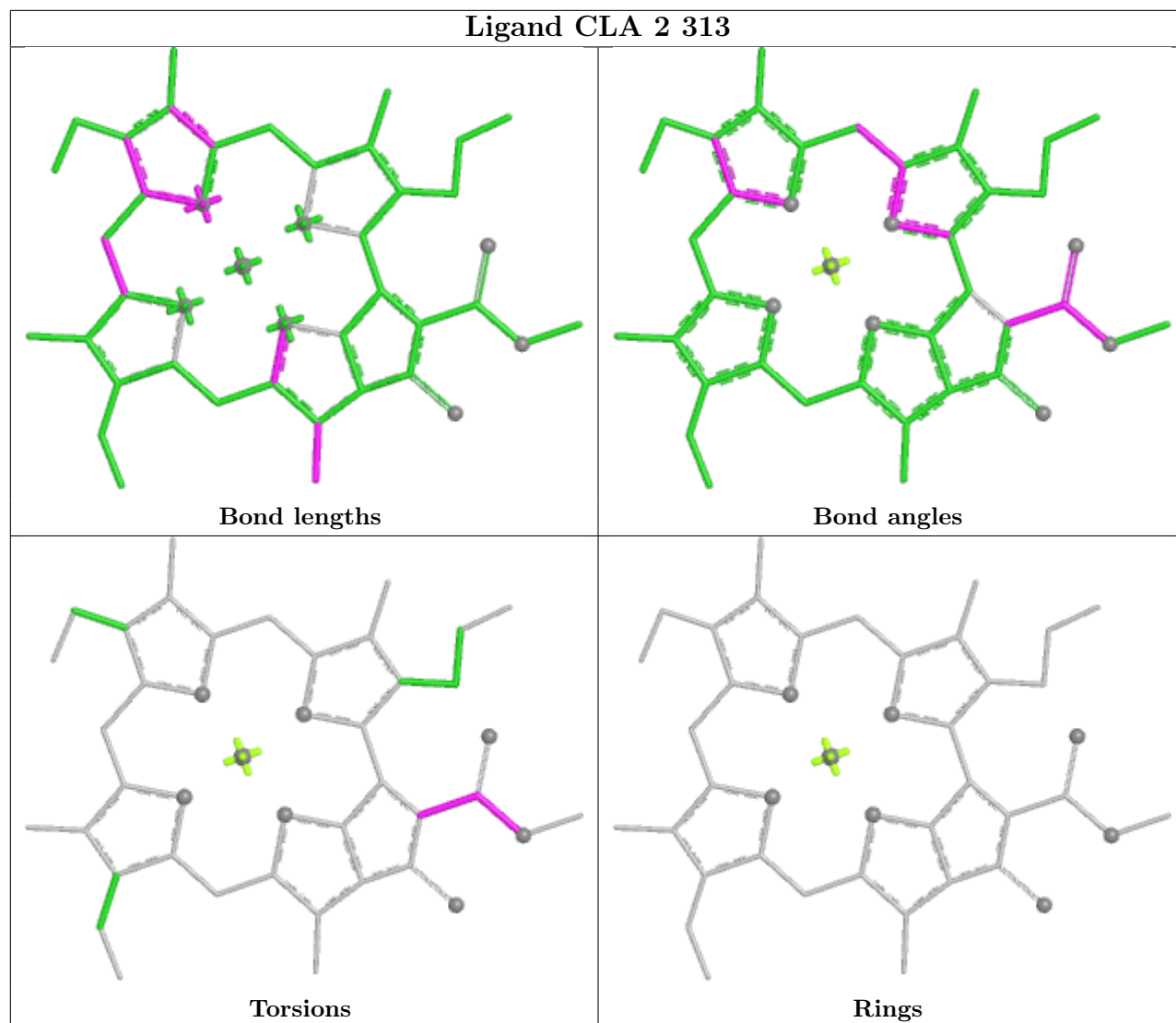
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

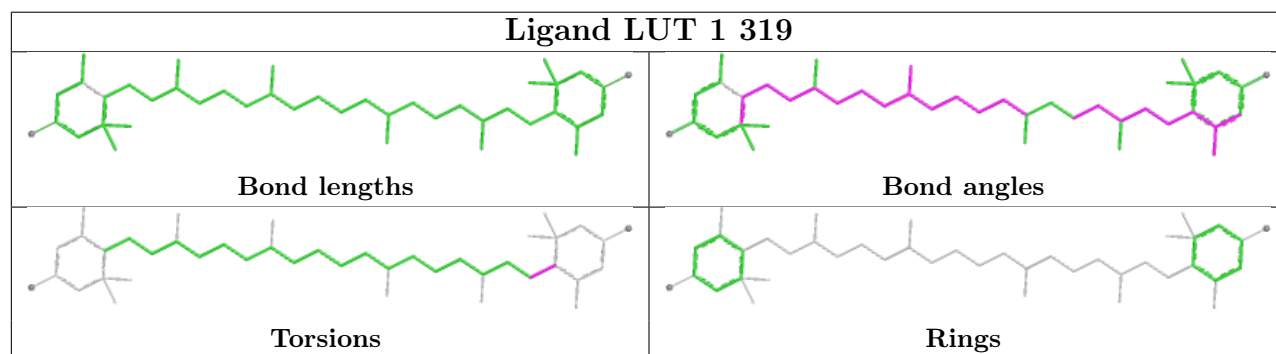




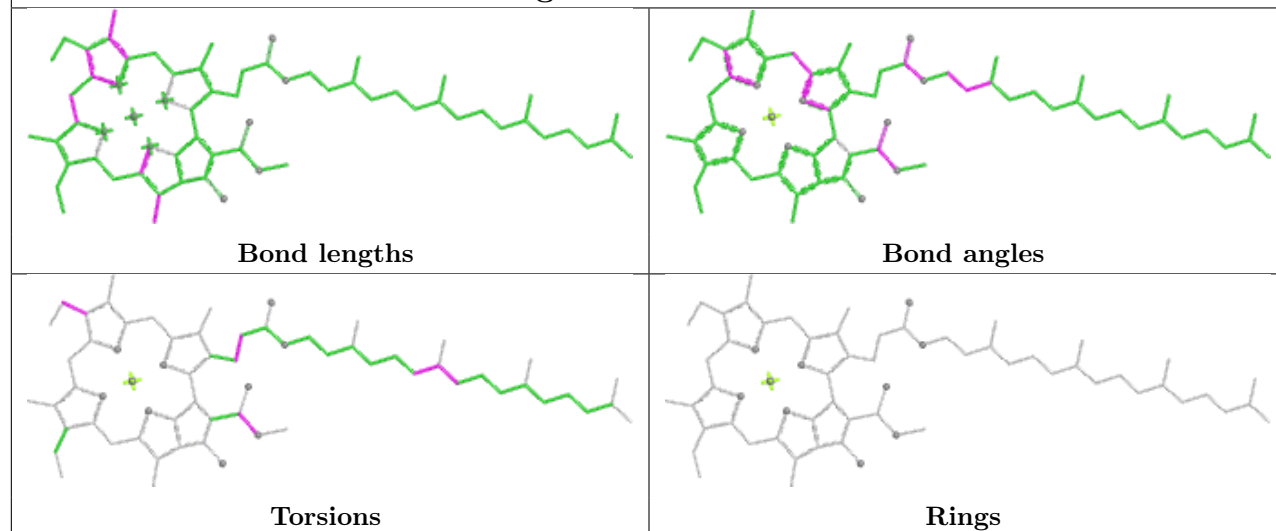
Ligand CLA 2 313



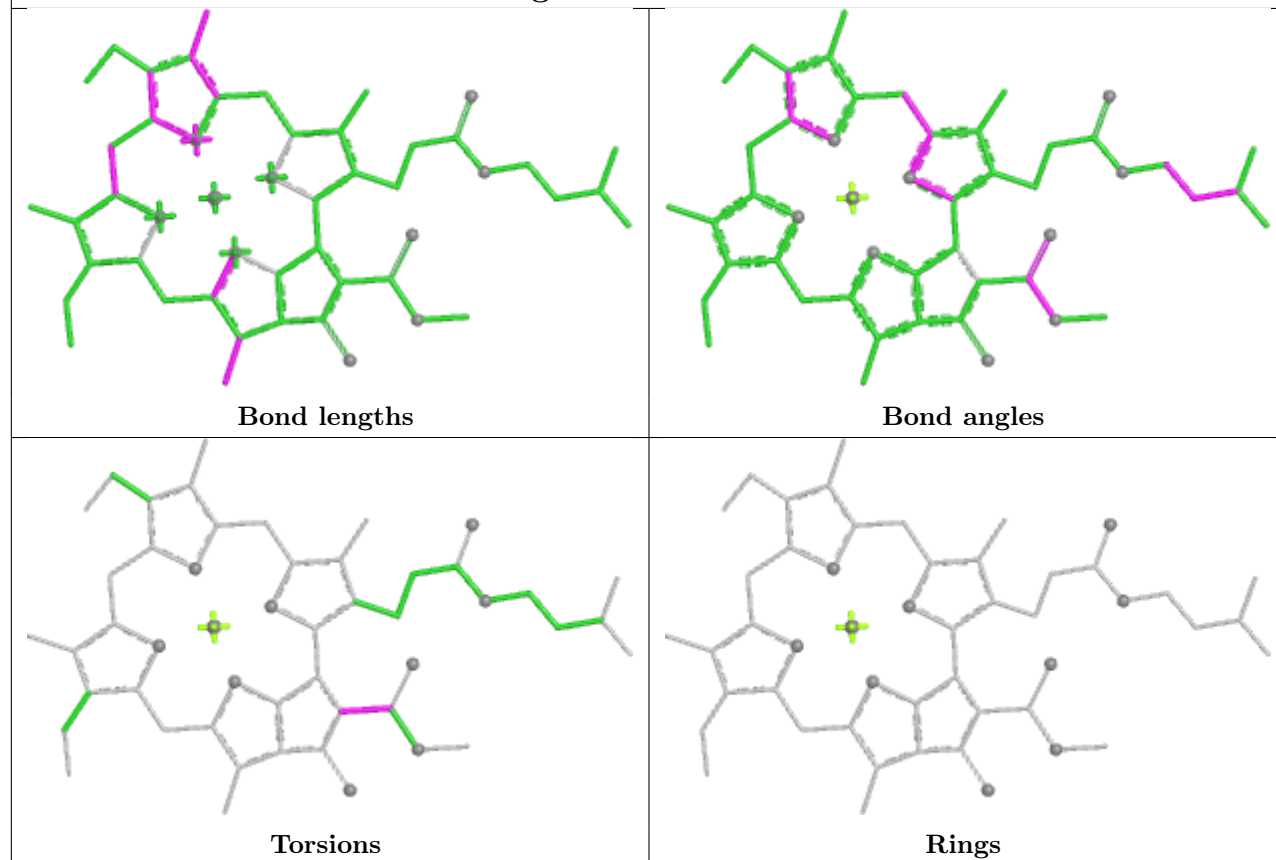
Ligand LUT 1 319



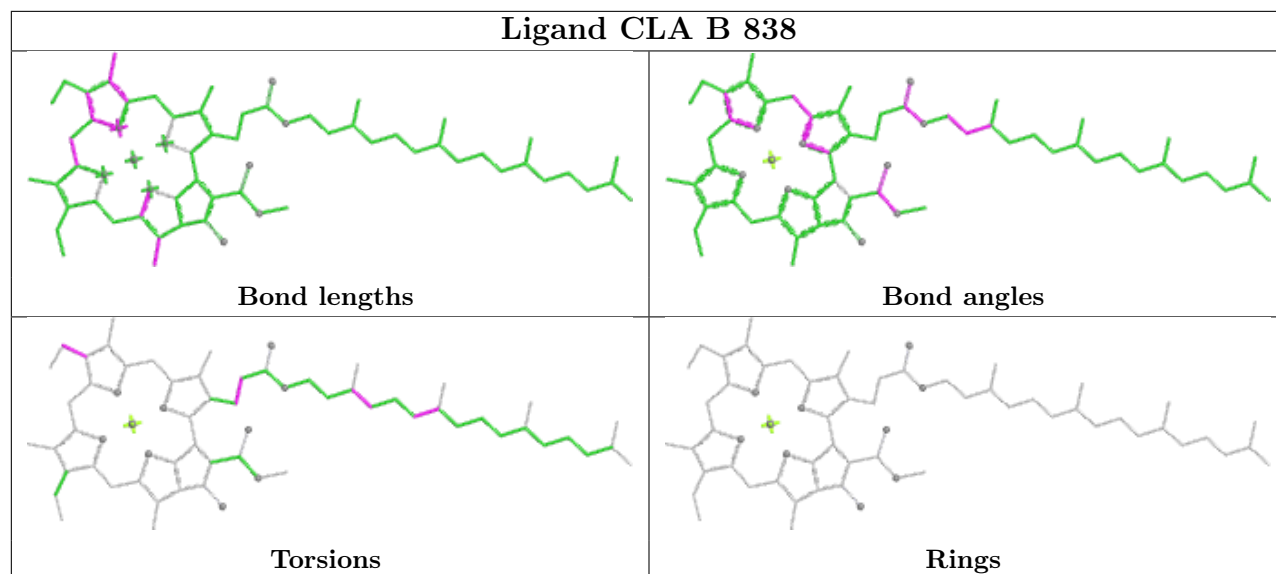
Ligand CLA 2 312



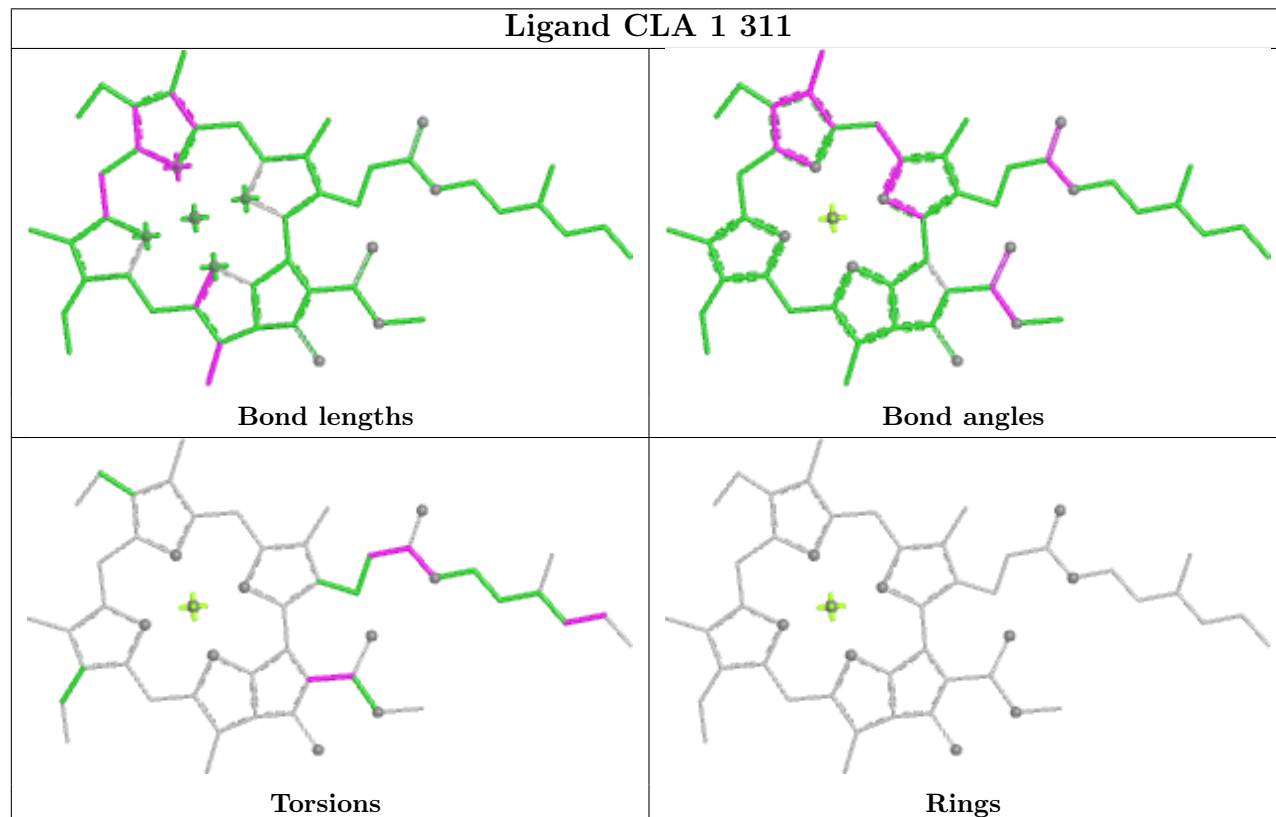
Ligand CLA A 830

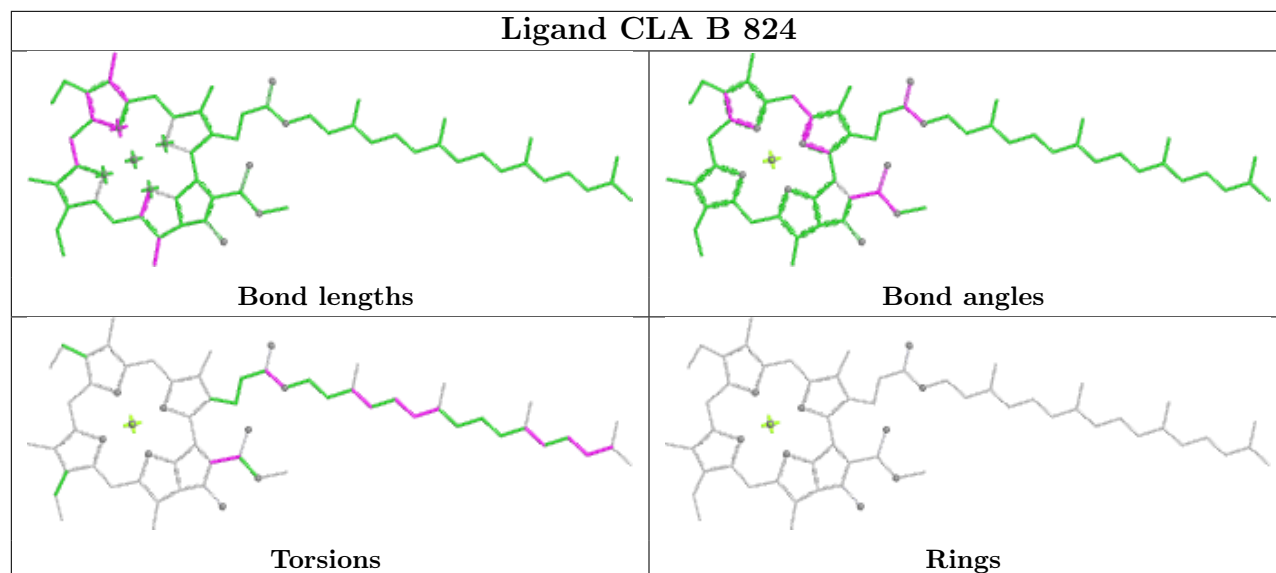
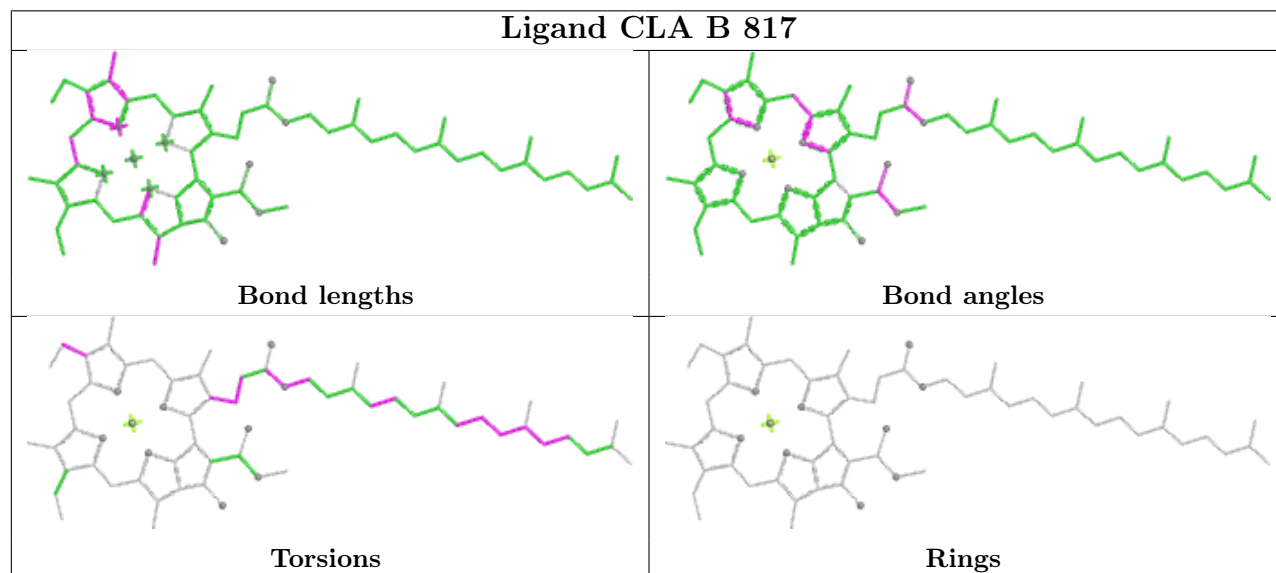
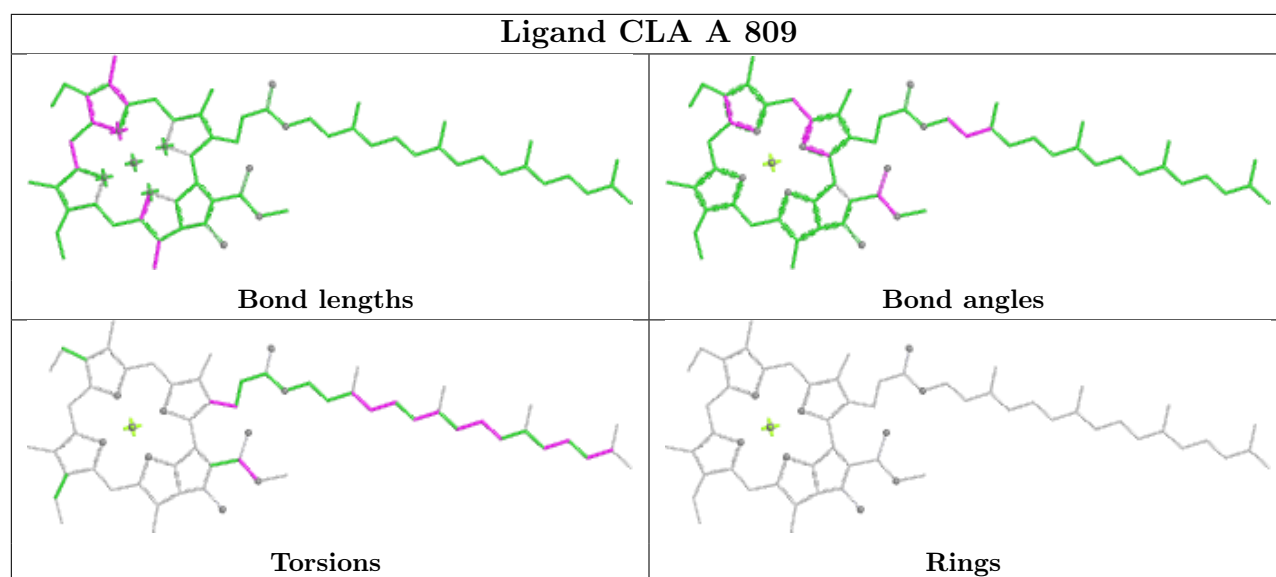


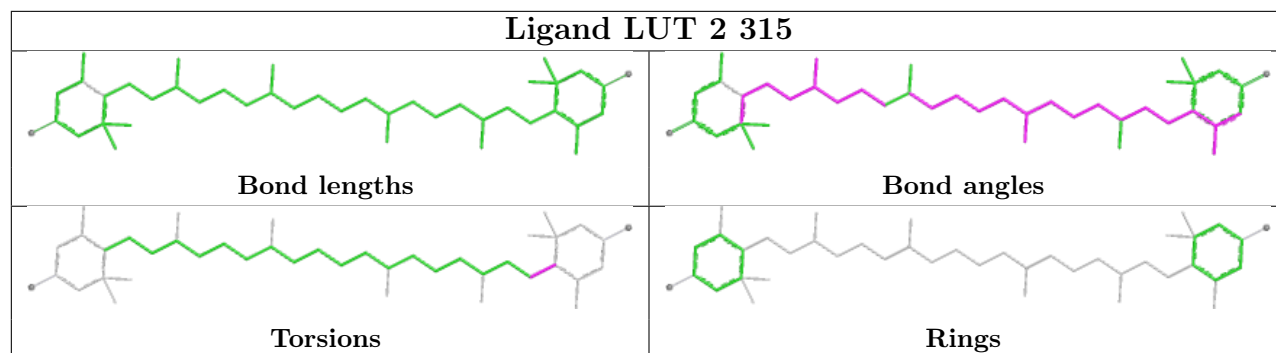
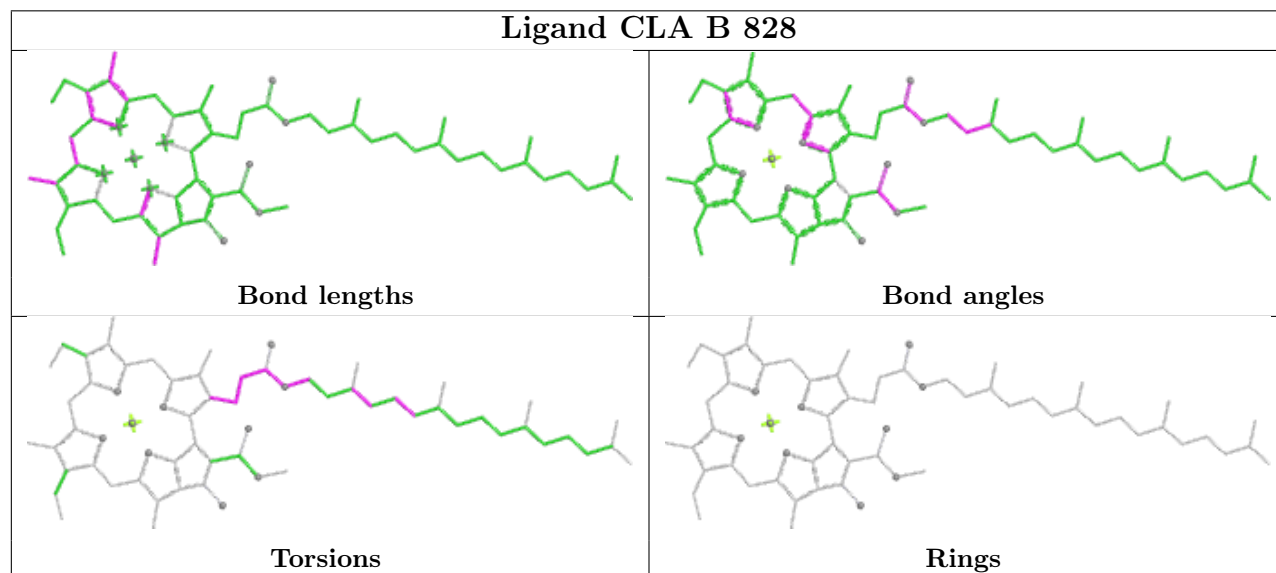
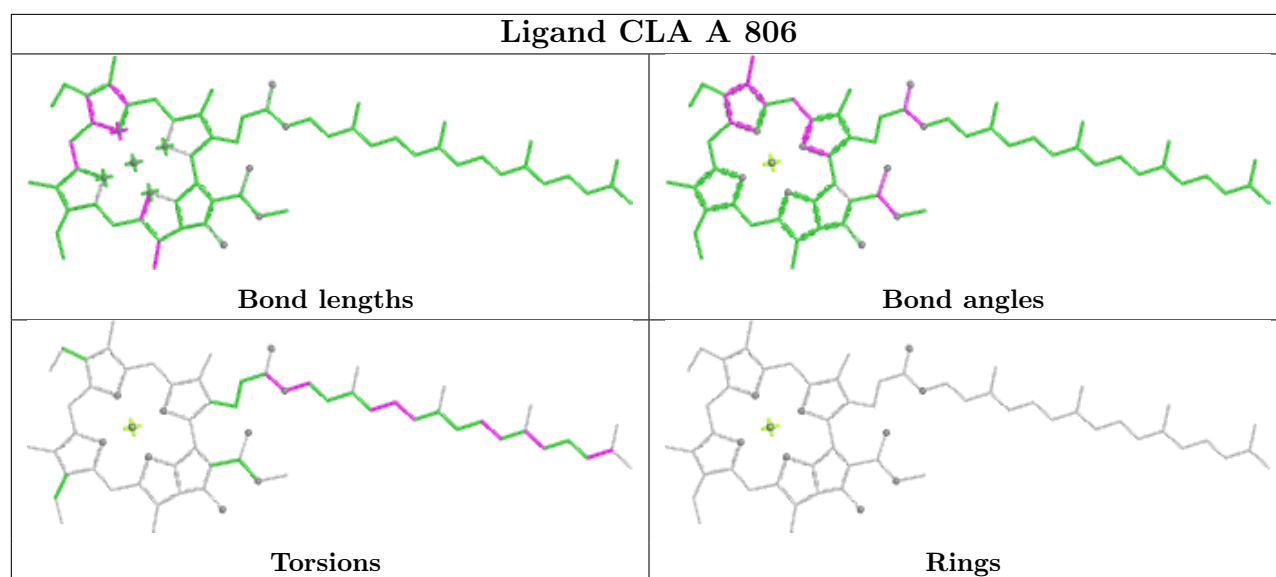
Ligand CLA B 838



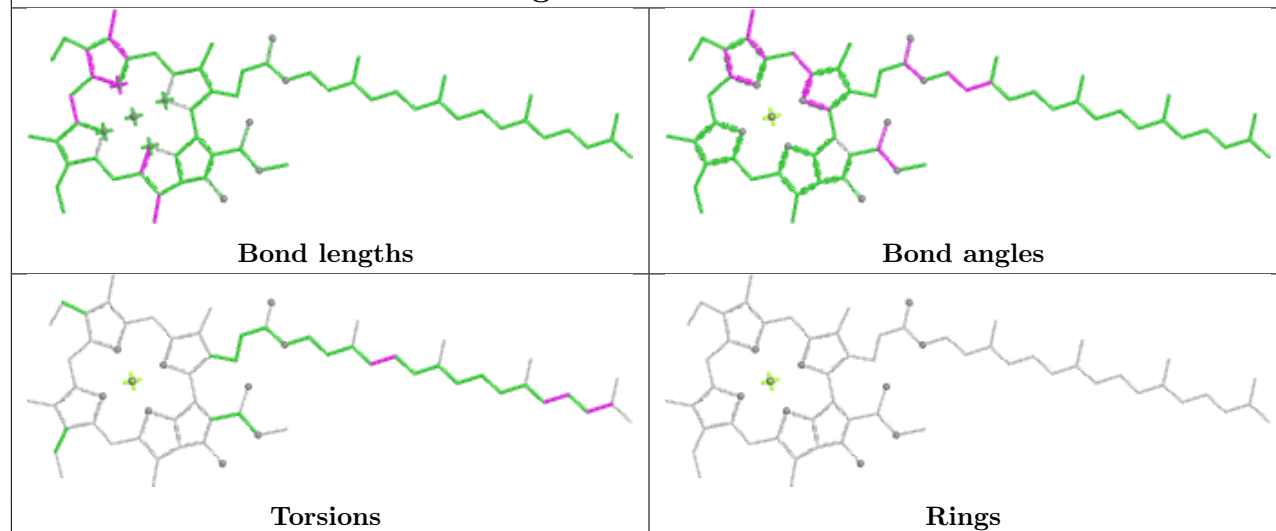
Ligand CLA 1 311



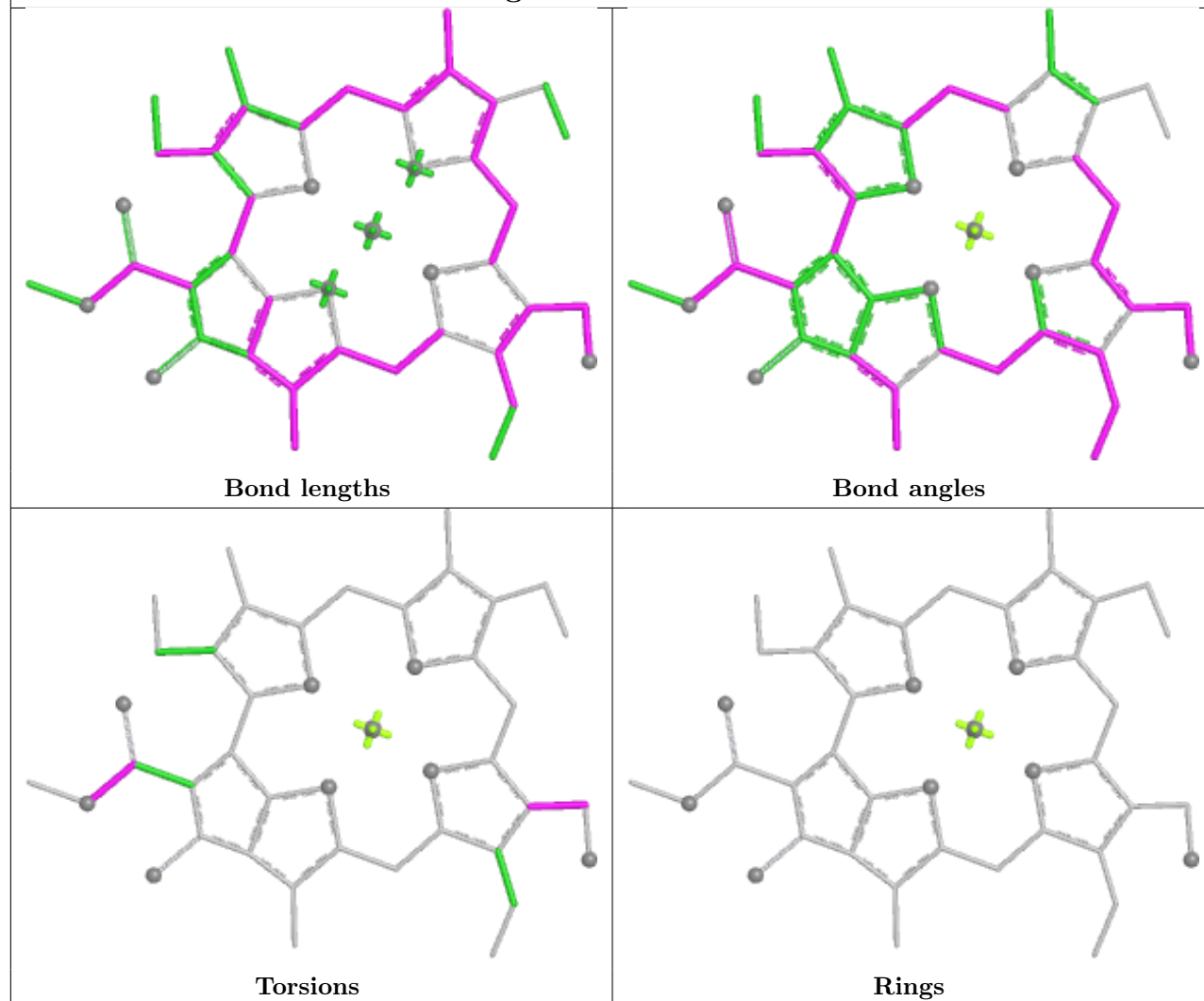


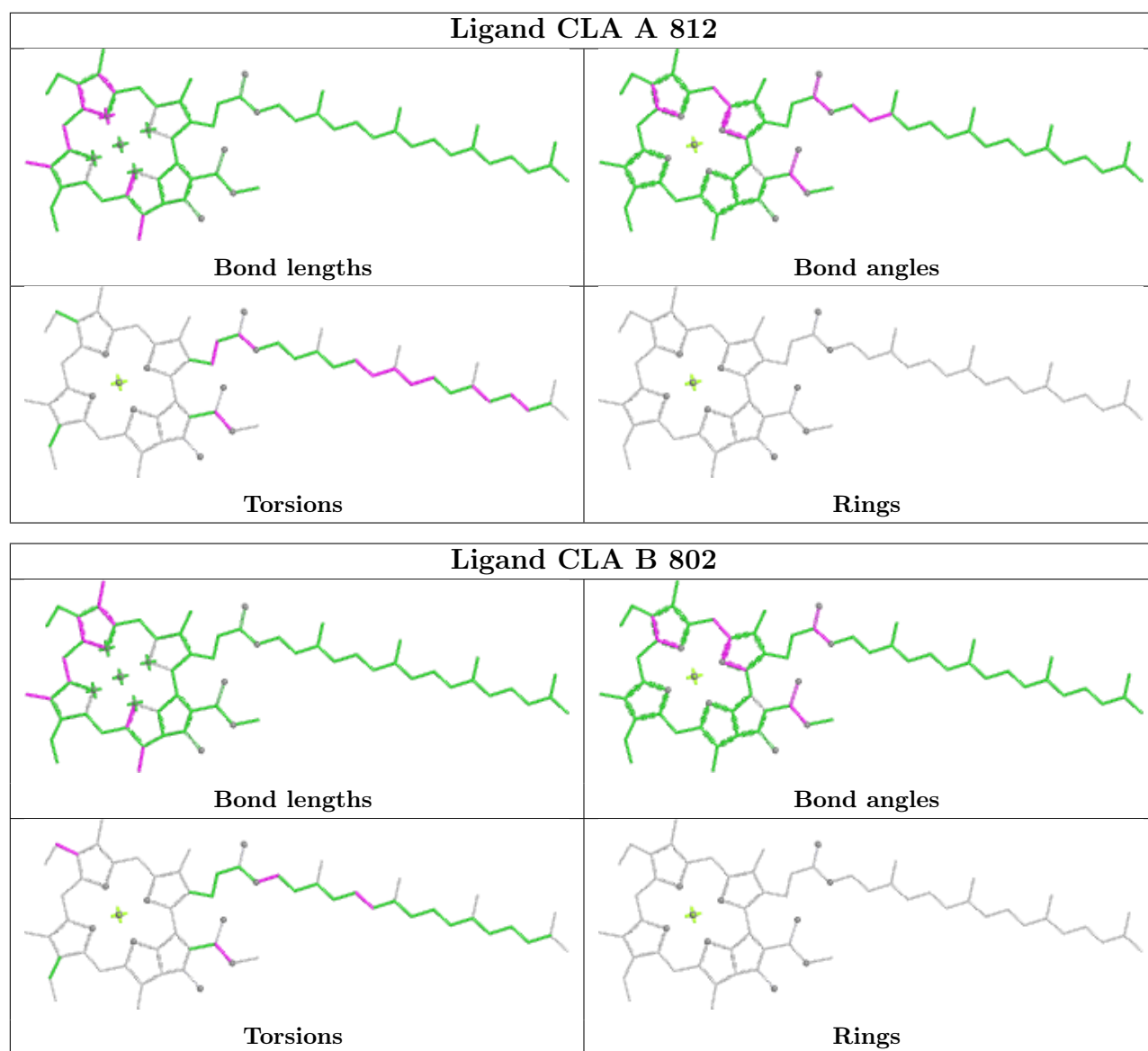


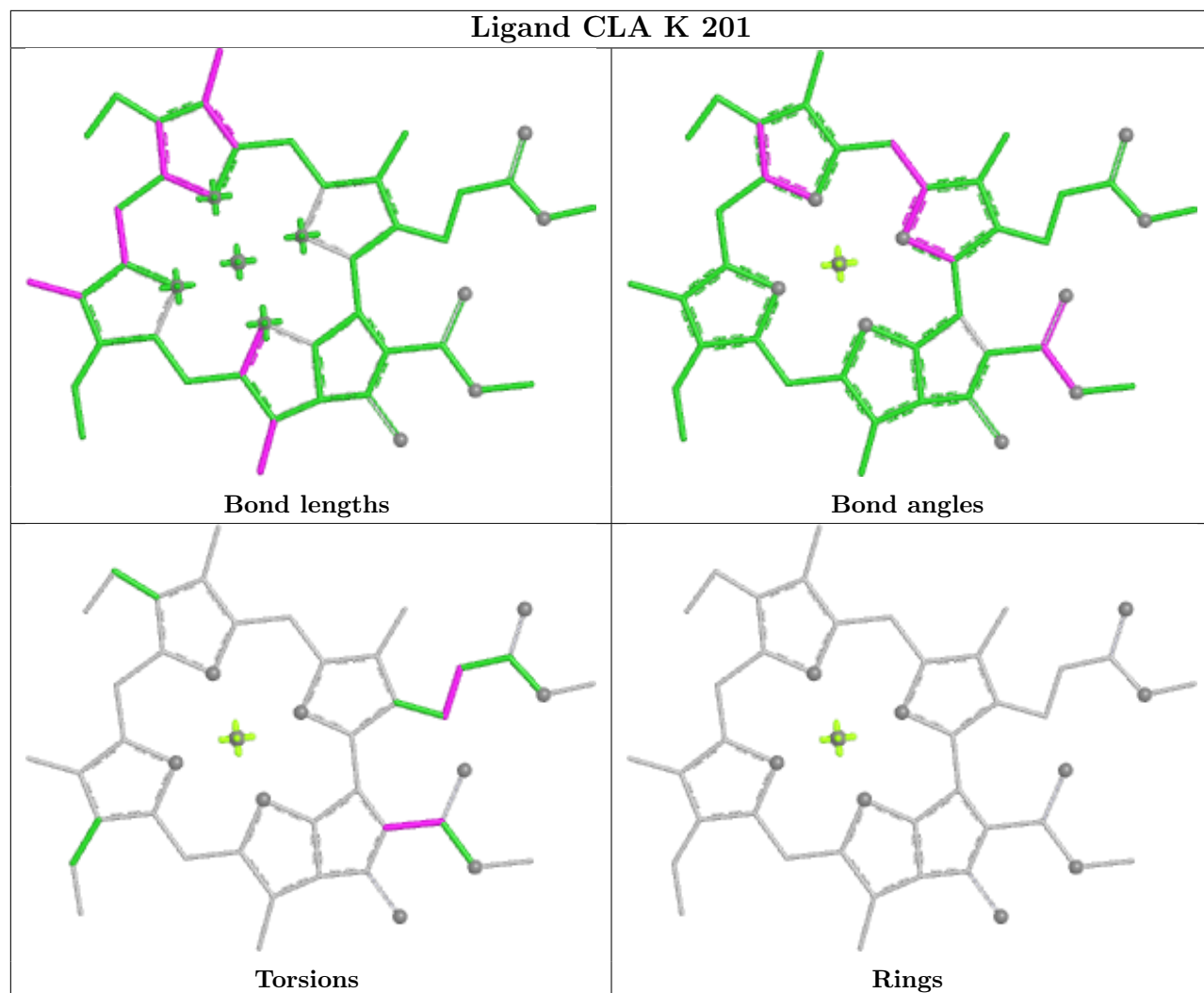
Ligand CLA B 809



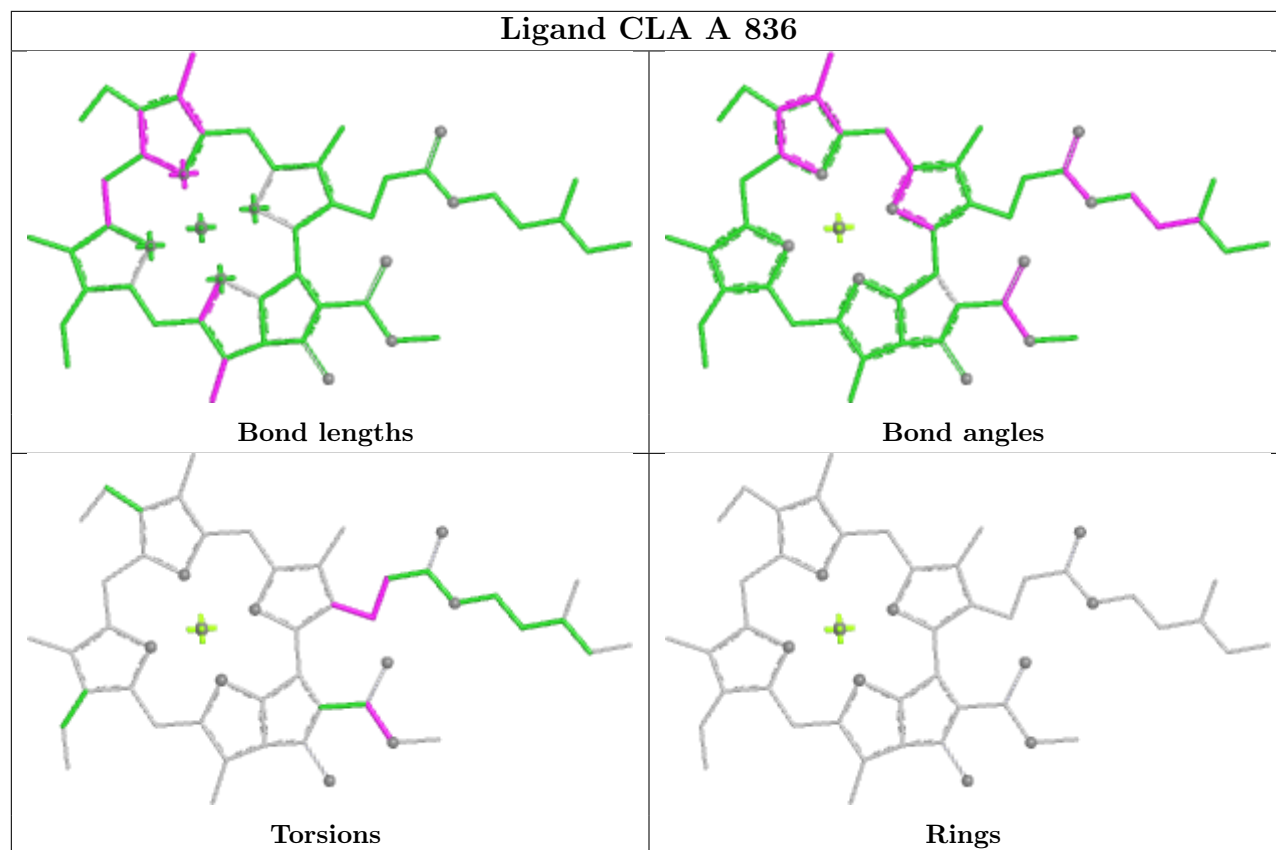
Ligand CHL 4 315



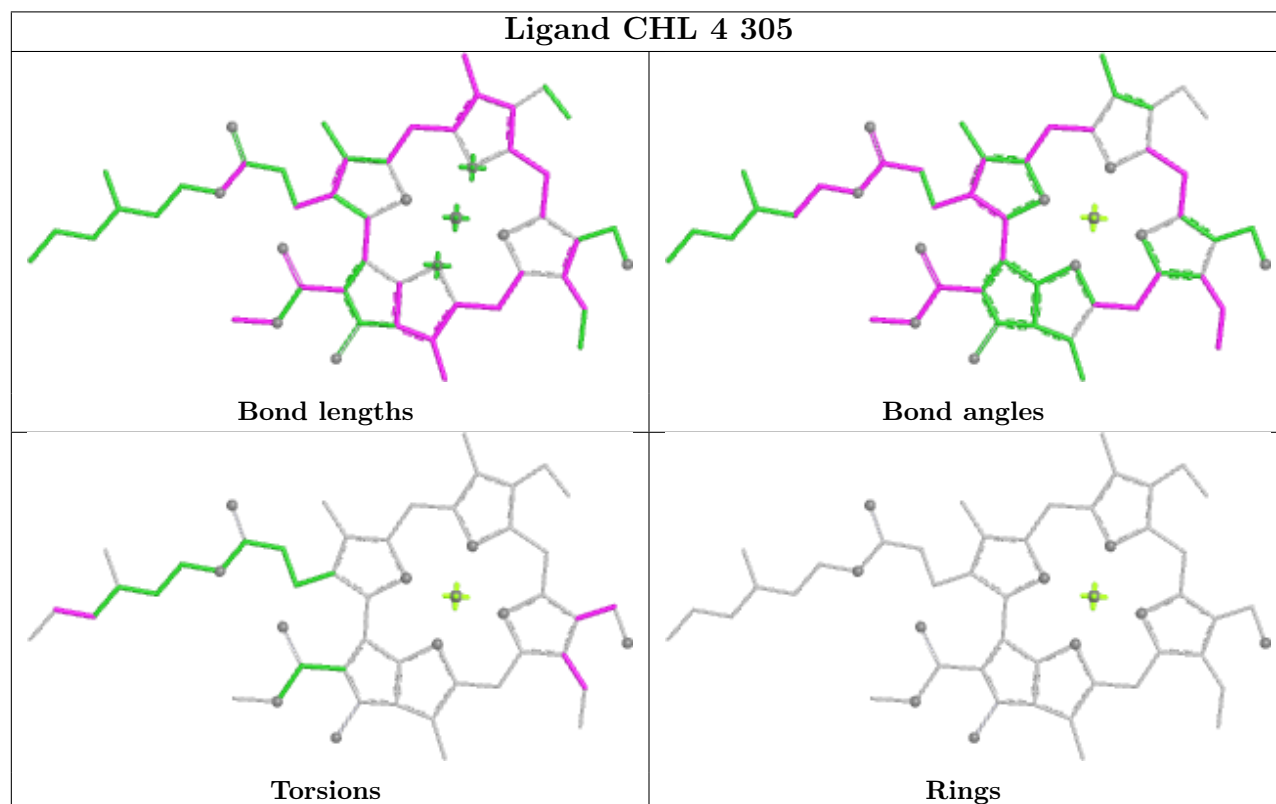


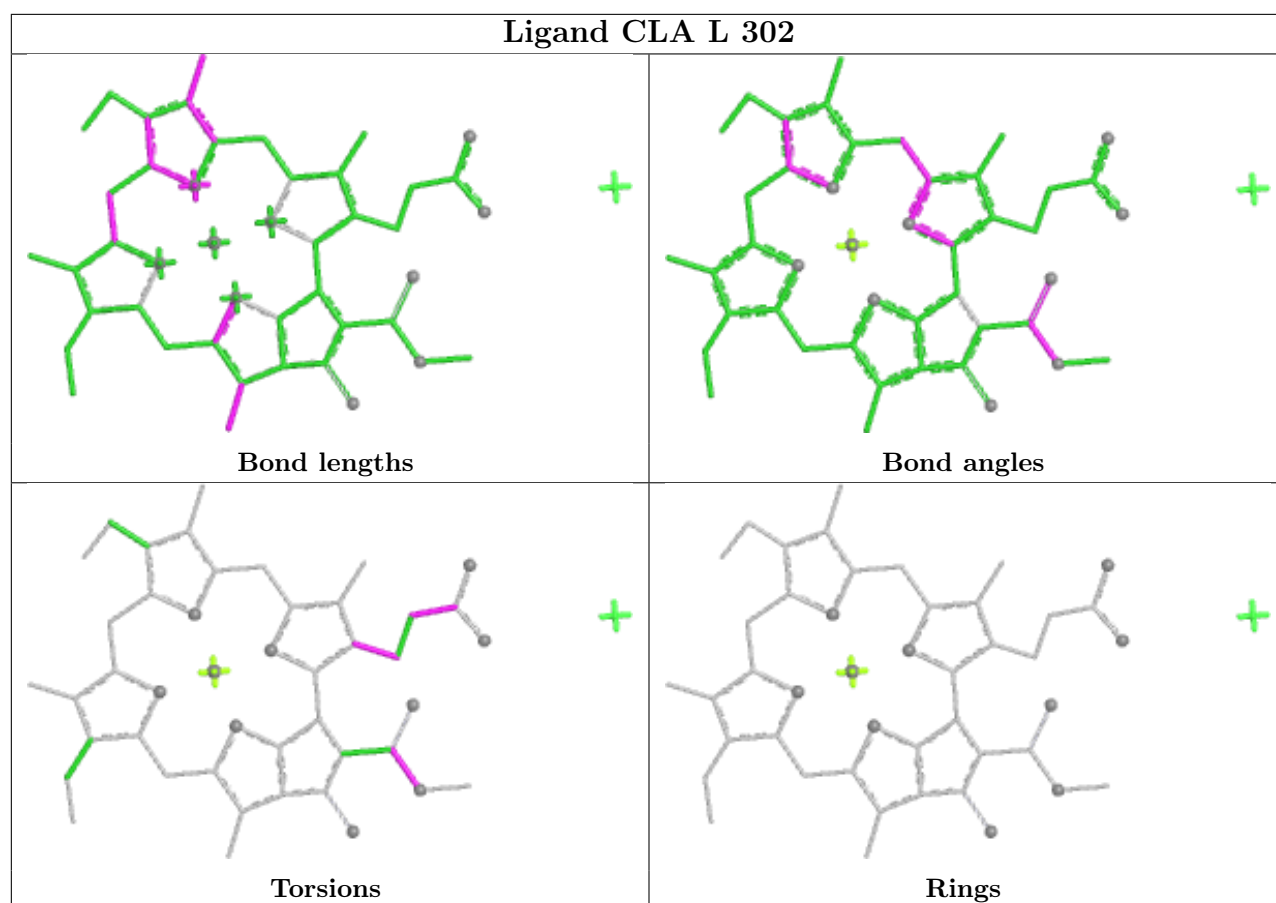


Ligand CLA A 836

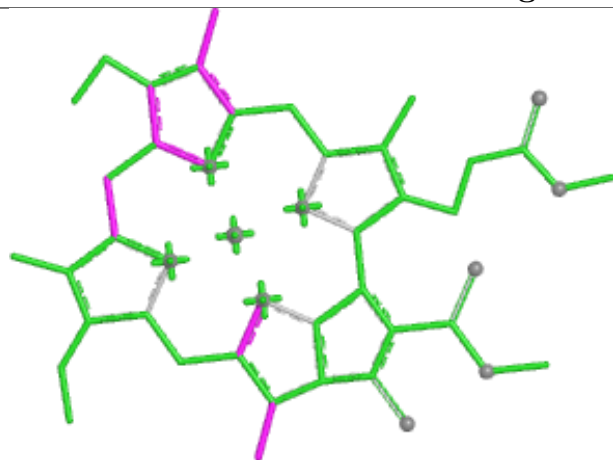


Ligand CHL 4 305

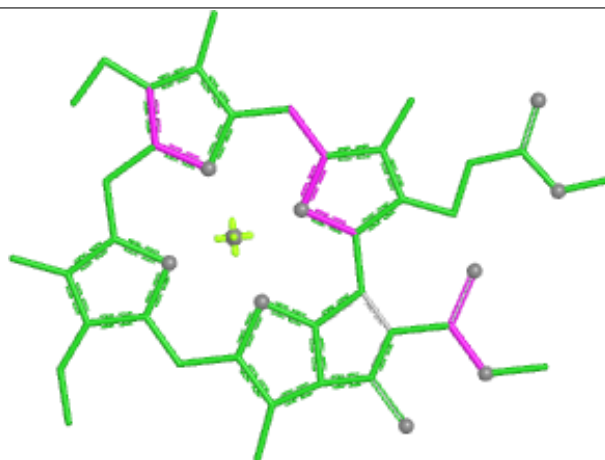




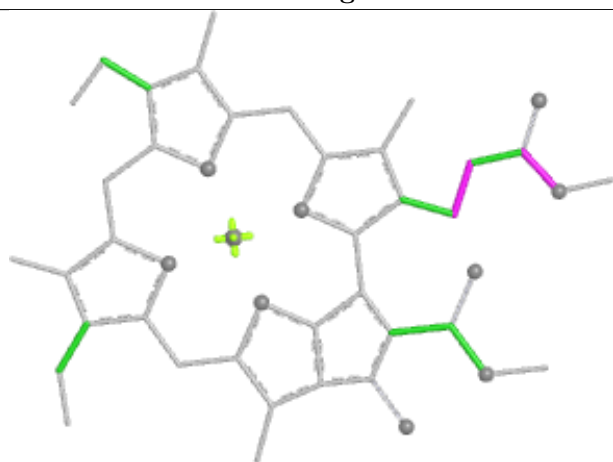
Ligand CLA 3 314



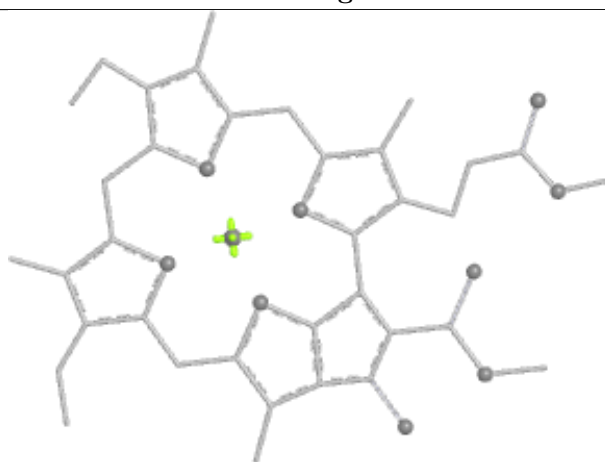
Bond lengths



Bond angles

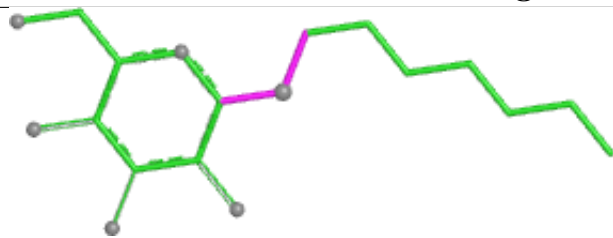


Torsions

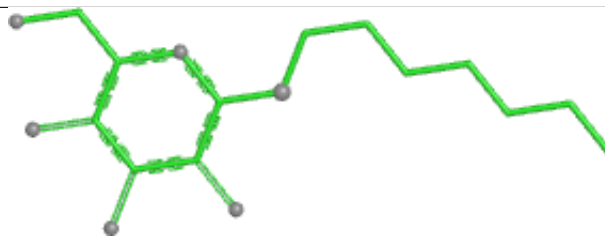


Rings

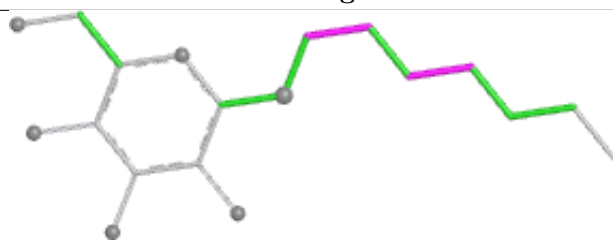
Ligand HTG 4 320



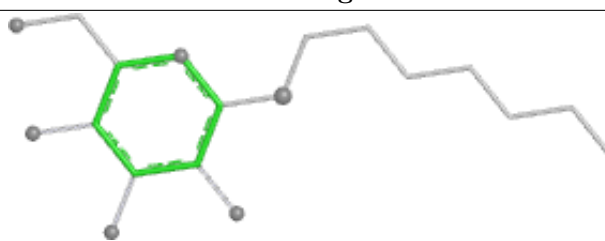
Bond lengths



Bond angles

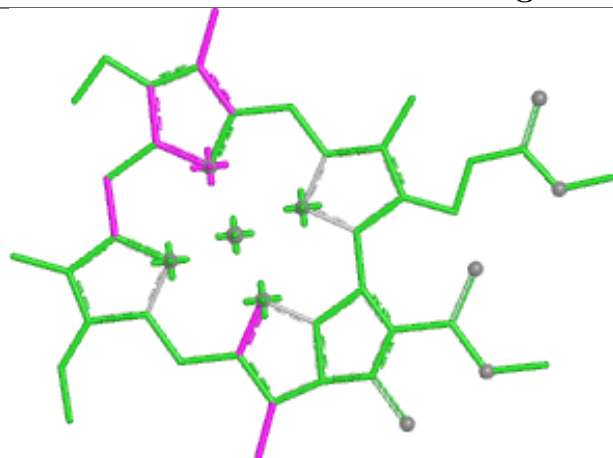


Torsions

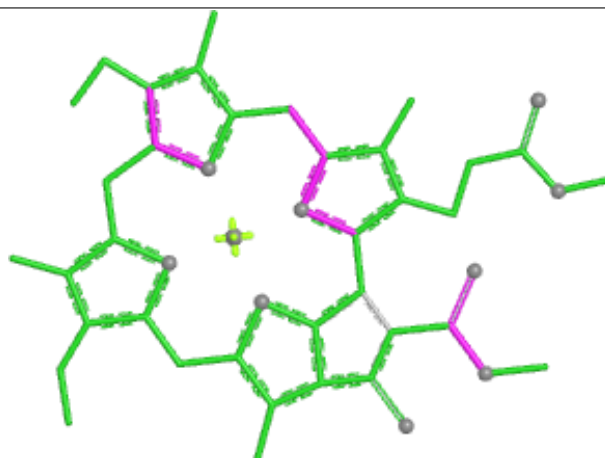


Rings

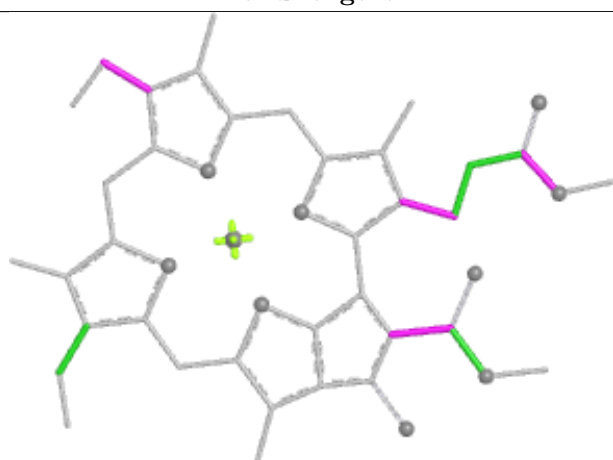
Ligand CLA F 805



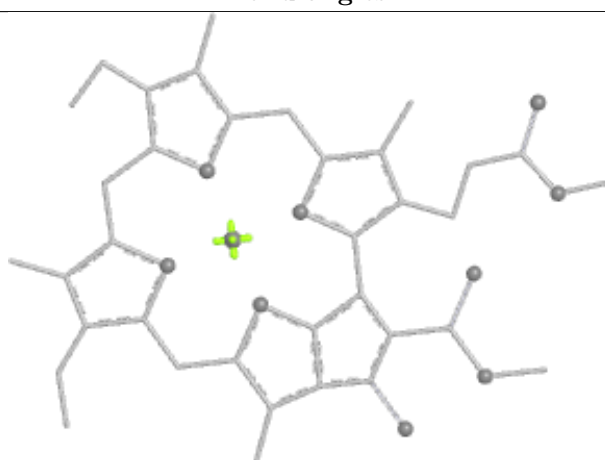
Bond lengths



Bond angles

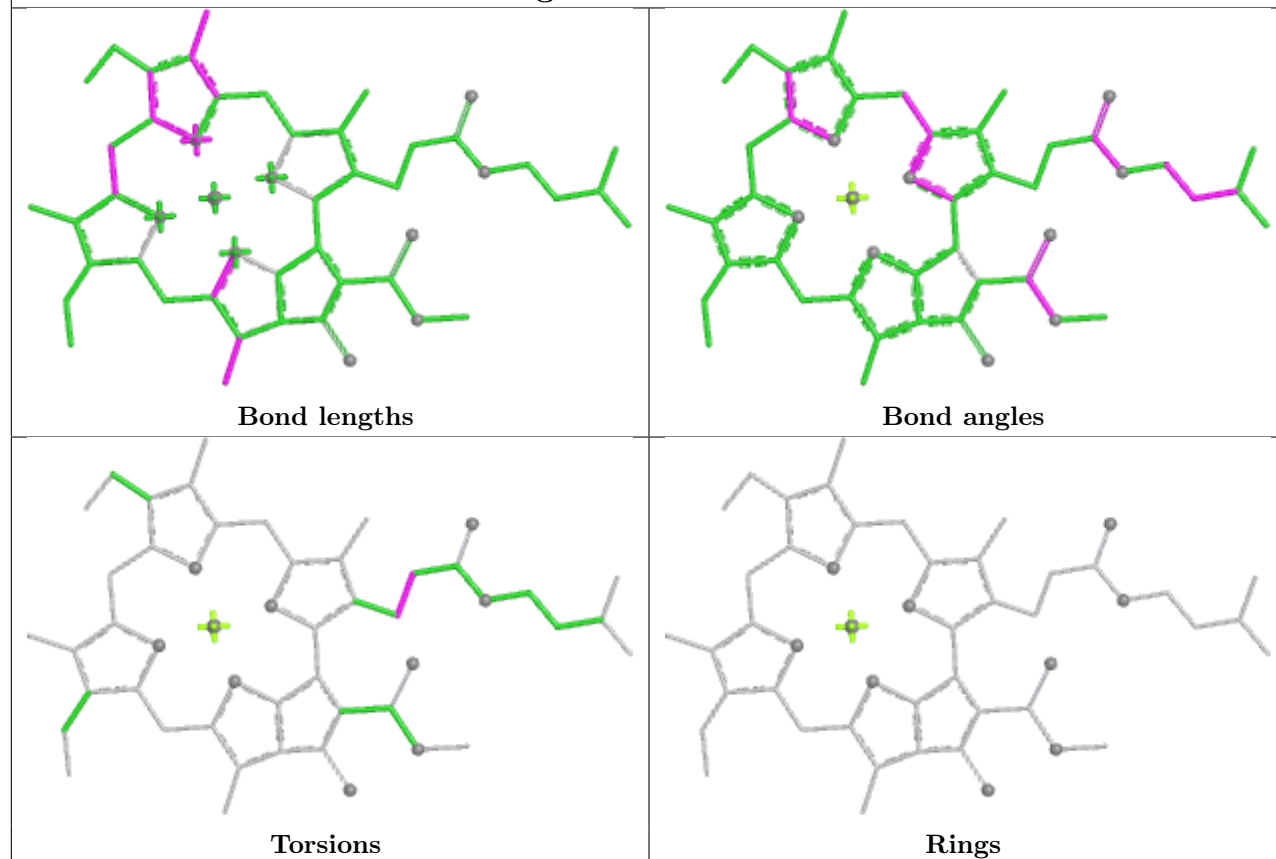


Torsions

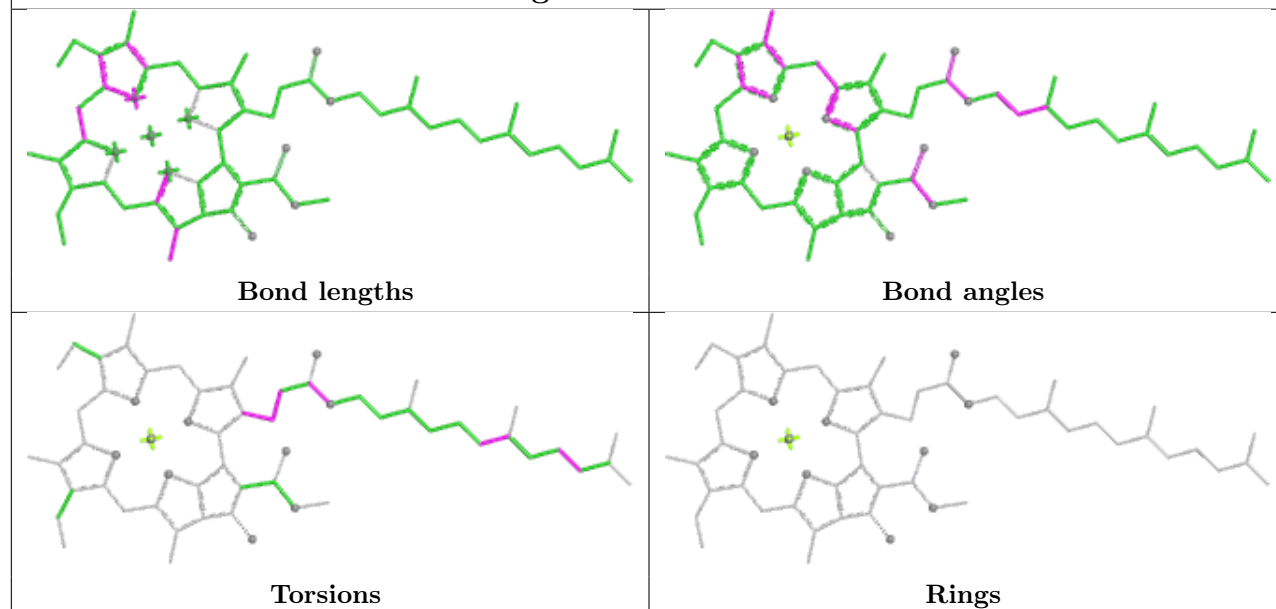


Rings

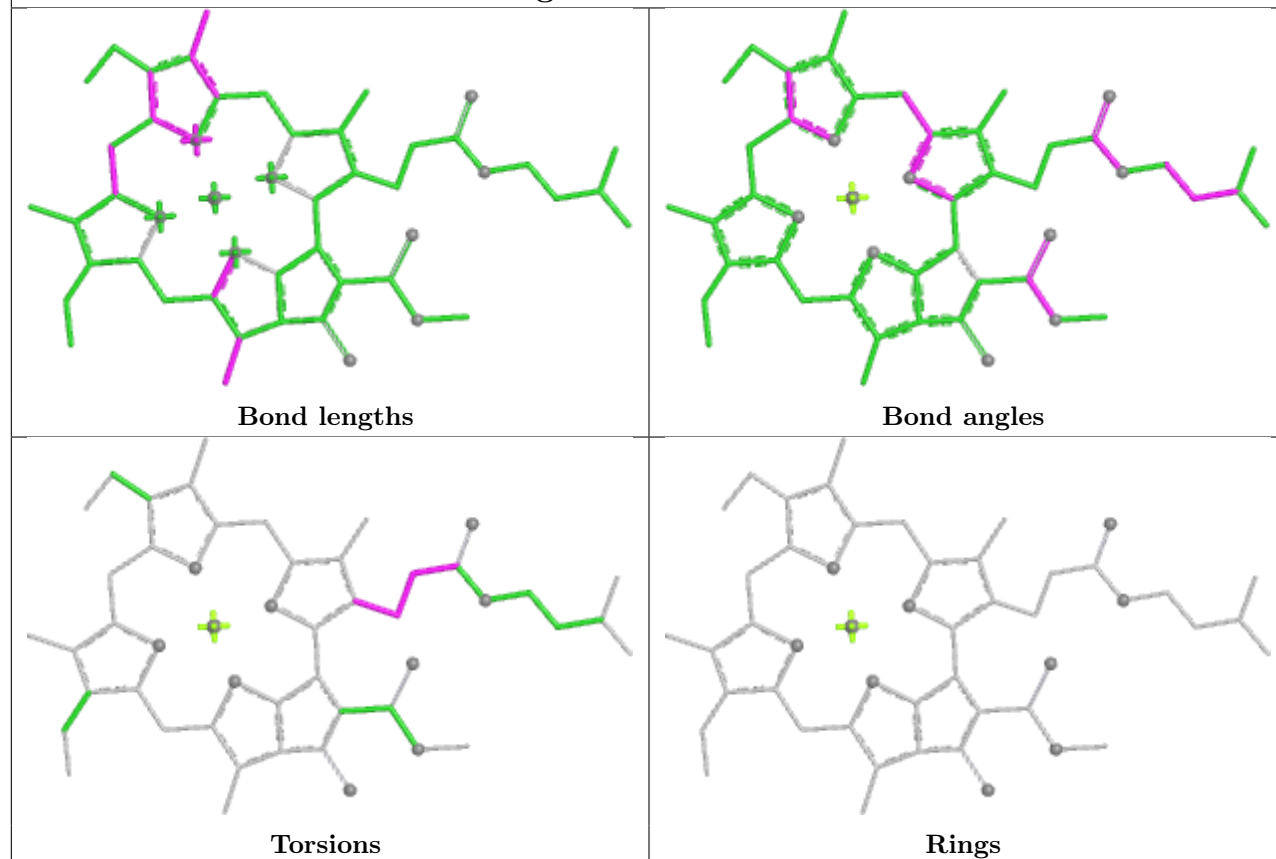
Ligand CLA 3 308



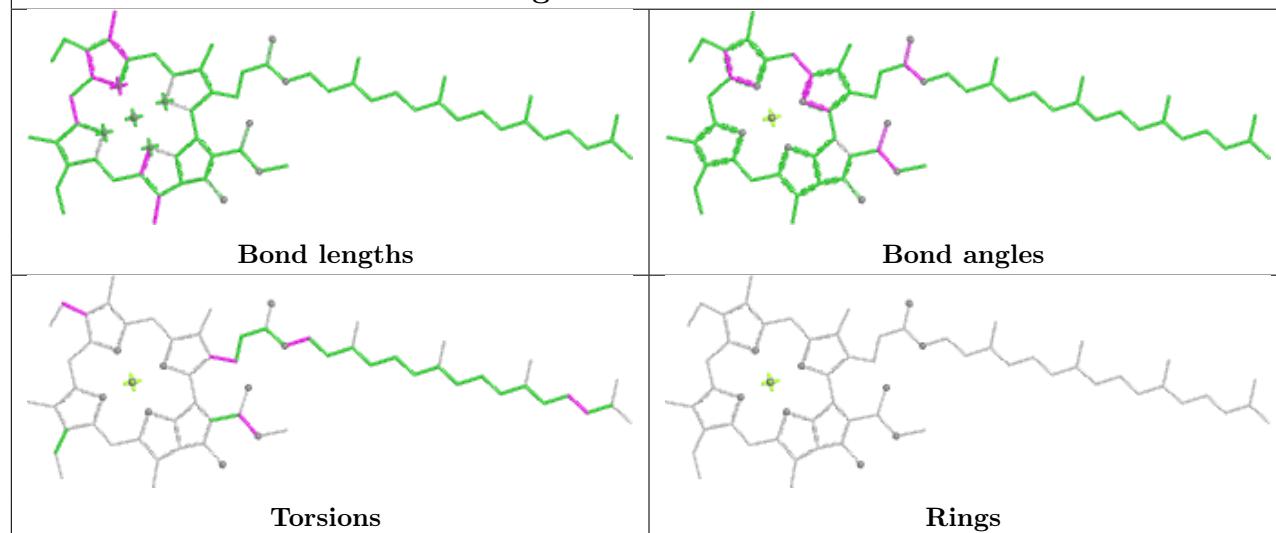
Ligand CLA O 203



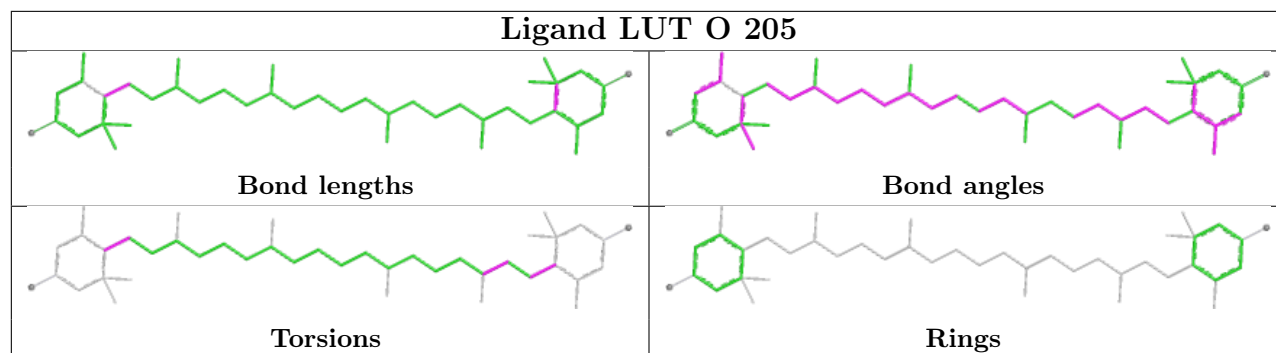
Ligand CLA 2 308



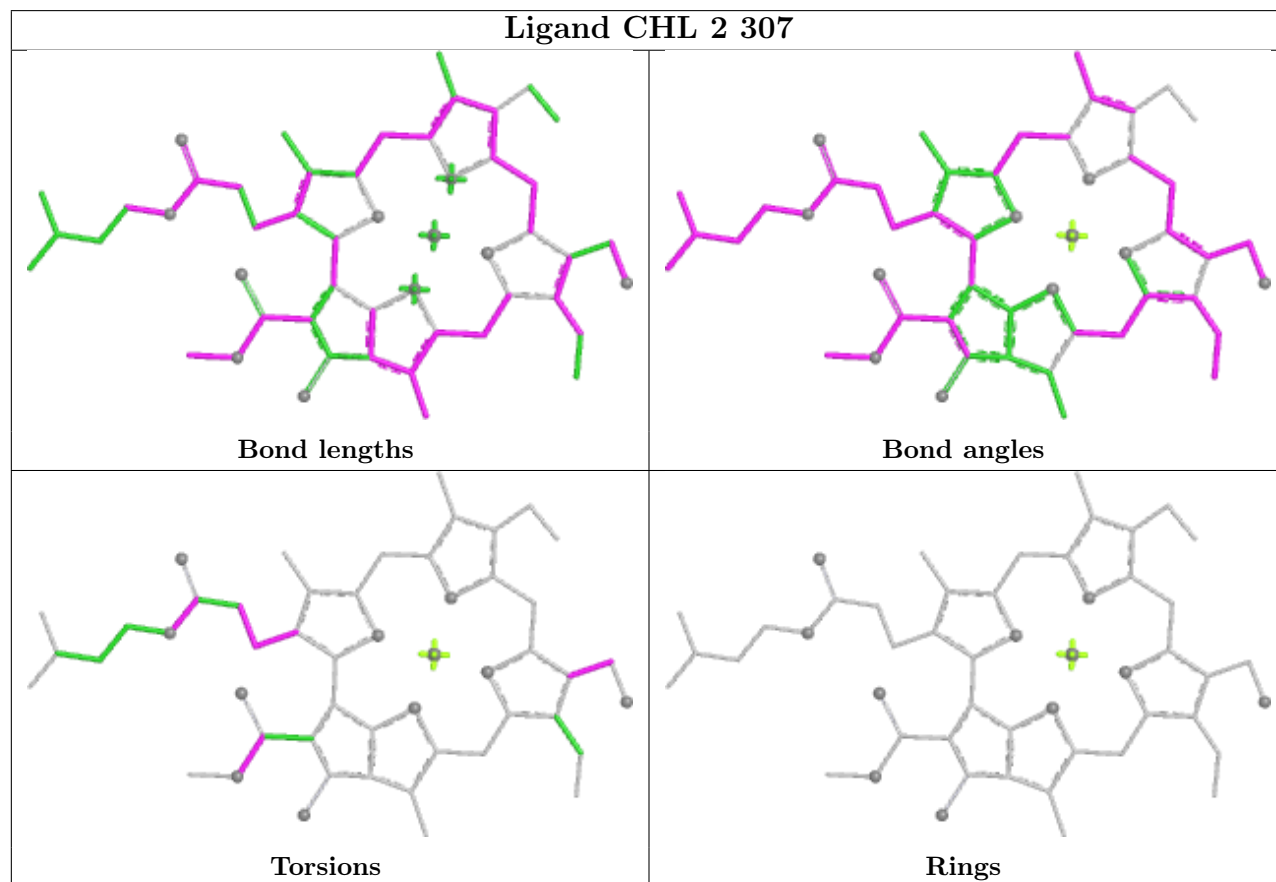
Ligand CLA B 839



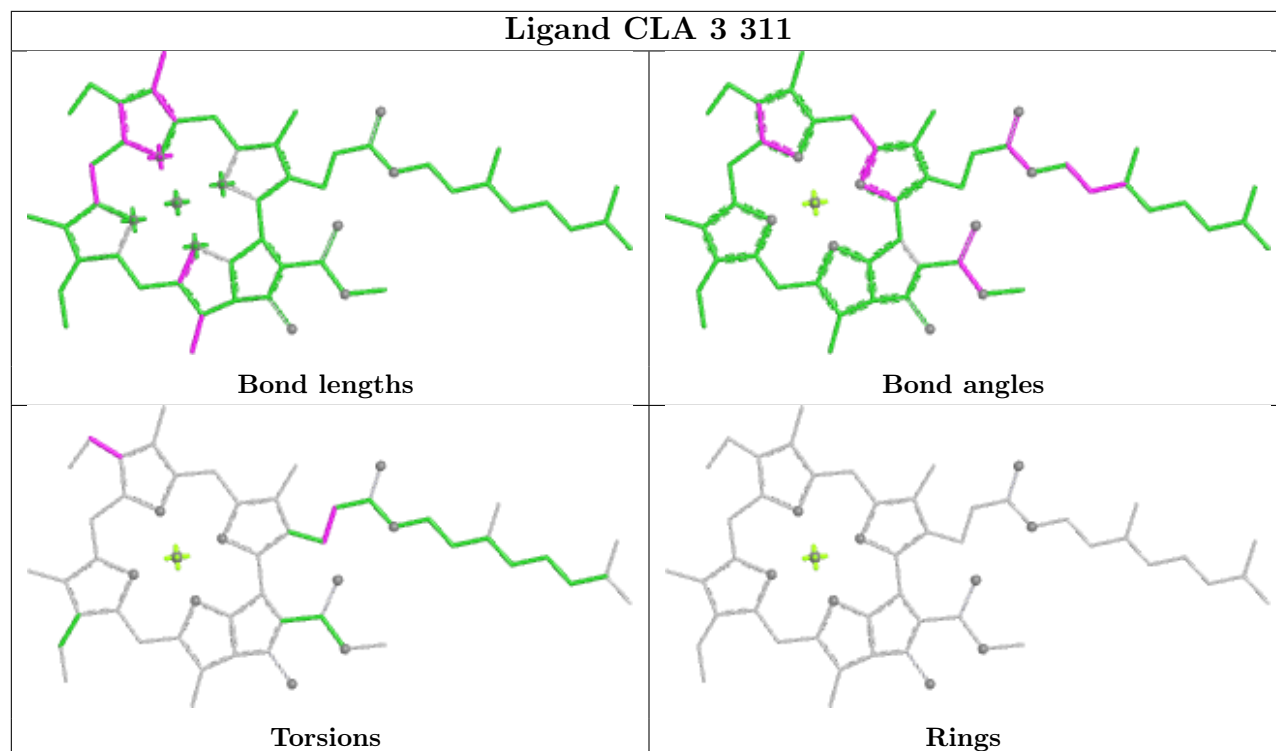
Ligand LUT O 205



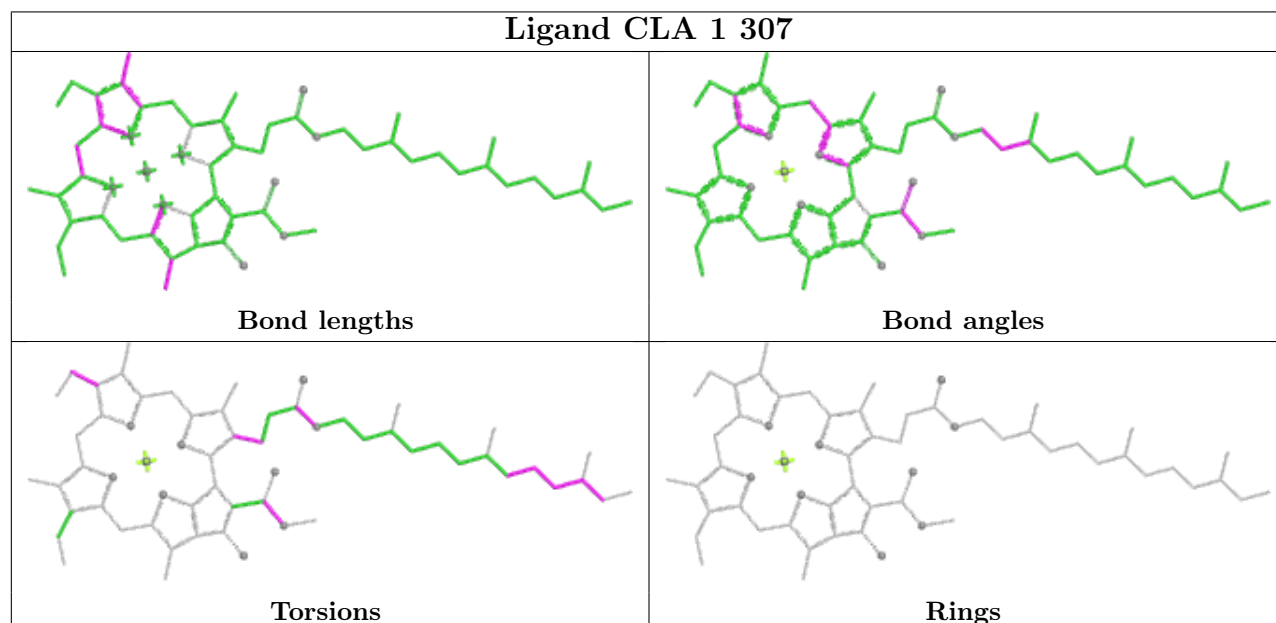
Ligand CHL 2 307



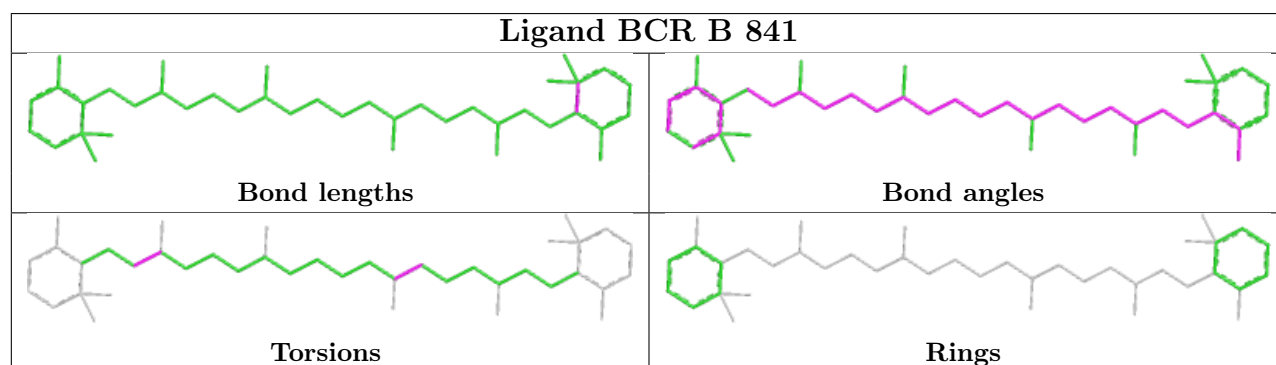
Ligand CLA 3 311

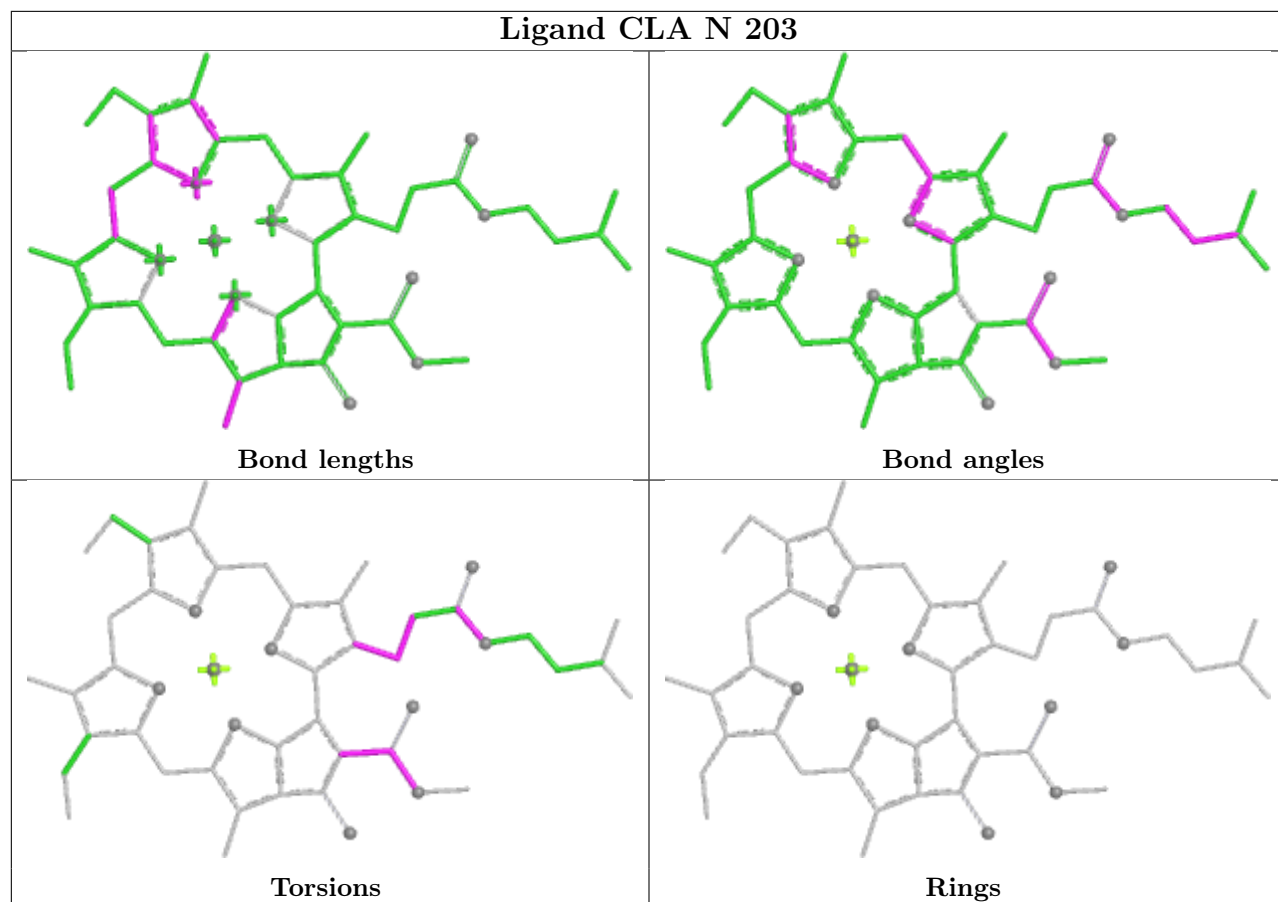


Ligand CLA 1 307

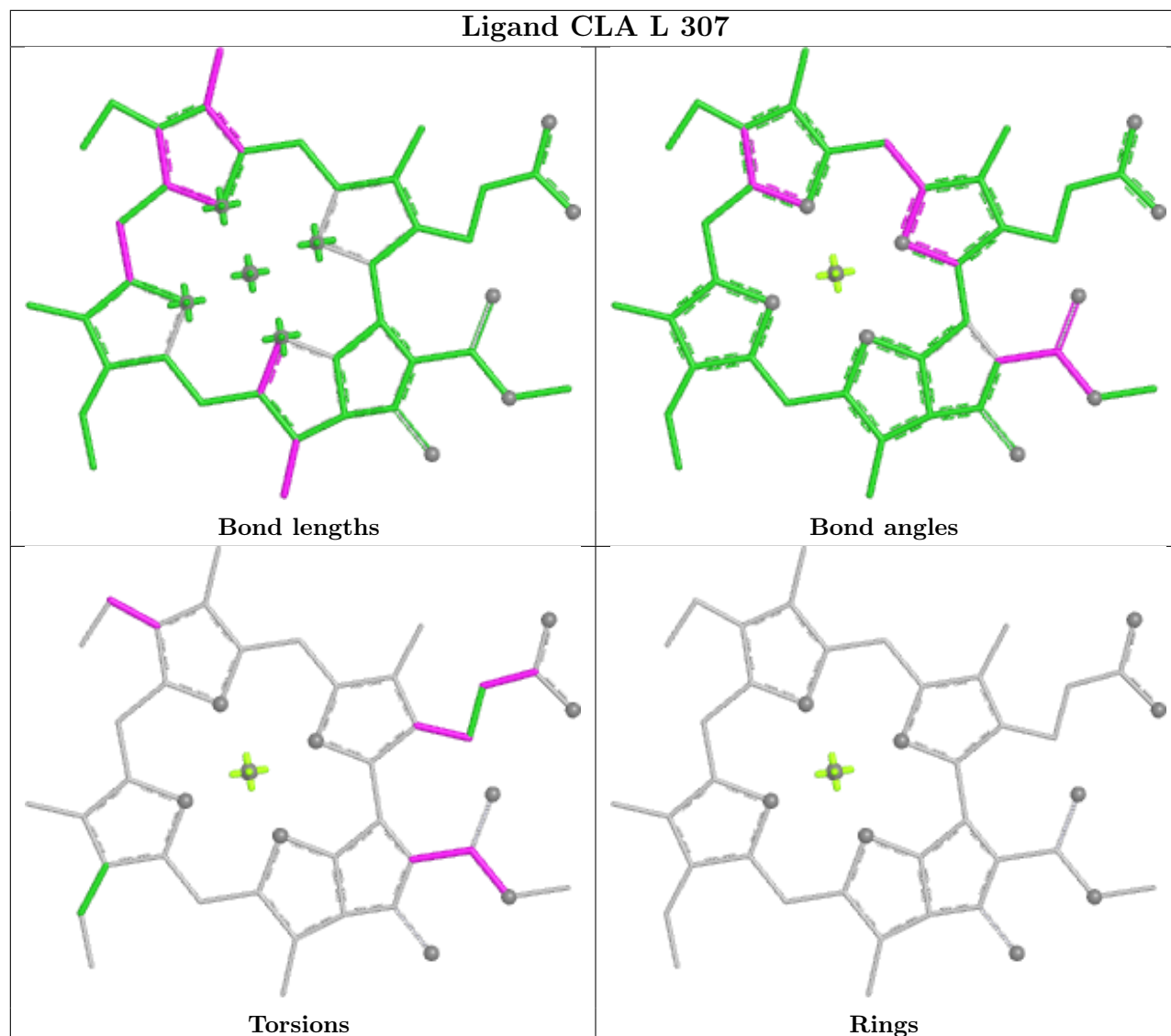


Ligand BCR B 841

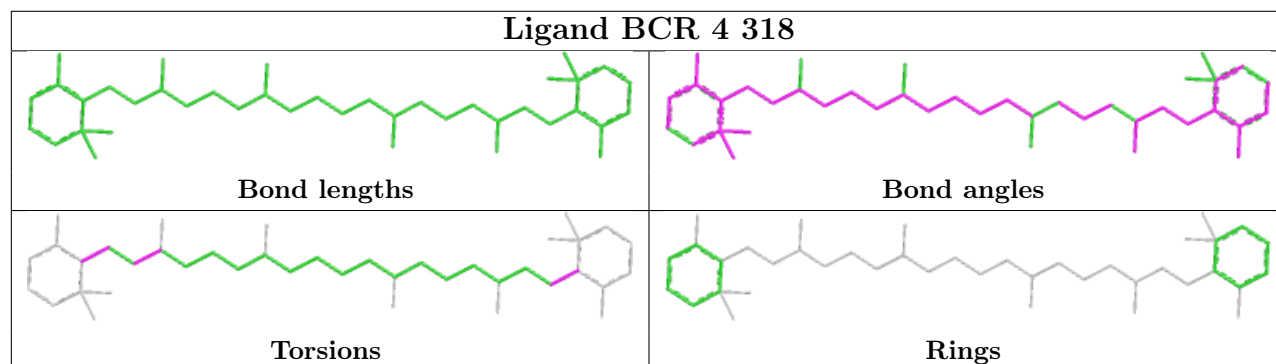


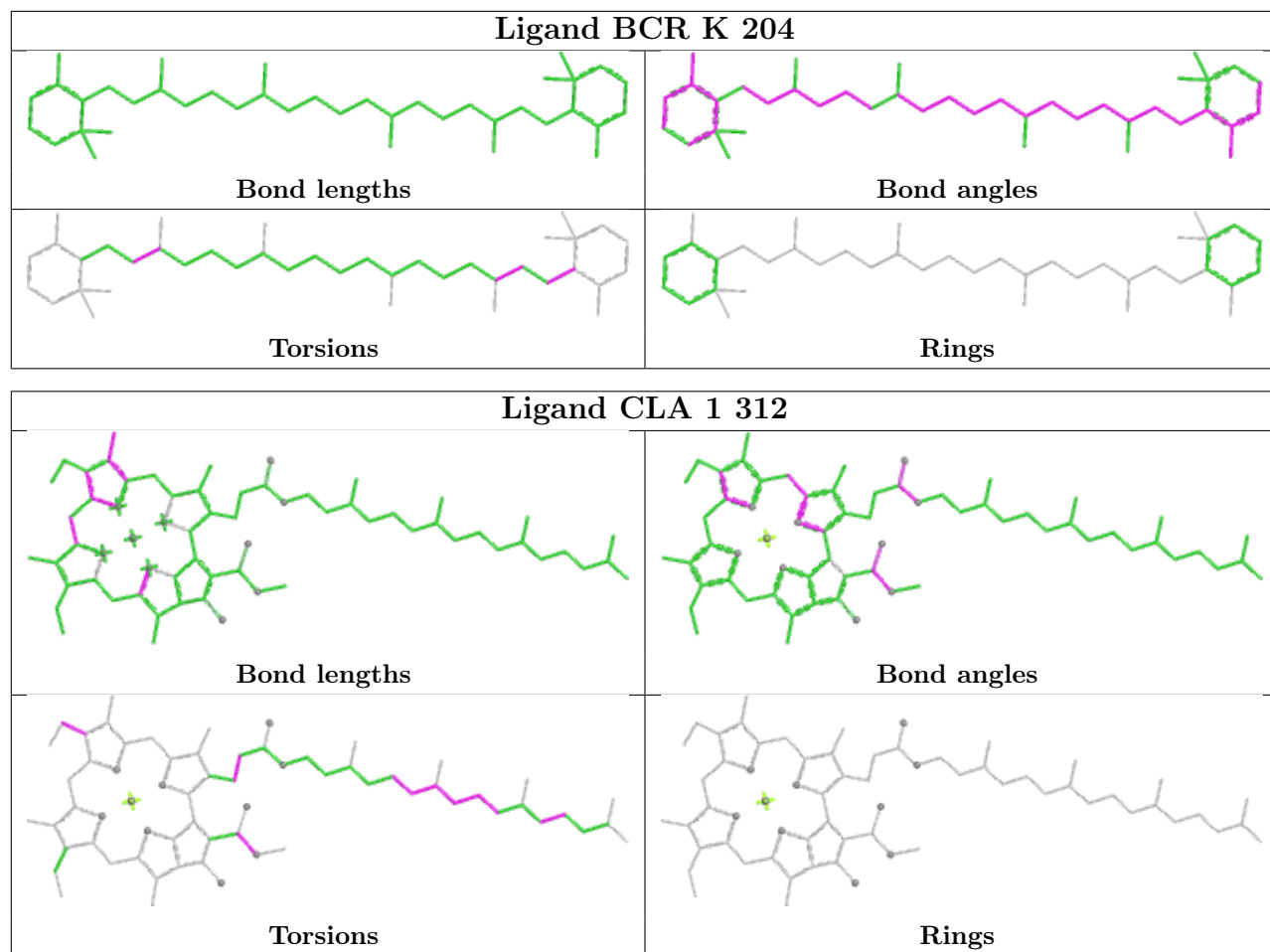


Ligand CLA L 307

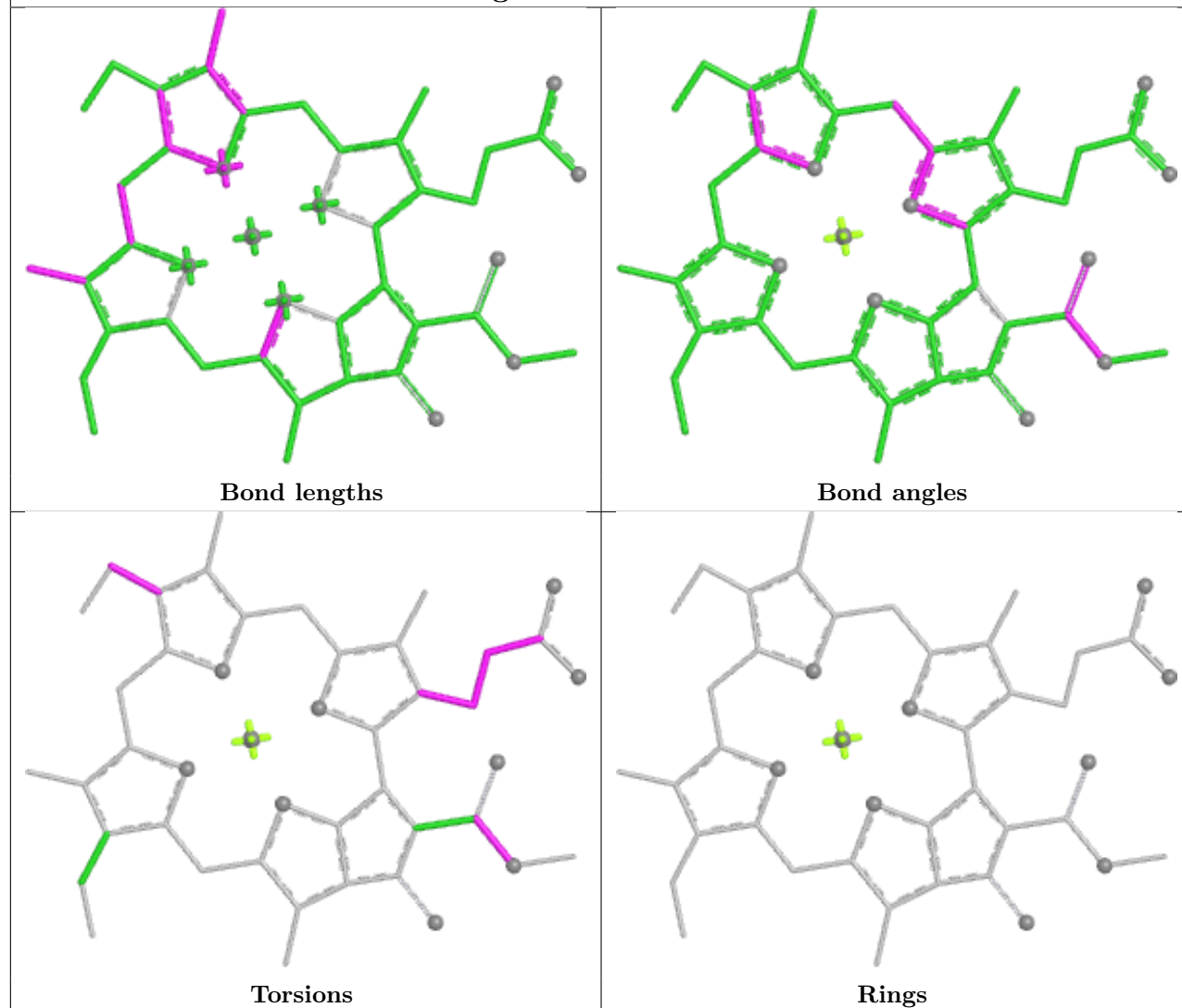


Ligand BCR 4 318

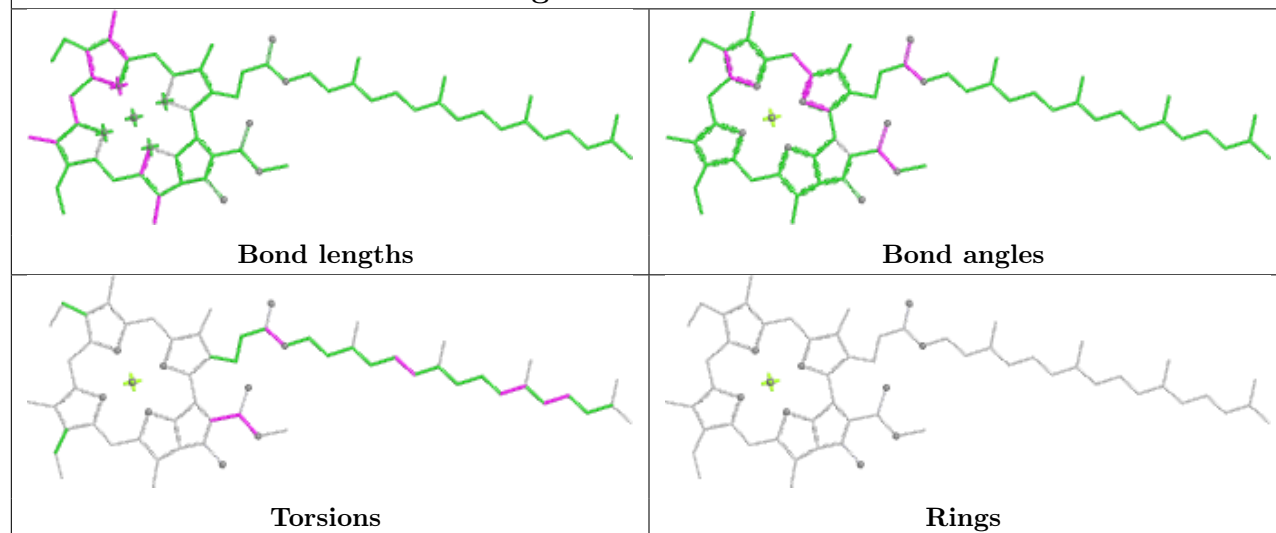




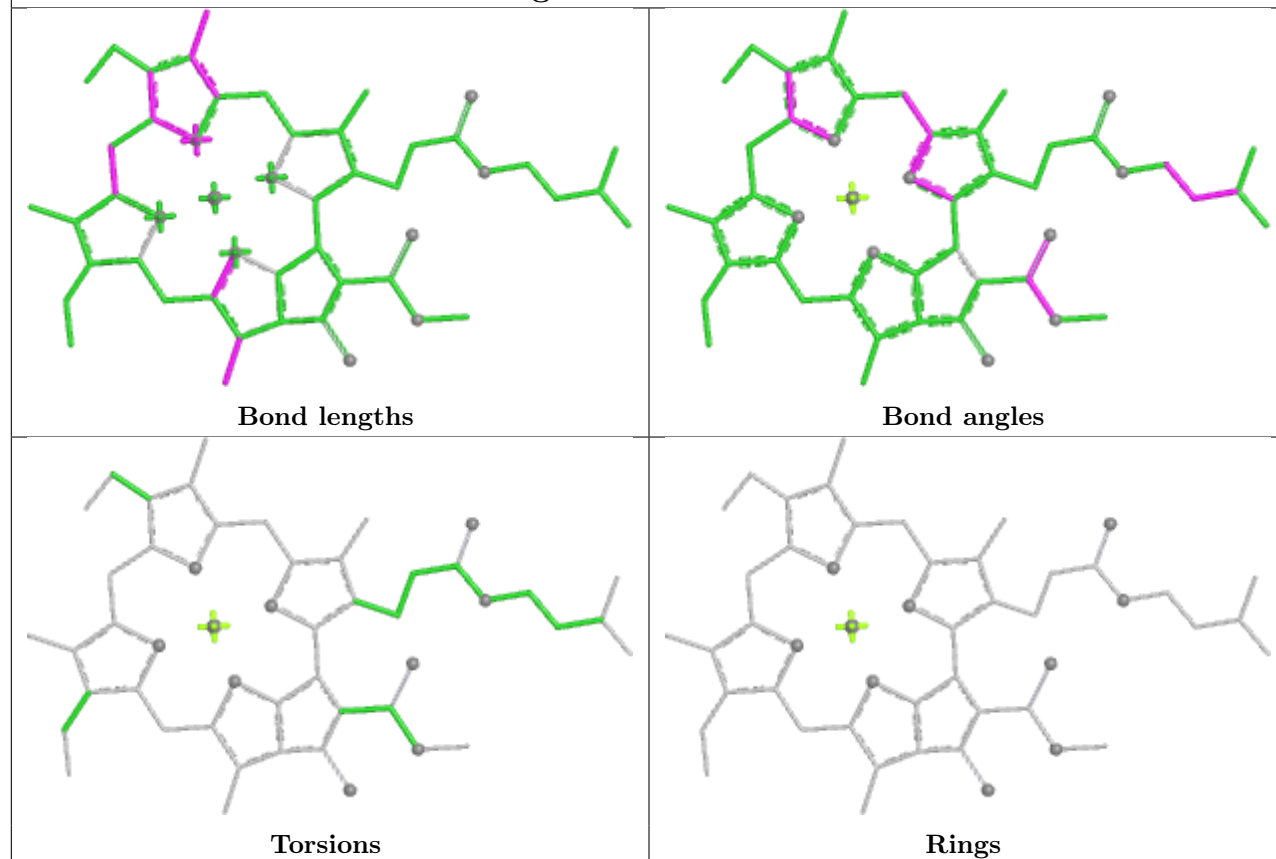
Ligand CLA A 835



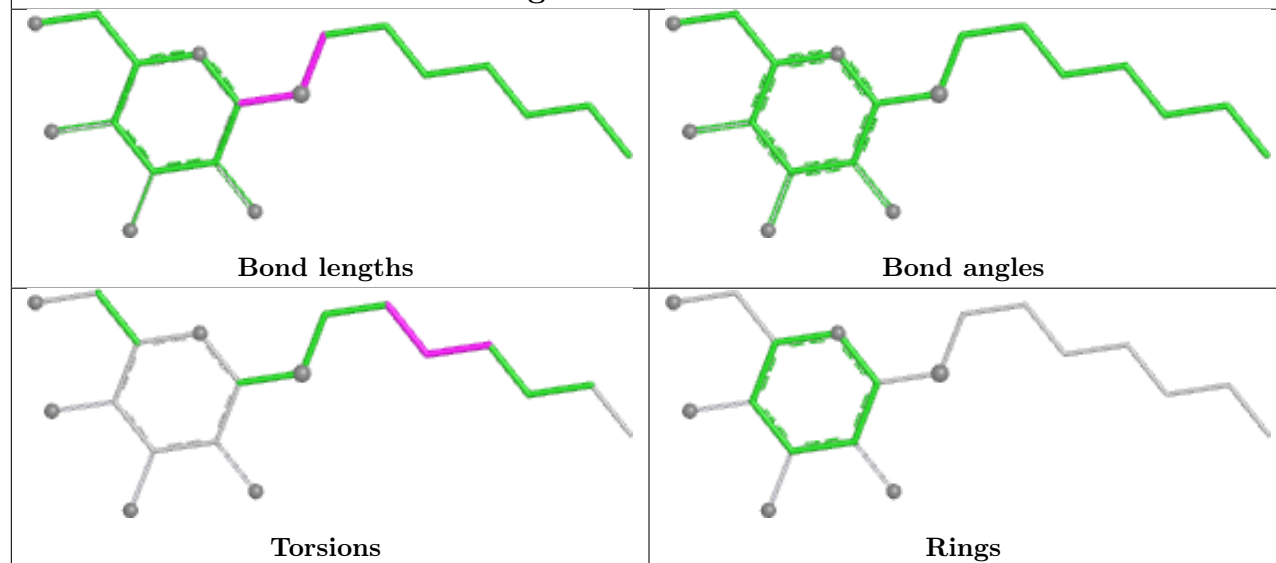
Ligand CLA A 833

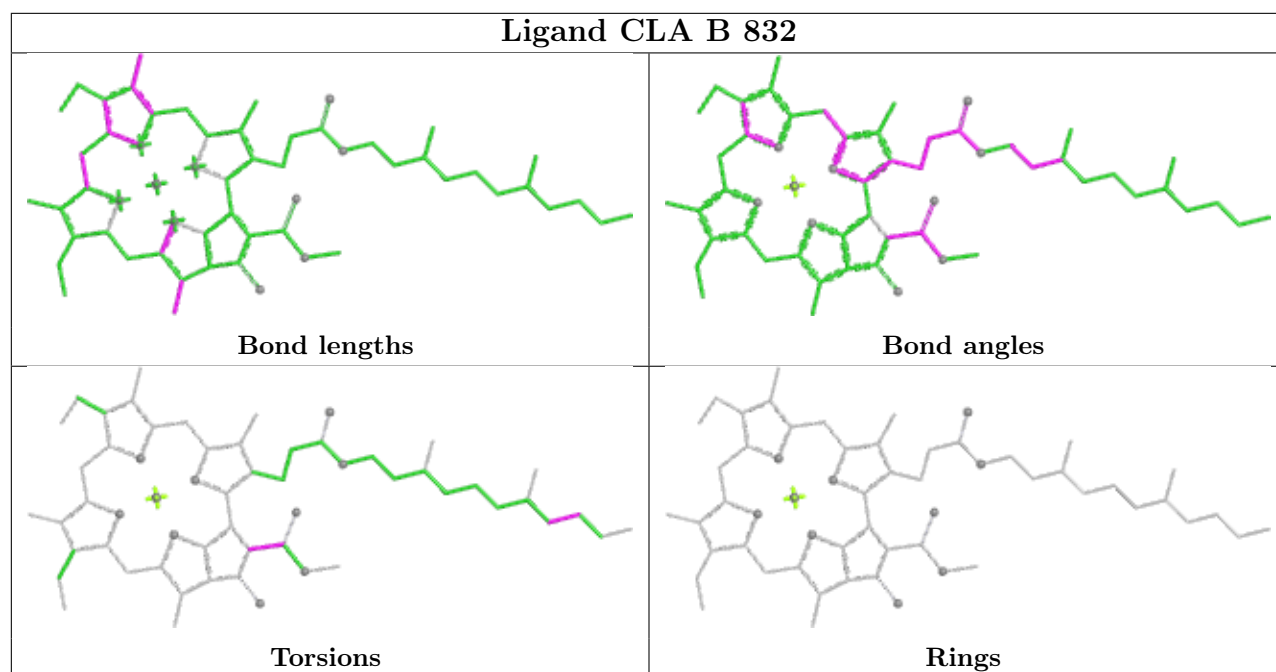
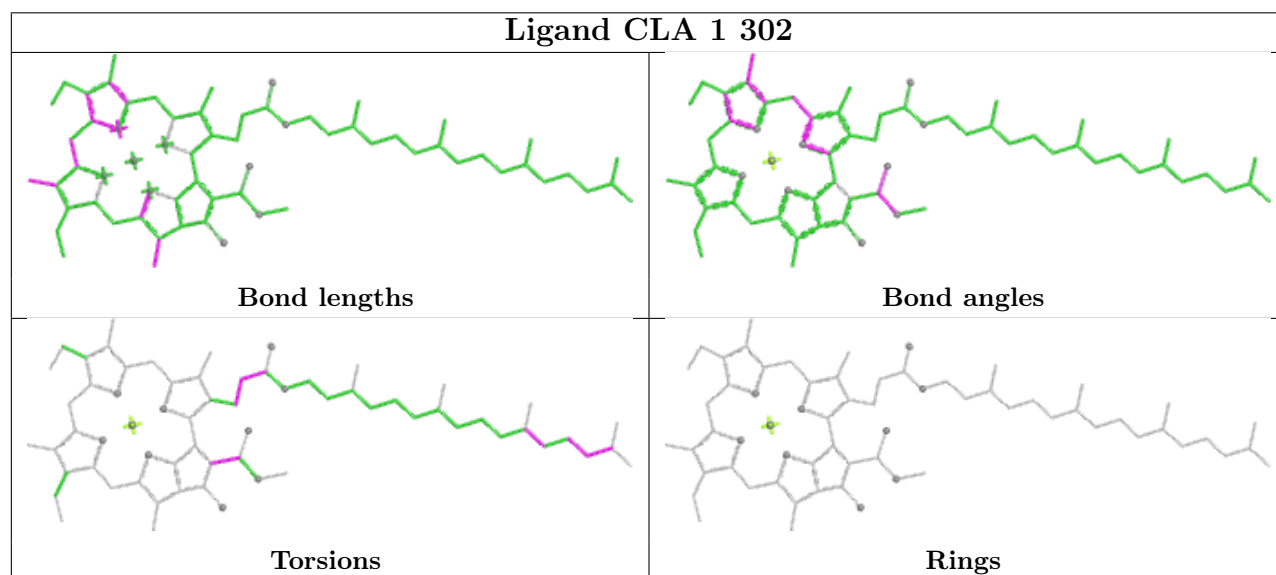
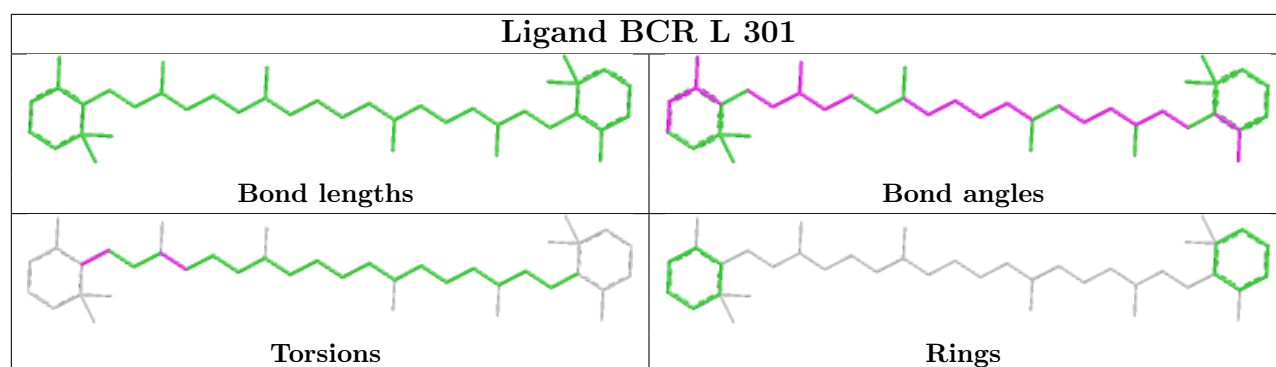


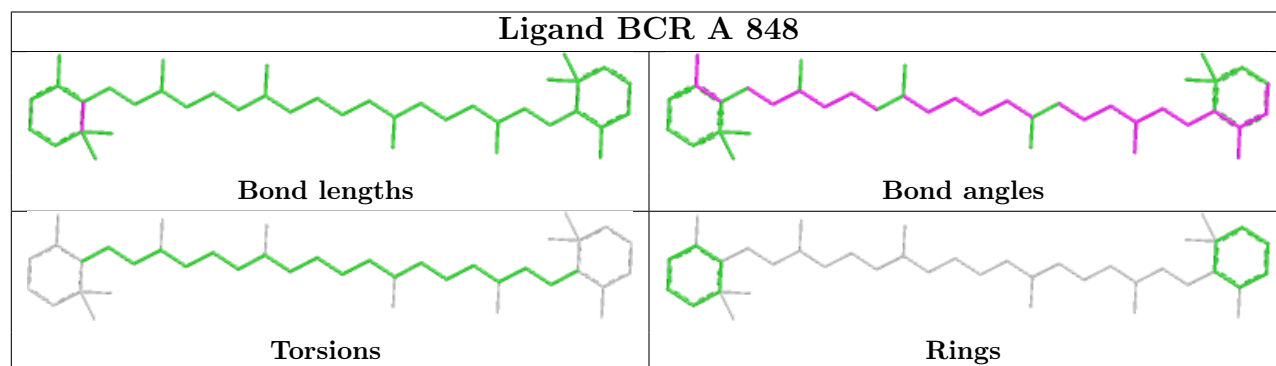
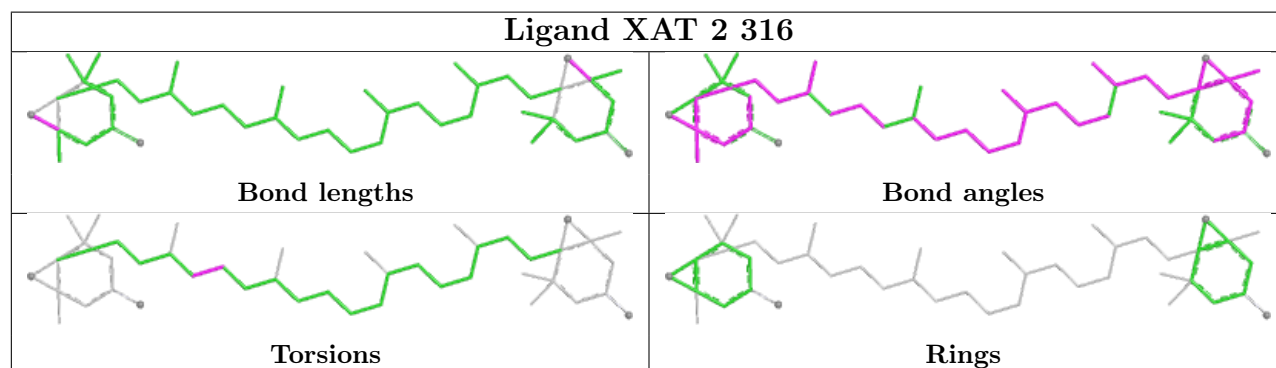
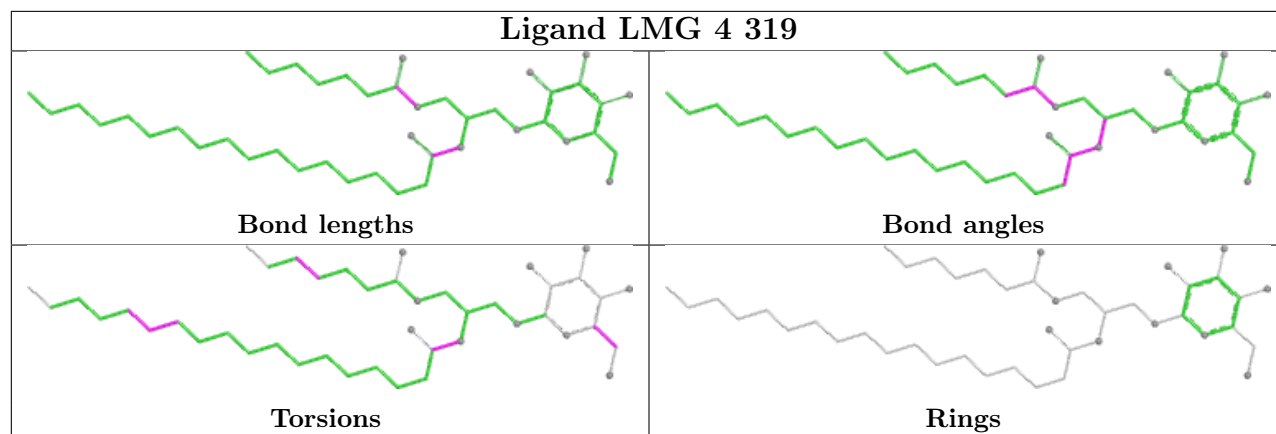
Ligand CLA B 820

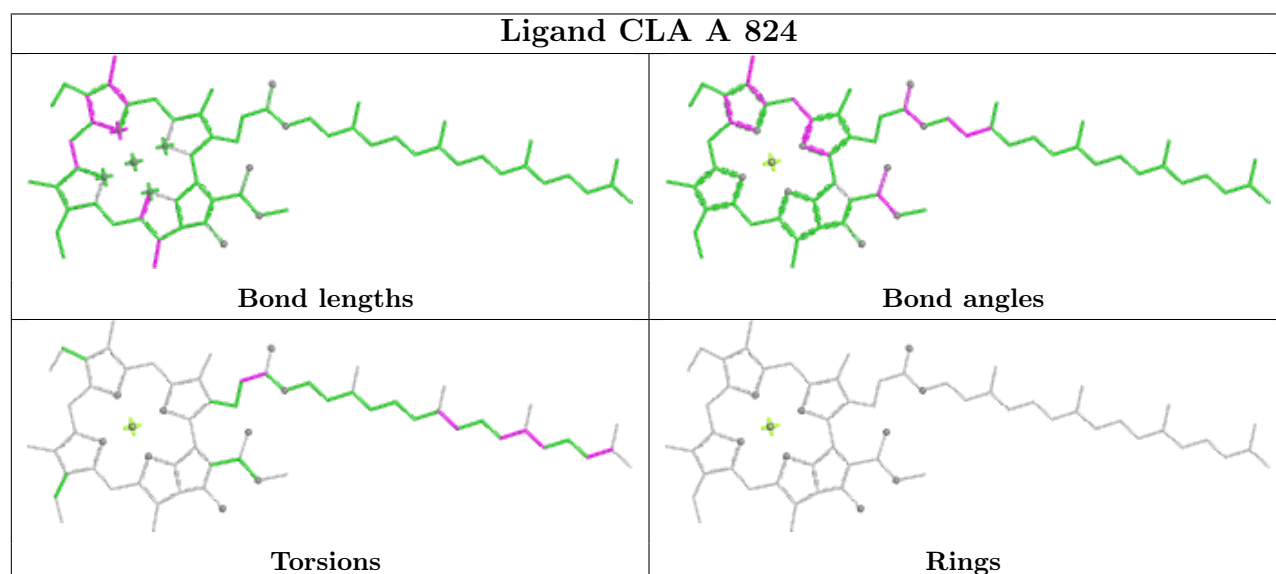
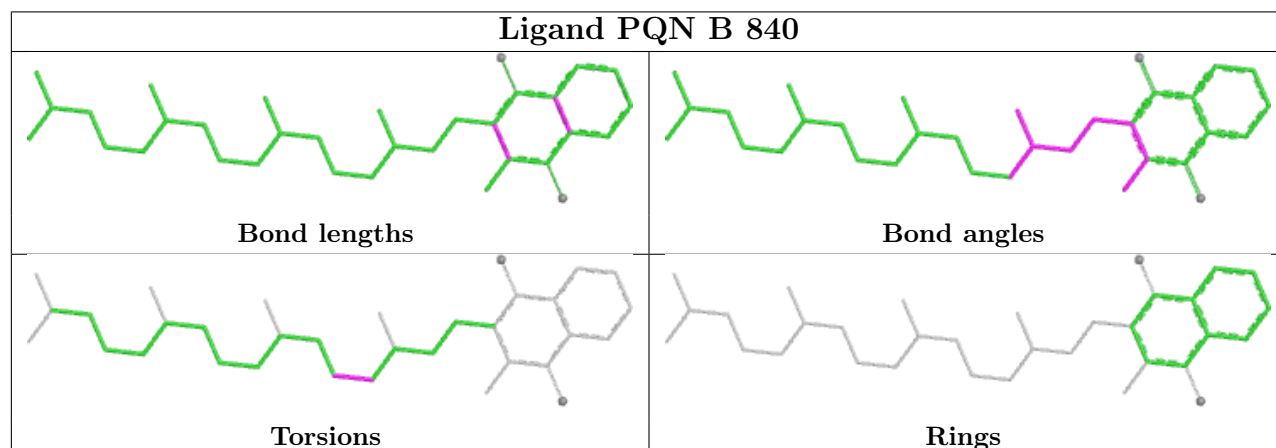
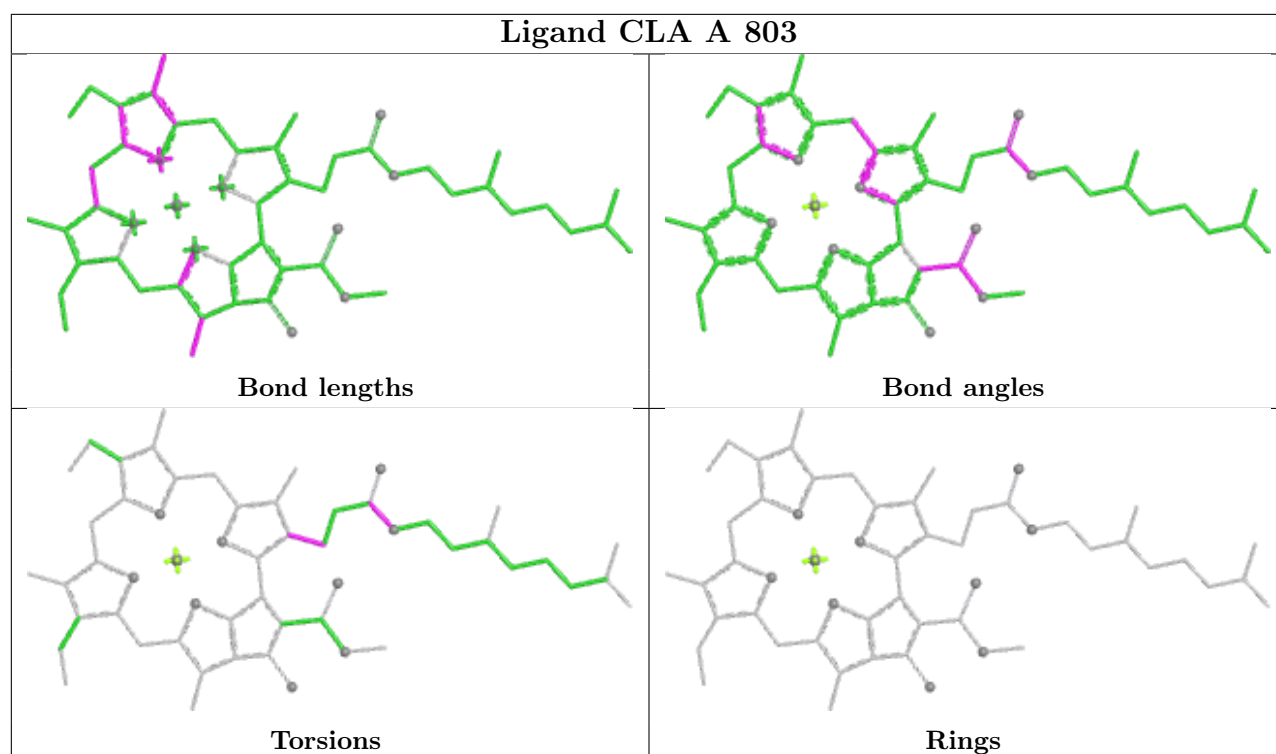


Ligand HTG N 201

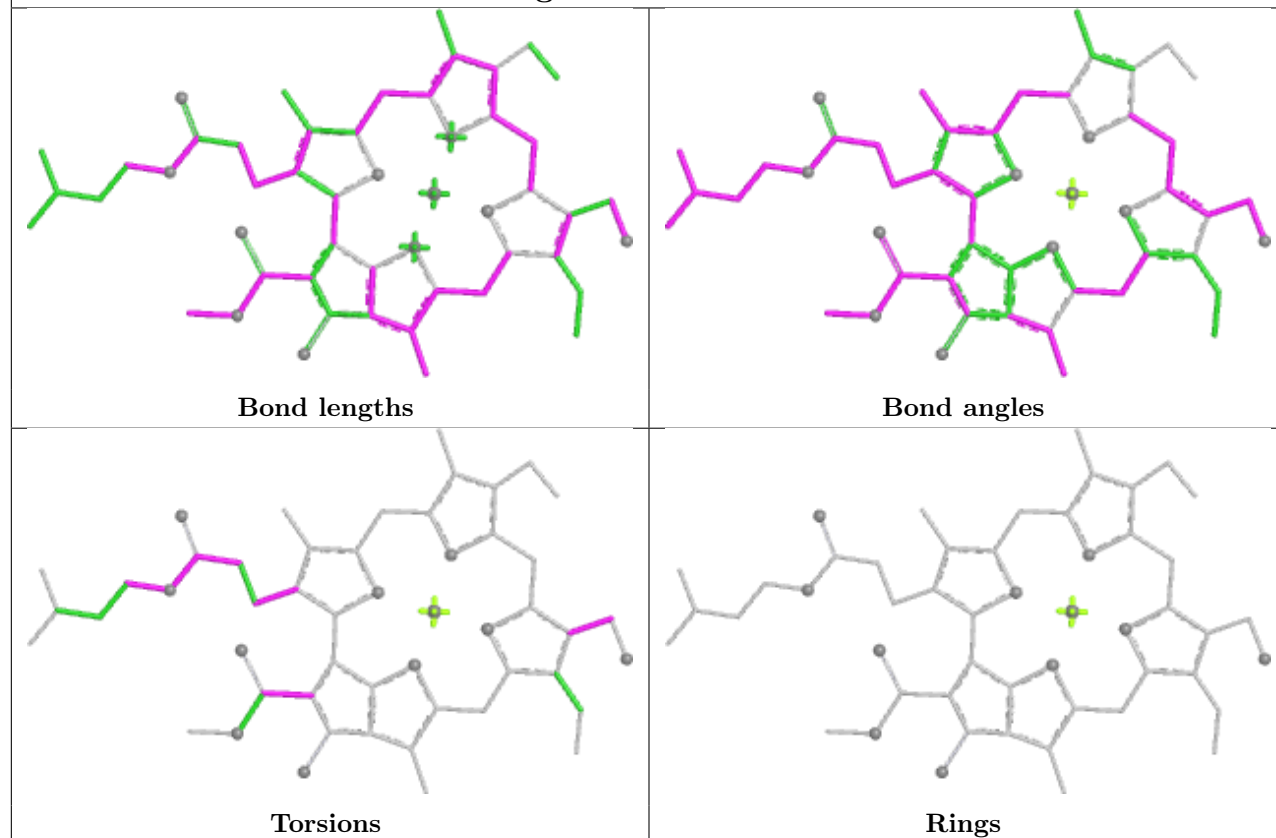




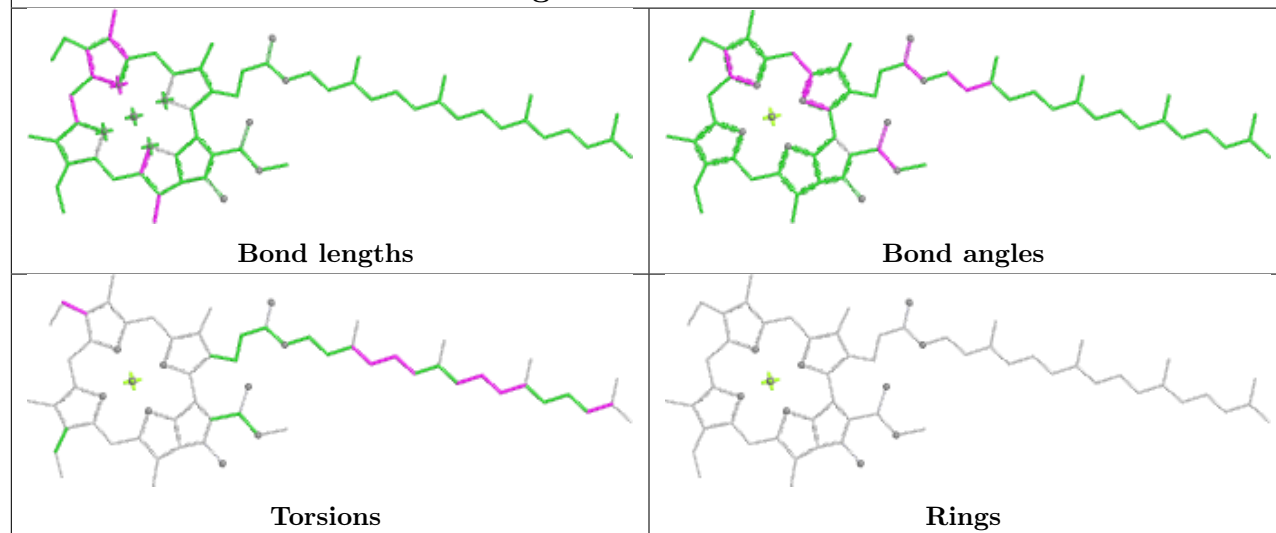


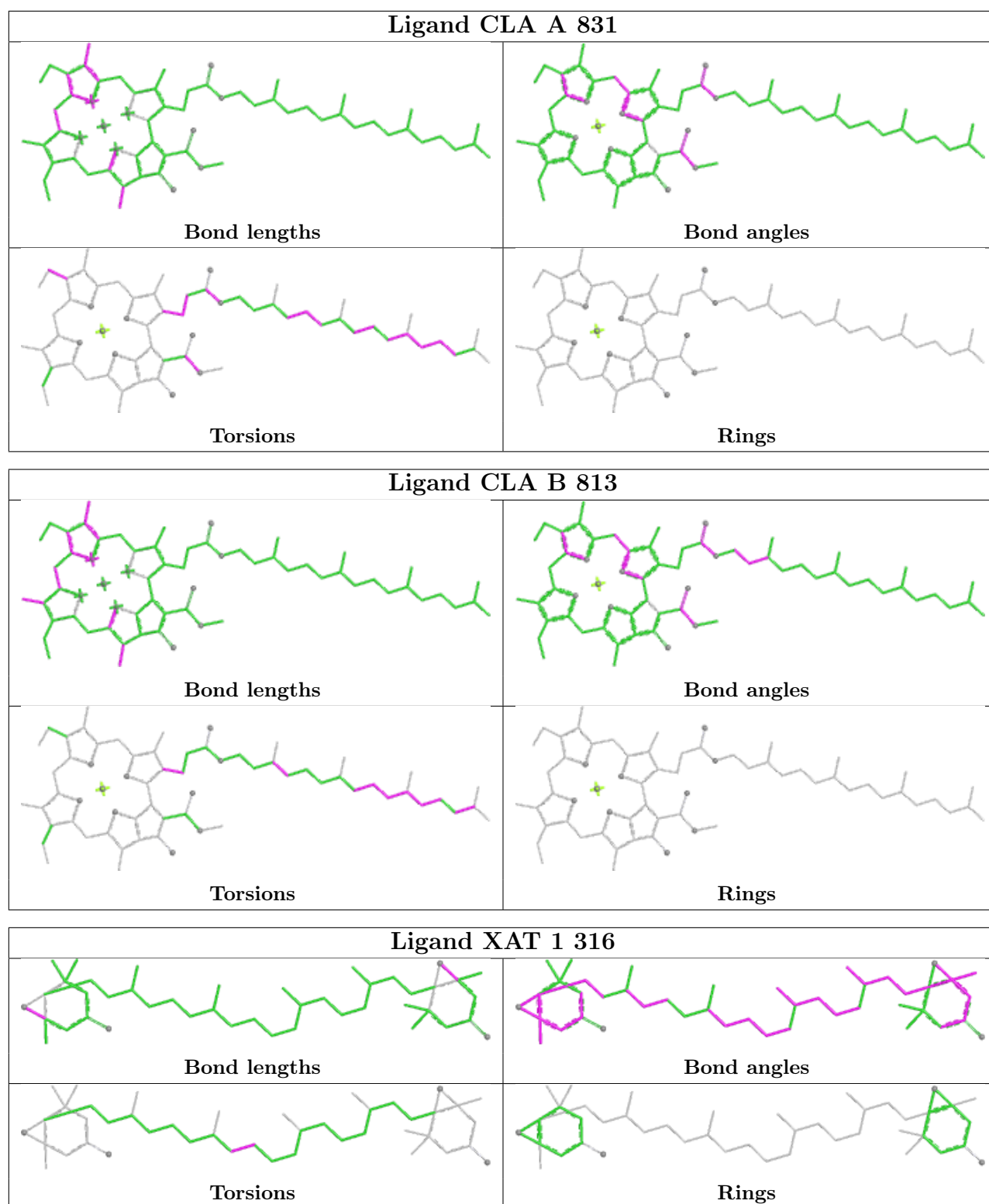


Ligand CHL 4 306

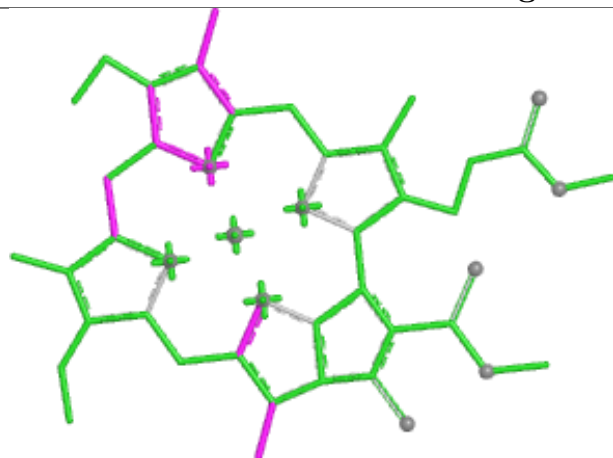


Ligand CLA B 833

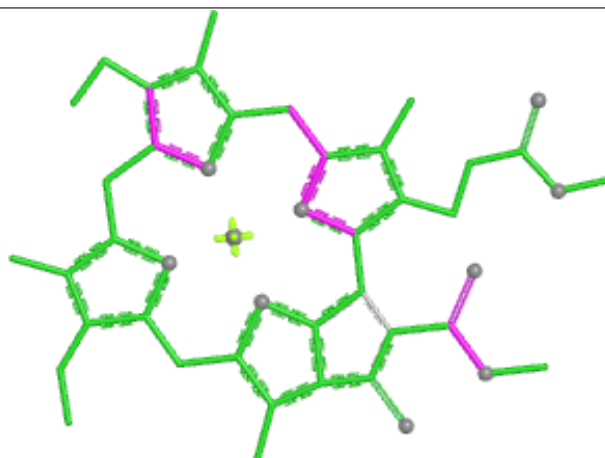




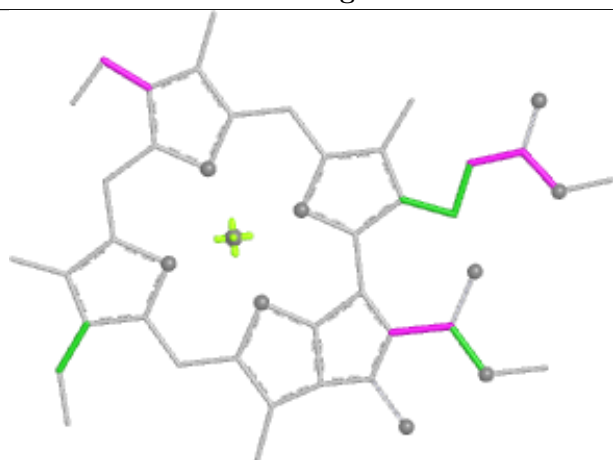
Ligand CLA 4 301



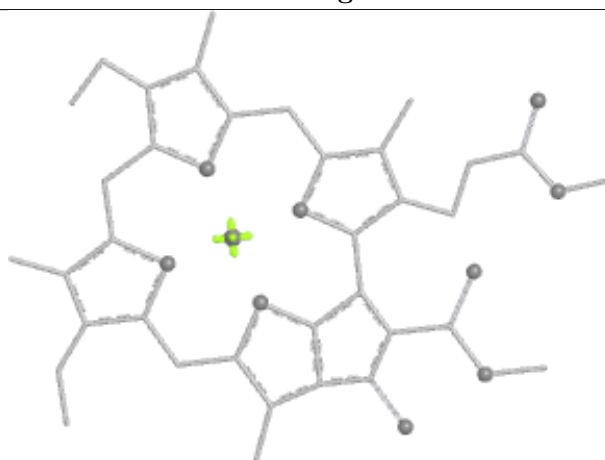
Bond lengths



Bond angles

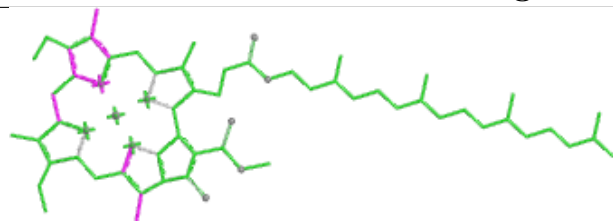


Torsions

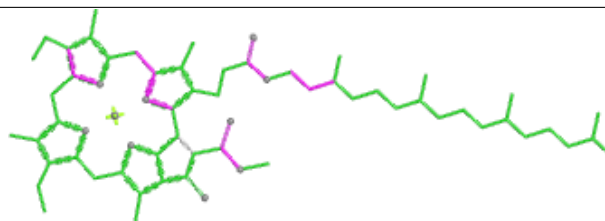


Rings

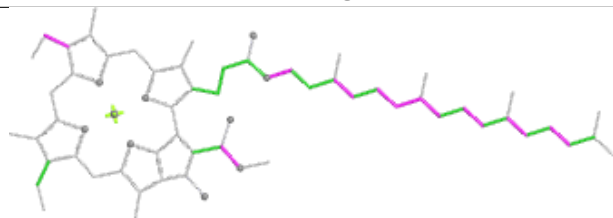
Ligand CLA A 853



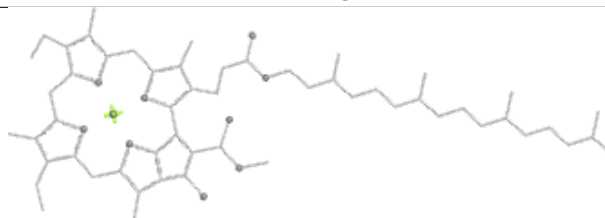
Bond lengths



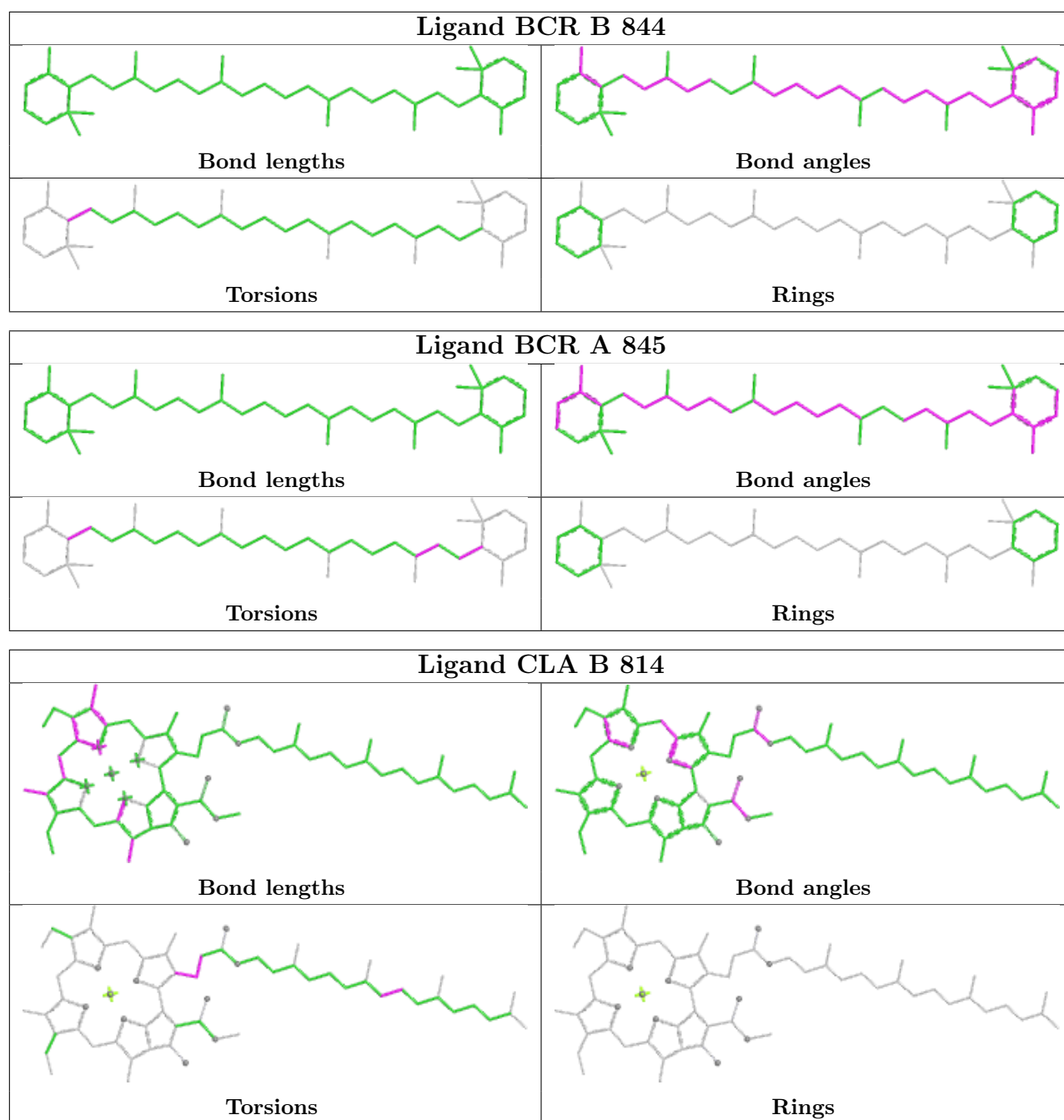
Bond angles



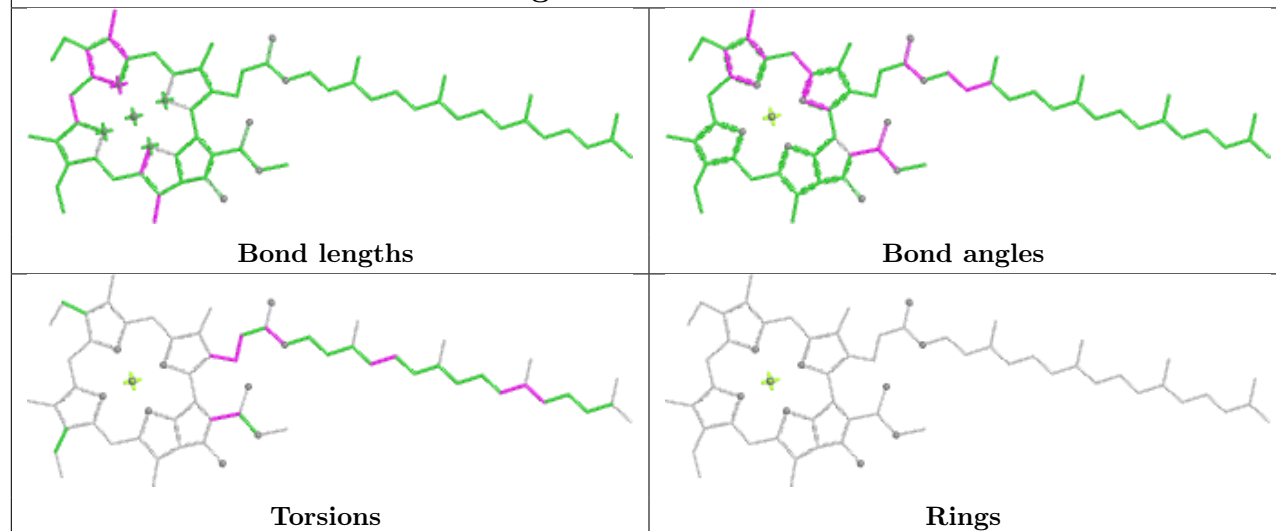
Torsions



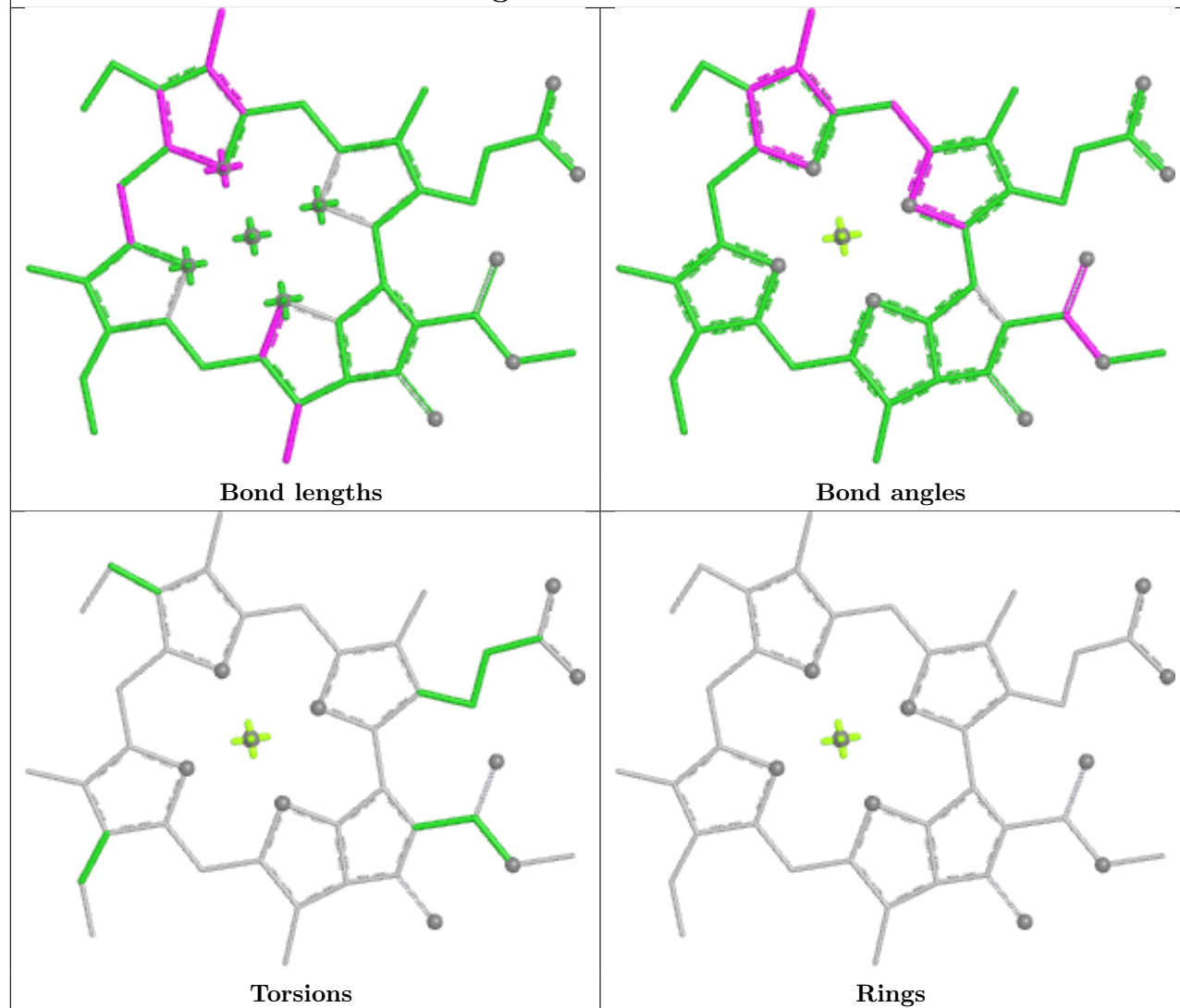
Rings

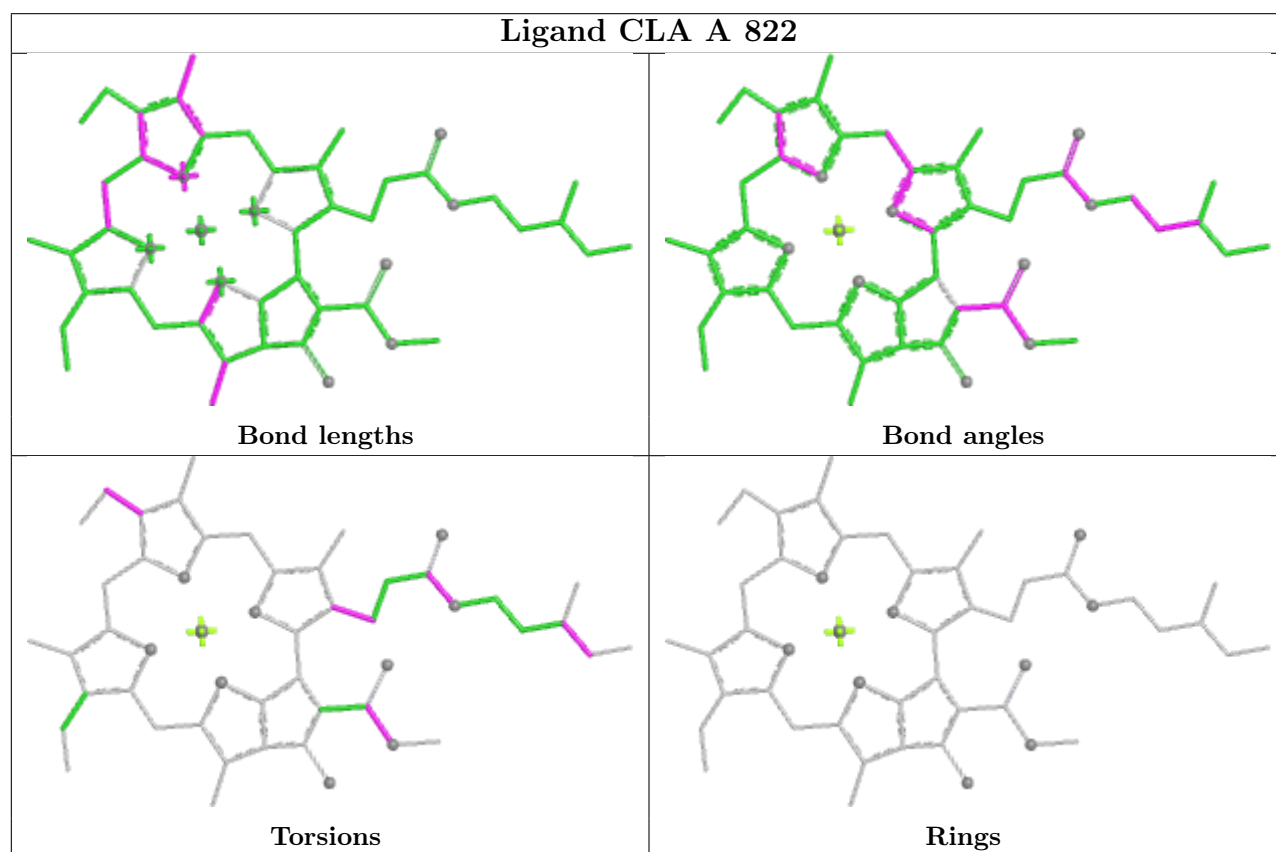
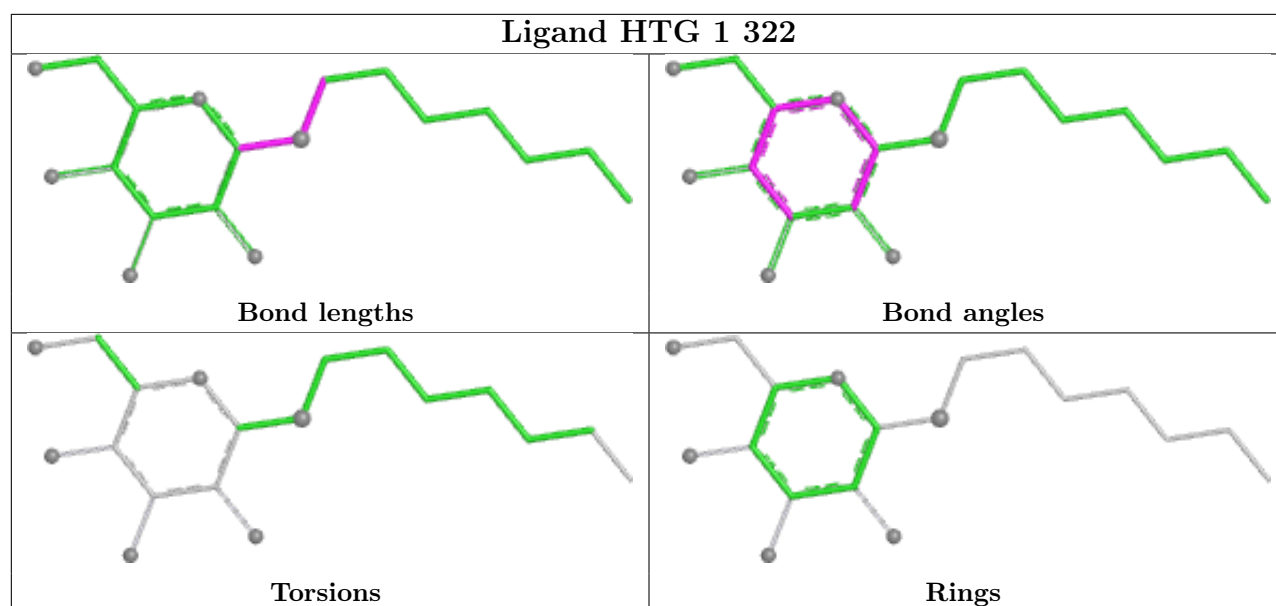


Ligand CLA A 807

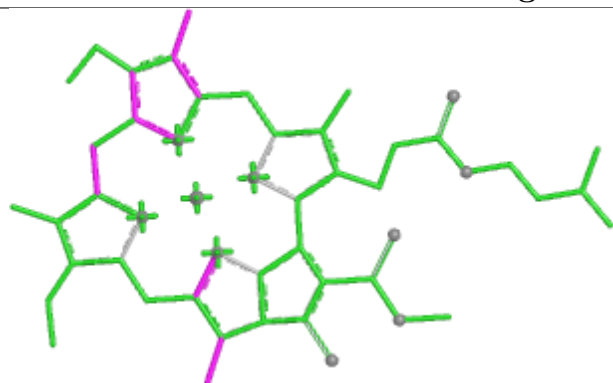


Ligand CLA B 834

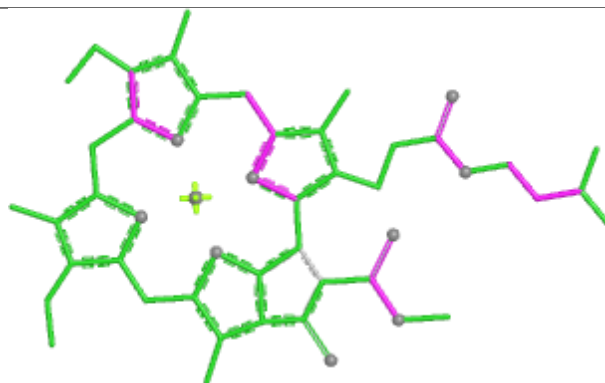




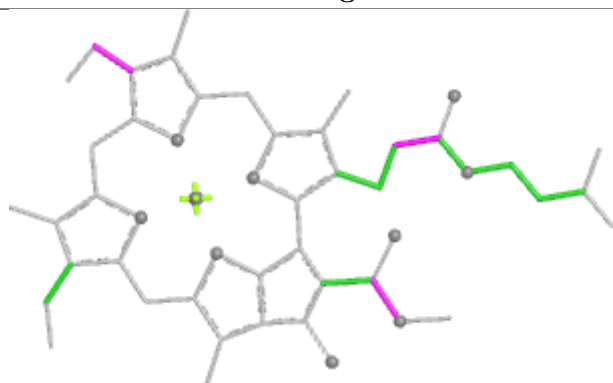
Ligand CLA 3 302



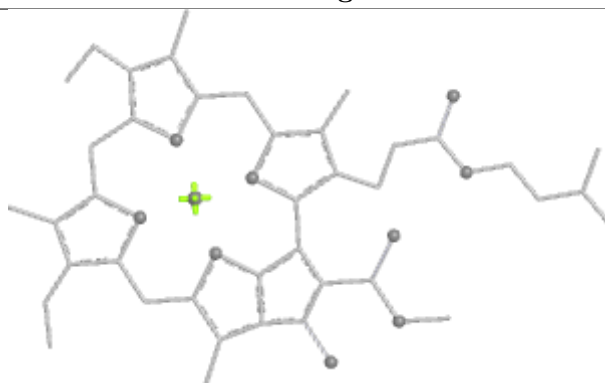
Bond lengths



Bond angles

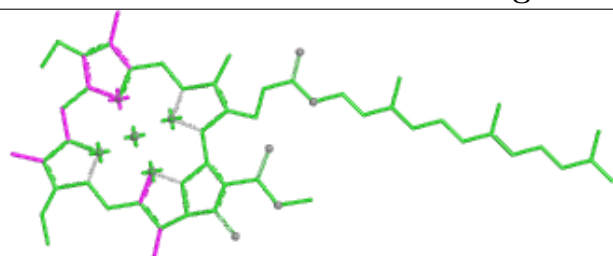


Torsions

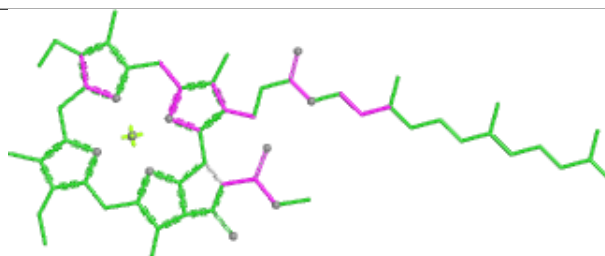


Rings

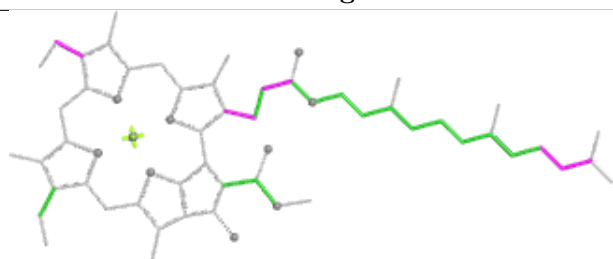
Ligand CLA K 202



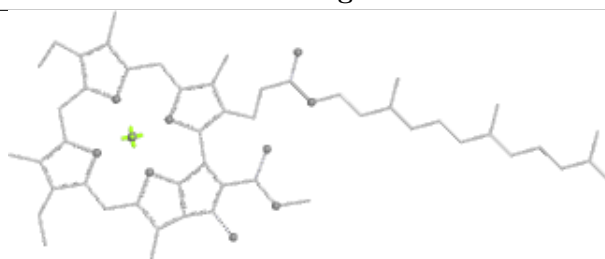
Bond lengths



Bond angles

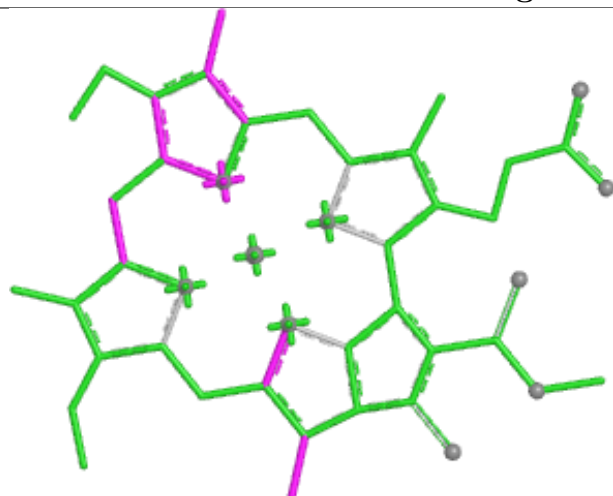


Torsions

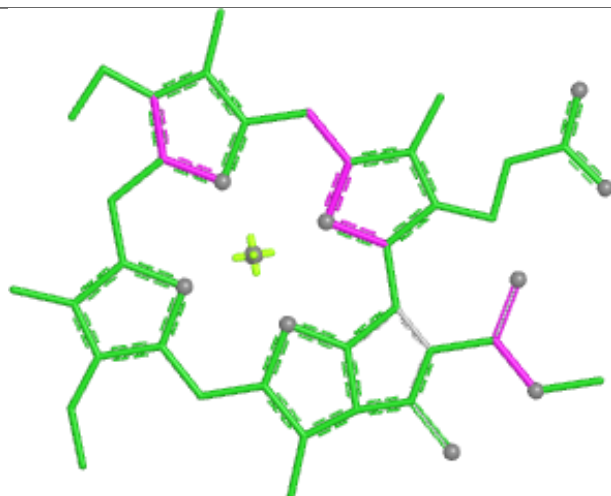


Rings

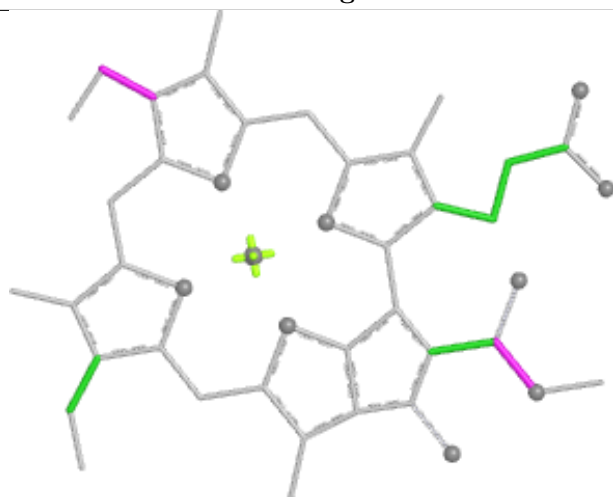
Ligand CLA F 804



Bond lengths



Bond angles

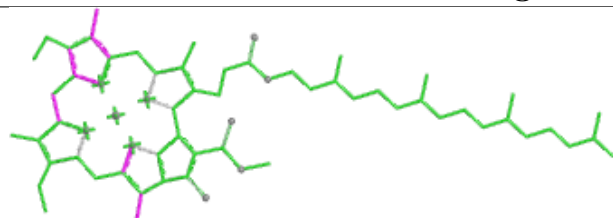


Torsions

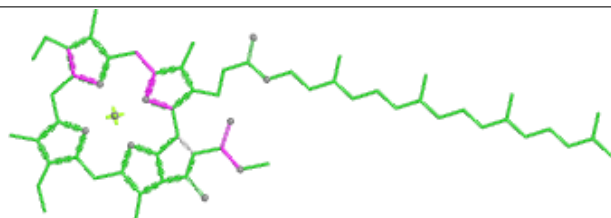


Rings

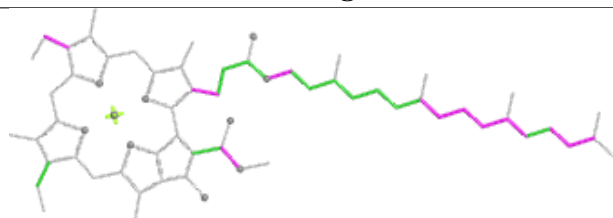
Ligand CLA A 810



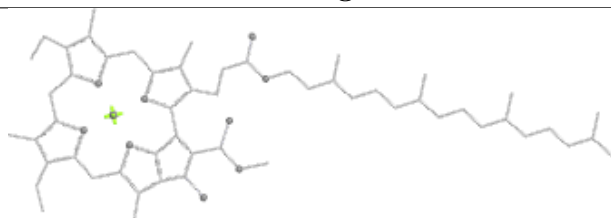
Bond lengths



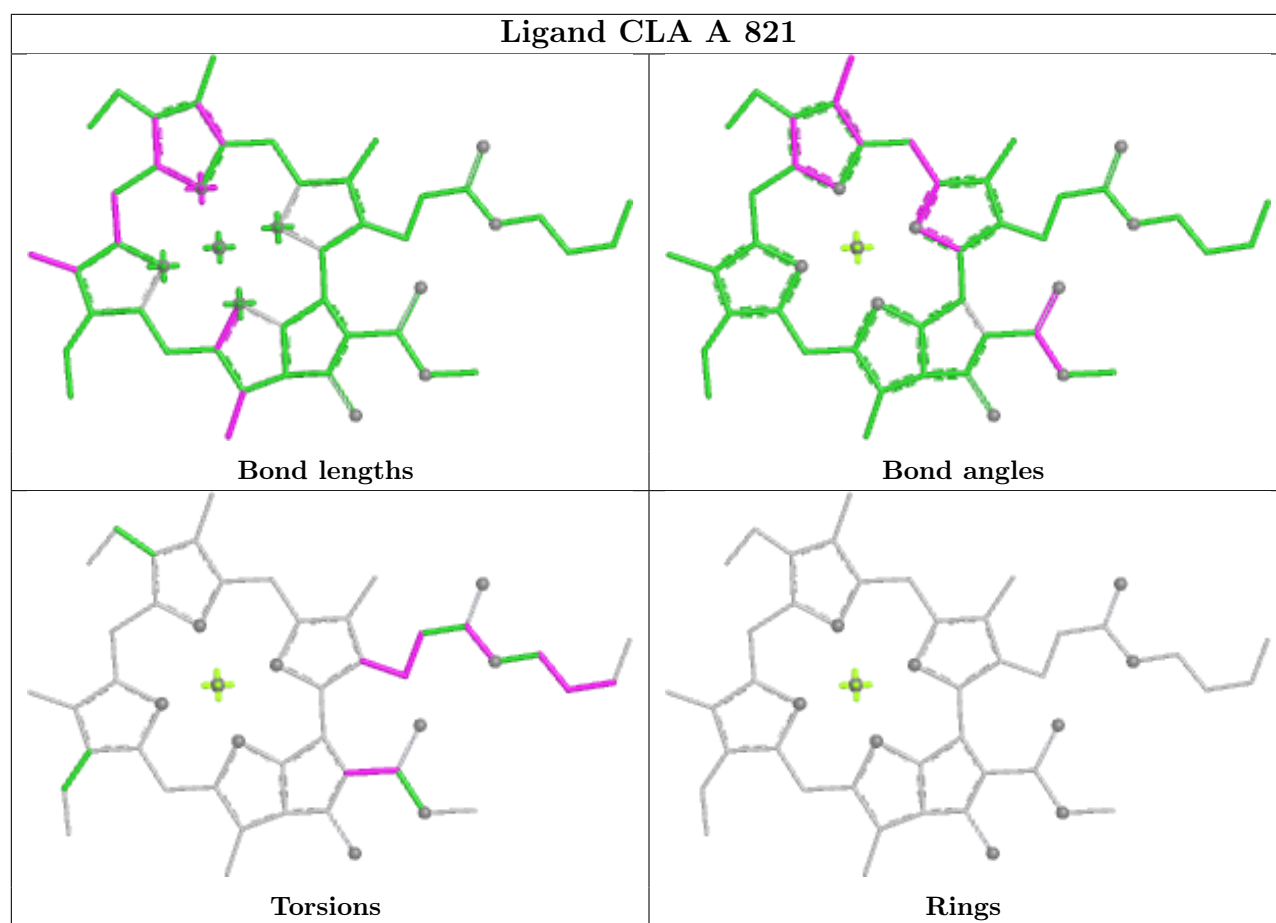
Bond angles



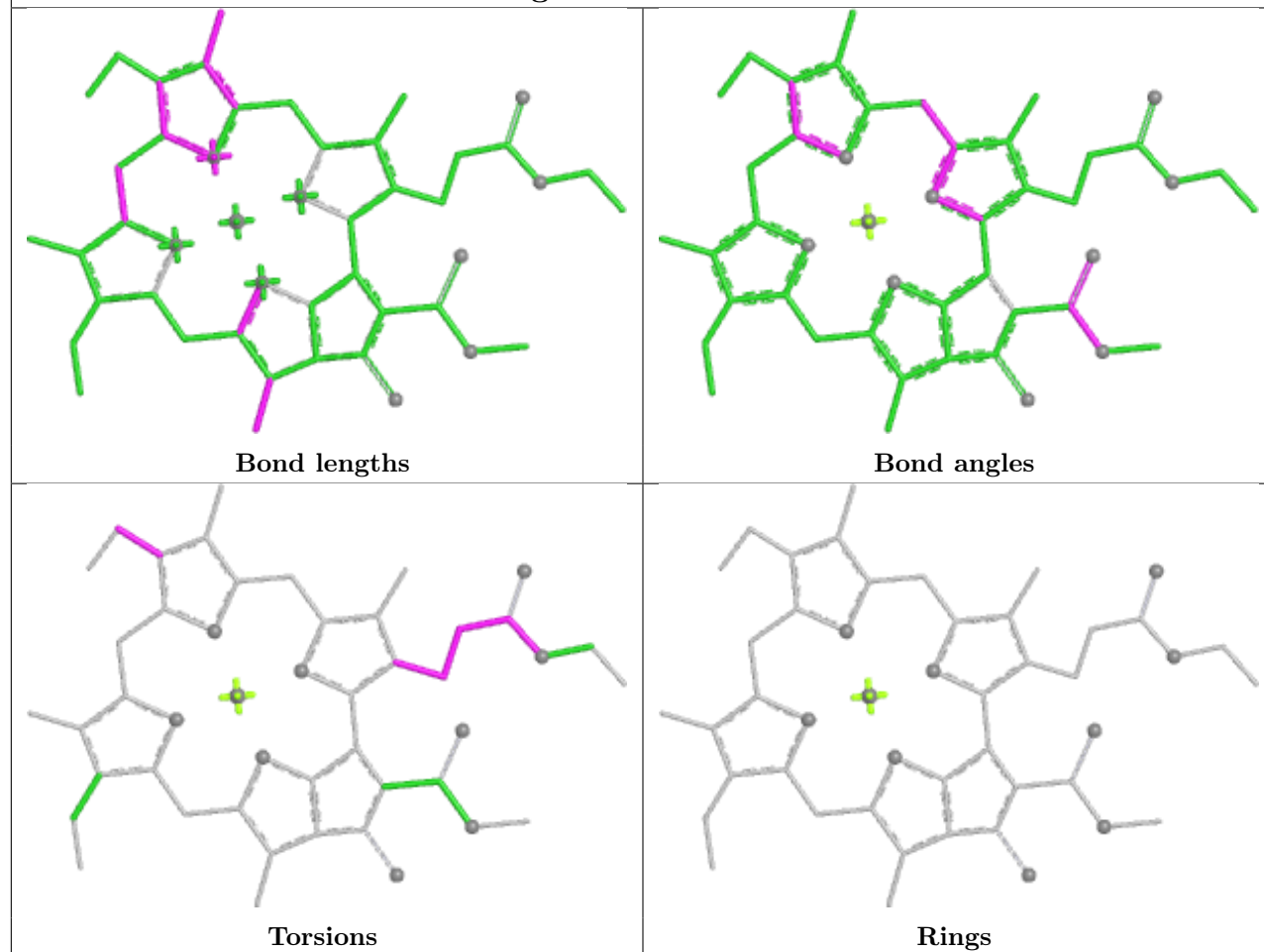
Torsions



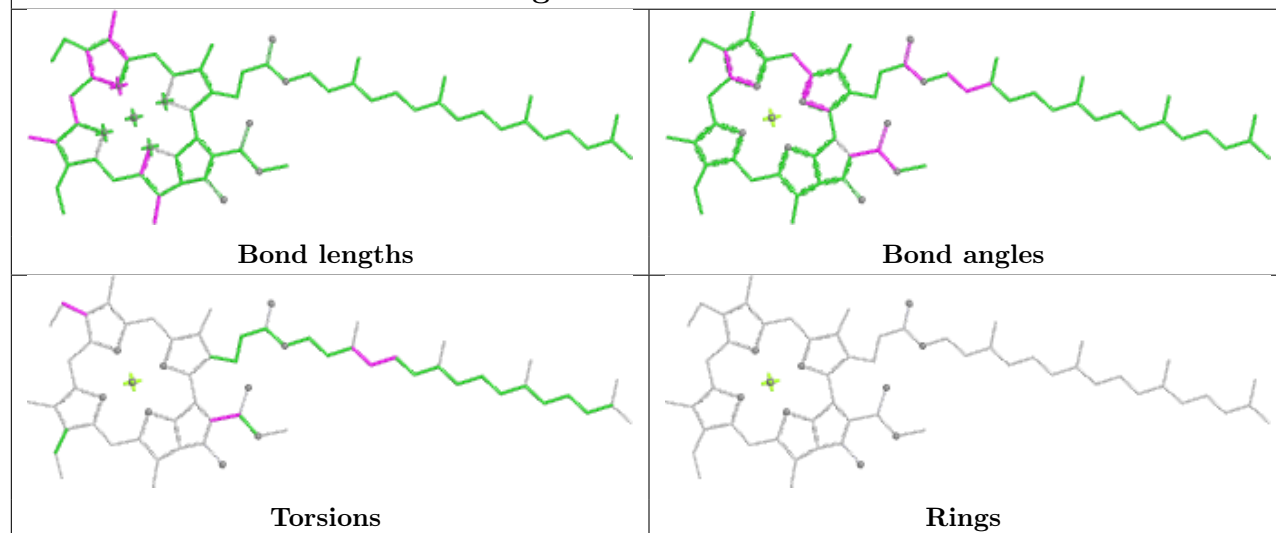
Rings



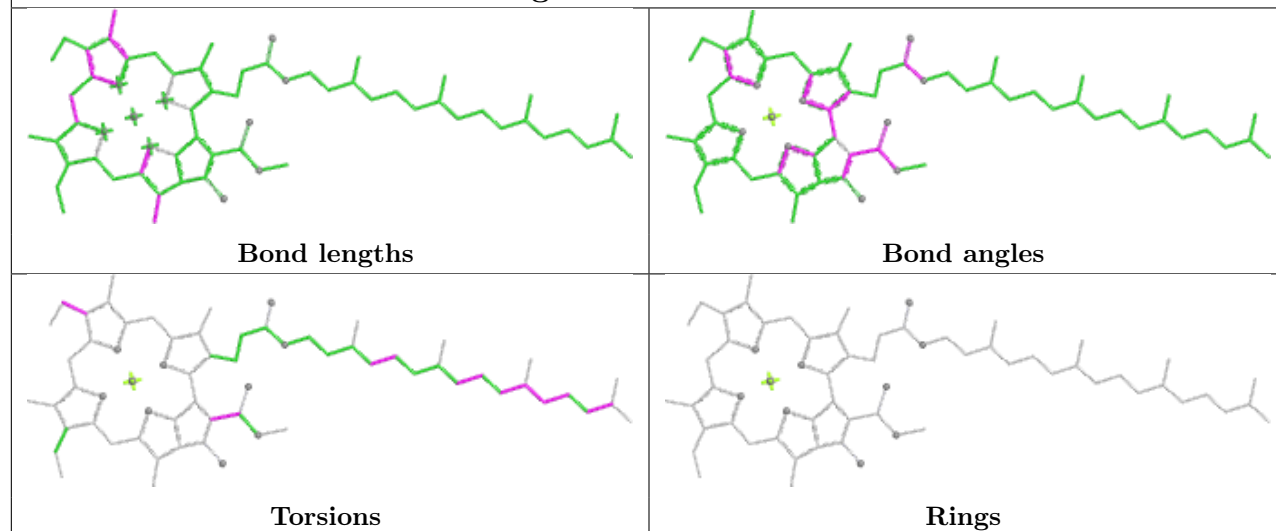
Ligand CLA 3 305



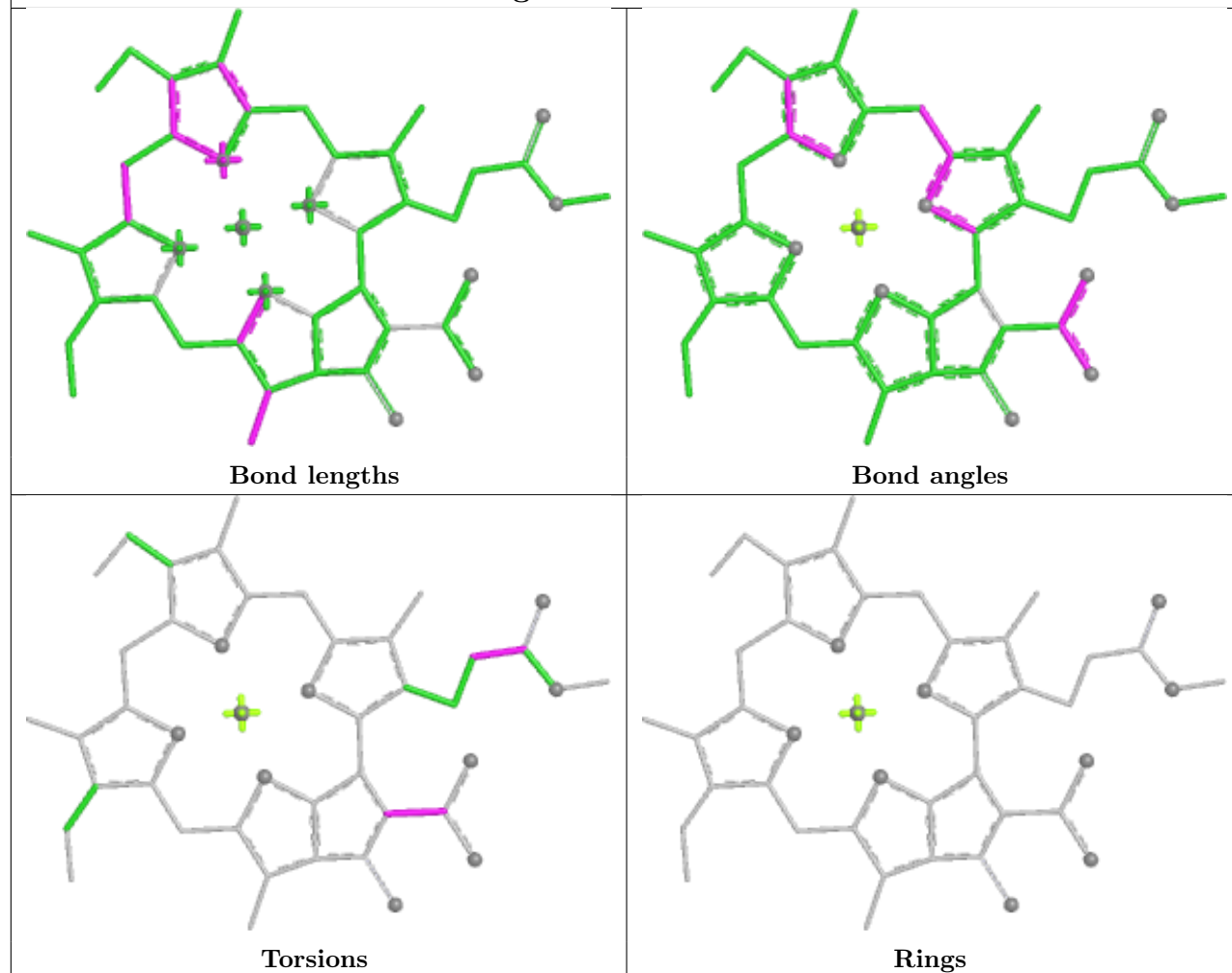
Ligand CLA B 808



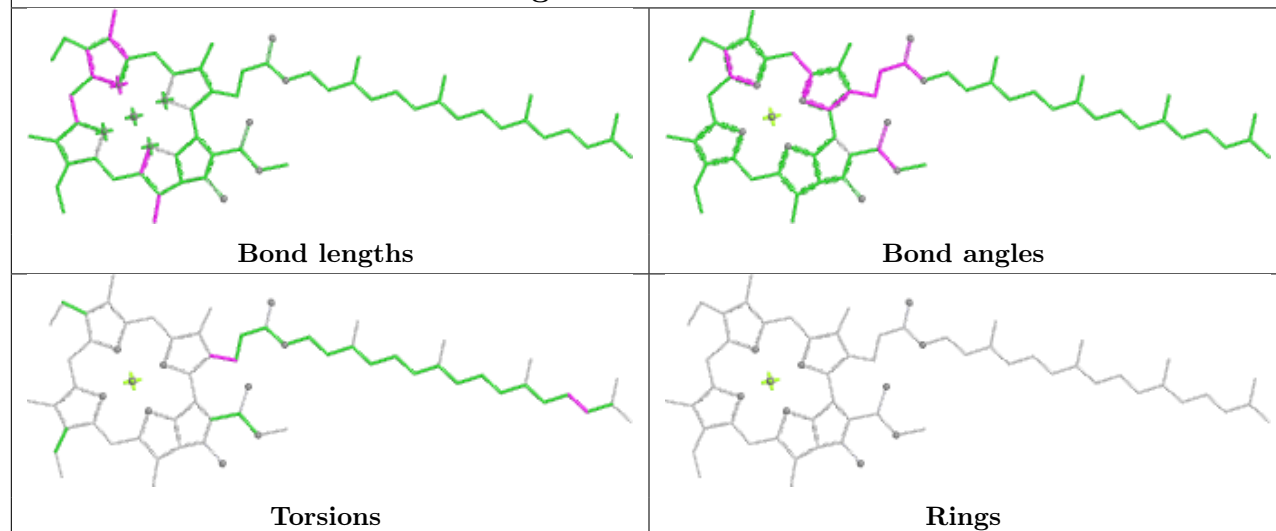
Ligand CLA A 801



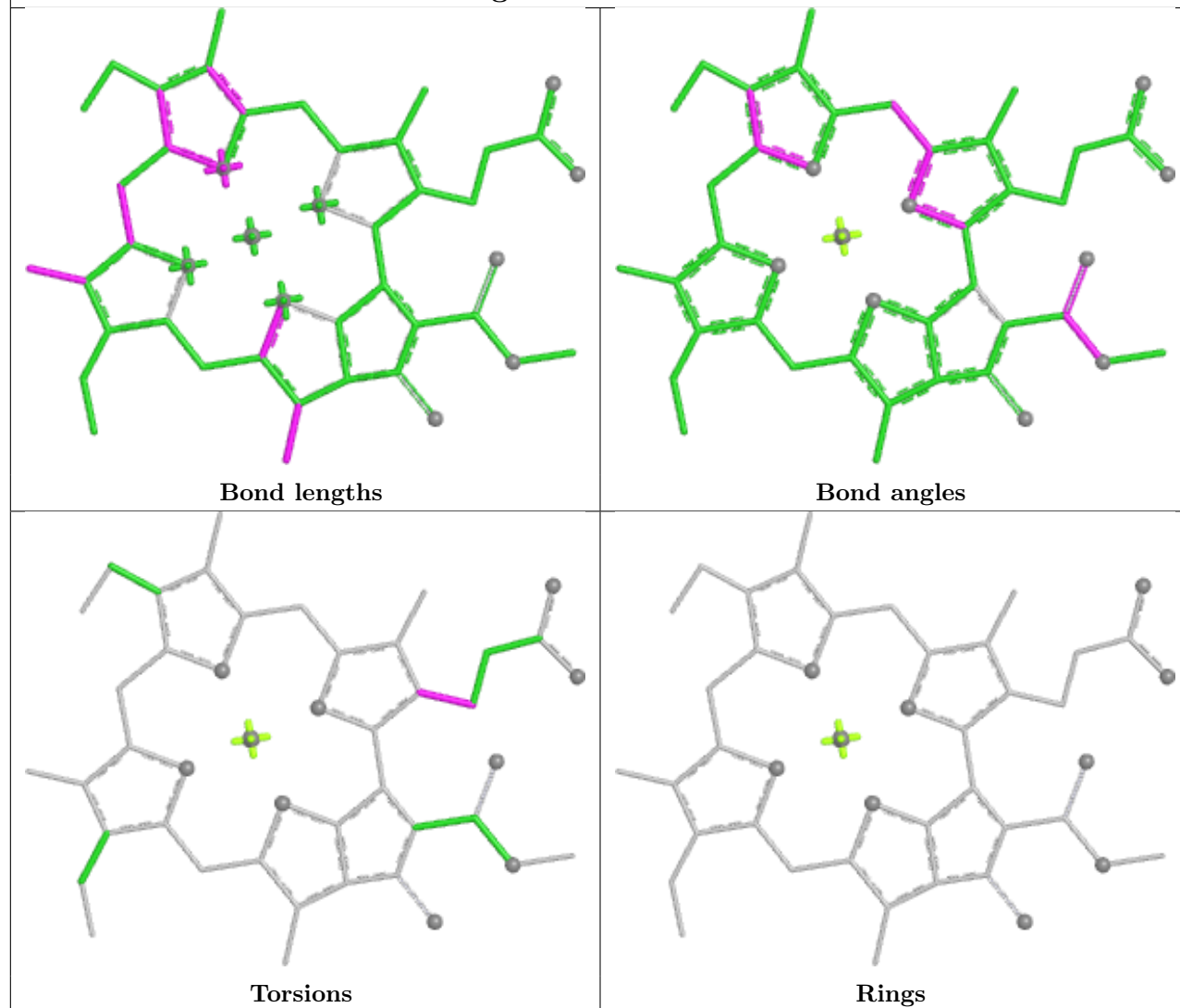
Ligand CLA N 202



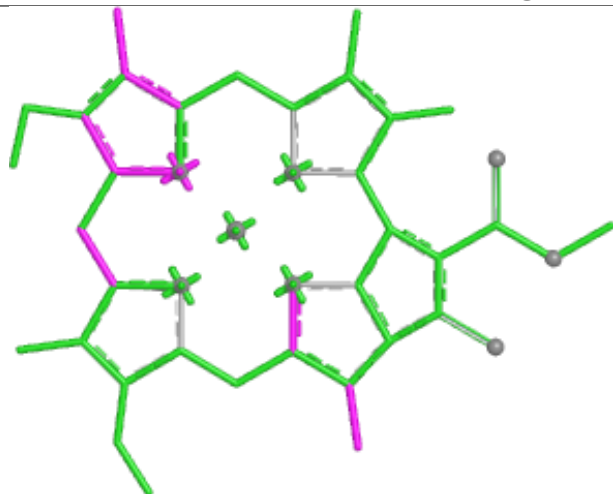
Ligand CLA A 825



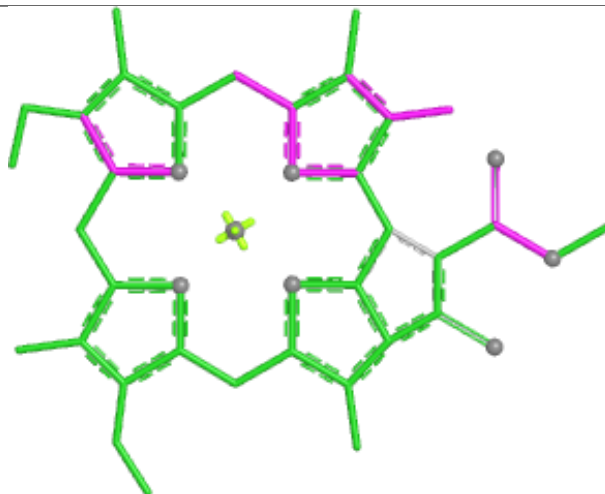
Ligand CLA A 813



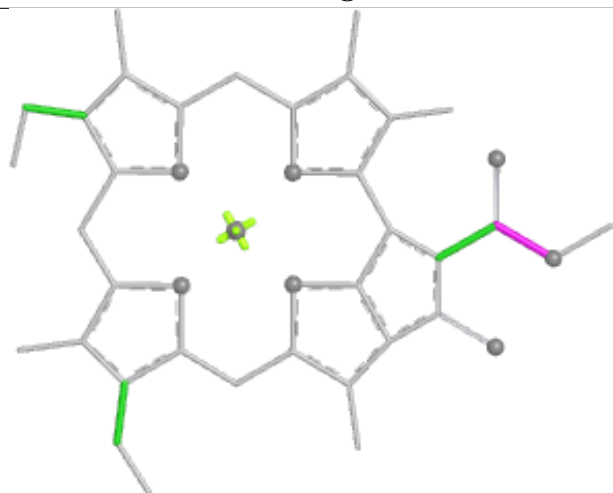
Ligand CLA 2 310



Bond lengths



Bond angles

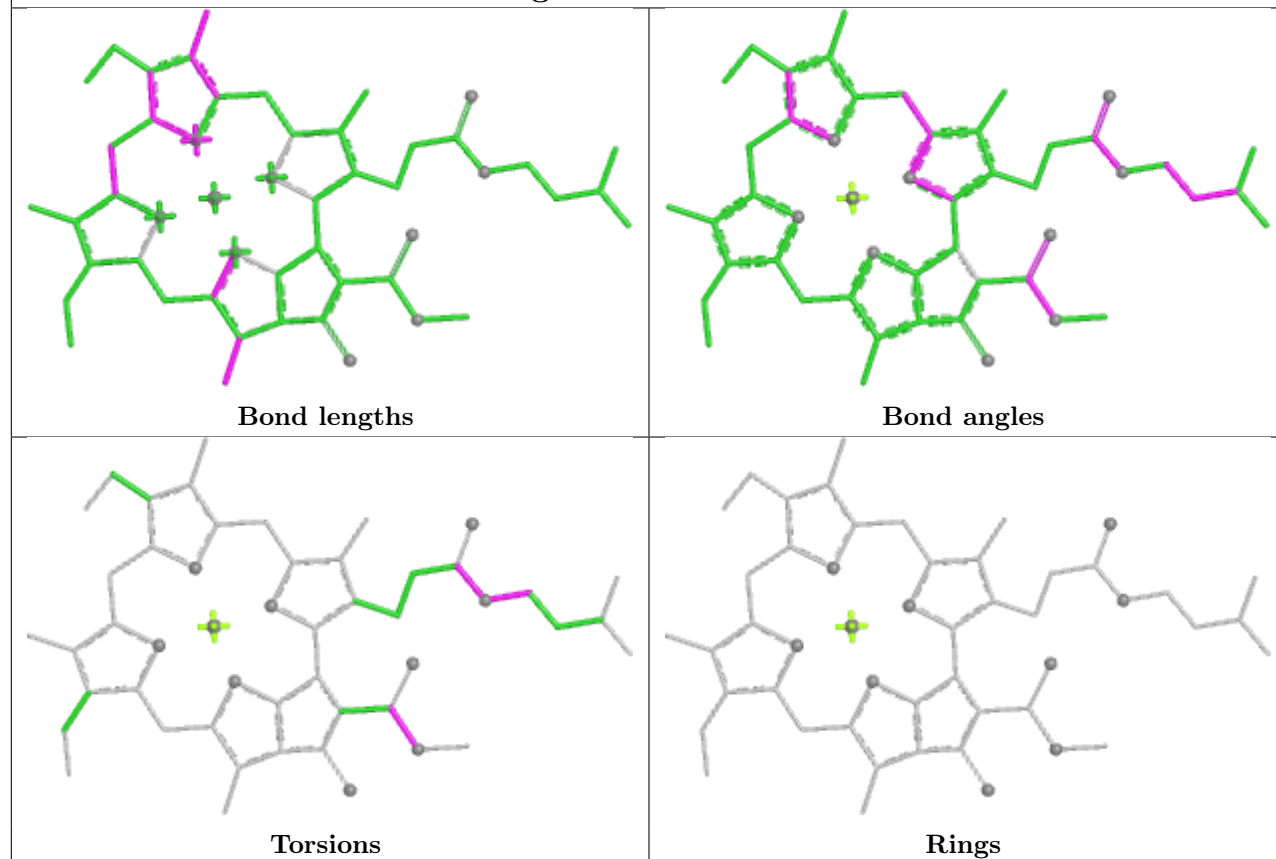


Torsions

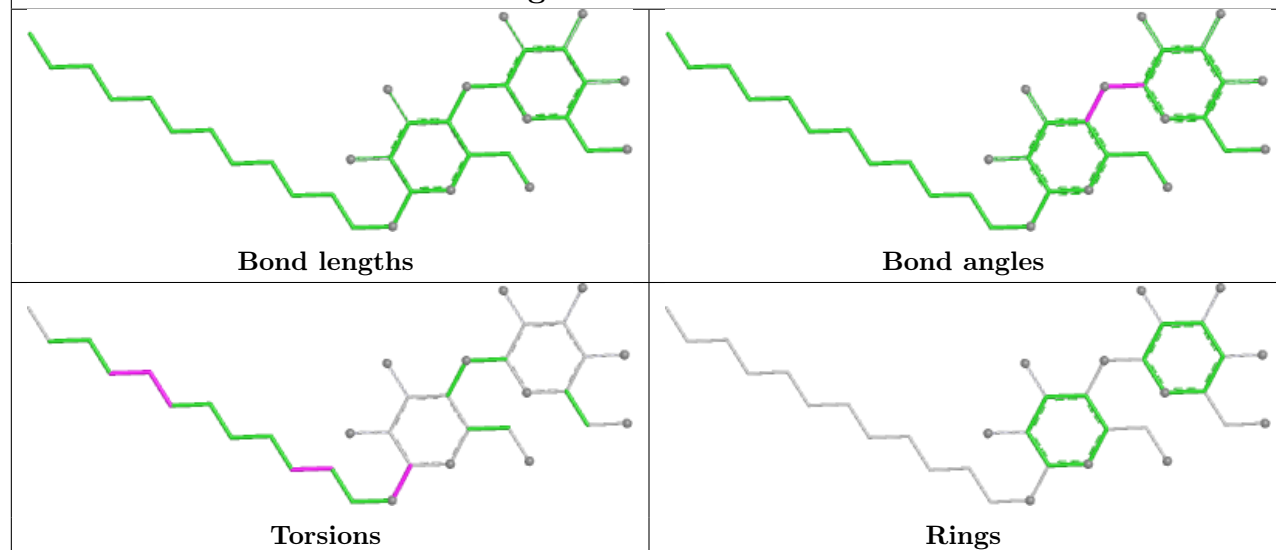


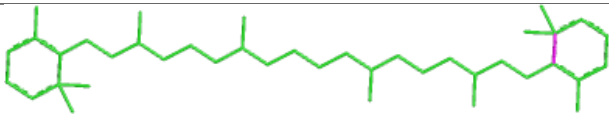
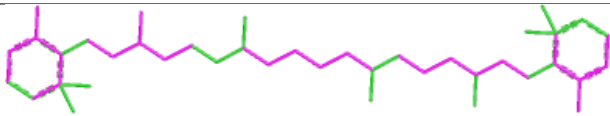
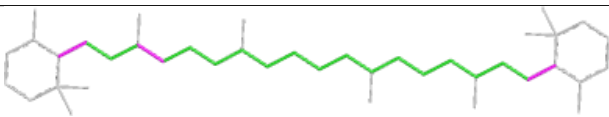
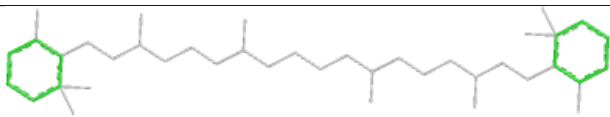
Rings

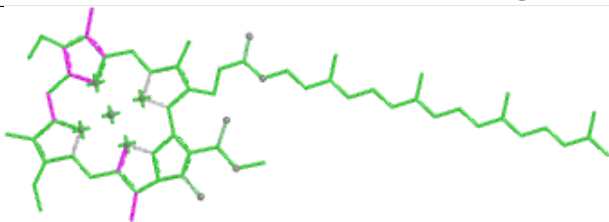
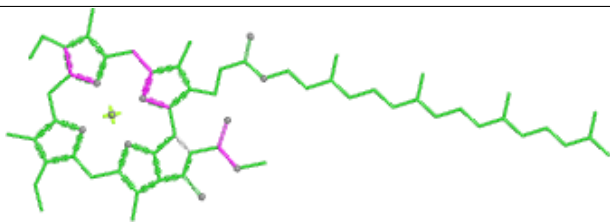
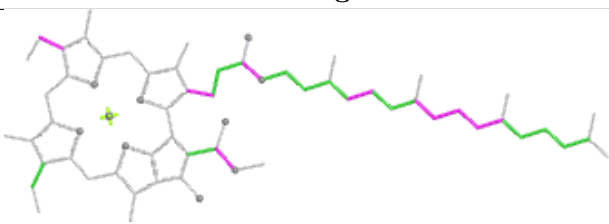
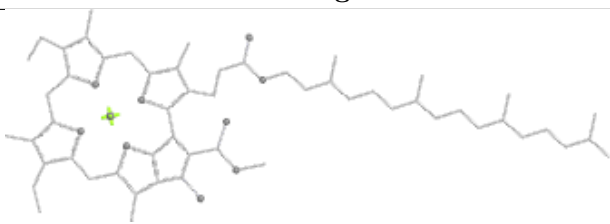
Ligand CLA A 814

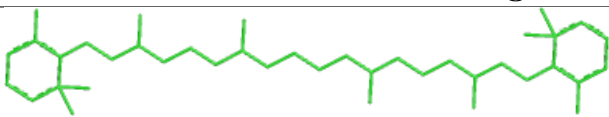
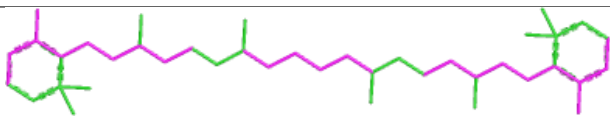
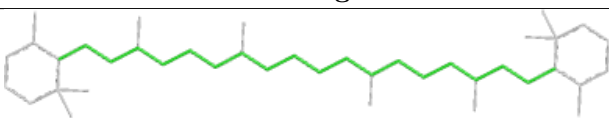
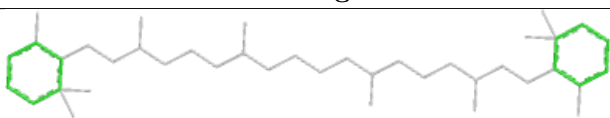


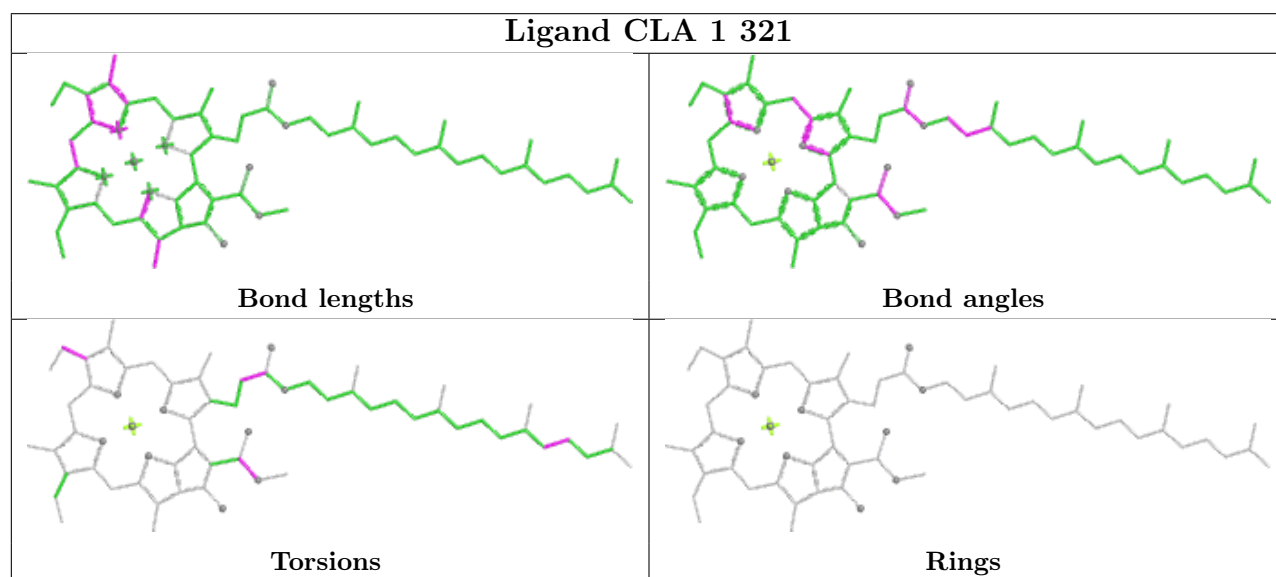
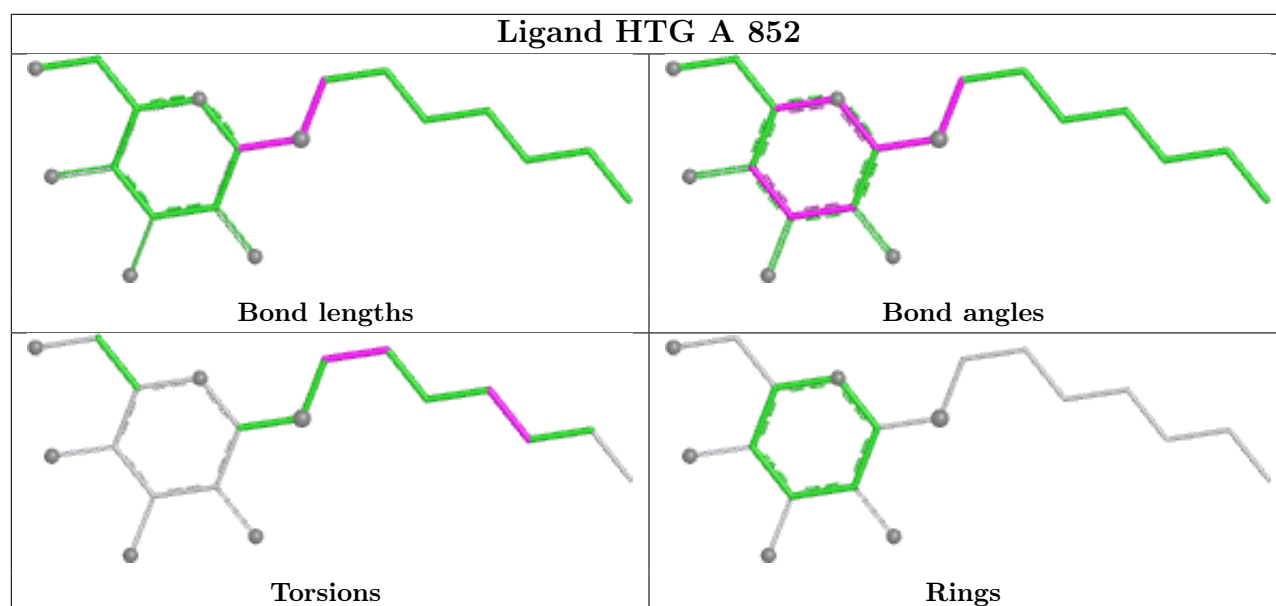
Ligand LMT G 601

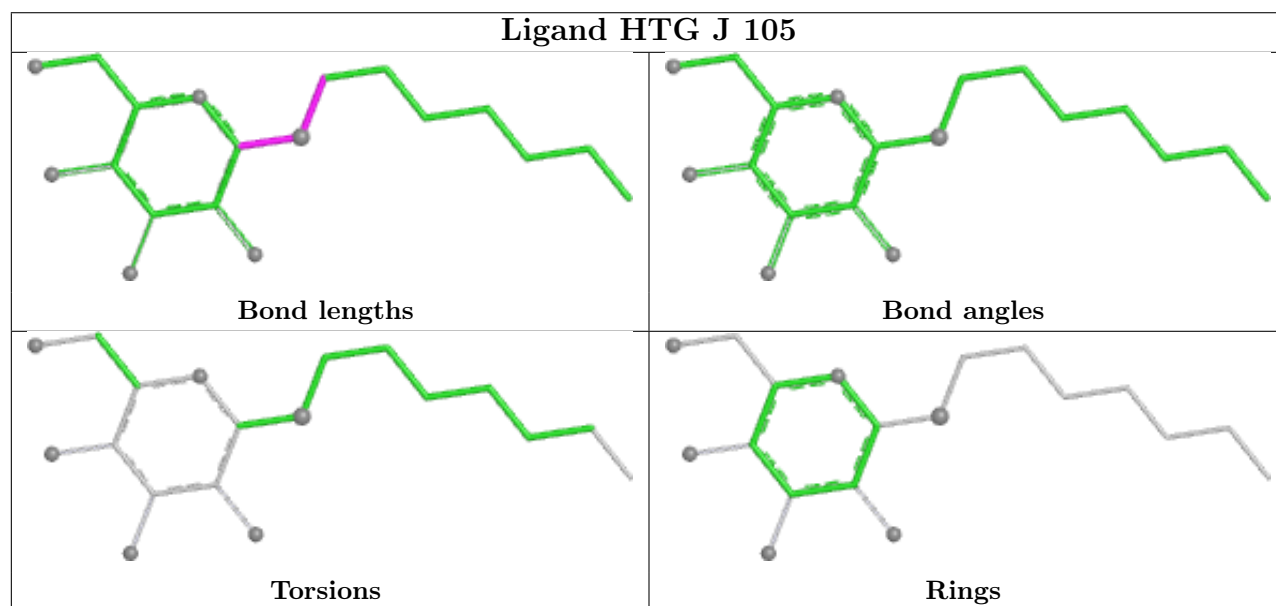
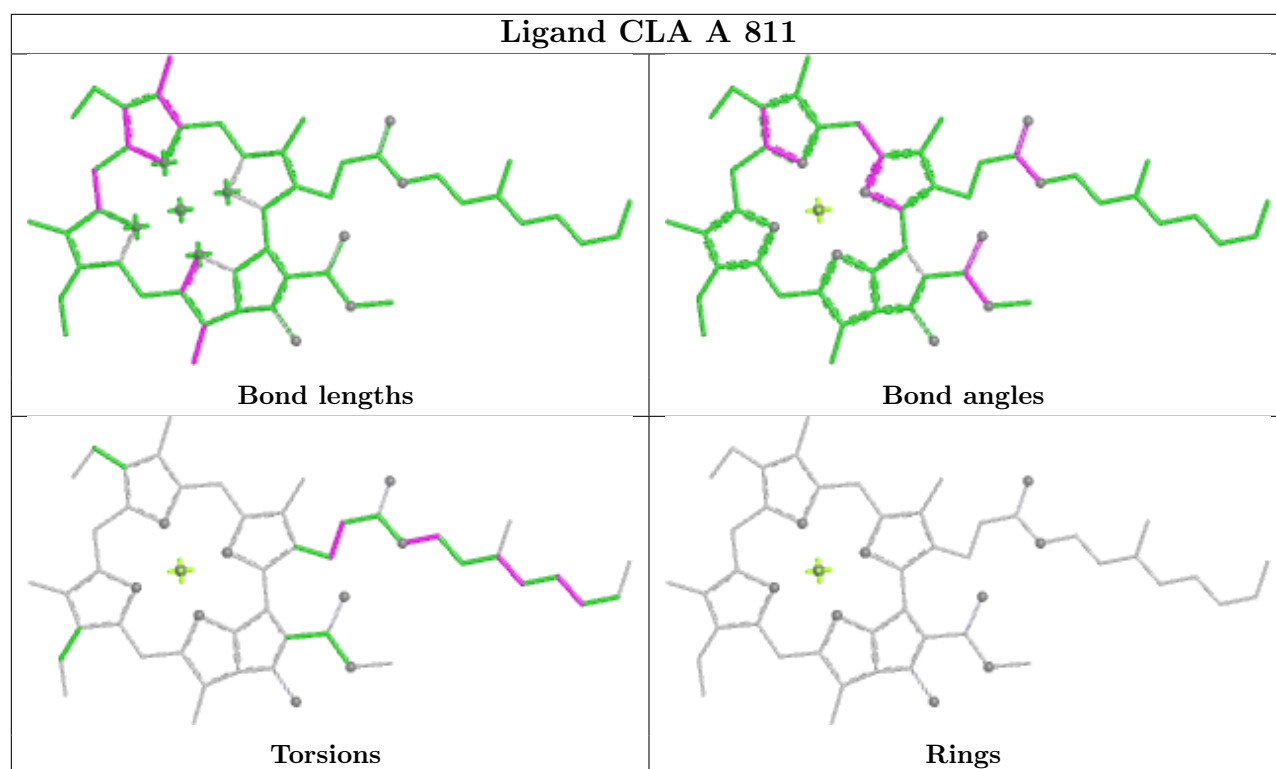


Ligand BCR B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

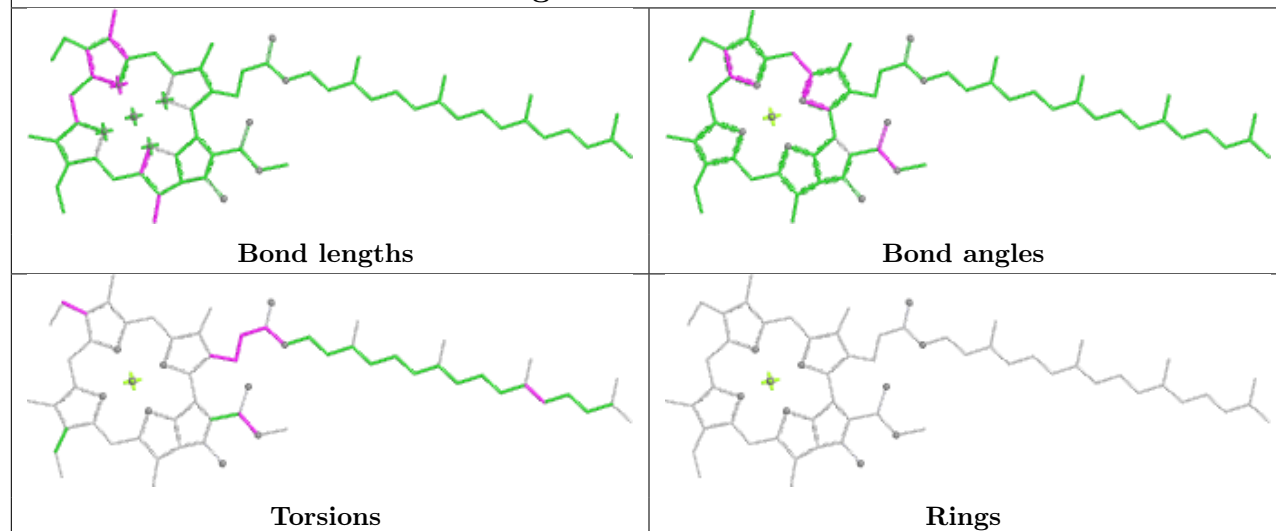
Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

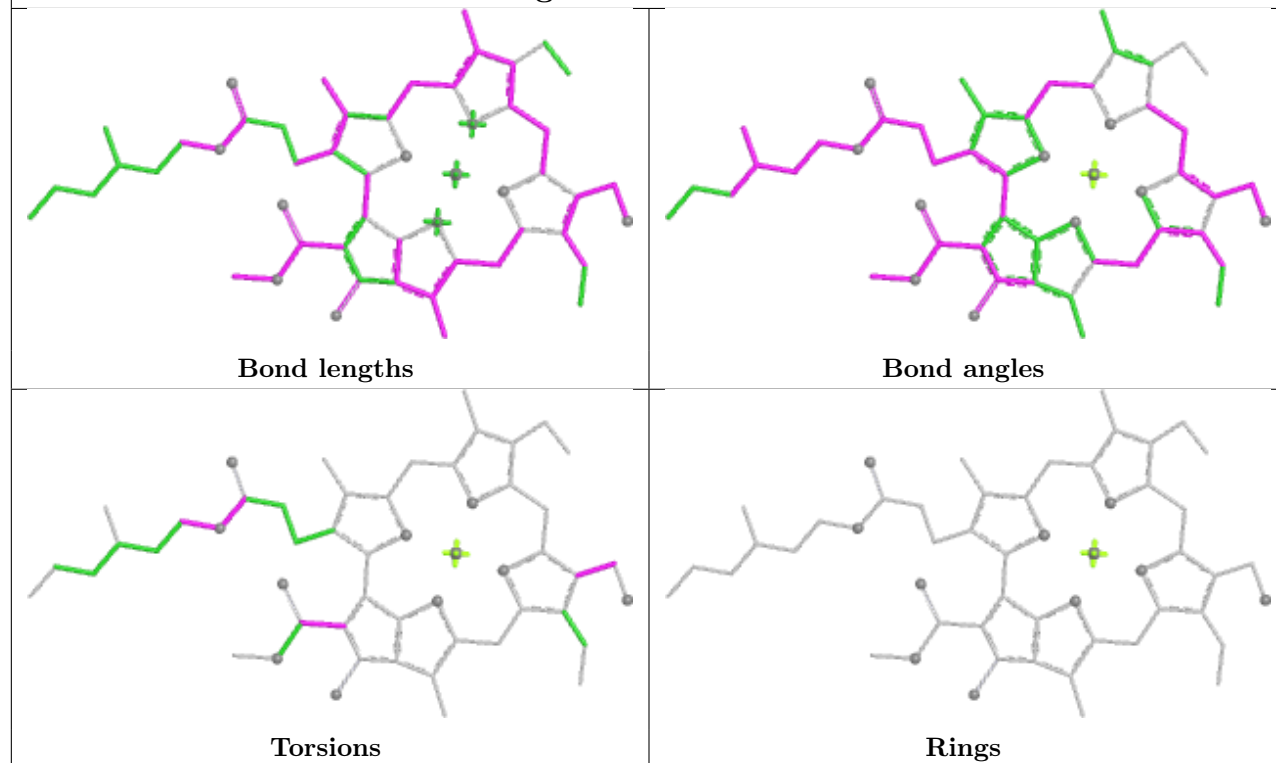




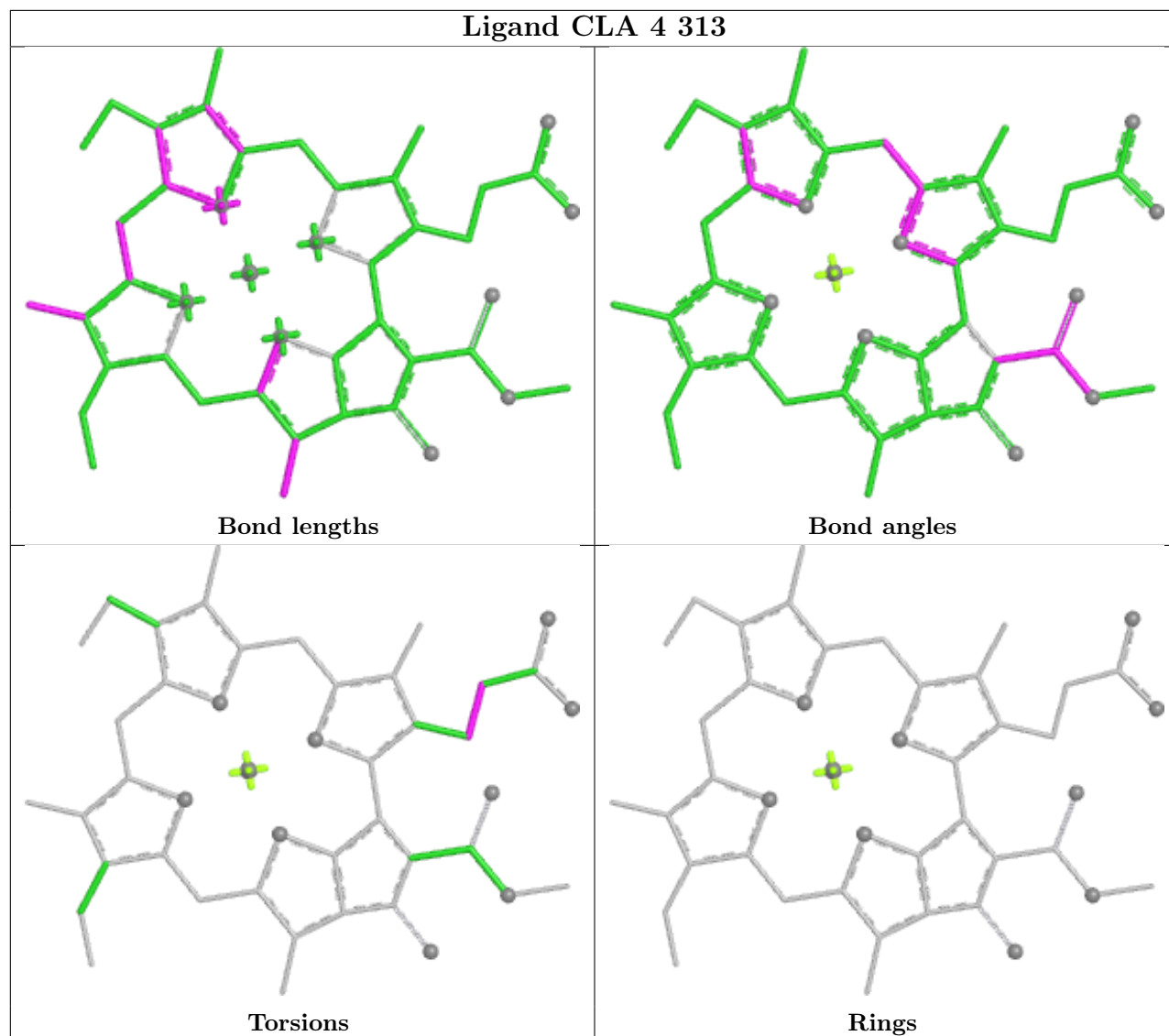
Ligand CLA B 831



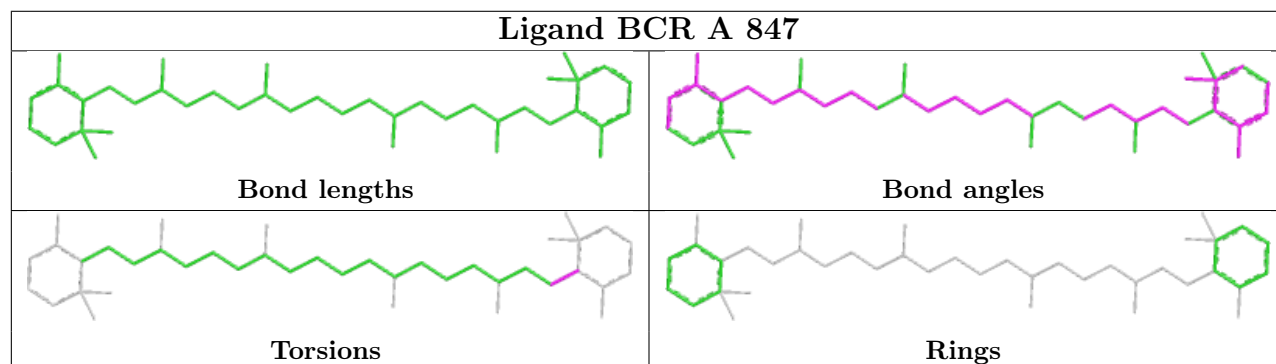
Ligand CHL 2 301

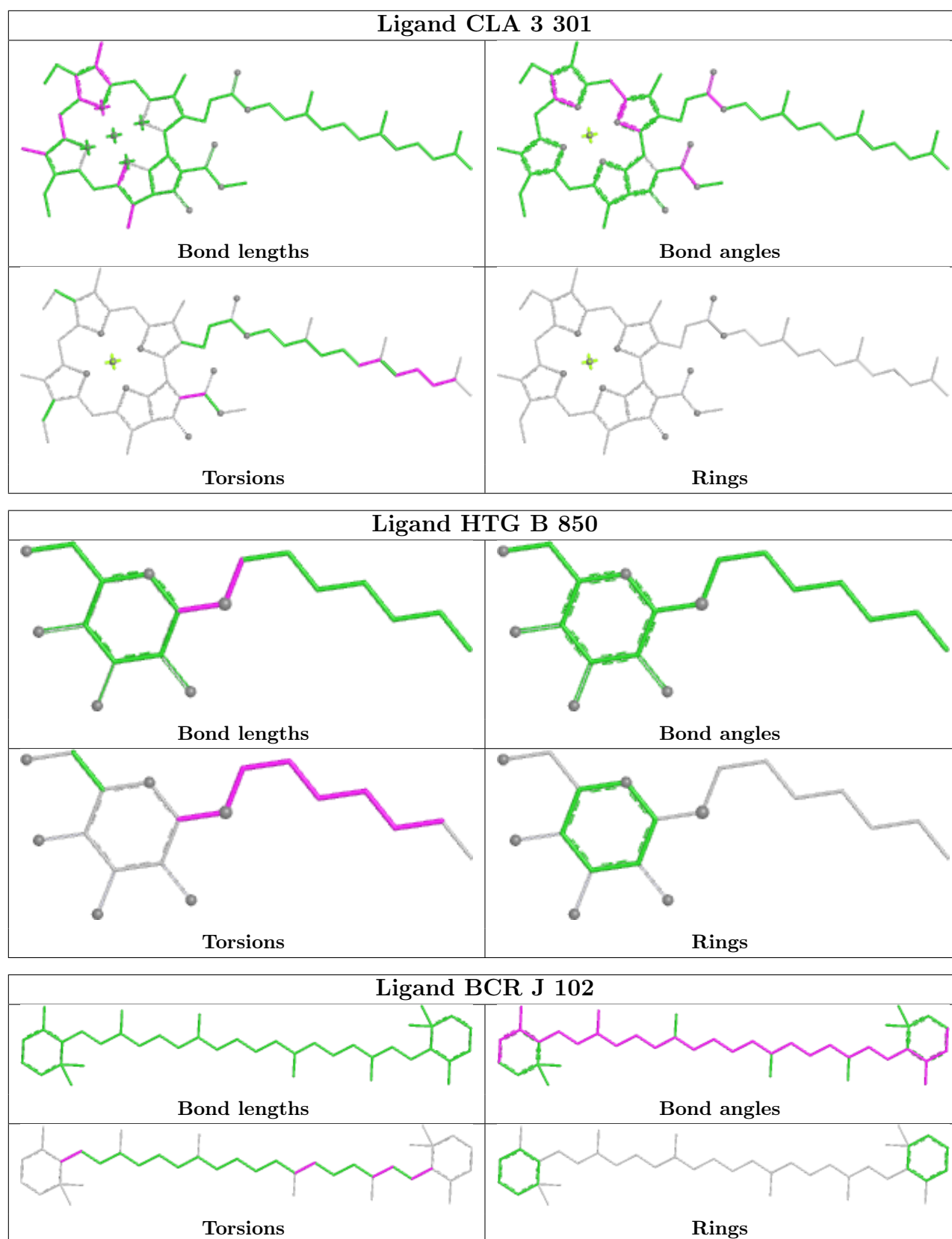


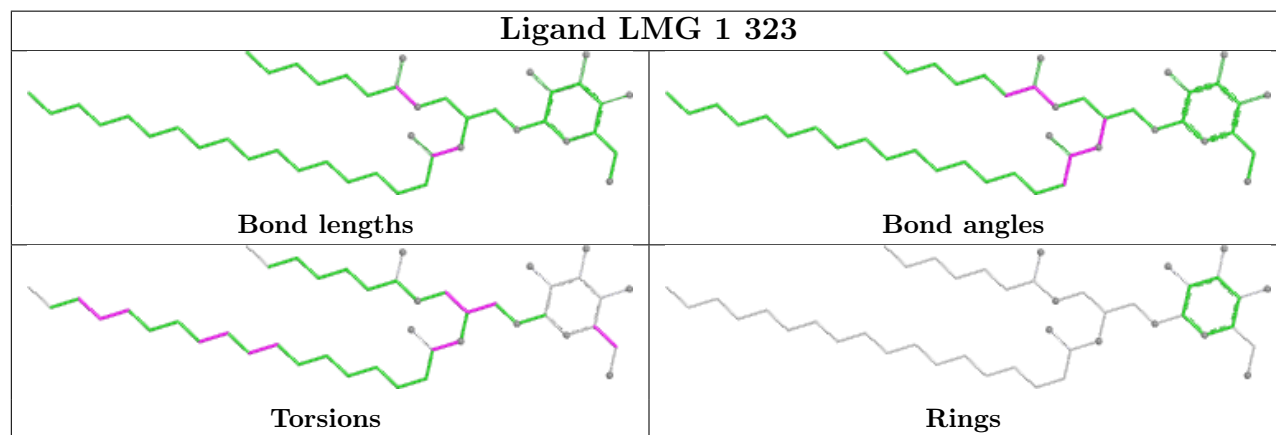
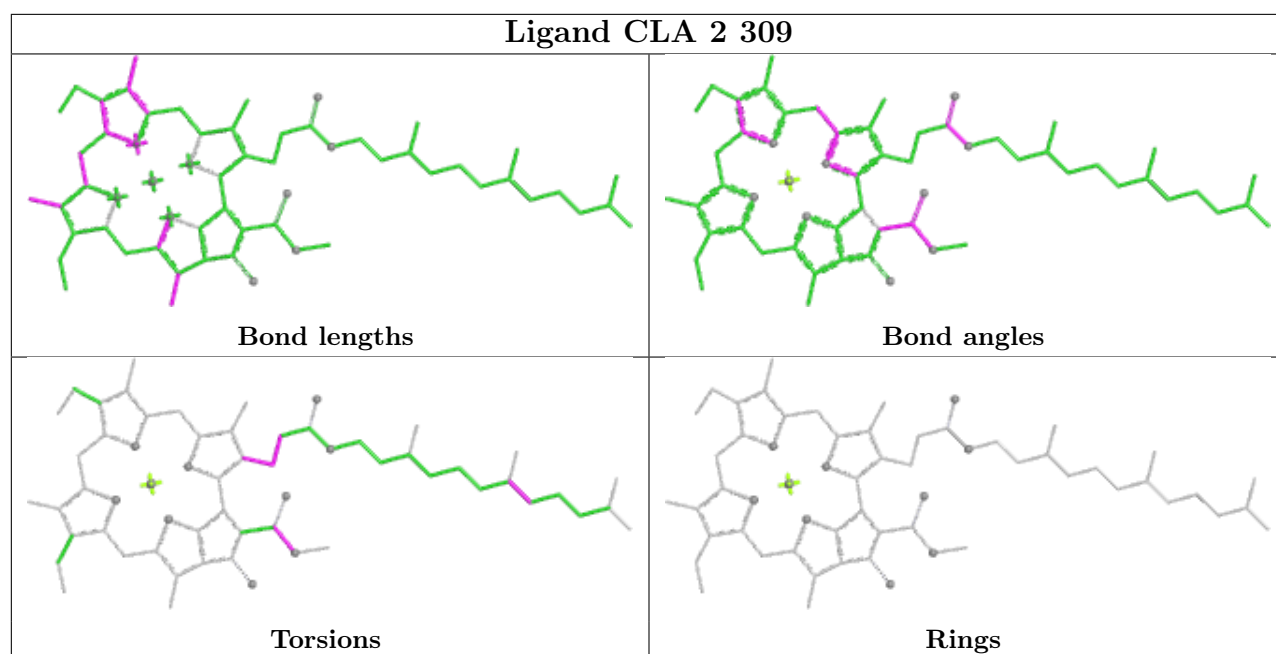
Ligand CLA 4 313



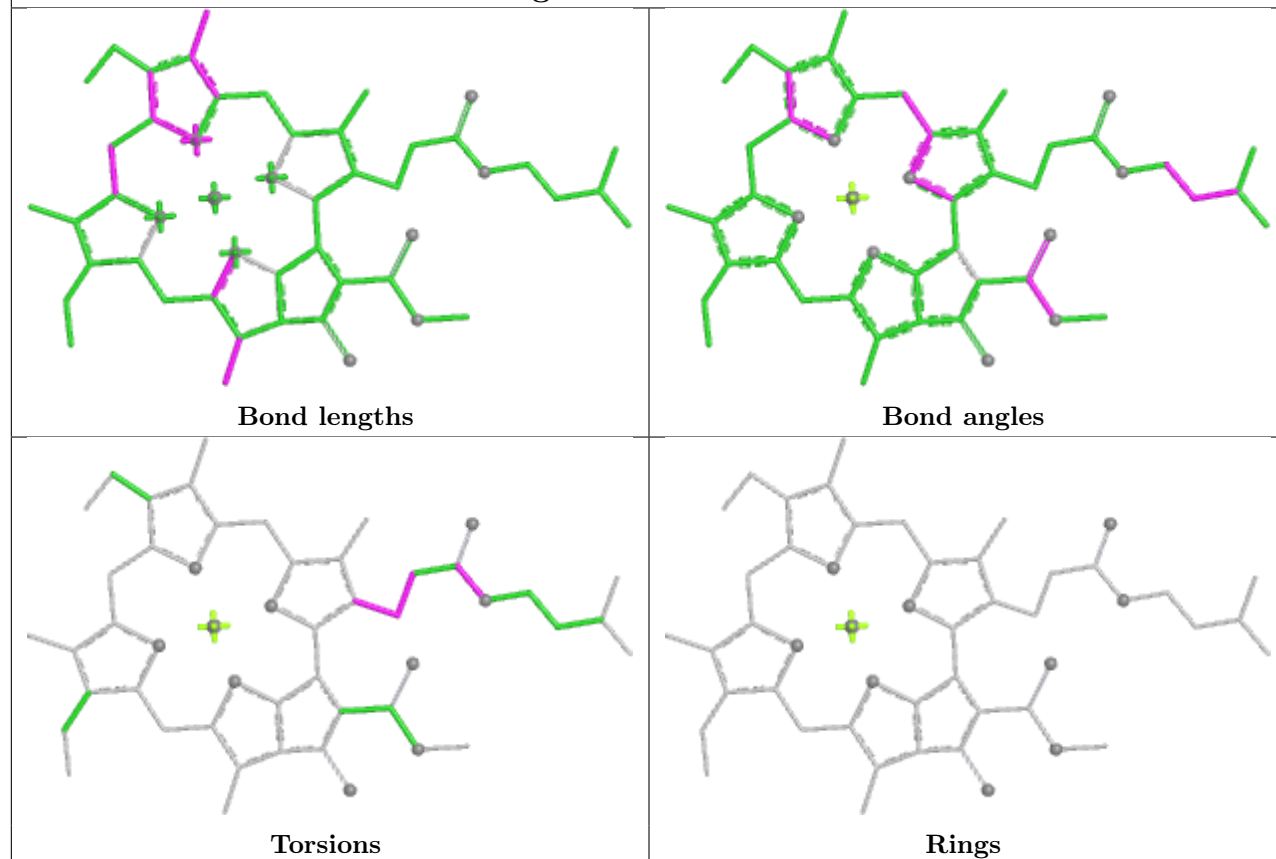
Ligand BCR A 847



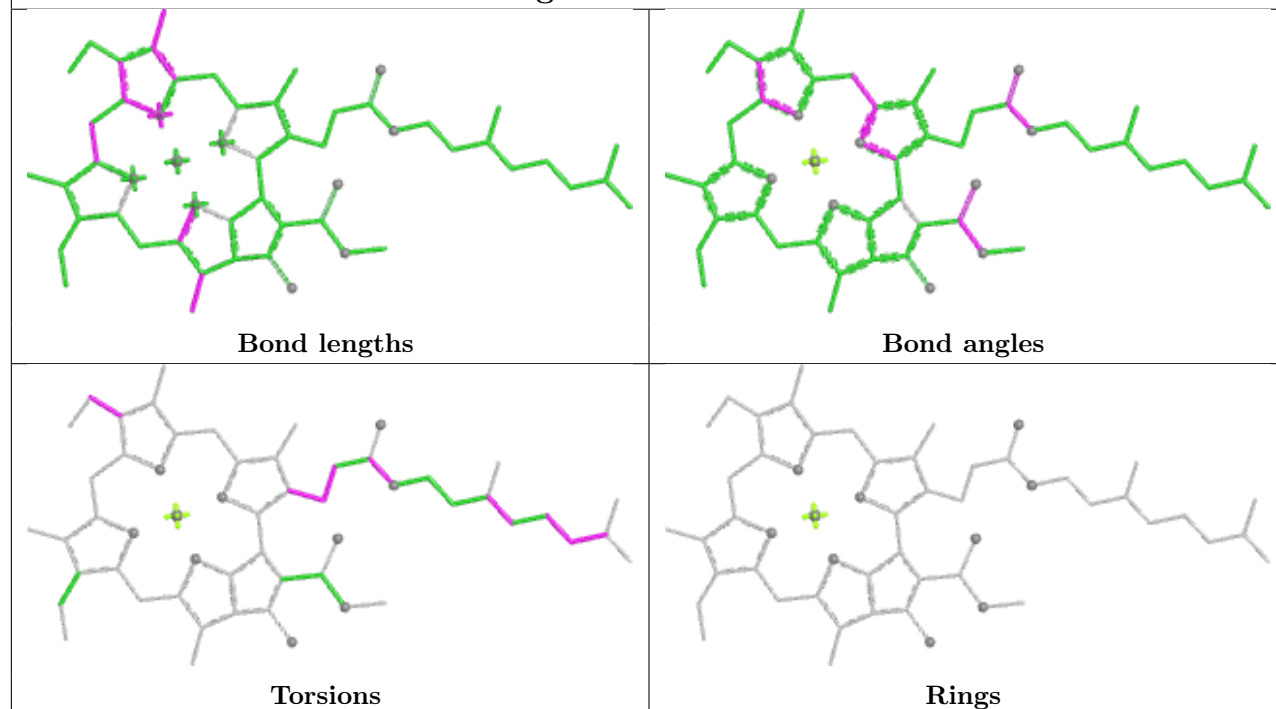




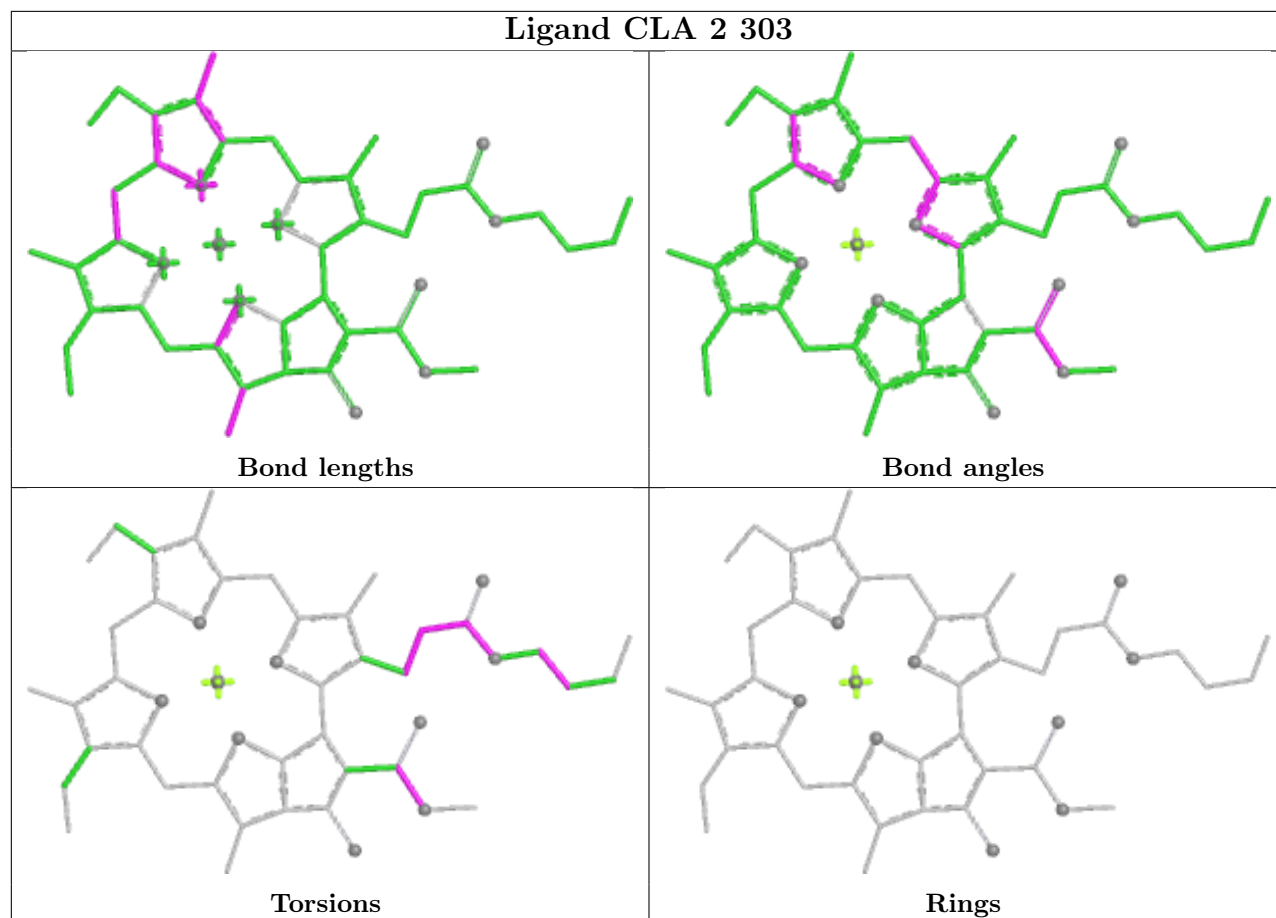
Ligand CLA B 830



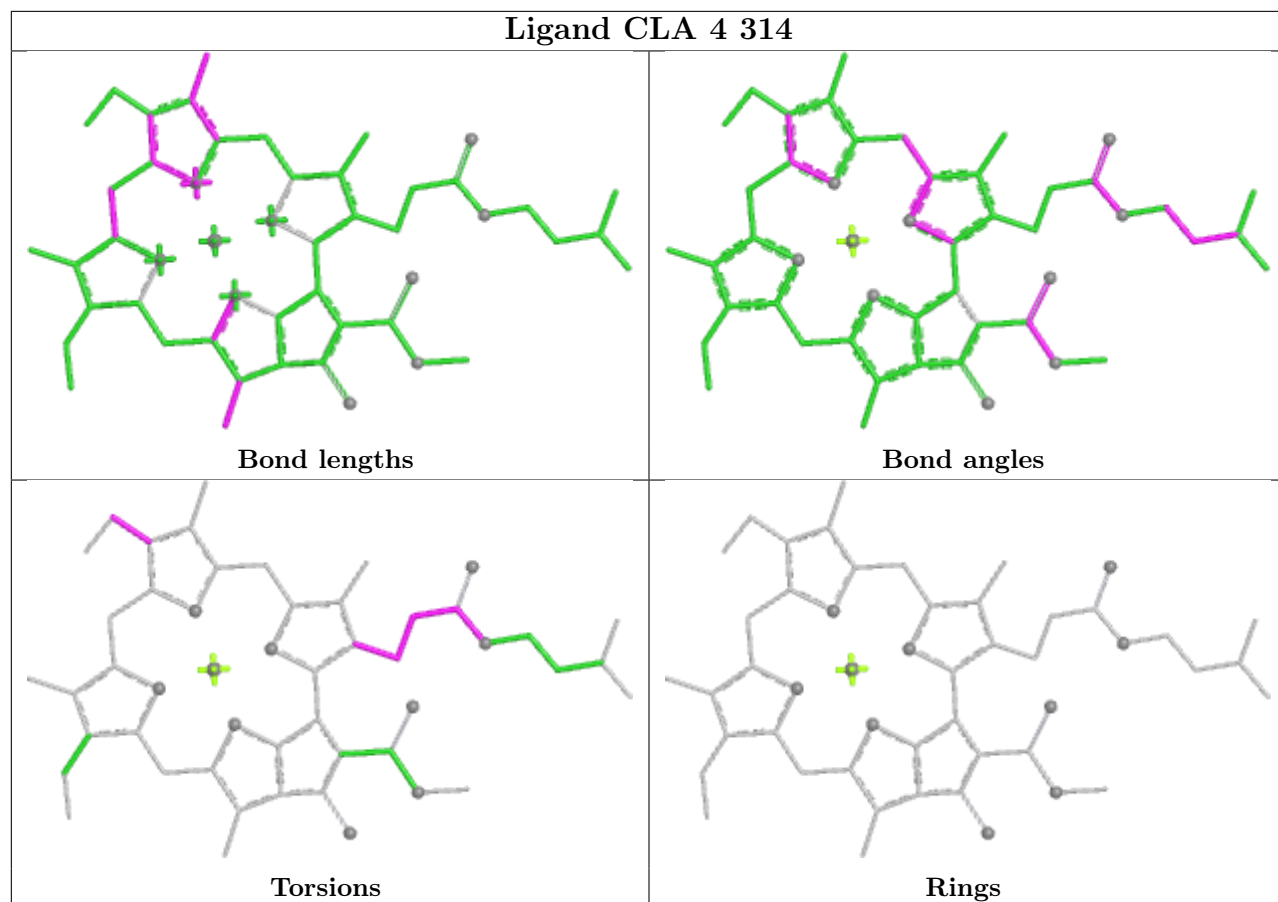
Ligand CLA 1 313

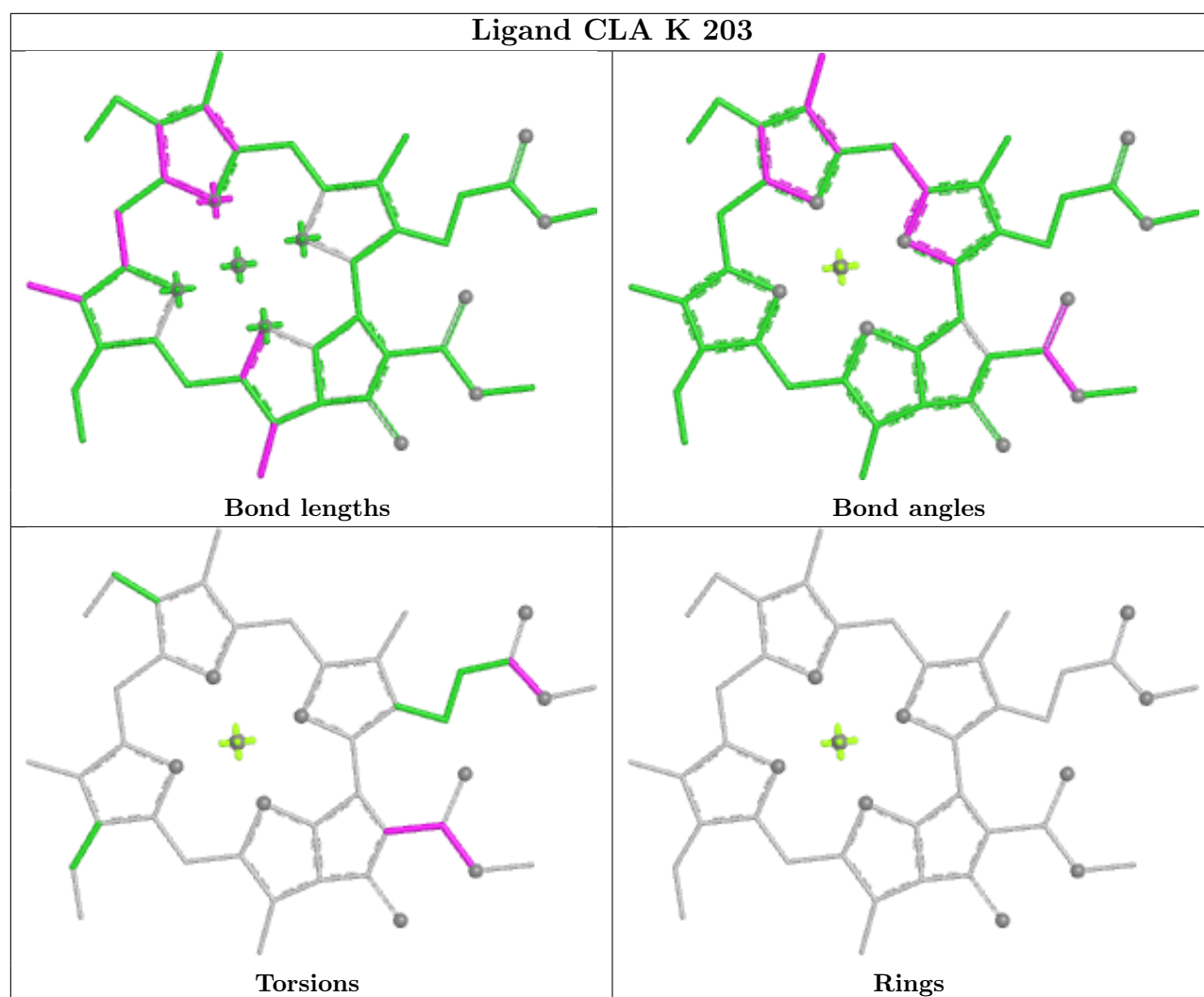


Ligand CLA 2 303

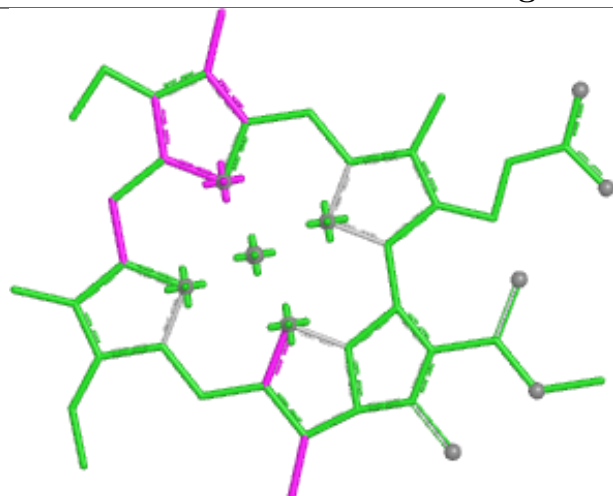


Ligand CLA 4 314

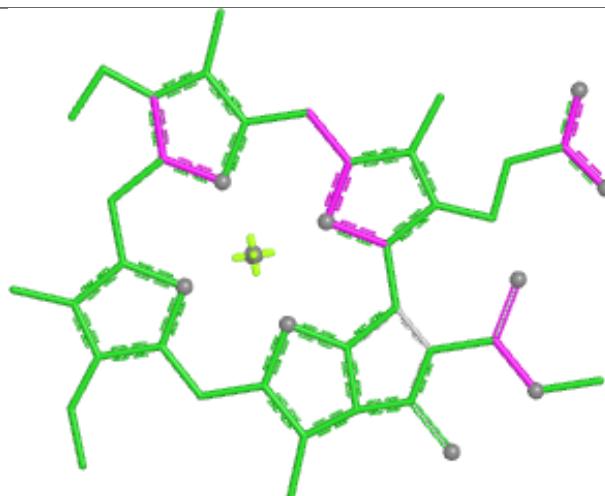




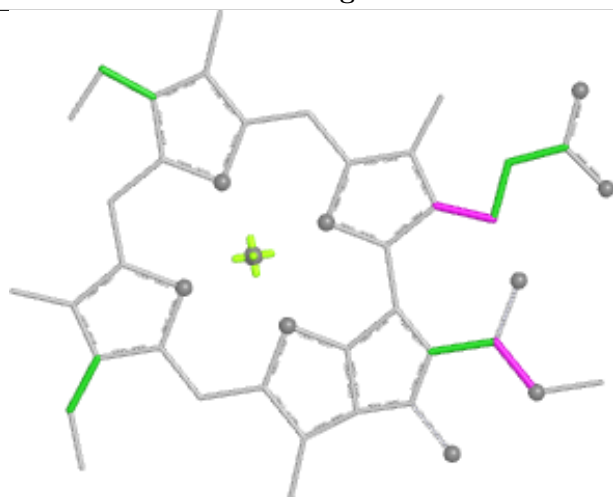
Ligand CLA 3 303



Bond lengths



Bond angles

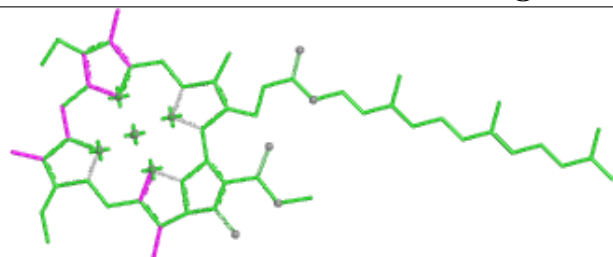


Torsions

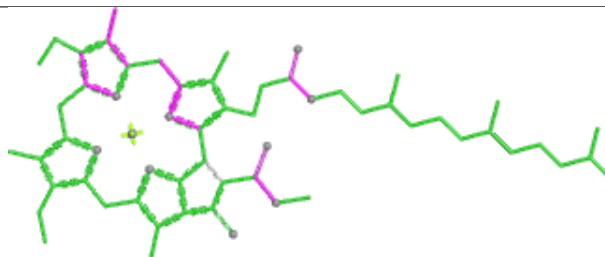


Rings

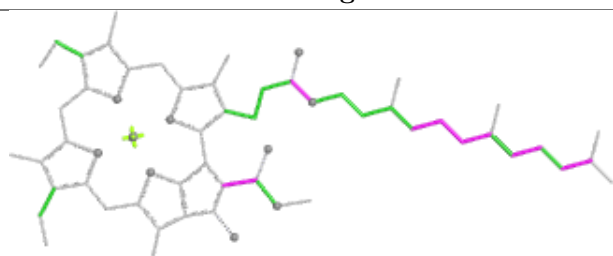
Ligand CLA B 815



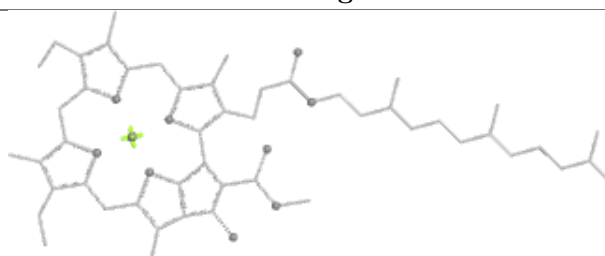
Bond lengths



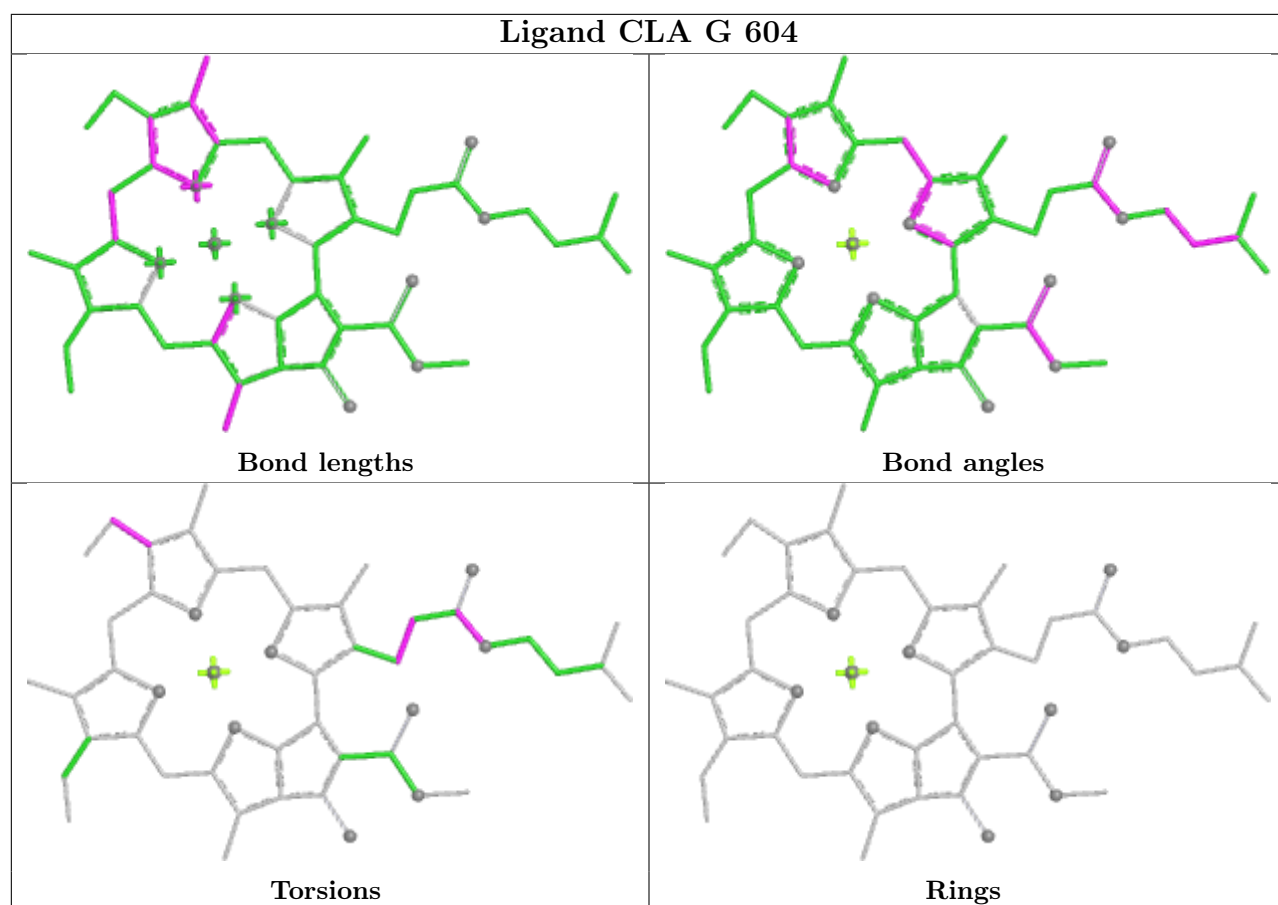
Bond angles



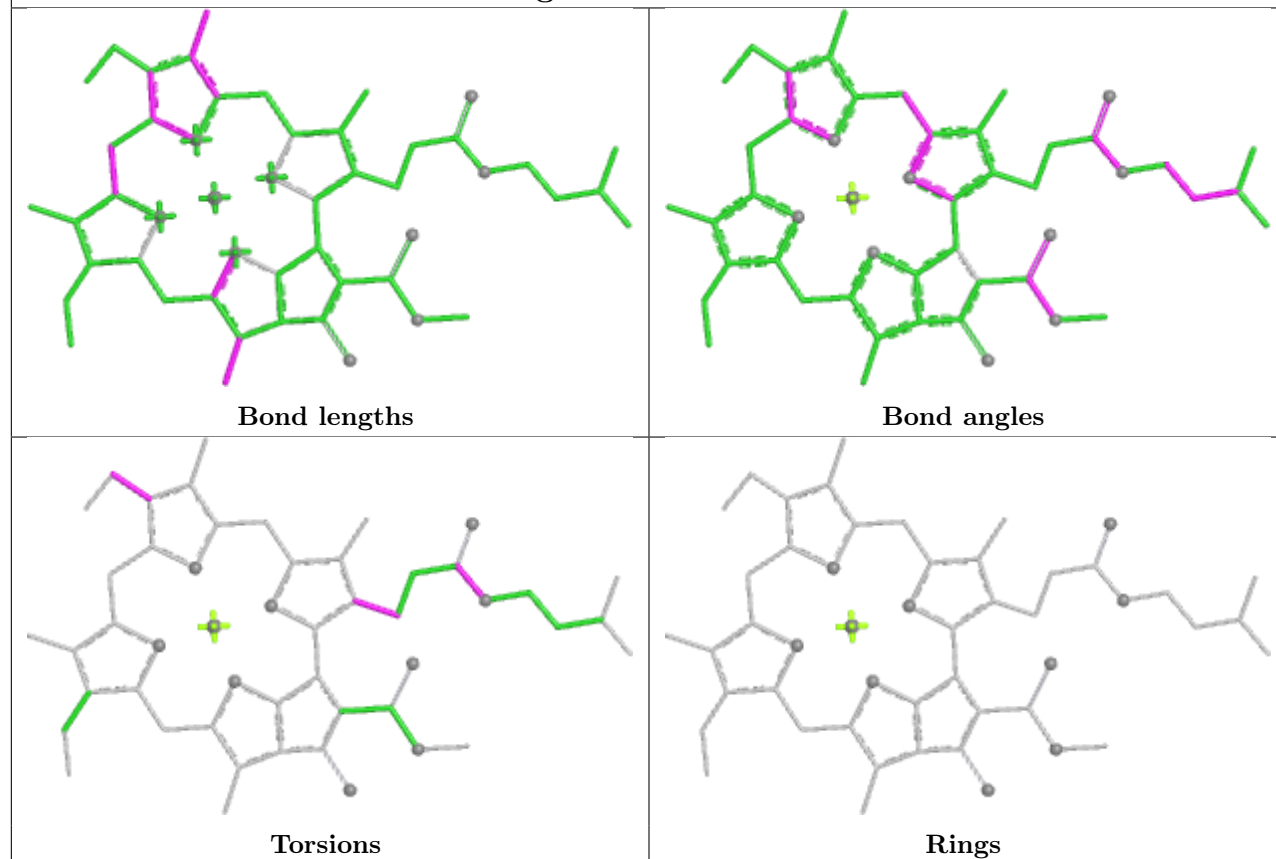
Torsions



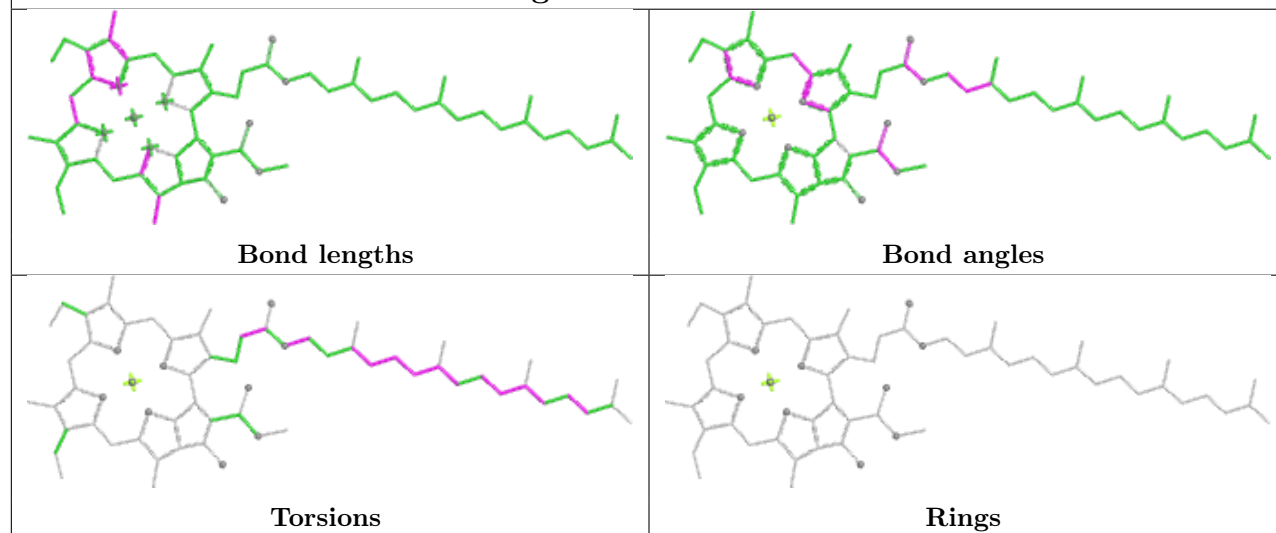
Rings



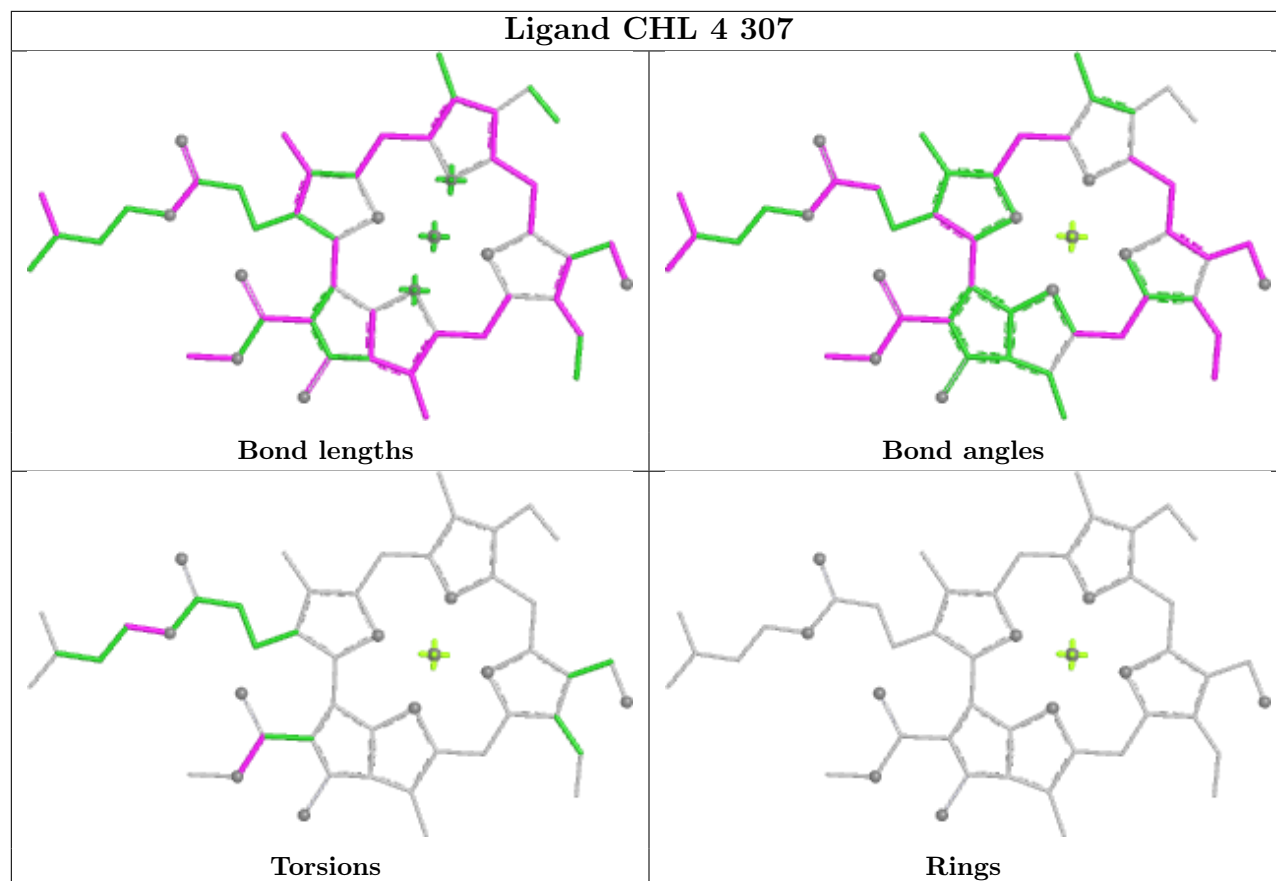
Ligand CLA 4 308



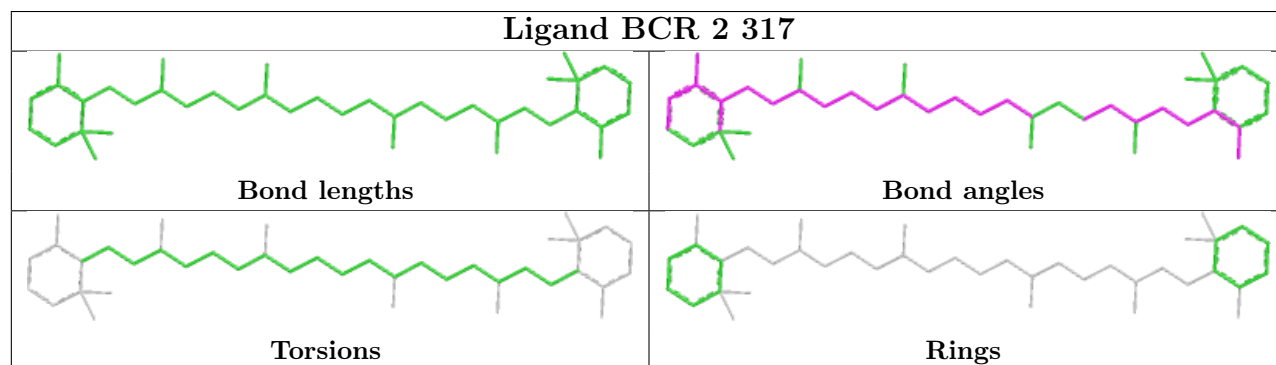
Ligand CLA A 805

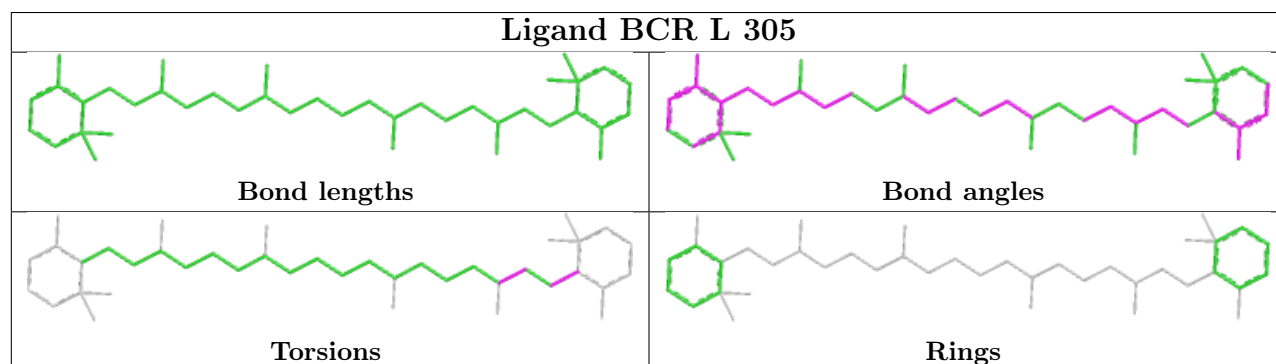
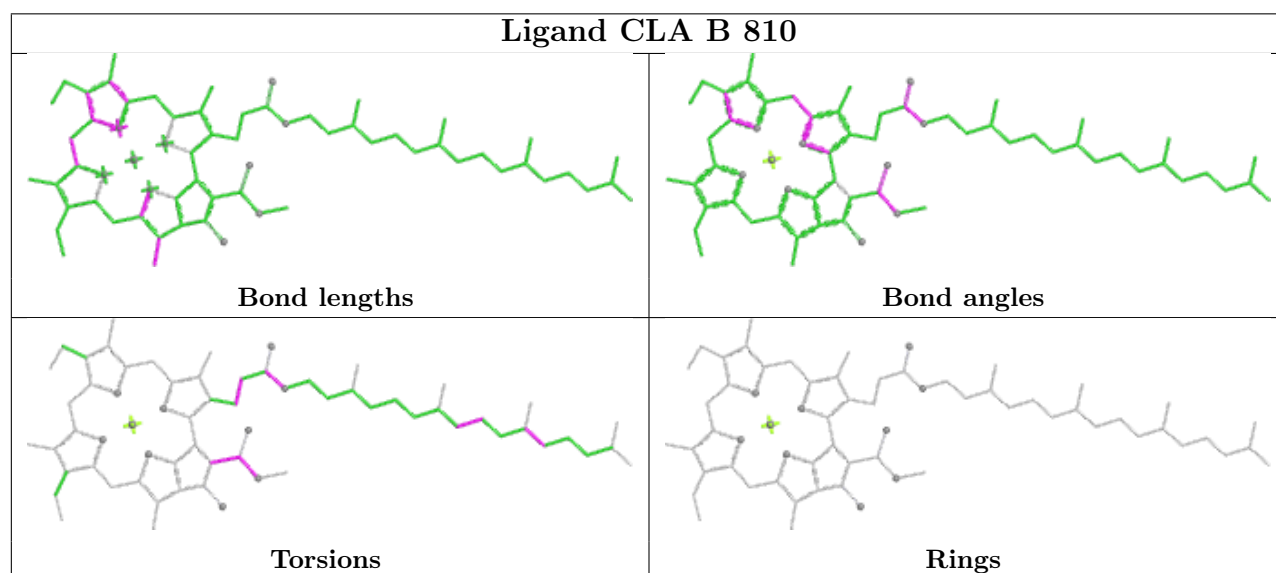
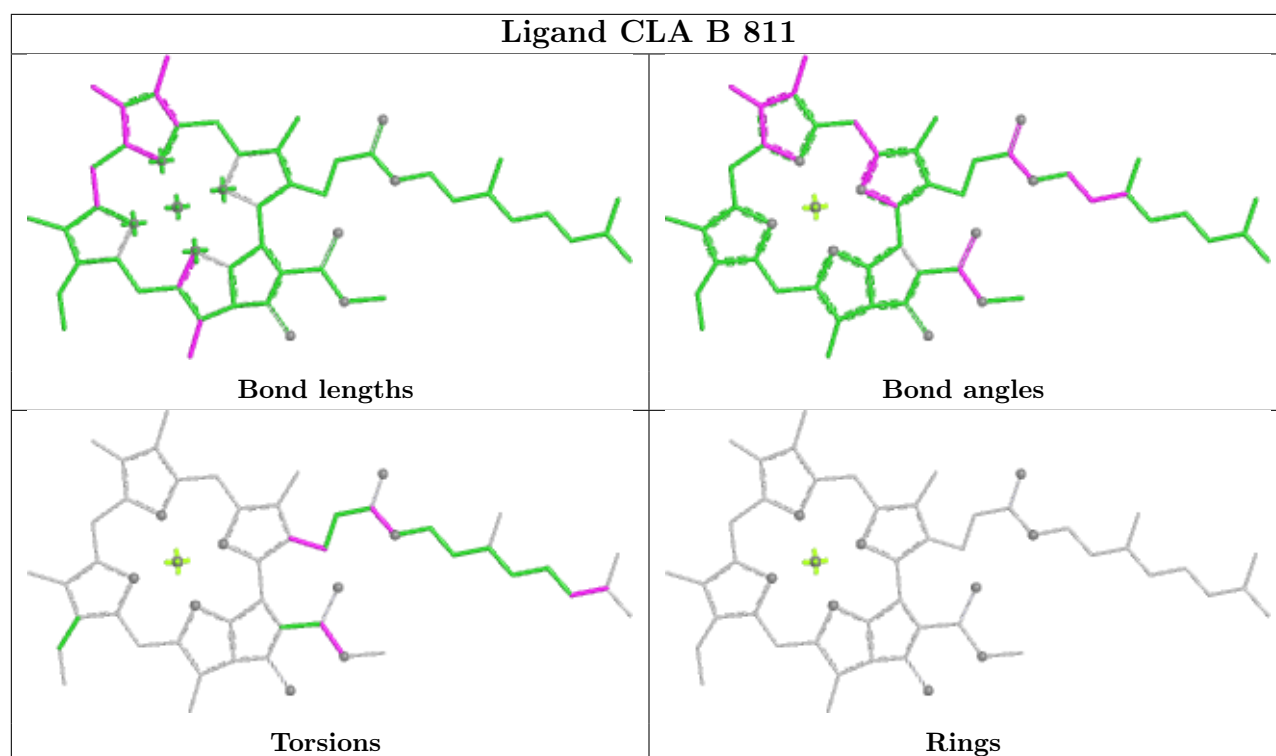


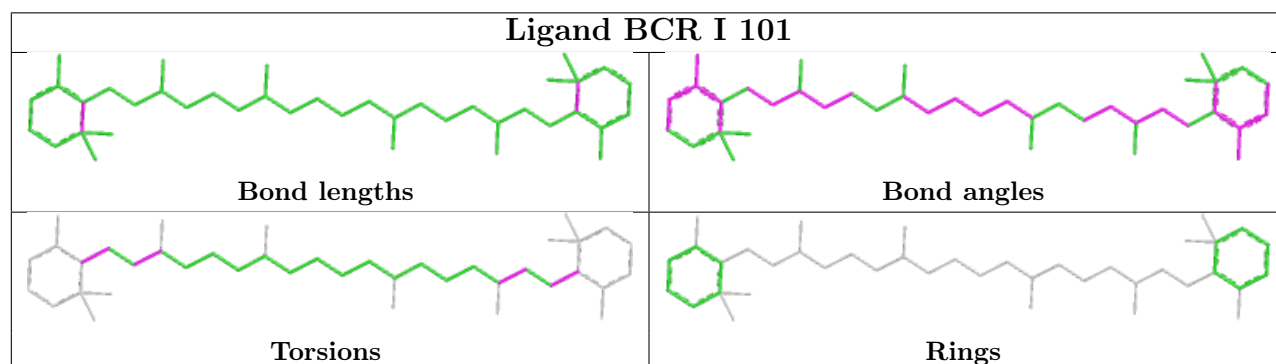
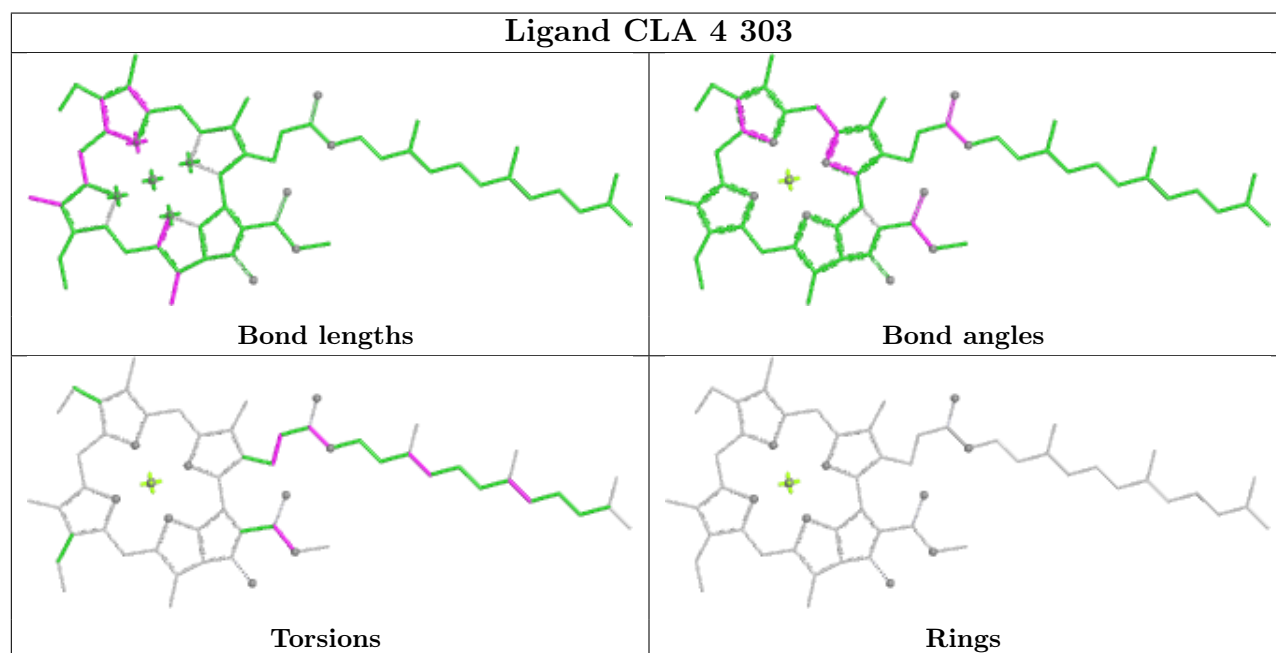
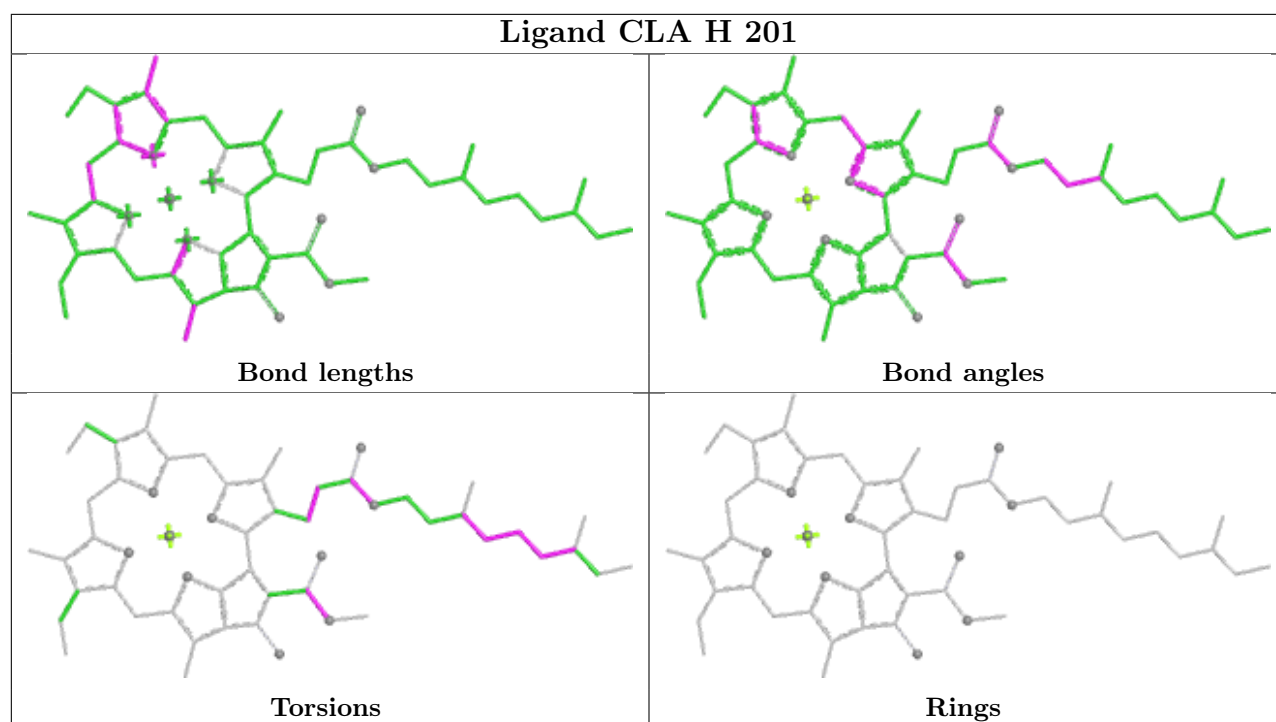
Ligand CHL 4 307

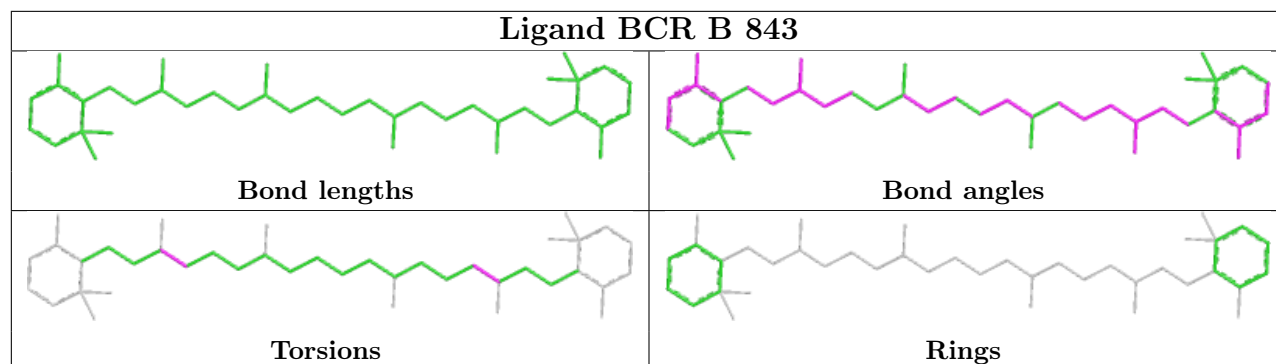
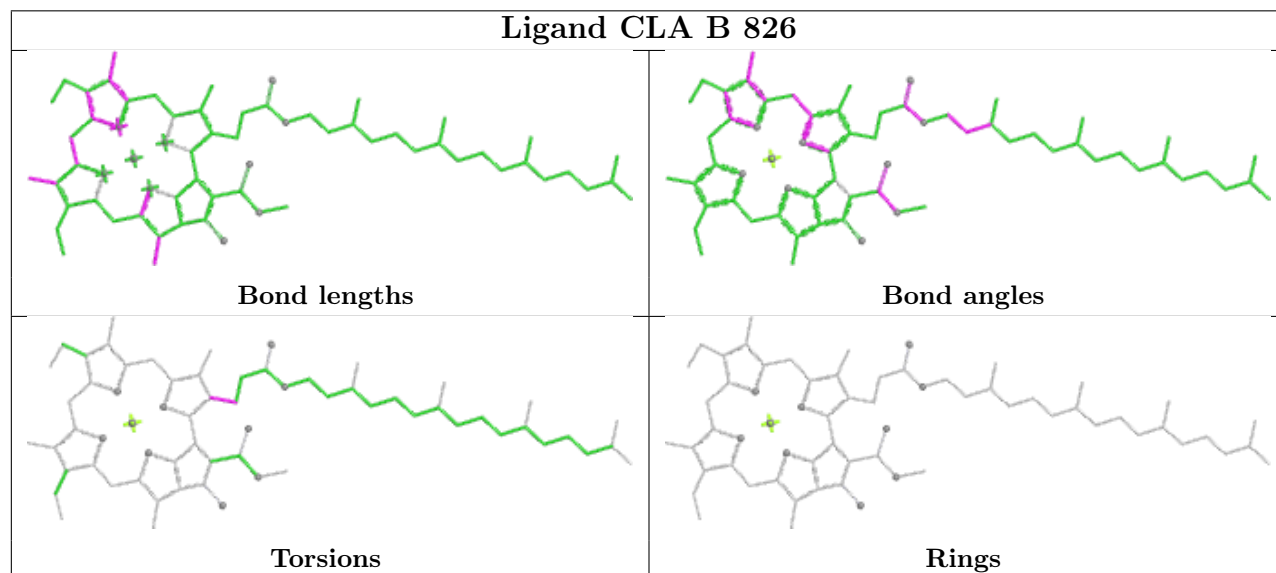
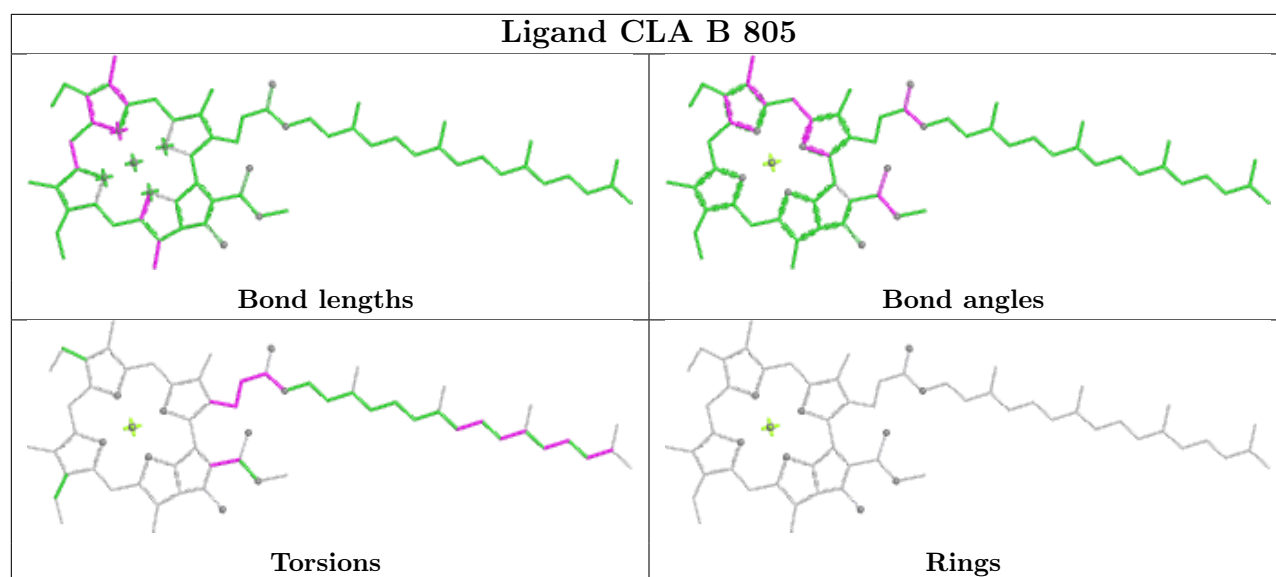


Ligand BCR 2 317

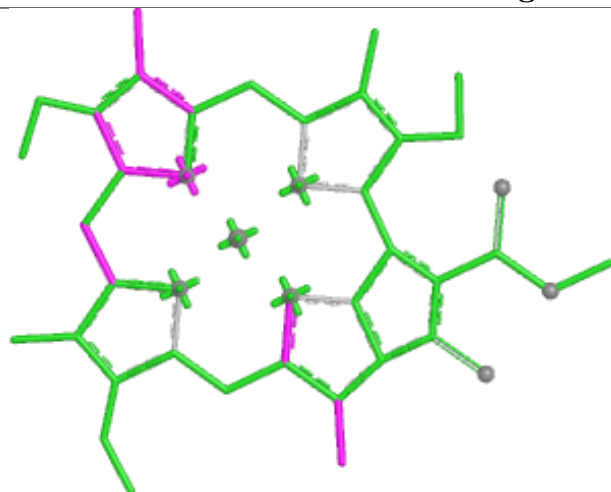




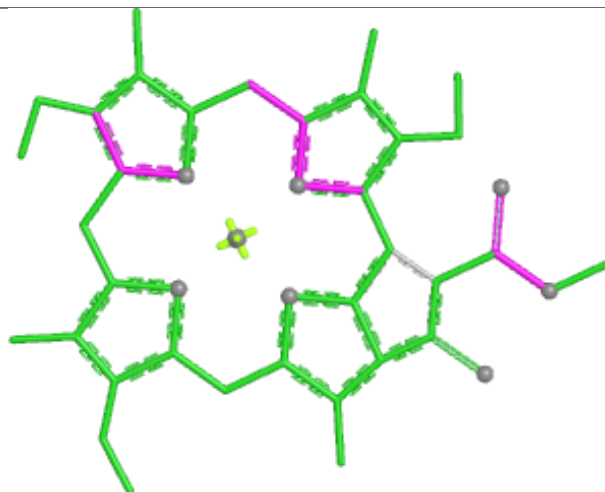




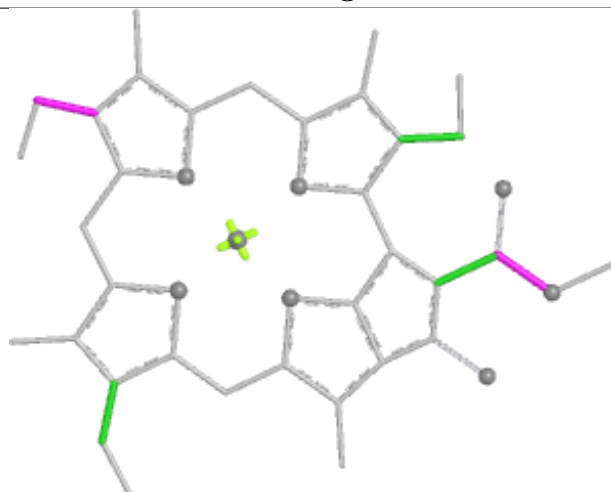
Ligand CLA J 103



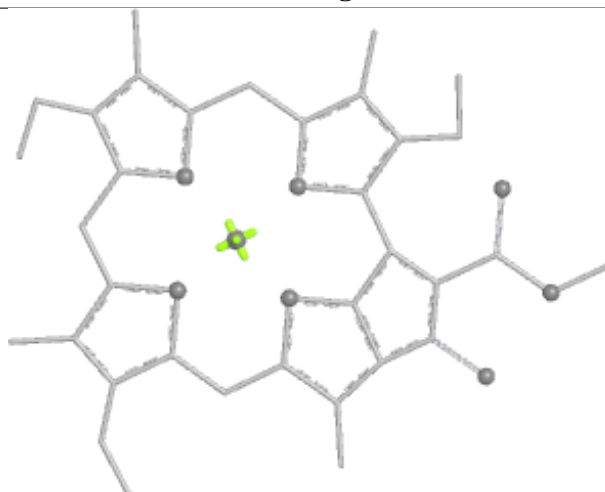
Bond lengths



Bond angles

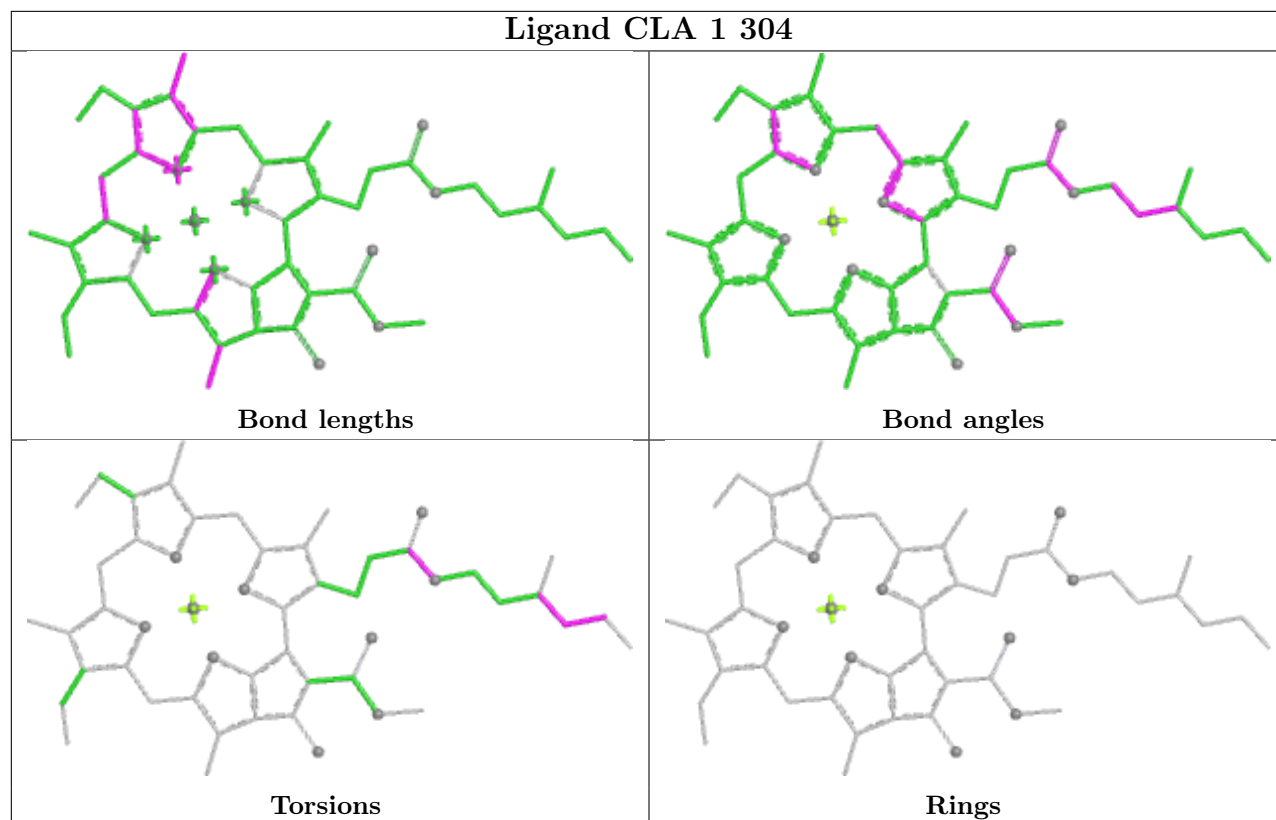


Torsions

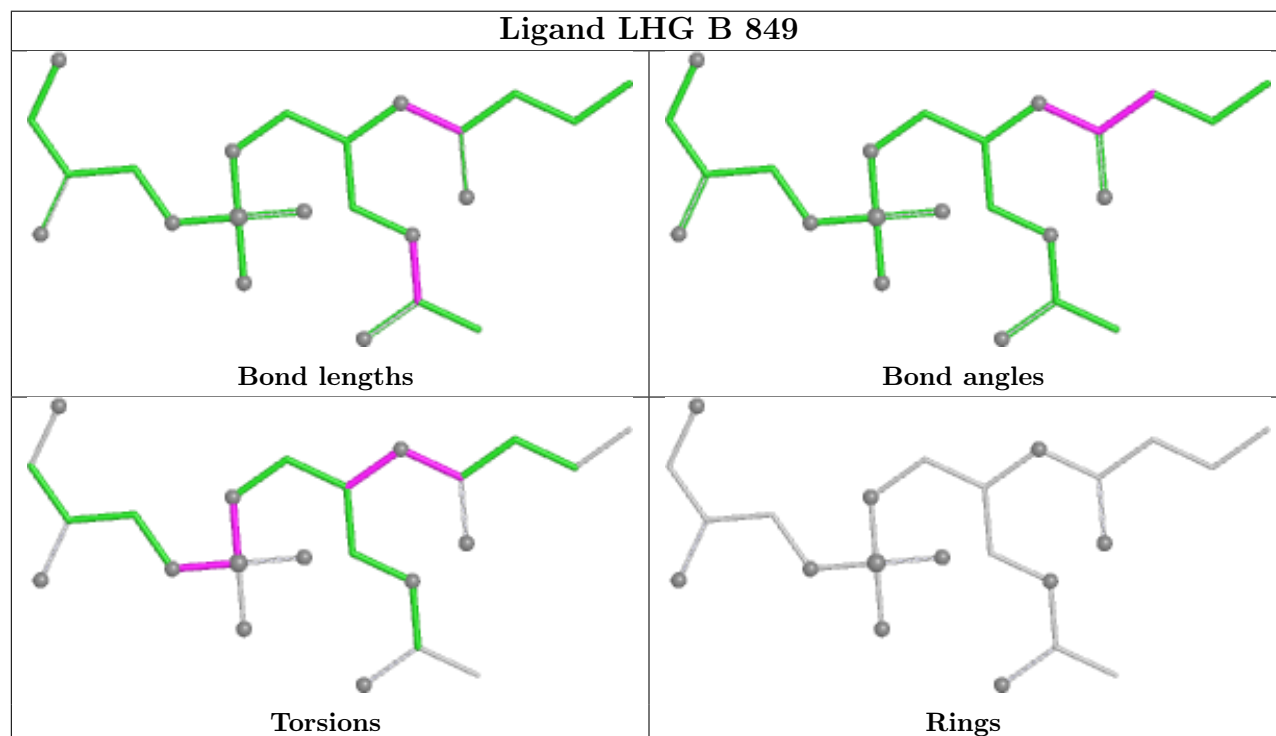


Rings

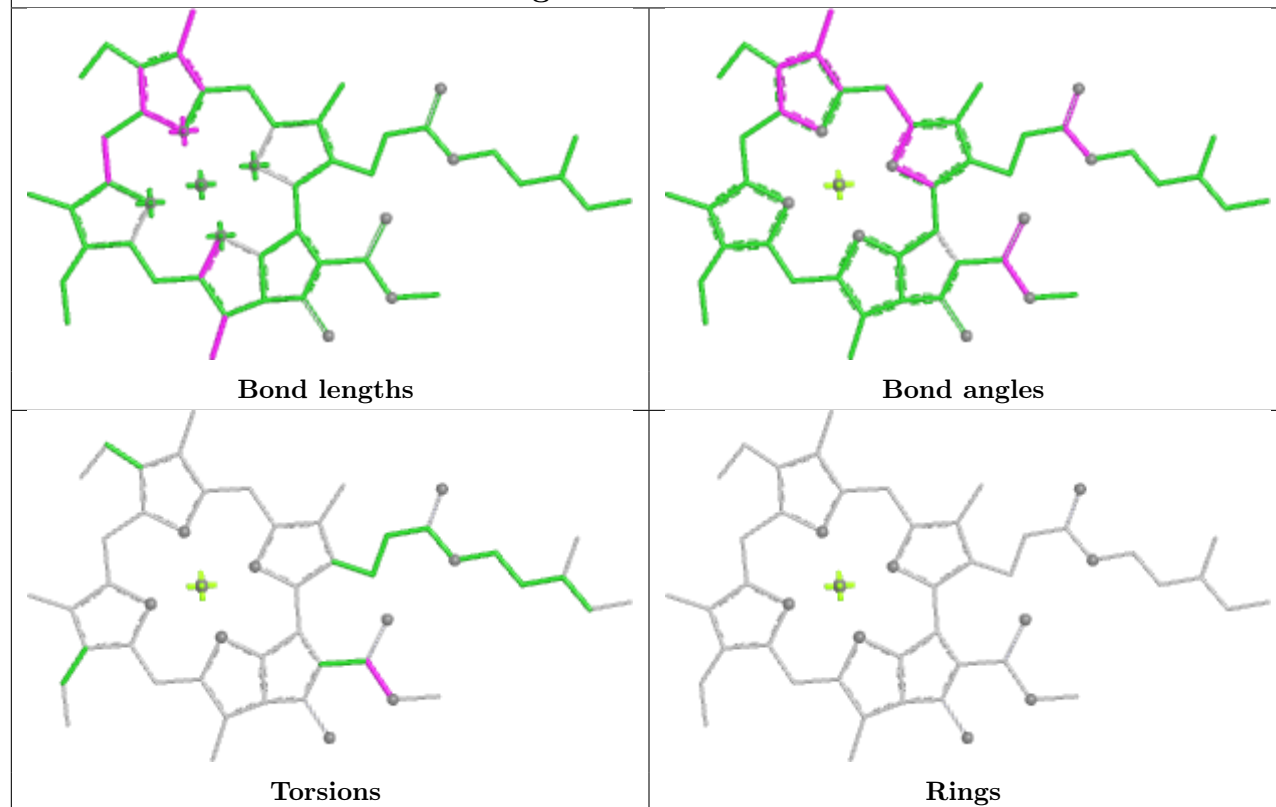
Ligand CLA 1 304



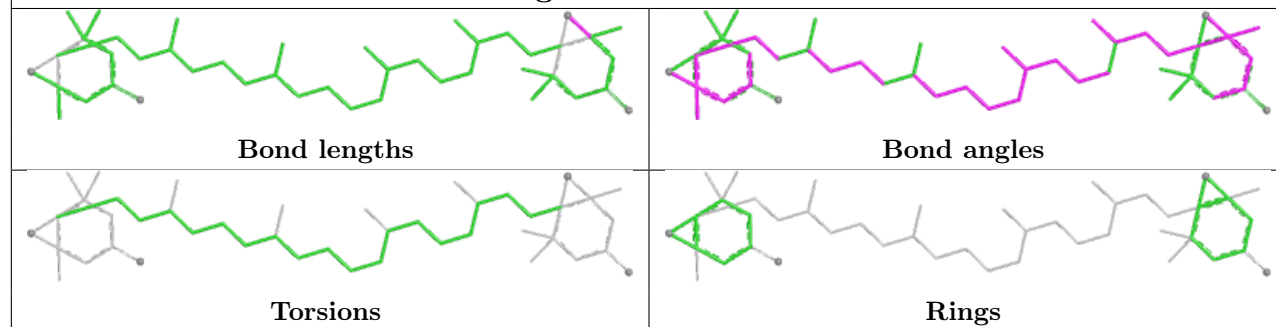
Ligand LHG B 849



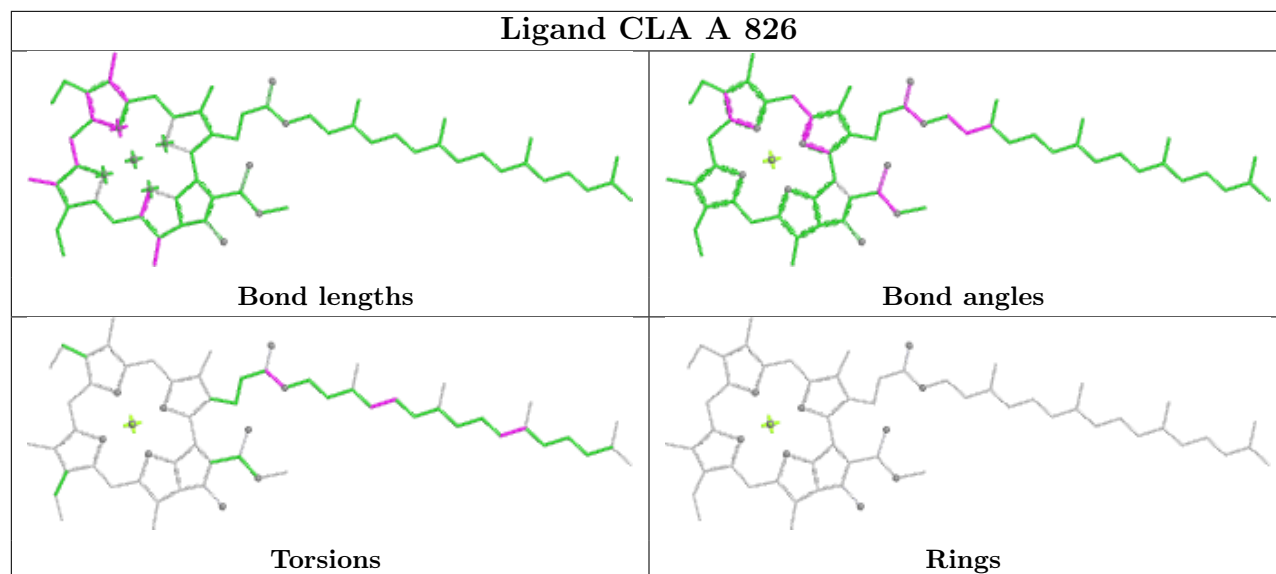
Ligand CLA B 835



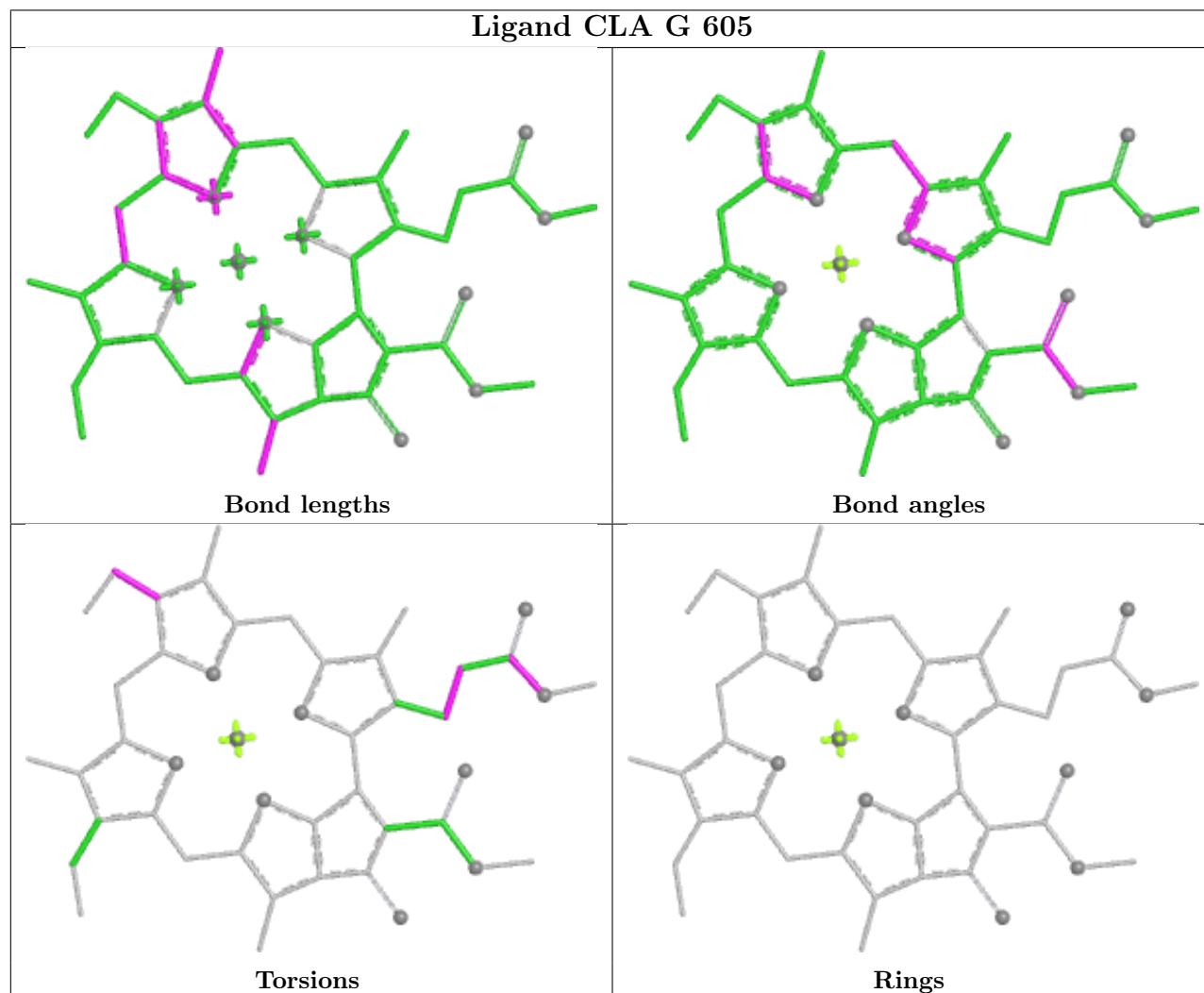
Ligand XAT 4 317

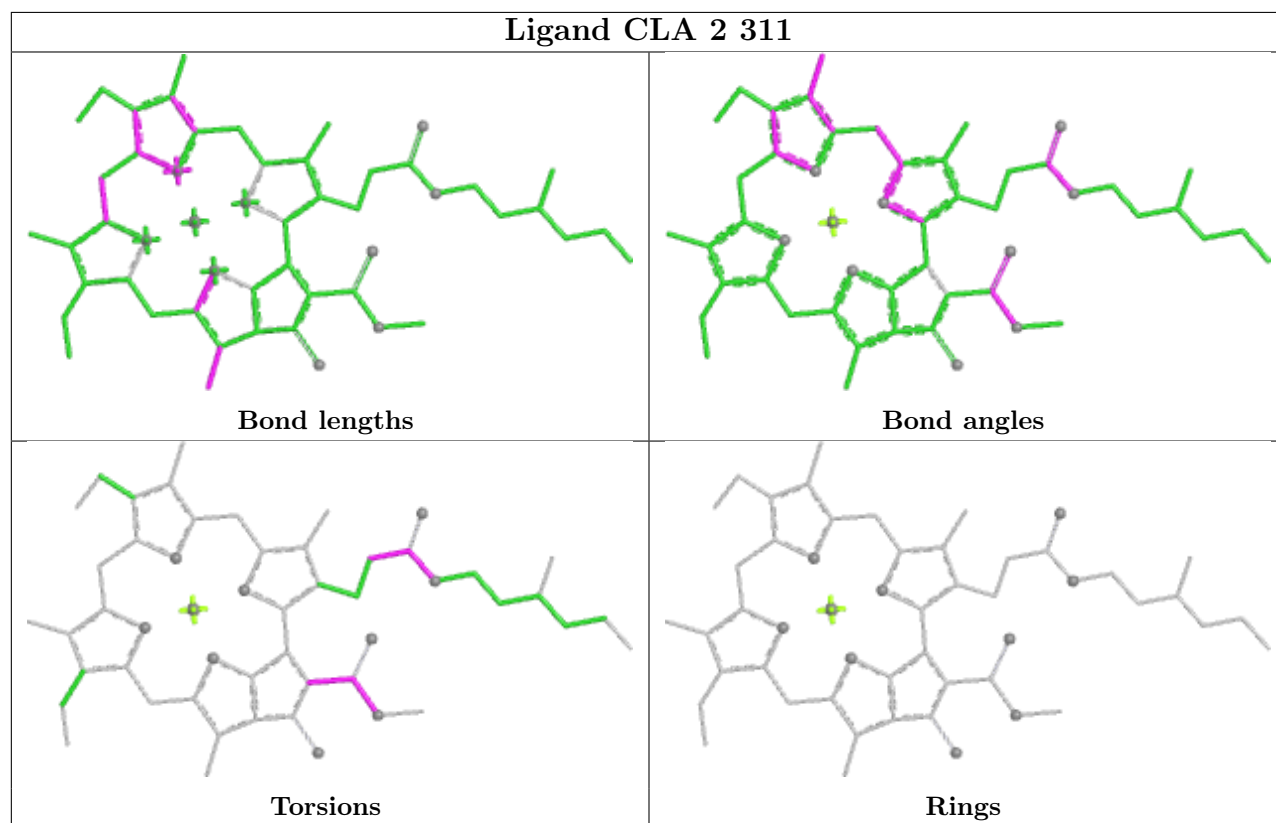
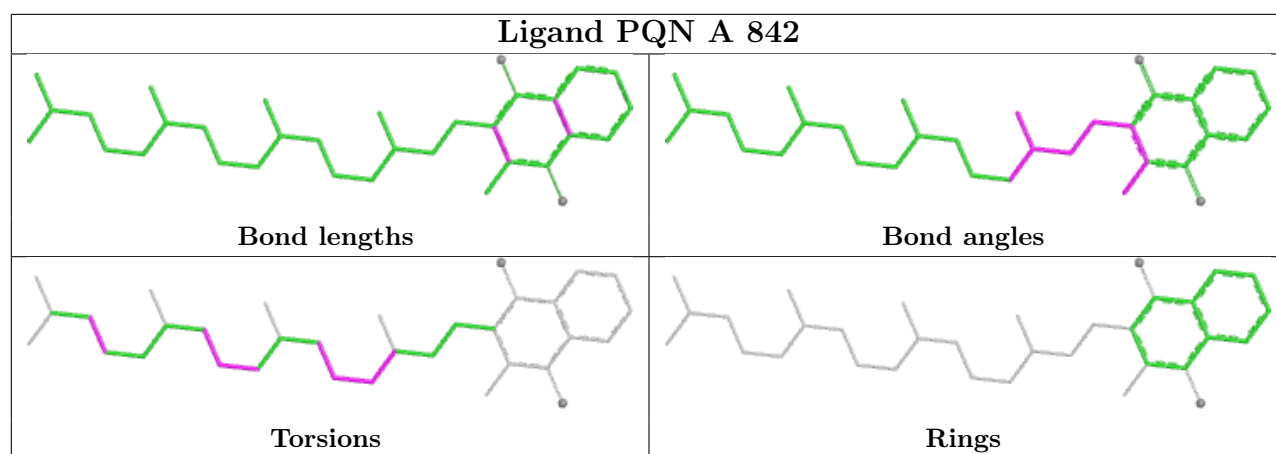


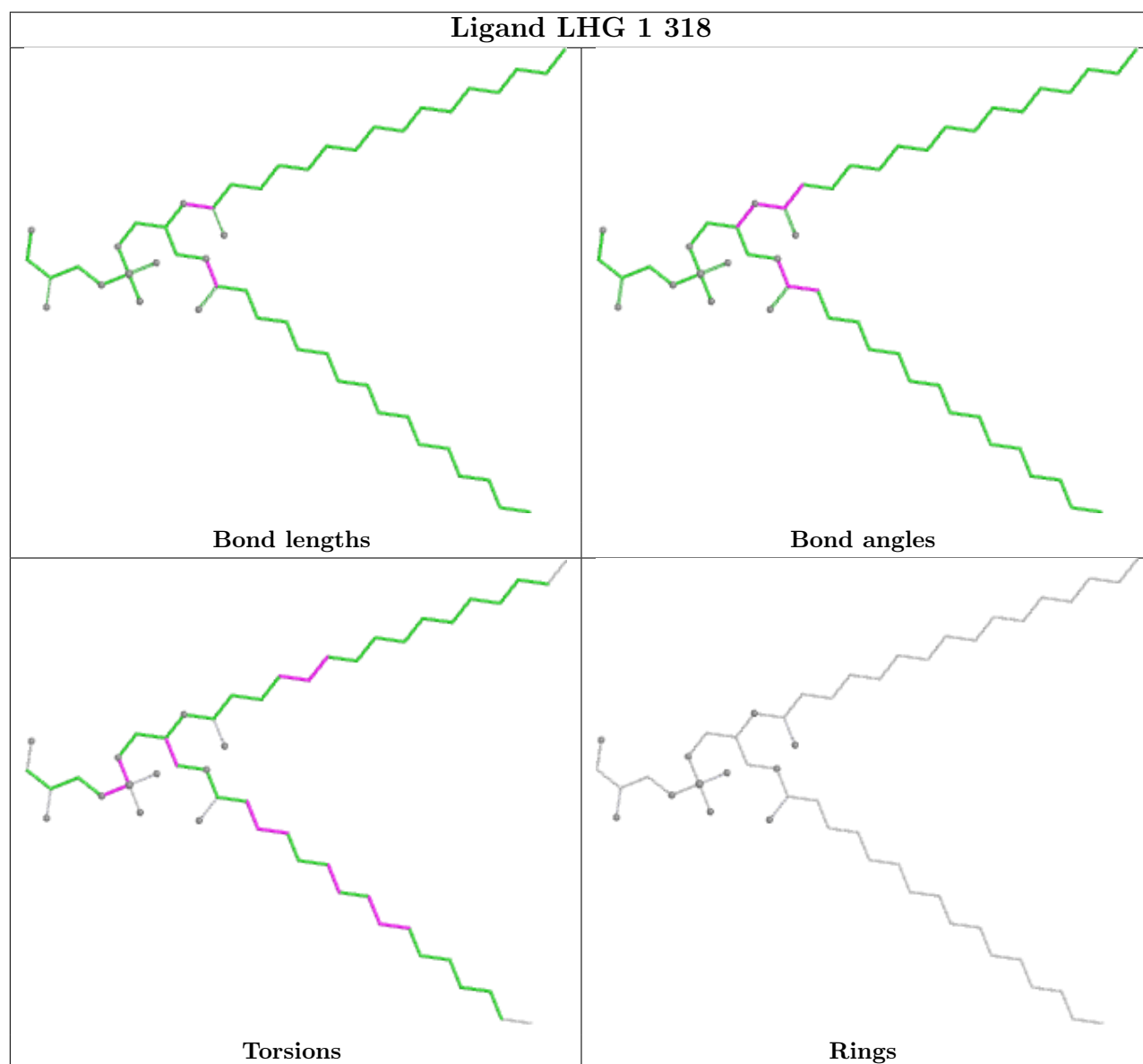
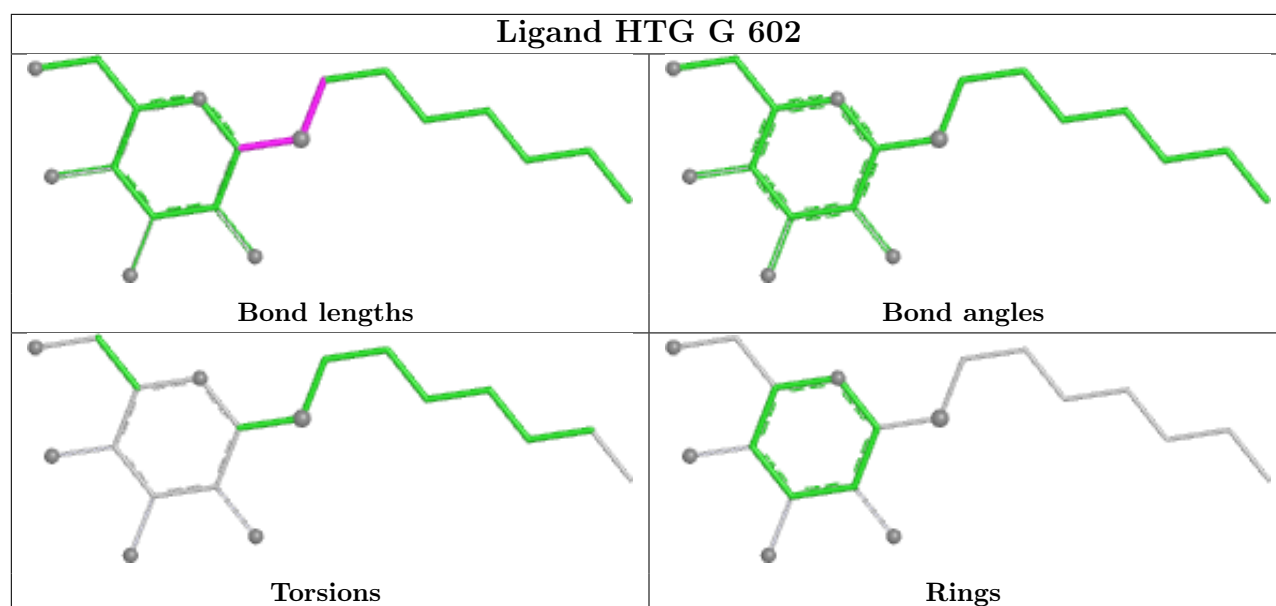
Ligand CLA A 826

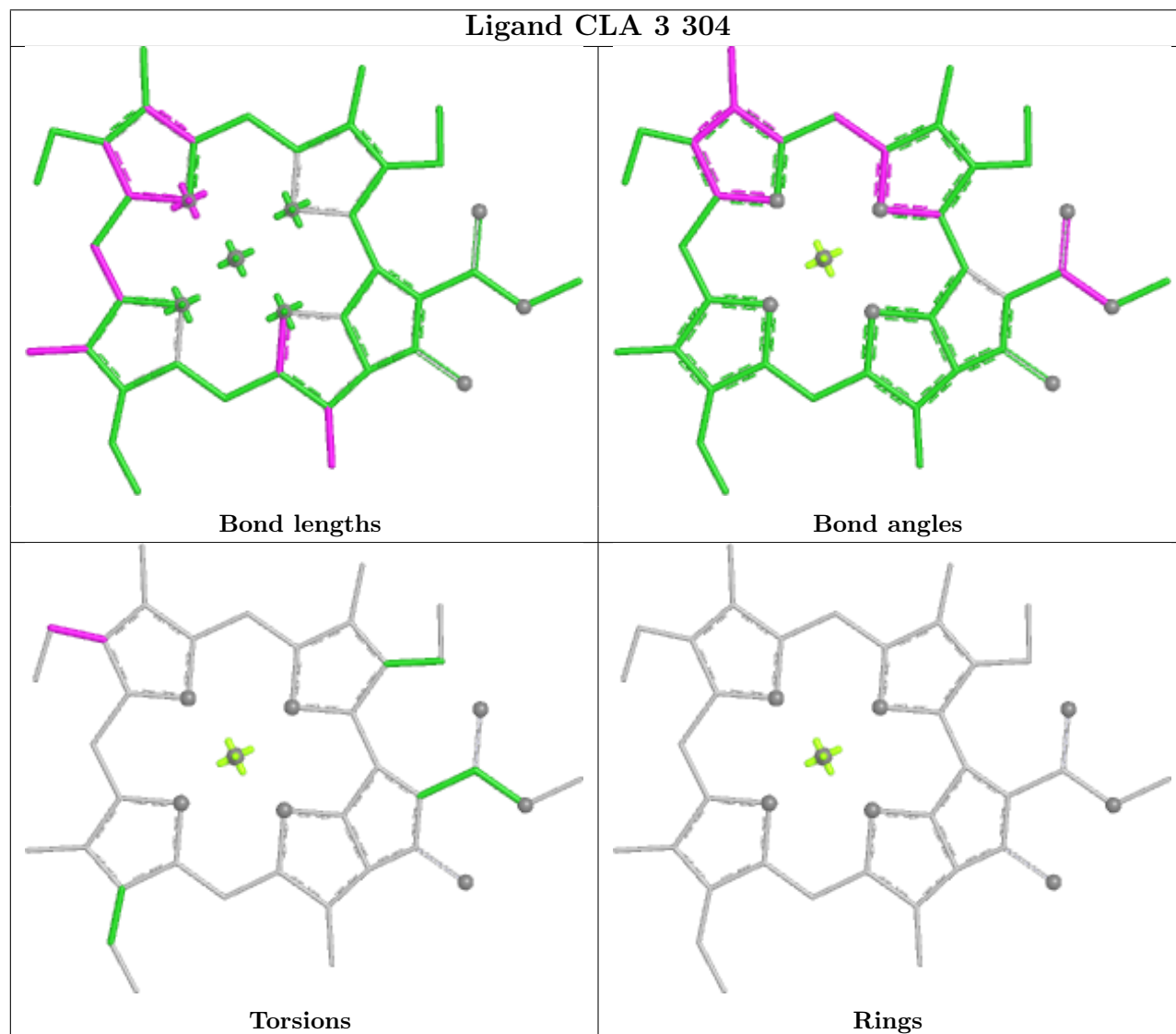
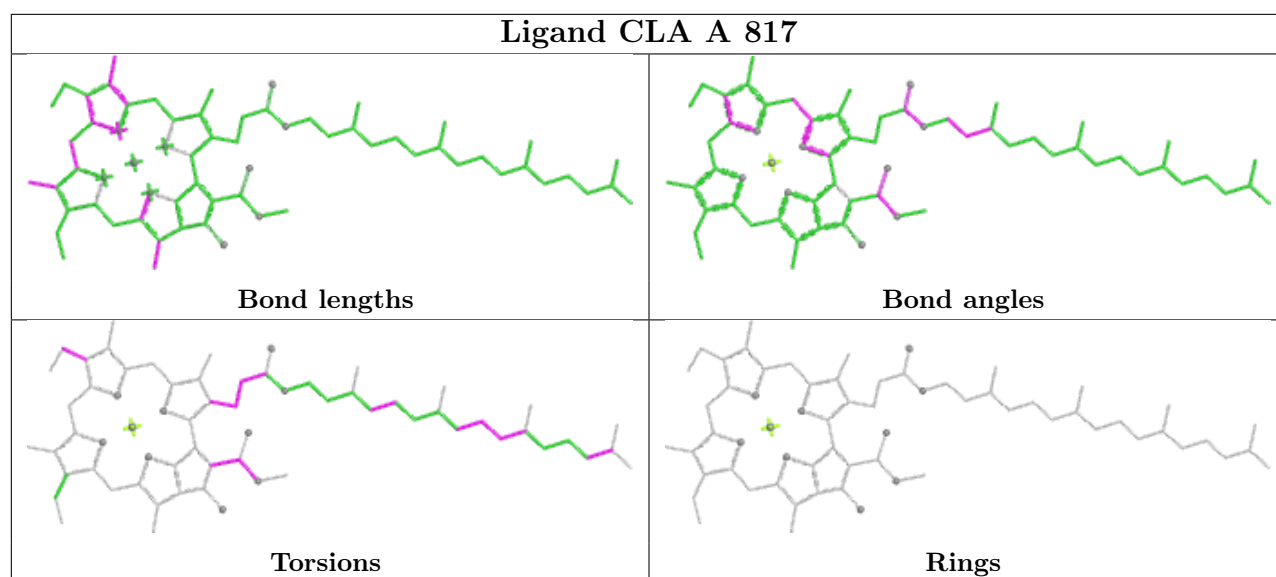


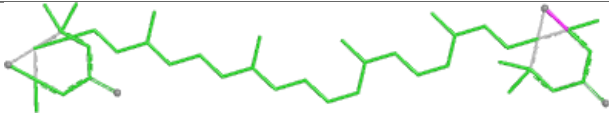
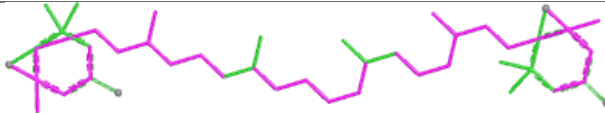
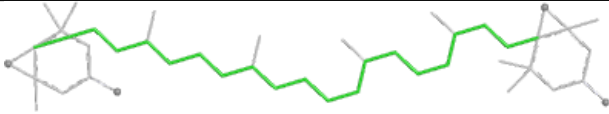
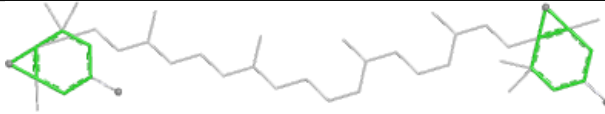
Ligand CLA G 605

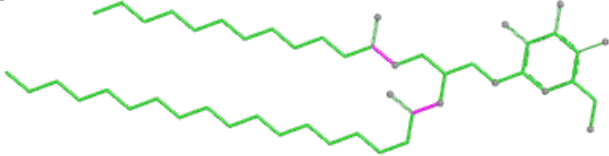
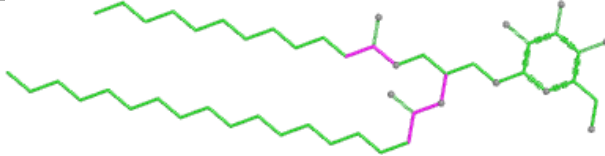
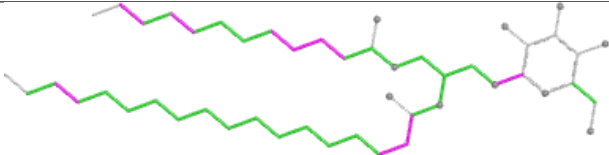


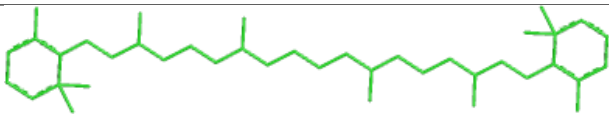
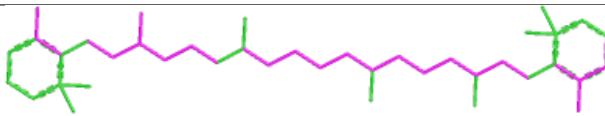
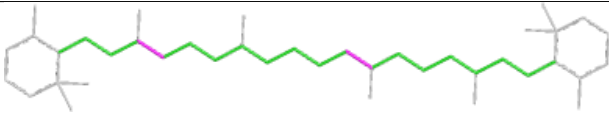
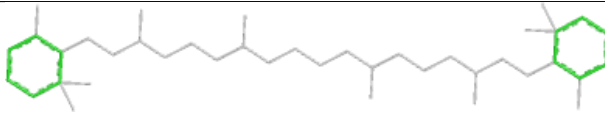




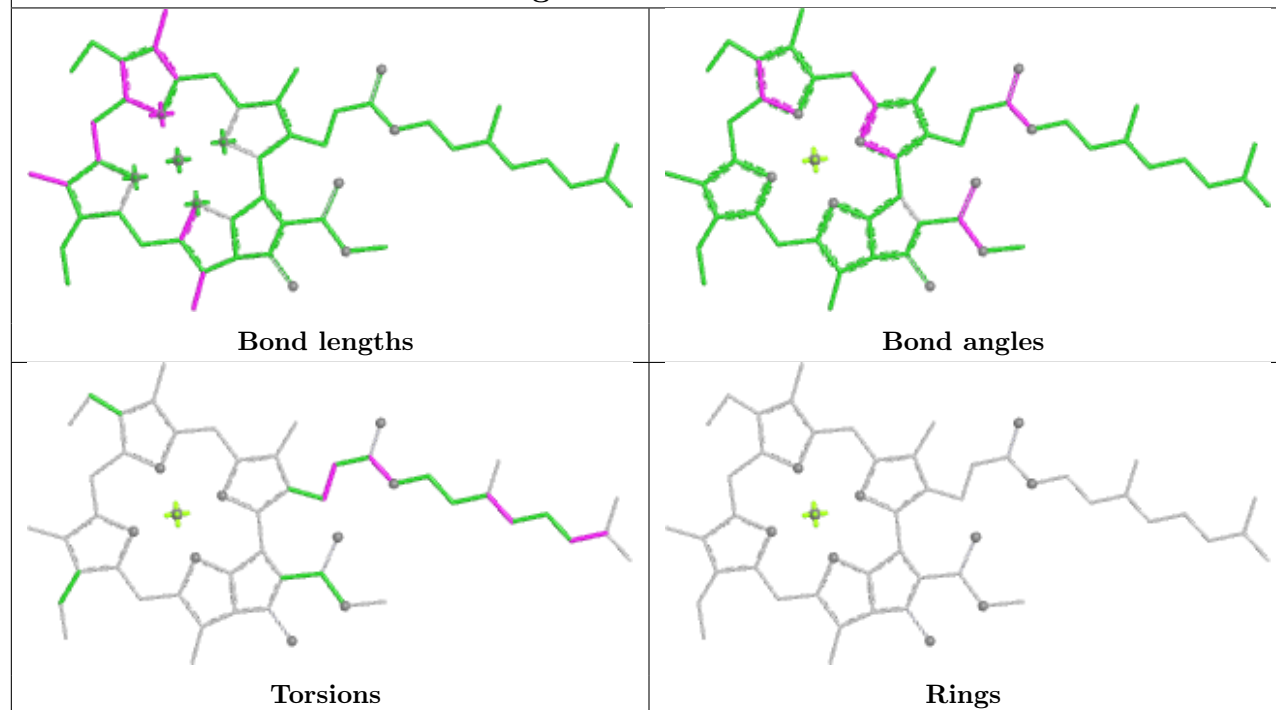


Ligand XAT 3 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

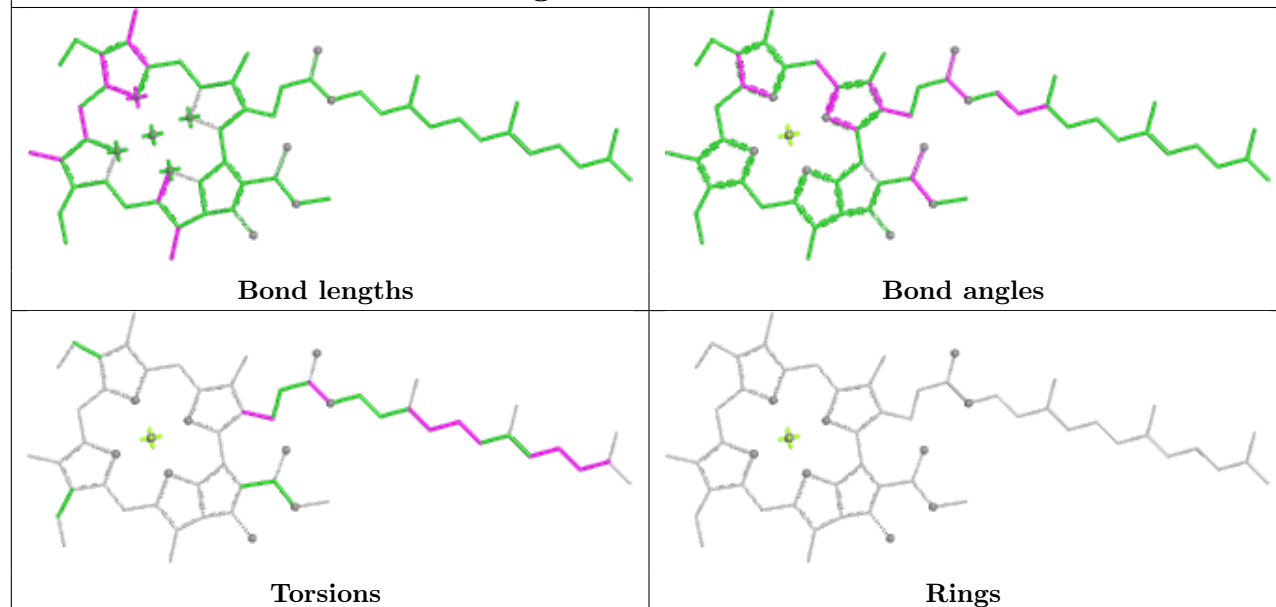
Ligand LMG 1 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

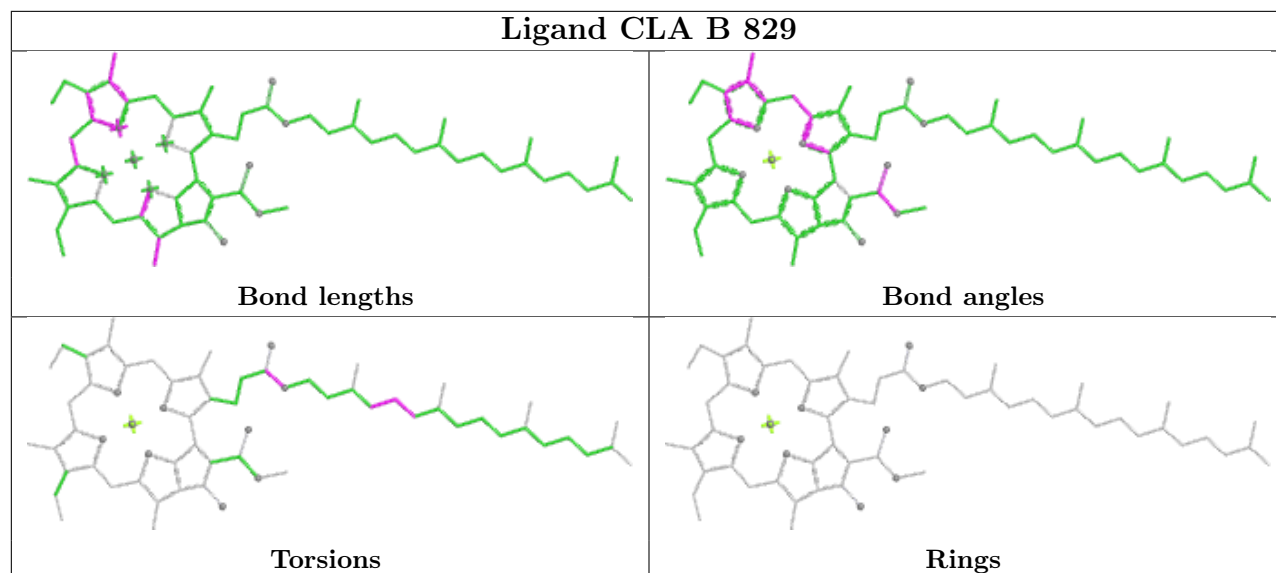
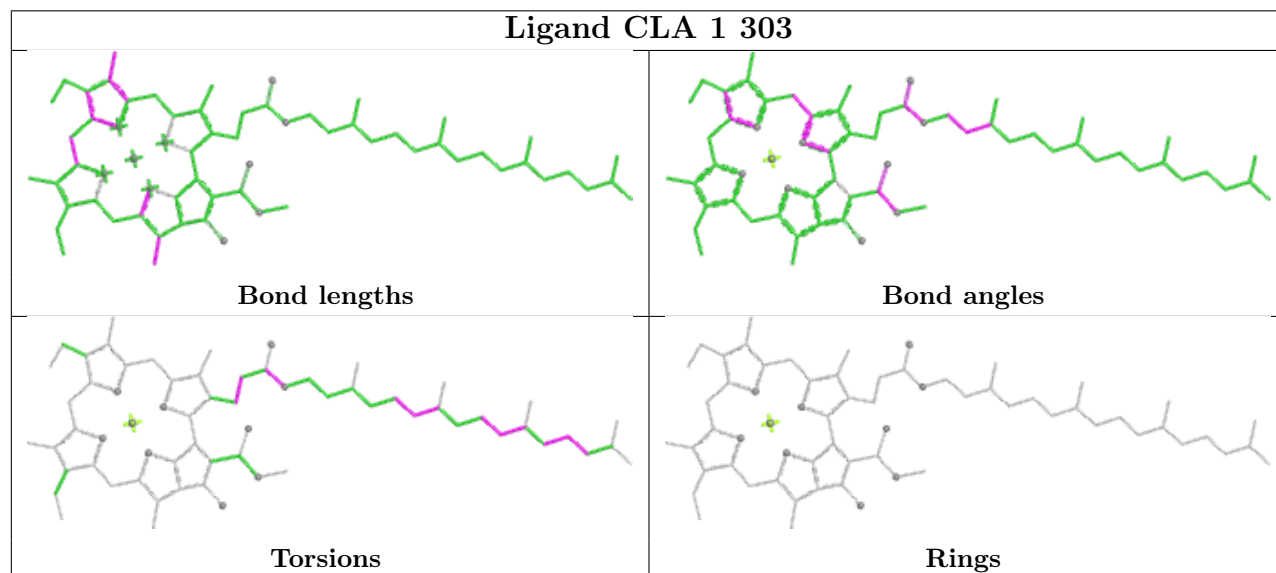
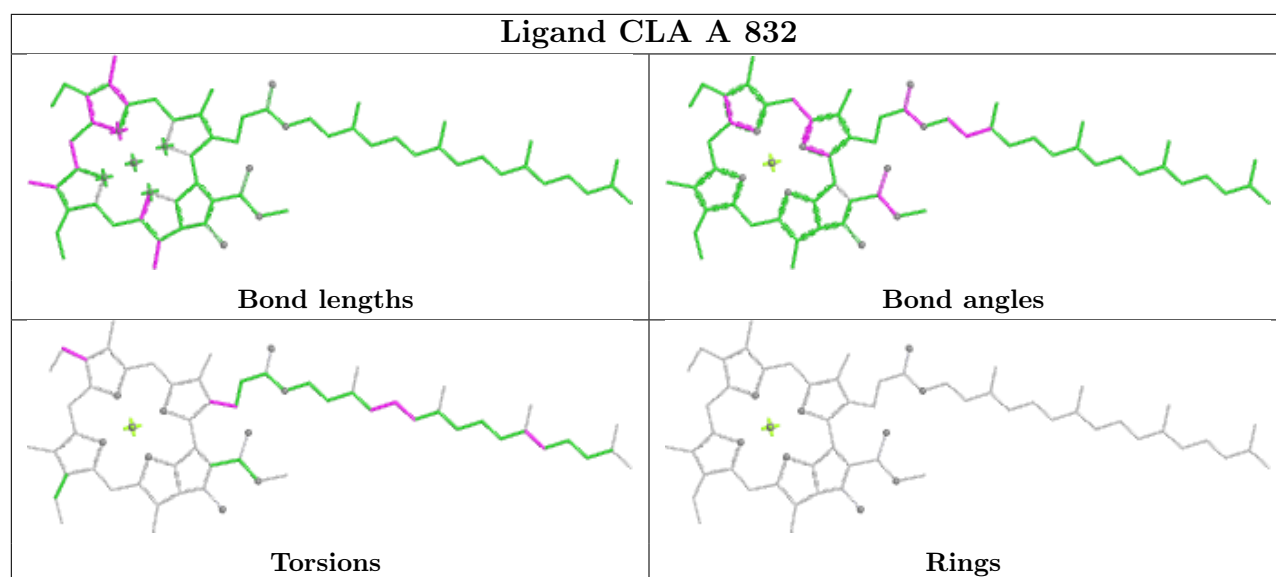
Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

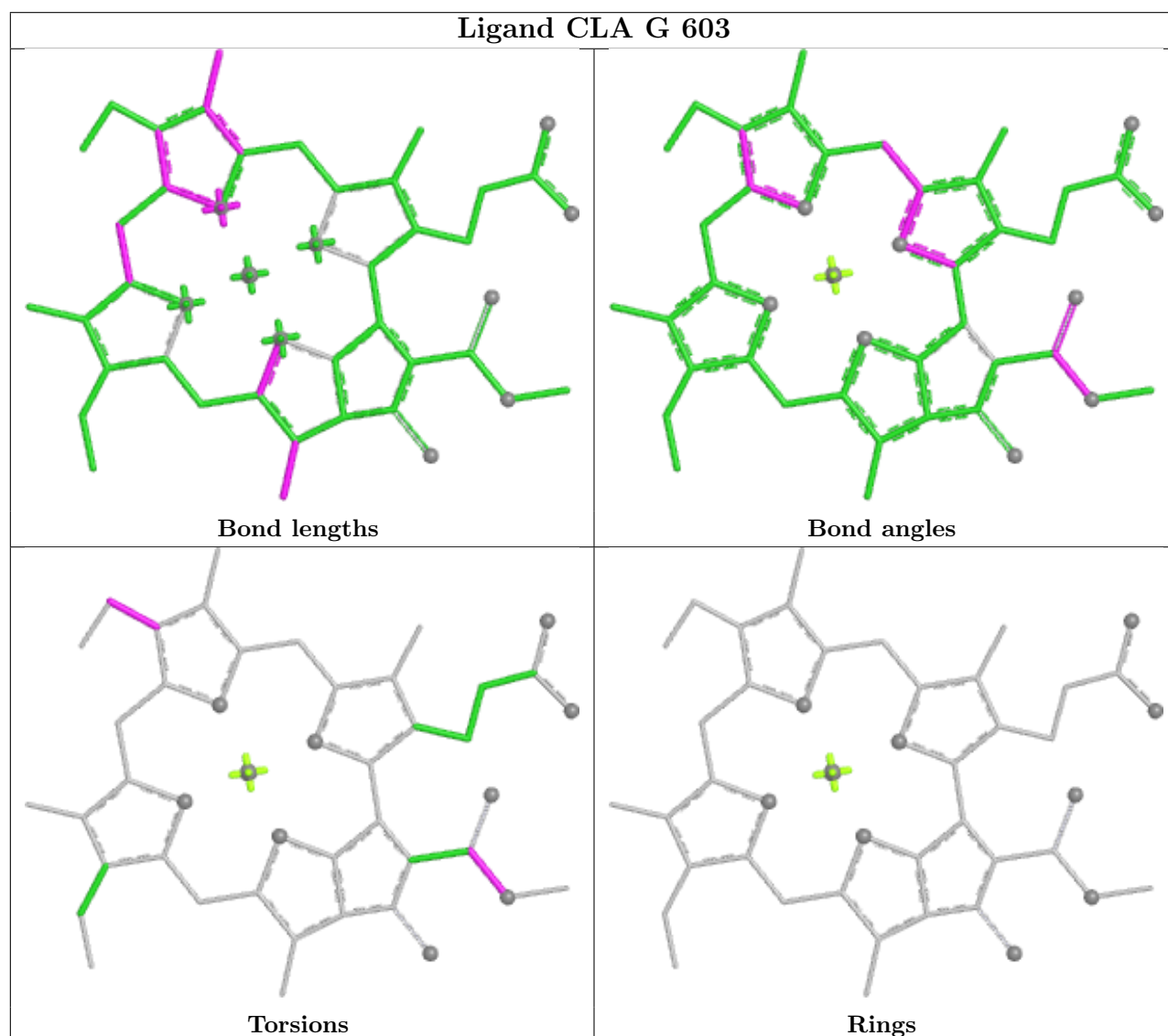
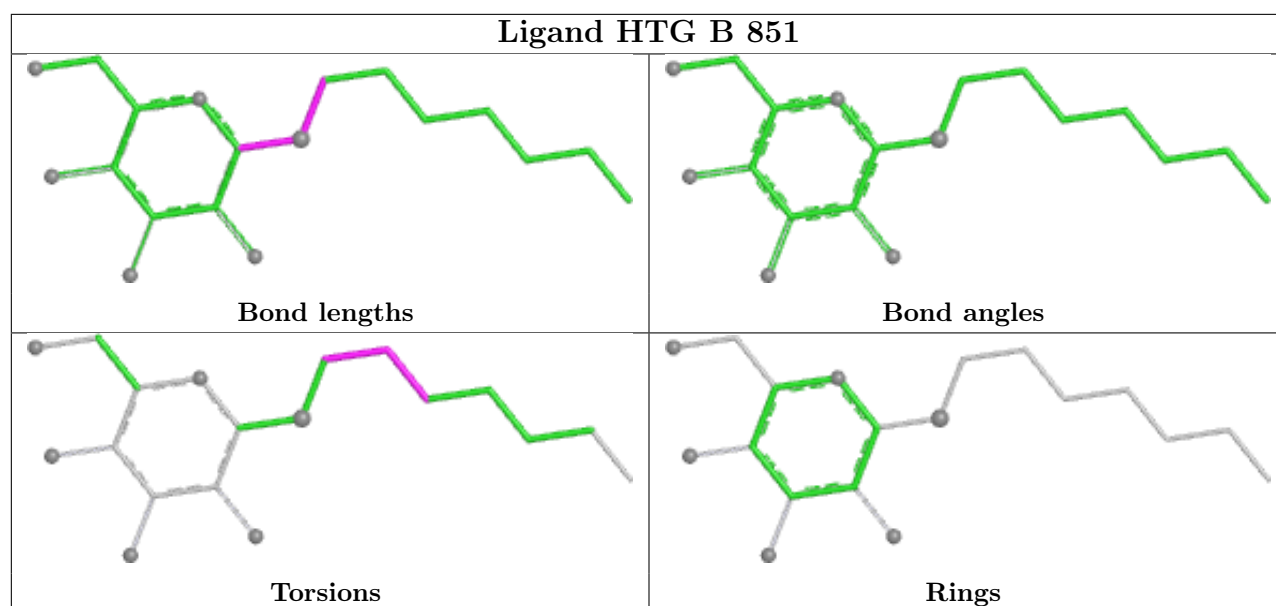
Ligand CLA B 816

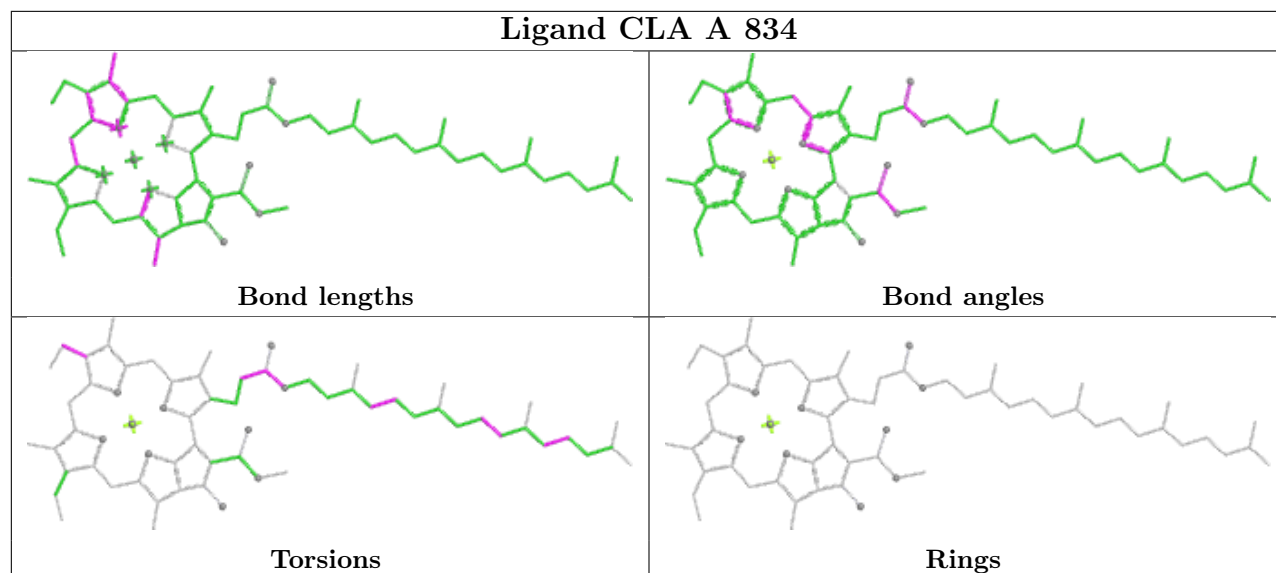
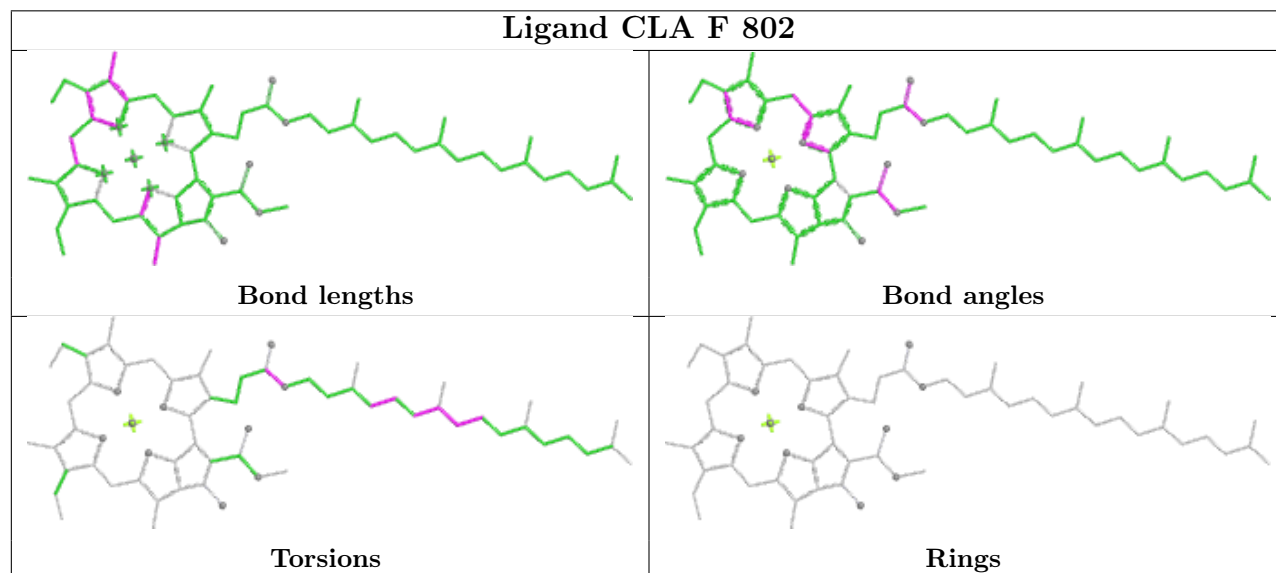
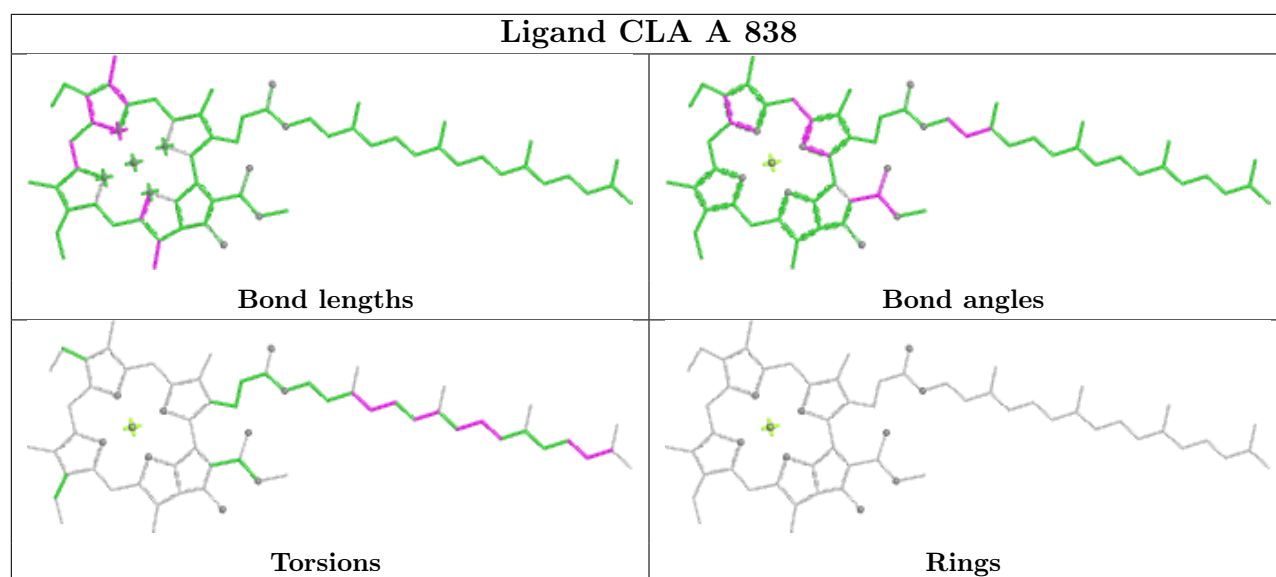


Ligand CLA B 823

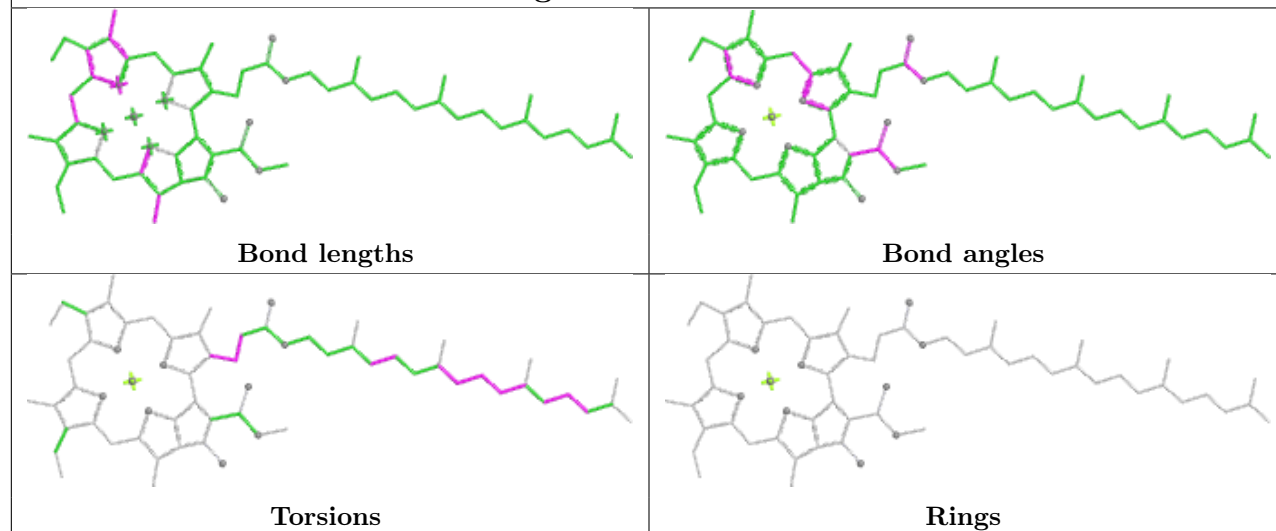




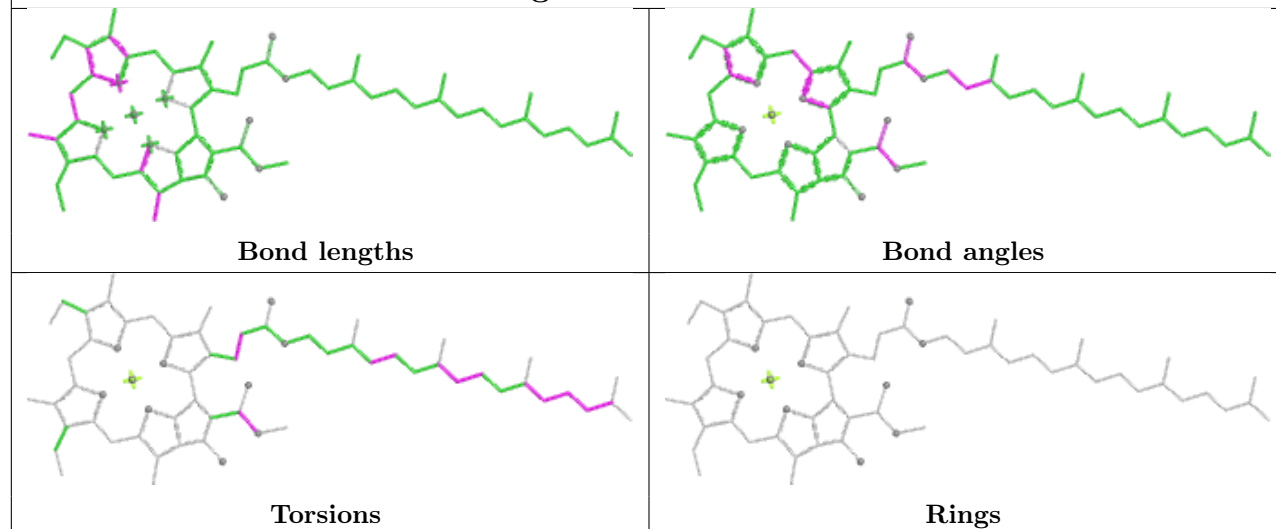




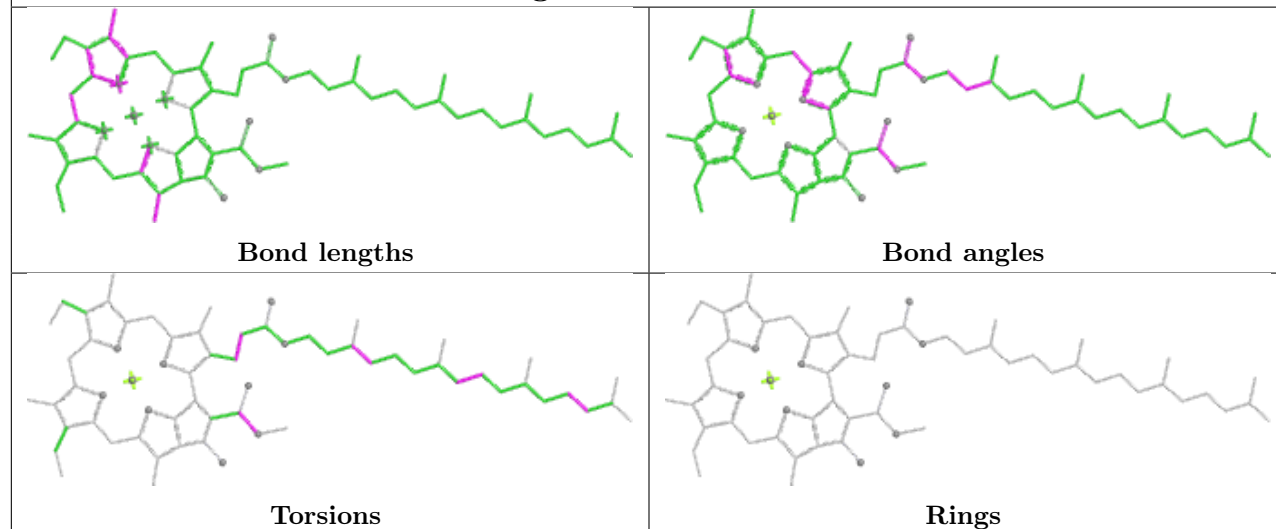
Ligand CLA L 303

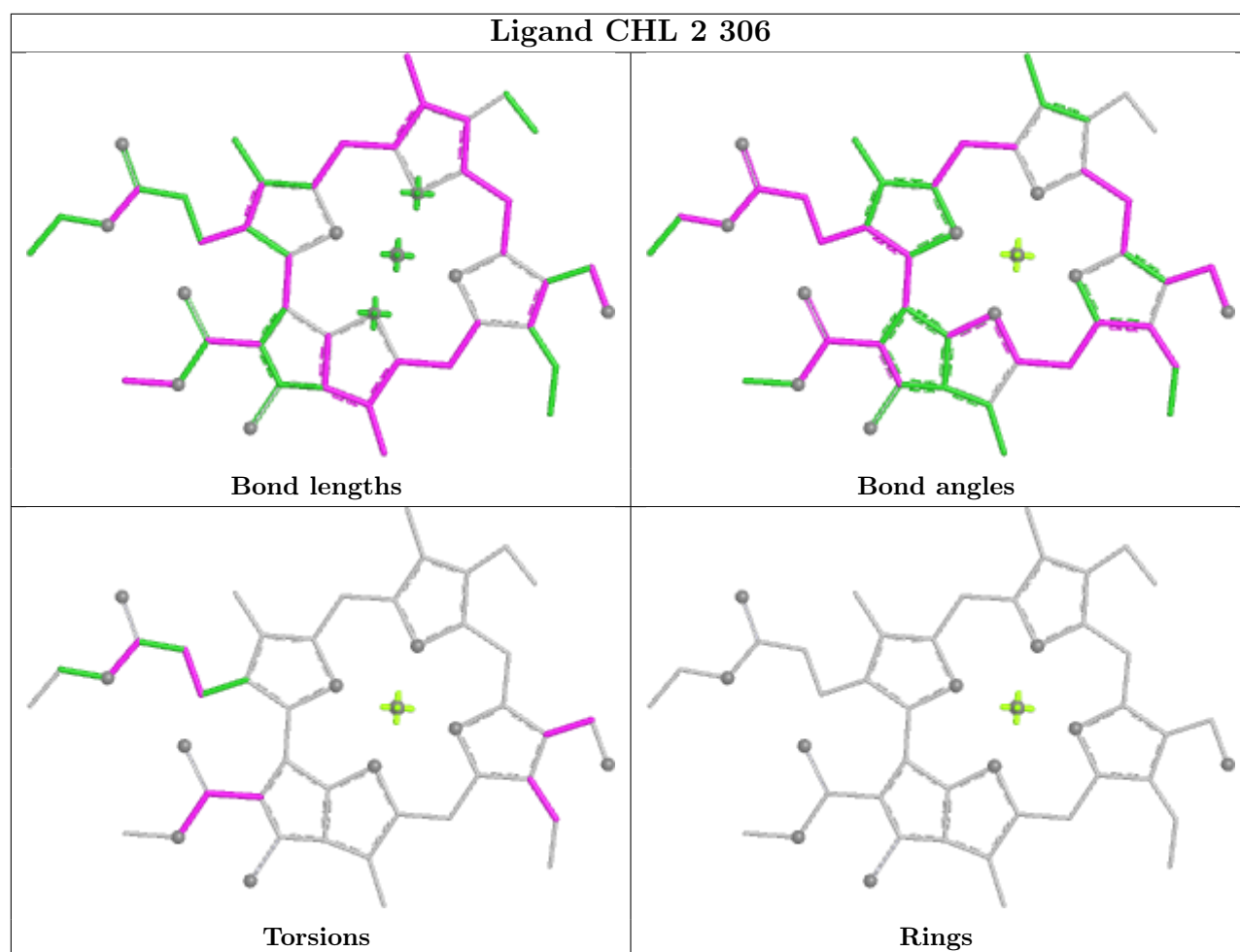


Ligand CLA A 802

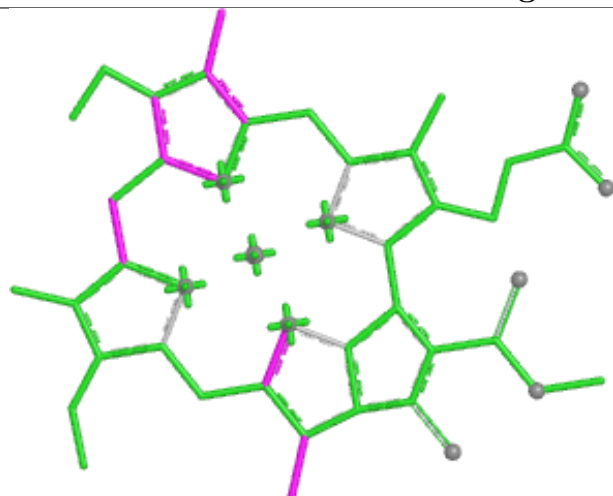


Ligand CLA A 818

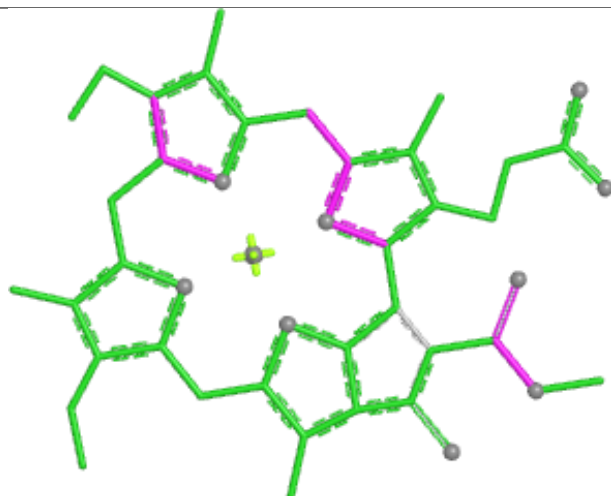




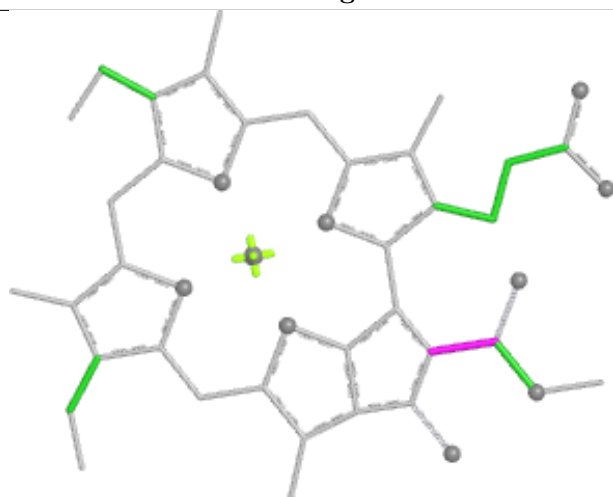
Ligand CLA 3 313



Bond lengths



Bond angles

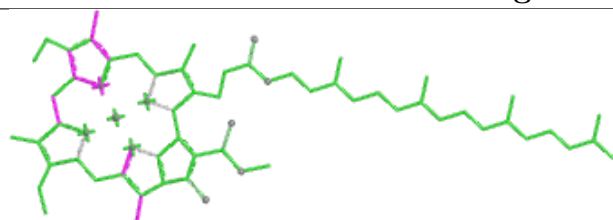


Torsions

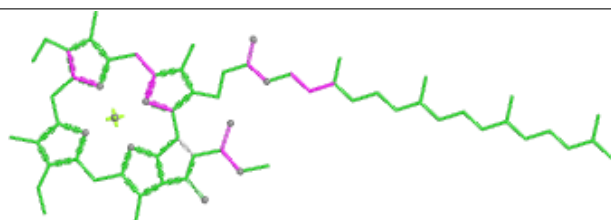


Rings

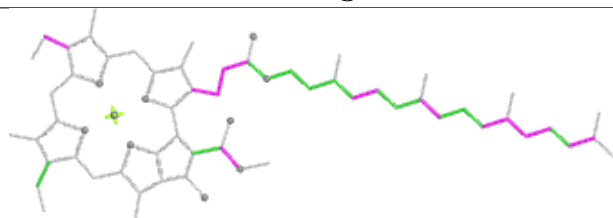
Ligand CLA A 808



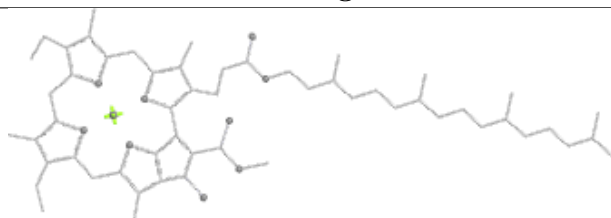
Bond lengths



Bond angles

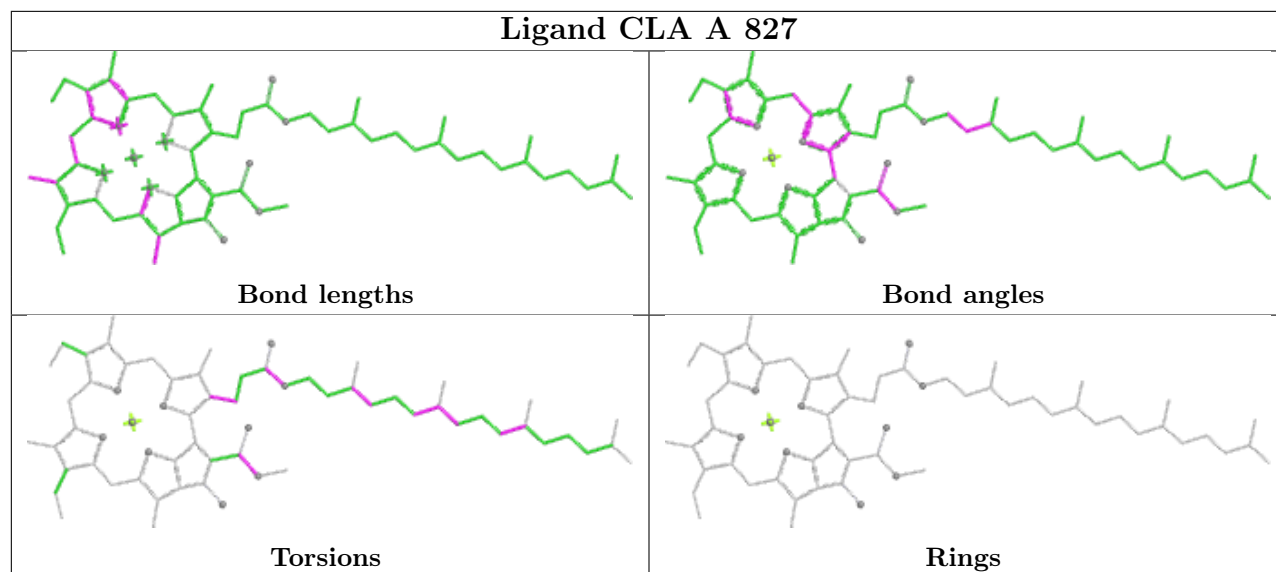


Torsions

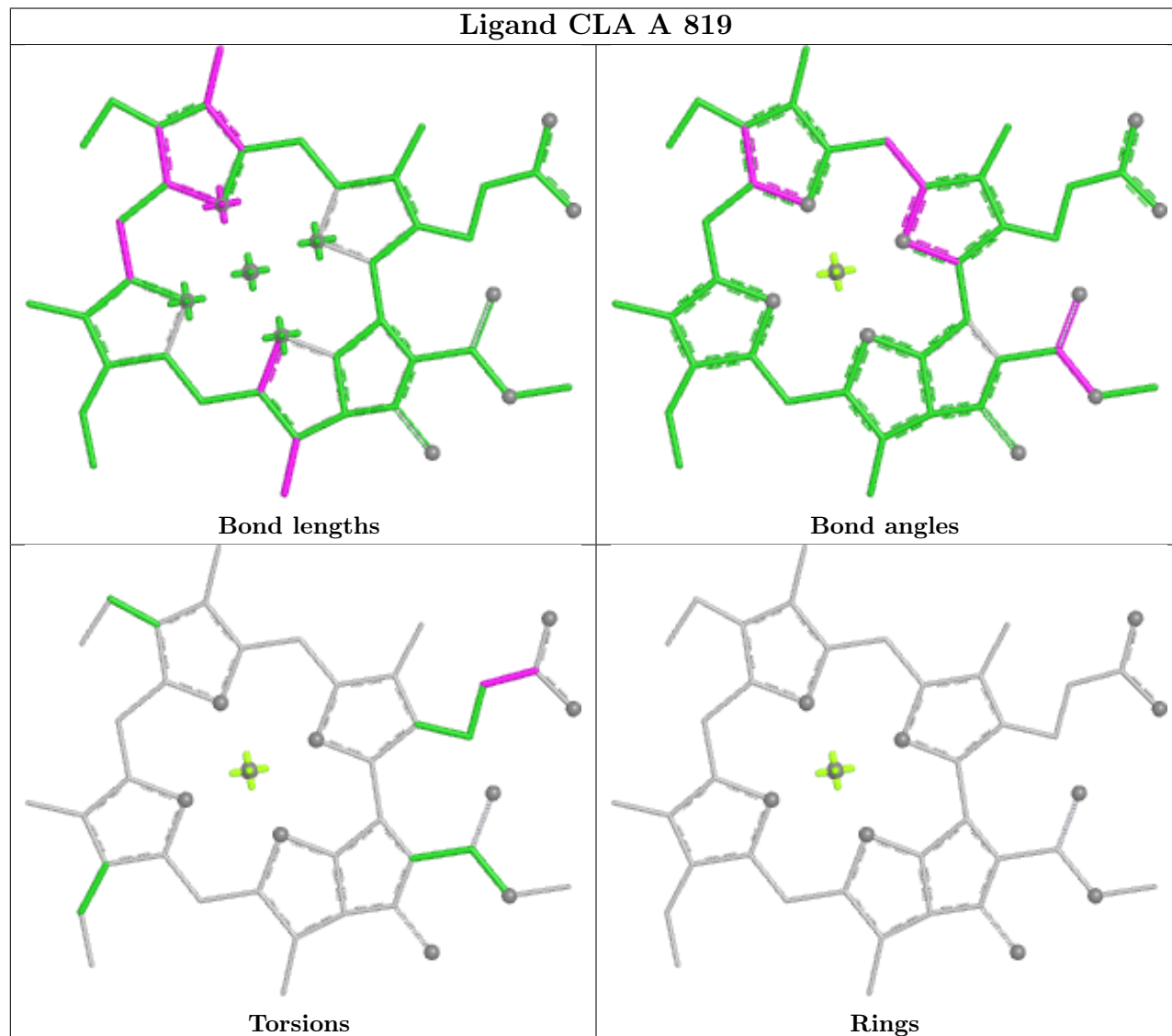


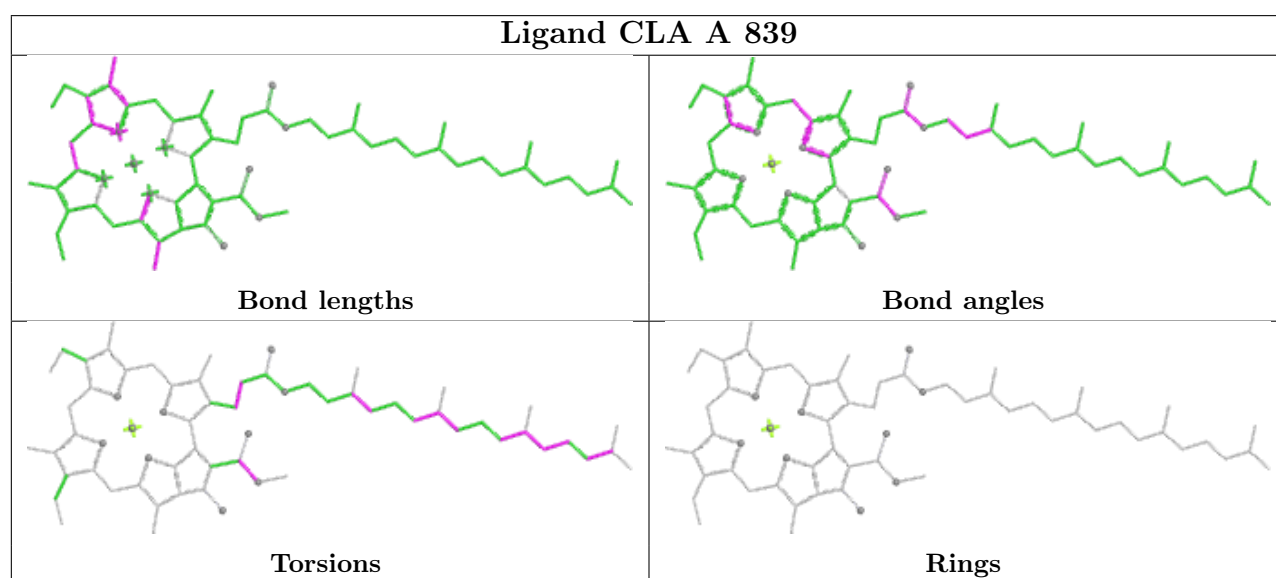
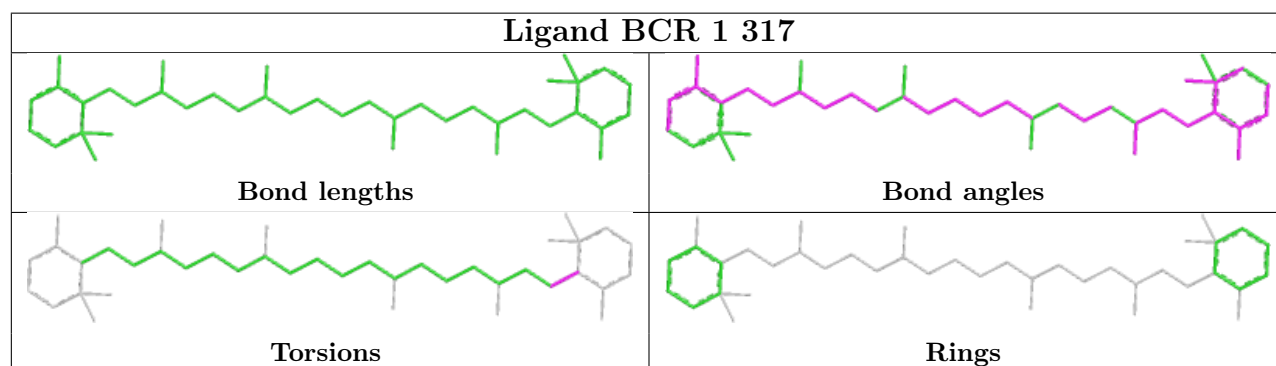
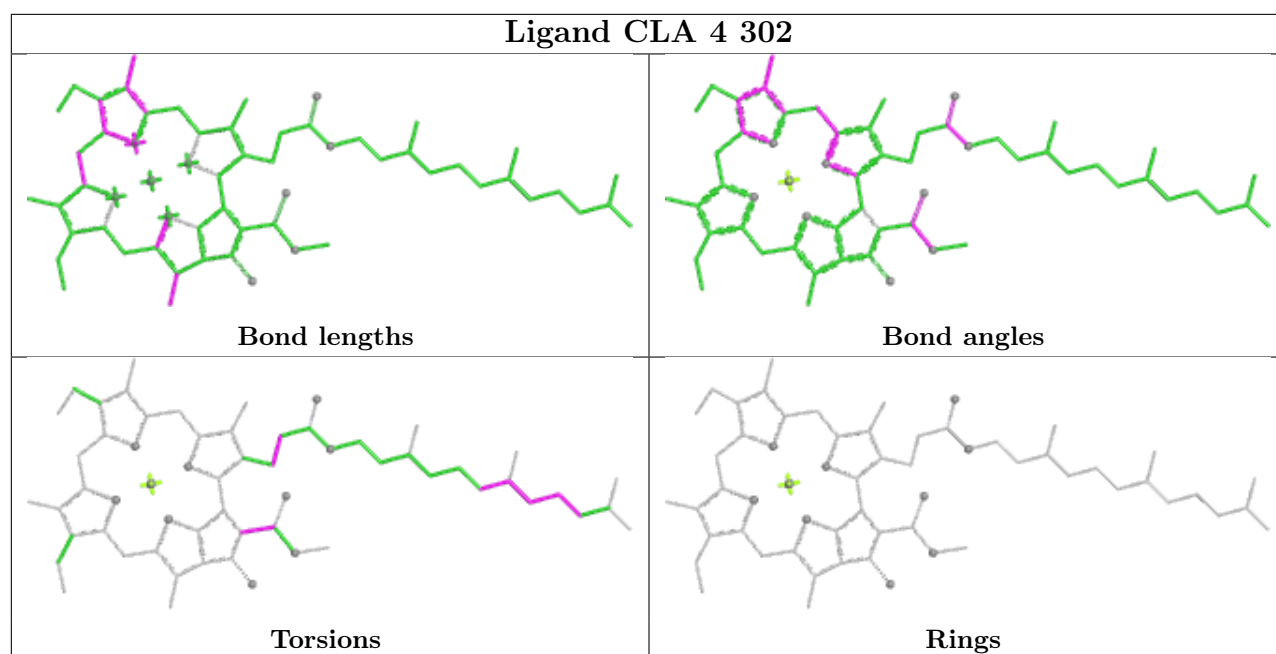
Rings

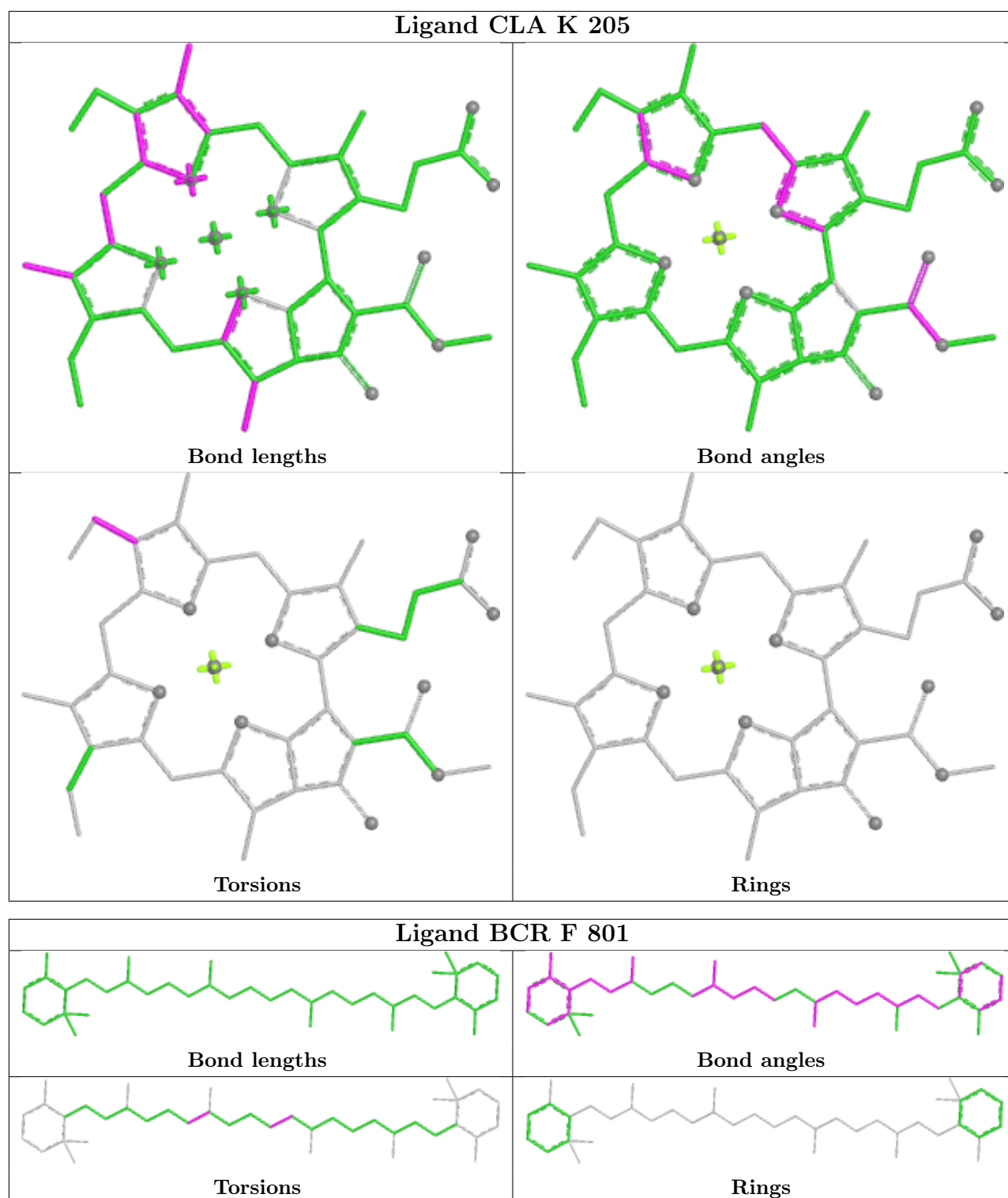
Ligand CLA A 827

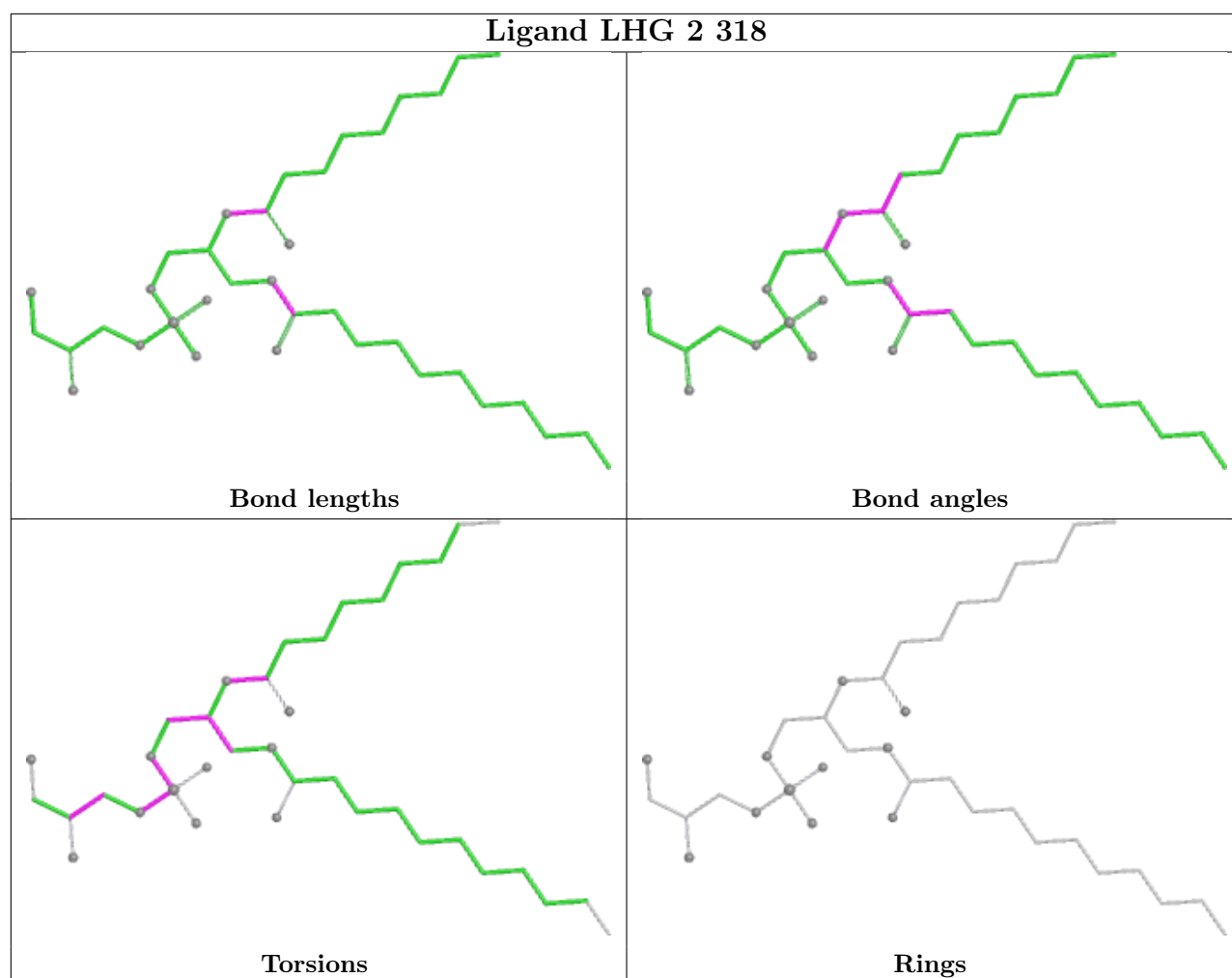


Ligand CLA A 819

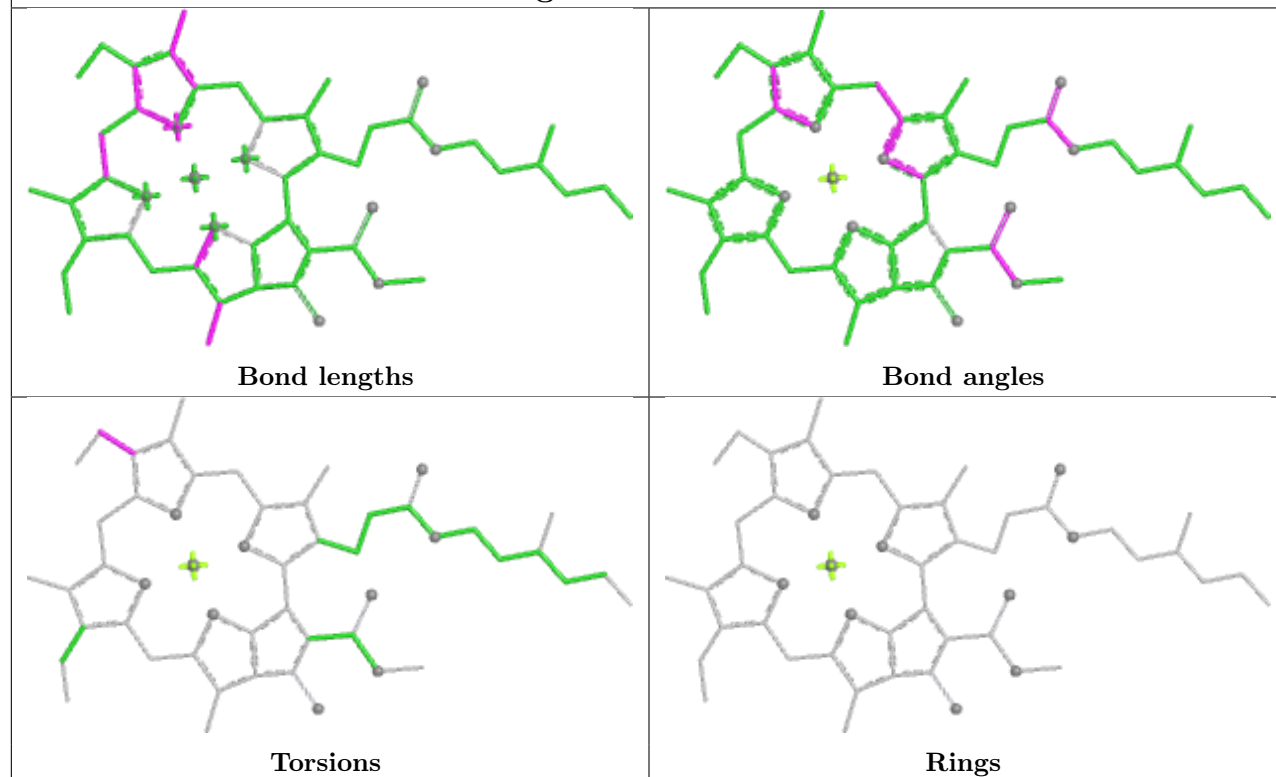




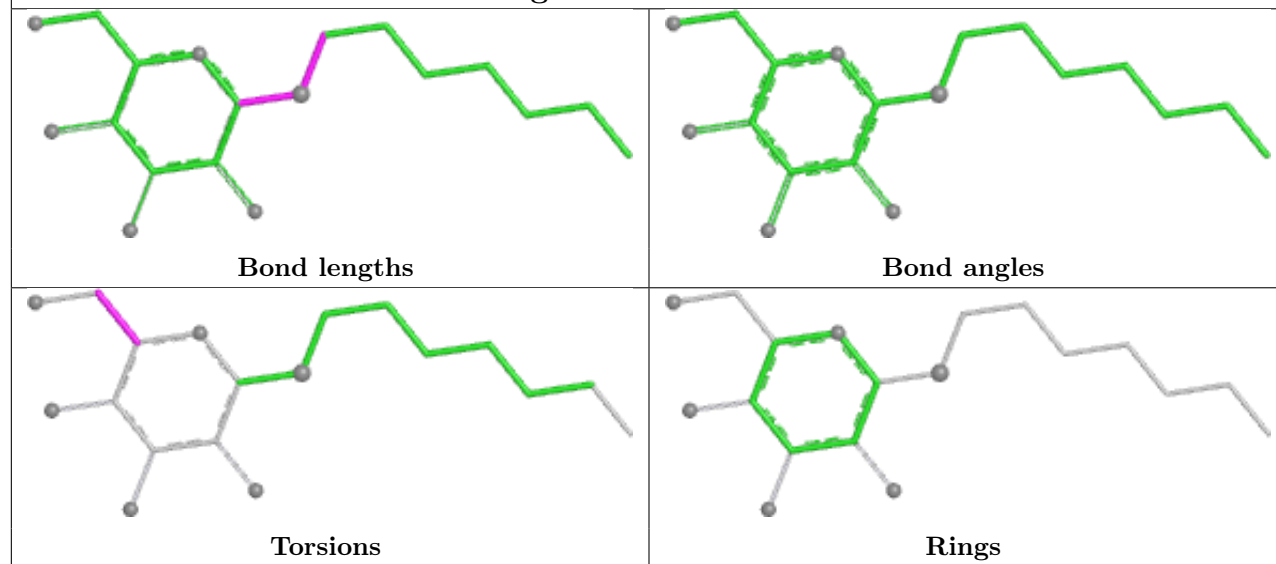




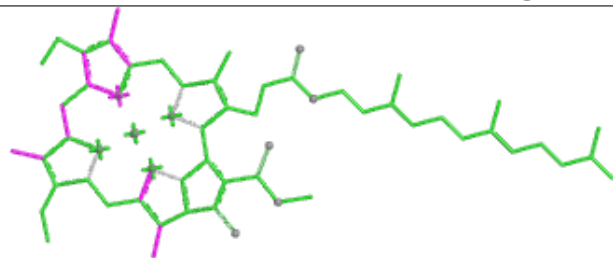
Ligand CLA 3 310



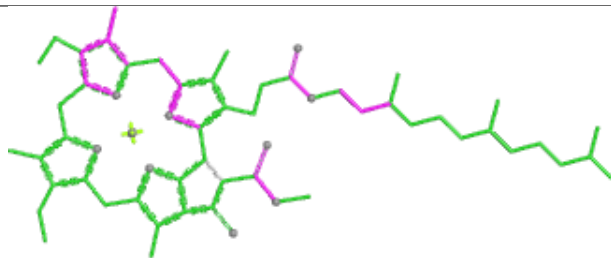
Ligand HTG F 803



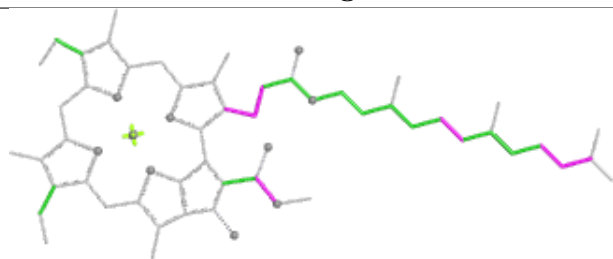
Ligand CLA 4 309



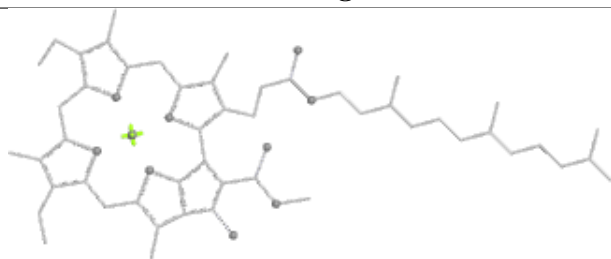
Bond lengths



Bond angles

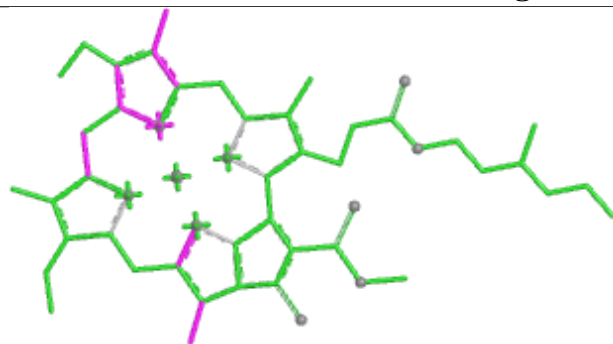


Torsions

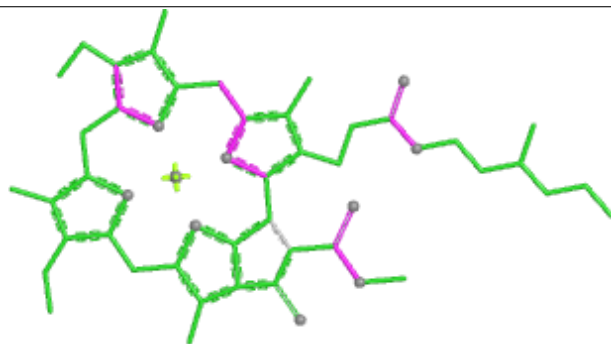


Rings

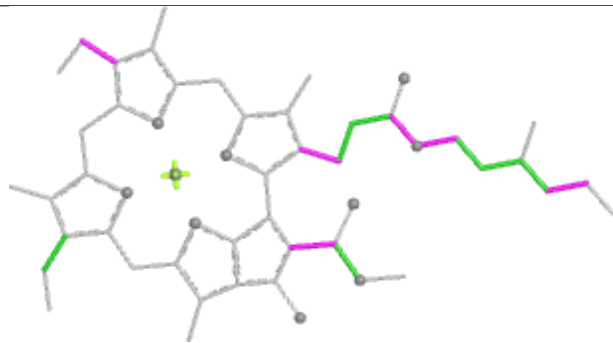
Ligand CLA O 201



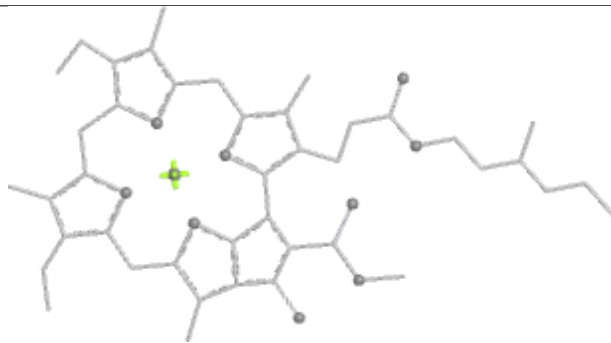
Bond lengths



Bond angles

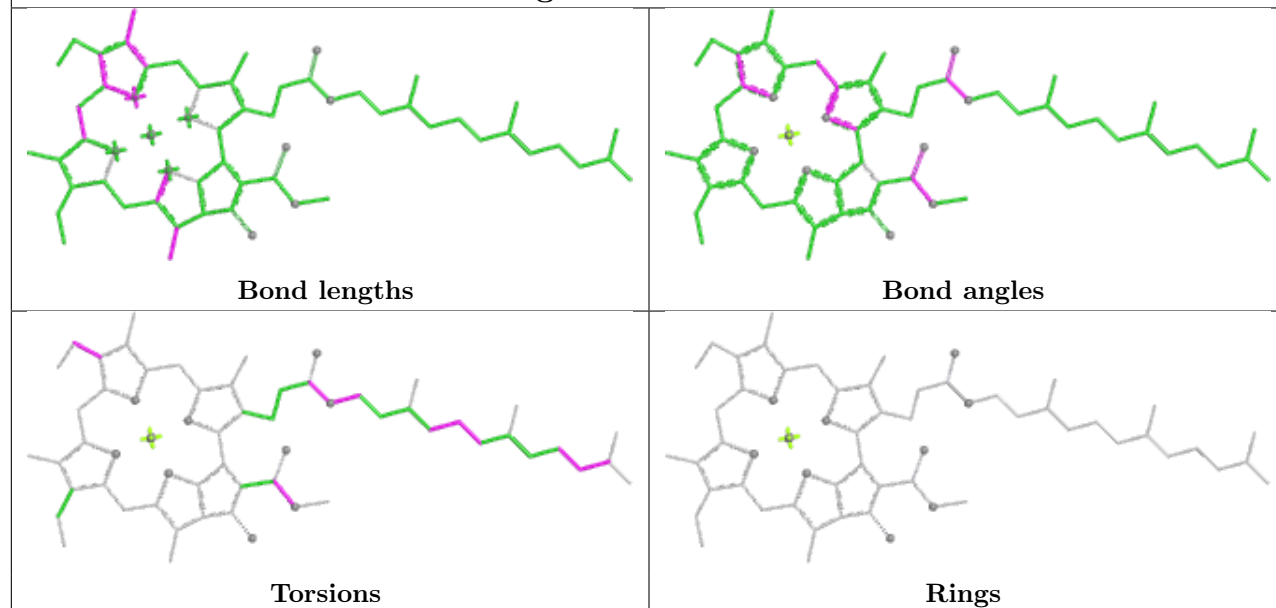


Torsions

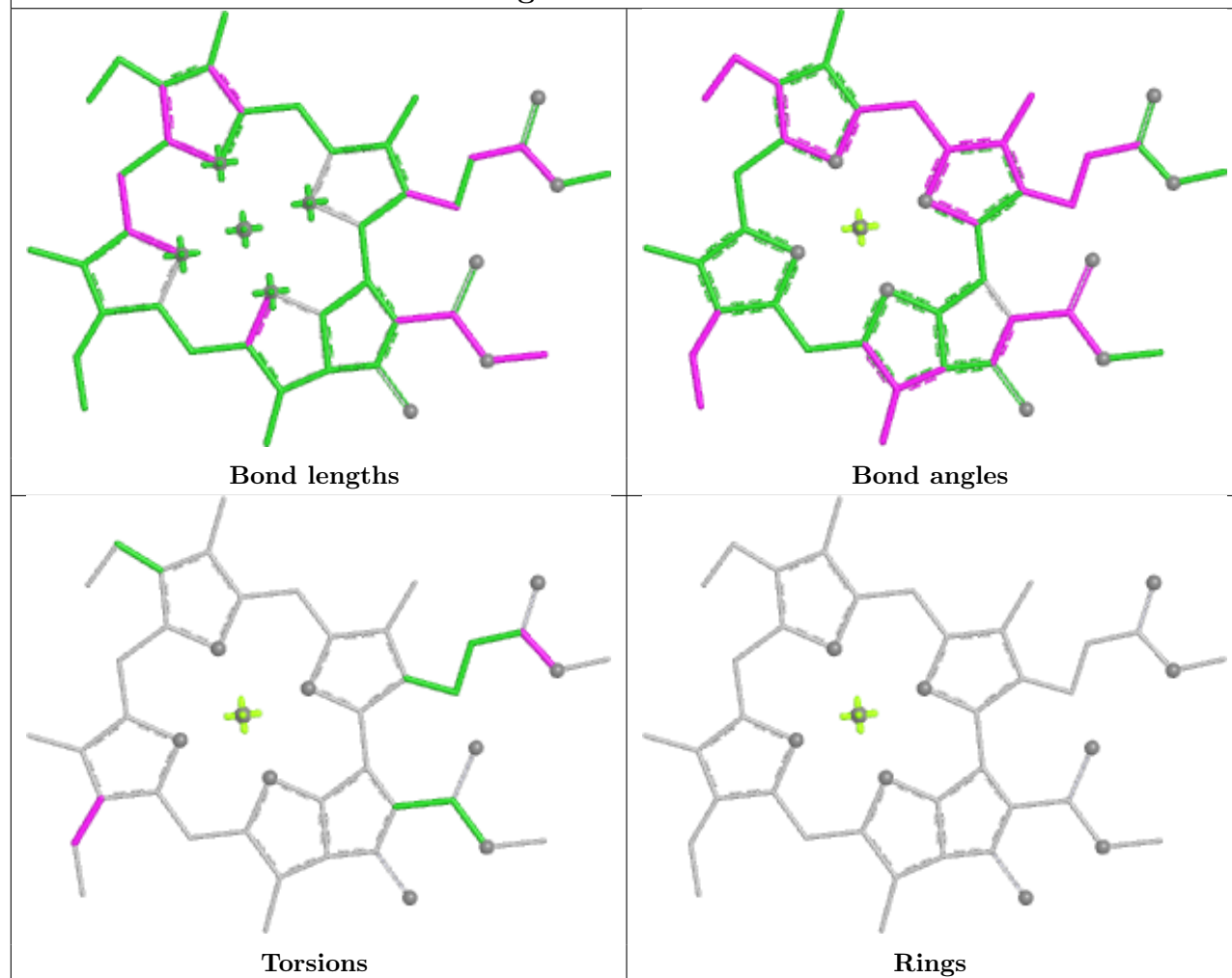


Rings

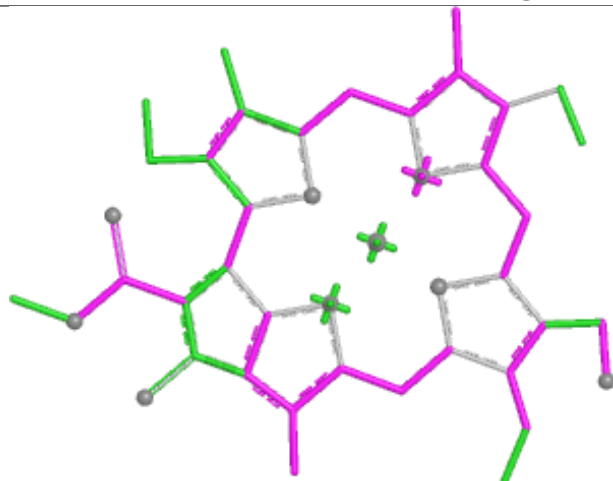
Ligand CLA 2 304



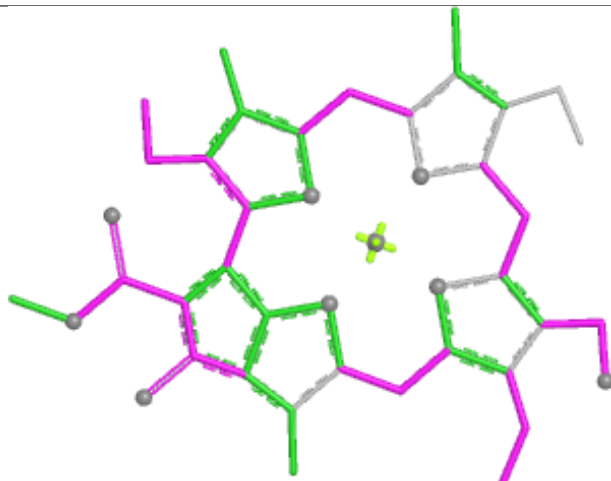
Ligand CLA 3 309



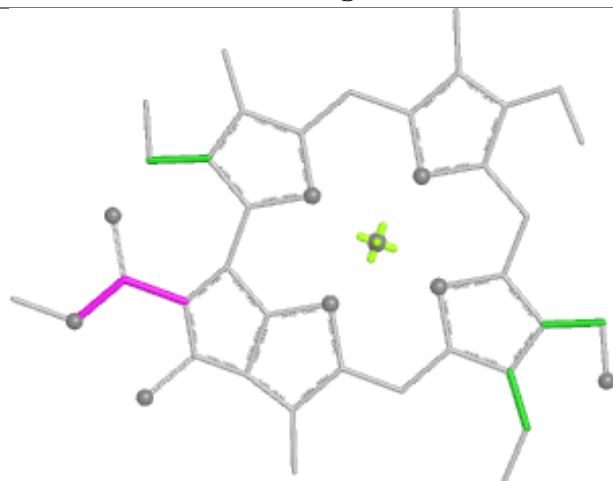
Ligand CHL 2 305



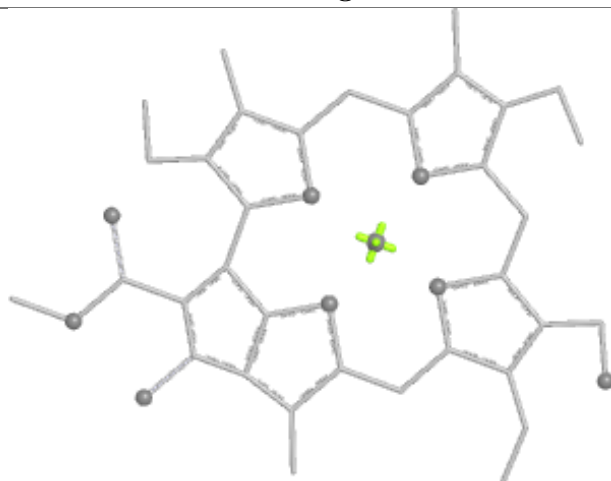
Bond lengths



Bond angles

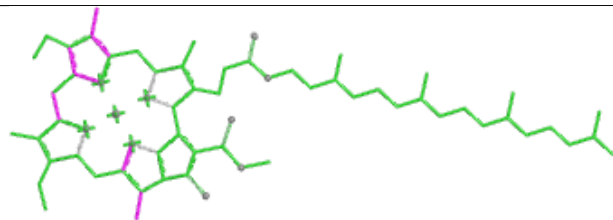


Torsions

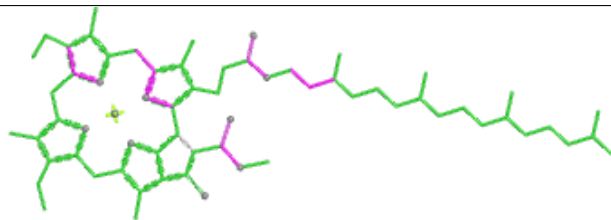


Rings

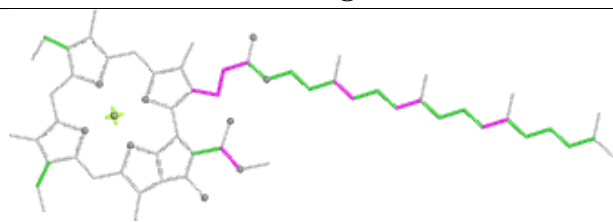
Ligand CLA B 827



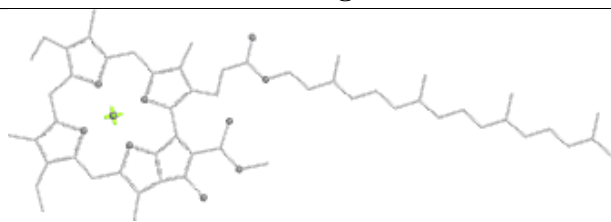
Bond lengths



Bond angles

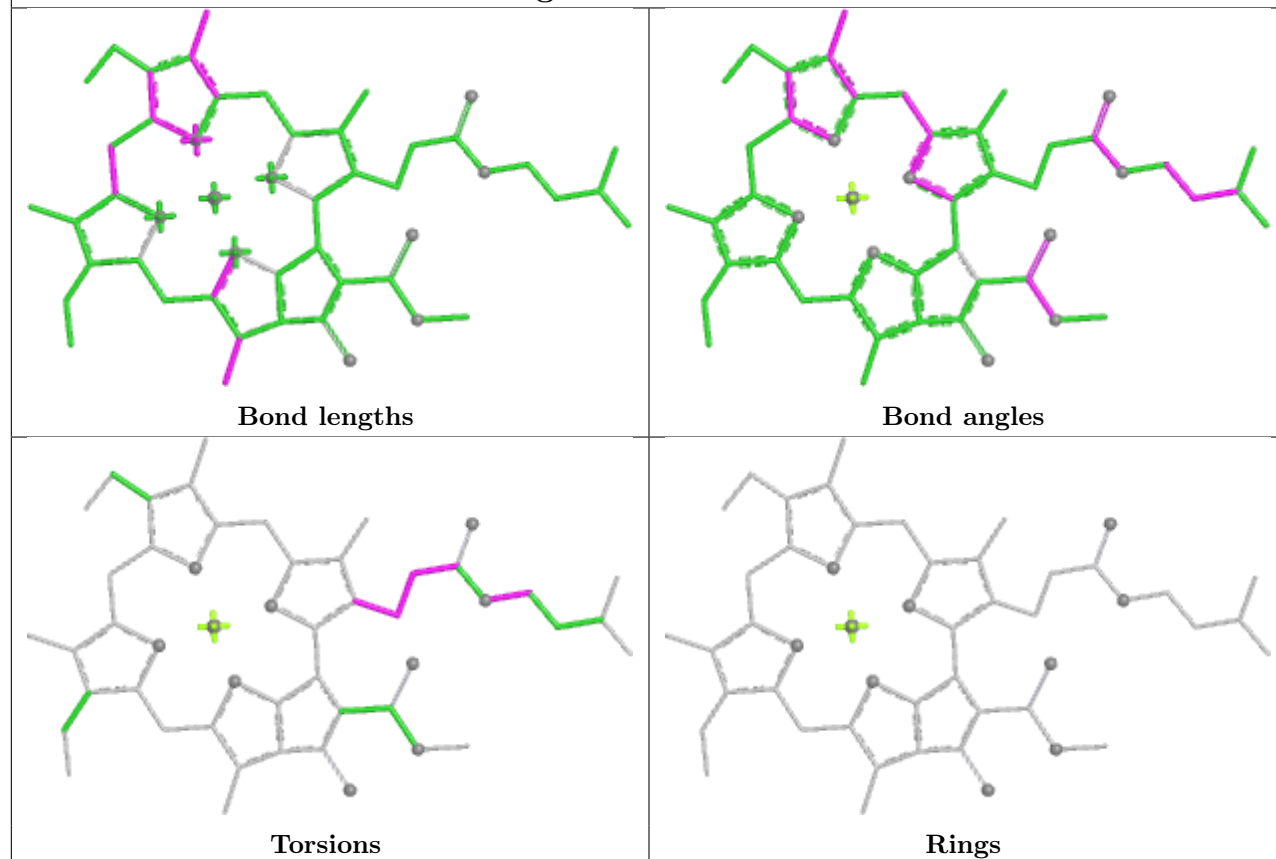


Torsions

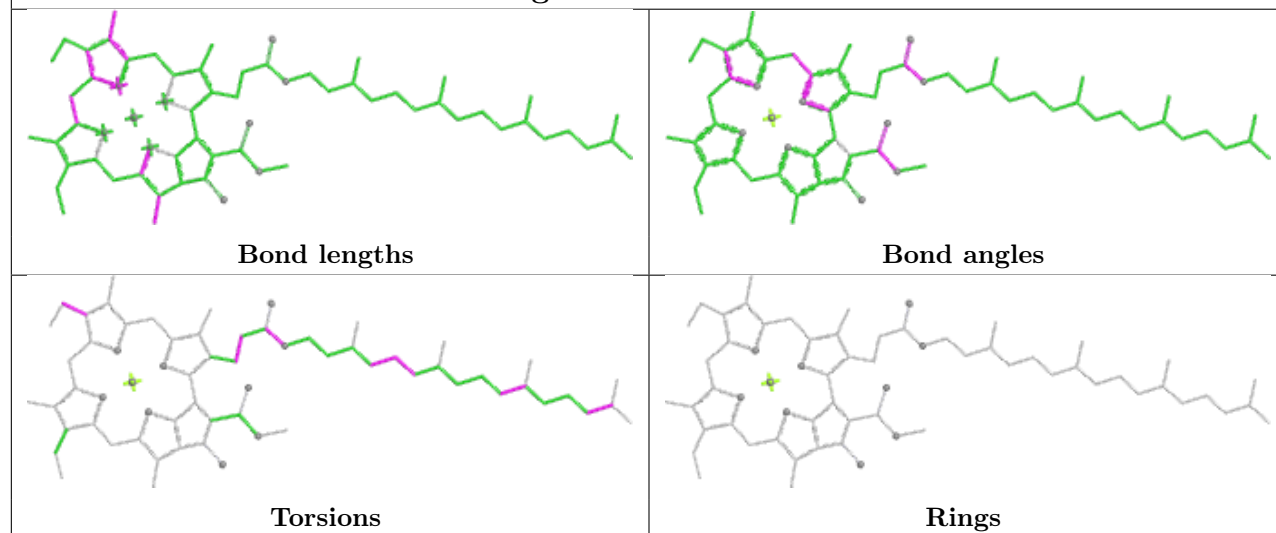


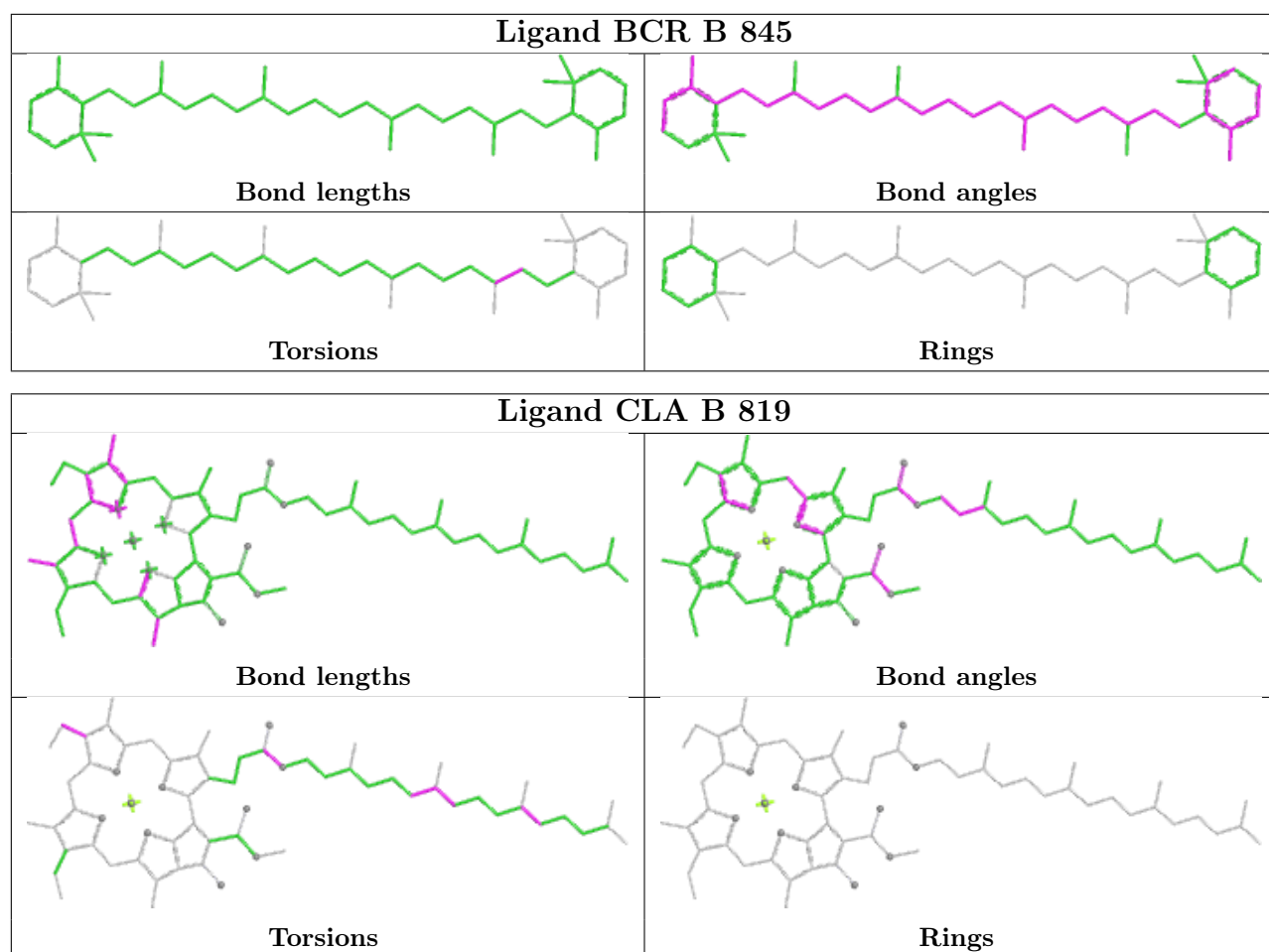
Rings

Ligand CLA 3 307

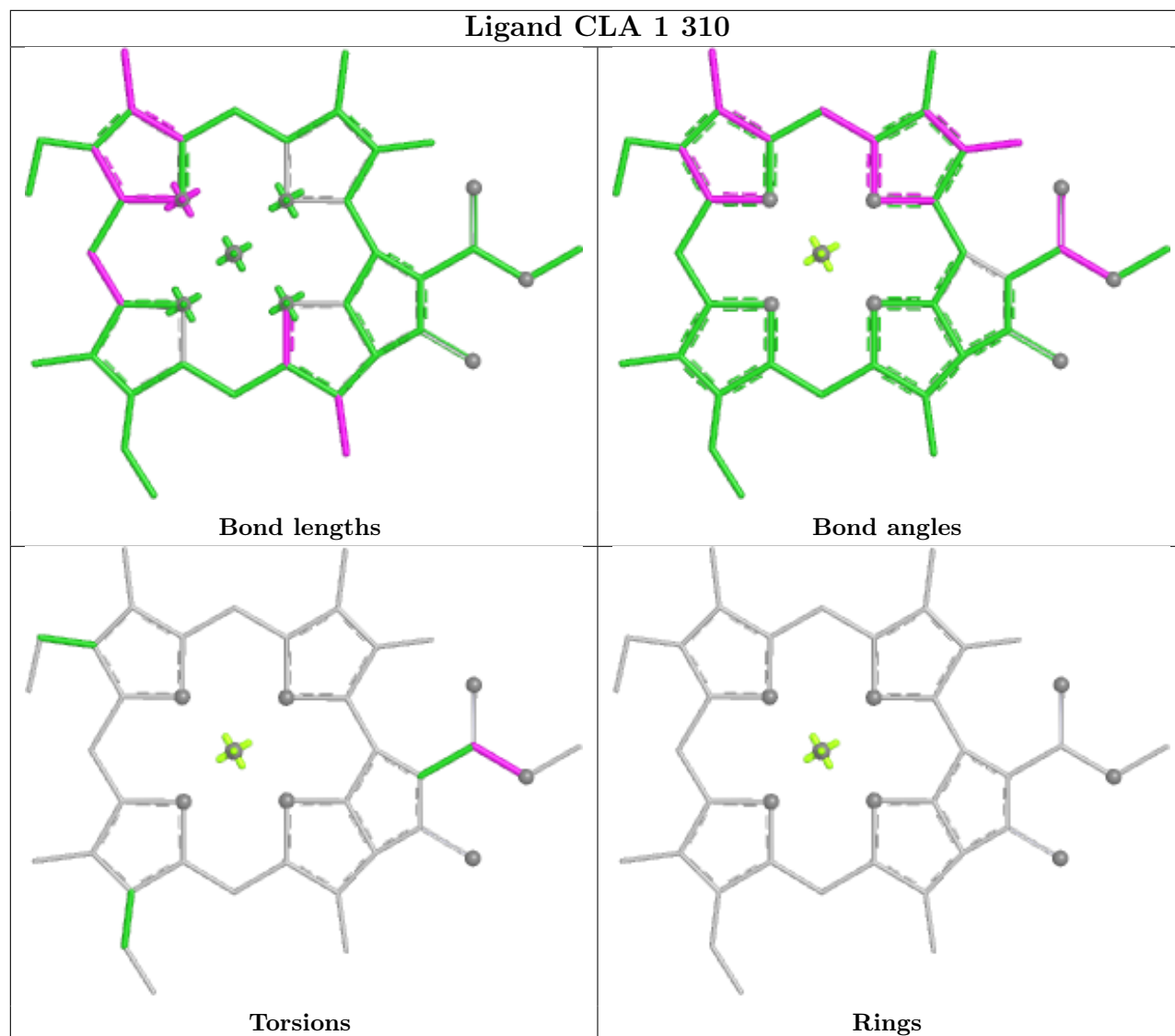


Ligand CLA A 820

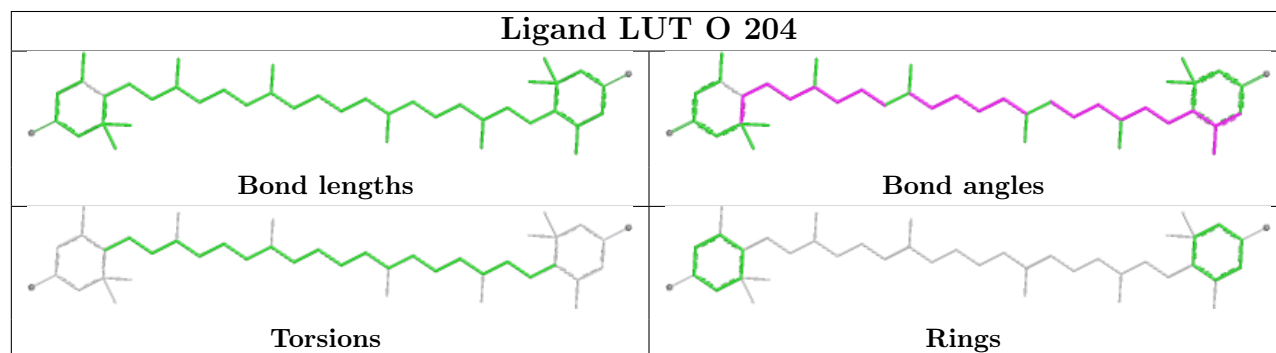


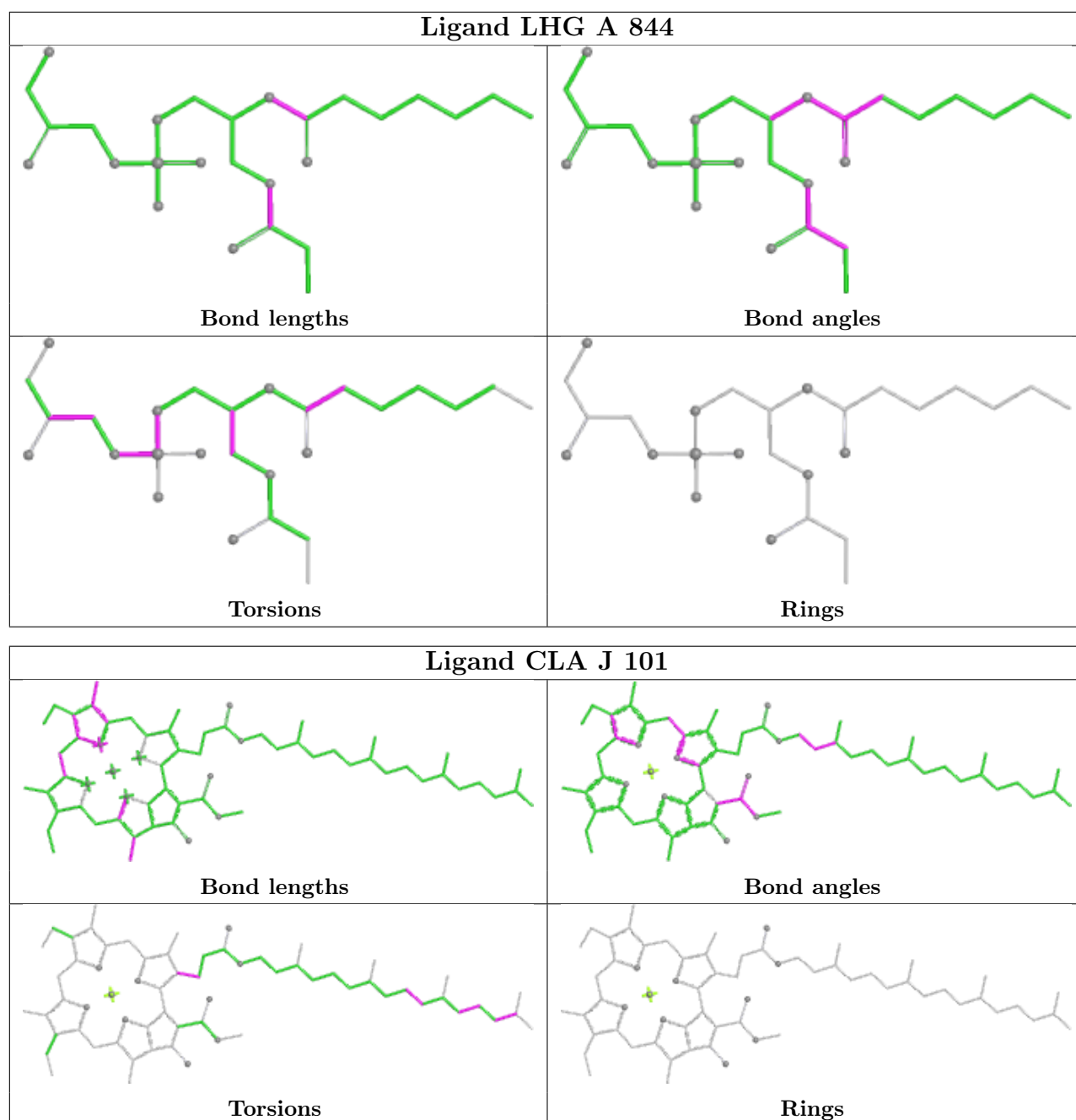


Ligand CLA 1 310

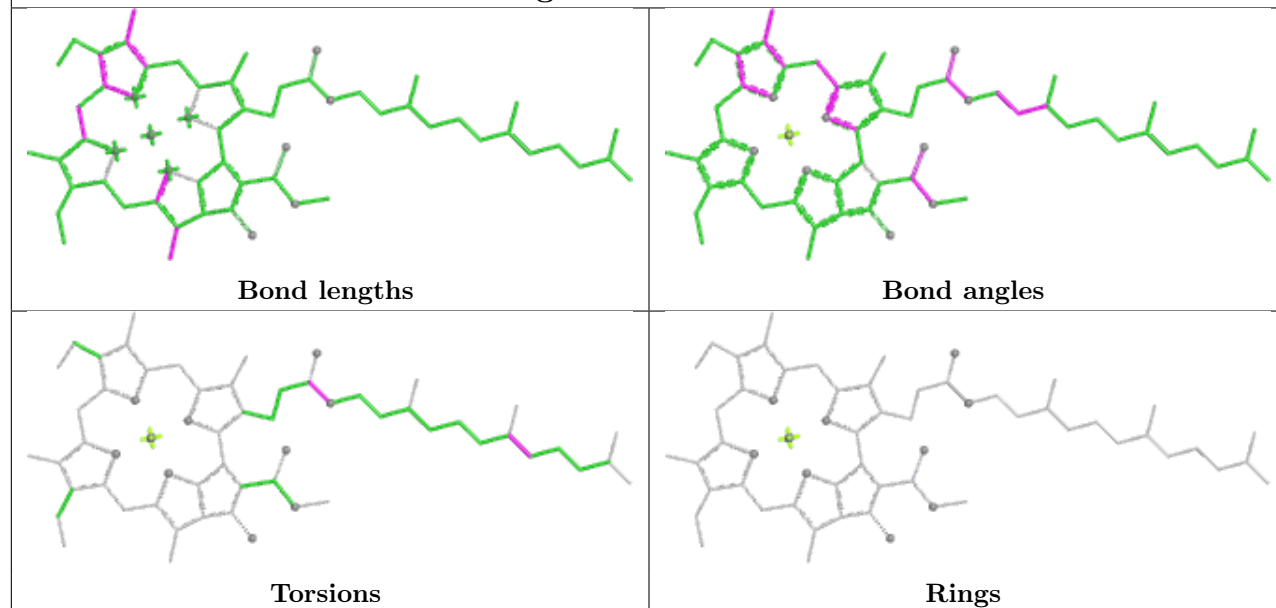


Ligand LUT O 204

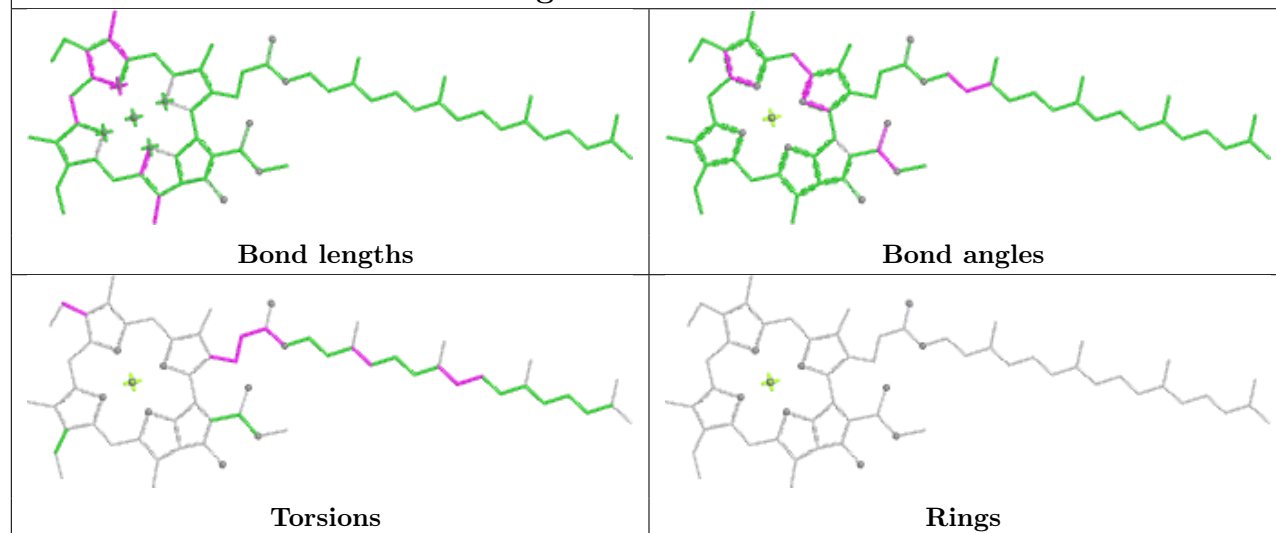


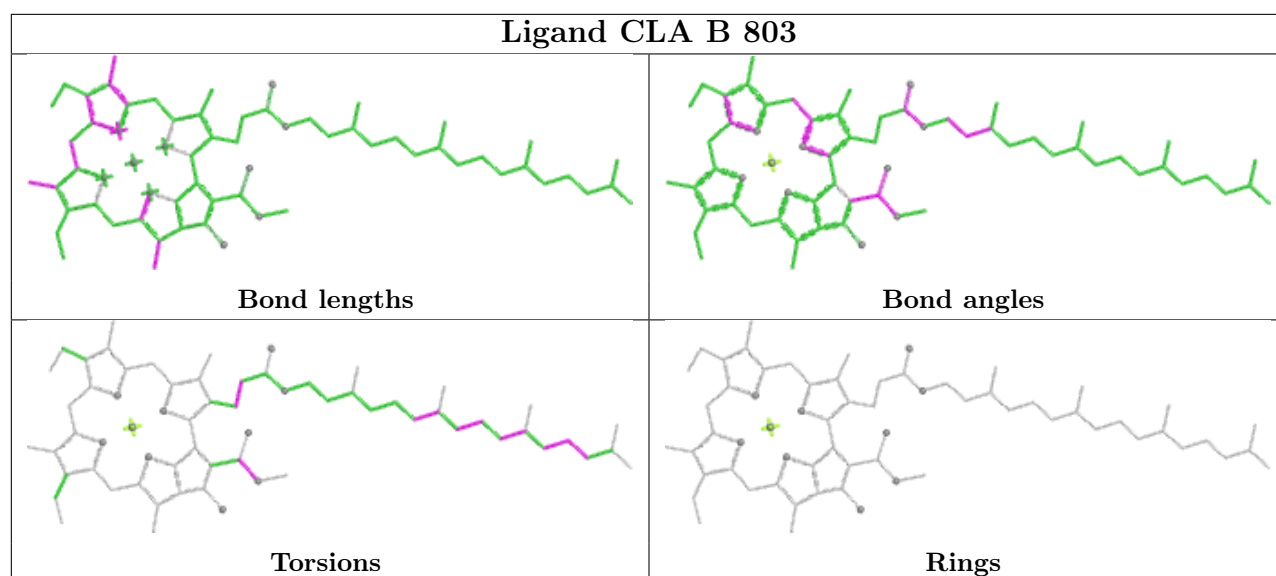
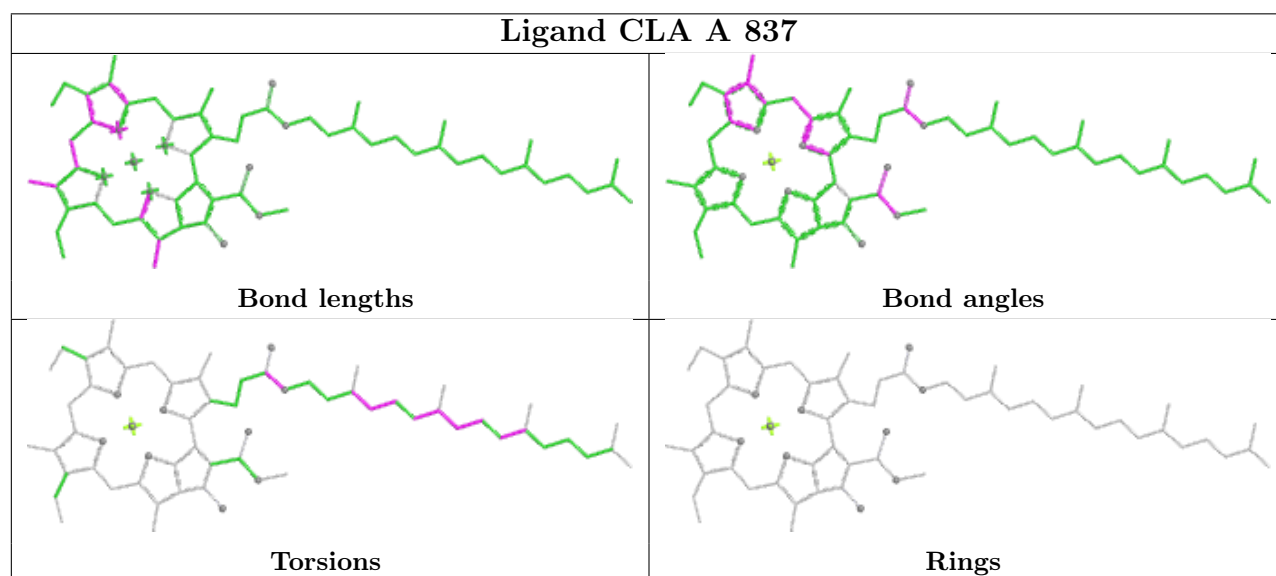
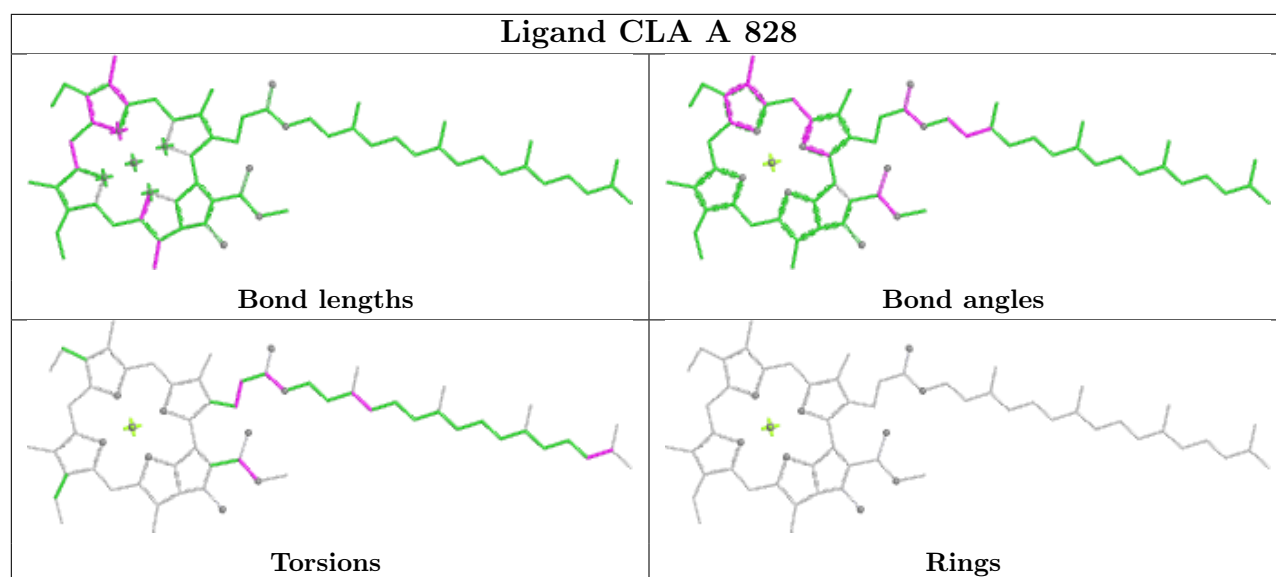


Ligand CLA 1 309

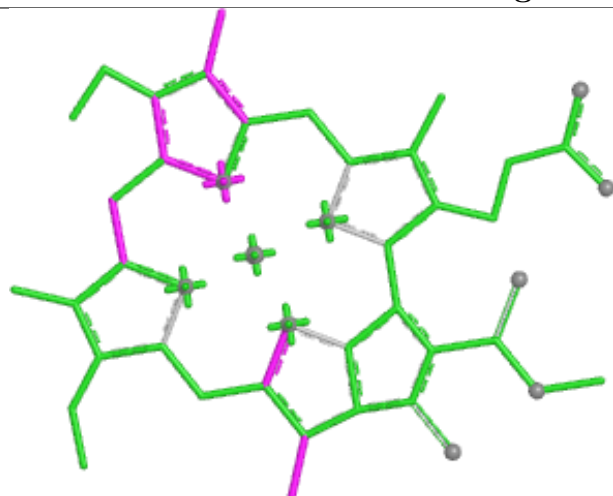


Ligand CLA 1 308

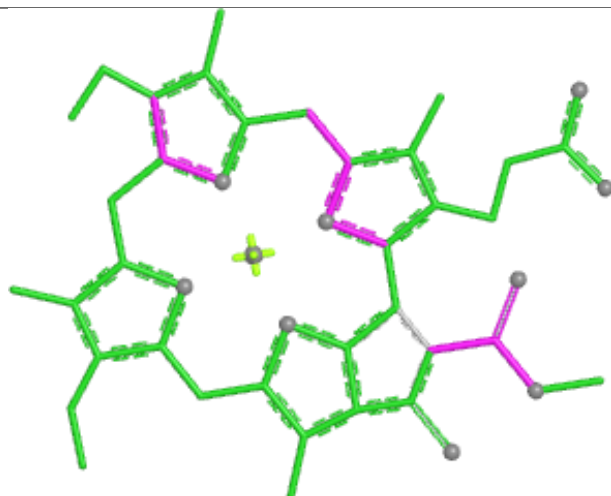




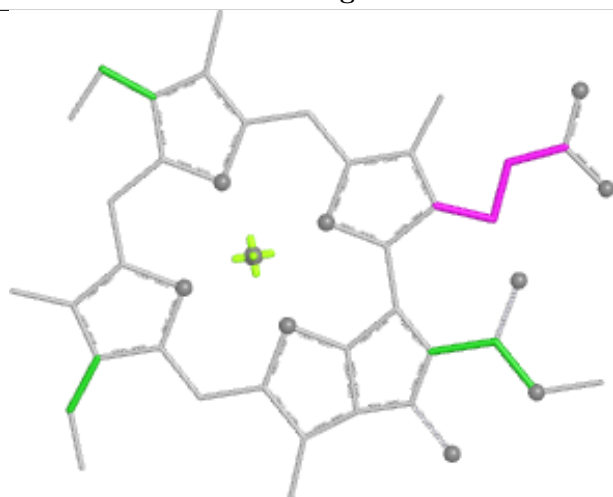
Ligand CLA B 804



Bond lengths



Bond angles

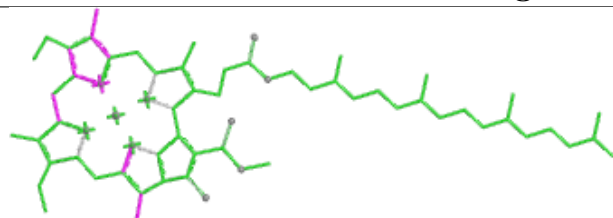


Torsions

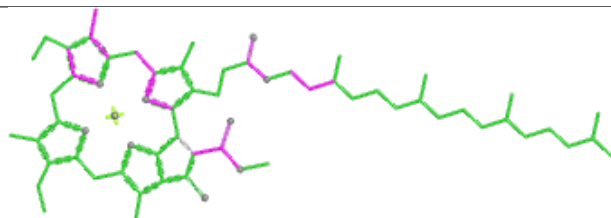


Rings

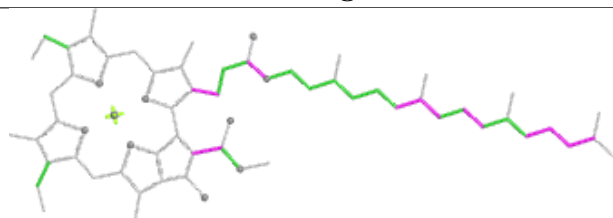
Ligand CLA B 825



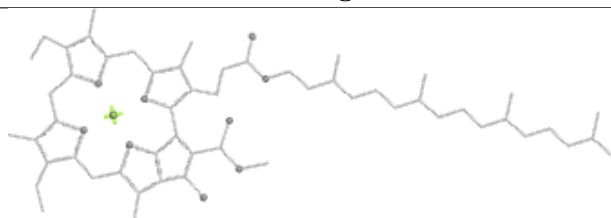
Bond lengths



Bond angles

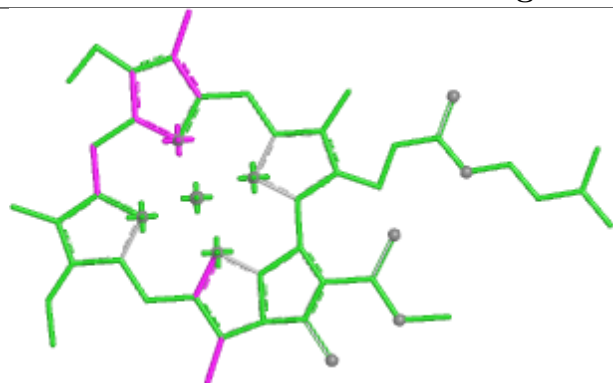


Torsions

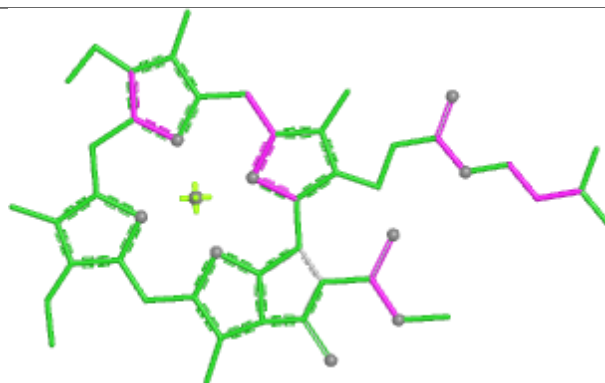


Rings

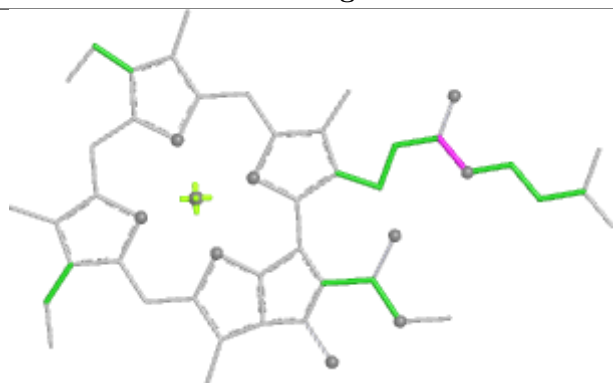
Ligand CLA L 304



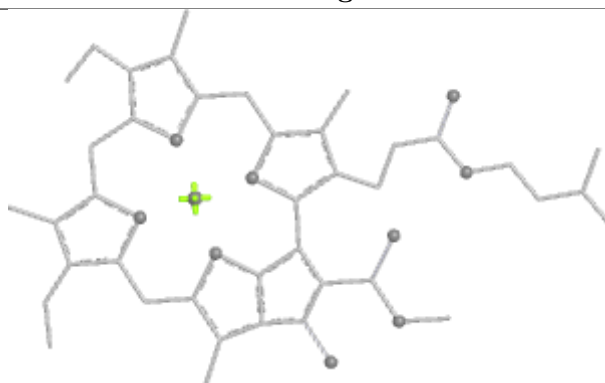
Bond lengths



Bond angles

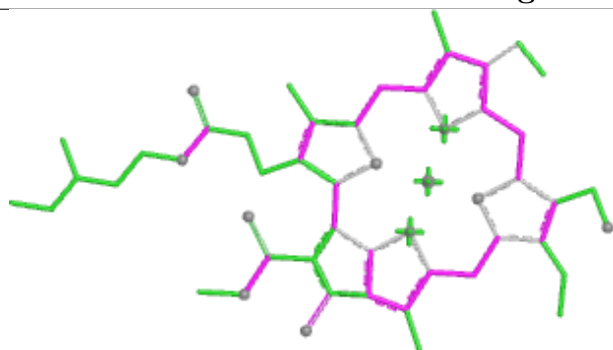


Torsions

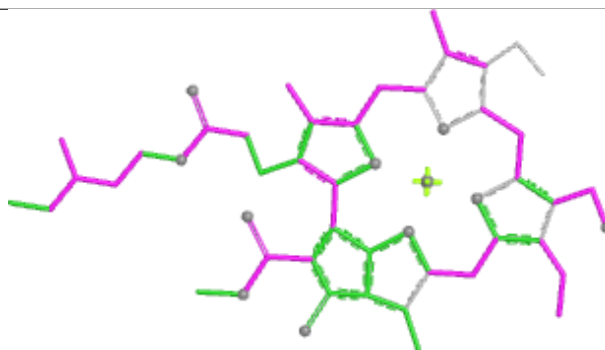


Rings

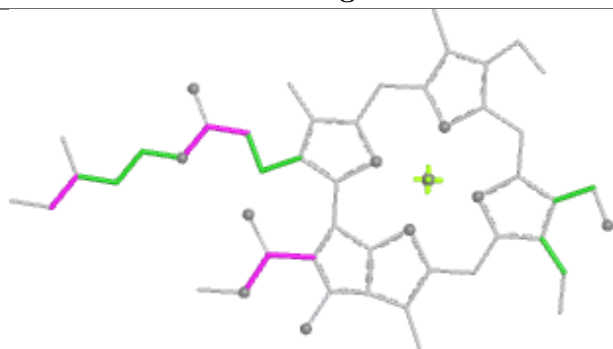
Ligand CHL 1 301



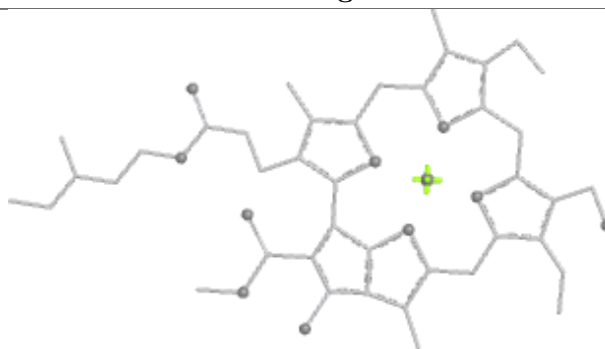
Bond lengths



Bond angles

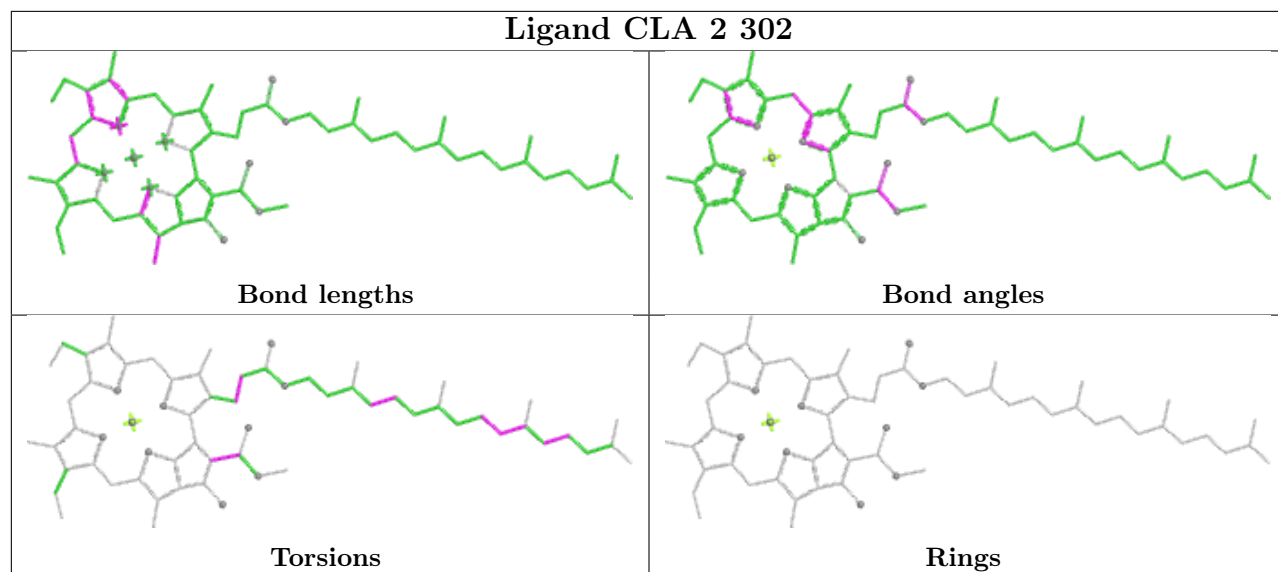


Torsions

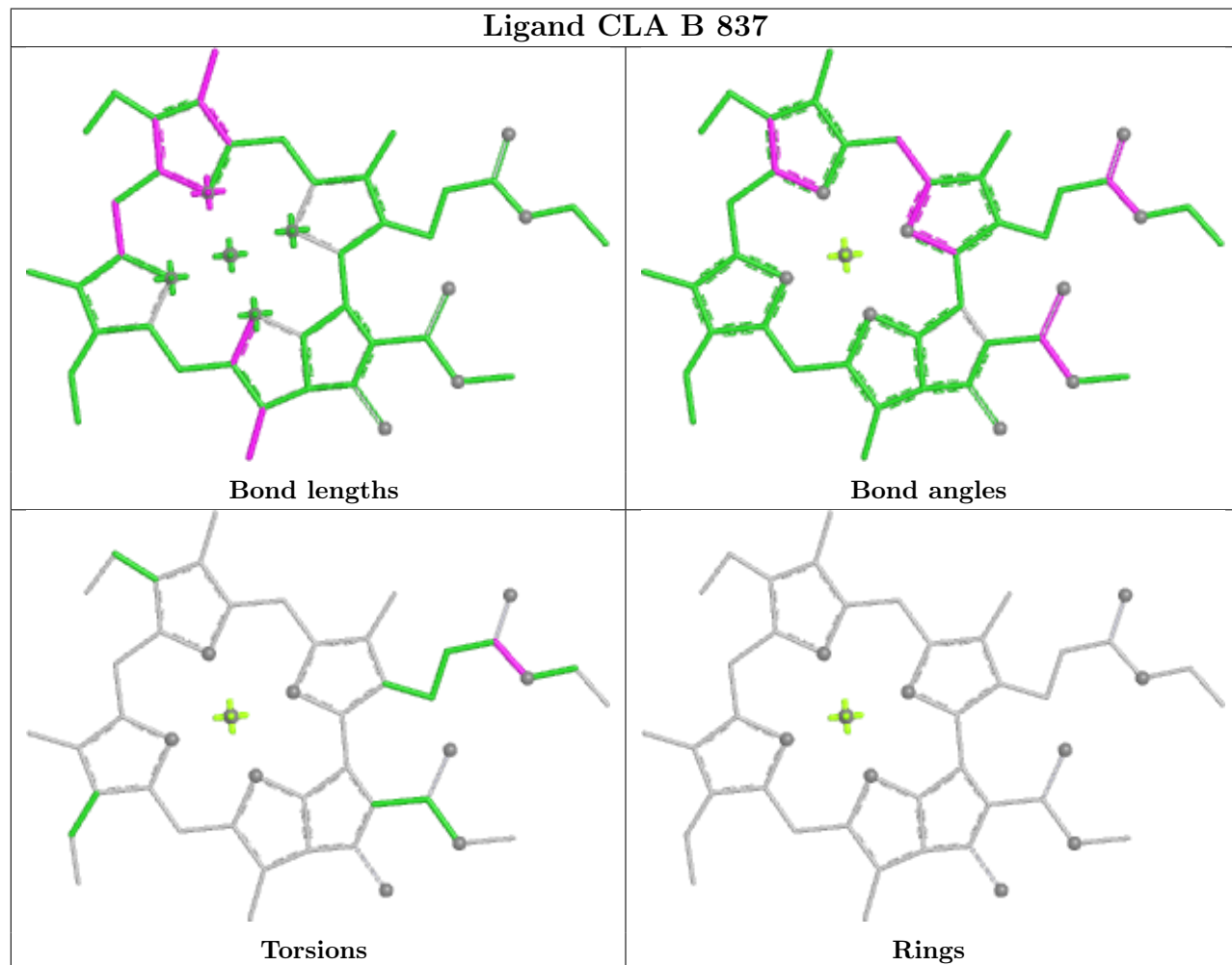


Rings

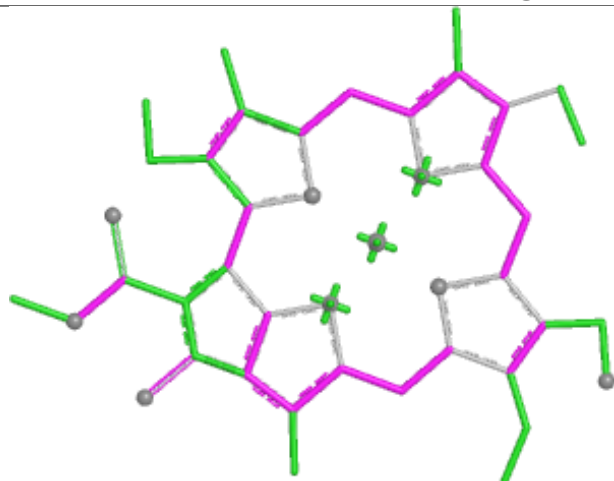
Ligand CLA 2 302



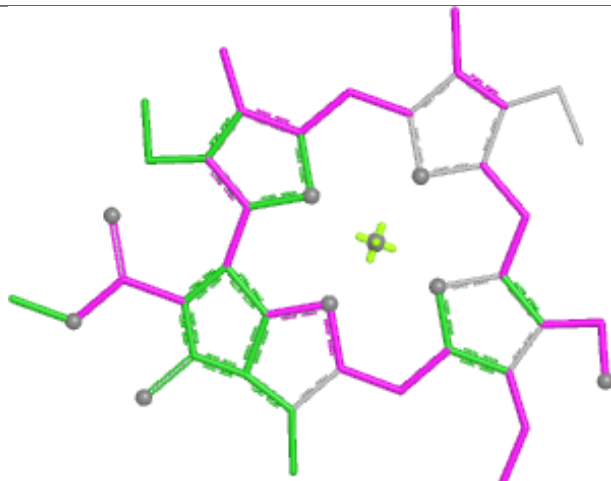
Ligand CLA B 837



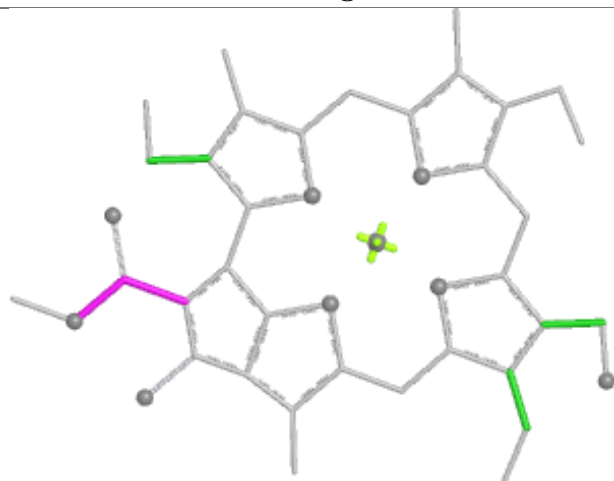
Ligand CHL 2 314



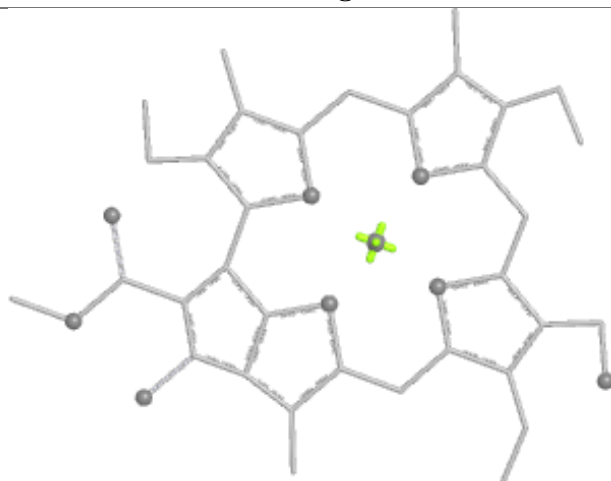
Bond lengths



Bond angles

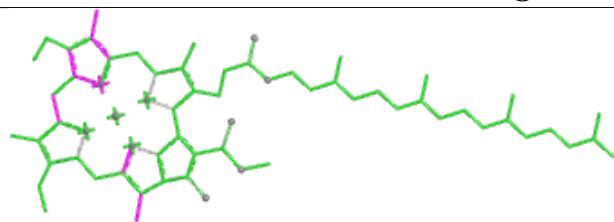


Torsions

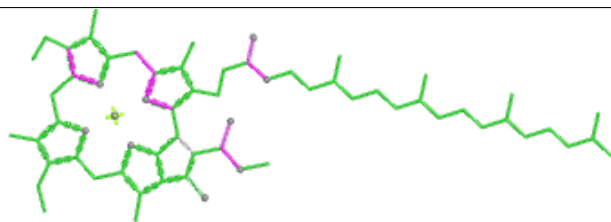


Rings

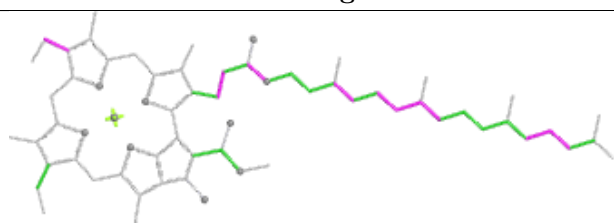
Ligand CLA A 816



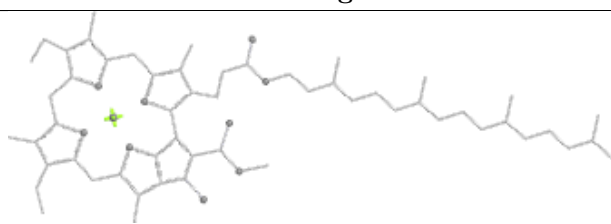
Bond lengths



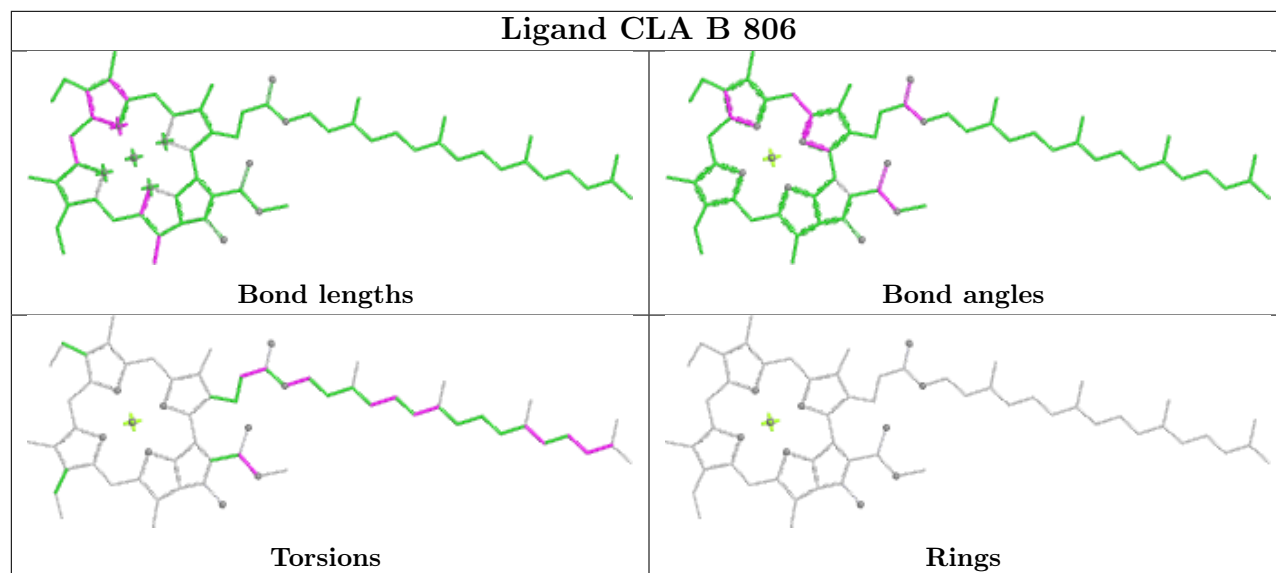
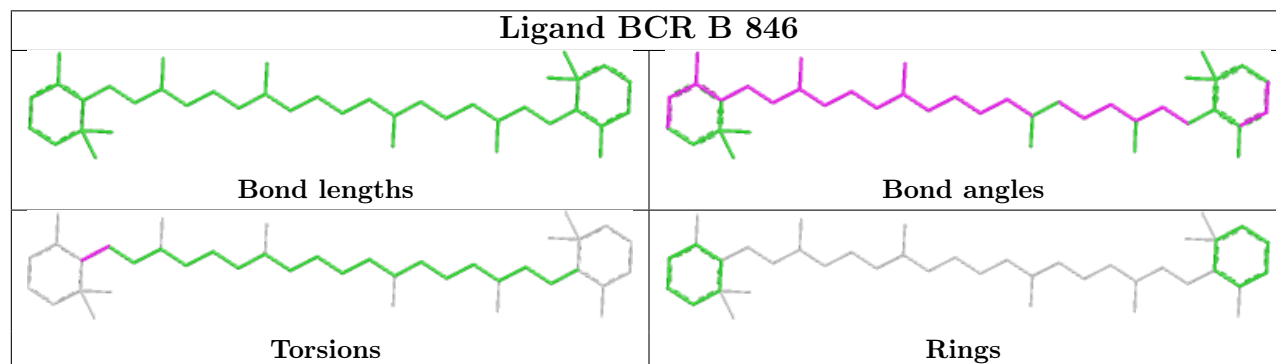
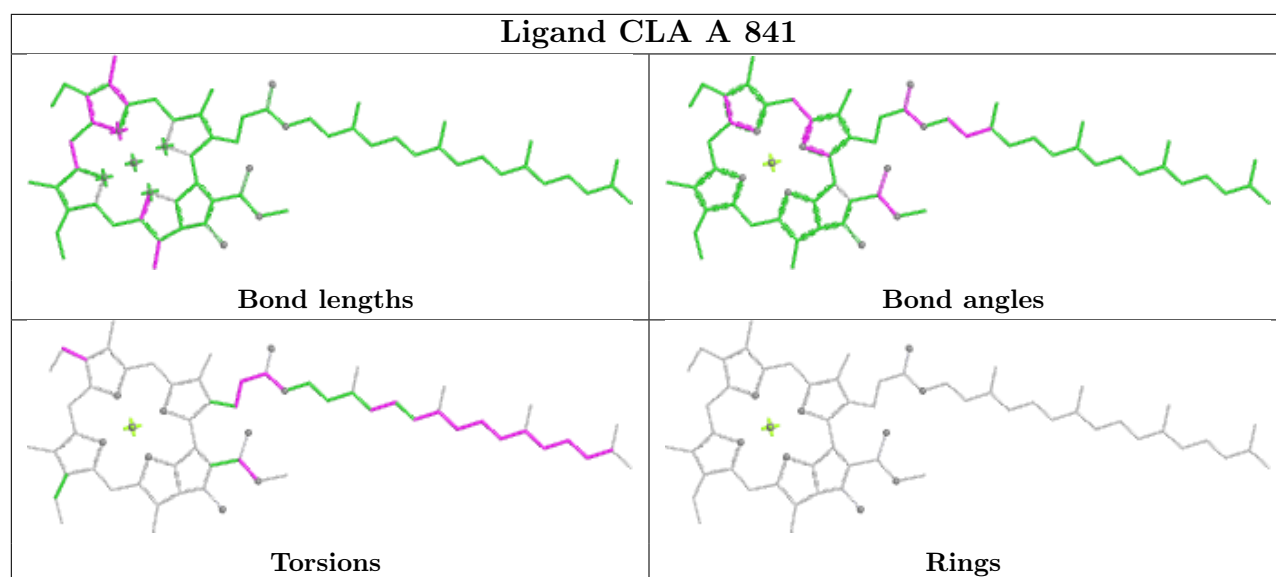
Bond angles

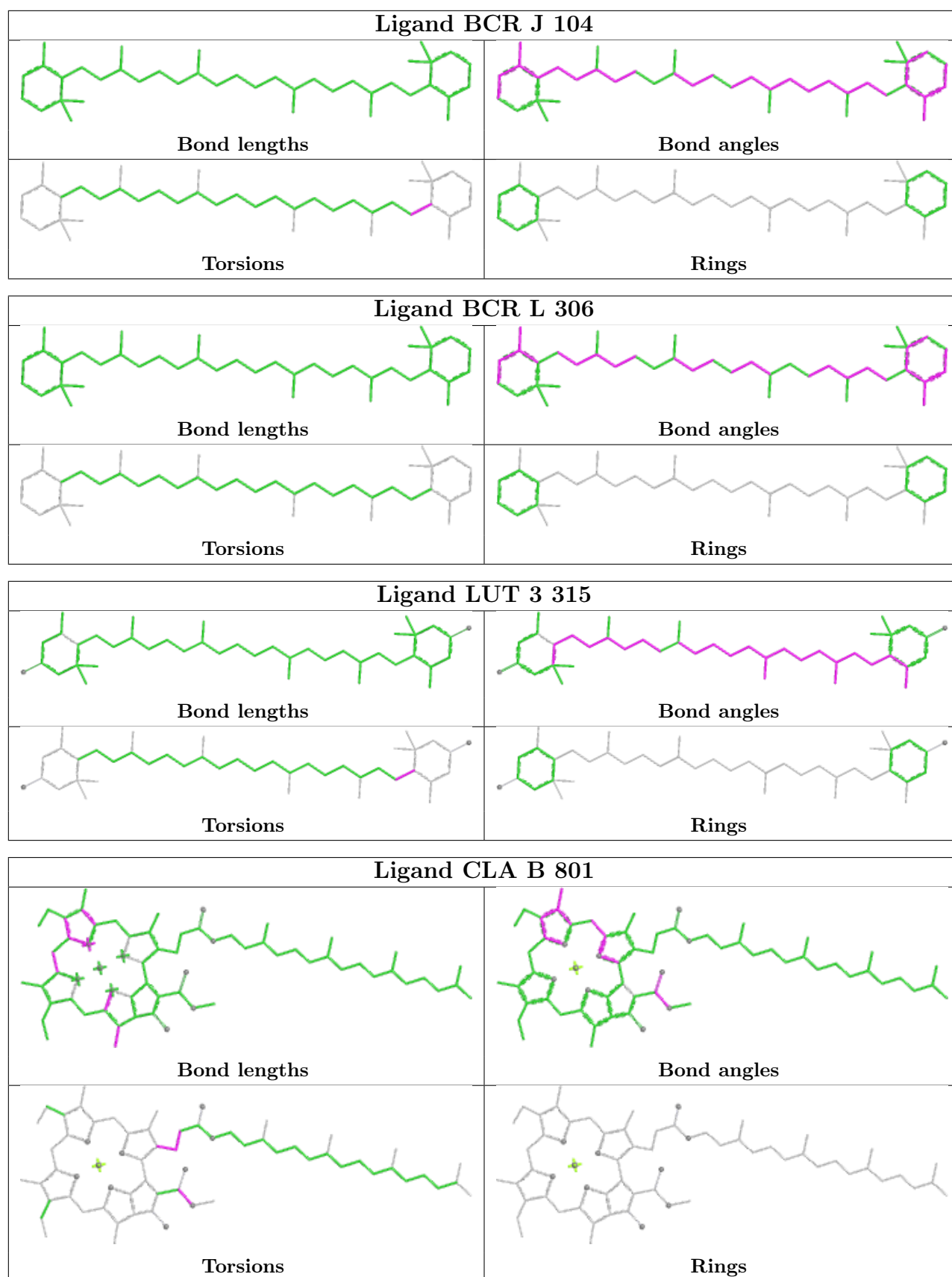


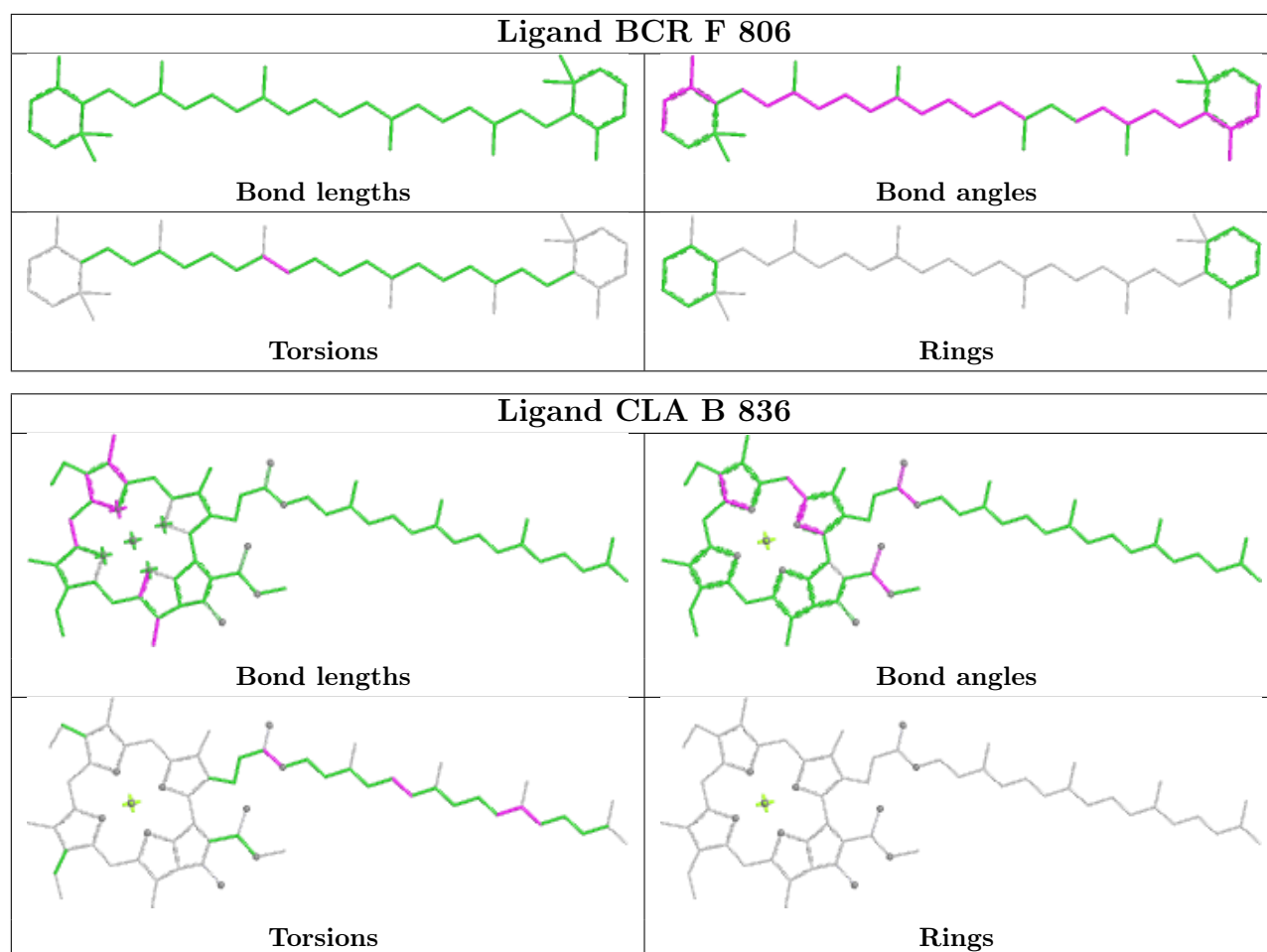
Torsions



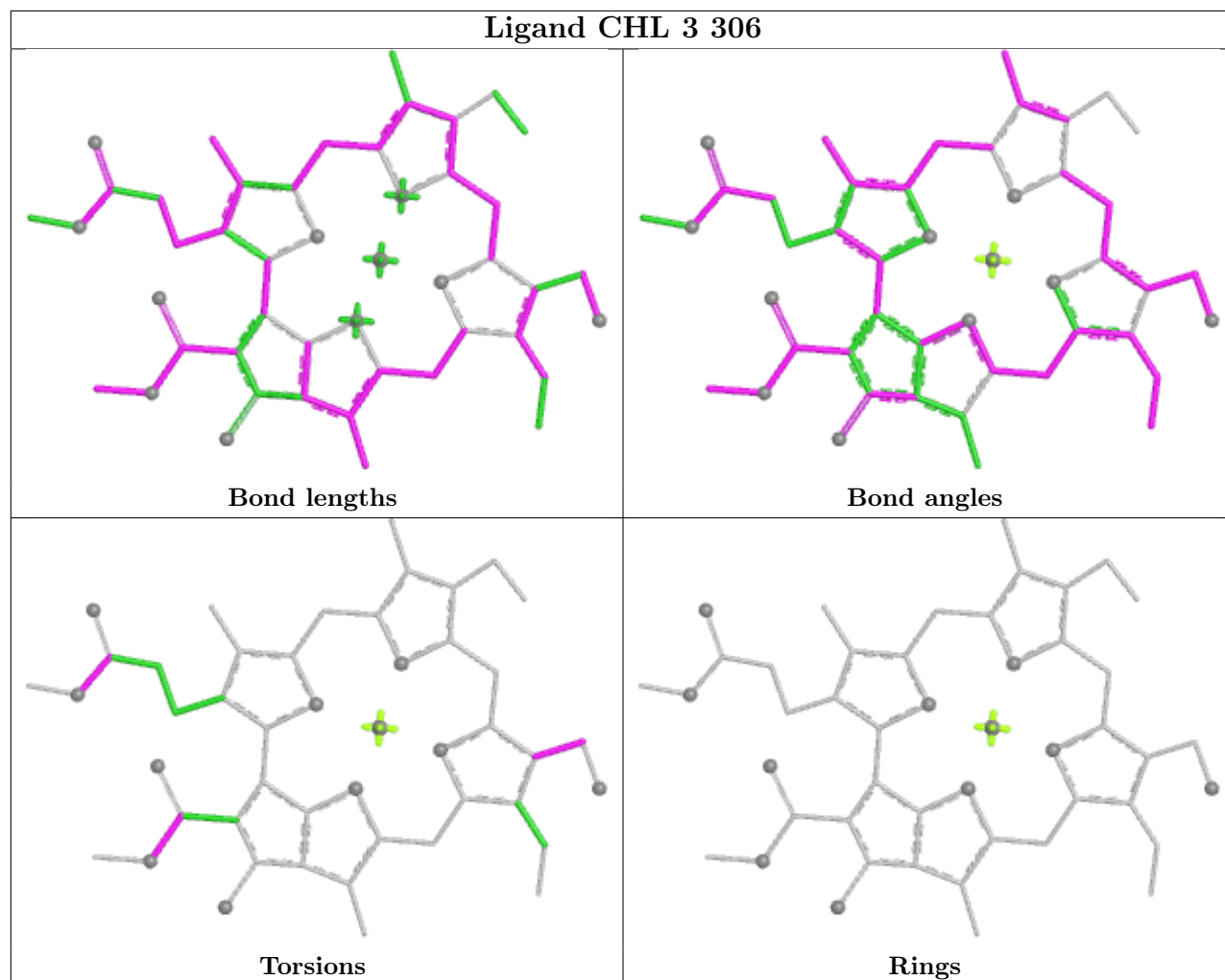
Rings



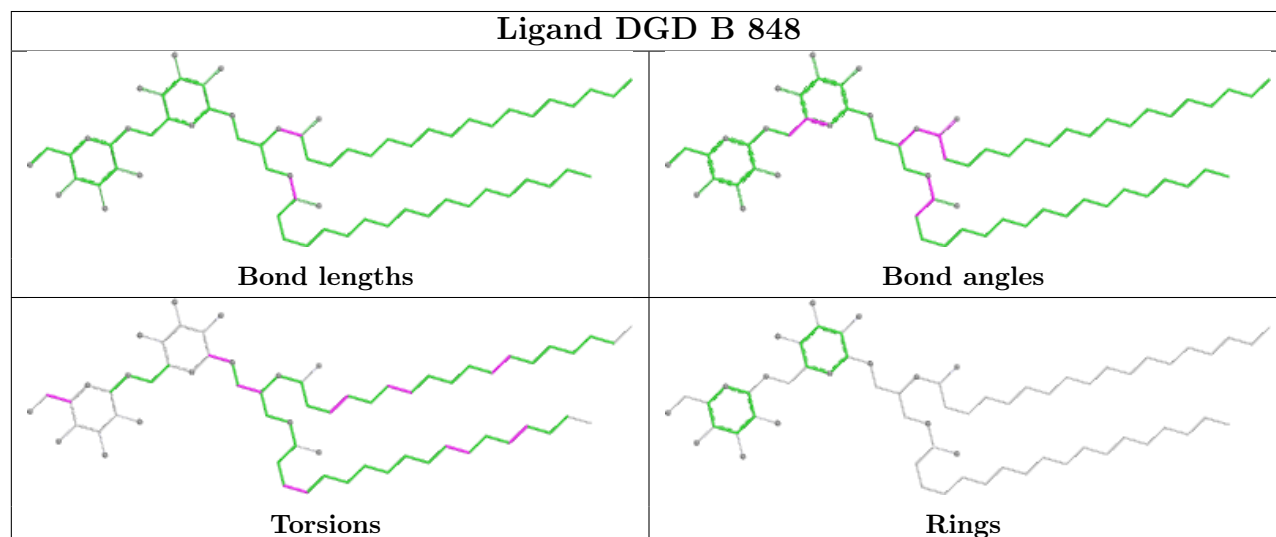


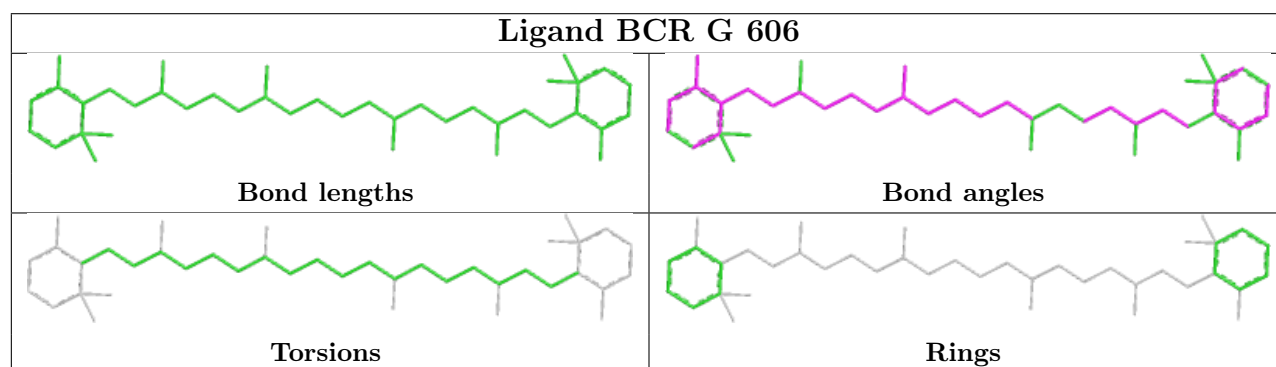
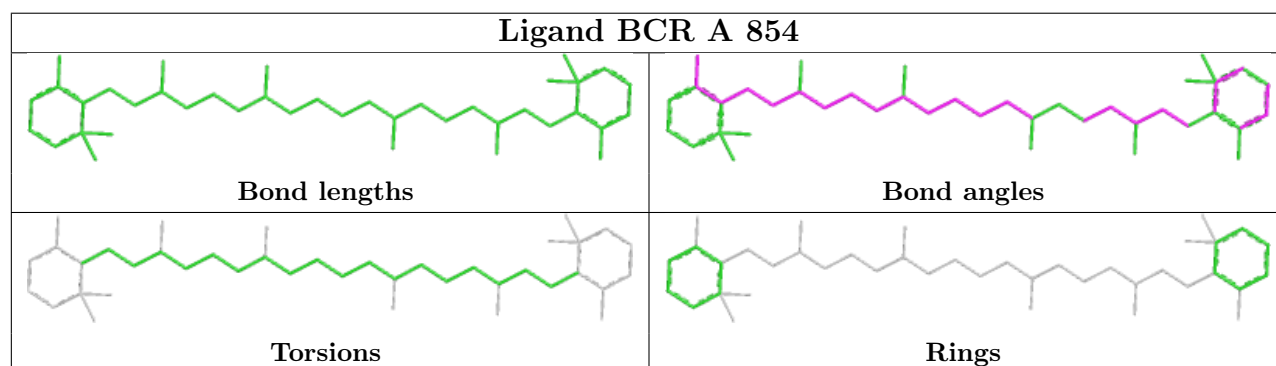
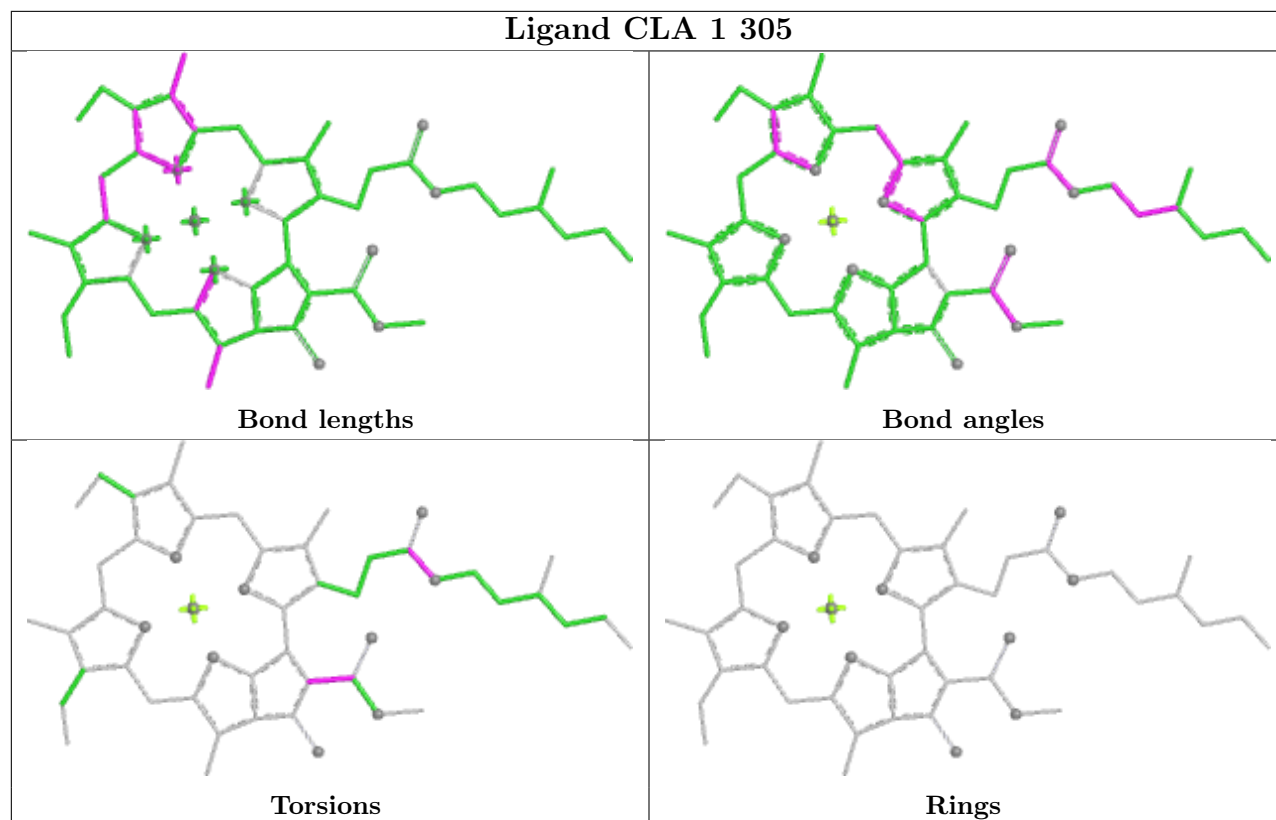


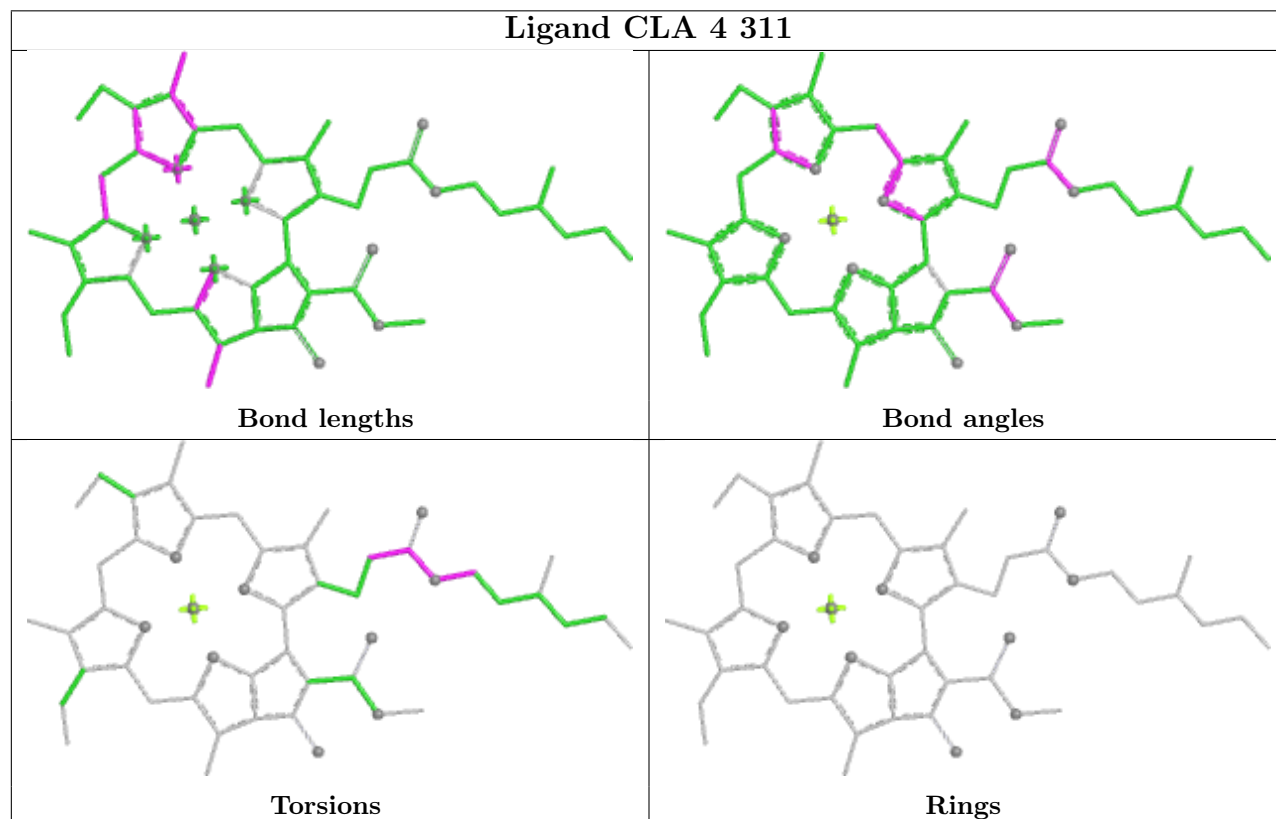
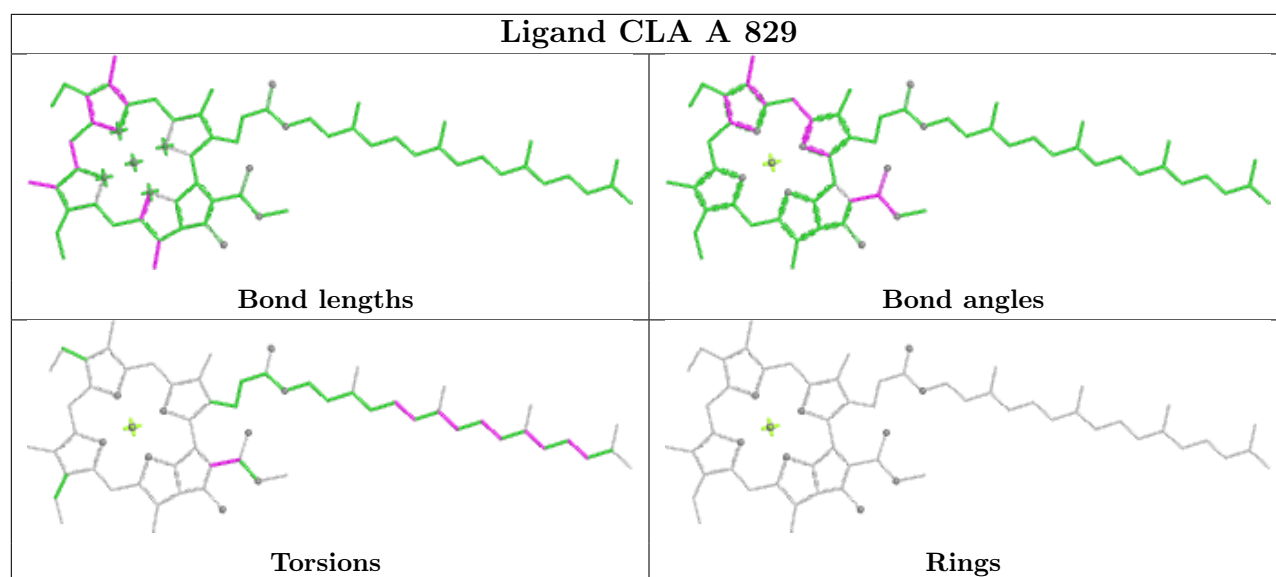
Ligand CHL 3 306

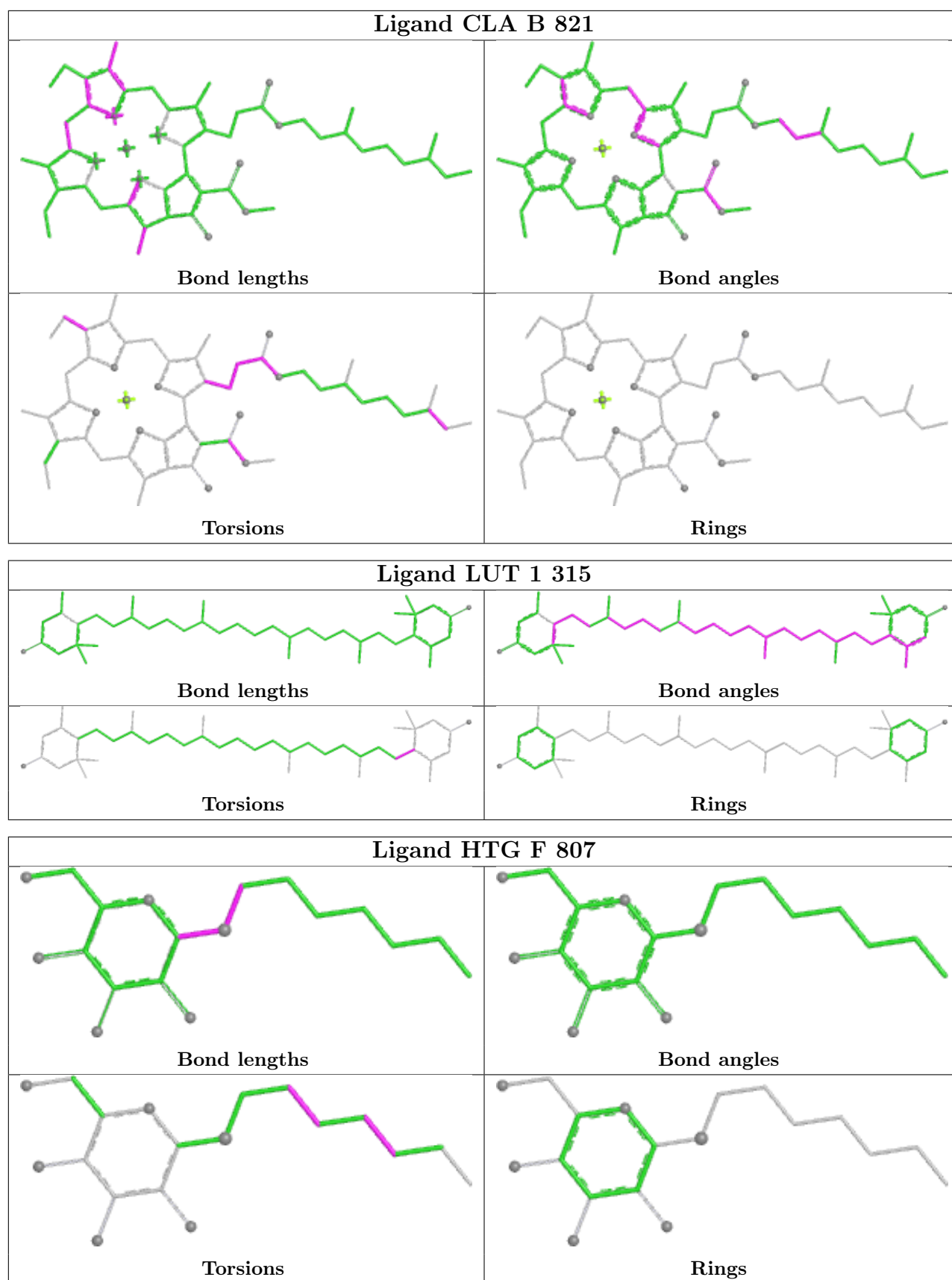


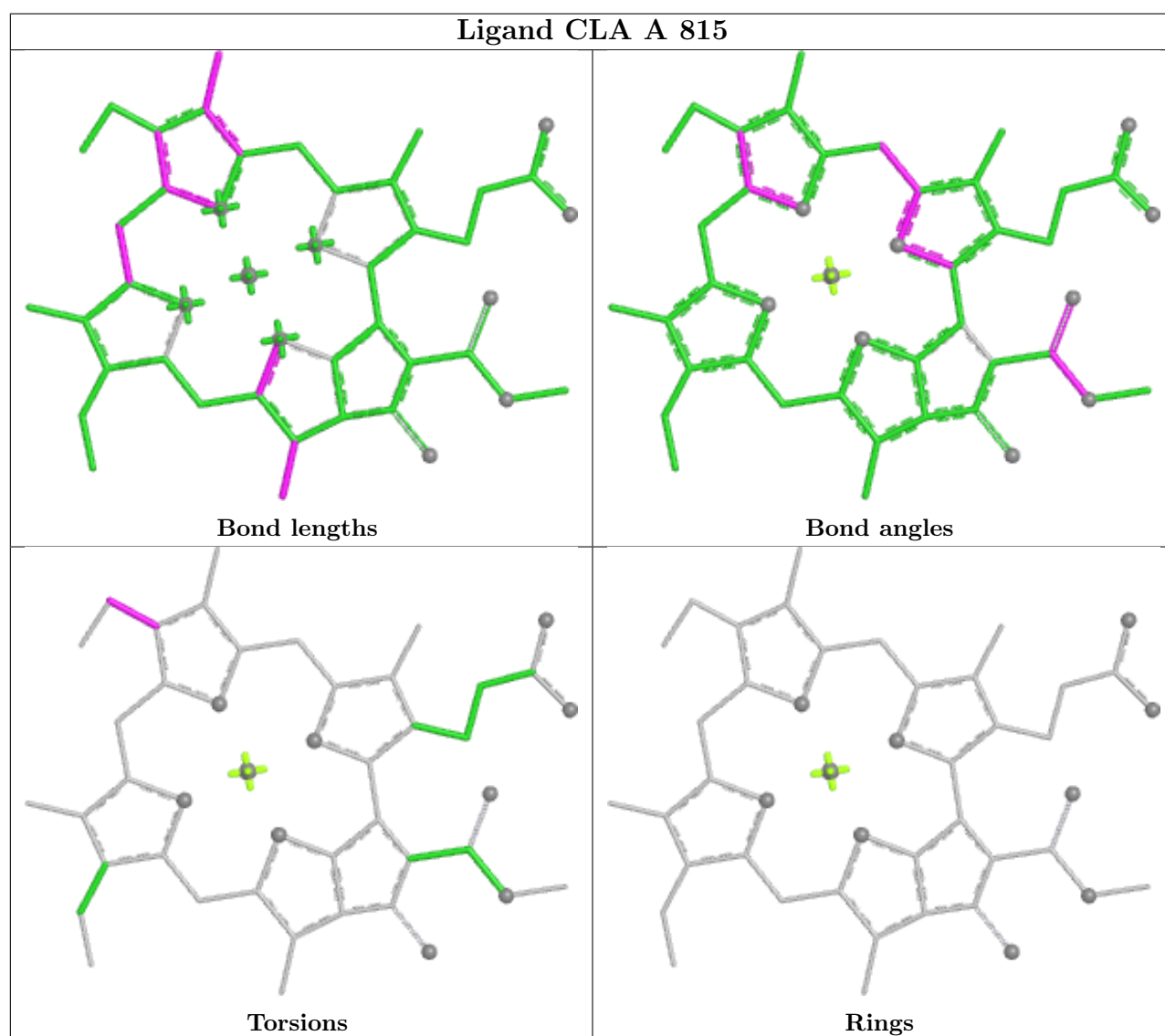
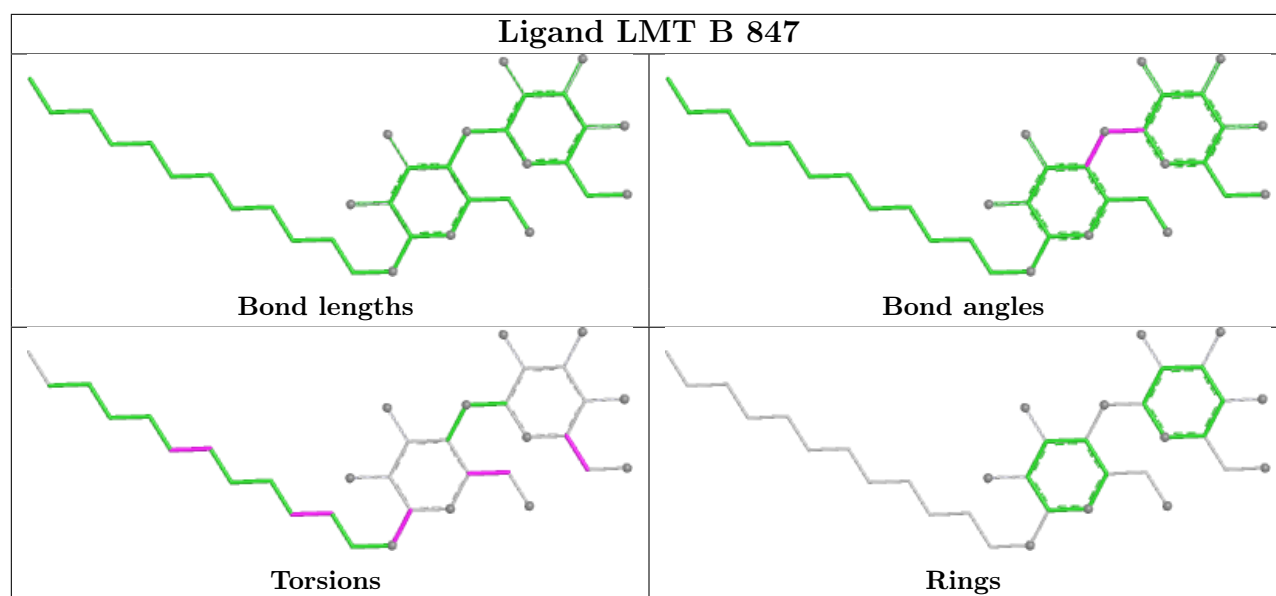
Ligand DGD B 848



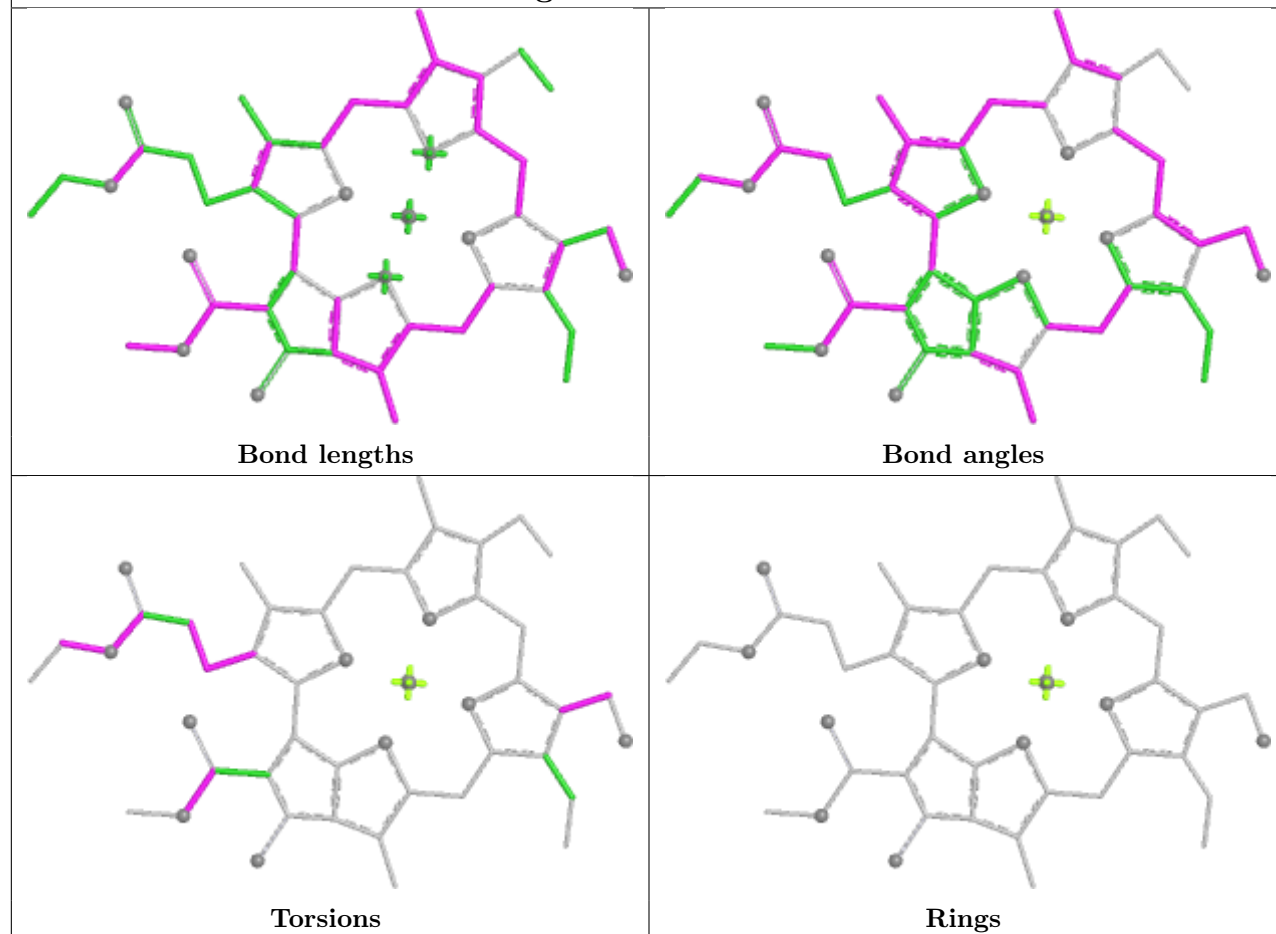




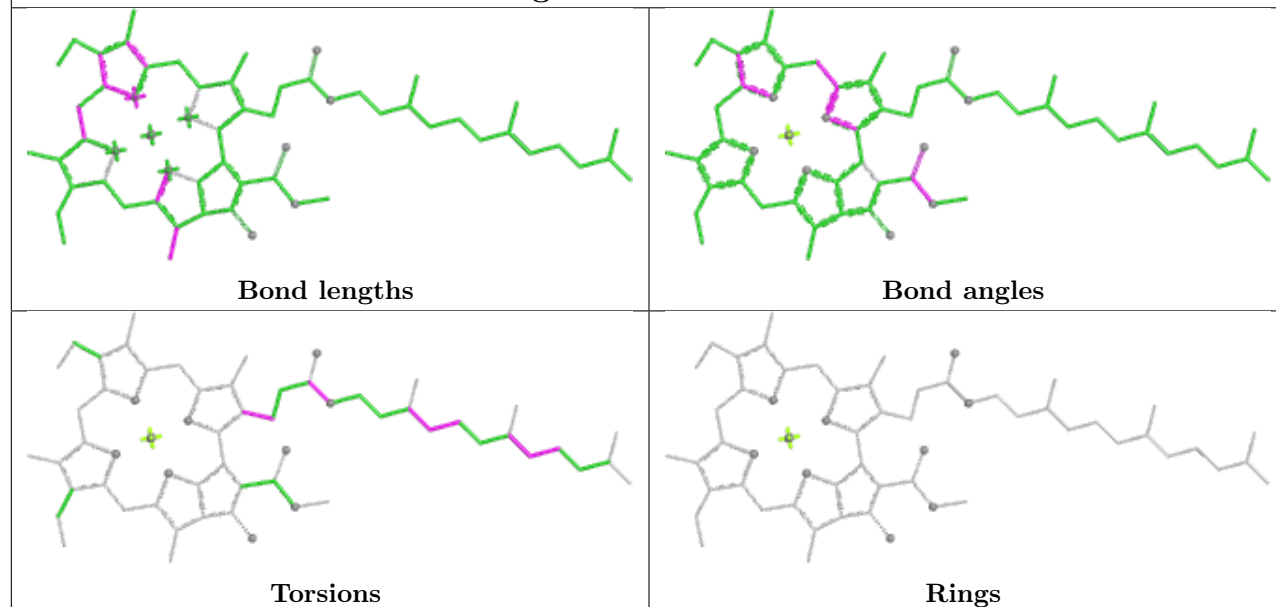




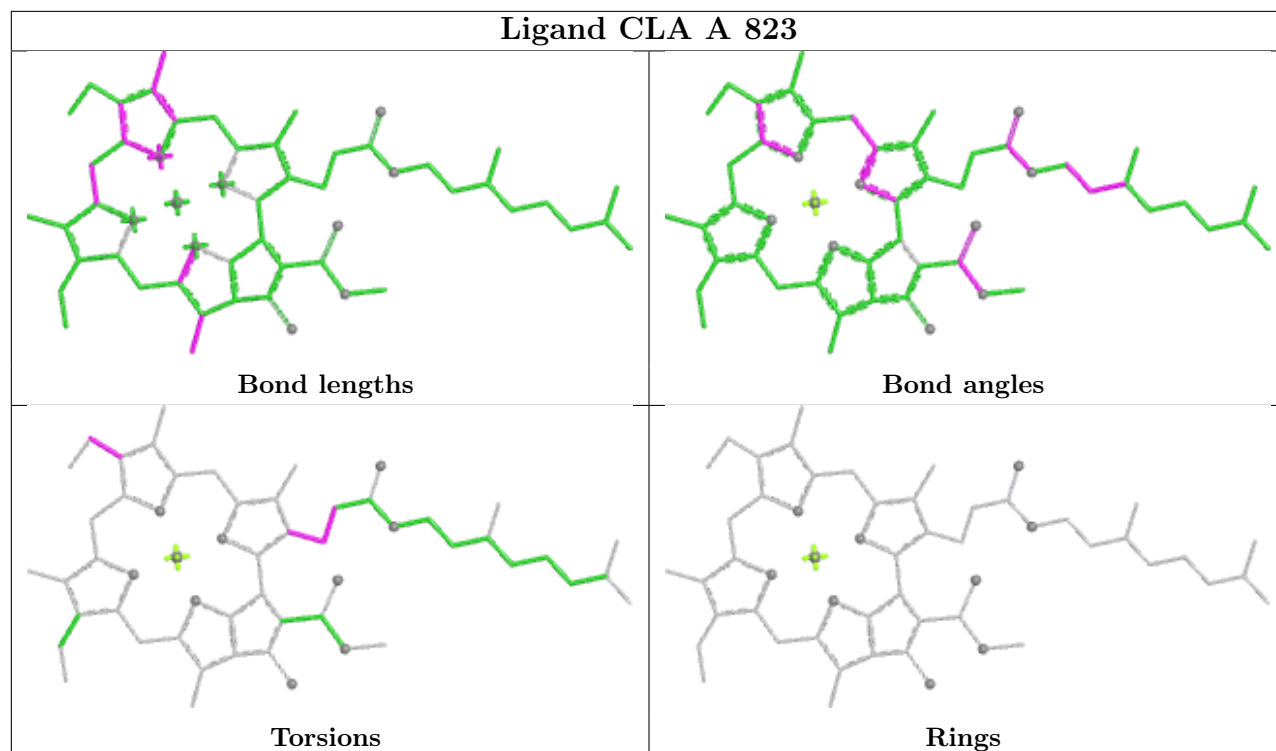
Ligand CHL 1 306



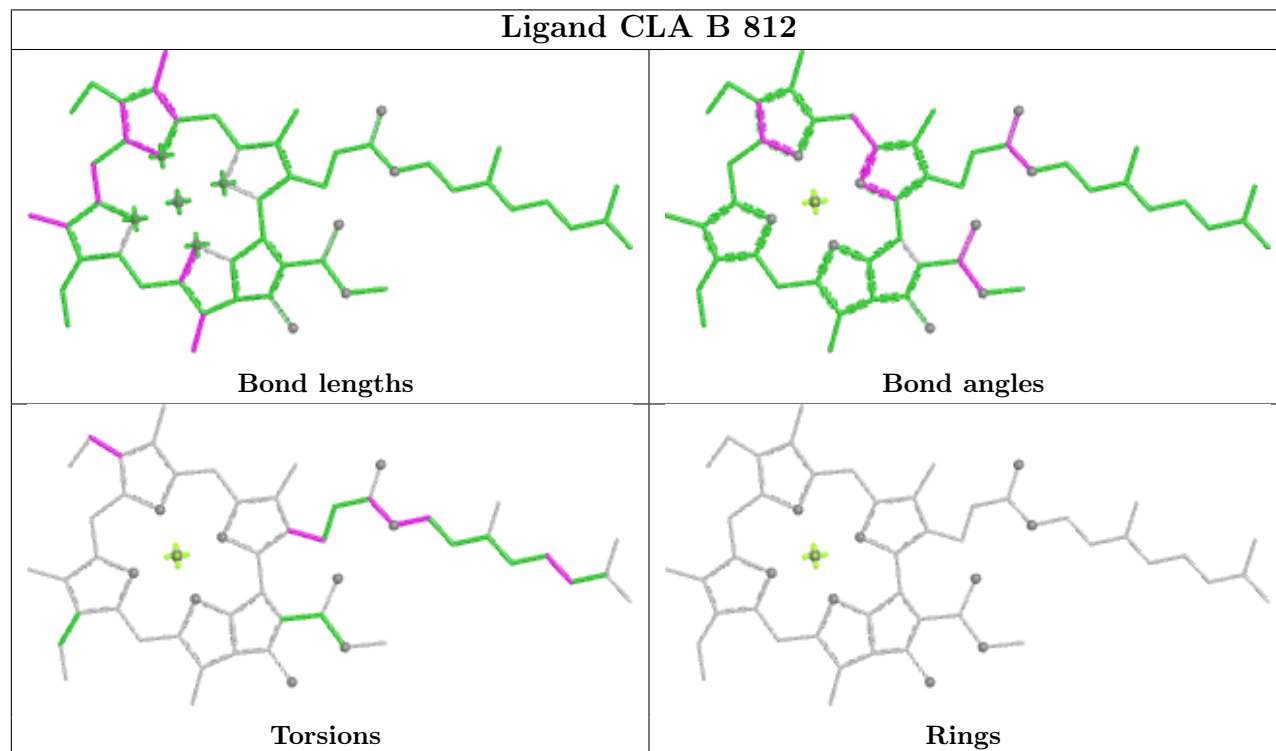
Ligand CLA B 818



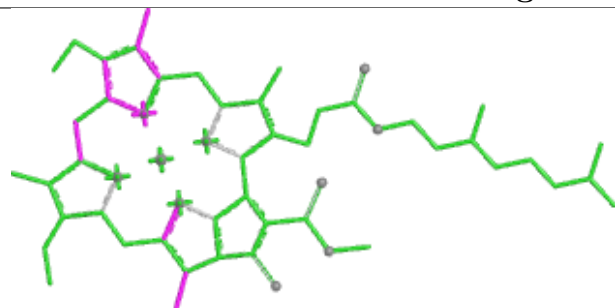
Ligand CLA A 823



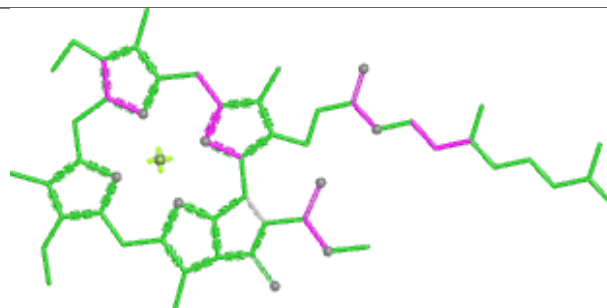
Ligand CLA B 812



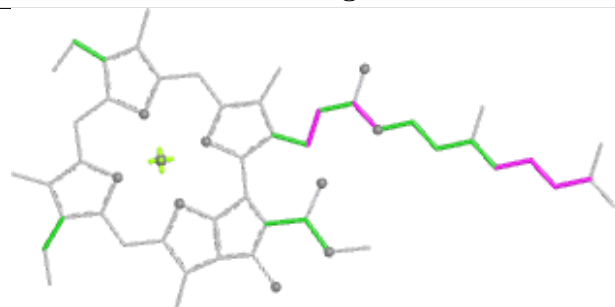
Ligand CLA B 807



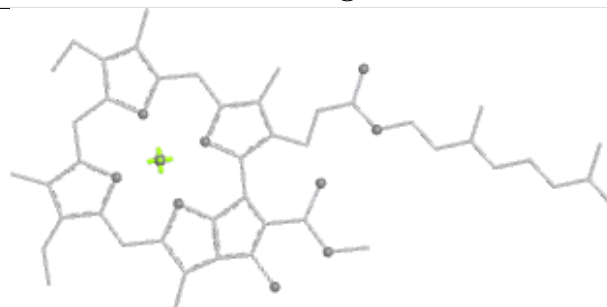
Bond lengths



Bond angles

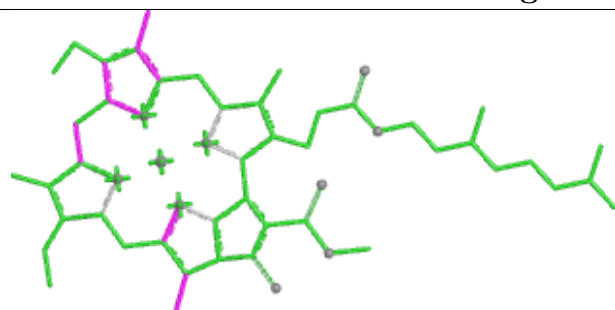


Torsions

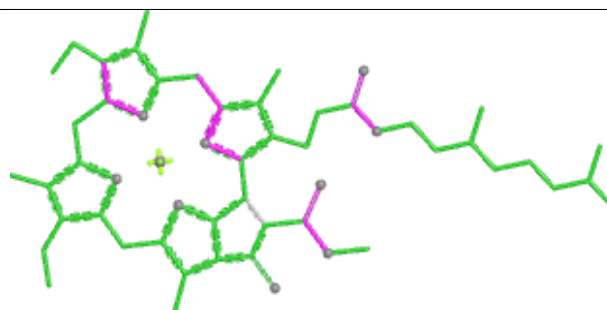


Rings

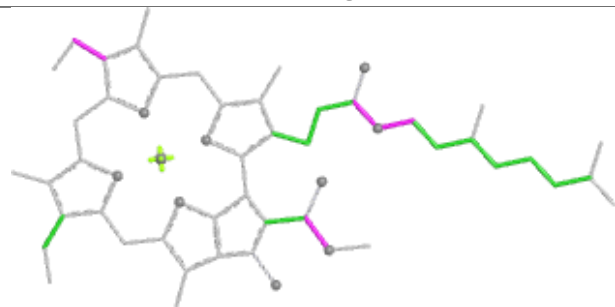
Ligand CLA 4 310



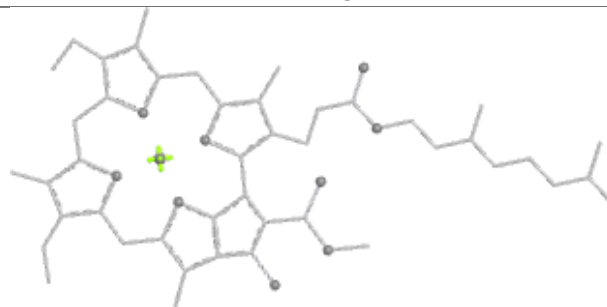
Bond lengths



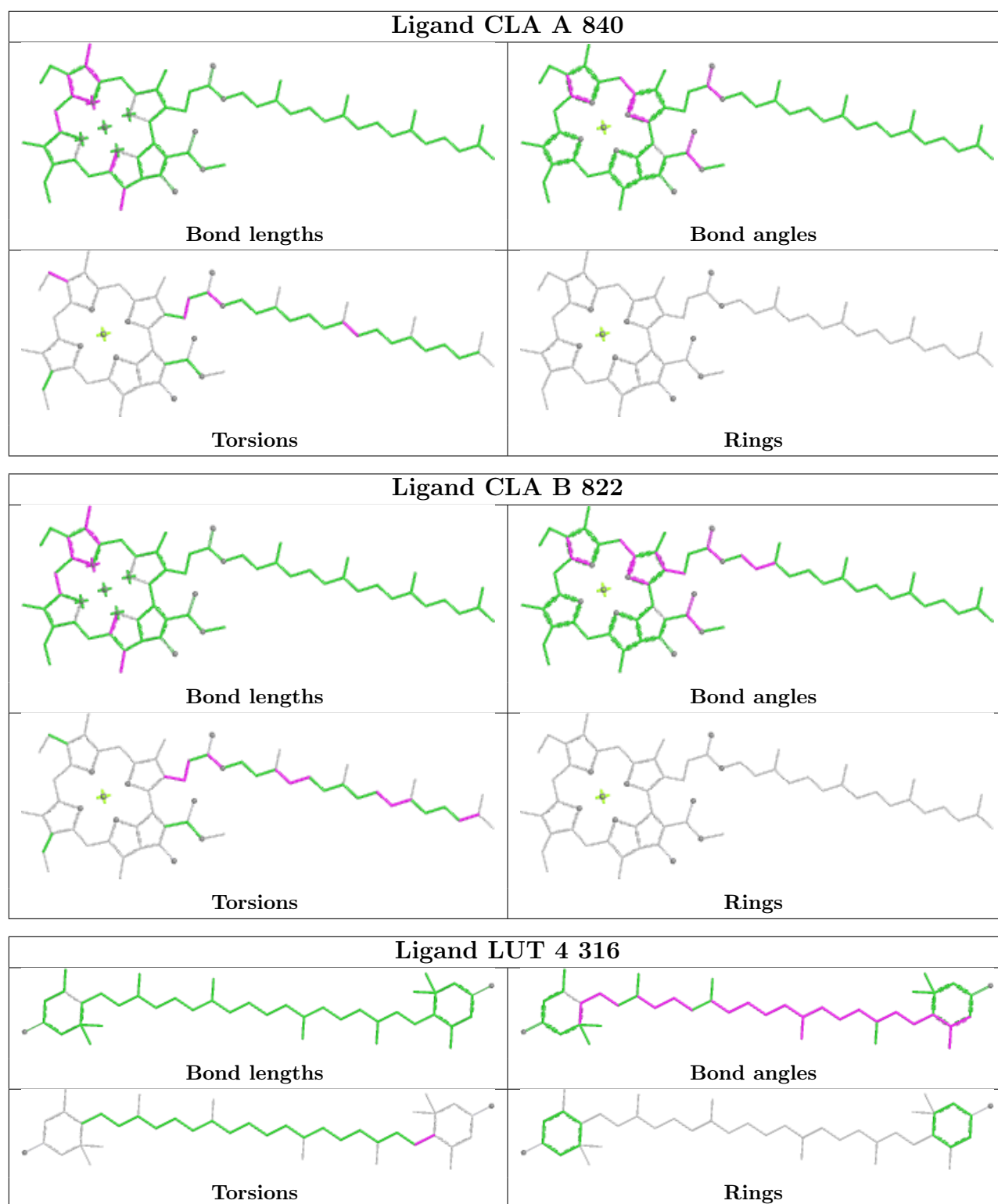
Bond angles

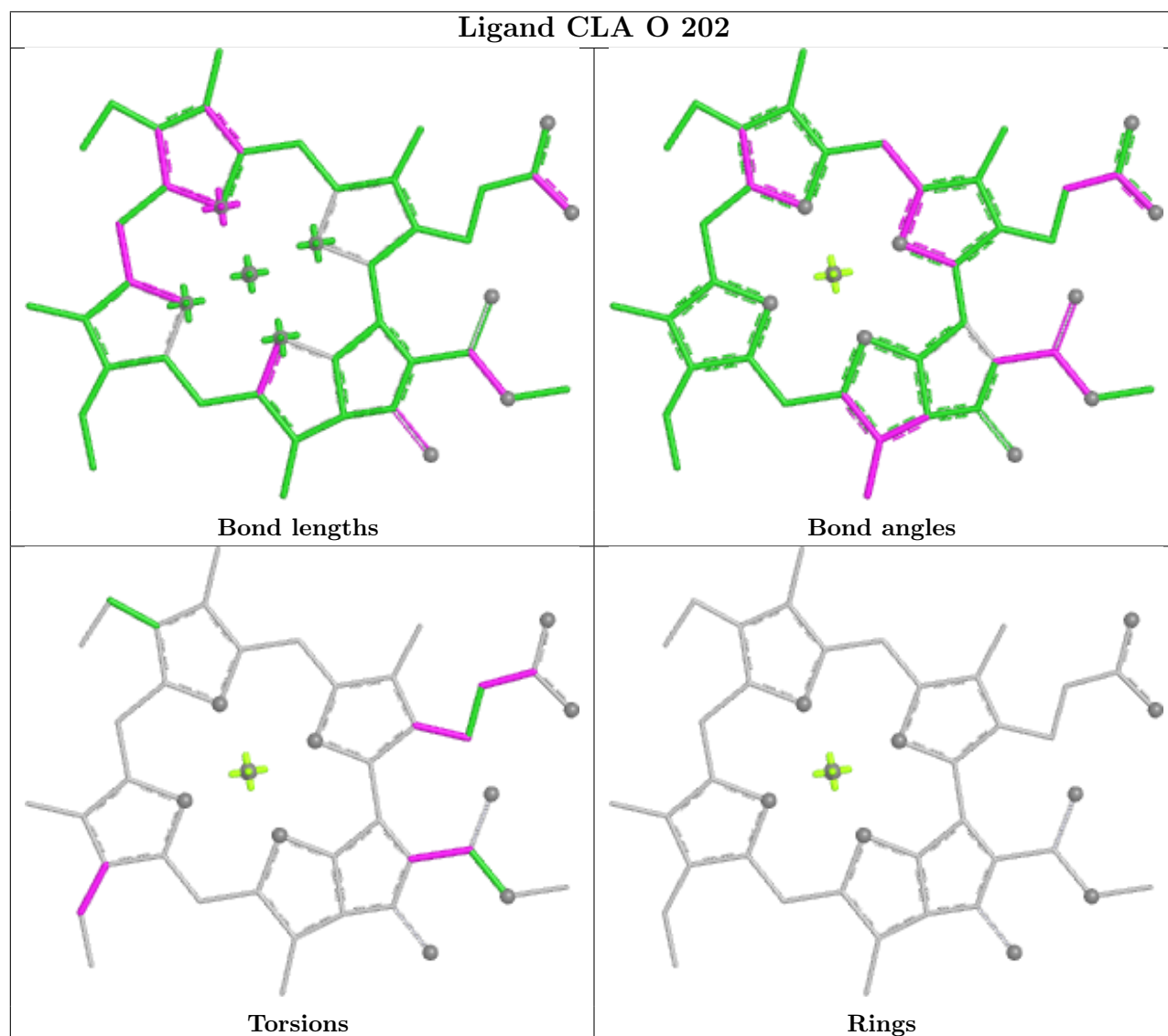
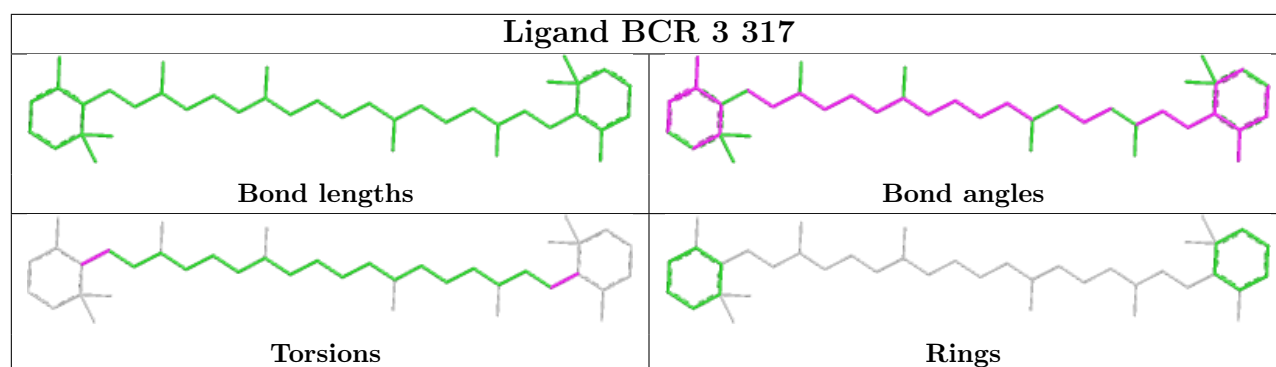


Torsions

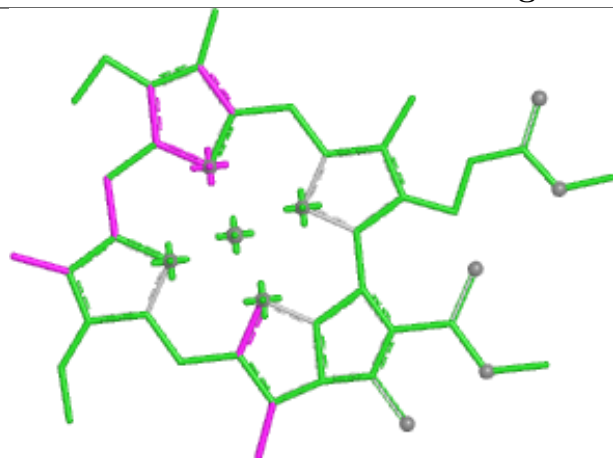


Rings

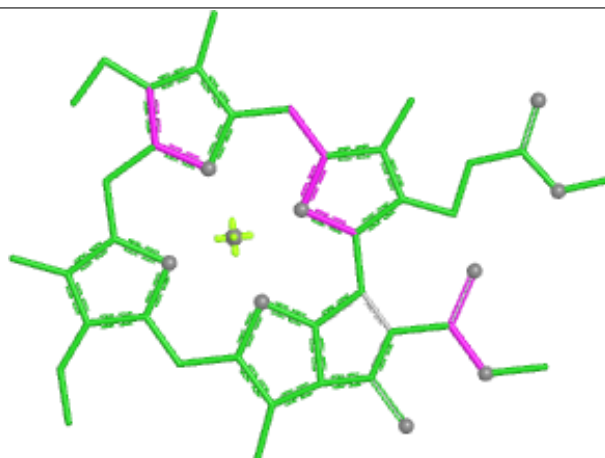




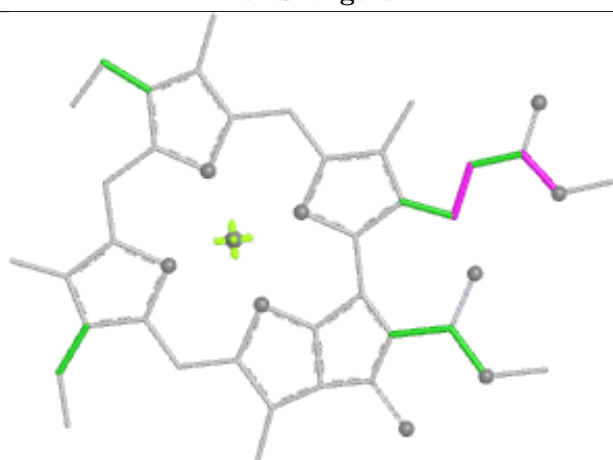
Ligand CLA 1 314



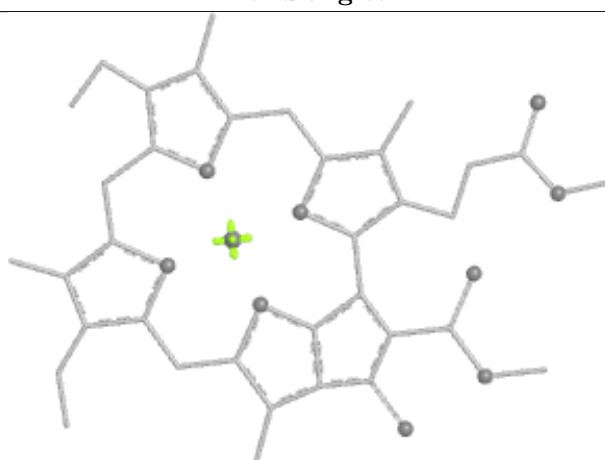
Bond lengths



Bond angles

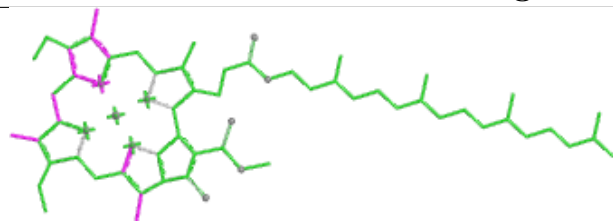


Torsions

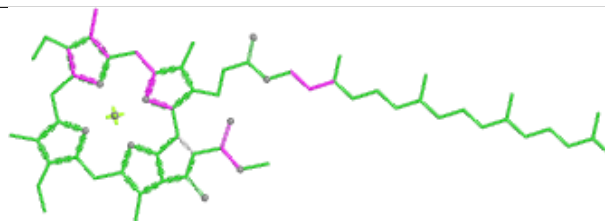


Rings

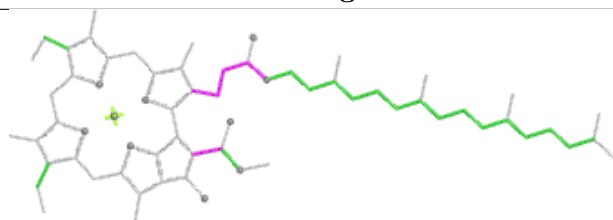
Ligand CLA A 804



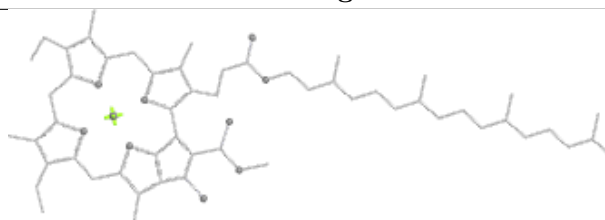
Bond lengths



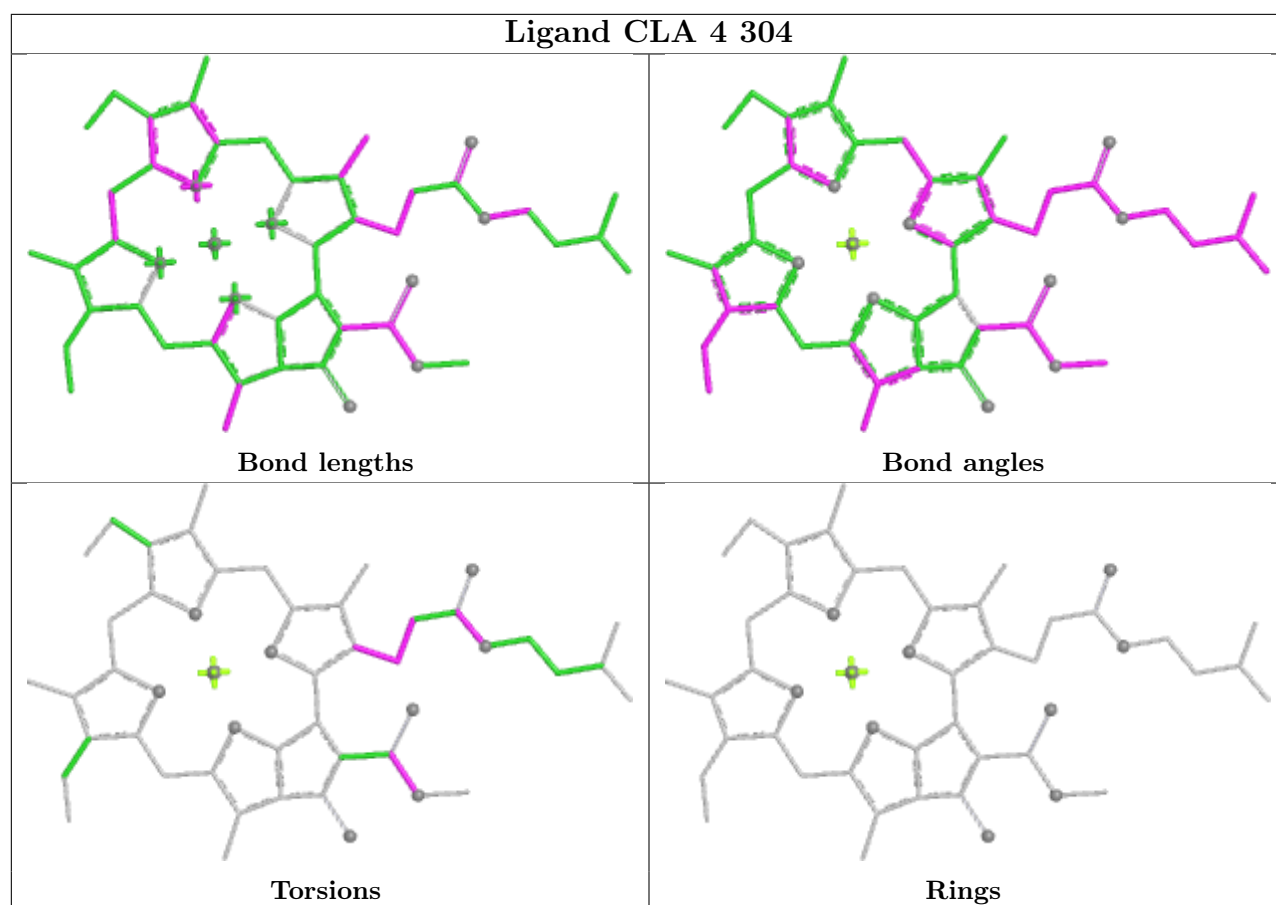
Bond angles



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.

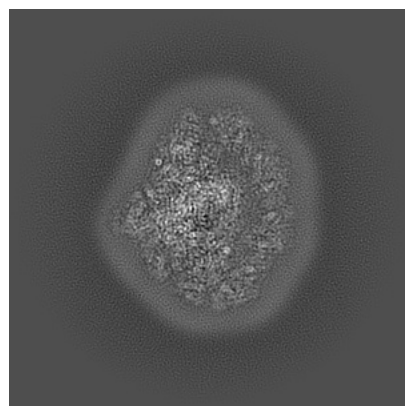
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37513. These allow visual inspection of the internal detail of the map and identification of artifacts.

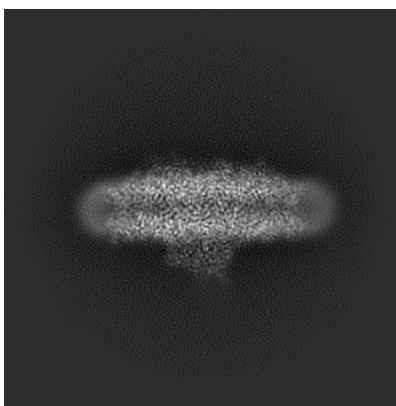
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

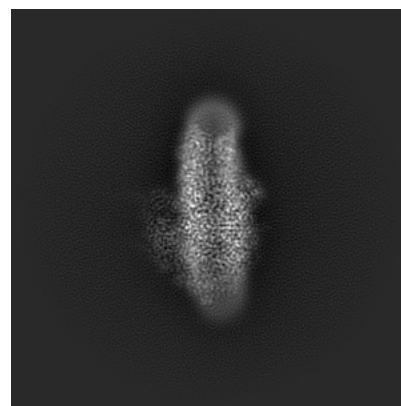
6.1.1 Primary map



X

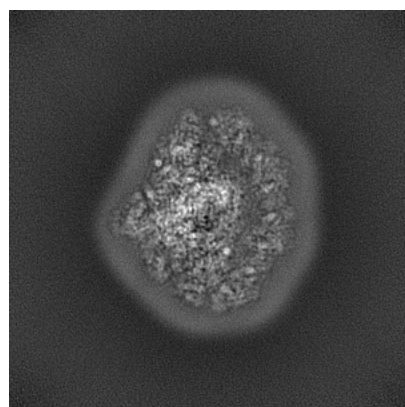


Y

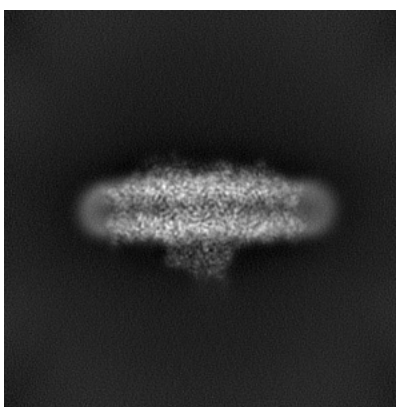


Z

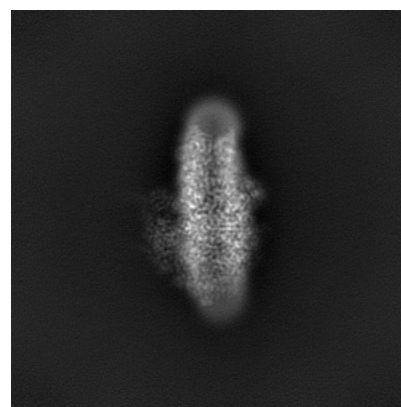
6.1.2 Raw map



X



Y

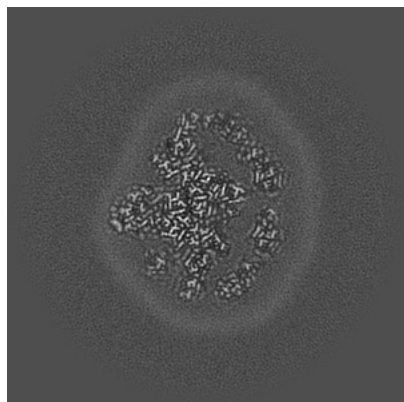


Z

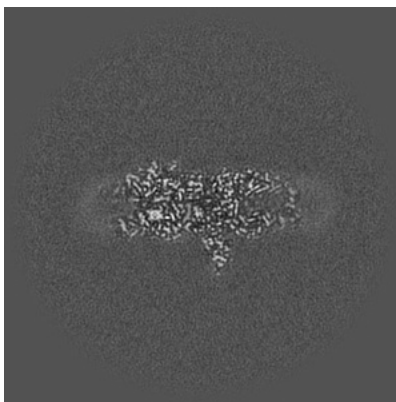
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

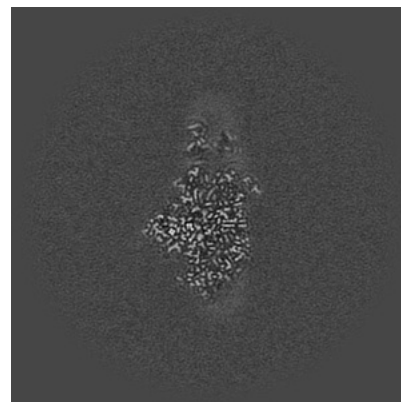
6.2.1 Primary map



X Index: 150

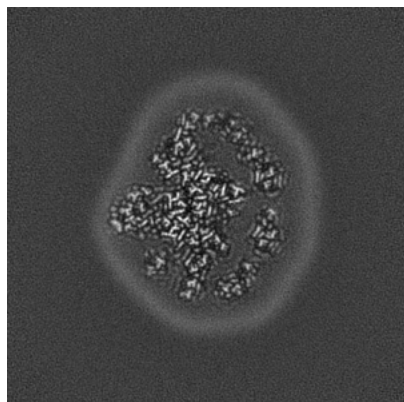


Y Index: 150

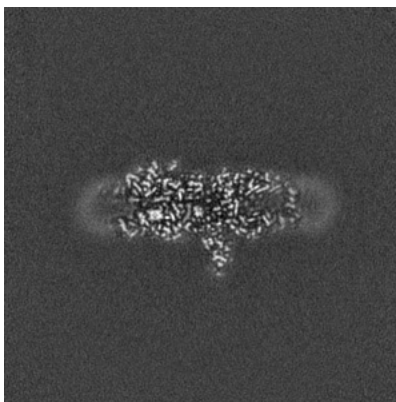


Z Index: 150

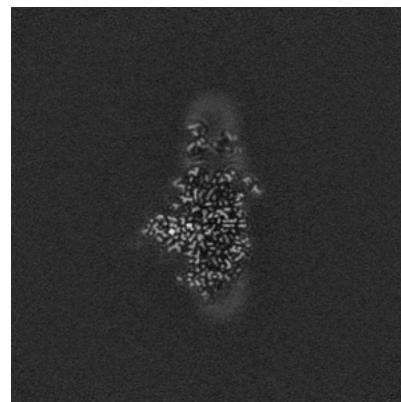
6.2.2 Raw map



X Index: 150



Y Index: 150

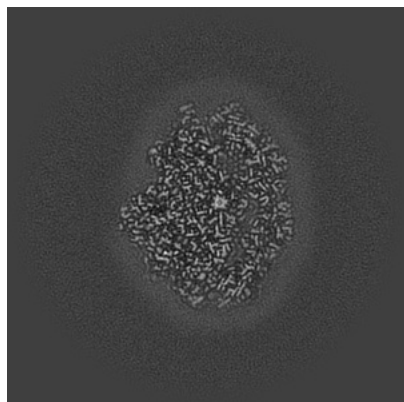


Z Index: 150

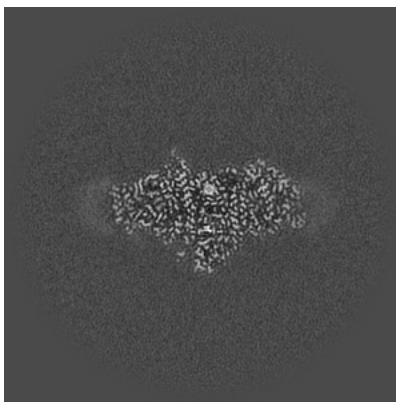
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

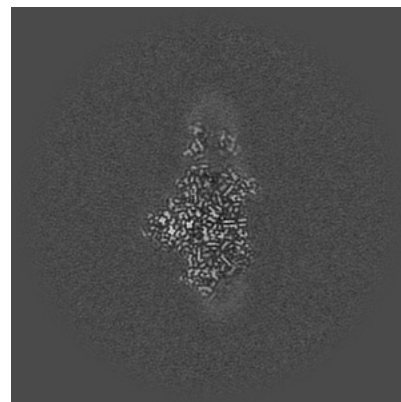
6.3.1 Primary map



X Index: 138

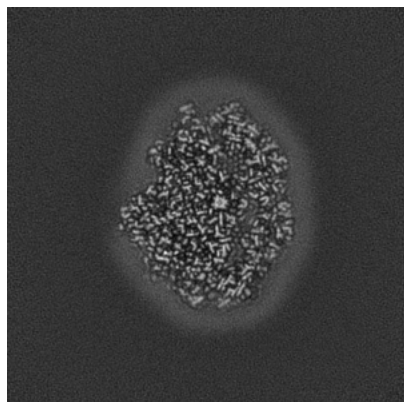


Y Index: 135

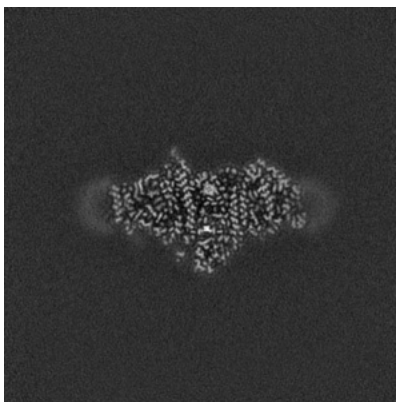


Z Index: 152

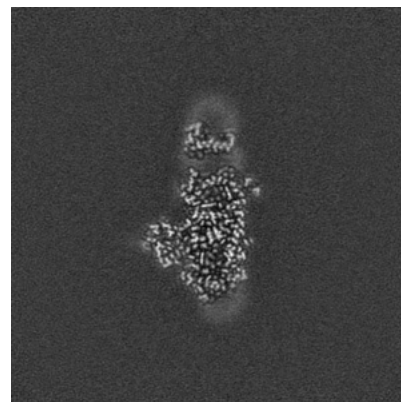
6.3.2 Raw map



X Index: 138



Y Index: 135

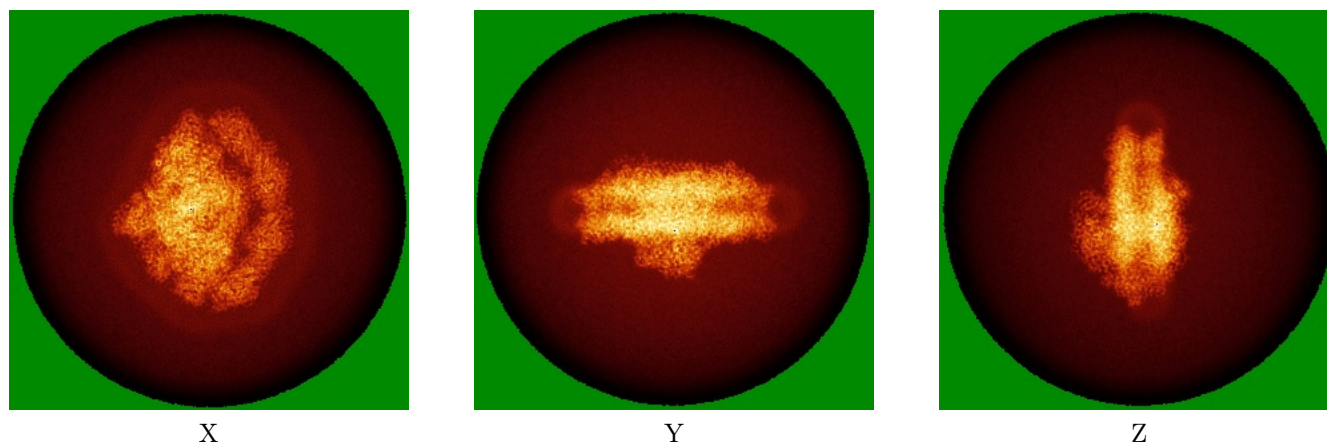


Z Index: 145

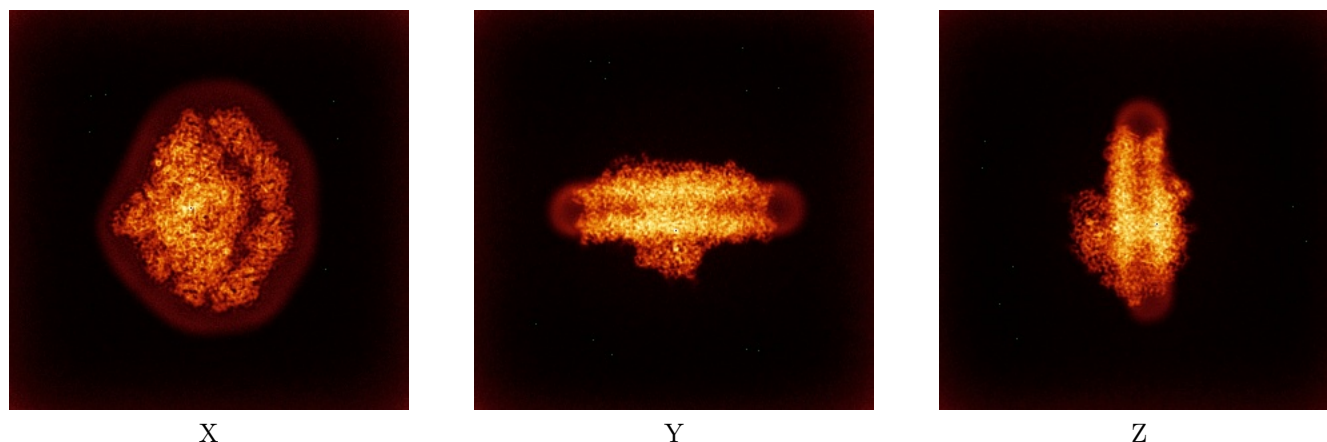
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

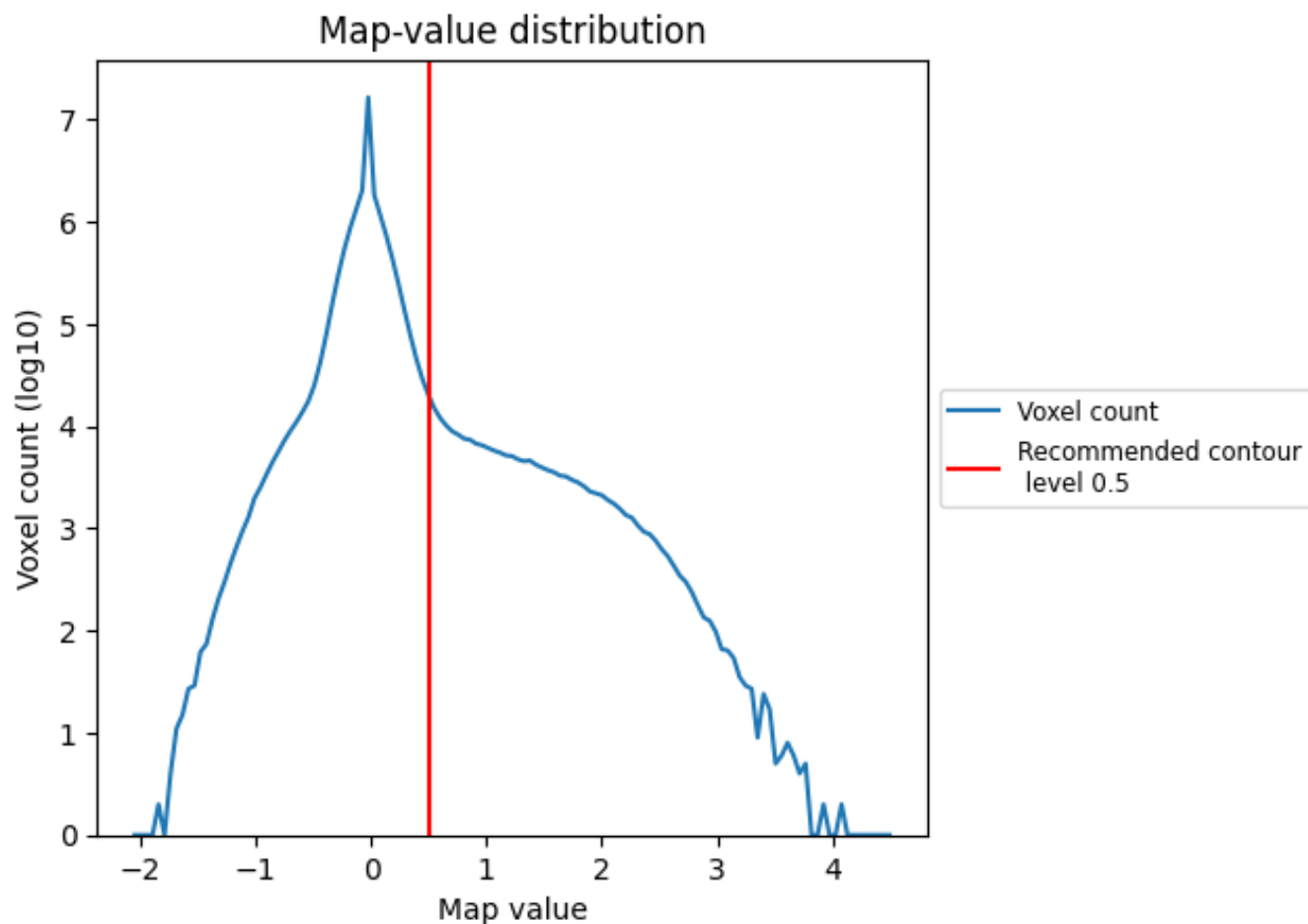
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

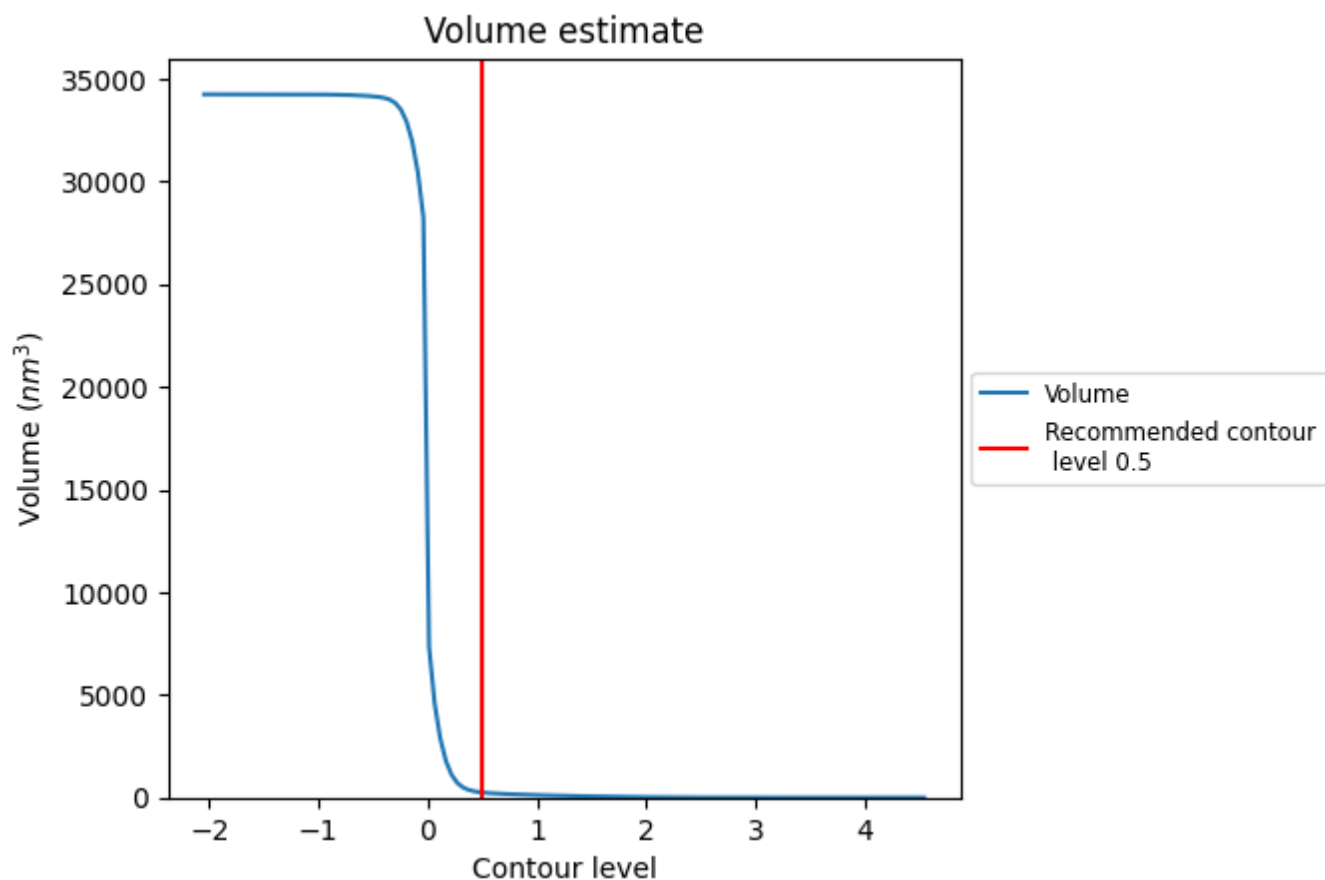
This section contains the results of statistical analysis of the map.

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.

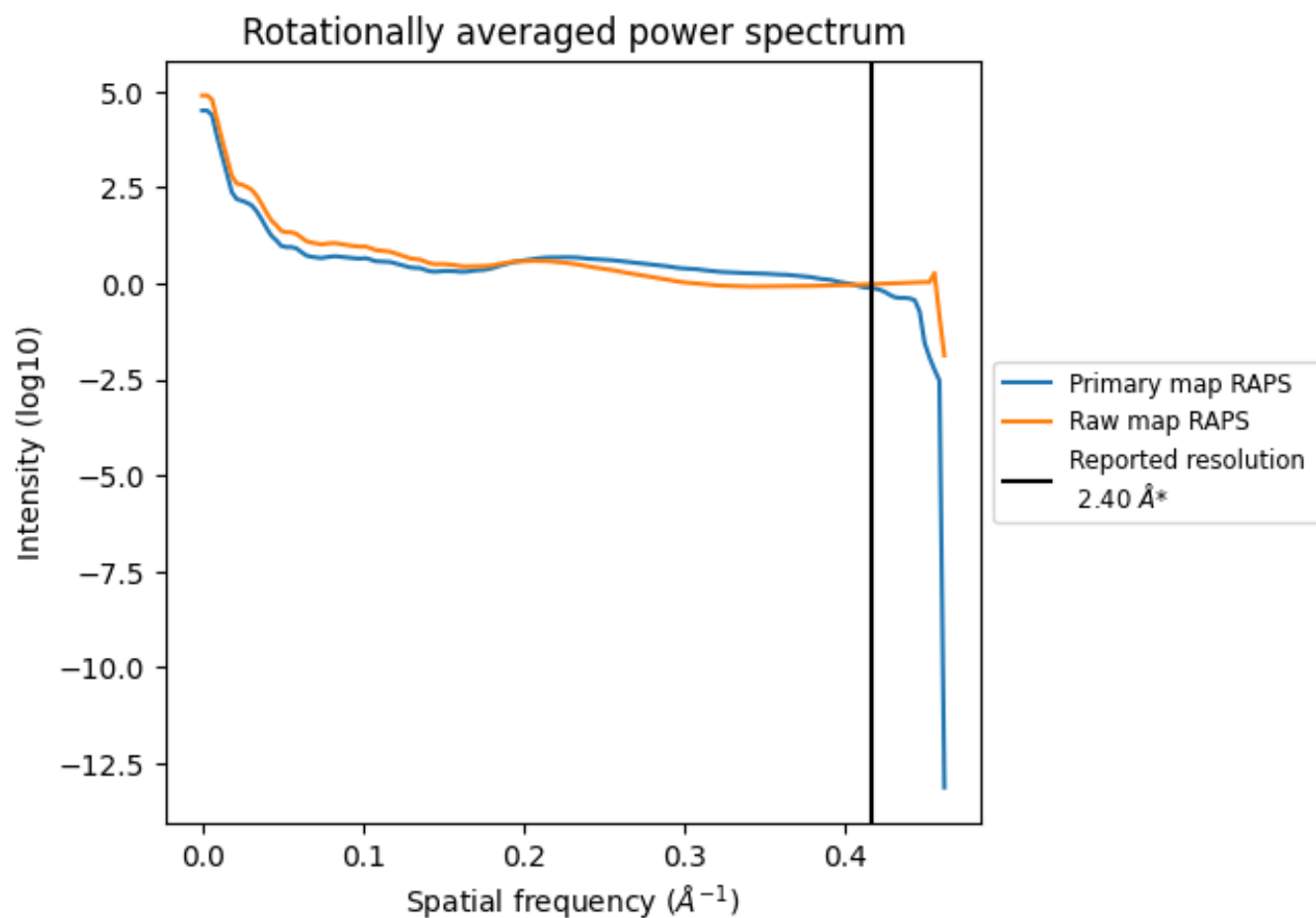
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 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 ⓘ

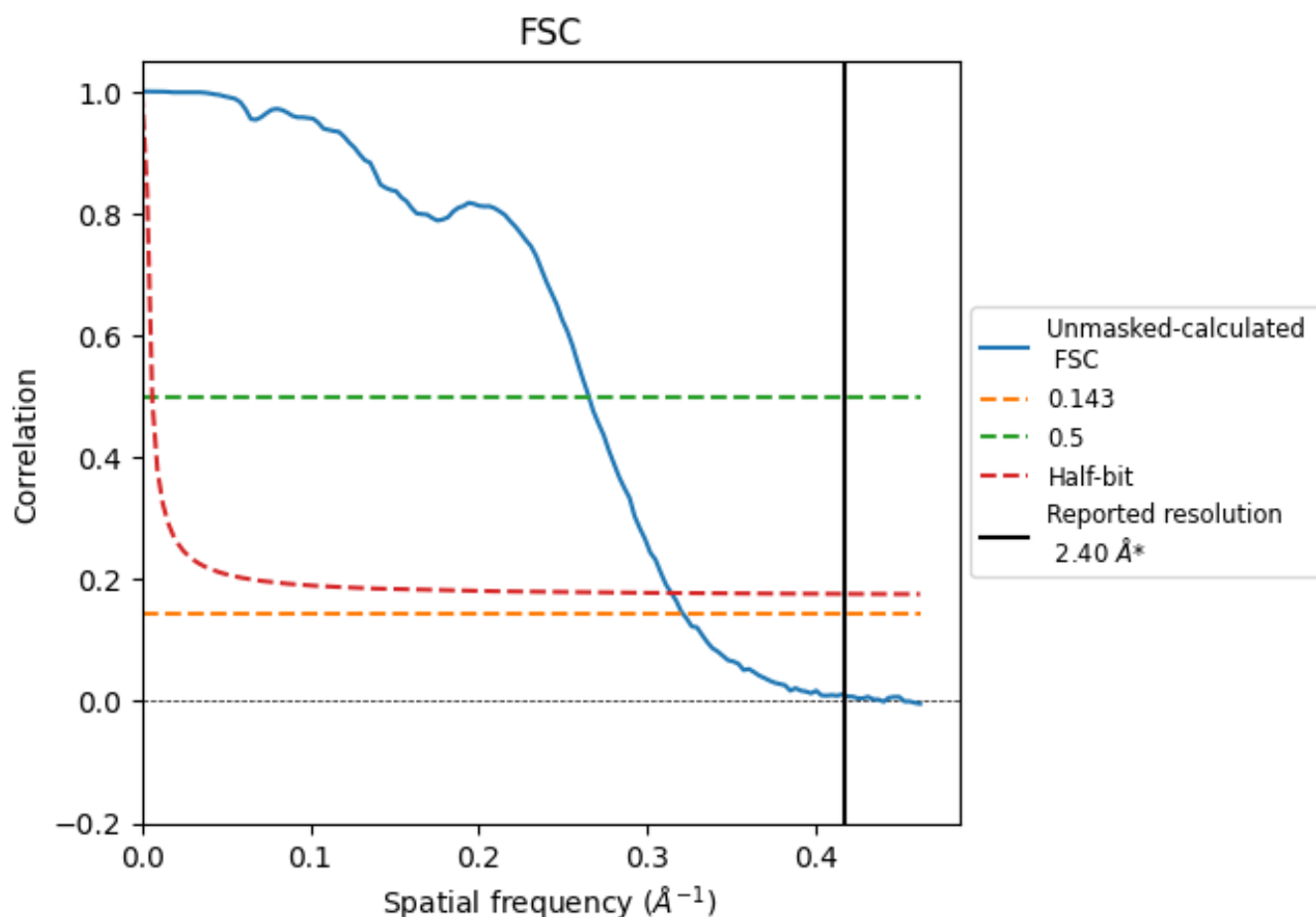


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 $0.417 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

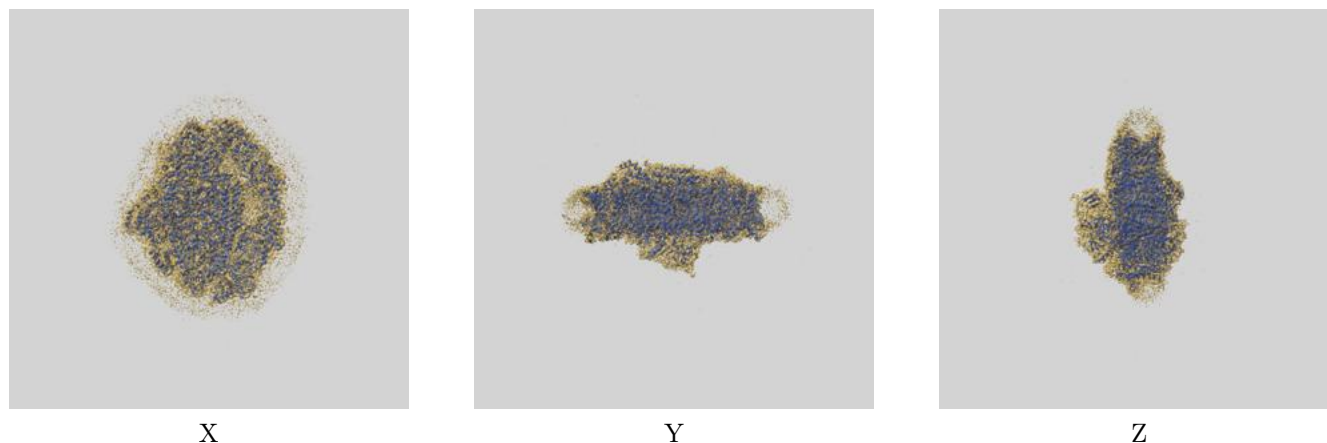
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.77	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

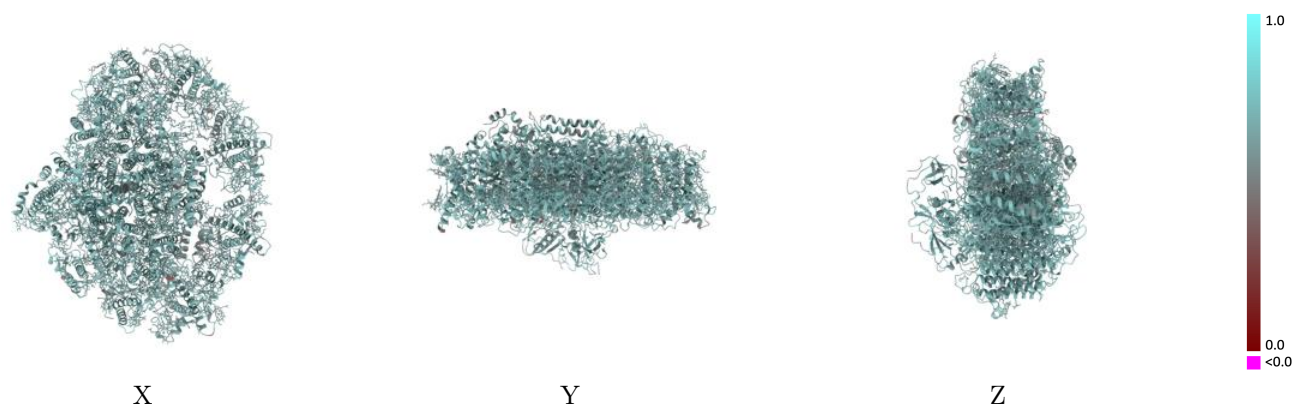
This section contains information regarding the fit between EMDB map EMD-37513 and PDB model 8WGH. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



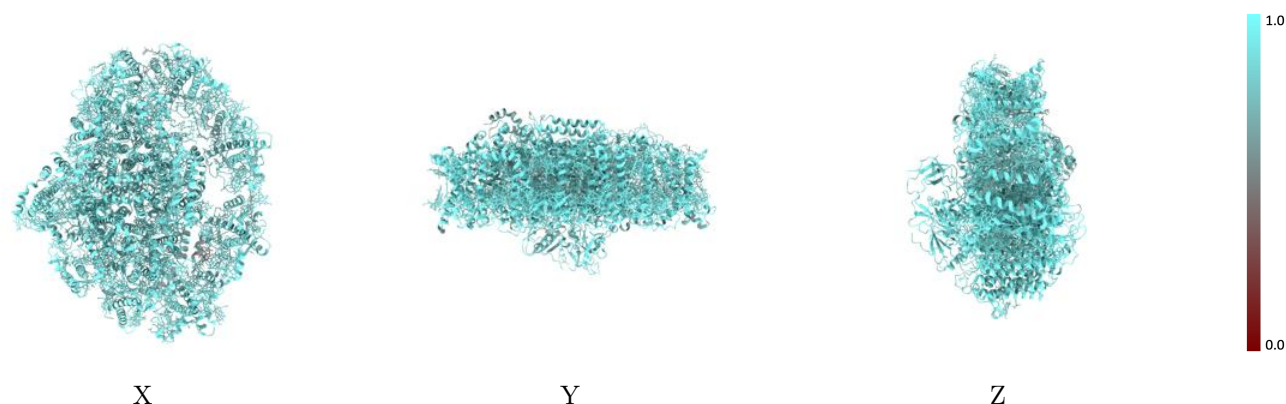
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



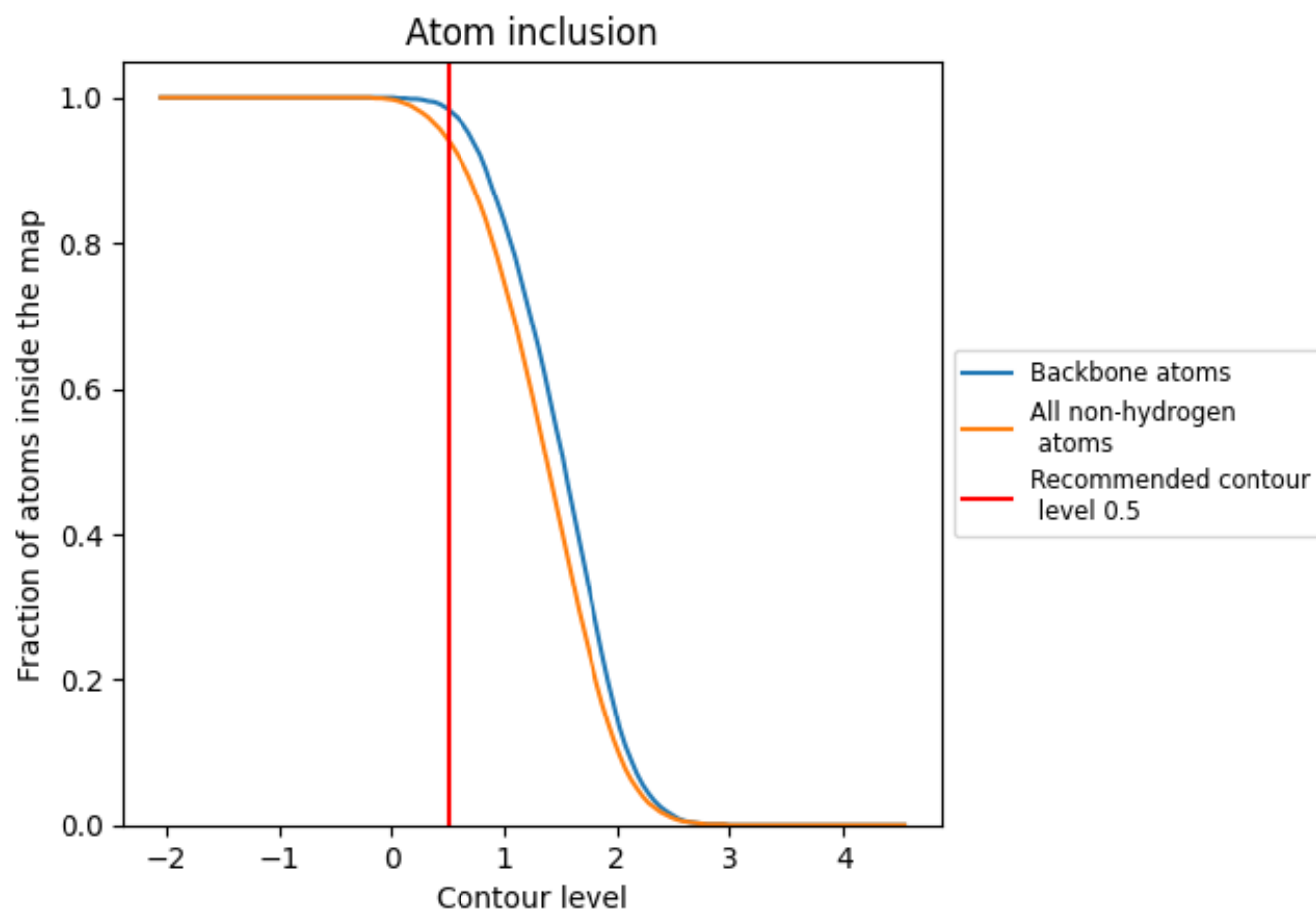
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.9420	0.6650
1	0.8880	0.6340
2	0.9220	0.6460
3	0.9360	0.6530
4	0.9280	0.6510
A	0.9670	0.6860
B	0.9650	0.6840
C	0.9850	0.6840
D	0.9580	0.6720
E	0.9390	0.6500
F	0.9160	0.6430
G	0.9150	0.6500
H	0.9320	0.6570
I	0.9660	0.6760
J	0.9490	0.6680
K	0.9180	0.6310
L	0.9580	0.6750
N	0.7530	0.5770
O	0.9270	0.6460

1.0

0.0

<0.0