



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:26 PM UTC

PDB ID : 9M4F / pdb_00009m4f
EMDB ID : EMD-63625
Title : Photosystem I from the eukaryotic filamentous algae
Authors : Shao, R.Q.; Pan, X.W.
Deposited on : 2025-03-04
Resolution : 2.82 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:

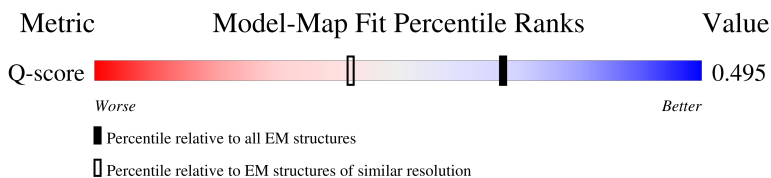
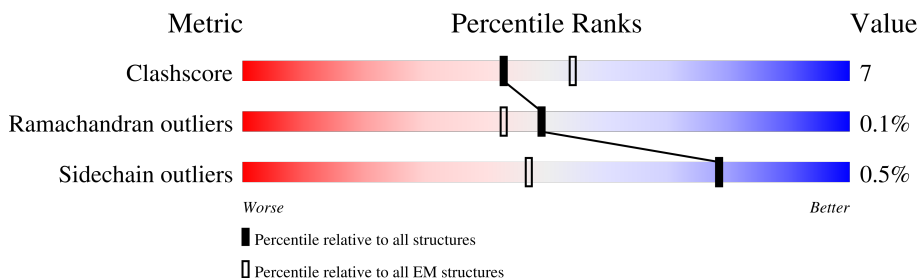
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.82 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	11795 (2.32 - 3.32)

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	220	
2	2	194	
3	3	205	
4	4	231	

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Mol	Chain	Length	Quality of chain
5	5	216	
6	6	212	
6	h	212	
7	7	207	
8	8	179	
9	9	215	
9	k	215	
10	c	210	
11	t	228	
12	A	749	
13	B	734	
14	C	81	
15	D	139	
16	E	61	
17	F	185	
18	I	36	
19	J	42	
20	L	149	
21	M	30	
22	R	87	
23	S	134	

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
24	CLA	1	301	X	-	-	-
24	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	1	303	X	-	-	-
24	CLA	1	304	X	-	-	-
24	CLA	1	305	X	-	-	-
24	CLA	1	306	X	-	-	-
24	CLA	1	307	X	-	-	-
24	CLA	1	308	X	-	-	-
24	CLA	1	309	X	-	-	-
24	CLA	1	317	X	-	-	-
24	CLA	2	201	X	-	-	-
24	CLA	2	202	X	-	-	-
24	CLA	2	203	X	-	-	-
24	CLA	2	204	X	-	-	-
24	CLA	2	206	X	-	-	-
24	CLA	2	207	X	-	-	-
24	CLA	2	208	X	-	-	-
24	CLA	2	209	X	-	-	-
24	CLA	3	302	X	-	-	-
24	CLA	3	303	X	-	-	-
24	CLA	3	304	X	-	-	-
24	CLA	3	305	X	-	-	-
24	CLA	3	306	X	-	-	-
24	CLA	3	307	X	-	-	-
24	CLA	3	308	X	-	-	-
24	CLA	3	309	X	-	-	-
24	CLA	4	601	X	-	-	-
24	CLA	4	602	X	-	-	-
24	CLA	4	603	X	-	-	-
24	CLA	4	604	X	-	-	-
24	CLA	4	605	X	-	-	-
24	CLA	4	606	X	-	-	-
24	CLA	4	607	X	-	-	-
24	CLA	4	608	X	-	-	-
24	CLA	4	609	X	-	-	-
24	CLA	4	610	X	-	-	-
24	CLA	4	611	X	-	-	-
24	CLA	4	612	X	-	-	-
24	CLA	4	613	X	-	-	-
24	CLA	5	601	X	-	-	-
24	CLA	5	602	X	-	-	-
24	CLA	5	603	X	-	-	-
24	CLA	5	604	X	-	-	-
24	CLA	5	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	5	606	X	-	-	-
24	CLA	5	607	X	-	-	-
24	CLA	6	601	X	-	-	-
24	CLA	6	602	X	-	-	-
24	CLA	6	603	X	-	-	-
24	CLA	6	604	X	-	-	-
24	CLA	6	606	X	-	-	-
24	CLA	6	607	X	-	-	-
24	CLA	6	608	X	-	-	-
24	CLA	6	609	X	-	-	-
24	CLA	6	610	X	-	-	-
24	CLA	6	611	X	-	-	-
24	CLA	6	612	X	-	-	-
24	CLA	7	601	X	-	-	-
24	CLA	7	602	X	-	-	-
24	CLA	7	603	X	-	-	-
24	CLA	7	604	X	-	-	-
24	CLA	7	605	X	-	-	-
24	CLA	7	606	X	-	-	-
24	CLA	7	607	X	-	-	-
24	CLA	7	608	X	-	-	-
24	CLA	7	609	X	-	-	-
24	CLA	7	610	X	-	-	-
24	CLA	7	611	X	-	-	-
24	CLA	7	612	X	-	-	-
24	CLA	8	201	X	-	-	-
24	CLA	8	202	X	-	-	-
24	CLA	8	203	X	-	-	-
24	CLA	8	204	X	-	-	-
24	CLA	8	205	X	-	-	-
24	CLA	8	206	X	-	-	-
24	CLA	8	207	X	-	-	-
24	CLA	8	208	X	-	-	-
24	CLA	8	209	X	-	-	-
24	CLA	9	301	X	-	-	-
24	CLA	9	302	X	-	-	-
24	CLA	9	303	X	-	-	-
24	CLA	9	304	X	-	-	-
24	CLA	9	306	X	-	-	-
24	CLA	9	307	X	-	-	-
24	CLA	9	308	X	-	-	-
24	CLA	9	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	9	310	X	-	-	-
24	CLA	9	311	X	-	-	-
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	806	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	814	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	818	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	847	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	A	857	X	-	-	-
24	CLA	A	860	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	801	X	-	-	-
24	CLA	B	802	X	-	-	-
24	CLA	B	803	X	-	-	-
24	CLA	B	804	X	-	-	-
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	817	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	819	X	-	-	-
24	CLA	B	820	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-
24	CLA	B	827	X	-	-	-
24	CLA	B	828	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	846	X	-	-	-
24	CLA	B	847	X	-	-	-
24	CLA	B	848	X	-	-	-
24	CLA	F	201	X	-	-	-
24	CLA	F	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	F	203	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	205	X	-	-	-
24	CLA	R	103	X	-	-	-
24	CLA	R	104	X	-	-	-
24	CLA	c	601	X	-	-	-
24	CLA	c	602	X	-	-	-
24	CLA	c	603	X	-	-	-
24	CLA	c	604	X	-	-	-
24	CLA	c	605	X	-	-	-
24	CLA	c	606	X	-	-	-
24	CLA	c	607	X	-	-	-
24	CLA	c	608	X	-	-	-
24	CLA	c	609	X	-	-	-
24	CLA	c	610	X	-	-	-
24	CLA	c	611	X	-	-	-
24	CLA	h	601	X	-	-	-
24	CLA	h	602	X	-	-	-
24	CLA	h	603	X	-	-	-
24	CLA	h	604	X	-	-	-
24	CLA	h	605	X	-	-	-
24	CLA	h	606	X	-	-	-
24	CLA	h	607	X	-	-	-
24	CLA	h	608	X	-	-	-
24	CLA	h	609	X	-	-	-
24	CLA	h	610	X	-	-	-
24	CLA	h	612	X	-	-	-
24	CLA	k	301	X	-	-	-
24	CLA	k	302	X	-	-	-
24	CLA	k	304	X	-	-	-
24	CLA	k	305	X	-	-	-
24	CLA	k	306	X	-	-	-
24	CLA	k	307	X	-	-	-
24	CLA	k	308	X	-	-	-
24	CLA	k	309	X	-	-	-
24	CLA	k	310	X	-	-	-
24	CLA	k	311	X	-	-	-
24	CLA	t	301	X	-	-	-
24	CLA	t	302	X	-	-	-
24	CLA	t	303	X	-	-	-
24	CLA	t	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	t	305	X	-	-	-
24	CLA	t	306	X	-	-	-
24	CLA	t	307	X	-	-	-
24	CLA	t	308	X	-	-	-
24	CLA	t	309	X	-	-	-
24	CLA	t	310	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 50344 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 Light-harvesting protein XLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	176	Total	C	N	O	S	0	0
			1328	865	221	237	5		

- Molecule 2 is a protein called light-harvesting protein XLH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	137	Total	C	N	O	S	0	0
			1080	695	187	191	7		

- Molecule 3 is a protein called light-harvesting protein XLH3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	158	Total	C	N	O	S	0	0
			1206	775	204	221	6		

- Molecule 4 is a protein called light-harvesting protein XLH4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	188	Total	C	N	O	S	0	0
			1396	894	240	251	11		

- Molecule 5 is a protein called light-harvesting protein XLH5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	167	Total	C	N	O	S	0	0
			1249	798	210	234	7		

- Molecule 6 is a protein called light-harvesting protein XLH6/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	163	Total	C	N	O	S	0	0
			1228	790	206	226	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	165	Total	C	N	O	S	0	0
			1244	801	209	228	6		

- Molecule 7 is a protein called light-harvesting protein XLH7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	166	Total	C	N	O	S	0	0
			1268	816	210	230	12		

- Molecule 8 is a protein called light-harvesting protein XLH8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	161	Total	C	N	O	S	0	0
			1240	794	208	229	9		

- Molecule 9 is a protein called light-harvesting protein XLH9/13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	149	Total	C	N	O	S	0	0
			1171	761	195	206	9		
9	k	154	Total	C	N	O	S	0	0
			1201	777	200	215	9		

- Molecule 10 is a protein called light-harvesting protein XLH11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	165	Total	C	N	O	S	0	0
			1231	787	209	225	10		

- Molecule 11 is a protein called light-harvesting protein XLH12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	t	159	Total	C	N	O	S	0	0
			1253	799	212	235	7		

- Molecule 12 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	741	Total	C	N	O	S	0	0
			5835	3825	992	996	22		

- Molecule 13 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	733	Total	C	N	O	S	0	0
			5822	3830	976	997	19		

- Molecule 14 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	80	Total	C	N	O	S	0	0
			592	363	103	115	11		

- Molecule 15 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	132	Total	C	N	O	S	0	0
			1030	668	171	188	3		

- Molecule 16 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	60	Total	C	N	O	S	0	0
			484	307	82	94	1		

- Molecule 17 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	161	Total	C	N	O	S	0	0
			1267	818	215	230	4		

- Molecule 18 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	33	Total	C	N	O	S	0	0
			252	174	34	43	1		

- Molecule 19 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	40	Total	C	N	O	S	0	0
			320	217	47	55	1		

- Molecule 20 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	137	Total	C	N	O	S	0	0
			1027	674	165	186	2		

- Molecule 21 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	30	Total	C	N	O	S	0	0
			227	153	35	38	1		

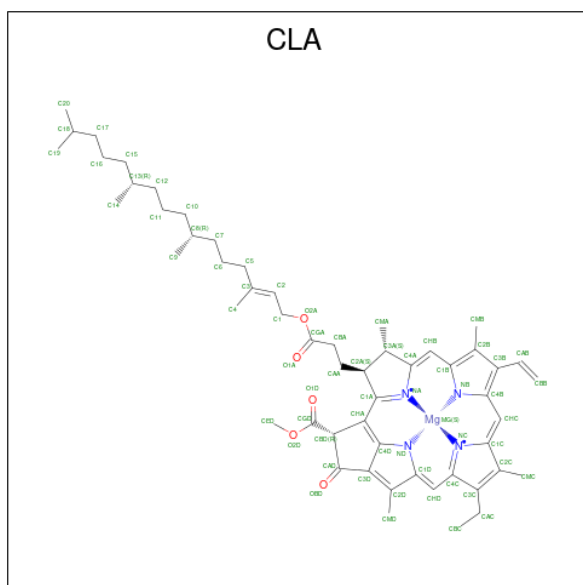
- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	81	Total	C	N	O	S	0	0
			608	397	99	111	1		

- Molecule 23 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	82	Total	C	N	O		0	0
			410	246	82	82			

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	h	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	h	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	c	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
24	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	c	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	c	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	k	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	k	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 54	C 44	Mg 1	N 4	O 5	0

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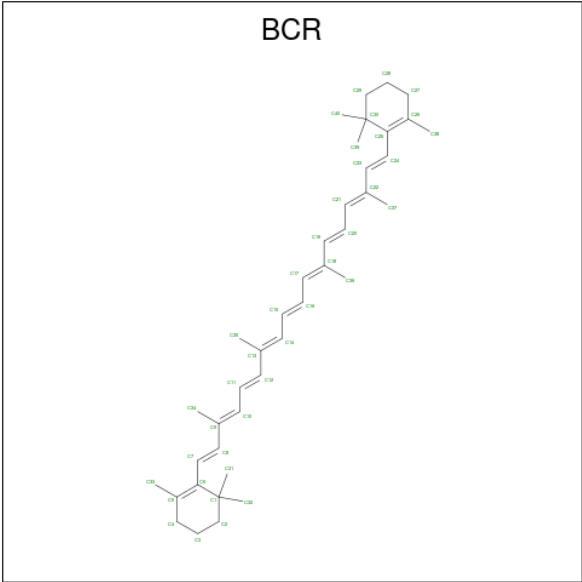
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



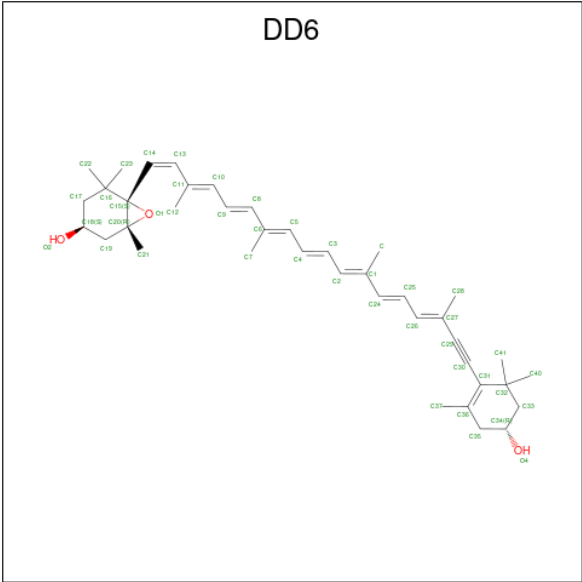
Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	1	1	Total	C	0
			40	40	
25	2	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	7	1	Total	C	0
			40	40	
25	9	1	Total	C	0
			40	40	
25	c	1	Total	C	0
			40	40	
25	t	1	Total	C	0
			40	40	
25	k	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			39	39	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	R	1	Total C 40 40	0
25	R	1	Total C 40 40	0

- Molecule 26 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			43	40	3	
26	1	1	Total	C	O	0
			43	40	3	
26	1	1	Total	C	O	0
			43	40	3	
26	2	1	Total	C	O	0
			43	40	3	
26	2	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	3	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	4	1	Total	C	O	0
			43	40	3	
26	5	1	Total	C	O	0
			43	40	3	
26	5	1	Total	C	O	0
			43	40	3	

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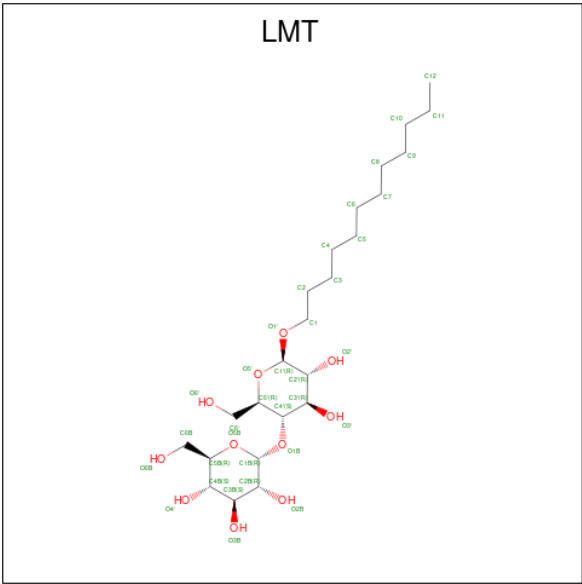
Mol	Chain	Residues	Atoms			AltConf
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	8	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	9	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	h	1	Total	C	O	0
			43	40	3	
26	c	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
26	c	1	Total	C	O	0
			43	40	3	
26	c	1	Total	C	O	0
			43	40	3	
26	t	1	Total	C	O	0
			43	40	3	
26	t	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	k	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	R	1	Total	C	O	0
			43	40	3	

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



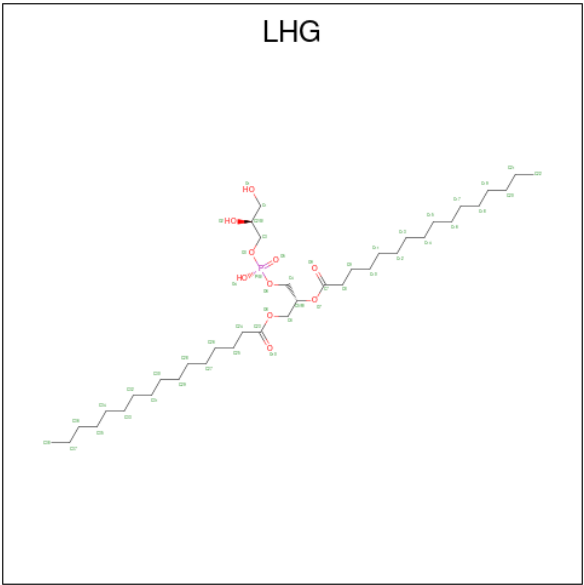
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	
27	3	1	Total	C	O	0
			30	19	11	
27	h	1	Total	C	O	0
			28	17	11	
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			25	14	11	
27	A	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



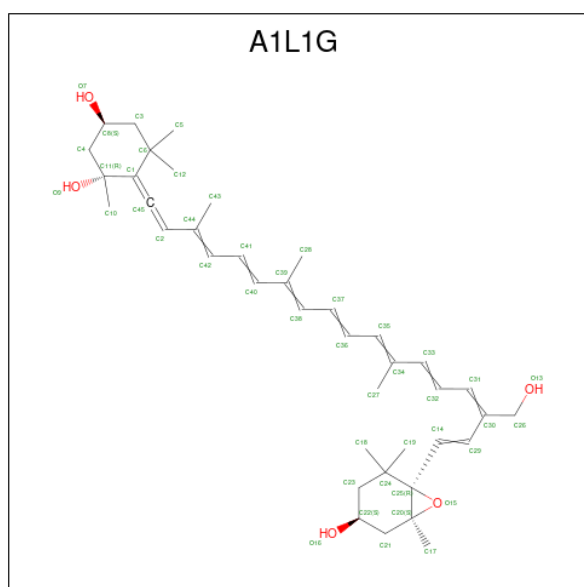
Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			31	20	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	4	1	Total	C	O	P	0
			39	28	10	1	
28	8	1	Total	C	O	P	0
			31	20	10	1	

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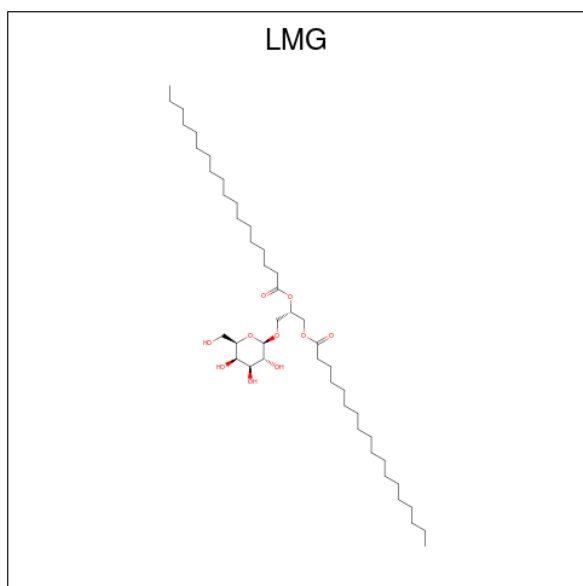
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	A	1	Total 48	37	10	1	0
28	A	1	Total 42	31	10	1	0
28	A	1	Total 41	30	10	1	0
28	A	1	Total 37	26	10	1	0
28	B	1	Total 49	38	10	1	0
28	B	1	Total 41	30	10	1	0
28	I	1	Total 40	29	10	1	0
28	J	1	Total 38	27	10	1	0
28	L	1	Total 29	18	10	1	0

- Molecule 29 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



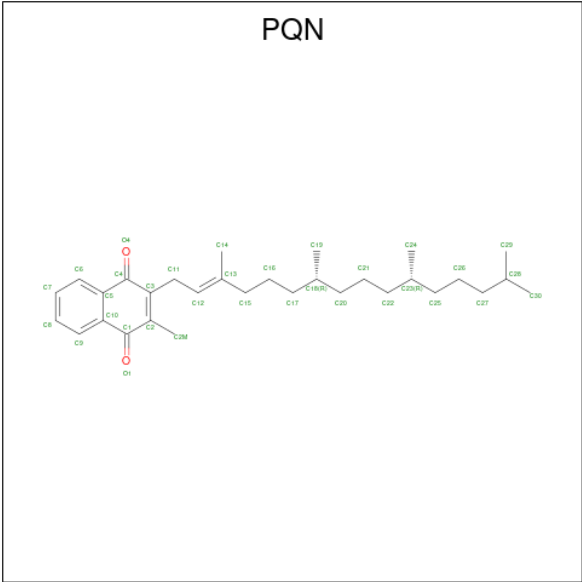
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			45	40	5	
29	3	1	Total	C	O	0
			45	40	5	
29	7	1	Total	C	O	0
			45	40	5	
29	9	1	Total	C	O	0
			45	40	5	
29	k	1	Total	C	O	0
			45	40	5	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



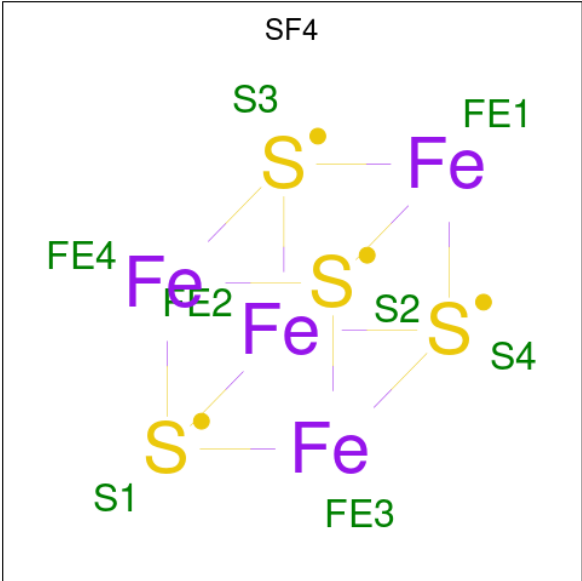
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			45	35	10	
30	t	1	Total	C	O	0
			34	24	10	
30	A	1	Total	C	O	0
			38	28	10	

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



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

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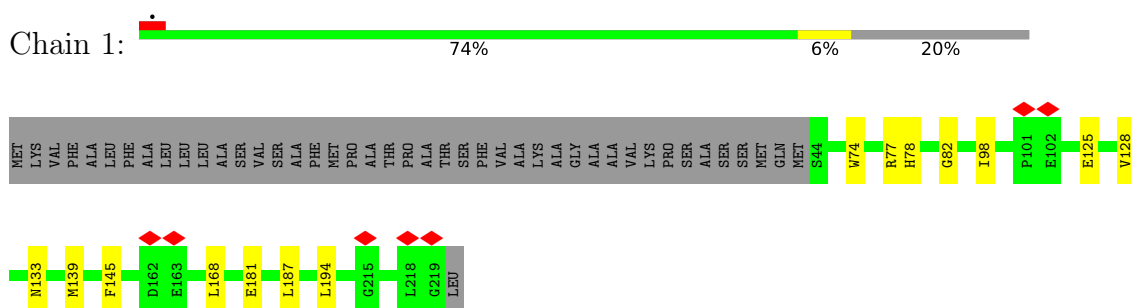
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Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

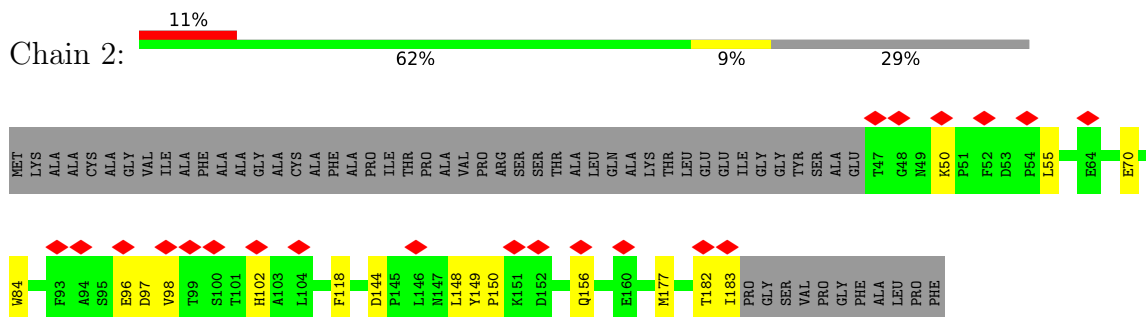
3 Residue-property plots [i](#)

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.

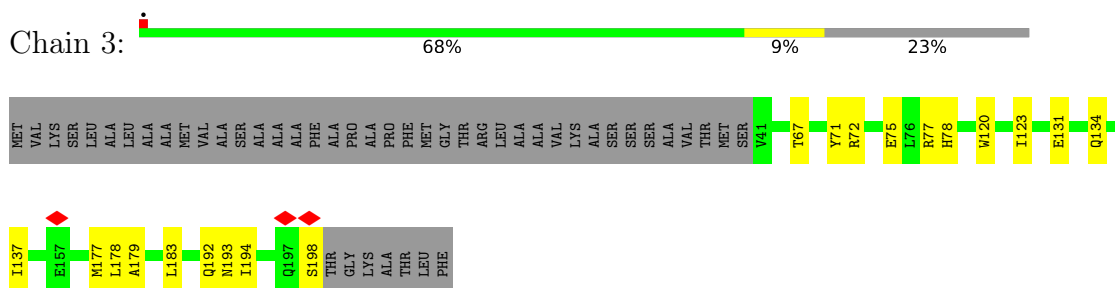
- Molecule 1: Light-harvesting protein XLH1



- Molecule 2: light-harvesting protein XLH2

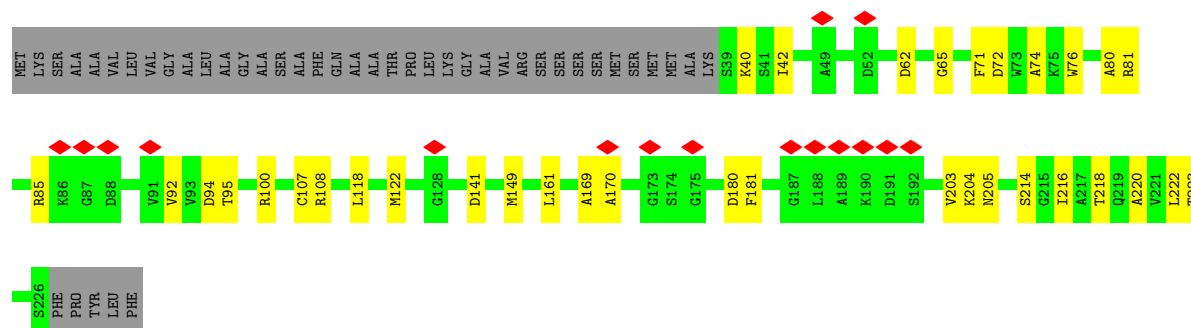


- Molecule 3: light-harvesting protein XLH3

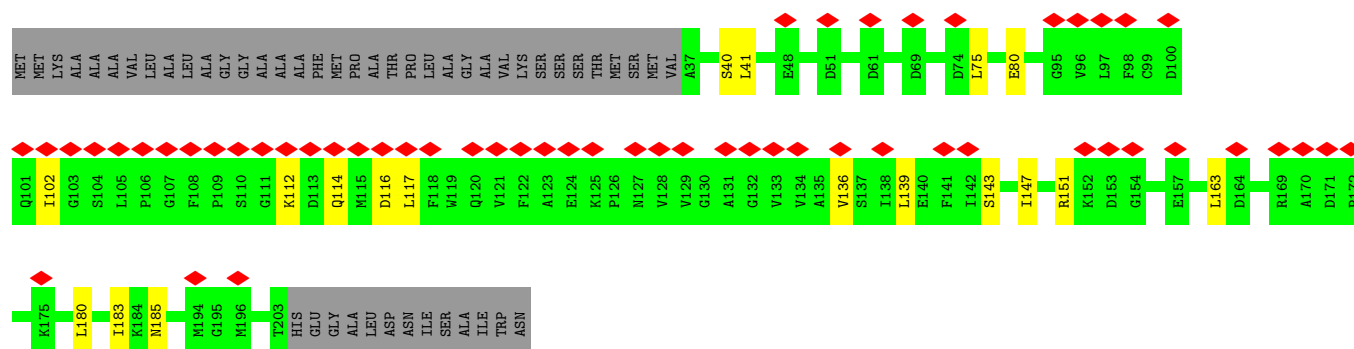


- Molecule 4: light-harvesting protein XLH4

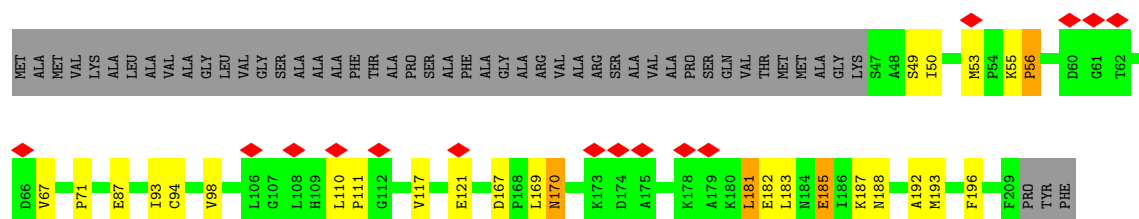




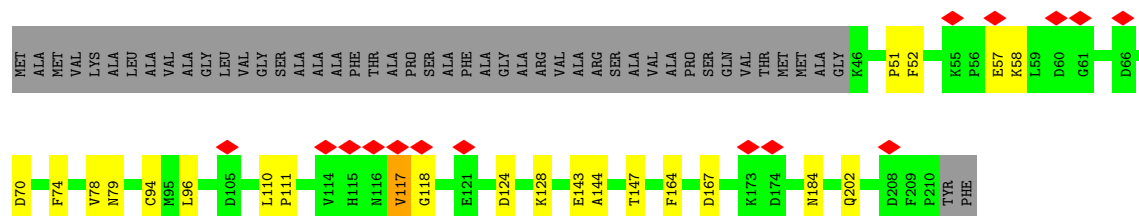
- Molecule 5: light-harvesting protein XLH5



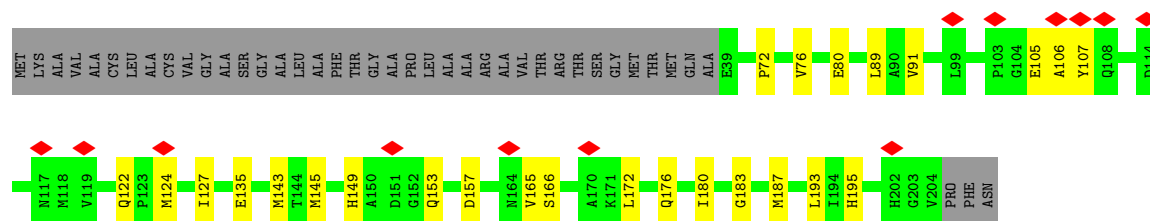
- Molecule 6: light-harvesting protein XLH6/10



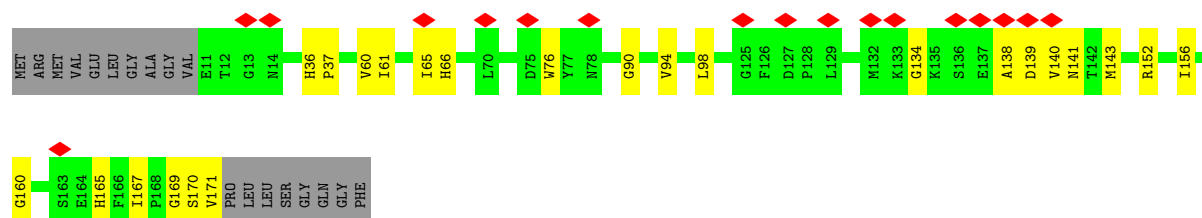
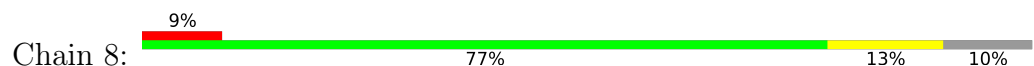
- Molecule 6: light-harvesting protein XLH6/10



- Molecule 7: light-harvesting protein XLH7



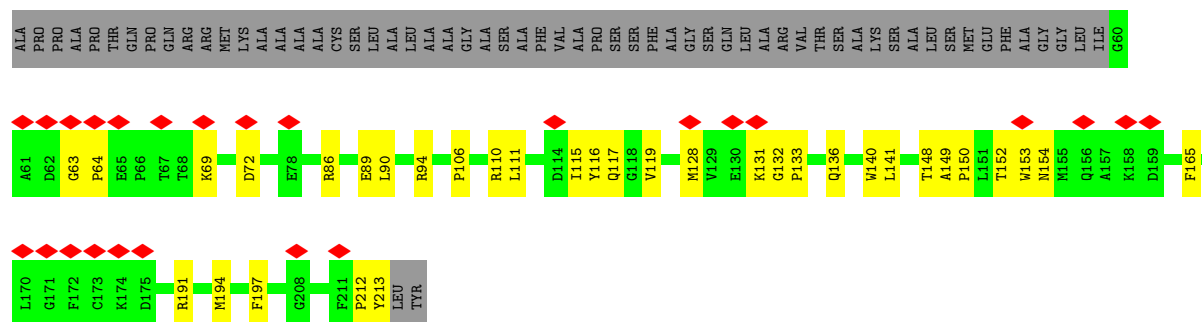
• Molecule 8: light-harvesting protein XLH8



• Molecule 9: light-harvesting protein XLH9/13

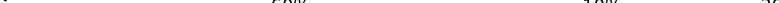


• Molecule 9: light-harvesting protein XLH9/13



• Molecule 10: light-harvesting protein XLH11

Amino Acid	Reference (%)	Variant (%)
MET	~1.5	~0.5
LYS	~0.5	~1.5
VAL	~1.5	~1.5
SER	~1.5	~1.5
ALA	~1.5	~1.5
THR	~1.5	~1.5
GLY	~1.5	~1.5
MET	~1.5	~0.5
ALA	~1.5	~1.5
SER	~1.5	~1.5
GLY	~1.5	~1.5
VAL	~1.5	~1.5
ALA	~1.5	~1.5
ALA	~1.5	~1.5
PHE	~1.5	~1.5
VAL	~1.5	~1.5
GLN	~1.5	~1.5
PRO	~1.5	~1.5
THR	~1.5	~1.5
ALA	~1.5	~1.5
PHE	~1.5	~1.5
ALA	~1.5	~1.5
GLY	~1.5	~1.5
SER	~1.5	~1.5
LYS	~0.5	~1.5
LEU	~1.5	~1.5
ALA	~1.5	~1.5
ALA	~1.5	~1.5
VAL	~1.5	~1.5
ALA	~1.5	~1.5
SER	~1.5	~1.5
GLY	~1.5	~1.5
SER	~1.5	~1.5
THR	~1.5	~1.5
MET	~1.5	~0.5
GLN	~1.5	~1.5
MET	~1.5	~0.5
ALA	~1.5	~1.5
ALA	~1.5	~1.5
ALA	~1.5	~1.5
GLU	~1.5	~1.5
PRO	~1.5	~1.5

- Chain t: 

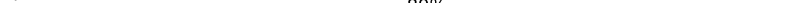
THR	ALA	LEU	ARG	HIS	PRO	HIS	LYS	MET	LYS	ALA	ALA	ALA	THR	VAL	ALA	LEU	ALA	VAL	GLY	SER	VAL	SER	ALA	PHE	ALA	PRO	ASN	ALA	PHE	THR	GLY	LYS	ALA	SER	THR	ALA	GLN	MET	ALA	ASP	ALA	SER	GLY	LEU	VAL	GLY	LYS
PRO	PHE	GLY	ALA	G65	S66	S67	V68	F69	D70	D71	L72	A75	T76	K77	A78	S79	D80	A81	I96	A97	M98	I101	M104	A105	V106	F110	S117	A118	E119	V120	A121	N122	I130	Y134	E149	T156	Y157	K158	P159	E160	S161	V164	Y167	D172	E183		

- Chain A: 92% 7%

Sequence logo for the 12th position of the 12-mer. The y-axis represents information content in bits (0 to 1.5). The x-axis lists amino acids. The logo shows a strong preference for Aspartic acid (D) and Glutamic acid (E) at this position, with D being the most frequent. Other amino acids like Asparagine (N), Glutamine (Q), and Lysine (K) also show some preference. The background is color-coded by amino acid families: yellow for hydrophobic, green for polar uncharged, blue for basic, red for acidic, and grey for sulfur-containing.

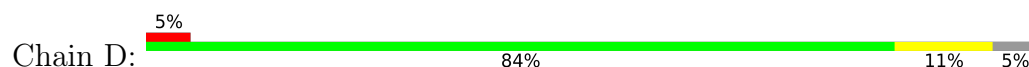
- Chain B: 93% 7%

A horizontal bar chart showing the distribution of 1000 samples across 48 categories. The categories are labeled with codes like MET, A2, E32, T33, H34, H53, Q76, T87, G108, A109, V113, H178, L182, S186, I199, P200, D238, G251, H276, R309, P310, R320, S329, T344, T348, D397, E401, N406, V407, R410, A417, L429, H432, and G434. The bars are color-coded: grey for MET, green for A2, yellow for most others, and red for G434. A red diamond marker is placed above the MET bar and below the G434 bar.

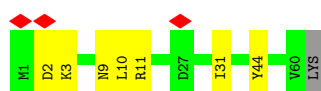
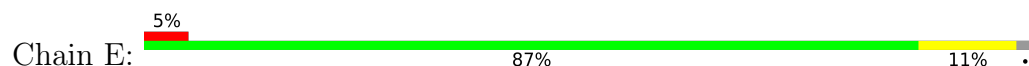
- Chain C: 



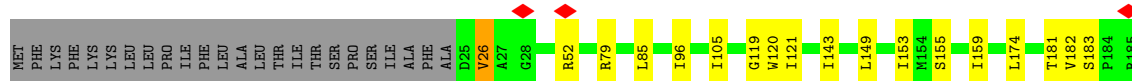
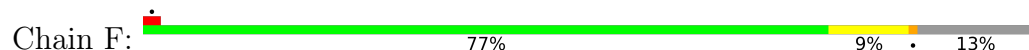
- Molecule 15: Psad



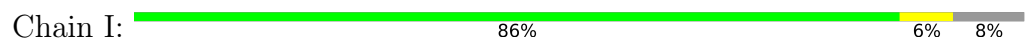
- Molecule 16: Psae



- Molecule 17: Psaf



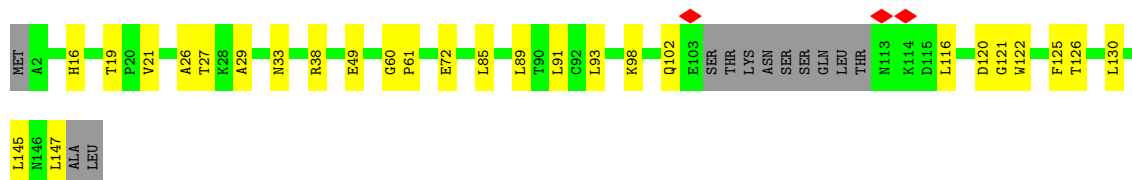
- Molecule 18: Psai



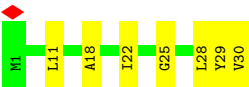
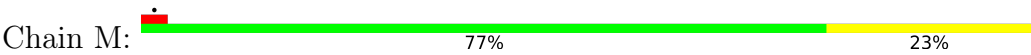
- Molecule 19: Psaj



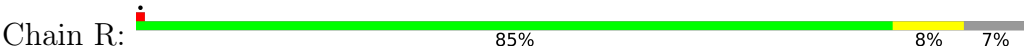
- Molecule 20: Psal



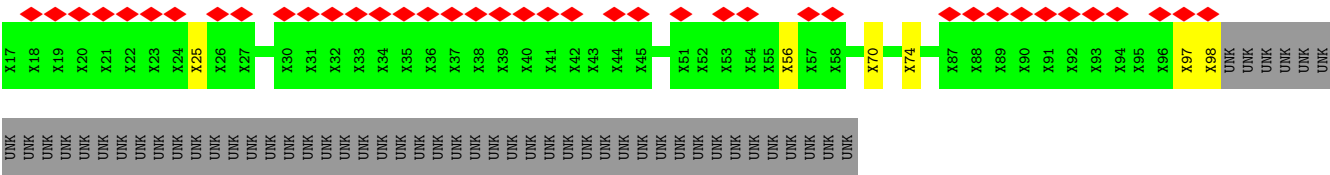
- Molecule 21: Psam



• Molecule 22: PsaR



• Molecule 23: PsaS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.857	Depositor
Minimum map value	-0.484	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	457.59998, 457.59998, 457.59998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, DD6, A1L1G, LHG, SF4, LMG, PQN, BCR, CLA

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	0.18	0/1363	0.30	0/1859
2	2	0.36	0/1109	0.60	0/1504
3	3	0.16	0/1238	0.31	0/1677
4	4	0.24	0/1427	0.38	0/1934
5	5	0.23	0/1274	0.43	0/1722
6	6	0.39	0/1257	0.64	0/1704
6	h	0.27	0/1274	0.46	0/1727
7	7	0.18	0/1298	0.36	0/1752
8	8	0.22	0/1276	0.41	0/1730
9	9	0.31	0/1200	0.48	0/1622
9	k	0.38	0/1231	0.57	0/1666
10	c	0.16	0/1255	0.32	0/1697
11	t	0.20	0/1285	0.37	0/1741
12	A	0.19	0/6030	0.33	0/8219
13	B	0.18	0/6034	0.31	0/8236
14	C	0.28	0/602	0.55	0/816
15	D	0.19	0/1059	0.36	0/1432
16	E	0.29	0/492	0.48	0/662
17	F	0.25	0/1297	0.44	0/1761
18	I	0.21	0/258	0.32	0/353
19	J	0.31	0/331	0.49	0/453
20	L	0.30	0/1051	0.45	0/1428
21	M	0.26	0/228	0.44	0/310
22	R	0.15	0/627	0.27	0/864
All	All	0.24	0/34496	0.40	0/46869

There are no bond length outliers.

There are no bond angle outliers.

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	1328	0	1344	24	0
2	2	1080	0	1061	16	0
3	3	1206	0	1171	18	0
4	4	1396	0	1415	32	0
5	5	1249	0	1255	15	0
6	6	1228	0	1215	41	0
6	h	1244	0	1236	16	0
7	7	1268	0	1265	27	0
8	8	1240	0	1195	17	0
9	9	1171	0	1187	28	0
9	k	1201	0	1207	30	0
10	c	1231	0	1259	12	0
11	t	1253	0	1213	15	0
12	A	5835	0	5718	48	0
13	B	5822	0	5629	43	0
14	C	592	0	569	5	0
15	D	1030	0	1028	11	0
16	E	484	0	486	5	0
17	F	1267	0	1290	14	0
18	I	252	0	272	1	0
19	J	320	0	313	9	0
20	L	1027	0	1037	27	0
21	M	227	0	262	5	0
22	R	608	0	612	5	0
23	S	410	0	86	3	0
24	1	507	0	427	16	0
24	2	440	0	345	13	0
24	3	468	0	413	8	0
24	4	607	0	454	27	0
24	5	328	0	247	7	0
24	6	554	0	401	12	0
24	7	564	0	428	23	0
24	8	409	0	299	9	0
24	9	505	0	363	18	0
24	A	2651	0	2720	33	0
24	B	2471	0	2526	59	0
24	F	161	0	144	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	42	0	31	1	0
24	L	166	0	154	6	0
24	R	110	0	105	1	0
24	c	548	0	460	7	0
24	h	553	0	405	5	0
24	k	513	0	387	10	0
24	t	477	0	369	8	0
25	1	80	0	112	7	0
25	2	40	0	56	4	0
25	4	40	0	56	7	0
25	7	40	0	56	2	0
25	9	40	0	56	9	0
25	A	199	0	277	8	0
25	B	200	0	280	11	0
25	F	40	0	56	2	0
25	I	80	0	112	3	0
25	J	80	0	112	5	0
25	L	80	0	112	2	0
25	M	40	0	56	2	0
25	R	80	0	112	2	0
25	c	40	0	56	7	0
25	k	40	0	56	2	0
25	t	40	0	56	2	0
26	1	129	0	0	7	0
26	2	86	0	0	2	0
26	3	129	0	0	1	0
26	4	172	0	0	2	0
26	5	86	0	0	3	0
26	6	215	0	0	2	0
26	7	172	0	0	3	0
26	8	129	0	0	2	0
26	9	172	0	0	6	0
26	A	43	0	0	0	0
26	J	43	0	0	0	0
26	R	43	0	0	0	0
26	c	129	0	0	3	0
26	h	172	0	0	1	0
26	k	129	0	0	4	0
26	t	86	0	0	0	0
27	1	70	0	92	2	0
27	3	30	0	33	1	0
27	A	95	0	115	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	h	28	0	29	1	0
28	1	43	0	56	2	0
28	2	31	0	32	0	0
28	3	43	0	59	1	0
28	4	39	0	48	1	0
28	8	31	0	32	1	0
28	A	168	0	222	2	0
28	B	90	0	129	0	0
28	I	40	0	50	1	0
28	J	38	0	46	1	0
28	L	29	0	28	4	0
29	2	45	0	0	0	0
29	3	45	0	0	2	0
29	7	45	0	0	0	0
29	9	45	0	0	1	0
29	k	45	0	0	2	0
30	2	45	0	60	1	0
30	A	38	0	46	0	0
30	t	34	0	38	0	0
31	A	33	0	46	1	0
31	B	33	0	46	0	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
All	All	50344	0	46831	640	0

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

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:147:LEU:HD23	24:L:205:CLA:C1	1.56	1.33
3:3:194:ILE:HD13	3:3:198:SER:OG	1.43	1.16
1:1:98:ILE:HG23	1:1:128:VAL:HG11	1.21	1.15
20:L:147:LEU:CD2	24:L:205:CLA:C1	2.31	1.07
6:6:50:ILE:HG21	6:6:53:MET:HG3	1.37	1.04
6:6:50:ILE:CG2	6:6:53:MET:HG3	1.92	0.99
24:9:301:CLA:H2A	24:9:301:CLA:HED2	1.45	0.98
6:6:50:ILE:HD12	6:6:53:MET:SD	2.08	0.93
7:7:165:VAL:HG12	7:7:166:SER:H	1.30	0.92
6:6:50:ILE:CD1	6:6:53:MET:SD	2.59	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:222:LEU:CD1	24:4:611:CLA:CMA	2.48	0.90
3:3:123:ILE:HG13	24:3:304:CLA:HAB	1.57	0.85
4:4:222:LEU:CD1	24:4:611:CLA:HMA1	2.07	0.84
6:6:53:MET:CE	6:6:71:PRO:HA	2.08	0.84
9:9:201:ILE:HD11	25:9:316:BCR:H383	1.58	0.84
13:B:320:ARG:NH1	22:R:6:TYR:CE2	2.46	0.84
4:4:222:LEU:HD11	24:4:611:CLA:CMA	2.08	0.84
1:1:125:GLU:O	1:1:128:VAL:HG12	1.79	0.82
7:7:165:VAL:HG12	7:7:166:SER:N	1.91	0.82
7:7:165:VAL:CG1	7:7:166:SER:H	1.94	0.81
6:6:50:ILE:HG21	6:6:53:MET:CG	2.09	0.80
6:6:53:MET:CE	6:6:71:PRO:CA	2.59	0.80
4:4:222:LEU:CD1	24:4:611:CLA:HMA2	2.09	0.80
10:c:194:ALA:O	10:c:198:MET:HG2	1.83	0.79
9:k:115:ILE:CG2	9:k:131:LYS:HD2	2.14	0.77
24:B:804:CLA:O1D	24:B:804:CLA:H2A	1.83	0.77
12:A:119:VAL:HG12	12:A:119:VAL:O	1.84	0.77
1:1:187:LEU:HG	25:1:1310:BCR:H14C	1.67	0.76
4:4:222:LEU:HD11	24:4:611:CLA:HMA1	1.63	0.76
1:1:98:ILE:CG2	1:1:128:VAL:HG11	2.11	0.76
24:7:602:CLA:H2A	24:7:602:CLA:HED3	1.68	0.74
9:k:115:ILE:HG22	9:k:131:LYS:HD2	1.70	0.74
24:B:823:CLA:HMA1	25:B:843:BCR:H14C	1.69	0.74
28:8:213:LHG:O3	28:8:213:LHG:O1	1.94	0.73
2:2:70:GLU:OE2	24:2:201:CLA:ND	2.21	0.73
7:7:135:GLU:OE1	24:7:606:CLA:NB	2.23	0.72
2:2:55:LEU:HD12	25:2:211:BCR:H313	1.70	0.71
7:7:165:VAL:CG1	7:7:172:LEU:HD13	2.20	0.71
15:D:22:ALA:O	15:D:26:GLU:N	2.22	0.71
3:3:194:ILE:CD1	3:3:198:SER:OG	2.33	0.71
13:B:186:SER:HB3	24:B:817:CLA:HBC1	1.73	0.70
11:t:159:PRO:O	11:t:164:VAL:HG21	1.93	0.69
14:C:24:ASP:OD2	15:D:96:HIS:ND1	2.23	0.69
23:S:25:UNK:O	23:S:56:UNK:CB	2.40	0.69
24:B:804:CLA:H3A	21:M:28:LEU:HD13	1.74	0.68
6:6:53:MET:HE1	6:6:71:PRO:CD	2.24	0.68
29:3:310:A1L1G:C2	24:A:840:CLA:H11	2.24	0.67
4:4:222:LEU:HD12	24:4:611:CLA:HMA2	1.76	0.67
6:6:53:MET:HE3	6:6:71:PRO:HB3	1.75	0.67
24:2:204:CLA:CGA	24:2:204:CLA:H3A	2.25	0.66
9:9:154:ASN:OD1	9:9:155:MET:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:29:ALA:O	20:L:33:ASN:ND2	2.28	0.66
20:L:147:LEU:HD21	24:L:205:CLA:O1A	1.96	0.66
24:A:830:CLA:NA	28:A:842:LHG:HC91	2.11	0.66
24:B:831:CLA:H93	25:B:843:BCR:HC42	1.77	0.66
15:D:62:ARG:NH2	15:D:64:GLU:OE1	2.28	0.66
12:A:119:VAL:CG1	24:B:830:CLA:HMD1	2.26	0.65
17:F:79:ARG:NH2	19:J:34:PRO:O	2.29	0.65
1:1:98:ILE:HG23	1:1:128:VAL:CG1	2.13	0.65
24:8:203:CLA:CGA	24:8:203:CLA:H3A	2.27	0.65
24:4:612:CLA:OBD	12:A:315:ILE:HD13	1.97	0.65
6:6:50:ILE:HD13	6:6:53:MET:SD	2.35	0.65
7:7:135:GLU:OE1	24:7:606:CLA:C1B	2.44	0.65
6:6:167:ASP:HB3	6:6:170:ASN:HA	1.79	0.65
2:2:183:ILE:HG22	2:2:183:ILE:O	1.96	0.64
12:A:69:LYS:NZ	24:A:810:CLA:OBD	2.29	0.64
12:A:315:ILE:HD11	24:A:819:CLA:HMA2	1.78	0.64
7:7:165:VAL:HG12	7:7:172:LEU:HD13	1.79	0.64
6:6:50:ILE:HG22	6:6:53:MET:HG3	1.79	0.64
24:4:607:CLA:O2A	24:4:607:CLA:H3A	1.97	0.64
6:h:184:ASN:ND2	24:h:610:CLA:O2D	2.31	0.63
24:9:301:CLA:HED2	24:9:301:CLA:C2A	2.26	0.63
9:9:72:ASP:HB2	24:9:301:CLA:HED1	1.81	0.63
27:A:854:LMT:O5B	27:A:854:LMT:O3'	2.14	0.63
2:2:183:ILE:HD13	24:2:209:CLA:CMD	2.28	0.63
15:D:55:GLU:N	15:D:55:GLU:OE1	2.32	0.62
24:k:304:CLA:HMB1	26:k:315:DD6:C3	2.29	0.62
9:9:95:LEU:HD21	26:9:315:DD6:C31	2.29	0.62
6:6:53:MET:HE1	6:6:71:PRO:CA	2.29	0.62
6:6:53:MET:HE3	6:6:71:PRO:HA	1.81	0.62
19:J:2:GLU:N	19:J:2:GLU:OE1	2.33	0.62
10:c:154:ASP:OD1	10:c:155:ALA:N	2.32	0.62
9:k:111:LEU:O	9:k:117:GLN:NE2	2.30	0.61
20:L:145:LEU:CD2	28:L:201:LHG:H102	2.30	0.61
24:3:304:CLA:H2A	24:3:304:CLA:HED3	1.83	0.60
13:B:309:ARG:NH1	13:B:310:PRO:O	2.33	0.60
24:1:317:CLA:H2A	24:1:317:CLA:O1D	2.00	0.60
24:7:602:CLA:HBC2	24:7:602:CLA:HHD	1.83	0.60
9:9:95:LEU:HD21	26:9:315:DD6:C40	2.32	0.60
20:L:145:LEU:HD21	28:L:201:LHG:H102	1.84	0.60
12:A:125:ASN:O	17:F:52:ARG:NH2	2.35	0.59
1:1:133:ASN:HB3	24:1:305:CLA:HBC1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:t:159:PRO:O	11:t:164:VAL:CG2	2.50	0.59
2:2:183:ILE:HD13	24:2:209:CLA:HMD2	1.84	0.59
24:8:206:CLA:H2A	24:8:206:CLA:HED3	1.85	0.59
6:h:164:PHE:N	24:h:608:CLA:OBD	2.34	0.59
12:A:254:PHE:O	12:A:257:GLY:N	2.35	0.59
27:A:854:LMT:H6B	27:A:854:LMT:H3O2	1.50	0.59
12:A:80:VAL:HG11	24:A:805:CLA:HMD2	1.84	0.59
24:2:201:CLA:HMD3	25:2:211:BCR:H12C	1.85	0.58
16:E:2:ASP:OD1	16:E:3:LYS:N	2.36	0.58
25:J:104:BCR:H382	25:J:104:BCR:H23C	1.84	0.58
24:B:831:CLA:O1A	24:B:832:CLA:HMB3	2.03	0.58
24:5:605:CLA:HED3	24:5:605:CLA:H2A	1.85	0.58
8:8:76:TRP:O	8:8:76:TRP:CD1	2.57	0.58
3:3:137:ILE:HD11	20:L:26:ALA:HA	1.86	0.58
6:6:53:MET:HE1	6:6:71:PRO:N	2.19	0.58
12:A:119:VAL:HG11	24:B:830:CLA:HMD1	1.85	0.58
24:2:201:CLA:HMD3	25:2:211:BCR:H10C	1.87	0.57
6:6:50:ILE:CG2	6:6:53:MET:CG	2.75	0.57
9:k:72:ASP:N	9:k:72:ASP:OD1	2.38	0.57
6:6:53:MET:CE	6:6:71:PRO:CB	2.83	0.57
9:k:63:GLY:HA2	9:k:69:LYS:O	2.05	0.57
12:A:119:VAL:HG11	24:B:830:CLA:CMD	2.35	0.57
24:1:305:CLA:HBB1	24:1:305:CLA:HHC	1.86	0.56
15:D:52:LEU:N	15:D:56:ASN:OD1	2.38	0.56
24:J:103:CLA:O1D	24:J:103:CLA:H2A	2.05	0.56
5:5:114:GLN:O	26:5:609:DD6:O4	2.23	0.56
28:1:318:LHG:H172	25:M:101:BCR:HC42	1.86	0.56
3:3:120:TRP:CE3	3:3:123:ILE:HD12	2.41	0.56
6:6:53:MET:HE1	6:6:71:PRO:HD3	1.87	0.55
24:6:603:CLA:H2A	24:6:603:CLA:HED2	1.87	0.55
24:A:818:CLA:H203	24:A:826:CLA:H3A	1.88	0.55
22:R:84:GLN:O	22:R:85:ASN:ND2	2.39	0.55
13:B:401:GLU:N	13:B:401:GLU:OE1	2.38	0.55
25:R:102:BCR:H331	25:R:102:BCR:HC8	1.89	0.55
24:4:607:CLA:H3A	24:4:607:CLA:C1	2.37	0.55
6:6:50:ILE:HG21	6:6:53:MET:SD	2.46	0.55
24:h:612:CLA:O1A	24:h:612:CLA:H2A	2.06	0.55
24:k:308:CLA:O1D	24:k:308:CLA:H2A	2.06	0.55
12:A:119:VAL:O	12:A:119:VAL:CG1	2.55	0.55
4:4:149:MET:HB3	24:4:605:CLA:HMD3	1.89	0.55
9:9:72:ASP:HB2	24:9:301:CLA:CED	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:429:ARG:NH1	15:D:14:GLY:O	2.39	0.55
6:6:53:MET:HE3	6:6:71:PRO:CB	2.37	0.54
12:A:367:HIS:ND1	24:A:817:CLA:OBD	2.40	0.54
24:A:816:CLA:O2D	24:A:816:CLA:H2A	2.06	0.54
9:k:154:ASN:OD1	9:k:154:ASN:O	2.25	0.54
9:k:194:MET:HE3	24:k:301:CLA:HMC2	1.88	0.54
12:A:330:PHE:O	12:A:426:ARG:NH1	2.40	0.54
5:5:163:LEU:HD12	24:5:605:CLA:HMD3	1.90	0.54
24:6:603:CLA:H2A	24:6:603:CLA:CED	2.37	0.54
24:c:607:CLA:HBB1	25:c:615:BCR:H362	1.89	0.54
12:A:233:GLU:N	12:A:233:GLU:OE1	2.40	0.54
24:4:613:CLA:H2A	24:4:613:CLA:O2A	2.07	0.54
5:5:180:LEU:O	5:5:183:ILE:HG22	2.08	0.54
1:1:139:MET:HE1	26:1:313:DD6:C28	2.37	0.54
24:A:814:CLA:HED3	24:A:814:CLA:H2A	1.90	0.54
6:6:53:MET:CE	6:6:71:PRO:HB3	2.36	0.54
12:A:693:GLU:OE1	13:B:536:LYS:NZ	2.40	0.54
3:3:192:GLN:O	3:3:193:ASN:CG	2.51	0.54
9:9:97:MET:SD	9:9:193:ALA:HB2	2.47	0.53
6:6:49:SER:OG	24:6:601:CLA:ND	2.42	0.53
6:6:53:MET:HE3	6:6:71:PRO:CA	2.36	0.53
1:1:125:GLU:O	1:1:128:VAL:CG1	2.53	0.53
24:4:602:CLA:H2A	24:4:602:CLA:HED3	1.91	0.53
9:9:160:ARG:NH1	6:h:52:PHE:O	2.41	0.53
24:5:604:CLA:O1D	24:5:604:CLA:H2A	2.08	0.53
28:J:105:LHG:O3	28:J:105:LHG:O1	2.23	0.53
2:2:183:ILE:O	2:2:183:ILE:CG2	2.57	0.53
17:F:143:ILE:O	19:J:11:ALA:N	2.41	0.53
1:1:125:GLU:C	1:1:128:VAL:HG12	2.33	0.53
1:1:133:ASN:ND2	26:1:311:DD6:O4	2.35	0.53
7:7:165:VAL:CG1	7:7:166:SER:N	2.58	0.53
7:7:145:MET:SD	17:F:155:SER:OG	2.66	0.53
3:3:77:ARG:NH1	3:3:134:GLN:OE1	2.41	0.52
5:5:80:GLU:HB2	24:5:604:CLA:HED1	1.91	0.52
8:8:140:VAL:HG11	8:8:143:MET:SD	2.49	0.52
6:6:187:LYS:HG2	26:6:615:DD6:C33	2.40	0.52
12:A:353:ASN:ND2	24:A:804:CLA:OBD	2.37	0.52
25:A:859:BCR:H23C	25:A:859:BCR:H382	1.90	0.52
24:2:207:CLA:H2A	24:2:207:CLA:O1A	2.08	0.52
27:3:314:LMT:O2'	27:A:851:LMT:O2B	2.28	0.52
4:4:76:TRP:NE1	24:4:606:CLA:O1A	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:607:CLA:HAB	26:7:613:DD6:C24	2.40	0.52
8:8:65:ILE:O	8:8:66:HIS:HB2	2.10	0.52
24:8:204:CLA:HAC2	26:8:212:DD6:C2	2.40	0.52
1:1:125:GLU:HA	1:1:128:VAL:HG12	1.90	0.52
13:B:542:ARG:NH2	15:D:125:ASN:OD1	2.40	0.52
5:5:163:LEU:O	26:5:608:DD6:O4	2.28	0.52
24:A:830:CLA:HMA2	20:L:19:THR:HG21	1.91	0.52
13:B:329:SER:OG	13:B:397:ASP:OD2	2.23	0.52
1:1:78:HIS:CE1	24:1:302:CLA:HMA1	2.45	0.52
24:1:306:CLA:O1D	24:1:306:CLA:H2A	2.10	0.52
7:7:149:HIS:HA	7:7:153:GLN:HB2	1.92	0.52
10:c:198:MET:SD	26:c:612:DD6:C40	2.98	0.52
2:2:150:PRO:O	2:2:156:GLN:NE2	2.42	0.51
24:4:608:CLA:HBC3	24:4:608:CLA:HHD	1.92	0.51
11:t:160:GLU:HA	11:t:164:VAL:HG23	1.92	0.51
9:k:63:GLY:N	9:k:64:PRO:CD	2.73	0.51
21:M:18:ALA:O	21:M:22:ILE:HG12	2.09	0.51
13:B:661:PHE:HB2	24:B:803:CLA:HMC2	1.91	0.51
24:B:801:CLA:H3A	25:L:202:BCR:C32	2.40	0.51
15:D:96:HIS:HB3	15:D:97:PRO:HD3	1.90	0.51
24:7:611:CLA:HMD3	25:7:617:BCR:H10C	1.93	0.51
12:A:515:GLY:O	12:A:516:SER:OG	2.21	0.51
24:B:829:CLA:HBA2	17:F:174:LEU:HD13	1.93	0.51
24:7:602:CLA:H2A	24:7:602:CLA:CGD	2.41	0.51
9:k:89:GLU:OE1	24:k:301:CLA:C1B	2.57	0.51
9:k:115:ILE:HG21	9:k:131:LYS:HD2	1.92	0.51
5:5:143:SER:O	5:5:147:ILE:HG12	2.10	0.51
9:9:160:ARG:NH2	6:h:51:PRO:O	2.44	0.51
24:1:304:CLA:NC	26:1:311:DD6:O4	2.43	0.51
11:t:202:GLU:OE1	24:t:306:CLA:C4A	2.57	0.51
24:A:838:CLA:O1D	24:A:838:CLA:H2A	2.10	0.51
17:F:105:ILE:HG23	19:J:39:PHE:HB3	1.93	0.51
20:L:120:ASP:OD1	20:L:121:GLY:N	2.43	0.51
1:1:82:GLY:HA2	26:1:311:DD6:C41	2.40	0.51
8:8:134:GLY:HA3	8:8:140:VAL:CG2	2.41	0.51
10:c:150:ASP:O	10:c:158:LYS:NZ	2.42	0.51
24:7:601:CLA:O2D	24:7:601:CLA:H2A	2.11	0.51
12:A:340:GLU:O	12:A:344:THR:OG1	2.21	0.51
14:C:13:GLY:O	14:C:38:GLN:NE2	2.37	0.51
10:c:151:ASP:OD1	10:c:151:ASP:N	2.44	0.51
25:c:615:BCR:HC8	25:c:615:BCR:H321	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:118:ILE:HG13	12:A:119:VAL:HG23	1.93	0.51
20:L:93:LEU:HB3	20:L:126:THR:HG22	1.92	0.50
9:9:72:ASP:OD1	26:9:313:DD6:O4	2.29	0.50
13:B:432:HIS:CG	25:J:101:BCR:H323	2.47	0.50
9:9:119:VAL:O	9:9:120:SER:HB2	2.11	0.50
24:9:302:CLA:HBB2	25:9:316:BCR:C16	2.41	0.50
12:A:403:ALA:HB2	25:A:846:BCR:H323	1.93	0.50
24:2:206:CLA:HMC2	26:2:210:DD6:C9	2.42	0.50
25:A:843:BCR:H362	25:A:844:BCR:H21C	1.93	0.50
4:4:72:ASP:O	4:4:74:ALA:N	2.45	0.50
25:c:615:BCR:H23C	25:c:615:BCR:H403	1.94	0.50
9:k:115:ILE:HB	9:k:131:LYS:HE3	1.94	0.50
13:B:182:LEU:HD11	24:B:812:CLA:H2	1.93	0.50
25:B:841:BCR:H23C	25:B:841:BCR:H382	1.94	0.50
4:4:222:LEU:HD13	24:4:611:CLA:HMA1	1.90	0.49
24:B:824:CLA:HHC	24:B:824:CLA:HBB1	1.94	0.49
9:k:116:TYR:HA	9:k:128:MET:HE1	1.94	0.49
24:5:606:CLA:CGA	24:5:606:CLA:H3A	2.42	0.49
4:4:181:PHE:HB2	24:4:607:CLA:HMD1	1.94	0.49
7:7:105:GLU:O	7:7:106:ALA:HB3	2.12	0.49
9:9:199:GLY:HA2	24:9:310:CLA:HMA2	1.95	0.49
9:k:197:PHE:CE2	26:k:313:DD6:C24	2.96	0.49
13:B:429:LEU:HD11	24:B:834:CLA:HMB1	1.95	0.49
13:B:545:LYS:NZ	17:F:181:THR:O	2.44	0.49
20:L:102:GLN:N	20:L:102:GLN:OE1	2.45	0.49
21:M:29:TYR:O	21:M:30:VAL:C	2.56	0.49
12:A:747:SER:O	12:A:748:VAL:HG23	2.13	0.49
6:6:117:VAL:CG1	6:6:121:GLU:HB2	2.42	0.49
11:t:104:MET:SD	11:t:216:ALA:HB1	2.53	0.49
9:k:213:TYR:HA	29:k:312:A1L1G:O16	2.13	0.49
9:9:194:MET:HB3	26:9:313:DD6:C3	2.43	0.49
24:A:832:CLA:H2A	24:A:832:CLA:O2D	2.12	0.49
25:B:849:BCR:H383	25:B:849:BCR:H23C	1.94	0.49
24:7:606:CLA:HBB1	24:7:612:CLA:HMC2	1.95	0.48
24:7:611:CLA:HED3	24:7:611:CLA:H2A	1.94	0.48
10:c:198:MET:SD	26:c:612:DD6:C41	3.01	0.48
12:A:119:VAL:HG12	24:B:830:CLA:HMD1	1.93	0.48
24:B:832:CLA:OBD	22:R:48:ASN:HB3	2.14	0.48
12:A:197:HIS:CD2	24:A:812:CLA:HMC2	2.47	0.48
13:B:571:SER:OG	13:B:574:ASP:OD2	2.28	0.48
24:4:611:CLA:NC	25:4:618:BCR:H17C	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:72:PRO:O	7:7:76:VAL:HG23	2.13	0.48
14:C:34:CYS:SG	14:C:35:LYS:N	2.86	0.48
4:4:204:LYS:HB2	24:4:608:CLA:HBC2	1.95	0.48
9:9:129:VAL:HG22	24:9:305:CLA:H3A	1.96	0.48
24:9:308:CLA:HHC	24:9:308:CLA:HBB1	1.95	0.48
13:B:716:GLY:O	13:B:720:THR:HG22	2.13	0.48
12:A:119:VAL:HG13	24:B:830:CLA:OBD	2.14	0.48
13:B:238:ASP:OD1	13:B:251:GLY:N	2.41	0.48
24:B:830:CLA:O1A	19:J:30:ASN:ND2	2.46	0.48
24:B:834:CLA:H152	25:F:204:BCR:H23C	1.95	0.48
4:4:220:ALA:HA	4:4:223:THR:O	2.14	0.48
24:2:205:CLA:HMB1	30:2:214:LMG:H331	1.96	0.48
4:4:214:SER:OG	25:4:618:BCR:H363	2.14	0.48
8:8:152:ARG:O	8:8:156:ILE:HG12	2.13	0.48
20:L:21:VAL:O	20:L:27:THR:HG21	2.14	0.48
6:h:117:VAL:HG23	6:h:118:GLY:H	1.79	0.48
11:t:130:ILE:O	11:t:134:TYR:N	2.45	0.48
11:t:156:THR:O	11:t:157:TYR:HB2	2.14	0.48
17:F:85:LEU:HD21	19:J:38:THR:HG21	1.94	0.48
20:L:72:GLU:OE1	20:L:72:GLU:N	2.41	0.48
22:R:48:ASN:N	22:R:51:HIS:O	2.43	0.48
24:3:308:CLA:HED2	28:3:315:LHG:H111	1.96	0.47
7:7:143:MET:CE	24:7:606:CLA:HMA1	2.44	0.47
9:9:66:PRO:HD2	9:9:69:LYS:HD2	1.95	0.47
6:h:124:ASP:O	6:h:128:LYS:HG2	2.14	0.47
27:h:617:LMT:O6'	27:h:617:LMT:O2B	2.30	0.47
12:A:192:GLU:OE1	12:A:192:GLU:N	2.43	0.47
18:I:1:ALA:O	18:I:2:SER:OG	2.26	0.47
24:8:206:CLA:H2A	24:8:206:CLA:CED	2.44	0.47
9:9:70:ASN:OD1	24:9:301:CLA:HED3	2.14	0.47
3:3:77:ARG:NH1	3:3:131:GLU:OE1	2.47	0.47
24:9:310:CLA:HBA2	24:9:310:CLA:H3A	1.59	0.47
24:B:810:CLA:O1D	24:B:810:CLA:H2A	2.14	0.47
24:B:830:CLA:HBB	25:J:101:BCR:H353	1.96	0.47
6:6:49:SER:OG	24:6:601:CLA:C4D	2.62	0.47
9:k:212:PRO:O	29:k:312:A1L1G:O16	2.33	0.47
6:6:53:MET:HE1	6:6:71:PRO:CB	2.45	0.47
24:t:307:CLA:H2A	24:t:307:CLA:HED3	1.96	0.47
12:A:485:GLN:NE2	24:A:835:CLA:OBD	2.46	0.47
25:B:843:BCR:H11C	25:B:843:BCR:H341	1.57	0.47
19:J:25:PHE:CD1	19:J:25:PHE:C	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:169:LEU:O	6:6:170:ASN:C	2.57	0.47
8:8:134:GLY:HA3	8:8:140:VAL:HG23	1.97	0.47
25:t:312:BCR:H403	25:t:312:BCR:H23C	1.97	0.47
9:k:110:ARG:HG2	9:k:117:GLN:HA	1.95	0.47
12:A:356:MET:HG3	24:A:824:CLA:HBB	1.97	0.47
12:A:696:GLU:OE2	16:E:44:TYR:OH	2.29	0.47
13:B:417:ALA:HB2	24:B:829:CLA:HED1	1.97	0.47
13:B:519:VAL:HG11	13:B:593:TYR:HB2	1.96	0.47
24:B:804:CLA:HHC	24:B:806:CLA:OBD	2.15	0.47
24:B:821:CLA:HBB	24:B:838:CLA:O1D	2.14	0.47
16:E:9:ASN:OD1	16:E:10:LEU:N	2.47	0.47
20:L:116:LEU:CD1	20:L:125:PHE:HB2	2.45	0.47
4:4:62:ASP:OD1	4:4:65:GLY:N	2.48	0.47
4:4:80:ALA:HB2	28:4:619:LHG:HC81	1.96	0.47
25:c:615:BCR:H11C	25:c:615:BCR:H341	1.76	0.47
24:t:308:CLA:HHC	24:t:308:CLA:HBB1	1.97	0.47
13:B:603:GLN:CD	13:B:732:LYS:HZ2	2.20	0.47
4:4:169:ALA:O	4:4:170:ALA:HB3	2.15	0.47
9:k:89:GLU:OE2	9:k:191:ARG:NH2	2.44	0.47
12:A:423:LEU:HD23	24:A:823:CLA:C1C	2.45	0.47
6:h:94:CYS:SG	26:h:614:DD6:C2	3.03	0.47
24:B:807:CLA:HBB	24:B:808:CLA:HMB3	1.97	0.47
20:L:38:ARG:NH2	20:L:49:GLU:OE1	2.48	0.47
1:1:74:TRP:CZ3	24:1:305:CLA:HAA1	2.49	0.46
24:7:602:CLA:H2A	24:7:602:CLA:CED	2.41	0.46
24:1:303:CLA:HMA2	26:1:312:DD6:C13	2.45	0.46
3:3:72:ARG:NH1	3:3:75:GLU:OE1	2.48	0.46
24:6:603:CLA:HMD3	24:6:607:CLA:HBD	1.98	0.46
8:8:61:ILE:CG2	8:8:76:TRP:HB2	2.46	0.46
10:c:49:ILE:HG12	24:c:601:CLA:HMA3	1.98	0.46
25:k:316:BCR:H11C	25:k:316:BCR:H341	1.75	0.46
25:1:314:BCR:H382	25:1:314:BCR:H23C	1.97	0.46
6:6:185:GLU:OE1	24:6:608:CLA:C1B	2.64	0.46
6:h:144:ALA:O	6:h:147:THR:OG1	2.21	0.46
9:k:141:LEU:HD21	26:k:315:DD6:C28	2.45	0.46
9:k:148:THR:C	9:k:150:PRO:HD2	2.40	0.46
13:B:594:TRP:HB2	24:B:833:CLA:HMC1	1.96	0.46
24:4:611:CLA:C4C	25:4:618:BCR:H17C	2.45	0.46
7:7:76:VAL:HG12	24:7:602:CLA:CGD	2.45	0.46
9:k:132:GLY:N	9:k:133:PRO:CD	2.79	0.46
8:8:60:VAL:HG11	24:8:203:CLA:HMB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:358:GLY:HA2	12:A:395:GLY:HA2	1.98	0.46
20:L:116:LEU:HD11	20:L:125:PHE:CB	2.46	0.46
24:1:301:CLA:H71	25:1:314:BCR:H363	1.97	0.46
24:3:305:CLA:HHC	24:3:305:CLA:HBB1	1.97	0.46
25:A:845:BCR:H11C	25:A:845:BCR:H341	1.74	0.46
24:B:825:CLA:H3A	24:B:825:CLA:CGA	2.44	0.46
4:4:94:ASP:OD1	4:4:95:THR:N	2.48	0.46
9:9:95:LEU:HD21	26:9:315:DD6:C30	2.46	0.46
6:h:70:ASP:OD1	6:h:74:PHE:N	2.48	0.46
8:8:160:GLY:HA2	24:8:209:CLA:HBC3	1.97	0.46
9:9:85:TYR:HB2	24:9:301:CLA:HMD3	1.98	0.46
24:B:835:CLA:O1D	24:B:835:CLA:H2A	2.16	0.46
2:2:182:THR:O	2:2:183:ILE:C	2.59	0.46
24:7:612:CLA:H3A	24:7:612:CLA:HBA2	1.69	0.46
11:t:106:VAL:O	11:t:110:PHE:N	2.49	0.46
11:t:149:GLU:OE1	24:t:305:CLA:C1B	2.64	0.46
2:2:183:ILE:CD1	24:2:209:CLA:CMD	2.94	0.45
4:4:141:ASP:OD1	4:4:141:ASP:N	2.49	0.45
25:7:617:BCR:H351	25:7:617:BCR:H15C	1.70	0.45
24:A:802:CLA:CGA	24:A:802:CLA:H3A	2.47	0.45
24:B:808:CLA:C1A	24:B:808:CLA:CGA	2.94	0.45
24:B:838:CLA:HMC3	24:R:103:CLA:H3A	1.98	0.45
1:1:194:LEU:HD12	25:1:310:BCR:H343	1.98	0.45
10:c:69:ASP:OD1	10:c:72:GLY:N	2.49	0.45
24:A:818:CLA:C20	24:A:826:CLA:H3A	2.45	0.45
13:B:178:HIS:CD2	24:B:812:CLA:NB	2.84	0.45
2:2:96:GLU:C	2:2:98:VAL:H	2.24	0.45
24:4:608:CLA:C5	24:4:609:CLA:HMC3	2.46	0.45
9:k:149:ALA:O	9:k:152:THR:HG22	2.17	0.45
12:A:569:ARG:NH1	24:A:829:CLA:O1D	2.50	0.45
24:A:829:CLA:O2D	24:A:829:CLA:H2A	2.15	0.45
5:5:180:LEU:HA	5:5:183:ILE:HG22	1.98	0.45
24:6:611:CLA:HBA2	24:6:611:CLA:H3A	1.73	0.45
8:8:140:VAL:HG12	8:8:143:MET:H	1.80	0.45
24:A:818:CLA:HBA2	24:A:818:CLA:H3A	1.80	0.45
27:1:316:LMT:H62	25:c:615:BCR:H17C	1.99	0.45
7:7:91:VAL:HG23	7:7:193:LEU:HD12	1.97	0.45
9:9:201:ILE:HD13	25:9:316:BCR:C22	2.47	0.45
14:C:14:CYS:O	14:C:15:THR:OG1	2.24	0.45
25:F:204:BCR:H11C	25:F:204:BCR:H341	1.76	0.45
28:1:318:LHG:H321	28:1:318:LHG:H292	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:9:316:BCR:H371	25:9:316:BCR:H24C	1.82	0.45
9:k:152:THR:HG23	9:k:153:TRP:N	2.31	0.45
12:A:259:VAL:N	12:A:260:PRO:HD2	2.32	0.45
12:A:321:GLU:OE1	12:A:321:GLU:N	2.49	0.45
3:3:67:THR:CG2	3:3:71:TYR:CZ	3.00	0.45
9:9:211:PHE:CD1	9:9:212:PRO:HD3	2.51	0.45
9:k:149:ALA:N	9:k:150:PRO:CD	2.80	0.45
9:k:165:PHE:O	24:k:307:CLA:OBD	2.33	0.45
9:k:149:ALA:O	9:k:150:PRO:C	2.60	0.45
9:k:149:ALA:N	9:k:150:PRO:HD2	2.32	0.45
12:A:747:SER:C	12:A:748:VAL:HG23	2.42	0.45
14:C:9:ASP:OD1	14:C:9:ASP:N	2.49	0.45
25:J:101:BCR:H341	25:J:101:BCR:H11C	1.83	0.45
6:6:94:CYS:SG	6:6:193:MET:HA	2.56	0.45
24:6:601:CLA:O1D	24:6:601:CLA:H2A	2.17	0.45
9:9:200:MET:HG3	29:9:312:A1L1G:C17	2.46	0.45
13:B:464:GLN:NE2	24:B:833:CLA:OBD	2.43	0.45
24:F:202:CLA:O1D	24:F:202:CLA:H2A	2.16	0.45
28:L:201:LHG:O3	28:L:201:LHG:O1	2.09	0.45
24:1:305:CLA:HHC	24:1:305:CLA:CBB	2.46	0.45
7:7:76:VAL:HG12	24:7:602:CLA:CBD	2.48	0.45
9:9:132:GLY:N	9:9:133:PRO:CD	2.79	0.45
10:c:66:VAL:CG2	24:c:602:CLA:HMD3	2.46	0.45
25:k:316:BCR:H351	25:k:316:BCR:H15C	1.68	0.45
24:1:304:CLA:O1D	24:1:304:CLA:H2A	2.18	0.44
2:2:84:TRP:CE3	2:2:177:MET:HB3	2.52	0.44
24:B:804:CLA:H12	21:M:25:GLY:C	2.42	0.44
5:5:116:ASP:OD1	5:5:116:ASP:N	2.48	0.44
5:5:136:VAL:O	5:5:139:LEU:HG	2.17	0.44
7:7:80:GLU:N	24:7:602:CLA:O1D	2.50	0.44
25:9:316:BCR:H341	25:9:316:BCR:H11C	1.67	0.44
24:B:831:CLA:HHC	24:B:831:CLA:HBB1	1.98	0.44
2:2:183:ILE:HD13	24:2:209:CLA:HMD3	1.96	0.44
5:5:75:LEU:O	5:5:75:LEU:HG	2.17	0.44
25:B:843:BCR:H351	25:B:843:BCR:H15C	1.66	0.44
22:R:57:THR:HG22	22:R:57:THR:O	2.17	0.44
4:4:161:LEU:HD13	24:4:612:CLA:HMB3	2.00	0.44
24:4:608:CLA:C5	24:4:609:CLA:CMC	2.96	0.44
8:8:167:ILE:O	8:8:169:GLY:N	2.50	0.44
9:9:125:HIS:CG	25:9:316:BCR:H393	2.53	0.44
9:9:191:ARG:HH22	24:9:301:CLA:HBA2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:207:HIS:C	10:c:209:LEU:H	2.25	0.44
11:t:67:SER:OG	24:t:307:CLA:HMA2	2.18	0.44
13:B:34:HIS:NE2	24:B:804:CLA:HED1	2.33	0.44
13:B:498:LEU:HA	13:B:501:ILE:HG22	1.98	0.44
20:L:61:PRO:HA	24:L:205:CLA:HMB2	2.00	0.44
4:4:218:THR:O	4:4:222:LEU:HD13	2.18	0.44
24:9:311:CLA:OBD	25:9:316:BCR:H402	2.18	0.44
6:6:55:LYS:O	6:6:56:PRO:C	2.61	0.44
13:B:87:ILE:HG23	13:B:113:VAL:CG2	2.48	0.44
15:D:35:SER:OG	15:D:37:LYS:O	2.35	0.44
25:I:102:BCR:HC8	25:I:102:BCR:H311	2.00	0.44
19:J:39:PHE:HA	25:J:101:BCR:H361	1.98	0.44
1:1:187:LEU:HD22	24:1:307:CLA:HMD2	1.98	0.44
24:4:611:CLA:C1D	25:4:618:BCR:H19C	2.47	0.44
6:6:181:LEU:HD12	6:6:181:LEU:HA	1.76	0.44
24:B:802:CLA:H2A	24:B:802:CLA:O2D	2.17	0.44
17:F:26:VAL:HG11	17:F:96:ILE:HD12	1.99	0.44
25:A:844:BCR:H15C	25:A:844:BCR:H351	1.78	0.44
23:S:97:UNK:O	23:S:98:UNK:C	2.65	0.44
24:8:201:CLA:H2A	24:8:201:CLA:O2D	2.16	0.44
24:A:830:CLA:H3A	24:A:830:CLA:HBA1	1.56	0.44
17:F:182:VAL:HG12	17:F:183:SER:H	1.81	0.44
1:1:82:GLY:CA	26:1:311:DD6:C41	2.96	0.43
7:7:176:GLN:O	7:7:180:ILE:HG12	2.18	0.43
24:A:853:CLA:HHB	13:B:685:THR:HG22	2.00	0.43
4:4:214:SER:OG	25:4:618:BCR:C16	2.66	0.43
6:6:94:CYS:SG	6:6:192:ALA:O	2.76	0.43
24:k:301:CLA:CGA	24:k:301:CLA:H3A	2.48	0.43
20:L:145:LEU:HD22	28:L:201:LHG:H102	1.99	0.43
24:3:308:CLA:CBB	29:3:310:A1L1G:C35	2.96	0.43
24:B:829:CLA:H92	24:B:829:CLA:H62	1.68	0.43
24:B:832:CLA:HMC1	24:B:832:CLA:HBC3	1.98	0.43
25:I:102:BCR:H392	25:I:102:BCR:H23C	2.00	0.43
21:M:11:LEU:HB3	25:M:101:BCR:H21C	1.99	0.43
1:1:145:PHE:HB2	20:L:130:LEU:HD22	2.00	0.43
25:9:316:BCR:H351	25:9:316:BCR:H15C	1.77	0.43
25:t:312:BCR:H11C	25:t:312:BCR:H341	1.84	0.43
9:k:90:LEU:O	9:k:94:ARG:HG2	2.18	0.43
9:k:136:GLN:NE2	9:k:140:TRP:CD1	2.86	0.43
24:A:847:CLA:O1D	24:A:847:CLA:H2A	2.18	0.43
1:1:77:ARG:NE	1:1:181:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:96:GLU:HG2	2:2:96:GLU:O	2.18	0.43
7:7:80:GLU:HB2	24:7:602:CLA:O1D	2.18	0.43
24:A:834:CLA:H2A	24:A:834:CLA:O2D	2.19	0.43
24:B:846:CLA:HBA2	24:B:846:CLA:H3A	1.81	0.43
1:1:145:PHE:HB2	20:L:130:LEU:CD2	2.48	0.43
3:3:137:ILE:HD13	20:L:29:ALA:CB	2.48	0.43
24:7:610:CLA:HBC3	26:7:615:DD6:C4	2.48	0.43
9:9:138:LEU:HB2	24:9:305:CLA:HMB2	2.00	0.43
11:t:75:ALA:O	11:t:76:THR:C	2.61	0.43
12:A:448:HIS:O	12:A:452:LEU:HG	2.18	0.43
24:B:805:CLA:HBA1	24:B:805:CLA:H3A	1.85	0.43
4:4:100:ARG:HH22	4:4:203:VAL:HG21	1.83	0.43
25:B:842:BCR:H24C	25:B:842:BCR:H371	1.59	0.43
4:4:81:ARG:O	4:4:85:ARG:HB3	2.19	0.43
7:7:143:MET:HG2	17:F:159:ILE:HG21	2.00	0.43
13:B:32:GLU:OE1	13:B:32:GLU:N	2.43	0.43
25:1:310:BCR:H11C	25:1:310:BCR:H341	1.83	0.43
3:3:178:LEU:HD13	26:3:312:DD6:C10	2.49	0.43
24:4:602:CLA:H102	26:4:615:DD6:C21	2.49	0.43
25:4:618:BCR:H24C	25:4:618:BCR:H371	1.84	0.43
8:8:36:HIS:CG	8:8:37:PRO:HD2	2.53	0.43
6:h:143:GLU:O	6:h:147:THR:HG23	2.18	0.43
24:A:853:CLA:HHB	13:B:685:THR:CG2	2.48	0.43
13:B:53:HIS:CE1	24:B:805:CLA:HMA2	2.53	0.43
13:B:76:GLN:OE1	13:B:76:GLN:N	2.50	0.43
1:1:187:LEU:CD2	24:1:307:CLA:HMD2	2.48	0.43
3:3:123:ILE:CG1	24:3:304:CLA:HAB	2.40	0.43
6:6:93:ILE:HD12	24:6:607:CLA:HMD2	2.00	0.43
9:9:116:TYR:HB3	24:9:303:CLA:HMB2	2.01	0.43
24:9:302:CLA:HBC2	24:9:305:CLA:HBC2	2.01	0.43
24:A:817:CLA:CGA	24:A:817:CLA:H3A	2.49	0.43
24:3:304:CLA:HMD1	24:L:205:CLA:HAA2	2.01	0.42
24:4:602:CLA:HBA2	24:4:602:CLA:H3A	1.75	0.42
8:8:170:SER:O	8:8:171:VAL:C	2.61	0.42
24:9:308:CLA:HHC	24:9:308:CLA:CBB	2.49	0.42
10:c:70:PRO:HD2	26:c:613:DD6:O4	2.19	0.42
13:B:636:ASN:HB2	13:B:637:PRO:HD2	2.00	0.42
28:I:103:LHG:O9	20:L:98:LYS:NZ	2.48	0.42
3:3:193:ASN:OD1	3:3:193:ASN:C	2.62	0.42
6:6:98:VAL:CG2	6:6:196:PHE:HB2	2.49	0.42
6:h:167:ASP:N	6:h:167:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:595:TRP:HE1	24:B:803:CLA:C1D	2.31	0.42
25:2:211:BCR:H15C	25:2:211:BCR:H351	1.77	0.42
4:4:107:CYS:SG	4:4:108:ARG:N	2.92	0.42
25:4:618:BCR:H351	25:4:618:BCR:H15C	1.77	0.42
7:7:76:VAL:HG12	24:7:602:CLA:OBD	2.19	0.42
7:7:157:ASP:O	24:7:607:CLA:OBD	2.38	0.42
11:t:98:MET:HA	11:t:101:ILE:HG22	2.00	0.42
9:k:150:PRO:O	9:k:154:ASN:OD1	2.37	0.42
12:A:702:HIS:HB3	12:A:707:VAL:O	2.18	0.42
13:B:494:LEU:N	13:B:495:PRO:HD2	2.34	0.42
25:1:310:BCR:H15C	25:1:310:BCR:H351	1.84	0.42
4:4:71:PHE:O	4:4:72:ASP:HB3	2.18	0.42
19:J:22:THR:HA	19:J:25:PHE:CE2	2.55	0.42
1:1:168:LEU:HA	24:1:301:CLA:HMD3	2.01	0.42
5:5:40:SER:C	5:5:41:LEU:HD12	2.44	0.42
13:B:344:ILE:O	13:B:348:THR:HG23	2.20	0.42
24:B:827:CLA:H2A	24:B:827:CLA:O2D	2.19	0.42
7:7:183:GLY:O	7:7:187:MET:HG3	2.19	0.42
24:c:601:CLA:O1D	24:c:601:CLA:H2A	2.19	0.42
11:t:96:ILE:HD12	24:t:305:CLA:HMD2	2.02	0.42
12:A:426:ARG:HD3	24:A:830:CLA:OBD	2.19	0.42
24:B:803:CLA:CGA	24:B:803:CLA:H3A	2.50	0.42
24:B:815:CLA:O1D	24:B:815:CLA:H2A	2.20	0.42
24:B:824:CLA:H152	25:B:843:BCR:H17C	2.00	0.42
25:L:202:BCR:H312	24:L:204:CLA:C1C	2.49	0.42
23:S:70:UNK:O	23:S:74:UNK:N	2.52	0.42
8:8:94:VAL:O	8:8:98:LEU:HG	2.20	0.42
9:k:86:ARG:NH2	24:k:301:CLA:O1D	2.48	0.42
24:k:304:CLA:CMB	26:k:315:DD6:C3	2.96	0.42
12:A:396:GLY:HA3	12:A:600:LEU:HD11	2.00	0.42
12:A:600:LEU:O	12:A:604:LEU:HG	2.20	0.42
24:B:805:CLA:H3A	24:B:805:CLA:CGA	2.49	0.42
17:F:120:TRP:O	17:F:121:ILE:C	2.62	0.42
6:h:202:GLN:HE21	6:h:202:GLN:HB3	1.64	0.42
11:t:216:ALA:O	11:t:219:GLN:N	2.43	0.42
25:B:841:BCR:H11C	25:B:841:BCR:H341	1.91	0.42
20:L:85:LEU:O	20:L:89:LEU:HG	2.19	0.42
3:3:179:ALA:O	3:3:183:LEU:HG	2.19	0.42
24:8:201:CLA:HMC1	26:8:211:DD6:C9	2.50	0.42
12:A:737:THR:HB	24:A:801:CLA:CED	2.50	0.42
24:A:830:CLA:C1A	28:A:842:LHG:HC91	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:406:ASN:OD1	13:B:407:VAL:N	2.52	0.42
24:1:317:CLA:HMB2	24:B:848:CLA:C9	2.50	0.41
8:8:138:ALA:O	8:8:141:ASN:N	2.53	0.41
24:B:829:CLA:HBB1	24:B:829:CLA:HMB3	2.02	0.41
24:1:304:CLA:C4B	26:1:311:DD6:C33	2.98	0.41
3:3:67:THR:HG22	3:3:71:TYR:CZ	2.55	0.41
24:5:607:CLA:HBA2	26:5:608:DD6:C9	2.50	0.41
6:6:94:CYS:SG	6:6:196:PHE:HB3	2.59	0.41
7:7:89:LEU:HD21	24:7:607:CLA:HMC3	2.02	0.41
24:k:305:CLA:O2A	24:k:305:CLA:H2A	2.18	0.41
13:B:182:LEU:HD13	24:B:812:CLA:HHB	2.01	0.41
25:1:314:BCR:H15C	25:1:314:BCR:H351	1.83	0.41
5:5:185:ASN:ND2	24:5:607:CLA:NA	2.64	0.41
6:6:67:VAL:HG22	24:6:602:CLA:HMD1	2.01	0.41
24:6:606:CLA:HHC	24:6:606:CLA:CBB	2.49	0.41
6:h:57:GLU:O	6:h:58:LYS:HB2	2.18	0.41
20:L:116:LEU:HD11	20:L:125:PHE:HB2	2.02	0.41
5:5:112:LYS:H	5:5:117:LEU:HD12	1.85	0.41
7:7:122:GLN:HG2	26:7:618:DD6:O4	2.19	0.41
24:c:602:CLA:CGA	24:c:602:CLA:H3A	2.50	0.41
12:A:331:THR:HA	24:A:830:CLA:OBD	2.21	0.41
13:B:199:ILE:HB	13:B:200:PRO:HD3	2.02	0.41
24:B:811:CLA:CGA	24:B:811:CLA:C1A	2.98	0.41
25:B:840:BCR:H383	25:B:840:BCR:H23C	2.02	0.41
2:2:148:LEU:O	2:2:149:TYR:HB3	2.21	0.41
6:6:98:VAL:HG11	26:6:613:DD6:C8	2.51	0.41
6:h:96:LEU:HD13	24:h:608:CLA:HMC1	2.03	0.41
27:A:854:LMT:O3'	27:A:854:LMT:O6B	2.33	0.41
1:1:98:ILE:CG2	1:1:125:GLU:HA	2.51	0.41
3:3:137:ILE:HD13	20:L:29:ALA:HB3	2.01	0.41
24:3:304:CLA:HHC	24:3:304:CLA:HBB1	2.02	0.41
4:4:118:LEU:O	4:4:122:MET:HG2	2.20	0.41
8:8:138:ALA:O	8:8:139:ASP:C	2.64	0.41
24:c:603:CLA:H3A	24:c:603:CLA:HBA1	1.79	0.41
24:t:302:CLA:O1D	24:t:302:CLA:H2A	2.20	0.41
4:4:40:LYS:C	4:4:42:ILE:H	2.28	0.41
25:c:615:BCR:H15C	25:c:615:BCR:H351	1.86	0.41
25:A:844:BCR:H11C	25:A:844:BCR:H341	1.90	0.41
13:B:108:GLY:O	13:B:109:ALA:HB3	2.20	0.41
1:1:125:GLU:CA	1:1:128:VAL:HG12	2.50	0.41
6:6:110:LEU:HB3	6:6:111:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:46:SER:O	10:c:47:LYS:C	2.64	0.41
12:A:157:TYR:O	12:A:161:ILE:HG12	2.21	0.41
25:A:843:BCR:H383	25:A:843:BCR:H23C	2.02	0.41
13:B:344:ILE:CG1	24:B:822:CLA:H42	2.51	0.41
24:B:803:CLA:H13	25:I:101:BCR:H271	2.03	0.41
2:2:97:ASP:O	2:2:98:VAL:CG2	2.69	0.41
24:2:206:CLA:HBA2	24:2:206:CLA:H3A	1.76	0.41
6:6:87:GLU:OE1	24:6:602:CLA:C4A	2.69	0.41
7:7:124:MET:HA	7:7:127:ILE:HG22	2.02	0.41
24:7:610:CLA:HBA1	24:7:610:CLA:H3A	1.84	0.41
24:c:610:CLA:H3A	24:c:610:CLA:HBA2	1.86	0.41
12:A:92:GLY:HA2	12:A:96:SER:HB3	2.01	0.41
12:A:581:CYS:HB2	13:B:667:TRP:HB3	2.02	0.41
12:A:696:GLU:CD	16:E:44:TYR:HH	2.28	0.41
13:B:276:HIS:CE1	24:B:817:CLA:HMB2	2.56	0.41
13:B:410:ARG:NE	24:B:828:CLA:OBD	2.42	0.41
13:B:546:LEU:HD23	13:B:570:ILE:HD12	2.03	0.41
13:B:720:THR:HG23	24:B:802:CLA:O1D	2.20	0.41
15:D:77:LYS:C	15:D:78:ILE:HG12	2.45	0.41
15:D:96:HIS:CB	15:D:97:PRO:HD3	2.50	0.41
4:4:92:VAL:HG21	4:4:170:ALA:O	2.20	0.41
24:4:613:CLA:H2A	24:4:613:CLA:O1D	2.20	0.41
24:9:301:CLA:HBB1	24:9:301:CLA:HMB3	2.02	0.41
24:k:308:CLA:C3D	24:k:309:CLA:HMA3	2.51	0.41
8:8:90:GLY:HA3	24:8:204:CLA:HBC3	2.02	0.40
16:E:9:ASN:OD1	16:E:11:ARG:N	2.45	0.40
2:2:118:PHE:HE1	26:2:212:DD6:C9	2.34	0.40
26:9:317:DD6:C11	24:h:612:CLA:HBB2	2.51	0.40
11:t:98:MET:HA	11:t:209:ALA:HB1	2.03	0.40
13:B:87:ILE:HG23	13:B:113:VAL:HG22	2.03	0.40
17:F:119:GLY:O	17:F:120:TRP:C	2.63	0.40
17:F:149:LEU:O	17:F:153:ILE:HG12	2.21	0.40
20:L:60:GLY:N	20:L:61:PRO:HD2	2.35	0.40
4:4:180:ASP:OD1	24:4:607:CLA:HED3	2.22	0.40
5:5:102:ILE:HG13	5:5:102:ILE:O	2.20	0.40
7:7:89:LEU:CD2	24:7:607:CLA:HMC3	2.52	0.40
9:9:198:SER:OG	25:9:316:BCR:C16	2.69	0.40
9:9:206:LEU:HD23	9:9:206:LEU:HA	1.90	0.40
6:h:110:LEU:HB3	6:h:111:PRO:HD2	2.04	0.40
12:A:747:SER:O	12:A:748:VAL:CG2	2.68	0.40
24:A:802:CLA:H171	31:A:839:PQN:H251	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:847:CLA:HHC	24:B:847:CLA:CBB	2.51	0.40
25:R:102:BCR:HC8	25:R:102:BCR:C33	2.51	0.40
3:3:78:HIS:HB3	3:3:177:MET:SD	2.62	0.40
4:4:42:ILE:O	4:4:42:ILE:HG23	2.22	0.40
4:4:216:ILE:HG13	26:4:614:DD6:C21	2.52	0.40
6:6:182:GLU:O	6:6:183:LEU:C	2.64	0.40
6:h:78:VAL:HG12	6:h:79:ASN:N	2.36	0.40
25:B:842:BCR:H341	25:B:842:BCR:H11C	1.79	0.40
20:L:122:TRP:O	20:L:126:THR:HG23	2.21	0.40
27:1:316:LMT:H2'	25:c:615:BCR:H393	2.03	0.40
24:2:202:CLA:O1A	24:2:202:CLA:H3A	2.21	0.40
5:5:147:ILE:O	5:5:151:ARG:HG2	2.21	0.40
24:t:305:CLA:O2D	24:t:305:CLA:H2A	2.22	0.40
25:A:846:BCR:H23C	25:A:846:BCR:H403	2.02	0.40
24:B:804:CLA:H2A	24:B:804:CLA:CGD	2.51	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	174/220 (79%)	169 (97%)	5 (3%)	0	100	100
2	2	135/194 (70%)	121 (90%)	13 (10%)	1 (1%)	18	45
3	3	156/205 (76%)	147 (94%)	9 (6%)	0	100	100
4	4	186/231 (80%)	172 (92%)	14 (8%)	0	100	100
5	5	165/216 (76%)	153 (93%)	12 (7%)	0	100	100
6	6	161/212 (76%)	148 (92%)	12 (8%)	1 (1%)	21	48
6	h	163/212 (77%)	154 (94%)	8 (5%)	1 (1%)	21	48
7	7	164/207 (79%)	149 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	8	159/179 (89%)	146 (92%)	13 (8%)	0	100	100
9	9	147/215 (68%)	142 (97%)	5 (3%)	0	100	100
9	k	152/215 (71%)	144 (95%)	7 (5%)	1 (1%)	18	45
10	c	163/210 (78%)	154 (94%)	9 (6%)	0	100	100
11	t	157/228 (69%)	143 (91%)	14 (9%)	0	100	100
12	A	739/749 (99%)	715 (97%)	24 (3%)	0	100	100
13	B	731/734 (100%)	706 (97%)	25 (3%)	0	100	100
14	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
15	D	130/139 (94%)	120 (92%)	10 (8%)	0	100	100
16	E	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	7	23
17	F	159/185 (86%)	153 (96%)	5 (3%)	1 (1%)	21	48
18	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
19	J	38/42 (90%)	38 (100%)	0	0	100	100
20	L	133/149 (89%)	130 (98%)	3 (2%)	0	100	100
21	M	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
22	R	79/87 (91%)	77 (98%)	2 (2%)	0	100	100
All	All	4286/5037 (85%)	4069 (95%)	211 (5%)	6 (0%)	49	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	6	56	PRO
16	E	31	ILE
9	k	119	VAL
6	h	117	VAL
17	F	26	VAL
2	2	50	LYS

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	137/169 (81%)	137 (100%)	0	100	100
2	2	112/149 (75%)	110 (98%)	2 (2%)	51	80
3	3	121/152 (80%)	121 (100%)	0	100	100
4	4	143/173 (83%)	142 (99%)	1 (1%)	76	91
5	5	130/162 (80%)	130 (100%)	0	100	100
6	6	129/159 (81%)	125 (97%)	4 (3%)	35	69
6	h	131/159 (82%)	131 (100%)	0	100	100
7	7	137/163 (84%)	135 (98%)	2 (2%)	57	83
8	8	127/141 (90%)	126 (99%)	1 (1%)	73	90
9	9	125/168 (74%)	124 (99%)	1 (1%)	73	90
9	k	128/168 (76%)	127 (99%)	1 (1%)	73	90
10	c	129/156 (83%)	128 (99%)	1 (1%)	73	90
11	t	133/178 (75%)	132 (99%)	1 (1%)	73	90
12	A	603/609 (99%)	601 (100%)	2 (0%)	86	95
13	B	597/598 (100%)	597 (100%)	0	100	100
14	C	66/67 (98%)	66 (100%)	0	100	100
15	D	110/117 (94%)	110 (100%)	0	100	100
16	E	55/56 (98%)	55 (100%)	0	100	100
17	F	138/159 (87%)	138 (100%)	0	100	100
18	I	28/31 (90%)	28 (100%)	0	100	100
19	J	32/34 (94%)	32 (100%)	0	100	100
20	L	108/119 (91%)	106 (98%)	2 (2%)	50	79
21	M	25/25 (100%)	25 (100%)	0	100	100
22	R	68/73 (93%)	67 (98%)	1 (2%)	57	83
All	All	3512/3985 (88%)	3493 (100%)	19 (0%)	78	93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	102	HIS
2	2	144	ASP
4	4	205	ASN
6	6	170	ASN
6	6	181	LEU
6	6	185	GLU

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Mol	Chain	Res	Type
6	6	188	ASN
7	7	107	TYR
7	7	195	HIS
8	8	165	HIS
9	9	189	ASN
10	c	183	GLN
11	t	167	TYR
9	k	106	PRO
12	A	96	SER
12	A	596	MET
20	L	16	HIS
20	L	91	LEU
22	R	76	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	198	HIS
2	2	72	HIS
2	2	73	ASN
2	2	132	HIS
2	2	166	ASN
3	3	166	GLN
5	5	120	GLN
6	6	184	ASN
6	6	188	ASN
7	7	202	HIS
8	8	66	HIS
9	9	92	HIS
6	h	123	HIS
6	h	184	ASN
6	h	202	GLN
10	c	83	GLN
10	c	187	ASN
10	c	207	HIS
11	t	148	HIS
9	k	70	ASN
9	k	203	GLN
12	A	197	HIS
12	A	214	GLN
12	A	421	ASN
12	A	486	ASN

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Mol	Chain	Res	Type
13	B	158	GLN
13	B	241	GLN
13	B	277	HIS
13	B	432	HIS
13	B	598	HIS
13	B	627	ASN
16	E	51	ASN
22	R	48	ASN
22	R	85	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](#)

338 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	$\# Z > 2$
26	DD6	7	615	-	40,45,45	1.21	8 (20%)	51,67,67	1.86	10 (19%)
29	A1L1G	2	213	-	40,47,47	1.16	8 (20%)	49,71,71	1.03	4 (8%)
24	CLA	9	304	9	50,54,73	1.34	6 (12%)	59,90,113	1.40	7 (11%)
27	LMT	h	617	-	29,29,36	0.73	0	40,40,47	0.86	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	4	608	-	54,58,73	1.31	5 (9%)	64,95,113	1.36	8 (12%)
24	CLA	B	813	13	50,54,73	1.34	5 (10%)	59,90,113	1.29	4 (6%)
24	CLA	A	817	12	69,73,73	1.15	6 (8%)	82,113,113	1.15	6 (7%)
25	BCR	F	204	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
26	DD6	3	311	-	40,45,45	1.20	8 (20%)	51,67,67	1.68	9 (17%)
24	CLA	6	610	6	50,54,73	1.36	5 (10%)	59,90,113	1.08	2 (3%)
24	CLA	2	203	-	54,58,73	1.30	5 (9%)	64,95,113	1.19	6 (9%)
24	CLA	7	608	-	49,53,73	1.39	6 (12%)	58,89,113	1.31	4 (6%)
24	CLA	1	307	1	49,53,73	1.39	5 (10%)	58,89,113	1.21	4 (6%)
24	CLA	2	209	-	50,54,73	1.36	5 (10%)	59,90,113	1.17	3 (5%)
24	CLA	9	303	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	5 (8%)
25	BCR	A	845	-	40,40,41	0.76	1 (2%)	52,54,56	2.24	18 (34%)
24	CLA	F	201	-	69,73,73	1.16	6 (8%)	82,113,113	1.12	6 (7%)
32	SF4	A	858	12,13	0,12,12	-	-	-	-	-
24	CLA	2	208	-	50,54,73	1.38	5 (10%)	59,90,113	1.21	3 (5%)
24	CLA	A	806	12	69,73,73	1.17	5 (7%)	82,113,113	1.10	5 (6%)
24	CLA	c	607	10	50,54,73	1.30	4 (8%)	59,90,113	1.27	7 (11%)
24	CLA	A	809	12	50,54,73	1.33	6 (12%)	59,90,113	1.20	5 (8%)
24	CLA	B	824	13	69,73,73	1.18	6 (8%)	82,113,113	1.26	8 (9%)
24	CLA	B	838	28	69,73,73	1.16	7 (10%)	82,113,113	1.27	7 (8%)
24	CLA	t	306	11	49,53,73	1.37	5 (10%)	58,89,113	1.25	4 (6%)
24	CLA	8	204	8	49,53,73	1.39	6 (12%)	58,89,113	1.30	5 (8%)
24	CLA	8	208	8	49,53,73	1.36	5 (10%)	58,89,113	1.34	5 (8%)
27	LMT	1	316	-	36,36,36	0.68	0	47,47,47	0.95	2 (4%)
24	CLA	4	604	-	50,54,73	1.37	6 (12%)	59,90,113	1.14	3 (5%)
24	CLA	B	818	-	69,73,73	1.16	6 (8%)	82,113,113	1.09	7 (8%)
27	LMT	A	851	-	26,26,36	0.80	0	37,37,47	1.06	5 (13%)
24	CLA	8	209	-	45,49,73	1.40	5 (11%)	54,84,113	1.24	4 (7%)
26	DD6	k	314	-	40,45,45	1.25	9 (22%)	51,67,67	1.84	8 (15%)
24	CLA	7	611	7	50,54,73	1.35	6 (12%)	59,90,113	1.21	3 (5%)
24	CLA	9	302	9	50,54,73	1.34	9 (18%)	59,90,113	1.37	6 (10%)
24	CLA	B	816	13	69,73,73	1.15	6 (8%)	82,113,113	1.24	7 (8%)
26	DD6	3	313	-	40,45,45	1.22	8 (20%)	51,67,67	1.62	10 (19%)
24	CLA	c	611	10	45,49,73	1.41	6 (13%)	54,84,113	1.27	4 (7%)
24	CLA	5	604	5	50,54,73	1.35	5 (10%)	59,90,113	1.16	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	821	13	57,61,73	1.27	6 (10%)	67,98,113	1.23	9 (13%)
24	CLA	B	819	13	50,54,73	1.36	6 (12%)	59,90,113	1.18	3 (5%)
24	CLA	B	834	13	69,73,73	1.15	5 (7%)	82,113,113	1.08	4 (4%)
24	CLA	B	804	13	69,73,73	1.18	6 (8%)	82,113,113	1.31	12 (14%)
24	CLA	8	203	-	54,58,73	1.32	7 (12%)	64,95,113	1.28	7 (10%)
26	DD6	R	105	-	40,45,45	1.28	10 (25%)	51,67,67	1.84	11 (21%)
24	CLA	3	308	3	50,54,73	1.34	8 (16%)	59,90,113	1.26	5 (8%)
24	CLA	5	603	5	49,53,73	1.39	5 (10%)	58,89,113	1.26	4 (6%)
24	CLA	c	601	10	47,51,73	1.39	6 (12%)	55,86,113	1.23	5 (9%)
26	DD6	7	616	-	40,45,45	1.25	7 (17%)	51,67,67	1.74	9 (17%)
24	CLA	6	607	6	50,54,73	1.35	6 (12%)	59,90,113	1.18	5 (8%)
26	DD6	6	617	-	40,45,45	1.27	10 (25%)	51,67,67	1.67	9 (17%)
26	DD6	h	613	-	40,45,45	1.24	8 (20%)	51,67,67	1.62	9 (17%)
24	CLA	4	607	4	50,54,73	1.34	7 (14%)	59,90,113	1.21	5 (8%)
30	LMG	A	855	-	38,38,55	1.08	2 (5%)	46,46,63	1.09	2 (4%)
24	CLA	A	840	28	69,73,73	1.15	6 (8%)	82,113,113	1.17	7 (8%)
26	DD6	2	212	-	40,45,45	1.22	8 (20%)	51,67,67	1.68	8 (15%)
25	BCR	M	101	-	41,41,41	0.68	0	56,56,56	2.14	14 (25%)
24	CLA	h	609	-	50,54,73	1.36	5 (10%)	59,90,113	1.18	4 (6%)
24	CLA	9	301	9	50,54,73	1.38	6 (12%)	59,90,113	1.33	6 (10%)
24	CLA	L	204	20	69,73,73	1.16	6 (8%)	82,113,113	1.13	7 (8%)
24	CLA	B	808	13	69,73,73	1.15	8 (11%)	82,113,113	1.17	7 (8%)
24	CLA	L	203	20	59,63,73	1.25	6 (10%)	70,101,113	1.32	7 (10%)
28	LHG	1	318	-	42,42,48	0.98	3 (7%)	45,48,54	1.41	4 (8%)
24	CLA	4	611	-	50,54,73	1.35	5 (10%)	59,90,113	1.20	5 (8%)
26	DD6	t	311	-	40,45,45	1.24	8 (20%)	51,67,67	1.59	9 (17%)
24	CLA	B	835	13	51,55,73	1.33	7 (13%)	60,91,113	1.36	7 (11%)
24	CLA	6	604	-	50,54,73	1.35	6 (12%)	59,90,113	1.17	3 (5%)
24	CLA	9	309	9	50,54,73	1.35	5 (10%)	59,90,113	1.30	6 (10%)
26	DD6	9	317	-	40,45,45	1.21	6 (15%)	51,67,67	2.13	16 (31%)
24	CLA	h	605	6	50,54,73	1.36	6 (12%)	59,90,113	1.20	6 (10%)
25	BCR	k	316	-	41,41,41	0.65	0	56,56,56	2.33	20 (35%)
26	DD6	9	315	-	40,45,45	1.25	9 (22%)	51,67,67	1.77	11 (21%)
24	CLA	3	306	3	69,73,73	1.15	6 (8%)	82,113,113	1.09	4 (4%)
25	BCR	B	843	-	41,41,41	0.82	1 (2%)	56,56,56	2.37	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	c	613	-	40,45,45	1.21	8 (20%)	51,67,67	1.75	9 (17%)
24	CLA	2	204	2	64,68,73	1.21	5 (7%)	76,107,113	1.21	5 (6%)
25	BCR	B	849	-	41,41,41	0.62	0	56,56,56	2.27	21 (37%)
24	CLA	5	605	5	50,54,73	1.35	5 (10%)	59,90,113	1.21	4 (6%)
24	CLA	1	304	26	59,63,73	1.24	6 (10%)	70,101,113	1.08	5 (7%)
24	CLA	B	803	-	69,73,73	1.13	8 (11%)	82,113,113	1.30	5 (6%)
24	CLA	8	206	8	50,54,73	1.33	5 (10%)	59,90,113	1.20	4 (6%)
27	LMT	A	850	-	36,36,36	0.67	0	47,47,47	0.65	0
24	CLA	A	830	12	59,63,73	1.23	8 (13%)	70,101,113	1.73	10 (14%)
28	LHG	J	105	-	37,37,48	1.06	2 (5%)	40,43,54	1.12	4 (10%)
25	BCR	A	859	-	41,41,41	0.69	0	56,56,56	1.82	14 (25%)
24	CLA	9	310	9	50,54,73	1.36	6 (12%)	59,90,113	1.30	3 (5%)
24	CLA	A	811	12	50,54,73	1.34	6 (12%)	59,90,113	1.20	4 (6%)
26	DD6	k	313	-	40,45,45	1.22	8 (20%)	51,67,67	1.78	14 (27%)
24	CLA	1	309	1	48,53,73	1.38	6 (12%)	56,89,113	1.17	4 (7%)
24	CLA	h	611	6	45,49,73	1.37	7 (15%)	54,84,113	1.55	6 (11%)
24	CLA	t	310	-	50,54,73	1.36	6 (12%)	59,90,113	1.21	3 (5%)
24	CLA	4	601	4	45,50,73	1.40	7 (15%)	52,85,113	1.07	3 (5%)
24	CLA	B	829	13	69,73,73	1.14	8 (11%)	82,113,113	1.36	10 (12%)
26	DD6	8	211	-	40,45,45	1.21	8 (20%)	51,67,67	1.76	10 (19%)
24	CLA	9	307	9	50,54,73	1.31	6 (12%)	59,90,113	1.32	4 (6%)
26	DD6	6	614	-	40,45,45	1.25	8 (20%)	51,67,67	1.49	6 (11%)
24	CLA	c	604	-	50,54,73	1.35	5 (10%)	59,90,113	1.16	3 (5%)
24	CLA	t	309	-	50,54,73	1.36	5 (10%)	59,90,113	1.17	3 (5%)
30	LMG	t	314	-	34,34,55	1.12	2 (5%)	42,42,63	1.22	4 (9%)
24	CLA	2	206	2	50,54,73	1.34	5 (10%)	59,90,113	1.27	6 (10%)
28	LHG	A	849	-	40,40,48	1.03	2 (5%)	43,46,54	1.06	2 (4%)
24	CLA	B	817	13	69,73,73	1.15	5 (7%)	82,113,113	1.13	7 (8%)
24	CLA	B	823	-	68,72,73	1.16	6 (8%)	80,111,113	1.14	9 (11%)
24	CLA	A	813	12	69,73,73	1.16	7 (10%)	82,113,113	1.09	6 (7%)
24	CLA	t	307	-	50,54,73	1.34	5 (10%)	59,90,113	1.15	2 (3%)
24	CLA	h	612	-	49,53,73	1.38	6 (12%)	58,89,113	1.27	4 (6%)
24	CLA	4	613	4	50,54,73	1.35	6 (12%)	59,90,113	1.16	4 (6%)
25	BCR	I	101	-	41,41,41	0.77	2 (4%)	56,56,56	2.30	25 (44%)
24	CLA	B	820	13	59,63,73	1.25	6 (10%)	70,101,113	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	6	613	-	40,45,45	1.23	8 (20%)	51,67,67	1.68	8 (15%)
24	CLA	B	827	13	69,73,73	1.16	7 (10%)	82,113,113	1.13	5 (6%)
24	CLA	t	301	11	49,53,73	1.40	5 (10%)	58,89,113	1.43	6 (10%)
24	CLA	A	825	-	69,73,73	1.15	6 (8%)	82,113,113	1.14	7 (8%)
28	LHG	L	201	-	28,28,48	1.22	2 (7%)	31,34,54	1.15	2 (6%)
24	CLA	t	308	11	50,54,73	1.37	5 (10%)	59,90,113	1.10	3 (5%)
24	CLA	8	202	8	50,54,73	1.35	5 (10%)	59,90,113	1.26	5 (8%)
24	CLA	A	824	-	69,73,73	1.16	6 (8%)	82,113,113	1.15	6 (7%)
24	CLA	A	838	12	69,73,73	1.16	7 (10%)	82,113,113	1.13	8 (9%)
24	CLA	A	831	12	69,73,73	1.16	6 (8%)	82,113,113	1.10	4 (4%)
24	CLA	h	604	-	50,54,73	1.34	5 (10%)	59,90,113	1.18	3 (5%)
24	CLA	B	807	13	69,73,73	1.17	6 (8%)	82,113,113	1.16	6 (7%)
24	CLA	B	828	13	54,58,73	1.31	7 (12%)	64,95,113	1.18	4 (6%)
26	DD6	c	614	-	40,45,45	1.22	8 (20%)	51,67,67	2.17	13 (25%)
24	CLA	A	818	12	69,73,73	1.15	6 (8%)	82,113,113	1.15	9 (10%)
24	CLA	B	802	13	69,73,73	1.14	7 (10%)	82,113,113	1.08	6 (7%)
25	BCR	I	102	-	41,41,41	0.67	0	56,56,56	2.35	28 (50%)
24	CLA	2	202	2	59,63,73	1.27	6 (10%)	70,101,113	1.18	5 (7%)
24	CLA	7	602	7	54,58,73	1.29	6 (11%)	64,95,113	1.47	11 (17%)
24	CLA	A	814	12	54,58,73	1.32	5 (9%)	64,95,113	1.25	5 (7%)
24	CLA	B	822	-	69,73,73	1.17	6 (8%)	82,113,113	1.25	7 (8%)
26	DD6	1	311	24	40,45,45	1.24	8 (20%)	51,67,67	1.59	11 (21%)
28	LHG	B	844	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
24	CLA	c	602	10	69,73,73	1.15	5 (7%)	82,113,113	1.14	6 (7%)
24	CLA	A	819	12	49,53,73	1.37	6 (12%)	58,89,113	1.25	4 (6%)
26	DD6	4	617	-	40,45,45	1.22	8 (20%)	51,67,67	1.84	12 (23%)
24	CLA	k	310	9	45,49,73	1.42	6 (13%)	54,84,113	1.29	6 (11%)
24	CLA	B	836	-	69,73,73	1.16	7 (10%)	82,113,113	1.06	5 (6%)
24	CLA	5	601	5	49,53,73	1.38	5 (10%)	58,89,113	1.20	3 (5%)
26	DD6	5	608	-	40,45,45	1.23	8 (20%)	51,67,67	1.76	10 (19%)
24	CLA	B	837	13	69,73,73	1.15	6 (8%)	82,113,113	1.23	5 (6%)
24	CLA	k	301	9	50,54,73	1.34	4 (8%)	59,90,113	1.21	3 (5%)
25	BCR	R	101	-	41,41,41	0.79	1 (2%)	56,56,56	2.04	21 (37%)
24	CLA	c	608	10	69,73,73	1.15	6 (8%)	82,113,113	1.09	6 (7%)
24	CLA	h	608	6	50,54,73	1.34	6 (12%)	59,90,113	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	4	612	4	50,54,73	1.33	5 (10%)	59,90,113	1.26	4 (6%)
24	CLA	B	806	13	69,73,73	1.16	5 (7%)	82,113,113	1.16	4 (4%)
24	CLA	B	832	-	49,53,73	1.39	6 (12%)	58,89,113	1.19	3 (5%)
24	CLA	3	307	-	49,53,73	1.37	6 (12%)	58,89,113	1.27	4 (6%)
24	CLA	A	835	12	55,59,73	1.30	7 (12%)	64,96,113	1.28	7 (10%)
24	CLA	5	607	5	49,53,73	1.39	5 (10%)	58,89,113	1.34	4 (6%)
24	CLA	A	847	-	59,63,73	1.25	5 (8%)	70,101,113	1.23	6 (8%)
24	CLA	t	305	11	50,54,73	1.34	6 (12%)	59,90,113	1.21	7 (11%)
24	CLA	k	306	9	50,54,73	1.33	7 (14%)	59,90,113	1.19	5 (8%)
24	CLA	6	611	6	47,52,73	1.40	7 (14%)	55,88,113	1.29	5 (9%)
26	DD6	9	313	-	40,45,45	1.23	8 (20%)	51,67,67	1.64	9 (17%)
24	CLA	h	601	6	49,53,73	1.37	4 (8%)	58,89,113	1.30	3 (5%)
24	CLA	B	812	13	69,73,73	1.17	6 (8%)	82,113,113	1.15	5 (6%)
25	BCR	J	101	-	41,41,41	0.88	0	56,56,56	2.38	20 (35%)
26	DD6	4	614	-	40,45,45	1.21	8 (20%)	51,67,67	1.77	10 (19%)
28	LHG	A	841	-	47,47,48	0.94	2 (4%)	50,53,54	0.99	3 (6%)
24	CLA	3	301	3	69,73,73	1.17	6 (8%)	82,113,113	1.20	4 (4%)
24	CLA	B	814	13	54,58,73	1.32	6 (11%)	64,95,113	1.24	7 (10%)
24	CLA	k	308	-	45,49,73	1.39	4 (8%)	54,84,113	1.46	7 (12%)
24	CLA	7	609	7	50,54,73	1.36	5 (10%)	59,90,113	1.27	4 (6%)
24	CLA	A	820	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	8 (9%)
24	CLA	A	805	12	69,73,73	1.16	5 (7%)	82,113,113	1.18	6 (7%)
32	SF4	C	102	14	0,12,12	-	-	-	-	-
28	LHG	A	852	-	36,36,48	1.08	2 (5%)	39,42,54	1.03	2 (5%)
24	CLA	4	602	4	64,68,73	1.19	6 (9%)	76,107,113	1.18	7 (9%)
24	CLA	B	810	13	58,62,73	1.32	7 (12%)	71,100,113	1.30	10 (14%)
24	CLA	c	609	-	64,68,73	1.23	5 (7%)	76,107,113	1.32	6 (7%)
24	CLA	k	303	-	59,63,73	1.24	5 (8%)	70,101,113	1.37	10 (14%)
24	CLA	h	607	6	50,54,73	1.35	6 (12%)	59,90,113	1.15	4 (6%)
24	CLA	B	833	13	62,66,73	1.22	7 (11%)	73,104,113	1.28	7 (9%)
26	DD6	t	313	-	40,45,45	1.20	5 (12%)	51,67,67	1.74	11 (21%)
27	LMT	A	854	-	36,36,36	0.67	0	47,47,47	0.89	1 (2%)
26	DD6	4	615	-	40,45,45	1.23	8 (20%)	51,67,67	1.65	9 (17%)
24	CLA	h	603	6	48,53,73	1.38	5 (10%)	56,89,113	1.23	6 (10%)
26	DD6	A	848	-	40,45,45	1.20	5 (12%)	51,67,67	1.99	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	1	303	1	50,54,73	1.34	5 (10%)	59,90,113	1.21	4 (6%)
25	BCR	1	310	-	41,41,41	0.73	0	56,56,56	2.18	22 (39%)
31	PQN	A	839	-	34,34,34	0.37	0	43,45,45	0.64	1 (2%)
25	BCR	A	844	-	41,41,41	0.75	1 (2%)	56,56,56	2.13	17 (30%)
24	CLA	A	815	-	49,53,73	1.39	7 (14%)	58,89,113	1.24	5 (8%)
24	CLA	h	606	6	50,54,73	1.35	7 (14%)	59,90,113	1.17	4 (6%)
24	CLA	A	801	12	69,73,73	1.16	6 (8%)	82,113,113	1.34	8 (9%)
26	DD6	7	618	-	40,45,45	1.30	6 (15%)	51,67,67	1.76	12 (23%)
24	CLA	B	848	13	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
29	A1L1G	9	312	-	40,47,47	1.17	8 (20%)	49,71,71	1.20	5 (10%)
24	CLA	7	606	7	64,68,73	1.22	6 (9%)	76,107,113	1.26	7 (9%)
24	CLA	B	830	13	62,66,73	1.22	6 (9%)	73,104,113	1.18	5 (6%)
24	CLA	9	306	9	50,54,73	1.36	7 (14%)	59,90,113	1.31	5 (8%)
25	BCR	B	842	-	41,41,41	0.73	1 (2%)	56,56,56	2.12	14 (25%)
24	CLA	6	601	6	49,53,73	1.38	5 (10%)	58,89,113	1.23	5 (8%)
24	CLA	4	605	4	50,54,73	1.33	5 (10%)	59,90,113	1.19	5 (8%)
26	DD6	7	613	-	40,45,45	1.21	8 (20%)	51,67,67	1.89	12 (23%)
24	CLA	F	202	-	50,54,73	1.36	6 (12%)	59,90,113	1.21	4 (6%)
24	CLA	2	201	2	49,53,73	1.38	5 (10%)	58,89,113	1.33	7 (12%)
24	CLA	3	303	-	59,63,73	1.25	7 (11%)	70,101,113	1.21	5 (7%)
24	CLA	t	303	11	69,73,73	1.15	5 (7%)	82,113,113	1.17	5 (6%)
24	CLA	7	605	7	50,54,73	1.35	5 (10%)	59,90,113	1.23	3 (5%)
24	CLA	7	612	7	50,54,73	1.38	5 (10%)	59,90,113	1.24	5 (8%)
24	CLA	R	104	22	49,53,73	1.35	7 (14%)	58,89,113	1.38	6 (10%)
29	A1L1G	7	614	-	40,47,47	1.16	8 (20%)	49,71,71	1.06	3 (6%)
24	CLA	1	302	1	49,53,73	1.36	5 (10%)	58,89,113	1.22	5 (8%)
25	BCR	4	618	-	41,41,41	0.76	1 (2%)	56,56,56	2.38	19 (33%)
24	CLA	1	305	1	49,53,73	1.36	6 (12%)	58,89,113	1.67	7 (12%)
24	CLA	6	603	6	50,54,73	1.35	6 (12%)	59,90,113	1.15	3 (5%)
28	LHG	3	315	-	42,42,48	0.99	2 (4%)	45,48,54	1.05	4 (8%)
24	CLA	F	203	17	54,58,73	1.30	6 (11%)	64,95,113	1.27	4 (6%)
24	CLA	3	304	3	50,54,73	1.34	5 (10%)	59,90,113	1.40	9 (15%)
24	CLA	3	305	3	64,68,73	1.19	6 (9%)	76,107,113	1.11	5 (6%)
24	CLA	t	304	-	50,54,73	1.36	6 (12%)	59,90,113	1.20	3 (5%)
24	CLA	h	602	6	59,63,73	1.27	6 (10%)	70,101,113	1.81	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	R	103	22	69,73,73	1.15	7 (10%)	82,113,113	1.13	6 (7%)
26	DD6	8	212	-	40,45,45	1.20	8 (20%)	51,67,67	1.66	9 (17%)
28	LHG	A	842	24	41,41,48	1.09	2 (4%)	44,47,54	1.29	5 (11%)
26	DD6	9	314	-	40,45,45	1.26	7 (17%)	51,67,67	2.23	12 (23%)
24	CLA	A	823	12	69,73,73	1.16	5 (7%)	82,113,113	1.09	6 (7%)
26	DD6	4	616	-	40,45,45	1.22	8 (20%)	51,67,67	1.83	13 (25%)
24	CLA	c	603	10	50,54,73	1.33	6 (12%)	59,90,113	1.29	5 (8%)
27	LMT	3	314	-	31,31,36	0.69	0	42,42,47	1.21	3 (7%)
24	CLA	t	302	11	50,54,73	1.36	6 (12%)	59,90,113	1.16	4 (6%)
24	CLA	6	612	-	50,54,73	1.36	5 (10%)	59,90,113	1.21	4 (6%)
26	DD6	8	210	-	40,45,45	1.30	8 (20%)	51,67,67	2.06	15 (29%)
24	CLA	2	205	2	50,54,73	1.35	6 (12%)	59,90,113	1.21	4 (6%)
26	DD6	h	616	-	40,45,45	1.22	8 (20%)	51,67,67	1.74	7 (13%)
24	CLA	2	207	-	50,54,73	1.35	5 (10%)	59,90,113	1.23	5 (8%)
24	CLA	A	816	12	69,73,73	1.15	5 (7%)	82,113,113	1.14	5 (6%)
24	CLA	4	606	4	50,54,73	1.33	6 (12%)	59,90,113	1.20	5 (8%)
24	CLA	B	825	13	59,63,73	1.24	6 (10%)	70,101,113	1.18	6 (8%)
26	DD6	2	210	-	40,45,45	1.20	8 (20%)	51,67,67	1.75	7 (13%)
24	CLA	A	857	12	69,73,73	1.13	7 (10%)	82,113,113	1.32	7 (8%)
26	DD6	6	615	-	40,45,45	1.20	5 (12%)	51,67,67	1.90	13 (25%)
25	BCR	B	841	-	41,41,41	0.72	0	56,56,56	2.10	22 (39%)
26	DD6	5	609	-	40,45,45	1.21	8 (20%)	51,67,67	1.78	10 (19%)
24	CLA	A	837	12	59,63,73	1.26	6 (10%)	70,101,113	1.25	7 (10%)
24	CLA	8	207	-	49,53,73	1.41	5 (10%)	58,89,113	1.22	3 (5%)
24	CLA	k	304	9	50,54,73	1.37	6 (12%)	59,90,113	1.30	3 (5%)
24	CLA	9	308	-	50,54,73	1.35	6 (12%)	59,90,113	1.20	4 (6%)
24	CLA	A	803	12	59,63,73	1.24	6 (10%)	70,101,113	1.25	9 (12%)
24	CLA	6	605	6	50,54,73	1.35	6 (12%)	59,90,113	1.21	4 (6%)
24	CLA	1	317	-	69,73,73	1.17	7 (10%)	82,113,113	1.07	4 (4%)
24	CLA	A	821	12	53,57,73	1.30	5 (9%)	61,93,113	1.21	5 (8%)
24	CLA	7	610	7	49,53,73	1.37	5 (10%)	58,89,113	1.18	3 (5%)
24	CLA	6	608	6	50,54,73	1.34	6 (12%)	59,90,113	1.20	4 (6%)
24	CLA	A	822	12	59,63,73	1.27	6 (10%)	70,101,113	1.18	5 (7%)
24	CLA	A	804	12	69,73,73	1.16	7 (10%)	82,113,113	1.16	6 (7%)
24	CLA	k	309	9	49,53,73	1.38	5 (10%)	58,89,113	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	610	10	47,52,73	1.41	6 (12%)	55,88,113	1.16	4 (7%)
26	DD6	1	313	-	40,45,45	1.22	8 (20%)	51,67,67	1.55	8 (15%)
24	CLA	h	610	6	50,54,73	1.37	5 (10%)	59,90,113	1.14	5 (8%)
24	CLA	4	603	4	50,54,73	1.37	7 (14%)	59,90,113	1.24	4 (6%)
24	CLA	A	836	12	69,73,73	1.16	5 (7%)	82,113,113	1.07	4 (4%)
28	LHG	2	215	-	30,30,48	1.16	2 (6%)	33,36,54	1.15	3 (9%)
25	BCR	A	843	-	41,41,41	0.73	0	56,56,56	2.35	21 (37%)
24	CLA	k	311	-	59,63,73	1.26	5 (8%)	70,101,113	1.19	6 (8%)
24	CLA	A	808	12	69,73,73	1.17	6 (8%)	82,113,113	1.12	4 (4%)
32	SF4	C	101	14	0,12,12	-	-	-	-	-
24	CLA	3	309	3	45,49,73	1.40	5 (11%)	54,84,113	1.28	5 (9%)
26	DD6	6	616	-	40,45,45	1.24	8 (20%)	51,67,67	2.05	13 (25%)
24	CLA	5	602	5	59,63,73	1.26	5 (8%)	70,101,113	1.23	8 (11%)
26	DD6	h	615	-	40,45,45	1.21	8 (20%)	51,67,67	1.73	9 (17%)
24	CLA	A	832	12	69,73,73	1.16	6 (8%)	82,113,113	1.14	7 (8%)
24	CLA	A	853	12	59,63,73	1.25	6 (10%)	70,101,113	1.24	6 (8%)
25	BCR	t	312	-	41,41,41	0.77	1 (2%)	56,56,56	1.79	9 (16%)
24	CLA	9	305	-	50,54,73	1.35	7 (14%)	59,90,113	1.39	5 (8%)
28	LHG	8	213	-	30,30,48	1.20	2 (6%)	33,36,54	1.50	4 (12%)
24	CLA	7	607	7	49,53,73	1.38	5 (10%)	58,89,113	1.25	8 (13%)
24	CLA	A	812	12	69,73,73	1.16	7 (10%)	82,113,113	1.19	7 (8%)
24	CLA	B	809	13	69,73,73	1.16	6 (8%)	82,113,113	1.19	6 (7%)
24	CLA	7	603	7	49,53,73	1.39	5 (10%)	58,89,113	1.27	8 (13%)
24	CLA	7	604	-	49,53,73	1.36	8 (16%)	58,89,113	1.33	5 (8%)
24	CLA	3	302	3	49,53,73	1.37	6 (12%)	58,89,113	1.34	5 (8%)
24	CLA	A	807	12	69,73,73	1.14	5 (7%)	82,113,113	1.15	7 (8%)
24	CLA	B	846	13	59,63,73	1.24	7 (11%)	70,101,113	1.14	4 (5%)
24	CLA	L	205	-	50,54,73	1.33	5 (10%)	59,90,113	1.15	5 (8%)
25	BCR	L	206	-	41,41,41	0.73	0	56,56,56	2.10	18 (32%)
24	CLA	A	810	12	66,70,73	1.18	6 (9%)	78,109,113	1.08	5 (6%)
24	CLA	4	610	4	45,49,73	1.42	5 (11%)	54,84,113	1.25	4 (7%)
28	LHG	I	103	-	39,39,48	1.03	2 (5%)	42,45,54	1.16	4 (9%)
25	BCR	R	102	-	41,41,41	0.74	0	56,56,56	2.17	21 (37%)
24	CLA	A	833	12	69,73,73	1.17	6 (8%)	82,113,113	1.13	6 (7%)
24	CLA	B	831	-	69,73,73	1.17	6 (8%)	82,113,113	1.12	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	1	312	-	40,45,45	1.23	9 (22%)	51,67,67	1.55	6 (11%)
24	CLA	7	601	7	49,53,73	1.38	7 (14%)	58,89,113	1.21	4 (6%)
25	BCR	B	840	-	41,41,41	0.78	2 (4%)	56,56,56	2.02	23 (41%)
25	BCR	1	314	-	41,41,41	0.72	0	56,56,56	2.16	17 (30%)
25	BCR	9	316	-	41,41,41	0.71	1 (2%)	56,56,56	2.37	18 (32%)
24	CLA	5	606	-	50,54,73	1.36	5 (10%)	59,90,113	1.22	4 (6%)
25	BCR	A	846	-	41,41,41	0.70	1 (2%)	56,56,56	2.41	26 (46%)
24	CLA	B	847	13	69,73,73	1.17	7 (10%)	82,113,113	1.12	6 (7%)
24	CLA	1	308	1	50,54,73	1.38	6 (12%)	59,90,113	1.14	3 (5%)
24	CLA	A	860	12	69,73,73	1.14	7 (10%)	82,113,113	1.36	11 (13%)
24	CLA	A	828	12	69,73,73	1.17	7 (10%)	82,113,113	1.12	4 (4%)
25	BCR	7	617	-	41,41,41	0.73	0	56,56,56	1.99	21 (37%)
24	CLA	k	305	9	50,54,73	1.35	5 (10%)	59,90,113	1.23	4 (6%)
24	CLA	c	606	10	50,54,73	1.35	5 (10%)	59,90,113	1.20	4 (6%)
25	BCR	c	615	-	41,41,41	0.69	0	56,56,56	2.65	20 (35%)
24	CLA	9	311	-	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
26	DD6	3	312	-	40,45,45	1.19	7 (17%)	51,67,67	1.91	10 (19%)
24	CLA	B	815	13	59,63,73	1.24	5 (8%)	70,101,113	1.21	7 (10%)
24	CLA	1	306	1	54,58,73	1.29	5 (9%)	64,95,113	1.24	6 (9%)
31	PQN	B	839	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
24	CLA	c	605	10	50,54,73	1.36	5 (10%)	59,90,113	1.20	2 (3%)
29	A1L1G	3	310	-	40,47,47	1.16	8 (20%)	49,71,71	0.93	1 (2%)
24	CLA	A	829	12	69,73,73	1.16	5 (7%)	82,113,113	1.14	6 (7%)
30	LMG	2	214	-	45,45,55	0.96	2 (4%)	53,53,63	1.37	5 (9%)
24	CLA	A	826	12	69,73,73	1.15	5 (7%)	82,113,113	1.21	10 (12%)
24	CLA	6	606	6	50,54,73	1.35	5 (10%)	59,90,113	1.15	3 (5%)
24	CLA	8	201	8	50,54,73	1.35	5 (10%)	59,90,113	1.17	4 (6%)
24	CLA	B	801	-	69,73,73	1.17	6 (8%)	82,113,113	1.20	4 (4%)
24	CLA	6	609	-	54,58,73	1.31	7 (12%)	64,95,113	1.29	5 (7%)
26	DD6	J	102	-	40,45,45	1.23	8 (20%)	51,67,67	1.66	11 (21%)
28	LHG	4	619	-	38,38,48	1.05	2 (5%)	41,44,54	1.00	2 (4%)
24	CLA	A	834	12	49,53,73	1.39	6 (12%)	58,89,113	1.28	6 (10%)
24	CLA	8	205	8	49,53,73	1.37	6 (12%)	58,89,113	1.17	4 (6%)
25	BCR	J	104	-	41,41,41	0.66	0	56,56,56	2.31	21 (37%)
25	BCR	L	202	-	41,41,41	0.68	0	56,56,56	2.29	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	k	302	9	50,54,73	1.34	5 (10%)	59,90,113	1.36	4 (6%)
24	CLA	4	609	4	50,54,73	1.35	6 (12%)	59,90,113	1.19	4 (6%)
27	LMT	1	315	-	36,36,36	0.66	0	47,47,47	0.80	1 (2%)
24	CLA	k	307	9	50,54,73	1.36	6 (12%)	59,90,113	1.20	3 (5%)
24	CLA	J	103	19	46,50,73	1.38	5 (10%)	53,85,113	1.24	4 (7%)
24	CLA	A	827	12	66,70,73	1.17	5 (7%)	78,109,113	1.13	6 (7%)
26	DD6	c	612	-	40,45,45	1.20	8 (20%)	51,67,67	2.05	12 (23%)
24	CLA	B	811	13	59,63,73	1.25	7 (11%)	70,101,113	1.24	8 (11%)
28	LHG	B	845	24	40,40,48	1.02	2 (5%)	43,46,54	0.98	2 (4%)
24	CLA	B	805	13	69,73,73	1.15	6 (8%)	82,113,113	1.16	7 (8%)
26	DD6	h	614	-	40,45,45	1.22	8 (20%)	51,67,67	1.60	9 (17%)
26	DD6	k	315	-	40,45,45	1.24	7 (17%)	51,67,67	2.04	12 (23%)
24	CLA	B	826	13	69,73,73	1.17	7 (10%)	82,113,113	1.08	7 (8%)
24	CLA	A	856	-	69,73,73	1.16	5 (7%)	82,113,113	1.14	7 (8%)
24	CLA	6	602	6	51,55,73	1.33	6 (11%)	60,91,113	1.20	7 (11%)
29	A1L1G	k	312	-	40,47,47	1.14	8 (20%)	49,71,71	1.02	5 (10%)
25	BCR	2	211	-	41,41,41	0.71	1 (2%)	56,56,56	2.14	22 (39%)
24	CLA	A	802	-	69,73,73	1.13	8 (11%)	82,113,113	1.29	9 (10%)
24	CLA	1	301	1	69,73,73	1.15	6 (8%)	82,113,113	1.08	5 (6%)

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
26	DD6	7	615	-	-	3/26/80/80	0/3/3/3
29	A1L1G	2	213	-	-	19/29/85/85	0/3/3/3
24	CLA	9	304	9	1/1/11/20	7/17/93/115	-
27	LMT	h	617	-	-	7/14/54/61	0/2/2/2
24	CLA	4	608	-	1/1/12/20	8/21/97/115	-
24	CLA	B	813	13	1/1/11/20	7/17/93/115	-
24	CLA	A	817	12	1/1/15/20	14/39/115/115	-
25	BCR	F	204	-	-	2/29/63/63	0/2/2/2
26	DD6	3	311	-	-	1/26/80/80	0/3/3/3
24	CLA	6	610	6	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	2	203	-	1/1/12/20	4/21/97/115	-
24	CLA	7	608	-	1/1/11/20	6/15/91/115	-
24	CLA	1	307	1	1/1/11/20	4/15/91/115	-
24	CLA	2	209	-	1/1/11/20	4/17/93/115	-
24	CLA	9	303	-	1/1/11/20	10/17/93/115	-
25	BCR	A	845	-	-	5/29/60/63	0/2/2/2
24	CLA	F	201	-	1/1/15/20	11/39/115/115	-
32	SF4	A	858	12,13	-	-	0/6/5/5
24	CLA	2	208	-	1/1/11/20	6/17/93/115	-
24	CLA	A	806	12	1/1/15/20	8/39/115/115	-
24	CLA	c	607	10	1/1/11/20	3/17/93/115	-
24	CLA	A	809	12	1/1/11/20	4/17/93/115	-
24	CLA	B	824	13	1/1/15/20	6/39/115/115	-
24	CLA	B	838	28	1/1/15/20	7/39/115/115	-
24	CLA	t	306	11	1/1/11/20	7/15/91/115	-
24	CLA	8	204	8	1/1/11/20	6/15/91/115	-
24	CLA	8	208	8	1/1/11/20	6/15/91/115	-
27	LMT	1	316	-	-	9/21/61/61	0/2/2/2
24	CLA	4	604	-	1/1/11/20	7/17/93/115	-
24	CLA	B	818	-	1/1/15/20	12/39/115/115	-
27	LMT	A	851	-	-	5/11/51/61	0/2/2/2
24	CLA	8	209	-	1/1/10/20	4/10/86/115	-
26	DD6	k	314	-	-	2/26/80/80	0/3/3/3
24	CLA	7	611	7	1/1/11/20	6/17/93/115	-
24	CLA	9	302	9	1/1/11/20	4/17/93/115	-
24	CLA	B	816	13	1/1/15/20	14/39/115/115	-
26	DD6	3	313	-	-	3/26/80/80	0/3/3/3
24	CLA	c	611	10	1/1/10/20	2/10/86/115	-
24	CLA	5	604	5	1/1/11/20	4/17/93/115	-
24	CLA	B	821	13	1/1/12/20	10/25/101/115	-
24	CLA	B	819	13	1/1/11/20	4/17/93/115	-
24	CLA	B	834	13	1/1/15/20	9/39/115/115	-
24	CLA	B	804	13	1/1/15/20	12/39/115/115	-
24	CLA	8	203	-	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	R	105	-	-	6/26/80/80	0/3/3/3
24	CLA	3	308	3	1/1/11/20	8/17/93/115	-
24	CLA	5	603	5	1/1/11/20	4/15/91/115	-
24	CLA	c	601	10	1/1/10/20	6/13/89/115	-
26	DD6	7	616	-	-	2/26/80/80	0/3/3/3
24	CLA	6	607	6	1/1/11/20	6/17/93/115	-
26	DD6	6	617	-	-	1/26/80/80	0/3/3/3
26	DD6	h	613	-	-	1/26/80/80	0/3/3/3
24	CLA	4	607	4	1/1/11/20	6/17/93/115	-
30	LMG	A	855	-	-	5/33/53/70	0/1/1/1
24	CLA	A	840	28	1/1/15/20	10/39/115/115	-
26	DD6	2	212	-	-	1/26/80/80	0/3/3/3
25	BCR	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	h	609	-	1/1/11/20	7/17/93/115	-
24	CLA	9	301	9	1/1/11/20	8/17/93/115	-
24	CLA	L	204	20	-	11/39/115/115	-
24	CLA	B	808	13	1/1/15/20	10/39/115/115	-
24	CLA	L	203	20	1/1/13/20	11/27/103/115	-
28	LHG	1	318	-	-	15/47/47/53	-
24	CLA	4	611	-	1/1/11/20	6/17/93/115	-
26	DD6	t	311	-	-	2/26/80/80	0/3/3/3
24	CLA	B	835	13	1/1/11/20	6/18/94/115	-
24	CLA	6	604	-	1/1/11/20	3/17/93/115	-
24	CLA	9	309	9	1/1/11/20	10/17/93/115	-
26	DD6	9	317	-	-	2/26/80/80	0/3/3/3
24	CLA	h	605	6	1/1/11/20	4/17/93/115	-
25	BCR	k	316	-	-	3/29/63/63	0/2/2/2
26	DD6	9	315	-	-	3/26/80/80	0/3/3/3
24	CLA	3	306	3	1/1/15/20	8/39/115/115	-
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	DD6	c	613	-	-	0/26/80/80	0/3/3/3
24	CLA	2	204	2	1/1/14/20	12/33/109/115	-
25	BCR	B	849	-	-	4/29/63/63	0/2/2/2
24	CLA	5	605	5	1/1/11/20	8/17/93/115	-
24	CLA	1	304	26	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	803	-	1/1/15/20	10/39/115/115	-
24	CLA	8	206	8	1/1/11/20	6/17/93/115	-
27	LMT	A	850	-	-	10/21/61/61	0/2/2/2
24	CLA	A	830	12	-	10/27/103/115	-
28	LHG	J	105	-	-	12/42/42/53	-
25	BCR	A	859	-	-	4/29/63/63	0/2/2/2
24	CLA	9	310	9	1/1/11/20	8/17/93/115	-
24	CLA	A	811	12	1/1/11/20	7/17/93/115	-
26	DD6	k	313	-	-	1/26/80/80	0/3/3/3
24	CLA	1	309	1	1/1/11/20	3/15/91/115	-
24	CLA	h	611	6	-	2/10/86/115	-
24	CLA	t	310	-	1/1/11/20	9/17/93/115	-
24	CLA	4	601	4	1/1/10/20	5/11/87/115	-
24	CLA	B	829	13	1/1/15/20	6/39/115/115	-
26	DD6	8	211	-	-	4/26/80/80	0/3/3/3
24	CLA	9	307	9	1/1/11/20	7/17/93/115	-
26	DD6	6	614	-	-	1/26/80/80	0/3/3/3
24	CLA	c	604	-	1/1/11/20	7/17/93/115	-
24	CLA	t	309	-	1/1/11/20	4/17/93/115	-
30	LMG	t	314	-	-	6/29/49/70	0/1/1/1
24	CLA	2	206	2	1/1/11/20	4/17/93/115	-
28	LHG	A	849	-	-	13/45/45/53	-
24	CLA	B	817	13	1/1/15/20	15/39/115/115	-
24	CLA	B	823	-	1/1/14/20	6/38/114/115	-
24	CLA	A	813	12	1/1/15/20	10/39/115/115	-
24	CLA	t	307	-	1/1/11/20	7/17/93/115	-
24	CLA	h	612	-	1/1/11/20	8/15/91/115	-
24	CLA	4	613	4	1/1/11/20	9/17/93/115	-
25	BCR	I	101	-	-	4/29/63/63	0/2/2/2
24	CLA	B	820	13	1/1/13/20	10/27/103/115	-
26	DD6	6	613	-	-	2/26/80/80	0/3/3/3
24	CLA	B	827	13	1/1/15/20	12/39/115/115	-
24	CLA	t	301	11	1/1/11/20	4/15/91/115	-
24	CLA	A	825	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	L	201	-	-	14/33/33/53	-
24	CLA	t	308	11	1/1/11/20	6/17/93/115	-
24	CLA	8	202	8	1/1/11/20	8/17/93/115	-
24	CLA	A	824	-	1/1/15/20	15/39/115/115	-
24	CLA	A	838	12	1/1/15/20	9/39/115/115	-
24	CLA	A	831	12	1/1/15/20	13/39/115/115	-
24	CLA	h	604	-	1/1/11/20	5/17/93/115	-
24	CLA	B	828	13	1/1/12/20	11/21/97/115	-
24	CLA	B	807	13	-	7/39/115/115	-
26	DD6	c	614	-	-	1/26/80/80	0/3/3/3
24	CLA	A	818	12	1/1/15/20	11/39/115/115	-
24	CLA	B	802	13	1/1/15/20	17/39/115/115	-
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
24	CLA	2	202	2	1/1/13/20	6/27/103/115	-
24	CLA	7	602	7	1/1/12/20	10/21/97/115	-
24	CLA	A	814	12	1/1/12/20	7/21/97/115	-
24	CLA	B	822	-	1/1/15/20	13/39/115/115	-
26	DD6	1	311	24	-	0/26/80/80	0/3/3/3
28	LHG	B	844	-	-	14/53/53/53	-
24	CLA	c	602	10	1/1/15/20	12/39/115/115	-
24	CLA	A	819	12	1/1/11/20	4/15/91/115	-
26	DD6	4	617	-	-	1/26/80/80	0/3/3/3
24	CLA	k	310	9	1/1/10/20	2/10/86/115	-
24	CLA	B	836	-	1/1/15/20	14/39/115/115	-
24	CLA	5	601	5	1/1/11/20	4/15/91/115	-
26	DD6	5	608	-	-	3/26/80/80	0/3/3/3
24	CLA	B	837	13	1/1/15/20	15/39/115/115	-
24	CLA	k	301	9	1/1/11/20	4/17/93/115	-
25	BCR	R	101	-	-	4/29/63/63	0/2/2/2
24	CLA	c	608	10	1/1/15/20	13/39/115/115	-
24	CLA	h	608	6	1/1/11/20	7/17/93/115	-
24	CLA	4	612	4	1/1/11/20	4/17/93/115	-
24	CLA	B	806	13	1/1/15/20	9/39/115/115	-
24	CLA	B	832	-	1/1/11/20	11/15/91/115	-
24	CLA	3	307	-	1/1/11/20	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	835	12	1/1/12/20	6/23/99/115	-
24	CLA	5	607	5	1/1/11/20	4/15/91/115	-
24	CLA	A	847	-	1/1/13/20	11/27/103/115	-
24	CLA	t	305	11	1/1/11/20	4/17/93/115	-
24	CLA	k	306	9	1/1/11/20	5/17/93/115	-
24	CLA	6	611	6	1/1/11/20	3/13/89/115	-
26	DD6	9	313	-	-	3/26/80/80	0/3/3/3
24	CLA	h	601	6	1/1/11/20	7/15/91/115	-
24	CLA	B	812	13	1/1/15/20	16/39/115/115	-
25	BCR	J	101	-	-	2/29/63/63	0/2/2/2
26	DD6	4	614	-	-	1/26/80/80	0/3/3/3
28	LHG	A	841	-	-	18/52/52/53	-
24	CLA	3	301	3	-	15/39/115/115	-
24	CLA	B	814	13	1/1/12/20	5/21/97/115	-
24	CLA	k	308	-	1/1/10/20	5/10/86/115	-
24	CLA	7	609	7	1/1/11/20	6/17/93/115	-
24	CLA	A	820	-	1/1/15/20	9/39/115/115	-
24	CLA	A	805	12	1/1/15/20	12/39/115/115	-
32	SF4	C	102	14	-	-	0/6/5/5
28	LHG	A	852	-	-	8/41/41/53	-
24	CLA	4	602	4	1/1/14/20	11/33/109/115	-
24	CLA	B	810	13	1/1/13/20	7/25/101/115	-
24	CLA	c	609	-	1/1/14/20	10/33/109/115	-
24	CLA	k	303	-	-	10/27/103/115	-
24	CLA	h	607	6	1/1/11/20	6/17/93/115	-
24	CLA	B	833	13	1/1/13/20	6/31/107/115	-
26	DD6	t	313	-	-	0/26/80/80	0/3/3/3
27	LMT	A	854	-	-	11/21/61/61	0/2/2/2
26	DD6	4	615	-	-	1/26/80/80	0/3/3/3
24	CLA	h	603	6	1/1/11/20	4/15/91/115	-
26	DD6	A	848	-	-	1/26/80/80	0/3/3/3
24	CLA	1	303	1	1/1/11/20	6/17/93/115	-
25	BCR	1	310	-	-	3/29/63/63	0/2/2/2
31	PQN	A	839	-	-	5/23/43/43	0/2/2/2
25	BCR	A	844	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	815	-	1/1/11/20	5/15/91/115	-
24	CLA	h	606	6	1/1/11/20	5/17/93/115	-
24	CLA	A	801	12	1/1/15/20	16/39/115/115	-
26	DD6	7	618	-	-	3/26/80/80	0/3/3/3
24	CLA	B	848	13	1/1/15/20	9/39/115/115	-
29	A1L1G	9	312	-	-	13/29/85/85	0/3/3/3
24	CLA	7	606	7	1/1/14/20	12/33/109/115	-
24	CLA	B	830	13	1/1/13/20	12/31/107/115	-
24	CLA	9	306	9	1/1/11/20	6/17/93/115	-
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
24	CLA	6	601	6	1/1/11/20	6/15/91/115	-
24	CLA	4	605	4	1/1/11/20	7/17/93/115	-
26	DD6	7	613	-	-	0/26/80/80	0/3/3/3
24	CLA	F	202	-	1/1/11/20	4/17/93/115	-
24	CLA	2	201	2	1/1/11/20	7/15/91/115	-
24	CLA	3	303	-	1/1/13/20	5/27/103/115	-
24	CLA	t	303	11	1/1/15/20	14/39/115/115	-
24	CLA	7	605	7	1/1/11/20	4/17/93/115	-
24	CLA	7	612	7	1/1/11/20	9/17/93/115	-
24	CLA	R	104	22	1/1/11/20	3/15/91/115	-
29	A1L1G	7	614	-	-	12/29/85/85	0/3/3/3
24	CLA	1	302	1	1/1/11/20	6/15/91/115	-
25	BCR	4	618	-	-	1/29/63/63	0/2/2/2
24	CLA	1	305	1	1/1/11/20	7/15/91/115	-
24	CLA	6	603	6	1/1/11/20	8/17/93/115	-
28	LHG	3	315	-	-	26/47/47/53	-
24	CLA	F	203	17	1/1/12/20	7/21/97/115	-
24	CLA	3	304	3	1/1/11/20	6/17/93/115	-
24	CLA	3	305	3	1/1/14/20	7/33/109/115	-
24	CLA	t	304	-	1/1/11/20	5/17/93/115	-
24	CLA	h	602	6	1/1/13/20	6/27/103/115	-
24	CLA	R	103	22	1/1/15/20	9/39/115/115	-
26	DD6	8	212	-	-	2/26/80/80	0/3/3/3
28	LHG	A	842	24	-	10/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	9	314	-	-	2/26/80/80	0/3/3/3
24	CLA	A	823	12	1/1/15/20	20/39/115/115	-
26	DD6	4	616	-	-	4/26/80/80	0/3/3/3
24	CLA	c	603	10	1/1/11/20	6/17/93/115	-
27	LMT	3	314	-	-	9/16/56/61	0/2/2/2
24	CLA	t	302	11	1/1/11/20	10/17/93/115	-
24	CLA	6	612	-	1/1/11/20	3/17/93/115	-
26	DD6	8	210	-	-	3/26/80/80	0/3/3/3
24	CLA	2	205	2	-	4/17/93/115	-
26	DD6	h	616	-	-	2/26/80/80	0/3/3/3
24	CLA	2	207	-	1/1/11/20	5/17/93/115	-
24	CLA	A	816	12	1/1/15/20	12/39/115/115	-
24	CLA	4	606	4	1/1/11/20	2/17/93/115	-
24	CLA	B	825	13	1/1/13/20	8/27/103/115	-
26	DD6	2	210	-	-	1/26/80/80	0/3/3/3
24	CLA	A	857	12	1/1/15/20	7/39/115/115	-
26	DD6	6	615	-	-	4/26/80/80	0/3/3/3
25	BCR	B	841	-	-	2/29/63/63	0/2/2/2
26	DD6	5	609	-	-	1/26/80/80	0/3/3/3
24	CLA	A	837	12	1/1/13/20	6/27/103/115	-
24	CLA	8	207	-	1/1/11/20	9/15/91/115	-
24	CLA	k	304	9	1/1/11/20	10/17/93/115	-
24	CLA	9	308	-	1/1/11/20	8/17/93/115	-
24	CLA	A	803	12	-	6/27/103/115	-
24	CLA	6	605	6	-	4/17/93/115	-
24	CLA	1	317	-	1/1/15/20	12/39/115/115	-
24	CLA	A	821	12	1/1/11/20	4/20/96/115	-
24	CLA	7	610	7	1/1/11/20	8/15/91/115	-
24	CLA	6	608	6	1/1/11/20	4/17/93/115	-
24	CLA	A	822	12	1/1/13/20	13/27/103/115	-
24	CLA	A	804	12	1/1/15/20	11/39/115/115	-
24	CLA	k	309	9	1/1/11/20	4/15/91/115	-
24	CLA	c	610	10	1/1/11/20	2/13/89/115	-
26	DD6	1	313	-	-	1/26/80/80	0/3/3/3
24	CLA	h	610	6	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	4	603	4	1/1/11/20	2/17/93/115	-
24	CLA	A	836	12	1/1/15/20	12/39/115/115	-
28	LHG	2	215	-	-	7/35/35/53	-
25	BCR	A	843	-	-	4/29/63/63	0/2/2/2
24	CLA	k	311	-	1/1/13/20	6/27/103/115	-
24	CLA	A	808	12	1/1/15/20	8/39/115/115	-
32	SF4	C	101	14	-	-	0/6/5/5
24	CLA	3	309	3	1/1/10/20	0/10/86/115	-
26	DD6	6	616	-	-	5/26/80/80	0/3/3/3
24	CLA	5	602	5	1/1/13/20	10/27/103/115	-
26	DD6	h	615	-	-	3/26/80/80	0/3/3/3
24	CLA	A	832	12	-	14/39/115/115	-
24	CLA	A	853	12	1/1/13/20	7/27/103/115	-
25	BCR	t	312	-	-	8/29/63/63	0/2/2/2
24	CLA	9	305	-	-	11/17/93/115	-
28	LHG	8	213	-	-	16/35/35/53	-
24	CLA	7	607	7	1/1/11/20	2/15/91/115	-
24	CLA	A	812	12	1/1/15/20	15/39/115/115	-
24	CLA	B	809	13	1/1/15/20	9/39/115/115	-
24	CLA	7	603	7	1/1/11/20	2/15/91/115	-
24	CLA	7	604	-	1/1/11/20	5/15/91/115	-
24	CLA	3	302	3	1/1/11/20	6/15/91/115	-
24	CLA	A	807	12	1/1/15/20	16/39/115/115	-
24	CLA	B	846	13	1/1/13/20	11/27/103/115	-
24	CLA	L	205	-	1/1/11/20	5/17/93/115	-
25	BCR	L	206	-	-	4/29/63/63	0/2/2/2
24	CLA	A	810	12	1/1/14/20	12/36/112/115	-
24	CLA	4	610	4	1/1/10/20	2/10/86/115	-
28	LHG	I	103	-	-	12/44/44/53	-
25	BCR	R	102	-	-	4/29/63/63	0/2/2/2
24	CLA	A	833	12	1/1/15/20	5/39/115/115	-
24	CLA	B	831	-	1/1/15/20	19/39/115/115	-
26	DD6	1	312	-	-	0/26/80/80	0/3/3/3
24	CLA	7	601	7	1/1/11/20	7/15/91/115	-
25	BCR	B	840	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	1	314	-	-	8/29/63/63	0/2/2/2
25	BCR	9	316	-	-	2/29/63/63	0/2/2/2
24	CLA	5	606	-	1/1/11/20	8/17/93/115	-
25	BCR	A	846	-	-	2/29/63/63	0/2/2/2
24	CLA	B	847	13	1/1/15/20	12/39/115/115	-
24	CLA	1	308	1	1/1/11/20	6/17/93/115	-
24	CLA	A	860	12	1/1/15/20	8/39/115/115	-
24	CLA	A	828	12	1/1/15/20	10/39/115/115	-
25	BCR	7	617	-	-	2/29/63/63	0/2/2/2
24	CLA	k	305	9	1/1/11/20	6/17/93/115	-
24	CLA	c	606	10	1/1/11/20	7/17/93/115	-
25	BCR	c	615	-	-	10/29/63/63	0/2/2/2
24	CLA	9	311	-	1/1/11/20	4/15/91/115	-
26	DD6	3	312	-	-	1/26/80/80	0/3/3/3
24	CLA	B	815	13	1/1/13/20	8/27/103/115	-
24	CLA	1	306	1	1/1/12/20	4/21/97/115	-
31	PQN	B	839	-	-	9/23/43/43	0/2/2/2
24	CLA	c	605	10	1/1/11/20	10/17/93/115	-
29	A1L1G	3	310	-	-	17/29/85/85	0/3/3/3
24	CLA	A	829	12	1/1/15/20	7/39/115/115	-
30	LMG	2	214	-	-	9/40/60/70	0/1/1/1
24	CLA	A	826	12	1/1/15/20	8/39/115/115	-
24	CLA	6	606	6	1/1/11/20	7/17/93/115	-
24	CLA	8	201	8	1/1/11/20	4/17/93/115	-
24	CLA	B	801	-	1/1/15/20	15/39/115/115	-
24	CLA	6	609	-	1/1/12/20	8/21/97/115	-
26	DD6	J	102	-	-	3/26/80/80	0/3/3/3
28	LHG	4	619	-	-	7/43/43/53	-
24	CLA	A	834	12	1/1/11/20	3/15/91/115	-
24	CLA	8	205	8	1/1/11/20	8/15/91/115	-
25	BCR	J	104	-	-	2/29/63/63	0/2/2/2
25	BCR	L	202	-	-	6/29/63/63	0/2/2/2
24	CLA	k	302	9	1/1/11/20	8/17/93/115	-
24	CLA	4	609	4	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	1	315	-	-	12/21/61/61	0/2/2/2
24	CLA	k	307	9	1/1/11/20	9/17/93/115	-
24	CLA	J	103	19	1/1/10/20	8/12/88/115	-
24	CLA	A	827	12	1/1/14/20	10/36/112/115	-
26	DD6	c	612	-	-	1/26/80/80	0/3/3/3
24	CLA	B	811	13	1/1/13/20	4/27/103/115	-
28	LHG	B	845	24	-	9/45/45/53	-
24	CLA	B	805	13	1/1/15/20	10/39/115/115	-
26	DD6	h	614	-	-	4/26/80/80	0/3/3/3
26	DD6	k	315	-	-	3/26/80/80	0/3/3/3
24	CLA	B	826	13	1/1/15/20	8/39/115/115	-
24	CLA	A	856	-	-	10/39/115/115	-
24	CLA	6	602	6	1/1/11/20	8/18/94/115	-
29	A1L1G	k	312	-	-	8/29/85/85	0/3/3/3
25	BCR	2	211	-	-	4/29/63/63	0/2/2/2
24	CLA	A	802	-	1/1/15/20	3/39/115/115	-
24	CLA	1	301	1	1/1/15/20	11/39/115/115	-

All (1786) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	842	LHG	O7-C7	4.82	1.47	1.34
28	8	213	LHG	O8-C23	4.39	1.46	1.33
28	L	201	LHG	O8-C23	4.30	1.45	1.33
28	A	849	LHG	O8-C23	4.29	1.45	1.33
28	4	619	LHG	O7-C7	4.26	1.46	1.34
28	B	845	LHG	O7-C7	4.25	1.46	1.34
28	3	315	LHG	O8-C23	4.24	1.45	1.33
28	A	852	LHG	O8-C23	4.23	1.45	1.33
30	A	855	LMG	O7-C10	4.23	1.46	1.34
30	t	314	LMG	O8-C28	4.20	1.45	1.33
28	2	215	LHG	O8-C23	4.20	1.45	1.33
28	I	103	LHG	O8-C23	4.19	1.45	1.33
28	B	844	LHG	O8-C23	4.19	1.45	1.33
28	J	105	LHG	O8-C23	4.17	1.45	1.33
28	A	852	LHG	O7-C7	4.17	1.46	1.34
28	4	619	LHG	O8-C23	4.16	1.45	1.33
28	A	849	LHG	O7-C7	4.16	1.46	1.34
30	A	855	LMG	O8-C28	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	201	LHG	O7-C7	4.15	1.46	1.34
28	A	841	LHG	O8-C23	4.14	1.45	1.33
28	1	318	LHG	O8-C23	4.13	1.45	1.33
30	2	214	LMG	O8-C28	4.10	1.45	1.33
28	A	842	LHG	O8-C23	4.08	1.45	1.33
28	B	845	LHG	O8-C23	4.08	1.45	1.33
28	A	841	LHG	O7-C7	4.07	1.45	1.34
28	B	844	LHG	O7-C7	4.07	1.45	1.34
28	J	105	LHG	O7-C7	4.04	1.45	1.34
28	2	215	LHG	O7-C7	4.03	1.45	1.34
28	I	103	LHG	O7-C7	4.02	1.45	1.34
28	8	213	LHG	O7-C7	4.01	1.45	1.34
30	t	314	LMG	O7-C10	3.98	1.45	1.34
24	A	801	CLA	C1D-ND	3.98	1.43	1.37
30	2	214	LMG	O7-C10	3.93	1.45	1.34
28	3	315	LHG	O7-C7	3.92	1.45	1.34
24	B	804	CLA	C1D-ND	3.91	1.43	1.37
24	2	208	CLA	C1D-ND	3.87	1.42	1.37
24	c	610	CLA	C1D-ND	3.87	1.42	1.37
24	8	207	CLA	C1D-ND	3.81	1.42	1.37
24	7	612	CLA	C1D-ND	3.80	1.42	1.37
24	k	308	CLA	C1D-ND	3.78	1.42	1.37
24	4	609	CLA	C1D-ND	3.78	1.42	1.37
24	B	816	CLA	C1D-ND	3.76	1.42	1.37
24	c	609	CLA	C1D-ND	3.76	1.42	1.37
28	1	318	LHG	O7-C7	3.75	1.44	1.34
24	k	305	CLA	C1D-ND	3.73	1.42	1.37
24	7	608	CLA	C1D-ND	3.73	1.42	1.37
24	7	601	CLA	C1D-ND	3.71	1.42	1.37
24	1	308	CLA	C1D-ND	3.70	1.42	1.37
24	7	611	CLA	C1D-ND	3.70	1.42	1.37
24	t	309	CLA	C1D-ND	3.69	1.42	1.37
24	2	207	CLA	C1D-ND	3.68	1.42	1.37
24	8	202	CLA	C1D-ND	3.68	1.42	1.37
24	h	604	CLA	C1D-ND	3.67	1.42	1.37
24	6	603	CLA	C1D-ND	3.67	1.42	1.37
24	9	309	CLA	C1D-ND	3.67	1.42	1.37
24	1	307	CLA	C1D-ND	3.67	1.42	1.37
24	8	203	CLA	C1D-ND	3.66	1.42	1.37
24	t	310	CLA	C1D-ND	3.65	1.42	1.37
24	7	605	CLA	C1D-ND	3.65	1.42	1.37
24	5	606	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	t	308	CLA	C1D-ND	3.64	1.42	1.37
24	5	601	CLA	C1D-ND	3.64	1.42	1.37
24	k	311	CLA	C1D-ND	3.64	1.42	1.37
24	h	610	CLA	C1D-ND	3.64	1.42	1.37
24	8	201	CLA	C1D-ND	3.63	1.42	1.37
24	2	202	CLA	C1D-ND	3.63	1.42	1.37
24	t	301	CLA	C1D-ND	3.63	1.42	1.37
24	2	209	CLA	C1D-ND	3.62	1.42	1.37
24	6	601	CLA	C1D-ND	3.62	1.42	1.37
24	h	609	CLA	C1D-ND	3.62	1.42	1.37
24	3	307	CLA	C1D-ND	3.61	1.42	1.37
24	6	605	CLA	C1D-ND	3.61	1.42	1.37
24	k	308	CLA	C4B-NB	3.61	1.42	1.37
24	6	610	CLA	C1D-ND	3.61	1.42	1.37
24	A	814	CLA	C1D-ND	3.61	1.42	1.37
24	F	203	CLA	C1D-ND	3.61	1.42	1.37
24	1	309	CLA	C1D-ND	3.61	1.42	1.37
24	A	829	CLA	C1D-ND	3.60	1.42	1.37
24	h	602	CLA	C1D-ND	3.60	1.42	1.37
24	c	604	CLA	C1D-ND	3.60	1.42	1.37
24	5	607	CLA	C1D-ND	3.60	1.42	1.37
24	k	301	CLA	C1D-ND	3.60	1.42	1.37
24	A	832	CLA	C1D-ND	3.60	1.42	1.37
24	c	605	CLA	C1D-ND	3.59	1.42	1.37
24	A	806	CLA	C1D-ND	3.59	1.42	1.37
24	8	204	CLA	C1D-ND	3.59	1.42	1.37
24	B	831	CLA	C1D-ND	3.59	1.42	1.37
24	2	206	CLA	C1D-ND	3.58	1.42	1.37
24	7	607	CLA	C1D-ND	3.58	1.42	1.37
24	A	856	CLA	C1D-ND	3.58	1.42	1.37
24	7	609	CLA	C1D-ND	3.58	1.42	1.37
24	B	824	CLA	C4B-NB	3.58	1.42	1.37
24	A	805	CLA	C1D-ND	3.58	1.42	1.37
24	t	302	CLA	C1D-ND	3.57	1.42	1.37
24	k	310	CLA	C1D-ND	3.57	1.42	1.37
24	9	301	CLA	C1D-ND	3.57	1.42	1.37
24	A	812	CLA	C1D-ND	3.57	1.42	1.37
24	5	604	CLA	C1D-ND	3.57	1.42	1.37
24	c	611	CLA	C1D-ND	3.57	1.42	1.37
24	4	610	CLA	C1D-ND	3.57	1.42	1.37
24	7	603	CLA	C1D-ND	3.57	1.42	1.37
24	2	203	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	612	CLA	C1D-ND	3.56	1.42	1.37
24	B	827	CLA	C1D-ND	3.56	1.42	1.37
24	h	601	CLA	C1D-ND	3.56	1.42	1.37
24	h	603	CLA	C1D-ND	3.56	1.42	1.37
24	c	606	CLA	C1D-ND	3.56	1.42	1.37
24	h	605	CLA	C1D-ND	3.56	1.42	1.37
24	A	816	CLA	C1D-ND	3.55	1.42	1.37
24	4	604	CLA	C4B-NB	3.55	1.42	1.37
24	B	806	CLA	C1D-ND	3.55	1.42	1.37
24	B	815	CLA	C1D-ND	3.55	1.42	1.37
24	4	611	CLA	C1D-ND	3.55	1.42	1.37
24	2	204	CLA	C1D-ND	3.55	1.42	1.37
24	A	837	CLA	C1D-ND	3.55	1.42	1.37
24	3	309	CLA	C1D-ND	3.55	1.42	1.37
24	A	834	CLA	C1D-ND	3.55	1.42	1.37
24	A	824	CLA	C1D-ND	3.55	1.42	1.37
24	B	819	CLA	C1D-ND	3.55	1.42	1.37
24	A	819	CLA	C1D-ND	3.54	1.42	1.37
24	1	303	CLA	C1D-ND	3.54	1.42	1.37
24	A	823	CLA	C1D-ND	3.54	1.42	1.37
24	h	611	CLA	C1D-ND	3.54	1.42	1.37
24	B	833	CLA	C1D-ND	3.54	1.42	1.37
24	t	308	CLA	C4B-NB	3.54	1.42	1.37
24	B	847	CLA	C1D-ND	3.53	1.42	1.37
24	6	609	CLA	C1D-ND	3.53	1.42	1.37
24	9	310	CLA	C1D-ND	3.53	1.42	1.37
24	A	815	CLA	C1D-ND	3.53	1.42	1.37
24	A	818	CLA	C1D-ND	3.53	1.42	1.37
24	A	833	CLA	C1D-ND	3.53	1.42	1.37
24	B	807	CLA	C1D-ND	3.53	1.42	1.37
24	3	301	CLA	C1D-ND	3.52	1.42	1.37
24	t	304	CLA	C1D-ND	3.52	1.42	1.37
24	B	834	CLA	C1D-ND	3.52	1.42	1.37
24	3	302	CLA	C1D-ND	3.52	1.42	1.37
24	7	610	CLA	C1D-ND	3.52	1.42	1.37
24	1	317	CLA	C1D-ND	3.52	1.42	1.37
24	6	612	CLA	C1D-ND	3.52	1.42	1.37
24	A	822	CLA	C1D-ND	3.52	1.42	1.37
24	B	813	CLA	C1D-ND	3.52	1.42	1.37
24	k	309	CLA	C1D-ND	3.51	1.42	1.37
24	4	613	CLA	C1D-ND	3.51	1.42	1.37
24	A	807	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	612	CLA	C1D-ND	3.51	1.42	1.37
24	3	303	CLA	C1D-ND	3.50	1.42	1.37
24	A	810	CLA	C1D-ND	3.50	1.42	1.37
24	A	840	CLA	C1D-ND	3.50	1.42	1.37
24	B	837	CLA	C1D-ND	3.50	1.42	1.37
24	B	826	CLA	C1D-ND	3.50	1.42	1.37
24	6	604	CLA	C1D-ND	3.49	1.42	1.37
24	B	822	CLA	C1D-ND	3.49	1.42	1.37
24	t	306	CLA	C1D-ND	3.49	1.42	1.37
24	6	607	CLA	C1D-ND	3.49	1.42	1.37
24	k	304	CLA	C1D-ND	3.49	1.42	1.37
24	B	820	CLA	C1D-ND	3.49	1.42	1.37
24	1	308	CLA	C4B-NB	3.49	1.42	1.37
24	J	103	CLA	C1D-ND	3.49	1.42	1.37
24	F	202	CLA	C1D-ND	3.48	1.42	1.37
24	t	307	CLA	C1D-ND	3.48	1.42	1.37
24	A	803	CLA	C1D-ND	3.48	1.42	1.37
24	A	817	CLA	C1D-ND	3.48	1.42	1.37
24	4	602	CLA	C1D-ND	3.48	1.42	1.37
24	5	603	CLA	C1D-ND	3.48	1.42	1.37
24	A	828	CLA	C1D-ND	3.48	1.42	1.37
24	A	808	CLA	C1D-ND	3.48	1.42	1.37
24	B	808	CLA	C1D-ND	3.47	1.42	1.37
24	A	827	CLA	C1D-ND	3.47	1.42	1.37
24	7	606	CLA	C1D-ND	3.47	1.42	1.37
24	A	835	CLA	C1D-ND	3.47	1.42	1.37
24	A	836	CLA	C1D-ND	3.47	1.42	1.37
24	B	805	CLA	C1D-ND	3.47	1.42	1.37
24	B	817	CLA	C1D-ND	3.47	1.42	1.37
24	1	306	CLA	C1D-ND	3.47	1.42	1.37
24	8	209	CLA	C1D-ND	3.47	1.42	1.37
24	B	812	CLA	C1D-ND	3.47	1.42	1.37
24	A	820	CLA	C1D-ND	3.47	1.42	1.37
24	B	824	CLA	C1D-ND	3.47	1.42	1.37
24	5	605	CLA	C1D-ND	3.46	1.42	1.37
24	A	831	CLA	C1D-ND	3.46	1.42	1.37
24	B	801	CLA	C1D-ND	3.46	1.42	1.37
24	A	809	CLA	C1D-ND	3.46	1.42	1.37
24	A	826	CLA	C1D-ND	3.46	1.42	1.37
24	4	603	CLA	C1D-ND	3.46	1.42	1.37
24	t	303	CLA	C1D-ND	3.46	1.42	1.37
24	4	605	CLA	C1D-ND	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	811	CLA	C1D-ND	3.45	1.42	1.37
24	h	607	CLA	C1D-ND	3.45	1.42	1.37
24	8	205	CLA	C1D-ND	3.45	1.42	1.37
24	2	205	CLA	C1D-ND	3.45	1.42	1.37
24	A	804	CLA	C1D-ND	3.44	1.42	1.37
24	A	825	CLA	C1D-ND	3.44	1.42	1.37
24	1	301	CLA	C1D-ND	3.43	1.42	1.37
24	B	838	CLA	C1D-ND	3.43	1.42	1.37
24	4	604	CLA	C1D-ND	3.43	1.42	1.37
24	9	302	CLA	C1D-ND	3.43	1.42	1.37
24	k	307	CLA	C1D-ND	3.43	1.42	1.37
24	h	610	CLA	C4B-NB	3.43	1.42	1.37
24	k	310	CLA	C4B-NB	3.42	1.42	1.37
24	B	823	CLA	C1D-ND	3.42	1.42	1.37
24	c	603	CLA	C1D-ND	3.42	1.42	1.37
24	A	838	CLA	C1D-ND	3.42	1.42	1.37
24	F	201	CLA	C1D-ND	3.42	1.42	1.37
24	L	203	CLA	C1D-ND	3.42	1.42	1.37
24	5	602	CLA	C1D-ND	3.41	1.42	1.37
24	A	821	CLA	C1D-ND	3.41	1.42	1.37
24	A	847	CLA	C1D-ND	3.41	1.42	1.37
24	c	608	CLA	C1D-ND	3.41	1.42	1.37
24	6	608	CLA	C1D-ND	3.41	1.42	1.37
24	k	303	CLA	C1D-ND	3.41	1.42	1.37
24	9	304	CLA	C1D-ND	3.41	1.42	1.37
24	B	830	CLA	C1D-ND	3.41	1.42	1.37
24	B	802	CLA	C1D-ND	3.41	1.42	1.37
24	9	303	CLA	C1D-ND	3.40	1.42	1.37
24	3	306	CLA	C1D-ND	3.40	1.42	1.37
24	k	302	CLA	C1D-ND	3.40	1.42	1.37
24	2	201	CLA	C1D-ND	3.40	1.42	1.37
24	6	602	CLA	C1D-ND	3.40	1.42	1.37
24	t	305	CLA	C1D-ND	3.40	1.42	1.37
24	B	809	CLA	C1D-ND	3.40	1.42	1.37
24	4	607	CLA	C1D-ND	3.39	1.42	1.37
24	B	811	CLA	C1D-ND	3.39	1.42	1.37
24	h	606	CLA	C1D-ND	3.39	1.42	1.37
24	3	305	CLA	C4B-NB	3.39	1.42	1.37
24	8	206	CLA	C1D-ND	3.39	1.42	1.37
24	A	860	CLA	C1D-ND	3.39	1.42	1.37
24	B	832	CLA	C1D-ND	3.39	1.42	1.37
24	9	308	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	305	CLA	C1D-ND	3.38	1.42	1.37
24	5	602	CLA	C4B-NB	3.38	1.42	1.37
24	3	304	CLA	C1D-ND	3.38	1.42	1.37
24	4	613	CLA	C4B-NB	3.38	1.42	1.37
24	c	607	CLA	C1D-ND	3.38	1.42	1.37
24	L	205	CLA	C1D-ND	3.38	1.42	1.37
24	6	606	CLA	C1D-ND	3.37	1.42	1.37
24	B	828	CLA	C4B-NB	3.37	1.42	1.37
24	7	605	CLA	C4B-NB	3.37	1.42	1.37
24	A	806	CLA	C4B-NB	3.37	1.42	1.37
24	8	206	CLA	C4B-NB	3.37	1.42	1.37
24	B	836	CLA	C1D-ND	3.37	1.42	1.37
24	1	304	CLA	C1D-ND	3.37	1.42	1.37
24	8	207	CLA	C4B-NB	3.37	1.42	1.37
24	L	204	CLA	C1D-ND	3.37	1.42	1.37
24	6	601	CLA	C4B-NB	3.37	1.42	1.37
24	1	307	CLA	C4B-NB	3.36	1.42	1.37
24	B	846	CLA	C1D-ND	3.36	1.42	1.37
24	8	208	CLA	C1D-ND	3.36	1.42	1.37
24	c	602	CLA	C1D-ND	3.36	1.42	1.37
24	B	835	CLA	C1D-ND	3.36	1.42	1.37
24	F	202	CLA	C4B-NB	3.36	1.42	1.37
24	7	602	CLA	C1D-ND	3.35	1.42	1.37
24	c	601	CLA	C4B-NB	3.35	1.42	1.37
24	h	608	CLA	C1D-ND	3.35	1.42	1.37
24	c	610	CLA	C4B-NB	3.35	1.42	1.37
24	c	601	CLA	C1D-ND	3.35	1.42	1.37
24	k	304	CLA	C4B-NB	3.35	1.42	1.37
24	5	607	CLA	C4B-NB	3.34	1.42	1.37
24	6	610	CLA	C4B-NB	3.34	1.42	1.37
24	2	208	CLA	C4B-NB	3.34	1.42	1.37
24	B	826	CLA	C4B-NB	3.34	1.42	1.37
24	t	307	CLA	C4B-NB	3.34	1.42	1.37
24	4	606	CLA	C1D-ND	3.34	1.42	1.37
24	B	836	CLA	C4B-NB	3.33	1.42	1.37
24	B	825	CLA	C1D-ND	3.33	1.42	1.37
24	B	821	CLA	C1D-ND	3.32	1.42	1.37
24	B	818	CLA	C1D-ND	3.32	1.42	1.37
24	A	833	CLA	C4B-NB	3.32	1.42	1.37
24	B	848	CLA	C1D-ND	3.32	1.42	1.37
24	B	831	CLA	C4B-NB	3.31	1.42	1.37
24	8	204	CLA	C4B-NB	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	304	CLA	C4B-NB	3.31	1.42	1.37
24	R	103	CLA	C1D-ND	3.31	1.42	1.37
24	9	308	CLA	C4B-NB	3.30	1.42	1.37
24	7	608	CLA	C4B-NB	3.30	1.42	1.37
24	6	611	CLA	C1D-ND	3.30	1.42	1.37
24	2	201	CLA	C4B-NB	3.30	1.42	1.37
24	t	302	CLA	C4B-NB	3.30	1.42	1.37
24	A	813	CLA	C1D-ND	3.30	1.42	1.37
24	1	302	CLA	C1D-ND	3.29	1.42	1.37
24	2	202	CLA	C4B-NB	3.29	1.42	1.37
24	k	307	CLA	C4B-NB	3.29	1.42	1.37
24	5	606	CLA	C4B-NB	3.29	1.42	1.37
24	7	611	CLA	C4B-NB	3.29	1.42	1.37
24	A	853	CLA	C1D-ND	3.29	1.42	1.37
24	A	836	CLA	C4B-NB	3.29	1.42	1.37
24	t	309	CLA	C4B-NB	3.29	1.42	1.37
24	1	301	CLA	C4B-NB	3.29	1.42	1.37
24	4	610	CLA	C4B-NB	3.29	1.42	1.37
24	8	201	CLA	C4B-NB	3.29	1.42	1.37
24	c	605	CLA	C4B-NB	3.29	1.42	1.37
24	k	302	CLA	C4B-NB	3.28	1.42	1.37
24	4	601	CLA	C1D-ND	3.28	1.42	1.37
24	B	828	CLA	C1D-ND	3.28	1.42	1.37
24	7	609	CLA	C4B-NB	3.28	1.42	1.37
24	k	306	CLA	C1D-ND	3.28	1.42	1.37
24	4	608	CLA	C1D-ND	3.28	1.42	1.37
24	B	834	CLA	C4B-NB	3.28	1.42	1.37
24	A	834	CLA	C4B-NB	3.28	1.42	1.37
24	A	838	CLA	C4B-NB	3.27	1.42	1.37
24	B	819	CLA	C4B-NB	3.27	1.42	1.37
24	B	818	CLA	C4B-NB	3.27	1.42	1.37
24	B	830	CLA	C4B-NB	3.27	1.42	1.37
24	7	604	CLA	C1D-ND	3.27	1.42	1.37
24	h	608	CLA	C4B-NB	3.27	1.42	1.37
24	8	209	CLA	C4B-NB	3.26	1.42	1.37
24	4	601	CLA	C4B-NB	3.26	1.42	1.37
24	R	104	CLA	C1D-ND	3.26	1.42	1.37
24	6	607	CLA	C4B-NB	3.26	1.42	1.37
24	c	604	CLA	C4B-NB	3.25	1.42	1.37
24	F	201	CLA	C4B-NB	3.25	1.42	1.37
24	7	601	CLA	C4B-NB	3.25	1.42	1.37
24	h	601	CLA	C4B-NB	3.25	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	811	CLA	C4B-NB	3.25	1.42	1.37
24	2	209	CLA	C4B-NB	3.24	1.42	1.37
24	h	605	CLA	C4B-NB	3.24	1.42	1.37
24	5	603	CLA	C4B-NB	3.24	1.42	1.37
24	6	604	CLA	C4B-NB	3.24	1.42	1.37
24	9	306	CLA	C4B-NB	3.24	1.42	1.37
24	h	609	CLA	C4B-NB	3.24	1.42	1.37
24	A	808	CLA	C4B-NB	3.24	1.42	1.37
24	A	847	CLA	C4B-NB	3.23	1.42	1.37
24	A	837	CLA	C4B-NB	3.23	1.42	1.37
24	1	309	CLA	C4B-NB	3.23	1.42	1.37
24	B	817	CLA	C4B-NB	3.23	1.42	1.37
24	6	605	CLA	C4B-NB	3.23	1.42	1.37
24	B	810	CLA	CAB-C3B	-3.22	1.44	1.50
24	A	815	CLA	C4B-NB	3.22	1.42	1.37
24	B	814	CLA	C1D-ND	3.22	1.42	1.37
24	1	317	CLA	C4B-NB	3.22	1.42	1.37
24	c	606	CLA	C4B-NB	3.22	1.42	1.37
24	3	305	CLA	C1D-ND	3.21	1.42	1.37
24	9	311	CLA	C1D-ND	3.21	1.42	1.37
24	3	308	CLA	C1D-ND	3.21	1.42	1.37
24	t	301	CLA	C4B-NB	3.21	1.42	1.37
24	6	612	CLA	C4B-NB	3.21	1.42	1.37
24	5	604	CLA	C4B-NB	3.21	1.42	1.37
24	8	202	CLA	C4B-NB	3.21	1.42	1.37
24	6	602	CLA	C4B-NB	3.21	1.42	1.37
24	B	808	CLA	C4B-NB	3.20	1.42	1.37
24	c	609	CLA	C4B-NB	3.20	1.42	1.37
24	k	309	CLA	C4B-NB	3.20	1.42	1.37
24	A	814	CLA	C4B-NB	3.20	1.42	1.37
24	7	607	CLA	C4B-NB	3.20	1.42	1.37
24	5	601	CLA	C4B-NB	3.20	1.42	1.37
24	A	810	CLA	C4B-NB	3.20	1.42	1.37
24	R	103	CLA	C4B-NB	3.19	1.42	1.37
24	A	829	CLA	C4B-NB	3.19	1.42	1.37
24	c	608	CLA	C4B-NB	3.19	1.42	1.37
24	B	813	CLA	C4B-NB	3.19	1.42	1.37
24	A	818	CLA	C4B-NB	3.19	1.42	1.37
24	9	301	CLA	C4B-NB	3.18	1.42	1.37
24	A	857	CLA	C1D-ND	3.18	1.42	1.37
24	4	611	CLA	C4B-NB	3.18	1.42	1.37
24	A	811	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	307	CLA	C4B-NB	3.18	1.42	1.37
24	h	607	CLA	C4B-NB	3.18	1.42	1.37
24	B	827	CLA	C4B-NB	3.18	1.42	1.37
24	2	206	CLA	C4B-NB	3.18	1.42	1.37
24	L	204	CLA	C4B-NB	3.18	1.42	1.37
24	J	103	CLA	C4B-NB	3.18	1.42	1.37
24	t	304	CLA	C4B-NB	3.18	1.42	1.37
24	A	822	CLA	C4B-NB	3.18	1.42	1.37
24	6	608	CLA	C4B-NB	3.18	1.42	1.37
24	t	305	CLA	C4B-NB	3.17	1.42	1.37
24	5	605	CLA	C4B-NB	3.17	1.42	1.37
24	4	607	CLA	C4B-NB	3.17	1.42	1.37
24	t	310	CLA	C4B-NB	3.16	1.42	1.37
24	7	603	CLA	C4B-NB	3.16	1.42	1.37
24	B	847	CLA	C4B-NB	3.16	1.42	1.37
24	A	804	CLA	C4B-NB	3.16	1.42	1.37
24	9	306	CLA	C1D-ND	3.16	1.42	1.37
24	t	306	CLA	C4B-NB	3.15	1.42	1.37
24	4	606	CLA	C4B-NB	3.15	1.42	1.37
24	9	310	CLA	C4B-NB	3.15	1.42	1.37
24	3	309	CLA	C4B-NB	3.15	1.42	1.37
24	8	203	CLA	C4B-NB	3.15	1.42	1.37
24	A	820	CLA	C4B-NB	3.15	1.42	1.37
24	B	810	CLA	C1D-ND	3.15	1.42	1.37
24	B	832	CLA	C4B-NB	3.15	1.42	1.37
24	A	830	CLA	C4B-NB	3.14	1.42	1.37
24	k	311	CLA	C4B-NB	3.14	1.42	1.37
24	9	303	CLA	C4B-NB	3.14	1.42	1.37
24	A	856	CLA	C4B-NB	3.14	1.42	1.37
24	c	611	CLA	C4B-NB	3.14	1.42	1.37
24	B	803	CLA	C1D-ND	3.14	1.42	1.37
24	1	306	CLA	C4B-NB	3.14	1.42	1.37
24	B	846	CLA	C4B-NB	3.14	1.42	1.37
24	4	603	CLA	C4B-NB	3.13	1.42	1.37
24	3	301	CLA	C4B-NB	3.13	1.42	1.37
24	F	203	CLA	C4B-NB	3.13	1.42	1.37
24	6	606	CLA	C4B-NB	3.13	1.42	1.37
24	A	805	CLA	C4B-NB	3.13	1.42	1.37
24	B	835	CLA	C4B-NB	3.13	1.42	1.37
24	2	205	CLA	C4B-NB	3.12	1.42	1.37
24	k	305	CLA	C4B-NB	3.12	1.42	1.37
24	B	814	CLA	C4B-NB	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	603	CLA	C4B-NB	3.12	1.42	1.37
24	A	821	CLA	C4B-NB	3.12	1.42	1.37
24	h	603	CLA	C4B-NB	3.12	1.42	1.37
24	A	801	CLA	C4B-NB	3.11	1.41	1.37
24	8	205	CLA	C4B-NB	3.11	1.41	1.37
24	B	816	CLA	C4B-NB	3.11	1.41	1.37
24	h	604	CLA	C4B-NB	3.11	1.41	1.37
24	A	819	CLA	C4B-NB	3.10	1.41	1.37
24	t	303	CLA	C4B-NB	3.10	1.41	1.37
24	3	303	CLA	C4B-NB	3.10	1.41	1.37
24	6	611	CLA	C4B-NB	3.10	1.41	1.37
24	2	203	CLA	C4B-NB	3.10	1.41	1.37
24	9	307	CLA	C1D-ND	3.10	1.41	1.37
24	A	816	CLA	C4B-NB	3.10	1.41	1.37
24	3	306	CLA	C4B-NB	3.10	1.41	1.37
24	7	610	CLA	C4B-NB	3.09	1.41	1.37
24	B	822	CLA	C4B-NB	3.09	1.41	1.37
24	4	612	CLA	C4B-NB	3.09	1.41	1.37
24	8	208	CLA	C4B-NB	3.09	1.41	1.37
24	B	820	CLA	C4B-NB	3.09	1.41	1.37
24	1	303	CLA	C4B-NB	3.08	1.41	1.37
24	B	815	CLA	C4B-NB	3.08	1.41	1.37
24	A	824	CLA	C4B-NB	3.08	1.41	1.37
24	4	608	CLA	C4B-NB	3.08	1.41	1.37
24	9	311	CLA	C4B-NB	3.08	1.41	1.37
24	k	301	CLA	C4B-NB	3.07	1.41	1.37
24	B	829	CLA	C1D-ND	3.07	1.41	1.37
24	A	809	CLA	C4B-NB	3.07	1.41	1.37
24	A	813	CLA	C4B-NB	3.07	1.41	1.37
24	B	807	CLA	C4B-NB	3.07	1.41	1.37
24	A	853	CLA	C4B-NB	3.07	1.41	1.37
24	h	612	CLA	C4B-NB	3.07	1.41	1.37
24	2	207	CLA	C4B-NB	3.06	1.41	1.37
24	A	803	CLA	C4B-NB	3.06	1.41	1.37
24	A	830	CLA	C1D-ND	3.06	1.41	1.37
24	A	826	CLA	C4B-NB	3.06	1.41	1.37
24	B	825	CLA	C4B-NB	3.06	1.41	1.37
24	A	835	CLA	C4B-NB	3.06	1.41	1.37
24	4	609	CLA	C4B-NB	3.06	1.41	1.37
24	h	602	CLA	C4B-NB	3.05	1.41	1.37
24	1	304	CLA	C4B-NB	3.05	1.41	1.37
24	7	606	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	809	CLA	C4B-NB	3.05	1.41	1.37
24	A	823	CLA	C4B-NB	3.05	1.41	1.37
24	B	806	CLA	C4B-NB	3.05	1.41	1.37
24	B	848	CLA	C4B-NB	3.04	1.41	1.37
24	A	828	CLA	C4B-NB	3.03	1.41	1.37
24	k	306	CLA	C4B-NB	3.03	1.41	1.37
24	A	832	CLA	C4B-NB	3.03	1.41	1.37
24	A	827	CLA	C4B-NB	3.02	1.41	1.37
24	4	605	CLA	C4B-NB	3.02	1.41	1.37
24	7	604	CLA	C4B-NB	3.01	1.41	1.37
24	B	805	CLA	C4B-NB	3.01	1.41	1.37
24	6	609	CLA	C4B-NB	3.01	1.41	1.37
24	k	303	CLA	C4B-NB	3.00	1.41	1.37
24	A	812	CLA	C4B-NB	3.00	1.41	1.37
24	h	611	CLA	C4B-NB	3.00	1.41	1.37
24	1	305	CLA	C4B-NB	3.00	1.41	1.37
24	A	840	CLA	C4B-NB	3.00	1.41	1.37
26	7	618	DD6	C9-C8	3.00	1.42	1.34
24	9	304	CLA	C4B-NB	2.99	1.41	1.37
24	B	802	CLA	C4B-NB	2.99	1.41	1.37
24	3	302	CLA	C4B-NB	2.99	1.41	1.37
24	9	305	CLA	C4B-NB	2.99	1.41	1.37
24	c	602	CLA	C4B-NB	2.99	1.41	1.37
24	A	807	CLA	C4B-NB	2.98	1.41	1.37
24	A	831	CLA	C4B-NB	2.98	1.41	1.37
24	B	801	CLA	C4B-NB	2.98	1.41	1.37
24	7	612	CLA	C4B-NB	2.98	1.41	1.37
24	7	602	CLA	C4B-NB	2.97	1.41	1.37
24	B	823	CLA	C4B-NB	2.97	1.41	1.37
24	A	825	CLA	C4B-NB	2.97	1.41	1.37
24	3	308	CLA	C4B-NB	2.96	1.41	1.37
24	B	812	CLA	C4B-NB	2.96	1.41	1.37
24	4	602	CLA	C4B-NB	2.96	1.41	1.37
24	2	204	CLA	C4B-NB	2.95	1.41	1.37
24	B	837	CLA	C4B-NB	2.95	1.41	1.37
24	B	838	CLA	C4B-NB	2.94	1.41	1.37
24	L	205	CLA	C4B-NB	2.94	1.41	1.37
24	9	302	CLA	C4B-NB	2.94	1.41	1.37
24	h	606	CLA	C4B-NB	2.94	1.41	1.37
24	B	833	CLA	C4B-NB	2.93	1.41	1.37
24	c	603	CLA	C4B-NB	2.93	1.41	1.37
24	9	307	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	821	CLA	C4B-NB	2.92	1.41	1.37
24	9	309	CLA	C4B-NB	2.91	1.41	1.37
24	2	208	CLA	C1B-C2B	2.90	1.49	1.43
24	L	203	CLA	C4B-NB	2.89	1.41	1.37
24	A	817	CLA	C4B-NB	2.88	1.41	1.37
24	R	104	CLA	C4B-NB	2.88	1.41	1.37
24	9	305	CLA	C1B-C2B	2.88	1.49	1.43
26	8	210	DD6	C9-C8	2.88	1.42	1.34
24	A	802	CLA	C4B-NB	2.87	1.41	1.37
24	6	601	CLA	C1B-C2B	2.87	1.49	1.43
26	7	618	DD6	C25-C24	2.86	1.42	1.34
24	4	608	CLA	C1B-C2B	2.85	1.49	1.43
24	A	857	CLA	C4B-NB	2.85	1.41	1.37
24	B	829	CLA	C4B-NB	2.85	1.41	1.37
24	A	860	CLA	C4B-NB	2.84	1.41	1.37
24	A	815	CLA	C1B-C2B	2.84	1.49	1.43
24	h	607	CLA	C1B-C2B	2.84	1.49	1.43
24	B	810	CLA	C4B-NB	2.83	1.41	1.37
24	h	601	CLA	C1B-C2B	2.80	1.49	1.43
24	1	302	CLA	C4B-NB	2.80	1.41	1.37
24	k	307	CLA	C1B-C2B	2.80	1.49	1.43
24	B	837	CLA	C1B-C2B	2.80	1.49	1.43
24	3	301	CLA	C1B-C2B	2.79	1.49	1.43
24	c	607	CLA	C1B-C2B	2.79	1.49	1.43
24	t	307	CLA	C1B-C2B	2.79	1.49	1.43
26	9	317	DD6	C24-C1	-2.79	1.40	1.46
26	7	618	DD6	C10-C11	2.78	1.42	1.35
24	B	802	CLA	C1B-C2B	2.78	1.49	1.43
26	7	618	DD6	C5-C6	2.78	1.42	1.35
24	k	310	CLA	C1B-C2B	2.78	1.49	1.43
24	6	606	CLA	C1B-C2B	2.78	1.49	1.43
24	A	836	CLA	C1B-C2B	2.78	1.49	1.43
24	8	209	CLA	C1B-C2B	2.77	1.49	1.43
24	2	207	CLA	C1B-C2B	2.77	1.49	1.43
24	8	207	CLA	C1B-C2B	2.77	1.49	1.43
24	h	611	CLA	C1B-C2B	2.77	1.49	1.43
24	4	602	CLA	C1B-C2B	2.77	1.49	1.43
24	6	607	CLA	C1B-C2B	2.77	1.49	1.43
24	k	301	CLA	C1B-C2B	2.77	1.49	1.43
24	1	305	CLA	C1D-ND	2.77	1.41	1.37
24	6	608	CLA	C1B-C2B	2.77	1.49	1.43
24	A	801	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	t	304	CLA	C1B-C2B	2.76	1.49	1.43
24	8	205	CLA	C1B-C2B	2.76	1.49	1.43
24	6	612	CLA	C1B-C2B	2.76	1.49	1.43
26	t	313	DD6	C24-C1	-2.75	1.40	1.46
24	A	832	CLA	C1B-C2B	2.75	1.49	1.43
24	1	309	CLA	C1B-C2B	2.75	1.49	1.43
24	A	814	CLA	C1B-C2B	2.75	1.49	1.43
26	6	615	DD6	C24-C1	-2.75	1.40	1.46
24	c	610	CLA	C1B-C2B	2.75	1.49	1.43
24	A	806	CLA	C1B-C2B	2.75	1.49	1.43
24	k	308	CLA	C1B-C2B	2.74	1.49	1.43
24	B	804	CLA	C4B-NB	2.74	1.41	1.37
26	8	210	DD6	C25-C24	2.74	1.41	1.34
24	4	606	CLA	C1B-C2B	2.74	1.49	1.43
26	7	616	DD6	C25-C24	2.74	1.41	1.34
26	9	314	DD6	C25-C24	2.74	1.41	1.34
24	4	607	CLA	C1B-C2B	2.74	1.49	1.43
24	c	602	CLA	C1B-C2B	2.74	1.49	1.43
24	4	601	CLA	C1B-C2B	2.74	1.49	1.43
24	3	307	CLA	C1B-C2B	2.74	1.49	1.43
24	3	302	CLA	C1B-C2B	2.74	1.49	1.43
24	t	309	CLA	C1B-C2B	2.74	1.49	1.43
24	7	605	CLA	C1B-C2B	2.73	1.49	1.43
24	A	816	CLA	C1B-C2B	2.73	1.49	1.43
24	5	606	CLA	C1B-C2B	2.73	1.49	1.43
24	B	821	CLA	C1B-C2B	2.73	1.49	1.43
25	B	843	BCR	C1-C6	-2.73	1.50	1.53
24	A	809	CLA	C1B-C2B	2.72	1.49	1.43
24	A	823	CLA	C1B-C2B	2.72	1.49	1.43
24	1	306	CLA	C1B-C2B	2.72	1.49	1.43
24	R	103	CLA	C1B-C2B	2.72	1.49	1.43
24	B	805	CLA	C1B-C2B	2.72	1.49	1.43
24	8	201	CLA	C1B-C2B	2.72	1.49	1.43
24	B	813	CLA	C1B-C2B	2.72	1.49	1.43
26	6	614	DD6	C9-C8	2.72	1.41	1.34
24	6	604	CLA	C1B-C2B	2.72	1.49	1.43
26	7	618	DD6	C2-C1	2.72	1.42	1.35
24	c	609	CLA	C1B-C2B	2.71	1.49	1.43
24	t	310	CLA	C1B-C2B	2.71	1.49	1.43
24	2	209	CLA	C1B-C2B	2.71	1.49	1.43
26	9	314	DD6	C9-C8	2.71	1.41	1.34
24	4	609	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	206	CLA	C1B-C2B	2.71	1.49	1.43
24	5	601	CLA	C1B-C2B	2.71	1.49	1.43
24	5	605	CLA	C1B-C2B	2.71	1.49	1.43
24	6	610	CLA	C1B-C2B	2.70	1.49	1.43
24	5	607	CLA	C1B-C2B	2.70	1.49	1.43
24	t	306	CLA	C1B-C2B	2.70	1.49	1.43
24	8	204	CLA	C1B-C2B	2.70	1.49	1.43
24	t	303	CLA	C1B-C2B	2.70	1.49	1.43
24	B	835	CLA	C1B-C2B	2.70	1.49	1.43
24	3	309	CLA	C1B-C2B	2.70	1.49	1.43
24	F	203	CLA	C1B-C2B	2.70	1.49	1.43
24	4	605	CLA	C1B-C2B	2.69	1.49	1.43
24	7	609	CLA	C1B-C2B	2.69	1.49	1.43
24	1	307	CLA	C1B-C2B	2.69	1.49	1.43
26	A	848	DD6	C8-C6	-2.69	1.40	1.46
26	1	311	DD6	C9-C8	2.69	1.41	1.34
24	A	804	CLA	C1B-C2B	2.69	1.49	1.43
24	A	805	CLA	C1B-C2B	2.69	1.49	1.43
24	A	807	CLA	C1B-C2B	2.69	1.49	1.43
24	7	608	CLA	C1B-C2B	2.69	1.49	1.43
24	k	309	CLA	C1B-C2B	2.69	1.49	1.43
24	2	204	CLA	C1B-C2B	2.69	1.49	1.43
24	5	603	CLA	C1B-C2B	2.69	1.49	1.43
24	c	611	CLA	C1B-C2B	2.69	1.49	1.43
24	c	607	CLA	C4B-NB	2.69	1.41	1.37
24	4	613	CLA	C1B-C2B	2.69	1.49	1.43
24	B	827	CLA	C1B-C2B	2.69	1.49	1.43
24	A	826	CLA	C1B-C2B	2.68	1.49	1.43
24	A	831	CLA	C1B-C2B	2.68	1.49	1.43
24	h	604	CLA	C1B-C2B	2.68	1.49	1.43
24	t	302	CLA	C1B-C2B	2.68	1.49	1.43
24	2	203	CLA	C1B-C2B	2.68	1.49	1.43
24	L	204	CLA	C1B-C2B	2.68	1.49	1.43
26	A	848	DD6	C13-C11	-2.68	1.40	1.46
24	c	605	CLA	C1B-C2B	2.68	1.49	1.43
24	A	810	CLA	C1B-C2B	2.68	1.49	1.43
24	9	309	CLA	C1B-C2B	2.67	1.49	1.43
24	1	308	CLA	C1B-C2B	2.67	1.49	1.43
24	B	801	CLA	C1B-C2B	2.67	1.49	1.43
24	B	825	CLA	C1B-C2B	2.67	1.49	1.43
24	t	301	CLA	C1B-C2B	2.67	1.49	1.43
24	B	807	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	203	CLA	C1B-C2B	2.67	1.49	1.43
24	B	834	CLA	C1B-C2B	2.67	1.49	1.43
24	5	604	CLA	C1B-C2B	2.67	1.49	1.43
24	h	609	CLA	C1B-C2B	2.67	1.49	1.43
24	h	605	CLA	C1B-C2B	2.67	1.49	1.43
24	A	829	CLA	C1B-C2B	2.67	1.49	1.43
26	k	315	DD6	C24-C1	-2.66	1.40	1.46
24	c	604	CLA	C1B-C2B	2.66	1.49	1.43
24	h	606	CLA	C1B-C2B	2.66	1.49	1.43
26	9	314	DD6	C2-C1	2.66	1.41	1.35
24	B	822	CLA	C1B-C2B	2.66	1.49	1.43
24	9	307	CLA	C1B-C2B	2.65	1.49	1.43
24	A	821	CLA	C1B-C2B	2.65	1.49	1.43
24	B	824	CLA	C3B-C4B	2.65	1.50	1.42
24	4	610	CLA	C1B-C2B	2.65	1.49	1.43
24	6	603	CLA	C1B-C2B	2.65	1.49	1.43
24	B	846	CLA	C1B-C2B	2.65	1.49	1.43
24	c	606	CLA	C1B-C2B	2.65	1.49	1.43
24	A	838	CLA	C1B-C2B	2.65	1.49	1.43
24	L	205	CLA	C1B-C2B	2.65	1.49	1.43
24	A	840	CLA	C1B-C2B	2.65	1.49	1.43
24	B	847	CLA	C1B-C2B	2.65	1.49	1.43
24	B	819	CLA	C1B-C2B	2.65	1.49	1.43
24	3	303	CLA	C1B-C2B	2.65	1.49	1.43
24	A	819	CLA	C1B-C2B	2.65	1.49	1.43
24	F	201	CLA	C1B-C2B	2.65	1.49	1.43
24	7	610	CLA	C1B-C2B	2.64	1.49	1.43
24	1	301	CLA	C1B-C2B	2.64	1.49	1.43
24	A	824	CLA	C1B-C2B	2.64	1.49	1.43
24	h	608	CLA	C1B-C2B	2.64	1.49	1.43
24	A	825	CLA	C1B-C2B	2.63	1.49	1.43
26	9	317	DD6	C13-C11	-2.63	1.40	1.46
24	6	602	CLA	C1B-C2B	2.63	1.49	1.43
24	t	308	CLA	C3B-C4B	2.63	1.50	1.42
24	6	605	CLA	C1B-C2B	2.63	1.49	1.43
24	h	602	CLA	C1B-C2B	2.63	1.49	1.43
24	A	837	CLA	C1B-C2B	2.63	1.49	1.43
24	7	601	CLA	C1B-C2B	2.63	1.49	1.43
24	h	610	CLA	C1B-C2B	2.63	1.49	1.43
26	1	311	DD6	C25-C24	2.63	1.41	1.34
24	B	817	CLA	C1B-C2B	2.63	1.49	1.43
24	A	828	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	206	CLA	C1B-C2B	2.63	1.49	1.43
24	J	103	CLA	C1B-C2B	2.62	1.49	1.43
24	1	303	CLA	C1B-C2B	2.62	1.49	1.43
24	A	833	CLA	C1B-C2B	2.62	1.49	1.43
24	B	828	CLA	C1B-C2B	2.62	1.49	1.43
24	B	814	CLA	CMB-C2B	-2.62	1.45	1.50
24	k	305	CLA	C1B-C2B	2.62	1.49	1.43
24	3	306	CLA	C1B-C2B	2.62	1.49	1.43
24	B	809	CLA	C1B-C2B	2.62	1.49	1.43
26	t	311	DD6	C25-C24	2.62	1.41	1.34
29	2	213	A1L1G	C33-C34	-2.62	1.40	1.46
26	c	614	DD6	C13-C11	-2.61	1.40	1.46
26	8	210	DD6	C2-C1	2.61	1.41	1.35
24	B	848	CLA	C1B-C2B	2.61	1.49	1.43
26	9	313	DD6	C9-C8	2.61	1.41	1.34
24	c	608	CLA	C1B-C2B	2.61	1.49	1.43
24	B	833	CLA	C1B-C2B	2.61	1.49	1.43
26	t	313	DD6	C8-C6	-2.61	1.40	1.46
24	1	317	CLA	C1B-C2B	2.61	1.49	1.43
26	9	315	DD6	C25-C24	2.61	1.41	1.34
24	2	205	CLA	C1B-C2B	2.61	1.49	1.43
29	7	614	A1L1G	C41-C40	2.61	1.41	1.34
26	8	210	DD6	C10-C11	2.61	1.41	1.35
24	A	822	CLA	C1B-C2B	2.60	1.49	1.43
24	B	808	CLA	C1B-C2B	2.60	1.49	1.43
24	A	835	CLA	C1B-C2B	2.60	1.49	1.43
24	A	808	CLA	C1B-C2B	2.60	1.49	1.43
24	9	308	CLA	C1B-C2B	2.60	1.49	1.43
24	B	820	CLA	C1B-C2B	2.60	1.49	1.43
24	1	302	CLA	C1B-C2B	2.60	1.49	1.43
26	7	616	DD6	C2-C1	2.60	1.41	1.35
26	k	315	DD6	C8-C6	-2.60	1.40	1.46
24	k	302	CLA	C1B-C2B	2.60	1.49	1.43
26	4	616	DD6	C13-C11	-2.60	1.40	1.46
26	A	848	DD6	C24-C1	-2.59	1.40	1.46
24	1	305	CLA	C1B-C2B	2.59	1.49	1.43
24	6	609	CLA	C1B-C2B	2.59	1.49	1.43
24	7	612	CLA	C1B-C2B	2.59	1.49	1.43
26	9	317	DD6	C8-C6	-2.59	1.40	1.46
26	6	614	DD6	C25-C24	2.59	1.41	1.34
24	4	612	CLA	C1B-C2B	2.59	1.49	1.43
24	A	802	CLA	C1D-ND	2.59	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	308	CLA	C3B-C4B	2.58	1.50	1.42
24	B	815	CLA	C1B-C2B	2.58	1.49	1.43
26	6	615	DD6	C8-C6	-2.58	1.40	1.46
24	2	201	CLA	C1B-C2B	2.58	1.49	1.43
26	6	613	DD6	C8-C6	-2.58	1.40	1.46
24	1	305	CLA	CMD-C2D	-2.58	1.45	1.50
26	7	616	DD6	C9-C8	2.58	1.41	1.34
24	4	603	CLA	C1B-C2B	2.58	1.49	1.43
24	B	806	CLA	C1B-C2B	2.58	1.49	1.43
24	k	311	CLA	C1B-C2B	2.58	1.49	1.43
24	8	208	CLA	C1B-C2B	2.58	1.49	1.43
24	9	304	CLA	C1B-C2B	2.57	1.49	1.43
24	6	611	CLA	C1B-C2B	2.57	1.49	1.43
26	1	312	DD6	C25-C24	2.57	1.41	1.34
26	4	617	DD6	C24-C1	-2.57	1.40	1.46
24	h	603	CLA	C1B-C2B	2.57	1.49	1.43
24	k	303	CLA	C1B-C2B	2.57	1.49	1.43
24	t	305	CLA	C1B-C2B	2.57	1.49	1.43
26	9	314	DD6	C10-C11	2.57	1.41	1.35
26	7	613	DD6	C24-C1	-2.57	1.40	1.46
26	4	615	DD6	C25-C24	2.57	1.41	1.34
26	h	615	DD6	C24-C1	-2.57	1.40	1.46
24	7	607	CLA	C1B-C2B	2.56	1.49	1.43
24	4	611	CLA	C1B-C2B	2.56	1.49	1.43
24	A	813	CLA	C1B-C2B	2.56	1.49	1.43
24	A	817	CLA	C1B-C2B	2.56	1.49	1.43
24	A	834	CLA	C1B-C2B	2.56	1.49	1.43
24	B	823	CLA	C1B-C2B	2.56	1.49	1.43
29	9	312	A1L1G	C41-C40	2.56	1.41	1.34
24	B	831	CLA	C3B-C4B	2.56	1.50	1.42
24	B	832	CLA	C1B-C2B	2.56	1.49	1.43
24	1	304	CLA	C1B-C2B	2.56	1.49	1.43
24	k	306	CLA	C1B-C2B	2.55	1.49	1.43
24	A	811	CLA	C1B-C2B	2.55	1.49	1.43
24	3	305	CLA	C3B-C4B	2.55	1.50	1.42
26	7	615	DD6	C24-C1	-2.55	1.40	1.46
24	A	812	CLA	C1B-C2B	2.55	1.49	1.43
24	B	810	CLA	C4B-C3B	2.55	1.49	1.43
26	6	613	DD6	C13-C11	-2.55	1.40	1.46
24	8	202	CLA	C1B-C2B	2.54	1.49	1.43
24	B	812	CLA	C1B-C2B	2.54	1.49	1.43
24	B	830	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	616	DD6	C13-C11	-2.54	1.40	1.46
26	t	313	DD6	C13-C11	-2.54	1.40	1.46
26	2	212	DD6	C25-C24	2.54	1.41	1.34
24	F	202	CLA	C1B-C2B	2.54	1.49	1.43
26	9	315	DD6	C9-C8	2.54	1.41	1.34
24	t	301	CLA	C3B-C4B	2.54	1.50	1.42
26	6	616	DD6	C25-C24	2.54	1.41	1.34
24	R	104	CLA	C1B-C2B	2.53	1.49	1.43
26	7	615	DD6	C8-C6	-2.53	1.40	1.46
26	7	616	DD6	C5-C6	2.53	1.41	1.35
26	8	210	DD6	C5-C6	2.53	1.41	1.35
26	c	613	DD6	C13-C11	-2.53	1.40	1.46
26	k	313	DD6	C24-C1	-2.53	1.40	1.46
26	h	614	DD6	C9-C8	2.53	1.41	1.34
26	t	311	DD6	C9-C8	2.53	1.41	1.34
24	A	830	CLA	C1B-C2B	2.53	1.49	1.43
24	9	306	CLA	C1B-C2B	2.53	1.49	1.43
24	A	847	CLA	C1B-C2B	2.53	1.49	1.43
24	2	202	CLA	C1B-C2B	2.53	1.49	1.43
24	8	203	CLA	C1B-C2B	2.53	1.49	1.43
26	3	312	DD6	C8-C6	-2.53	1.40	1.46
26	2	210	DD6	C13-C11	-2.53	1.40	1.46
24	7	611	CLA	C1B-C2B	2.53	1.49	1.43
26	c	612	DD6	C25-C24	2.53	1.41	1.34
26	6	614	DD6	C5-C6	2.52	1.41	1.35
24	4	610	CLA	C3B-C4B	2.52	1.50	1.42
29	7	614	A1L1G	C42-C44	2.52	1.41	1.35
24	B	838	CLA	C1B-C2B	2.52	1.49	1.43
24	B	804	CLA	C3B-C4B	2.52	1.50	1.42
24	A	860	CLA	C1B-C2B	2.52	1.49	1.43
24	5	602	CLA	C3B-C4B	2.52	1.50	1.42
26	4	616	DD6	C8-C6	-2.51	1.40	1.46
24	B	831	CLA	C1B-C2B	2.51	1.49	1.43
29	9	312	A1L1G	C42-C44	2.51	1.41	1.35
26	h	616	DD6	C9-C8	2.51	1.41	1.34
24	t	308	CLA	C1B-C2B	2.51	1.49	1.43
24	B	811	CLA	C1B-C2B	2.51	1.49	1.43
26	7	613	DD6	C13-C11	-2.51	1.40	1.46
24	B	803	CLA	CMC-C2C	-2.51	1.45	1.50
26	c	614	DD6	C8-C6	-2.51	1.40	1.46
24	7	606	CLA	C1B-C2B	2.51	1.49	1.43
26	8	211	DD6	C8-C6	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	310	CLA	C1B-C2B	2.51	1.49	1.43
24	A	818	CLA	C1B-C2B	2.51	1.49	1.43
24	k	304	CLA	C1B-C2B	2.51	1.49	1.43
24	F	202	CLA	C3B-C4B	2.50	1.50	1.42
24	A	853	CLA	C1B-C2B	2.50	1.49	1.43
26	3	312	DD6	C13-C11	-2.50	1.40	1.46
26	1	312	DD6	C9-C8	2.50	1.41	1.34
26	4	617	DD6	C13-C11	-2.50	1.40	1.46
24	t	303	CLA	C3B-C4B	2.50	1.50	1.42
26	8	211	DD6	C25-C24	2.50	1.41	1.34
26	4	615	DD6	C9-C8	2.50	1.41	1.34
26	c	612	DD6	C24-C1	-2.50	1.40	1.46
26	6	613	DD6	C24-C1	-2.49	1.40	1.46
26	5	609	DD6	C8-C6	-2.49	1.40	1.46
26	3	313	DD6	C25-C24	2.49	1.41	1.34
24	3	305	CLA	C1B-C2B	2.49	1.49	1.43
24	A	803	CLA	C1B-C2B	2.49	1.49	1.43
26	2	210	DD6	C25-C24	2.49	1.41	1.34
26	h	613	DD6	C24-C1	-2.49	1.40	1.46
26	c	613	DD6	C24-C1	-2.49	1.40	1.46
24	c	601	CLA	C3B-C4B	2.49	1.50	1.42
26	5	609	DD6	C24-C1	-2.49	1.40	1.46
26	3	313	DD6	C9-C8	2.49	1.41	1.34
26	7	613	DD6	C8-C6	-2.49	1.40	1.46
24	A	857	CLA	C1B-C2B	2.49	1.49	1.43
24	7	603	CLA	C3B-C4B	2.49	1.50	1.42
25	R	101	BCR	C30-C25	-2.49	1.50	1.53
26	h	613	DD6	C8-C6	-2.48	1.40	1.46
26	R	105	DD6	C25-C24	2.48	1.41	1.34
24	9	308	CLA	C3B-C4B	2.48	1.50	1.42
24	A	856	CLA	C1B-C2B	2.48	1.48	1.43
29	3	310	A1L1G	C33-C34	-2.48	1.40	1.46
24	B	810	CLA	C1B-C2B	2.48	1.48	1.43
24	7	602	CLA	C1B-C2B	2.47	1.48	1.43
26	9	313	DD6	C25-C24	2.47	1.41	1.34
26	8	211	DD6	C13-C11	-2.47	1.40	1.46
24	9	302	CLA	C1B-C2B	2.47	1.48	1.43
26	5	608	DD6	C13-C11	-2.47	1.40	1.46
29	2	213	A1L1G	C41-C40	2.47	1.41	1.34
24	7	604	CLA	C1B-C2B	2.47	1.48	1.43
24	9	301	CLA	C1B-C2B	2.47	1.48	1.43
24	9	311	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	312	DD6	C24-C1	-2.47	1.40	1.46
26	4	617	DD6	C8-C6	-2.47	1.40	1.46
26	6	615	DD6	C13-C11	-2.47	1.40	1.46
24	B	811	CLA	C3B-C4B	2.47	1.49	1.42
29	9	312	A1L1G	C32-C33	2.46	1.41	1.34
26	c	613	DD6	C8-C6	-2.46	1.40	1.46
26	7	615	DD6	C13-C11	-2.46	1.40	1.46
24	B	836	CLA	C1B-C2B	2.46	1.48	1.43
26	5	608	DD6	C24-C1	-2.46	1.40	1.46
26	k	313	DD6	C13-C11	-2.46	1.40	1.46
29	k	312	A1L1G	C41-C40	2.46	1.41	1.34
26	9	314	DD6	C5-C6	2.46	1.41	1.35
26	J	102	DD6	C9-C8	2.46	1.41	1.34
24	7	607	CLA	C3B-C4B	2.46	1.49	1.42
26	6	613	DD6	C25-C24	2.46	1.41	1.34
24	c	601	CLA	C1B-C2B	2.46	1.48	1.43
29	7	614	A1L1G	C33-C34	-2.46	1.40	1.46
26	2	212	DD6	C13-C11	-2.46	1.40	1.46
26	5	608	DD6	C8-C6	-2.46	1.40	1.46
29	3	310	A1L1G	C40-C39	-2.46	1.40	1.46
24	B	816	CLA	C1B-C2B	2.45	1.48	1.43
24	A	827	CLA	C1B-C2B	2.45	1.48	1.43
24	B	803	CLA	C4B-NB	2.45	1.41	1.37
26	4	614	DD6	C13-C11	-2.45	1.40	1.46
24	3	308	CLA	C1B-C2B	2.45	1.48	1.43
24	B	826	CLA	C1B-C2B	2.45	1.48	1.43
24	1	305	CLA	CMB-C2B	-2.45	1.45	1.50
26	6	614	DD6	C10-C11	2.45	1.41	1.35
24	B	829	CLA	C1B-C2B	2.45	1.48	1.43
24	7	608	CLA	C3B-C4B	2.45	1.49	1.42
26	4	614	DD6	C9-C8	2.45	1.41	1.34
24	8	202	CLA	C3B-C4B	2.45	1.49	1.42
24	9	301	CLA	C3B-C4B	2.44	1.49	1.42
24	B	803	CLA	C1B-C2B	2.44	1.48	1.43
26	6	617	DD6	C24-C1	-2.44	1.40	1.46
24	1	307	CLA	C3B-C4B	2.44	1.49	1.42
26	h	615	DD6	C8-C6	-2.44	1.40	1.46
26	1	311	DD6	C10-C11	2.44	1.41	1.35
24	c	603	CLA	C1B-C2B	2.44	1.48	1.43
26	6	614	DD6	C2-C1	2.44	1.41	1.35
26	k	313	DD6	C8-C6	-2.44	1.40	1.46
24	h	602	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	609	DD6	C13-C11	-2.43	1.40	1.46
26	R	105	DD6	C8-C6	-2.43	1.40	1.46
26	h	613	DD6	C25-C24	2.43	1.41	1.34
26	1	311	DD6	C2-C1	2.43	1.41	1.35
26	5	608	DD6	C9-C8	2.43	1.41	1.34
26	c	614	DD6	C24-C1	-2.43	1.40	1.46
26	7	616	DD6	C10-C11	2.43	1.41	1.35
26	3	311	DD6	C8-C6	-2.43	1.40	1.46
24	A	820	CLA	C1B-C2B	2.43	1.48	1.43
24	7	603	CLA	CHC-C1C	2.43	1.43	1.38
24	A	838	CLA	C3B-C4B	2.43	1.49	1.42
26	k	315	DD6	C25-C24	2.43	1.41	1.34
26	J	102	DD6	C24-C1	-2.43	1.40	1.46
24	A	833	CLA	C3B-C4B	2.43	1.49	1.42
26	1	313	DD6	C25-C24	2.43	1.41	1.34
26	3	311	DD6	C13-C11	-2.43	1.40	1.46
26	2	210	DD6	C8-C6	-2.42	1.40	1.46
26	6	616	DD6	C9-C8	2.42	1.41	1.34
26	6	617	DD6	C9-C8	2.42	1.41	1.34
26	R	105	DD6	C24-C1	-2.42	1.40	1.46
26	h	614	DD6	C24-C1	-2.42	1.40	1.46
24	A	802	CLA	C3B-C4B	2.42	1.49	1.42
26	1	313	DD6	C8-C6	-2.42	1.40	1.46
26	8	212	DD6	C8-C6	-2.42	1.40	1.46
24	4	611	CLA	C3B-C4B	2.42	1.49	1.42
26	h	613	DD6	C13-C11	-2.42	1.40	1.46
26	k	314	DD6	C8-C6	-2.42	1.40	1.46
29	2	213	A1L1G	C42-C44	2.41	1.41	1.35
26	1	313	DD6	C24-C1	-2.41	1.40	1.46
26	h	616	DD6	C25-C24	2.41	1.41	1.34
24	t	302	CLA	C3B-C4B	2.41	1.49	1.42
26	6	616	DD6	C24-C1	-2.41	1.40	1.46
24	B	826	CLA	C3B-C4B	2.41	1.49	1.42
24	B	824	CLA	C1B-C2B	2.41	1.48	1.43
24	A	853	CLA	CMD-C2D	-2.41	1.45	1.50
24	A	857	CLA	CMD-C2D	-2.41	1.45	1.50
24	3	304	CLA	C3B-C4B	2.41	1.49	1.42
26	k	314	DD6	C13-C11	-2.40	1.40	1.46
24	A	830	CLA	CMB-C2B	-2.40	1.45	1.50
24	k	302	CLA	C3B-C4B	2.40	1.49	1.42
26	6	616	DD6	C8-C6	-2.40	1.40	1.46
24	B	818	CLA	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	311	DD6	C2-C1	2.40	1.41	1.35
26	6	617	DD6	C25-C24	2.40	1.40	1.34
24	9	303	CLA	C3B-C4B	2.40	1.49	1.42
26	J	102	DD6	C13-C11	-2.40	1.40	1.46
24	A	860	CLA	CMC-C2C	-2.40	1.45	1.50
26	1	311	DD6	C5-C6	2.39	1.41	1.35
29	k	312	A1L1G	C32-C33	2.39	1.40	1.34
26	c	612	DD6	C8-C6	-2.39	1.40	1.46
26	5	609	DD6	C25-C24	2.39	1.40	1.34
26	8	212	DD6	C24-C1	-2.39	1.40	1.46
29	k	312	A1L1G	C42-C44	2.39	1.41	1.35
26	9	315	DD6	C2-C1	2.39	1.41	1.35
29	2	213	A1L1G	C40-C39	-2.39	1.40	1.46
24	A	834	CLA	C3B-C4B	2.39	1.49	1.42
26	8	211	DD6	C9-C8	2.39	1.40	1.34
29	3	310	A1L1G	C42-C44	2.39	1.41	1.35
26	4	616	DD6	C25-C24	2.39	1.40	1.34
24	k	311	CLA	C3B-C4B	2.39	1.49	1.42
29	3	310	A1L1G	C41-C40	2.39	1.40	1.34
24	B	804	CLA	CHC-C1C	2.39	1.43	1.38
26	c	612	DD6	C13-C11	-2.39	1.40	1.46
24	5	602	CLA	C1B-C2B	2.39	1.48	1.43
26	4	614	DD6	C24-C1	-2.39	1.40	1.46
26	k	315	DD6	C13-C11	-2.39	1.40	1.46
26	J	102	DD6	C8-C6	-2.39	1.40	1.46
24	A	811	CLA	C3B-C4B	2.39	1.49	1.42
24	4	604	CLA	C3B-C4B	2.39	1.49	1.42
26	3	311	DD6	C25-C24	2.39	1.40	1.34
26	J	102	DD6	C25-C24	2.38	1.40	1.34
26	t	311	DD6	C10-C11	2.38	1.41	1.35
26	8	210	DD6	C13-C11	-2.38	1.40	1.46
26	h	613	DD6	C9-C8	2.38	1.40	1.34
26	6	617	DD6	C8-C6	-2.38	1.40	1.46
26	1	312	DD6	C2-C1	2.38	1.41	1.35
26	1	313	DD6	C9-C8	2.38	1.40	1.34
24	9	303	CLA	C1B-C2B	2.38	1.48	1.43
26	2	212	DD6	C9-C8	2.38	1.40	1.34
26	2	210	DD6	C24-C1	-2.38	1.40	1.46
24	B	805	CLA	C3B-C4B	2.38	1.49	1.42
26	2	212	DD6	C8-C6	-2.38	1.40	1.46
24	7	612	CLA	C3B-C4B	2.38	1.49	1.42
24	2	201	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	616	DD6	C5-C6	2.38	1.41	1.35
24	B	812	CLA	C3B-C4B	2.37	1.49	1.42
24	2	201	CLA	C3B-C4B	2.37	1.49	1.42
26	9	317	DD6	C9-C8	2.37	1.40	1.34
24	h	609	CLA	C3B-C4B	2.37	1.49	1.42
24	2	202	CLA	C3B-C4B	2.37	1.49	1.42
24	B	812	CLA	CHC-C1C	2.37	1.43	1.38
26	k	313	DD6	C9-C8	2.37	1.40	1.34
26	9	313	DD6	C5-C6	2.37	1.41	1.35
26	3	312	DD6	C25-C24	2.37	1.40	1.34
29	k	312	A1L1G	C33-C34	-2.37	1.40	1.46
24	k	310	CLA	C3B-C4B	2.37	1.49	1.42
24	A	808	CLA	C3B-C4B	2.37	1.49	1.42
24	8	206	CLA	C3B-C4B	2.37	1.49	1.42
26	4	616	DD6	C9-C8	2.37	1.40	1.34
24	h	612	CLA	C1B-C2B	2.37	1.48	1.43
26	k	314	DD6	C25-C24	2.37	1.40	1.34
26	4	617	DD6	C9-C8	2.37	1.40	1.34
26	h	615	DD6	C13-C11	-2.37	1.40	1.46
24	A	826	CLA	C3B-C4B	2.36	1.49	1.42
24	A	820	CLA	C3B-C4B	2.36	1.49	1.42
24	7	612	CLA	CHC-C1C	2.36	1.43	1.38
24	A	837	CLA	C3B-C4B	2.36	1.49	1.42
24	h	603	CLA	C3B-C4B	2.36	1.49	1.42
24	c	603	CLA	C3B-C4B	2.36	1.49	1.42
26	3	313	DD6	C2-C1	2.36	1.41	1.35
26	c	614	DD6	C9-C8	2.36	1.40	1.34
24	A	803	CLA	C3B-C4B	2.36	1.49	1.42
26	8	211	DD6	C24-C1	-2.36	1.40	1.46
26	h	616	DD6	C10-C11	2.36	1.41	1.35
24	5	602	CLA	CHC-C1C	2.36	1.43	1.38
24	1	304	CLA	C3B-C4B	2.36	1.49	1.42
26	8	212	DD6	C25-C24	2.36	1.40	1.34
26	c	613	DD6	C25-C24	2.36	1.40	1.34
26	1	312	DD6	C5-C6	2.36	1.41	1.35
24	A	805	CLA	C3B-C4B	2.36	1.49	1.42
24	A	818	CLA	C3B-C4B	2.36	1.49	1.42
24	7	609	CLA	C3B-C4B	2.35	1.49	1.42
24	k	309	CLA	C3B-C4B	2.35	1.49	1.42
26	9	315	DD6	C10-C11	2.35	1.41	1.35
24	9	303	CLA	CMB-C2B	-2.35	1.45	1.50
24	1	317	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	612	DD6	C9-C8	2.35	1.40	1.34
24	5	607	CLA	C3B-C4B	2.35	1.49	1.42
24	B	819	CLA	C3B-C4B	2.35	1.49	1.42
29	7	614	A1L1G	C32-C33	2.35	1.40	1.34
24	A	812	CLA	C3B-C4B	2.35	1.49	1.42
24	9	311	CLA	C3B-C4B	2.35	1.49	1.42
24	5	603	CLA	C3B-C4B	2.35	1.49	1.42
29	k	312	A1L1G	C40-C39	-2.35	1.40	1.46
24	A	806	CLA	C3B-C4B	2.34	1.49	1.42
26	h	614	DD6	C10-C11	2.34	1.41	1.35
26	8	212	DD6	C9-C8	2.34	1.40	1.34
26	9	315	DD6	C5-C6	2.34	1.41	1.35
24	A	804	CLA	C3B-C4B	2.34	1.49	1.42
24	A	827	CLA	C3B-C4B	2.34	1.49	1.42
26	k	313	DD6	C25-C24	2.34	1.40	1.34
24	4	604	CLA	C1B-C2B	2.34	1.48	1.43
26	3	311	DD6	C9-C8	2.34	1.40	1.34
26	5	608	DD6	C25-C24	2.34	1.40	1.34
24	2	207	CLA	C3B-C4B	2.34	1.49	1.42
24	c	604	CLA	C3B-C4B	2.34	1.49	1.42
26	k	314	DD6	C9-C8	2.34	1.40	1.34
29	3	310	A1L1G	C32-C33	2.34	1.40	1.34
24	B	806	CLA	CHC-C1C	2.34	1.43	1.38
24	6	612	CLA	C3B-C4B	2.34	1.49	1.42
24	A	824	CLA	C3B-C4B	2.34	1.49	1.42
26	c	614	DD6	C25-C24	2.34	1.40	1.34
24	B	825	CLA	C3B-C4B	2.33	1.49	1.42
26	4	615	DD6	C10-C11	2.33	1.41	1.35
26	6	613	DD6	C9-C8	2.33	1.40	1.34
24	7	606	CLA	CMB-C2B	-2.33	1.46	1.50
24	9	302	CLA	C3B-C4B	2.33	1.49	1.42
24	7	602	CLA	C3B-C4B	2.33	1.49	1.42
24	F	201	CLA	C3B-C4B	2.33	1.49	1.42
26	k	314	DD6	C24-C1	-2.33	1.41	1.46
26	4	617	DD6	C25-C24	2.33	1.40	1.34
26	R	105	DD6	C9-C8	2.33	1.40	1.34
24	t	305	CLA	C3B-C4B	2.33	1.49	1.42
24	A	853	CLA	C3B-C4B	2.33	1.49	1.42
24	B	836	CLA	C3B-C4B	2.33	1.49	1.42
26	5	609	DD6	C9-C8	2.33	1.40	1.34
26	6	617	DD6	C13-C11	-2.33	1.41	1.46
24	B	828	CLA	CMD-C2D	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	614	DD6	C13-C11	-2.33	1.41	1.46
24	4	604	CLA	CMB-C2B	-2.33	1.46	1.50
24	B	817	CLA	C3B-C4B	2.33	1.49	1.42
24	6	611	CLA	CMD-C2D	-2.33	1.46	1.50
24	B	813	CLA	C3B-C4B	2.33	1.49	1.42
26	1	313	DD6	C13-C11	-2.33	1.41	1.46
26	4	614	DD6	C8-C6	-2.33	1.41	1.46
24	7	603	CLA	C1B-C2B	2.33	1.48	1.43
26	4	616	DD6	C24-C1	-2.33	1.41	1.46
24	B	806	CLA	C3B-C4B	2.32	1.49	1.42
24	B	815	CLA	C3B-C4B	2.32	1.49	1.42
24	6	609	CLA	CHC-C1C	2.32	1.43	1.38
26	2	210	DD6	C9-C8	2.32	1.40	1.34
24	B	818	CLA	C3B-C4B	2.32	1.49	1.42
24	A	815	CLA	C3B-C4B	2.32	1.49	1.42
26	h	615	DD6	C9-C8	2.32	1.40	1.34
26	6	616	DD6	C10-C11	2.32	1.41	1.35
24	h	610	CLA	C3B-C4B	2.32	1.49	1.42
24	A	802	CLA	CMC-C2C	-2.32	1.46	1.50
29	2	213	A1L1G	C32-C33	2.32	1.40	1.34
24	6	602	CLA	C3B-C4B	2.32	1.49	1.42
26	3	311	DD6	C24-C1	-2.32	1.41	1.46
24	t	301	CLA	CHC-C1C	2.32	1.43	1.38
24	6	606	CLA	C3B-C4B	2.32	1.49	1.42
26	c	613	DD6	C9-C8	2.31	1.40	1.34
24	k	303	CLA	C3B-C4B	2.31	1.49	1.42
24	4	611	CLA	CHC-C1C	2.31	1.43	1.38
24	4	609	CLA	C3B-C4B	2.31	1.49	1.42
24	k	311	CLA	CHC-C1C	2.31	1.43	1.38
24	B	808	CLA	C3B-C4B	2.31	1.49	1.42
24	B	835	CLA	C3B-C4B	2.31	1.49	1.42
24	t	309	CLA	C3B-C4B	2.31	1.49	1.42
26	h	614	DD6	C25-C24	2.31	1.40	1.34
26	9	315	DD6	C24-C1	-2.31	1.41	1.46
26	4	614	DD6	C25-C24	2.31	1.40	1.34
24	4	602	CLA	C3B-C4B	2.31	1.49	1.42
24	5	604	CLA	C3B-C4B	2.31	1.49	1.42
24	5	605	CLA	C3B-C4B	2.31	1.49	1.42
24	5	606	CLA	C3B-C4B	2.31	1.49	1.42
24	B	809	CLA	CMB-C2B	-2.31	1.46	1.50
24	6	604	CLA	C3B-C4B	2.30	1.49	1.42
26	1	312	DD6	C10-C11	2.30	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	312	DD6	C8-C6	-2.30	1.41	1.46
26	t	311	DD6	C5-C6	2.30	1.41	1.35
26	7	613	DD6	C9-C8	2.30	1.40	1.34
24	t	304	CLA	C3B-C4B	2.30	1.49	1.42
24	1	303	CLA	C3B-C4B	2.30	1.49	1.42
24	4	609	CLA	CMC-C2C	-2.30	1.46	1.50
24	8	207	CLA	C3B-C4B	2.30	1.49	1.42
24	B	848	CLA	C3B-C4B	2.30	1.49	1.42
26	9	313	DD6	C2-C1	2.30	1.41	1.35
24	h	604	CLA	C3B-C4B	2.30	1.49	1.42
24	9	306	CLA	C3B-C4B	2.30	1.49	1.42
24	k	307	CLA	C3B-C4B	2.30	1.49	1.42
24	2	209	CLA	C3B-C4B	2.30	1.49	1.42
24	c	603	CLA	CHC-C1C	2.29	1.43	1.38
24	A	813	CLA	C3B-C4B	2.29	1.49	1.42
24	9	301	CLA	CMD-C2D	-2.29	1.46	1.50
24	A	822	CLA	C3B-C4B	2.29	1.49	1.42
26	7	618	DD6	C13-C14	2.29	1.37	1.32
24	4	612	CLA	C3B-C4B	2.29	1.49	1.42
26	9	313	DD6	C10-C11	2.29	1.41	1.35
24	7	602	CLA	CHC-C1C	2.29	1.43	1.38
26	3	312	DD6	C9-C8	2.29	1.40	1.34
24	B	814	CLA	C1B-C2B	2.29	1.48	1.43
24	B	832	CLA	C3B-C4B	2.29	1.49	1.42
24	k	306	CLA	C3B-C4B	2.29	1.49	1.42
26	7	615	DD6	C9-C8	2.29	1.40	1.34
24	c	606	CLA	C3B-C4B	2.29	1.49	1.42
24	A	847	CLA	C3B-C4B	2.29	1.49	1.42
24	5	601	CLA	C3B-C4B	2.29	1.49	1.42
24	c	605	CLA	C3B-C4B	2.29	1.49	1.42
26	2	212	DD6	C2-C1	2.29	1.41	1.35
24	8	208	CLA	C3B-C4B	2.29	1.49	1.42
24	6	601	CLA	C3B-C4B	2.29	1.49	1.42
24	L	203	CLA	C3B-C4B	2.29	1.49	1.42
24	k	302	CLA	CHC-C1C	2.29	1.43	1.38
24	7	607	CLA	CHC-C1C	2.28	1.43	1.38
26	7	613	DD6	C25-C24	2.28	1.40	1.34
26	R	105	DD6	C2-C1	2.28	1.41	1.35
24	3	308	CLA	C3B-C4B	2.28	1.49	1.42
26	8	212	DD6	C13-C11	-2.28	1.41	1.46
25	I	101	BCR	C30-C25	-2.28	1.50	1.53
24	B	826	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	103	CLA	C3B-C4B	2.28	1.49	1.42
26	4	615	DD6	C5-C6	2.28	1.41	1.35
24	6	610	CLA	C3B-C4B	2.28	1.49	1.42
24	A	820	CLA	CHC-C1C	2.28	1.43	1.38
24	6	605	CLA	C3B-C4B	2.28	1.49	1.42
24	c	609	CLA	C3B-C4B	2.28	1.49	1.42
26	9	313	DD6	C24-C1	-2.28	1.41	1.46
24	B	817	CLA	CHC-C1C	2.28	1.43	1.38
24	7	601	CLA	C3B-C4B	2.28	1.49	1.42
24	B	834	CLA	C3B-C4B	2.28	1.49	1.42
24	3	309	CLA	C3B-C4B	2.28	1.49	1.42
24	R	103	CLA	C3B-C4B	2.28	1.49	1.42
26	6	617	DD6	C5-C6	2.28	1.41	1.35
24	h	605	CLA	C3B-C4B	2.28	1.49	1.42
24	B	847	CLA	C3B-C4B	2.27	1.49	1.42
24	2	205	CLA	CMB-C2B	-2.27	1.46	1.50
24	c	610	CLA	C3B-C4B	2.27	1.49	1.42
26	6	617	DD6	C2-C1	2.27	1.41	1.35
26	h	616	DD6	C2-C1	2.27	1.41	1.35
24	8	201	CLA	C3B-C4B	2.27	1.49	1.42
24	A	821	CLA	C3B-C4B	2.27	1.49	1.42
24	t	310	CLA	C3B-C4B	2.27	1.49	1.42
24	9	301	CLA	CHC-C1C	2.27	1.43	1.38
24	B	828	CLA	C3B-C4B	2.27	1.49	1.42
24	t	306	CLA	C3B-C4B	2.27	1.49	1.42
24	k	305	CLA	C3B-C4B	2.27	1.49	1.42
24	3	306	CLA	C3B-C4B	2.27	1.49	1.42
26	h	616	DD6	C13-C11	-2.27	1.41	1.46
24	A	809	CLA	C3B-C4B	2.27	1.49	1.42
24	A	810	CLA	C3B-C4B	2.27	1.49	1.42
24	A	802	CLA	CMD-C2D	-2.27	1.46	1.50
24	7	610	CLA	C3B-C4B	2.26	1.49	1.42
24	F	203	CLA	C3B-C4B	2.26	1.49	1.42
24	B	832	CLA	CHC-C1C	2.26	1.43	1.38
24	A	802	CLA	CMB-C2B	-2.26	1.46	1.50
26	9	313	DD6	C8-C6	-2.26	1.41	1.46
26	9	315	DD6	C13-C11	-2.26	1.41	1.46
24	t	307	CLA	C3B-C4B	2.26	1.49	1.42
24	9	310	CLA	CMB-C2B	-2.26	1.46	1.50
24	2	203	CLA	C3B-C4B	2.26	1.49	1.42
24	c	608	CLA	C3B-C4B	2.26	1.49	1.42
26	7	615	DD6	C25-C24	2.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	313	DD6	C8-C6	-2.26	1.41	1.46
24	8	209	CLA	C3B-C4B	2.26	1.49	1.42
26	4	615	DD6	C2-C1	2.26	1.41	1.35
24	4	613	CLA	C3B-C4B	2.26	1.49	1.42
26	h	616	DD6	C8-C6	-2.26	1.41	1.46
24	A	814	CLA	C3B-C4B	2.26	1.49	1.42
24	A	835	CLA	C3B-C4B	2.26	1.49	1.42
29	9	312	A1L1G	C38-C39	2.26	1.41	1.35
24	h	607	CLA	C3B-C4B	2.26	1.49	1.42
24	A	805	CLA	CHC-C1C	2.25	1.43	1.38
26	R	105	DD6	C5-C6	2.25	1.41	1.35
24	h	611	CLA	CMD-C2D	-2.25	1.46	1.50
26	h	614	DD6	C8-C6	-2.25	1.41	1.46
24	k	307	CLA	CHC-C1C	2.25	1.43	1.38
26	3	313	DD6	C13-C11	-2.25	1.41	1.46
24	B	829	CLA	CMD-C2D	-2.25	1.46	1.50
26	t	311	DD6	C13-C11	-2.25	1.41	1.46
26	h	616	DD6	C24-C1	-2.25	1.41	1.46
26	h	615	DD6	C25-C24	2.25	1.40	1.34
26	h	614	DD6	C5-C6	2.25	1.41	1.35
24	B	831	CLA	CHC-C1C	2.25	1.43	1.38
26	3	311	DD6	C2-C1	2.25	1.41	1.35
26	4	614	DD6	C10-C11	2.25	1.41	1.35
29	9	312	A1L1G	C33-C34	-2.25	1.41	1.46
24	A	826	CLA	CHC-C1C	2.25	1.43	1.38
24	B	801	CLA	CMD-C2D	-2.25	1.46	1.50
24	c	611	CLA	C3B-C4B	2.25	1.49	1.42
24	A	825	CLA	C3B-C4B	2.25	1.49	1.42
24	A	840	CLA	C3B-C4B	2.24	1.49	1.42
24	A	829	CLA	CMB-C2B	-2.24	1.46	1.50
26	k	315	DD6	C2-C1	2.24	1.41	1.35
24	c	601	CLA	CHC-C1C	2.24	1.43	1.38
24	9	302	CLA	CMD-C2D	-2.24	1.46	1.50
24	h	608	CLA	C3B-C4B	2.24	1.49	1.42
26	1	312	DD6	C24-C1	-2.24	1.41	1.46
24	2	206	CLA	C3B-C4B	2.24	1.49	1.42
24	7	605	CLA	C3B-C4B	2.24	1.49	1.42
24	B	825	CLA	CHC-C1C	2.24	1.43	1.38
24	B	820	CLA	C3B-C4B	2.24	1.49	1.42
26	3	313	DD6	C10-C11	2.24	1.41	1.35
24	5	603	CLA	CHC-C1C	2.24	1.43	1.38
26	2	210	DD6	C2-C1	2.24	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	829	CLA	C3B-C4B	2.24	1.49	1.42
26	3	313	DD6	C24-C1	-2.24	1.41	1.46
26	k	314	DD6	C26-C27	2.24	1.41	1.37
24	1	301	CLA	C3B-C4B	2.24	1.49	1.42
24	7	611	CLA	C3B-C4B	2.24	1.49	1.42
24	1	309	CLA	C3B-C4B	2.24	1.49	1.42
24	A	816	CLA	C3B-C4B	2.24	1.49	1.42
24	B	830	CLA	C3B-C4B	2.24	1.49	1.42
26	8	212	DD6	C2-C1	2.24	1.41	1.35
24	A	817	CLA	C3B-C4B	2.24	1.49	1.42
24	L	204	CLA	C3B-C4B	2.24	1.49	1.42
24	1	302	CLA	CMB-C2B	-2.24	1.46	1.50
24	6	603	CLA	C3B-C4B	2.24	1.49	1.42
24	6	611	CLA	C3B-C4B	2.24	1.49	1.42
24	B	829	CLA	C3B-C4B	2.23	1.49	1.42
24	B	827	CLA	C3B-C4B	2.23	1.49	1.42
26	A	848	DD6	C9-C8	2.23	1.40	1.34
24	3	301	CLA	C3B-C4B	2.23	1.49	1.42
26	3	313	DD6	C5-C6	2.23	1.41	1.35
26	6	613	DD6	C2-C1	2.23	1.41	1.35
26	4	615	DD6	C8-C6	-2.23	1.41	1.46
24	A	856	CLA	C3B-C4B	2.23	1.49	1.42
24	B	833	CLA	C3B-C4B	2.23	1.49	1.42
24	8	203	CLA	C3B-C4B	2.23	1.49	1.42
26	5	608	DD6	C5-C6	2.23	1.41	1.35
26	t	311	DD6	C8-C6	-2.23	1.41	1.46
24	9	304	CLA	C3B-C4B	2.23	1.49	1.42
24	B	823	CLA	C3B-C4B	2.23	1.49	1.42
29	7	614	A1L1G	C38-C39	2.23	1.41	1.35
24	L	205	CLA	C3B-C4B	2.23	1.49	1.42
25	A	846	BCR	C1-C6	-2.23	1.50	1.53
24	A	860	CLA	C3B-C4B	2.23	1.49	1.42
24	B	830	CLA	CMB-C2B	-2.23	1.46	1.50
24	4	603	CLA	CMB-C2B	-2.23	1.46	1.50
24	h	608	CLA	CMB-C2B	-2.22	1.46	1.50
24	6	607	CLA	C3B-C4B	2.22	1.49	1.42
24	A	822	CLA	CHC-C1C	2.22	1.42	1.38
24	A	830	CLA	CMD-C2D	-2.22	1.46	1.50
24	6	611	CLA	CMC-C2C	-2.22	1.46	1.50
24	3	302	CLA	C3B-C4B	2.22	1.49	1.42
24	h	611	CLA	C3B-C4B	2.22	1.49	1.42
24	A	828	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	612	CLA	CHC-C1C	2.22	1.42	1.38
24	7	611	CLA	CMB-C2B	-2.22	1.46	1.50
24	h	612	CLA	CMB-C2B	-2.22	1.46	1.50
24	1	302	CLA	CMD-C2D	-2.22	1.46	1.50
24	B	819	CLA	CHC-C1C	2.22	1.42	1.38
26	4	615	DD6	C24-C1	-2.22	1.41	1.46
24	3	303	CLA	C3B-C4B	2.22	1.49	1.42
24	h	606	CLA	C3B-C4B	2.22	1.49	1.42
26	2	212	DD6	C10-C11	2.22	1.40	1.35
24	5	604	CLA	CHC-C1C	2.22	1.42	1.38
24	A	804	CLA	CHC-C1C	2.22	1.42	1.38
24	2	208	CLA	C3B-C4B	2.22	1.49	1.42
24	8	204	CLA	C3B-C4B	2.22	1.49	1.42
24	c	604	CLA	CHC-C1C	2.22	1.42	1.38
24	h	609	CLA	CHC-C1C	2.22	1.42	1.38
24	B	807	CLA	C3B-C4B	2.22	1.49	1.42
24	4	603	CLA	C3B-C4B	2.22	1.49	1.42
26	8	211	DD6	C2-C1	2.21	1.40	1.35
24	A	808	CLA	CHC-C1C	2.21	1.42	1.38
26	2	212	DD6	C24-C1	-2.21	1.41	1.46
29	7	614	A1L1G	C35-C34	2.21	1.40	1.35
26	t	313	DD6	C25-C24	2.21	1.40	1.34
24	B	822	CLA	C3B-C4B	2.21	1.49	1.42
24	A	802	CLA	CHC-C1C	2.21	1.42	1.38
24	B	805	CLA	CHC-C1C	2.21	1.42	1.38
26	J	102	DD6	C10-C11	2.21	1.40	1.35
26	R	105	DD6	C13-C14	2.21	1.37	1.32
26	h	614	DD6	C2-C1	2.21	1.40	1.35
24	4	607	CLA	C3B-C4B	2.21	1.49	1.42
24	A	827	CLA	CHC-C1C	2.21	1.42	1.38
24	L	203	CLA	CHC-C1C	2.21	1.42	1.38
24	4	608	CLA	C3B-C4B	2.21	1.49	1.42
24	B	818	CLA	CMB-C2B	-2.21	1.46	1.50
26	6	615	DD6	C9-C8	2.21	1.40	1.34
24	B	835	CLA	CHC-C1C	2.21	1.42	1.38
24	B	838	CLA	C3B-C4B	2.21	1.49	1.42
29	3	310	A1L1G	C29-C30	-2.21	1.40	1.45
24	h	601	CLA	C3B-C4B	2.21	1.49	1.42
24	1	306	CLA	C3B-C4B	2.21	1.49	1.42
26	4	614	DD6	C5-C6	2.21	1.40	1.35
24	h	605	CLA	CMB-C2B	-2.21	1.46	1.50
26	k	315	DD6	C9-C8	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	t	306	CLA	CHC-C1C	2.21	1.42	1.38
26	1	313	DD6	C5-C6	2.20	1.40	1.35
26	J	102	DD6	C5-C6	2.20	1.40	1.35
24	1	308	CLA	CHC-C1C	2.20	1.42	1.38
24	2	207	CLA	CHC-C1C	2.20	1.42	1.38
26	6	617	DD6	C10-C11	2.20	1.40	1.35
29	9	312	A1L1G	C35-C34	2.20	1.40	1.35
24	A	803	CLA	CHC-C1C	2.20	1.42	1.38
24	A	807	CLA	C3B-C4B	2.20	1.49	1.42
24	B	824	CLA	CHC-C1C	2.20	1.42	1.38
24	4	601	CLA	C3B-C4B	2.20	1.49	1.42
24	B	832	CLA	CMB-C2B	-2.20	1.46	1.50
26	2	212	DD6	C5-C6	2.20	1.40	1.35
24	4	603	CLA	CHC-C1C	2.20	1.42	1.38
24	B	808	CLA	CHC-C1C	2.20	1.42	1.38
24	A	831	CLA	C3B-C4B	2.20	1.49	1.42
24	B	815	CLA	CHC-C1C	2.20	1.42	1.38
24	A	860	CLA	CMD-C2D	-2.20	1.46	1.50
26	c	614	DD6	C10-C11	2.20	1.40	1.35
24	B	816	CLA	C3B-C4B	2.20	1.49	1.42
24	L	204	CLA	CMB-C2B	-2.20	1.46	1.50
24	2	209	CLA	CHC-C1C	2.20	1.42	1.38
26	t	313	DD6	C9-C8	2.20	1.40	1.34
24	k	304	CLA	CMB-C2B	-2.19	1.46	1.50
26	A	848	DD6	C25-C24	2.19	1.40	1.34
26	4	617	DD6	C5-C6	2.19	1.40	1.35
24	k	310	CLA	CHC-C1C	2.19	1.42	1.38
24	k	301	CLA	C3B-C4B	2.19	1.49	1.42
24	B	836	CLA	CHC-C1C	2.19	1.42	1.38
24	2	205	CLA	C3B-C4B	2.19	1.49	1.42
24	7	601	CLA	CMD-C2D	-2.19	1.46	1.50
24	1	308	CLA	C3B-C4B	2.19	1.49	1.42
24	A	834	CLA	CHC-C1C	2.19	1.42	1.38
26	8	212	DD6	C5-C6	2.19	1.40	1.35
24	B	814	CLA	C3B-C4B	2.19	1.49	1.42
24	B	838	CLA	CHC-C1C	2.19	1.42	1.38
24	A	812	CLA	CMC-C2C	-2.19	1.46	1.50
24	3	307	CLA	C3B-C4B	2.19	1.49	1.42
26	h	615	DD6	C2-C1	2.19	1.40	1.35
26	9	313	DD6	C13-C11	-2.18	1.41	1.46
26	4	616	DD6	C2-C1	2.18	1.40	1.35
26	8	211	DD6	C10-C11	2.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	609	CLA	C3B-C4B	2.18	1.49	1.42
24	9	310	CLA	C3B-C4B	2.18	1.49	1.42
24	A	821	CLA	CHC-C1C	2.18	1.42	1.38
26	4	615	DD6	C13-C11	-2.18	1.41	1.46
24	A	818	CLA	CMB-C2B	-2.18	1.46	1.50
24	t	305	CLA	CHC-C1C	2.18	1.42	1.38
26	7	616	DD6	C13-C11	-2.18	1.41	1.46
24	F	202	CLA	CHC-C1C	2.18	1.42	1.38
24	9	309	CLA	C3B-C4B	2.18	1.49	1.42
24	B	847	CLA	CMB-C2B	-2.18	1.46	1.50
24	B	848	CLA	CHC-C1C	2.18	1.42	1.38
24	4	604	CLA	CHC-C1C	2.18	1.42	1.38
24	B	833	CLA	CMB-C2B	-2.18	1.46	1.50
24	k	304	CLA	C3B-C4B	2.18	1.49	1.42
24	4	606	CLA	CHC-C1C	2.18	1.42	1.38
29	2	213	A1L1G	C38-C39	2.18	1.40	1.35
24	9	305	CLA	CMB-C2B	-2.18	1.46	1.50
24	7	604	CLA	C3B-C4B	2.17	1.49	1.42
24	A	812	CLA	CHC-C1C	2.17	1.42	1.38
24	A	840	CLA	CHC-C1C	2.17	1.42	1.38
26	4	614	DD6	C2-C1	2.17	1.40	1.35
24	A	837	CLA	CHC-C1C	2.17	1.42	1.38
24	1	317	CLA	CHC-C1C	2.17	1.42	1.38
26	1	313	DD6	C2-C1	2.17	1.40	1.35
24	3	309	CLA	CHC-C1C	2.17	1.42	1.38
24	A	838	CLA	CHC-C1C	2.17	1.42	1.38
24	R	104	CLA	CMC-C2C	-2.17	1.46	1.50
26	4	616	DD6	C5-C6	2.17	1.40	1.35
29	7	614	A1L1G	C40-C39	-2.17	1.41	1.46
24	6	602	CLA	CHC-C1C	2.17	1.42	1.38
24	9	308	CLA	CMB-C2B	-2.17	1.46	1.50
26	8	210	DD6	C13-C14	2.17	1.37	1.32
24	t	309	CLA	CHC-C1C	2.17	1.42	1.38
24	A	847	CLA	CHC-C1C	2.17	1.42	1.38
26	1	313	DD6	C10-C11	2.17	1.40	1.35
24	A	819	CLA	C3B-C4B	2.17	1.49	1.42
24	B	846	CLA	C3B-C4B	2.16	1.49	1.42
26	6	613	DD6	C5-C6	2.16	1.40	1.35
24	B	829	CLA	CMB-C2B	-2.16	1.46	1.50
24	4	608	CLA	CHC-C1C	2.16	1.42	1.38
26	9	314	DD6	C13-C14	2.16	1.37	1.32
26	1	312	DD6	C13-C11	-2.16	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	606	CLA	C3B-C4B	2.16	1.49	1.42
24	6	608	CLA	C3B-C4B	2.16	1.49	1.42
24	c	602	CLA	C3B-C4B	2.16	1.49	1.42
24	c	602	CLA	CHC-C1C	2.16	1.42	1.38
24	B	834	CLA	CHC-C1C	2.16	1.42	1.38
24	4	605	CLA	C3B-C4B	2.16	1.49	1.42
24	B	810	CLA	CMB-C2B	-2.16	1.46	1.50
24	8	208	CLA	CMD-C2D	-2.16	1.46	1.50
24	h	605	CLA	CHC-C1C	2.16	1.42	1.38
24	A	853	CLA	CHC-C1C	2.16	1.42	1.38
24	7	604	CLA	CMB-C2B	-2.16	1.46	1.50
26	6	615	DD6	C25-C24	2.16	1.40	1.34
24	B	813	CLA	CHC-C1C	2.16	1.42	1.38
26	3	311	DD6	C5-C6	2.16	1.40	1.35
24	h	603	CLA	CHC-C1C	2.16	1.42	1.38
26	6	614	DD6	C13-C11	-2.16	1.41	1.46
24	1	308	CLA	CMB-C2B	-2.16	1.46	1.50
26	9	315	DD6	C8-C6	-2.16	1.41	1.46
24	A	815	CLA	CHC-C1C	2.16	1.42	1.38
24	B	818	CLA	CHC-C1C	2.16	1.42	1.38
24	7	610	CLA	CHC-C1C	2.16	1.42	1.38
24	B	821	CLA	CMD-C2D	-2.15	1.46	1.50
24	t	303	CLA	CHC-C1C	2.15	1.42	1.38
26	J	102	DD6	C2-C1	2.15	1.40	1.35
24	A	836	CLA	C3B-C4B	2.15	1.49	1.42
26	h	613	DD6	C2-C1	2.15	1.40	1.35
24	A	832	CLA	C3B-C4B	2.15	1.49	1.42
24	R	104	CLA	CMD-C2D	-2.15	1.46	1.50
24	4	606	CLA	C3B-C4B	2.15	1.49	1.42
24	A	820	CLA	CMB-C2B	-2.15	1.46	1.50
26	8	210	DD6	C24-C1	-2.15	1.41	1.46
24	1	305	CLA	C3B-C4B	2.15	1.49	1.42
26	k	314	DD6	C10-C11	2.15	1.40	1.35
24	A	836	CLA	CMB-C2B	-2.15	1.46	1.50
24	R	104	CLA	C3B-C4B	2.15	1.49	1.42
26	R	105	DD6	C36-C31	-2.15	1.32	1.35
29	7	614	A1L1G	C29-C30	-2.15	1.40	1.45
26	h	613	DD6	C10-C11	2.15	1.40	1.35
24	A	814	CLA	CHC-C1C	2.15	1.42	1.38
24	A	856	CLA	CHC-C1C	2.15	1.42	1.38
24	4	612	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	824	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	306	CLA	CHC-C1C	2.15	1.42	1.38
24	2	204	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	828	CLA	CHC-C1C	2.15	1.42	1.38
26	3	311	DD6	C10-C11	2.15	1.40	1.35
24	2	206	CLA	CHC-C1C	2.15	1.42	1.38
24	B	823	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	801	CLA	C3B-C4B	2.15	1.49	1.42
24	4	601	CLA	CMD-C2D	-2.15	1.46	1.50
25	2	211	BCR	C1-C6	-2.15	1.51	1.53
24	t	304	CLA	CHC-C1C	2.15	1.42	1.38
24	B	821	CLA	CHC-C1C	2.15	1.42	1.38
24	B	810	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	823	CLA	CHC-C1C	2.15	1.42	1.38
24	B	809	CLA	C3B-C4B	2.14	1.49	1.42
24	c	611	CLA	CMB-C2B	-2.14	1.46	1.50
24	6	607	CLA	CHC-C1C	2.14	1.42	1.38
24	k	309	CLA	CHC-C1C	2.14	1.42	1.38
24	3	308	CLA	CMB-C2B	-2.14	1.46	1.50
24	9	305	CLA	C3B-C4B	2.14	1.49	1.42
24	c	606	CLA	CHC-C1C	2.14	1.42	1.38
24	B	811	CLA	CMD-C2D	-2.14	1.46	1.50
24	9	307	CLA	C3B-C4B	2.14	1.49	1.42
24	A	813	CLA	CHC-C1C	2.14	1.42	1.38
24	B	801	CLA	CMB-C2B	-2.14	1.46	1.50
24	A	857	CLA	C3B-C4B	2.14	1.49	1.42
24	A	806	CLA	CHC-C1C	2.14	1.42	1.38
24	9	302	CLA	CHC-C1C	2.14	1.42	1.38
26	9	317	DD6	C25-C24	2.14	1.40	1.34
26	c	613	DD6	C2-C1	2.14	1.40	1.35
29	9	312	A1L1G	C40-C39	-2.14	1.41	1.46
24	3	306	CLA	CHC-C1C	2.14	1.42	1.38
26	R	105	DD6	C13-C11	-2.14	1.41	1.46
24	5	606	CLA	CHC-C1C	2.14	1.42	1.38
26	3	312	DD6	C2-C1	2.14	1.40	1.35
26	5	608	DD6	C2-C1	2.14	1.40	1.35
24	9	311	CLA	CMD-C2D	-2.14	1.46	1.50
24	9	304	CLA	CHC-C1C	2.14	1.42	1.38
24	c	605	CLA	CHC-C1C	2.14	1.42	1.38
24	A	824	CLA	CHC-C1C	2.14	1.42	1.38
24	t	304	CLA	CMD-C2D	-2.14	1.46	1.50
24	h	604	CLA	CHC-C1C	2.14	1.42	1.38
26	5	608	DD6	C10-C11	2.14	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	829	CLA	CHC-C1C	2.14	1.42	1.38
28	1	318	LHG	O7-C5	-2.14	1.41	1.46
24	A	813	CLA	CMD-C2D	-2.14	1.46	1.50
24	h	612	CLA	C3B-C4B	2.14	1.49	1.42
24	c	608	CLA	CHC-C1C	2.14	1.42	1.38
24	6	605	CLA	CHC-C1C	2.14	1.42	1.38
24	B	837	CLA	C3B-C4B	2.14	1.49	1.42
24	L	204	CLA	CHC-C1C	2.14	1.42	1.38
24	5	605	CLA	CHC-C1C	2.13	1.42	1.38
24	A	817	CLA	CHC-C1C	2.13	1.42	1.38
25	A	845	BCR	C30-C25	-2.13	1.51	1.53
24	B	811	CLA	CHC-C1C	2.13	1.42	1.38
24	8	207	CLA	CHC-C1C	2.13	1.42	1.38
24	c	611	CLA	CHC-C1C	2.13	1.42	1.38
24	F	201	CLA	CHC-C1C	2.13	1.42	1.38
24	J	103	CLA	CHC-C1C	2.13	1.42	1.38
24	A	801	CLA	C3B-C4B	2.13	1.49	1.42
24	4	610	CLA	CHC-C1C	2.13	1.42	1.38
24	4	607	CLA	CHC-C1C	2.13	1.42	1.38
24	3	302	CLA	CHC-C1C	2.13	1.42	1.38
24	9	303	CLA	CMD-C2D	-2.13	1.46	1.50
24	B	827	CLA	CHC-C1C	2.13	1.42	1.38
26	t	311	DD6	C24-C1	-2.13	1.41	1.46
26	c	612	DD6	C10-C11	2.13	1.40	1.35
26	6	616	DD6	C2-C1	2.13	1.40	1.35
24	t	305	CLA	CMB-C2B	-2.13	1.46	1.50
24	B	821	CLA	C3B-C4B	2.13	1.48	1.42
24	B	822	CLA	CMB-C2B	-2.13	1.46	1.50
24	A	818	CLA	CHC-C1C	2.13	1.42	1.38
24	A	823	CLA	C3B-C4B	2.12	1.48	1.42
26	k	313	DD6	C5-C6	2.12	1.40	1.35
24	B	847	CLA	CHC-C1C	2.12	1.42	1.38
26	2	210	DD6	C5-C6	2.12	1.40	1.35
29	k	312	A1L1G	C38-C39	2.12	1.40	1.35
24	1	301	CLA	CHC-C1C	2.12	1.42	1.38
24	A	809	CLA	CHC-C1C	2.12	1.42	1.38
24	7	608	CLA	CHC-C1C	2.12	1.42	1.38
24	9	307	CLA	CMC-C2C	-2.12	1.46	1.50
24	A	832	CLA	CMB-C2B	-2.12	1.46	1.50
26	5	609	DD6	C5-C6	2.12	1.40	1.35
26	9	317	DD6	C5-C6	2.12	1.40	1.35
24	R	103	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	803	CLA	CMB-C2B	-2.12	1.46	1.50
26	k	314	DD6	C5-C6	2.12	1.40	1.35
26	7	616	DD6	C8-C6	-2.12	1.41	1.46
26	7	615	DD6	C5-C6	2.12	1.40	1.35
24	B	803	CLA	CMD-C2D	-2.12	1.46	1.50
24	9	311	CLA	CHC-C1C	2.12	1.42	1.38
24	B	826	CLA	CHC-C1C	2.12	1.42	1.38
24	8	205	CLA	C3B-C4B	2.12	1.48	1.42
24	6	604	CLA	CHC-C1C	2.12	1.42	1.38
26	h	613	DD6	C5-C6	2.12	1.40	1.35
25	4	618	BCR	C30-C25	-2.12	1.51	1.53
24	h	607	CLA	CHC-C1C	2.12	1.42	1.38
24	k	303	CLA	CHC-C1C	2.12	1.42	1.38
24	A	828	CLA	CHC-C1C	2.12	1.42	1.38
24	A	822	CLA	CMB-C2B	-2.12	1.46	1.50
24	t	310	CLA	CHC-C1C	2.12	1.42	1.38
26	6	616	DD6	C5-C6	2.12	1.40	1.35
24	k	305	CLA	CHC-C1C	2.11	1.42	1.38
24	2	203	CLA	CHC-C1C	2.11	1.42	1.38
24	9	308	CLA	CMD-C2D	-2.11	1.46	1.50
24	4	601	CLA	CHC-C1C	2.11	1.42	1.38
24	B	808	CLA	CMC-C2C	-2.11	1.46	1.50
29	2	213	A1L1G	C35-C34	2.11	1.40	1.35
26	5	609	DD6	C2-C1	2.11	1.40	1.35
26	c	613	DD6	C5-C6	2.11	1.40	1.35
24	9	307	CLA	CMD-C2D	-2.11	1.46	1.50
24	1	304	CLA	CHC-C1C	2.11	1.42	1.38
24	1	304	CLA	CMD-C2D	-2.11	1.46	1.50
24	9	306	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	860	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	823	CLA	CHC-C1C	2.11	1.42	1.38
24	3	301	CLA	CHC-C1C	2.11	1.42	1.38
25	B	840	BCR	C30-C25	-2.11	1.51	1.53
24	B	846	CLA	CMB-C2B	-2.11	1.46	1.50
26	4	617	DD6	C10-C11	2.11	1.40	1.35
24	7	604	CLA	CMD-C2D	-2.11	1.46	1.50
24	9	304	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	801	CLA	CMD-C2D	-2.11	1.46	1.50
24	B	804	CLA	CMB-C2B	-2.11	1.46	1.50
26	5	609	DD6	C10-C11	2.11	1.40	1.35
26	8	211	DD6	C5-C6	2.11	1.40	1.35
24	B	814	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	602	CLA	CHC-C1C	2.10	1.42	1.38
24	8	203	CLA	CMB-C2B	-2.10	1.46	1.50
24	3	308	CLA	CHC-C1C	2.10	1.42	1.38
24	4	602	CLA	CHC-C1C	2.10	1.42	1.38
24	B	820	CLA	CHC-C1C	2.10	1.42	1.38
24	B	829	CLA	CMC-C2C	-2.10	1.46	1.50
24	L	205	CLA	CMD-C2D	-2.10	1.46	1.50
24	h	608	CLA	CHC-C1C	2.10	1.42	1.38
26	k	313	DD6	C2-C1	2.10	1.40	1.35
24	1	317	CLA	CMB-C2B	-2.10	1.46	1.50
24	A	833	CLA	CHC-C1C	2.10	1.42	1.38
25	t	312	BCR	C1-C6	-2.10	1.51	1.53
24	A	824	CLA	CMD-C2D	-2.10	1.46	1.50
26	6	614	DD6	C24-C1	-2.10	1.41	1.46
26	2	210	DD6	C10-C11	2.10	1.40	1.35
26	k	313	DD6	C10-C11	2.10	1.40	1.35
24	6	604	CLA	CMD-C2D	-2.10	1.46	1.50
24	B	836	CLA	CMB-C2B	-2.10	1.46	1.50
25	A	844	BCR	C1-C6	-2.09	1.51	1.53
25	B	842	BCR	C1-C6	-2.09	1.51	1.53
24	k	307	CLA	CMD-C2D	-2.09	1.46	1.50
24	B	820	CLA	CMB-C2B	-2.09	1.46	1.50
24	6	609	CLA	CMC-C2C	-2.09	1.46	1.50
24	h	607	CLA	CMB-C2B	-2.09	1.46	1.50
24	A	857	CLA	CMC-C2C	-2.09	1.46	1.50
24	5	607	CLA	MG-NC	2.09	2.11	2.06
26	k	314	DD6	C2-C1	2.09	1.40	1.35
24	h	606	CLA	CMB-C2B	-2.09	1.46	1.50
24	k	306	CLA	CMB-C2B	-2.09	1.46	1.50
24	9	310	CLA	CMD-C2D	-2.09	1.46	1.50
24	R	103	CLA	CMD-C2D	-2.09	1.46	1.50
24	6	603	CLA	CHC-C1C	2.09	1.42	1.38
26	c	614	DD6	C2-C1	2.09	1.40	1.35
24	A	831	CLA	CHC-C1C	2.09	1.42	1.38
24	1	309	CLA	CHC-C1C	2.09	1.42	1.38
24	3	305	CLA	CHC-C1C	2.09	1.42	1.38
24	2	204	CLA	C3B-C4B	2.09	1.48	1.42
26	1	311	DD6	C8-C6	-2.09	1.41	1.46
26	c	613	DD6	C10-C11	2.09	1.40	1.35
24	A	813	CLA	CMB-C2B	-2.08	1.46	1.50
26	1	311	DD6	C13-C11	-2.08	1.41	1.46
24	A	835	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	201	CLA	CHC-C1C	2.08	1.42	1.38
24	t	308	CLA	CHC-C1C	2.08	1.42	1.38
24	B	803	CLA	CHC-C1C	2.08	1.42	1.38
26	h	615	DD6	C5-C6	2.08	1.40	1.35
24	1	307	CLA	CHC-C1C	2.08	1.42	1.38
26	6	613	DD6	C10-C11	2.08	1.40	1.35
24	8	206	CLA	CHC-C1C	2.08	1.42	1.38
24	3	307	CLA	CMD-C2D	-2.08	1.46	1.50
24	A	834	CLA	CMB-C2B	-2.08	1.46	1.50
26	h	615	DD6	C10-C11	2.08	1.40	1.35
24	F	203	CLA	CHC-C1C	2.08	1.42	1.38
24	3	308	CLA	CMD-C2D	-2.08	1.46	1.50
24	5	601	CLA	CHC-C1C	2.08	1.42	1.38
26	k	315	DD6	C36-C31	-2.08	1.32	1.35
24	2	202	CLA	CHC-C1C	2.08	1.42	1.38
24	t	307	CLA	CHC-C1C	2.08	1.42	1.38
24	7	601	CLA	CMB-C2B	-2.08	1.46	1.50
24	A	857	CLA	CMB-C2B	-2.08	1.46	1.50
24	A	807	CLA	CHC-C1C	2.08	1.42	1.38
24	8	204	CLA	CMD-C2D	-2.08	1.46	1.50
26	8	212	DD6	C10-C11	2.08	1.40	1.35
24	3	303	CLA	CHC-C1C	2.07	1.42	1.38
24	A	810	CLA	CHC-C1C	2.07	1.42	1.38
24	1	309	CLA	CMD-C2D	-2.07	1.46	1.50
26	7	615	DD6	C10-C11	2.07	1.40	1.35
29	k	312	A1L1G	C35-C34	2.07	1.40	1.35
29	3	310	A1L1G	C38-C39	2.07	1.40	1.35
24	B	802	CLA	CMD-C2D	-2.07	1.46	1.50
24	L	203	CLA	CMB-C2B	-2.07	1.46	1.50
24	A	828	CLA	CMD-C2D	-2.07	1.46	1.50
24	B	808	CLA	CMD-C2D	-2.07	1.46	1.50
24	8	203	CLA	CHC-C1C	2.07	1.42	1.38
24	B	827	CLA	CMD-C2D	-2.07	1.46	1.50
24	R	104	CLA	CMB-C2B	-2.07	1.46	1.50
24	9	306	CLA	CMB-C2B	-2.07	1.46	1.50
24	A	833	CLA	CMB-C2B	-2.07	1.46	1.50
24	B	831	CLA	CMD-C2D	-2.07	1.46	1.50
26	6	617	DD6	C13-C14	2.07	1.37	1.32
24	c	607	CLA	CMD-C2D	-2.07	1.46	1.50
24	A	811	CLA	CHC-C1C	2.07	1.42	1.38
24	B	807	CLA	CHC-C1C	2.07	1.42	1.38
24	3	301	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	846	CLA	CMD-C2D	-2.07	1.46	1.50
24	h	610	CLA	CHC-C1C	2.06	1.42	1.38
24	B	828	CLA	CMB-C2B	-2.06	1.46	1.50
26	7	613	DD6	C10-C11	2.06	1.40	1.35
24	B	803	CLA	C3B-C4B	2.06	1.48	1.42
24	1	301	CLA	CMD-C2D	-2.06	1.46	1.50
24	F	202	CLA	CMB-C2B	-2.06	1.46	1.50
24	4	605	CLA	CHC-C1C	2.06	1.42	1.38
24	B	826	CLA	CMD-C2D	-2.06	1.46	1.50
24	B	833	CLA	CHC-C1C	2.06	1.42	1.38
24	h	602	CLA	CMD-C2D	-2.06	1.46	1.50
24	8	203	CLA	CMC-C2C	-2.06	1.46	1.50
24	9	303	CLA	CMC-C2C	-2.06	1.46	1.50
24	A	838	CLA	CMD-C2D	-2.06	1.46	1.50
24	h	606	CLA	CMD-C2D	-2.06	1.46	1.50
24	A	817	CLA	CMD-C2D	-2.06	1.46	1.50
26	6	614	DD6	C8-C6	-2.06	1.41	1.46
24	9	311	CLA	CMB-C2B	-2.06	1.46	1.50
24	6	608	CLA	CMB-C2B	-2.06	1.46	1.50
24	A	816	CLA	CHC-C1C	2.06	1.42	1.38
24	3	303	CLA	CMB-C2B	-2.06	1.46	1.50
24	B	807	CLA	CMB-C2B	-2.06	1.46	1.50
26	4	616	DD6	C10-C11	2.06	1.40	1.35
24	c	610	CLA	CMC-C2C	-2.06	1.46	1.50
29	2	213	A1L1G	C29-C30	-2.06	1.40	1.45
24	1	303	CLA	CHC-C1C	2.06	1.42	1.38
24	A	803	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	614	DD6	C5-C6	2.05	1.40	1.35
24	8	209	CLA	CHC-C1C	2.05	1.42	1.38
24	A	804	CLA	CMB-C2B	-2.05	1.46	1.50
24	B	808	CLA	CMB-C2B	-2.05	1.46	1.50
26	7	615	DD6	C2-C1	2.05	1.40	1.35
24	3	306	CLA	CMB-C2B	-2.05	1.46	1.50
24	h	611	CLA	CMB-C2B	-2.05	1.46	1.50
24	B	837	CLA	CMB-C2B	-2.05	1.46	1.50
24	7	604	CLA	CHC-C1C	2.05	1.42	1.38
24	B	837	CLA	CHC-C1C	2.05	1.42	1.38
24	7	604	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	840	CLA	CMB-C2B	-2.05	1.46	1.50
24	A	831	CLA	CMD-C2D	-2.05	1.46	1.50
24	A	838	CLA	CMB-C2B	-2.05	1.46	1.50
26	c	612	DD6	C5-C6	2.05	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	835	CLA	CMD-C2D	-2.05	1.46	1.50
24	B	822	CLA	CHC-C1C	2.05	1.42	1.38
24	B	835	CLA	CMD-C2D	-2.05	1.46	1.50
26	3	312	DD6	C5-C6	2.05	1.40	1.35
24	4	609	CLA	CHC-C1C	2.05	1.42	1.38
24	B	825	CLA	CMD-C2D	-2.04	1.46	1.50
24	B	838	CLA	CMB-C2B	-2.04	1.46	1.50
26	7	613	DD6	C2-C1	2.04	1.40	1.35
24	k	306	CLA	CMD-C2D	-2.04	1.46	1.50
24	B	802	CLA	C3B-C4B	2.04	1.48	1.42
24	9	302	CLA	MG-NB	-2.04	2.01	2.05
26	7	613	DD6	C5-C6	2.04	1.40	1.35
24	6	603	CLA	CMD-C2D	-2.04	1.46	1.50
24	4	603	CLA	CMD-C2D	-2.04	1.46	1.50
24	B	816	CLA	CMB-C2B	-2.04	1.46	1.50
24	7	606	CLA	CHC-C1C	2.04	1.42	1.38
24	B	833	CLA	CMD-C2D	-2.04	1.46	1.50
24	c	603	CLA	CMB-C2B	-2.04	1.46	1.50
24	A	810	CLA	CMB-C2B	-2.04	1.46	1.50
24	A	835	CLA	CMB-C2B	-2.04	1.46	1.50
24	3	304	CLA	CHC-C1C	2.04	1.42	1.38
24	F	201	CLA	CMB-C2B	-2.04	1.46	1.50
24	4	613	CLA	CHC-C1C	2.04	1.42	1.38
24	2	202	CLA	CMB-C2B	-2.04	1.46	1.50
24	t	302	CLA	CHC-C1C	2.04	1.42	1.38
24	A	825	CLA	CMB-C2B	-2.04	1.46	1.50
24	B	848	CLA	CMB-C2B	-2.04	1.46	1.50
25	I	101	BCR	C1-C6	-2.04	1.51	1.53
24	A	832	CLA	CHC-C1C	2.04	1.42	1.38
24	4	606	CLA	CMD-C2D	-2.04	1.46	1.50
24	t	310	CLA	CMB-C2B	-2.04	1.46	1.50
26	1	311	DD6	C24-C1	-2.04	1.41	1.46
26	R	105	DD6	C10-C11	2.04	1.40	1.35
24	8	202	CLA	CHC-C1C	2.04	1.42	1.38
26	9	314	DD6	C13-C11	-2.03	1.41	1.46
26	c	612	DD6	C2-C1	2.03	1.40	1.35
24	9	305	CLA	CMD-C2D	-2.03	1.46	1.50
24	B	847	CLA	CMD-C2D	-2.03	1.46	1.50
24	4	607	CLA	CMB-C2B	-2.03	1.46	1.50
24	6	609	CLA	CMB-C2B	-2.03	1.46	1.50
24	3	305	CLA	CMD-C2D	-2.03	1.46	1.50
24	6	610	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	830	CLA	C3B-C4B	2.03	1.48	1.42
29	3	310	A1L1G	C35-C34	2.03	1.40	1.35
24	k	310	CLA	CMD-C2D	-2.03	1.46	1.50
24	8	205	CLA	CHC-C1C	2.03	1.42	1.38
24	B	804	CLA	C1B-C2B	2.03	1.47	1.43
24	6	601	CLA	CHC-C1C	2.03	1.42	1.38
24	B	811	CLA	CMB-C2B	-2.03	1.46	1.50
24	B	812	CLA	CMC-C2C	-2.03	1.46	1.50
24	F	203	CLA	CMD-C2D	-2.03	1.46	1.50
24	c	610	CLA	CMD-C2D	-2.03	1.46	1.50
24	4	607	CLA	CMD-C2D	-2.03	1.46	1.50
24	h	606	CLA	CHC-C1C	2.03	1.42	1.38
24	h	612	CLA	CHC-C1C	2.03	1.42	1.38
24	7	608	CLA	CMD-C2D	-2.02	1.46	1.50
24	9	306	CLA	CMC-C2C	-2.02	1.46	1.50
24	B	835	CLA	CMB-C2B	-2.02	1.46	1.50
24	8	204	CLA	CMB-C2B	-2.02	1.46	1.50
24	B	805	CLA	CMD-C2D	-2.02	1.46	1.50
24	4	601	CLA	CMB-C2B	-2.02	1.46	1.50
24	c	601	CLA	CMB-C2B	-2.02	1.46	1.50
24	2	205	CLA	CHC-C1C	2.02	1.42	1.38
24	A	812	CLA	CMB-C2B	-2.02	1.46	1.50
24	A	802	CLA	C1B-C2B	2.02	1.47	1.43
24	1	306	CLA	CMD-C2D	-2.02	1.46	1.50
25	9	316	BCR	C1-C6	-2.02	1.51	1.53
24	3	302	CLA	CMB-C2B	-2.02	1.46	1.50
26	4	617	DD6	C2-C1	2.02	1.40	1.35
24	c	609	CLA	CHC-C1C	2.02	1.42	1.38
24	B	816	CLA	CHC-C1C	2.02	1.42	1.38
24	7	602	CLA	CMD-C2D	-2.02	1.46	1.50
24	7	611	CLA	CMD-C2D	-2.02	1.46	1.50
24	9	302	CLA	CMB-C2B	-2.02	1.46	1.50
24	3	304	CLA	C1B-C2B	2.02	1.47	1.43
24	7	609	CLA	CHC-C1C	2.02	1.42	1.38
25	B	840	BCR	C1-C6	-2.02	1.51	1.53
24	9	305	CLA	CMC-C2C	-2.02	1.46	1.50
24	9	302	CLA	CMC-C2C	-2.02	1.46	1.50
24	A	809	CLA	CMB-C2B	-2.02	1.46	1.50
24	A	815	CLA	CMB-C2B	-2.02	1.46	1.50
24	A	828	CLA	CMB-C2B	-2.02	1.46	1.50
24	B	838	CLA	MG-NB	-2.02	2.01	2.05
24	6	605	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	205	CLA	CMB-C2B	-2.01	1.46	1.50
26	9	315	DD6	C13-C14	2.01	1.37	1.32
24	6	611	CLA	CHC-C1C	2.01	1.42	1.38
24	3	308	CLA	MG-NB	-2.01	2.01	2.05
29	k	312	A1L1G	C29-C30	-2.01	1.40	1.45
24	B	846	CLA	CHC-C1C	2.01	1.42	1.38
24	4	602	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	802	CLA	CHC-C1C	2.01	1.42	1.38
24	6	602	CLA	CMB-C2B	-2.01	1.46	1.50
24	R	103	CLA	CMB-C2B	-2.01	1.46	1.50
24	A	819	CLA	CMB-C2B	-2.01	1.46	1.50
26	1	312	DD6	C13-C14	2.01	1.37	1.32
24	c	608	CLA	CMB-C2B	-2.01	1.46	1.50
24	t	302	CLA	CMD-C2D	-2.01	1.46	1.50
24	7	605	CLA	CHC-C1C	2.01	1.42	1.38
24	A	815	CLA	CMD-C2D	-2.01	1.46	1.50
26	6	617	DD6	C28-C27	-2.01	1.49	1.50
24	A	819	CLA	CHC-C1C	2.01	1.42	1.38
24	4	613	CLA	CMB-C2B	-2.01	1.46	1.50
24	B	836	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	830	CLA	CHC-C1C	2.01	1.42	1.38
24	A	808	CLA	CMB-C2B	-2.01	1.46	1.50
24	B	848	CLA	CMD-C2D	-2.01	1.46	1.50
24	7	601	CLA	CHC-C1C	2.01	1.42	1.38
24	A	811	CLA	CMB-C2B	-2.01	1.46	1.50
24	A	830	CLA	CMC-C2C	-2.01	1.46	1.50
24	1	317	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	827	CLA	CMB-C2B	-2.01	1.46	1.50
29	9	312	A1L1G	C29-C30	-2.00	1.40	1.45
24	B	819	CLA	CMB-C2B	-2.00	1.46	1.50
24	B	809	CLA	CHC-C1C	2.00	1.42	1.38
24	6	608	CLA	CHC-C1C	2.00	1.42	1.38
24	A	801	CLA	CHC-C1C	2.00	1.42	1.38
24	6	607	CLA	CMD-C2D	-2.00	1.46	1.50
24	h	611	CLA	CMC-C2C	-2.00	1.46	1.50
24	B	802	CLA	CMB-C2B	-2.00	1.46	1.50
24	A	837	CLA	CMB-C2B	-2.00	1.46	1.50
24	3	307	CLA	CHC-C1C	2.00	1.42	1.38
24	2	208	CLA	CHC-C1C	2.00	1.42	1.38
24	k	304	CLA	CHC-C1C	2.00	1.42	1.38
24	A	830	CLA	MG-NA	2.00	2.11	2.06
24	9	309	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	804	CLA	CMD-C2D	-2.00	1.46	1.50
24	A	825	CLA	CMD-C2D	-2.00	1.46	1.50
24	3	303	CLA	CMD-C2D	-2.00	1.46	1.50
24	6	606	CLA	CMB-C2B	-2.00	1.46	1.50

All (2352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	830	CLA	C4A-NA-C1A	9.25	110.90	106.68
26	9	314	DD6	C3-C2-C1	-9.05	114.58	127.28
25	c	615	BCR	C20-C21-C22	-8.79	114.95	127.28
26	8	210	DD6	C14-C13-C11	-8.74	111.97	125.53
26	k	315	DD6	C3-C2-C1	-8.73	115.04	127.28
24	1	305	CLA	C4A-NA-C1A	7.84	110.26	106.68
25	B	843	BCR	C11-C10-C9	-7.26	117.09	127.28
26	6	616	DD6	C3-C2-C1	-7.24	117.13	127.28
26	R	105	DD6	C9-C10-C11	-7.07	117.36	127.28
26	9	315	DD6	C3-C2-C1	-7.06	117.37	127.28
25	k	316	BCR	C15-C14-C13	-6.97	117.51	127.28
26	4	617	DD6	C4-C5-C6	-6.86	117.66	127.28
24	9	305	CLA	C4A-NA-C1A	6.85	109.80	106.68
26	7	613	DD6	C3-C2-C1	-6.82	117.72	127.28
25	M	101	BCR	C20-C21-C22	-6.81	117.72	127.28
26	c	612	DD6	C9-C10-C11	-6.80	117.74	127.28
25	A	843	BCR	C28-C27-C26	-6.74	102.03	114.06
25	c	615	BCR	C16-C17-C18	-6.74	117.83	127.28
25	B	842	BCR	C24-C23-C22	-6.69	116.34	126.23
26	k	314	DD6	C3-C2-C1	-6.68	117.91	127.28
26	9	317	DD6	C4-C5-C6	-6.64	117.97	127.28
25	A	846	BCR	C28-C27-C26	-6.60	102.29	114.06
26	2	210	DD6	C3-C2-C1	-6.54	118.11	127.28
24	h	602	CLA	C5-C3-C2	6.42	135.57	121.17
25	9	316	BCR	C7-C8-C9	-6.38	116.79	126.23
26	h	615	DD6	C3-C2-C1	-6.34	118.39	127.28
25	4	618	BCR	C16-C17-C18	-6.32	118.42	127.28
25	L	202	BCR	C28-C27-C26	-6.31	102.80	114.06
25	1	314	BCR	C16-C17-C18	-6.31	118.43	127.28
26	A	848	DD6	C4-C5-C6	-6.31	118.43	127.28
26	6	617	DD6	C3-C2-C1	-6.25	118.51	127.28
26	c	614	DD6	C3-C2-C1	-6.21	118.57	127.28
26	t	313	DD6	C3-C2-C1	-6.21	118.57	127.28
24	R	104	CLA	C4A-NA-C1A	6.17	109.50	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	609	DD6	C3-C2-C1	-6.16	118.64	127.28
25	J	104	BCR	C28-C27-C26	-6.11	103.16	114.06
25	B	849	BCR	C28-C27-C26	-6.10	103.18	114.06
24	h	611	CLA	C4A-NA-C1A	6.10	109.46	106.68
24	A	860	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	9	310	CLA	C4A-NA-C1A	6.06	109.45	106.68
26	6	613	DD6	C3-C2-C1	-6.04	118.81	127.28
24	B	803	CLA	C4A-NA-C1A	6.02	109.43	106.68
25	4	618	BCR	C20-C21-C22	-6.01	118.85	127.28
26	c	612	DD6	C3-C2-C1	-6.01	118.85	127.28
26	5	608	DD6	C3-C2-C1	-5.99	118.87	127.28
24	L	203	CLA	C4A-NA-C1A	5.93	109.38	106.68
24	h	602	CLA	C1-C2-C3	5.91	135.89	126.20
26	9	317	DD6	C3-C2-C1	-5.91	119.00	127.28
26	3	313	DD6	C3-C2-C1	-5.89	119.01	127.28
26	c	613	DD6	C3-C2-C1	-5.83	119.10	127.28
26	6	615	DD6	C9-C10-C11	-5.82	119.12	127.28
24	B	837	CLA	C4A-NA-C1A	5.79	109.32	106.68
25	9	316	BCR	C11-C10-C9	-5.78	119.17	127.28
25	B	843	BCR	C15-C14-C13	-5.77	119.18	127.28
24	k	302	CLA	C4A-NA-C1A	5.77	109.31	106.68
25	M	101	BCR	C16-C17-C18	-5.75	119.21	127.28
24	9	304	CLA	C4A-NA-C1A	5.72	109.29	106.68
24	3	301	CLA	C4A-NA-C1A	5.72	109.29	106.68
24	A	857	CLA	C4A-NA-C1A	5.70	109.28	106.68
24	h	601	CLA	C4A-NA-C1A	5.69	109.28	106.68
24	B	829	CLA	C4A-NA-C1A	5.65	109.26	106.68
25	B	841	BCR	C33-C5-C6	-5.64	118.33	124.48
26	A	848	DD6	C3-C2-C1	-5.61	119.40	127.28
26	5	608	DD6	C4-C5-C6	-5.60	119.42	127.28
25	1	314	BCR	C11-C10-C9	-5.57	119.46	127.28
25	7	617	BCR	C15-C14-C13	-5.56	119.48	127.28
25	J	101	BCR	C1-C6-C5	-5.55	115.05	122.64
25	A	845	BCR	C11-C10-C9	-5.54	119.51	127.28
26	7	615	DD6	C3-C2-C1	-5.54	119.51	127.28
25	L	202	BCR	C3-C4-C5	-5.53	104.20	114.06
25	1	310	BCR	C16-C17-C18	-5.50	119.56	127.28
24	B	835	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	t	312	BCR	C38-C26-C25	-5.49	118.50	124.48
26	J	102	DD6	C3-C2-C1	-5.48	119.59	127.28
25	B	843	BCR	C24-C23-C22	-5.48	118.13	126.23
24	B	809	CLA	C4A-NA-C1A	5.46	109.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	BCR	C3-C4-C5	-5.45	104.33	114.06
25	A	844	BCR	C16-C17-C18	-5.45	119.64	127.28
25	M	101	BCR	C15-C14-C13	-5.44	119.65	127.28
24	A	837	CLA	C4A-NA-C1A	5.43	109.16	106.68
24	3	302	CLA	C4A-NA-C1A	5.43	109.16	106.68
26	7	616	DD6	C9-C10-C11	-5.42	119.68	127.28
26	h	613	DD6	C3-C2-C1	-5.41	119.70	127.28
24	9	307	CLA	C4A-NA-C1A	5.39	109.14	106.68
24	B	822	CLA	C4A-NA-C1A	5.39	109.14	106.68
24	t	301	CLA	C4A-NA-C1A	5.38	109.14	106.68
24	9	302	CLA	C4A-NA-C1A	5.38	109.13	106.68
25	9	316	BCR	C16-C17-C18	-5.35	119.78	127.28
24	F	203	CLA	C4A-NA-C1A	5.34	109.12	106.68
26	t	311	DD6	C3-C2-C1	-5.34	119.79	127.28
24	6	611	CLA	C4A-NA-C1A	5.34	109.12	106.68
24	9	303	CLA	C4A-NA-C1A	5.34	109.11	106.68
26	3	311	DD6	C3-C2-C1	-5.34	119.79	127.28
24	B	806	CLA	C4A-NA-C1A	5.34	109.11	106.68
26	c	612	DD6	C14-C13-C11	-5.34	117.25	125.53
24	2	204	CLA	C4A-NA-C1A	5.33	109.11	106.68
26	6	615	DD6	C3-C2-C1	-5.32	119.81	127.28
25	J	101	BCR	C4-C5-C6	-5.32	115.52	122.70
25	c	615	BCR	C7-C8-C9	-5.32	118.37	126.23
24	k	304	CLA	C4A-NA-C1A	5.31	109.10	106.68
26	2	212	DD6	C3-C2-C1	-5.30	119.84	127.28
25	9	316	BCR	C15-C14-C13	-5.30	119.85	127.28
25	I	102	BCR	C28-C27-C26	-5.29	104.62	114.06
26	k	315	DD6	C14-C13-C11	-5.29	117.33	125.53
26	4	616	DD6	C3-C2-C1	-5.28	119.88	127.28
25	F	204	BCR	C15-C14-C13	-5.27	119.89	127.28
26	6	616	DD6	C9-C10-C11	-5.26	119.89	127.28
26	9	314	DD6	C9-C10-C11	-5.26	119.91	127.28
25	J	104	BCR	C3-C4-C5	-5.25	104.70	114.06
24	8	204	CLA	C4A-NA-C1A	5.24	109.07	106.68
24	B	838	CLA	C4A-NA-C1A	5.24	109.07	106.68
26	1	313	DD6	C3-C2-C1	-5.23	119.95	127.28
24	h	602	CLA	C4-C3-C2	-5.22	110.22	123.63
25	L	206	BCR	C28-C27-C26	-5.22	104.75	114.06
25	4	618	BCR	C24-C23-C22	-5.20	118.53	126.23
26	4	614	DD6	C3-C2-C1	-5.20	119.98	127.28
24	B	833	CLA	C4A-NA-C1A	5.19	109.05	106.68
26	7	616	DD6	C3-C2-C1	-5.19	119.99	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	849	BCR	C3-C4-C5	-5.19	104.80	114.06
24	B	801	CLA	C4A-NA-C1A	5.18	109.04	106.68
24	5	603	CLA	C4A-NA-C1A	5.17	109.04	106.68
24	7	604	CLA	C4A-NA-C1A	5.17	109.04	106.68
25	c	615	BCR	C38-C26-C25	-5.16	118.85	124.48
26	3	312	DD6	C4-C5-C6	-5.16	120.04	127.28
26	c	612	DD6	C4-C5-C6	-5.14	120.07	127.28
26	8	211	DD6	C3-C2-C1	-5.12	120.10	127.28
24	A	814	CLA	C4A-NA-C1A	5.11	109.01	106.68
24	B	805	CLA	C4A-NA-C1A	5.11	109.01	106.68
24	7	605	CLA	C4A-NA-C1A	5.11	109.01	106.68
26	3	312	DD6	C3-C2-C1	-5.10	120.13	127.28
24	A	815	CLA	C4A-NA-C1A	5.09	109.00	106.68
24	8	203	CLA	C4A-NA-C1A	5.09	109.00	106.68
24	c	602	CLA	C4A-NA-C1A	5.08	109.00	106.68
25	k	316	BCR	C20-C21-C22	-5.07	120.17	127.28
25	L	206	BCR	C30-C25-C26	-5.07	115.71	122.64
26	9	313	DD6	C4-C5-C6	-5.07	120.17	127.28
26	4	614	DD6	C4-C5-C6	-5.04	120.21	127.28
25	J	101	BCR	C7-C8-C9	-5.04	118.78	126.23
24	5	606	CLA	C4A-NA-C1A	5.04	108.98	106.68
26	A	848	DD6	C15-C14-C13	-5.04	115.35	125.99
24	B	807	CLA	C4A-NA-C1A	5.03	108.97	106.68
24	6	601	CLA	C4A-NA-C1A	5.03	108.97	106.68
24	A	808	CLA	C4A-NA-C1A	5.03	108.97	106.68
26	4	615	DD6	C3-C2-C1	-5.02	120.23	127.28
26	h	616	DD6	C4-C5-C6	-5.02	120.24	127.28
24	R	103	CLA	C4A-NA-C1A	5.02	108.97	106.68
26	8	212	DD6	C3-C2-C1	-5.01	120.25	127.28
26	c	614	DD6	C4-C5-C6	-5.01	120.25	127.28
25	J	101	BCR	C11-C10-C9	-4.99	120.27	127.28
24	k	310	CLA	C4A-NA-C1A	4.99	108.96	106.68
25	B	842	BCR	C7-C8-C9	-4.99	118.86	126.23
25	2	211	BCR	C15-C14-C13	-4.98	120.30	127.28
25	9	316	BCR	C20-C21-C22	-4.96	120.32	127.28
25	B	849	BCR	C27-C26-C25	-4.95	116.01	122.70
25	B	842	BCR	C11-C10-C9	-4.95	120.34	127.28
24	B	812	CLA	C4A-NA-C1A	4.95	108.94	106.68
24	4	608	CLA	C4A-NA-C1A	4.94	108.94	106.68
24	6	612	CLA	C4A-NA-C1A	4.94	108.93	106.68
25	A	846	BCR	C7-C8-C9	-4.94	118.92	126.23
24	A	826	CLA	C4A-NA-C1A	4.94	108.93	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	805	CLA	C4A-NA-C1A	4.93	108.93	106.68
24	A	804	CLA	C4A-NA-C1A	4.92	108.92	106.68
26	8	211	DD6	C15-C14-C13	-4.92	115.60	125.99
24	9	301	CLA	C4A-NA-C1A	4.91	108.92	106.68
26	1	312	DD6	C3-C2-C1	-4.90	120.41	127.28
25	A	845	BCR	C7-C8-C9	-4.90	118.99	126.23
26	8	210	DD6	C3-C2-C1	-4.90	120.41	127.28
24	A	832	CLA	C4A-NA-C1A	4.89	108.91	106.68
26	h	616	DD6	C9-C10-C11	-4.88	120.43	127.28
26	4	616	DD6	C4-C5-C6	-4.88	120.43	127.28
24	c	609	CLA	C1-C2-C3	-4.87	118.21	126.20
26	2	212	DD6	C9-C10-C11	-4.87	120.45	127.28
24	t	304	CLA	C4A-NA-C1A	4.86	108.89	106.68
26	k	313	DD6	C3-C2-C1	-4.86	120.47	127.28
24	A	817	CLA	C4A-NA-C1A	4.85	108.89	106.68
25	B	842	BCR	C16-C17-C18	-4.84	120.49	127.28
24	B	848	CLA	C4A-NA-C1A	4.84	108.89	106.68
25	c	615	BCR	C24-C23-C22	-4.83	119.09	126.23
26	6	616	DD6	C14-C13-C11	-4.83	118.04	125.53
24	A	812	CLA	C4A-NA-C1A	4.81	108.88	106.68
25	k	316	BCR	C11-C10-C9	-4.80	120.55	127.28
26	k	314	DD6	C9-C10-C11	-4.80	120.55	127.28
26	9	317	DD6	C15-C14-C13	-4.80	115.85	125.99
24	7	609	CLA	C4A-NA-C1A	4.80	108.87	106.68
24	B	825	CLA	C4A-NA-C1A	4.80	108.87	106.68
24	3	309	CLA	C4A-NA-C1A	4.79	108.86	106.68
24	6	609	CLA	C4A-NA-C1A	4.79	108.86	106.68
24	t	310	CLA	C4A-NA-C1A	4.78	108.86	106.68
24	k	307	CLA	C4A-NA-C1A	4.78	108.86	106.68
26	6	615	DD6	C4-C5-C6	-4.77	120.59	127.28
26	1	311	DD6	C3-C2-C1	-4.76	120.60	127.28
25	c	615	BCR	C33-C5-C6	-4.75	119.30	124.48
26	3	311	DD6	C15-C14-C13	-4.75	115.95	125.99
24	A	835	CLA	C4A-NA-C1A	4.75	108.84	106.68
25	I	101	BCR	C4-C5-C6	-4.74	116.29	122.70
24	4	608	CLA	C1-C2-C3	-4.73	119.11	126.76
24	B	820	CLA	C4A-NA-C1A	4.71	108.83	106.68
24	8	208	CLA	C4A-NA-C1A	4.71	108.83	106.68
26	9	314	DD6	C25-C24-C1	-4.70	113.46	126.36
24	2	206	CLA	C4A-NA-C1A	4.70	108.82	106.68
24	A	834	CLA	C4A-NA-C1A	4.70	108.82	106.68
26	7	615	DD6	C4-C5-C6	-4.70	120.69	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	844	BCR	C24-C23-C22	-4.70	119.28	126.23
25	A	845	BCR	C15-C14-C13	-4.69	120.70	127.28
24	2	207	CLA	C4A-NA-C1A	4.69	108.82	106.68
24	9	309	CLA	C4A-NA-C1A	4.68	108.81	106.68
30	2	214	LMG	O1-C1-C2	4.68	115.37	108.27
24	A	816	CLA	C4A-NA-C1A	4.67	108.81	106.68
25	B	841	BCR	C37-C22-C23	4.67	125.22	118.09
25	J	101	BCR	C36-C18-C19	4.66	125.21	118.09
26	2	210	DD6	C9-C10-C11	-4.66	120.74	127.28
24	6	608	CLA	C4A-NA-C1A	4.66	108.81	106.68
24	7	608	CLA	C4A-NA-C1A	4.66	108.80	106.68
24	B	847	CLA	C4A-NA-C1A	4.65	108.80	106.68
24	B	827	CLA	C4A-NA-C1A	4.65	108.80	106.68
24	c	607	CLA	C4A-NA-C1A	4.65	108.80	106.68
26	c	614	DD6	C9-C10-C11	-4.64	120.76	127.28
24	B	824	CLA	C4A-NA-C1A	4.64	108.80	106.68
25	A	845	BCR	C24-C23-C22	-4.64	119.37	126.23
26	9	313	DD6	C3-C2-C1	-4.63	120.79	127.28
25	R	102	BCR	C38-C26-C25	-4.62	119.44	124.48
24	A	801	CLA	O2D-CGD-CBD	4.62	119.31	111.23
24	B	802	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	c	615	BCR	C11-C10-C9	-4.60	120.83	127.28
26	h	614	DD6	C3-C2-C1	-4.60	120.83	127.28
26	6	613	DD6	C15-C14-C13	-4.60	116.27	125.99
24	1	309	CLA	C4A-NA-C1A	4.60	108.78	106.68
25	I	102	BCR	C37-C22-C23	4.59	125.10	118.09
25	A	846	BCR	C37-C22-C23	4.59	125.10	118.09
24	2	208	CLA	C4A-NA-C1A	4.59	108.77	106.68
24	k	305	CLA	C4A-NA-C1A	4.58	108.77	106.68
26	7	615	DD6	C9-C10-C11	-4.58	120.85	127.28
24	F	201	CLA	C4A-NA-C1A	4.58	108.77	106.68
24	A	806	CLA	C4A-NA-C1A	4.58	108.77	106.68
25	4	618	BCR	C28-C27-C26	-4.58	105.89	114.06
24	k	311	CLA	C4A-NA-C1A	4.57	108.76	106.68
25	A	845	BCR	C8-C7-C6	-4.55	119.61	126.94
26	7	618	DD6	C4-C5-C6	-4.55	120.90	127.28
24	A	831	CLA	C4A-NA-C1A	4.54	108.75	106.68
24	7	602	CLA	CAC-C3C-C4C	4.53	130.69	124.79
24	4	610	CLA	C4A-NA-C1A	4.53	108.75	106.68
24	9	308	CLA	C4A-NA-C1A	4.53	108.74	106.68
25	F	204	BCR	C7-C8-C9	-4.52	119.55	126.23
24	8	207	CLA	C4A-NA-C1A	4.52	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	315	DD6	C9-C10-C11	-4.51	120.95	127.28
25	F	204	BCR	C11-C10-C9	-4.51	120.95	127.28
24	A	807	CLA	C4A-NA-C1A	4.51	108.74	106.68
26	c	614	DD6	C15-C14-C13	-4.50	116.48	125.99
24	t	306	CLA	C4A-NA-C1A	4.50	108.73	106.68
24	A	803	CLA	C4A-NA-C1A	4.49	108.73	106.68
26	c	613	DD6	C15-C14-C13	-4.49	116.50	125.99
24	4	607	CLA	C4A-NA-C1A	4.48	108.72	106.68
24	A	821	CLA	C4A-NA-C1A	4.48	108.72	106.68
24	A	820	CLA	C4A-NA-C1A	4.48	108.72	106.68
24	A	829	CLA	C4A-NA-C1A	4.47	108.72	106.68
26	3	312	DD6	C9-C10-C11	-4.47	121.01	127.28
26	1	312	DD6	C9-C10-C11	-4.46	121.03	127.28
25	1	314	BCR	C33-C5-C6	-4.45	119.62	124.48
24	k	301	CLA	C4A-NA-C1A	4.45	108.71	106.68
26	A	848	DD6	C9-C10-C11	-4.45	121.04	127.28
25	B	849	BCR	C37-C22-C23	4.45	124.88	118.09
24	A	809	CLA	C4A-NA-C1A	4.45	108.71	106.68
25	4	618	BCR	C15-C14-C13	-4.44	121.05	127.28
24	5	601	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	t	307	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	A	801	CLA	C1D-ND-C4D	-4.44	103.20	106.31
24	A	825	CLA	C4A-NA-C1A	4.44	108.70	106.68
26	3	312	DD6	C14-C13-C11	-4.44	118.65	125.53
25	A	843	BCR	C16-C17-C18	-4.43	121.06	127.28
25	I	102	BCR	C4-C5-C6	-4.43	116.72	122.70
24	4	603	CLA	C4A-NA-C1A	4.43	108.70	106.68
25	A	844	BCR	C15-C14-C13	-4.43	121.07	127.28
24	A	828	CLA	C4A-NA-C1A	4.43	108.70	106.68
24	A	819	CLA	C4A-NA-C1A	4.43	108.70	106.68
26	7	618	DD6	C3-C2-C1	-4.42	121.07	127.28
25	R	102	BCR	C37-C22-C23	4.42	124.84	118.09
24	6	604	CLA	C4A-NA-C1A	4.41	108.69	106.68
24	7	611	CLA	C4A-NA-C1A	4.41	108.69	106.68
25	J	101	BCR	C36-C18-C17	-4.40	115.68	122.82
26	k	314	DD6	C4-C5-C6	-4.40	121.11	127.28
24	c	611	CLA	C4A-NA-C1A	4.39	108.68	106.68
25	1	310	BCR	C28-C27-C26	-4.39	106.23	114.06
24	A	824	CLA	C4A-NA-C1A	4.39	108.68	106.68
25	A	844	BCR	C11-C10-C9	-4.38	121.13	127.28
24	L	204	CLA	C4A-NA-C1A	4.38	108.68	106.68
26	7	613	DD6	C15-C14-C13	-4.38	116.73	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	602	CLA	C4A-NA-C1A	4.38	108.67	106.68
25	M	101	BCR	C24-C23-C22	-4.36	119.79	126.23
28	1	318	LHG	C5-O7-C7	-4.35	107.38	117.80
24	4	605	CLA	C4A-NA-C1A	4.35	108.66	106.68
24	c	603	CLA	C4A-NA-C1A	4.35	108.66	106.68
26	4	617	DD6	C3-C2-C1	-4.34	121.19	127.28
28	A	842	LHG	O7-C7-C8	4.34	120.86	111.48
24	5	605	CLA	C4A-NA-C1A	4.33	108.66	106.68
25	A	859	BCR	C20-C21-C22	-4.33	121.20	127.28
28	I	103	LHG	O7-C7-C8	4.33	120.85	111.48
24	A	840	CLA	C4A-NA-C1A	4.32	108.65	106.68
24	B	819	CLA	C4A-NA-C1A	4.32	108.65	106.68
24	h	604	CLA	C4A-NA-C1A	4.30	108.64	106.68
26	8	211	DD6	C4-C5-C6	-4.30	121.25	127.28
25	A	846	BCR	C1-C6-C5	-4.29	116.77	122.64
25	A	844	BCR	C20-C21-C22	-4.29	121.26	127.28
24	2	205	CLA	C4A-NA-C1A	4.27	108.63	106.68
24	A	827	CLA	C4A-NA-C1A	4.27	108.63	106.68
25	J	104	BCR	C37-C22-C23	4.27	124.61	118.09
25	k	316	BCR	C3-C4-C5	-4.26	106.47	114.06
24	1	303	CLA	C4A-NA-C1A	4.25	108.62	106.68
26	c	613	DD6	C4-C5-C6	-4.24	121.33	127.28
26	8	212	DD6	C15-C14-C13	-4.24	117.03	125.99
24	3	303	CLA	C4A-NA-C1A	4.24	108.61	106.68
25	A	845	BCR	C16-C17-C18	-4.23	121.34	127.28
24	1	301	CLA	C4A-NA-C1A	4.23	108.61	106.68
24	B	831	CLA	C4A-NA-C1A	4.23	108.61	106.68
25	1	314	BCR	C7-C8-C9	-4.22	119.99	126.23
24	7	601	CLA	C4A-NA-C1A	4.22	108.61	106.68
25	B	840	BCR	C16-C17-C18	-4.22	121.36	127.28
25	R	102	BCR	C23-C24-C25	-4.22	115.73	127.00
26	R	105	DD6	C3-C2-C1	-4.21	121.37	127.28
26	9	314	DD6	C25-C26-C27	-4.21	114.84	126.61
24	8	209	CLA	C4A-NA-C1A	4.21	108.60	106.68
24	B	846	CLA	C4A-NA-C1A	4.20	108.60	106.68
24	F	202	CLA	C4A-NA-C1A	4.20	108.59	106.68
27	3	314	LMT	C1-O1'-C1'	4.19	120.84	113.68
26	c	614	DD6	O1-C20-C19	-4.19	109.56	113.49
25	B	849	BCR	C16-C17-C18	-4.19	121.40	127.28
25	B	840	BCR	C20-C21-C22	-4.19	121.40	127.28
26	h	614	DD6	C4-C5-C6	-4.19	121.41	127.28
25	B	843	BCR	C38-C26-C25	-4.18	119.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	206	BCR	C27-C26-C25	-4.18	117.05	122.70
25	A	844	BCR	C33-C5-C6	-4.18	119.92	124.48
28	J	105	LHG	O7-C7-C8	4.18	120.52	111.48
24	h	609	CLA	C4A-NA-C1A	4.18	108.58	106.68
25	I	102	BCR	C36-C18-C19	4.17	124.46	118.09
25	1	310	BCR	C33-C5-C6	-4.16	119.94	124.48
26	2	212	DD6	C4-C5-C6	-4.16	121.45	127.28
25	2	211	BCR	C28-C27-C26	-4.16	106.64	114.06
24	c	606	CLA	C4A-NA-C1A	4.16	108.58	106.68
26	7	613	DD6	C4-C5-C6	-4.15	121.45	127.28
24	4	606	CLA	C4A-NA-C1A	4.15	108.57	106.68
26	h	613	DD6	C15-C14-C13	-4.15	117.22	125.99
24	8	201	CLA	C4A-NA-C1A	4.15	108.57	106.68
24	c	601	CLA	C4A-NA-C1A	4.15	108.57	106.68
25	I	101	BCR	C3-C4-C5	-4.15	106.66	114.06
24	1	307	CLA	C4A-NA-C1A	4.14	108.57	106.68
26	k	315	DD6	C9-C10-C11	-4.13	121.49	127.28
24	c	604	CLA	C4A-NA-C1A	4.13	108.56	106.68
24	8	206	CLA	C4A-NA-C1A	4.12	108.56	106.68
24	B	813	CLA	C4A-NA-C1A	4.12	108.56	106.68
25	J	101	BCR	C15-C14-C13	-4.12	121.51	127.28
24	8	202	CLA	C4A-NA-C1A	4.11	108.56	106.68
25	A	846	BCR	C36-C18-C19	4.11	124.36	118.09
25	J	104	BCR	C27-C26-C25	-4.11	117.16	122.70
24	h	605	CLA	C4A-NA-C1A	4.10	108.55	106.68
25	k	316	BCR	C38-C26-C25	-4.10	120.01	124.48
24	A	853	CLA	C4A-NA-C1A	4.10	108.55	106.68
25	L	202	BCR	C37-C22-C23	4.10	124.35	118.09
26	R	105	DD6	C4-C5-C6	-4.09	121.54	127.28
24	A	801	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
25	I	101	BCR	C30-C25-C26	-4.09	117.05	122.64
24	4	611	CLA	C4A-NA-C1A	4.09	108.55	106.68
28	8	213	LHG	O7-C7-C8	4.09	120.33	111.48
24	c	609	CLA	C4A-NA-C1A	4.09	108.54	106.68
24	4	609	CLA	C4A-NA-C1A	4.08	108.54	106.68
24	A	847	CLA	C4A-NA-C1A	4.08	108.54	106.68
24	3	307	CLA	C4A-NA-C1A	4.08	108.54	106.68
24	4	602	CLA	C4A-NA-C1A	4.08	108.54	106.68
28	B	844	LHG	O7-C7-C8	4.07	120.30	111.48
24	J	103	CLA	C4A-NA-C1A	4.07	108.54	106.68
26	1	312	DD6	C4-C5-C6	-4.07	121.57	127.28
24	B	816	CLA	O2D-CGD-O1D	-4.07	115.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	816	CLA	O2D-CGD-CBD	4.06	118.33	111.23
28	B	845	LHG	O7-C7-C8	4.06	120.27	111.48
24	1	308	CLA	C4A-NA-C1A	4.06	108.53	106.68
25	B	842	BCR	C15-C14-C13	-4.06	121.59	127.28
25	R	102	BCR	C34-C9-C8	-4.06	111.89	118.09
24	B	808	CLA	C4A-NA-C1A	4.06	108.53	106.68
28	1	318	LHG	O7-C7-C8	4.04	120.23	111.48
26	7	615	DD6	C15-C14-C13	-4.04	117.46	125.99
24	A	838	CLA	C4A-NA-C1A	4.04	108.52	106.68
24	B	816	CLA	C4A-NA-C1A	4.04	108.52	106.68
24	h	602	CLA	C4A-NA-C1A	4.04	108.52	106.68
24	7	610	CLA	C4A-NA-C1A	4.03	108.52	106.68
25	k	316	BCR	C24-C23-C22	-4.03	120.27	126.23
24	A	810	CLA	C4A-NA-C1A	4.03	108.52	106.68
24	h	607	CLA	C4A-NA-C1A	4.03	108.52	106.68
24	5	607	CLA	C4A-NA-C1A	4.02	108.52	106.68
24	8	205	CLA	C4A-NA-C1A	4.02	108.51	106.68
25	7	617	BCR	C33-C5-C6	-4.02	120.10	124.48
24	2	203	CLA	C4A-NA-C1A	4.02	108.51	106.68
24	9	311	CLA	C4A-NA-C1A	4.01	108.51	106.68
25	B	840	BCR	C37-C22-C23	4.01	124.21	118.09
25	A	843	BCR	C27-C26-C25	-4.01	117.29	122.70
25	J	104	BCR	C4-C5-C6	-4.01	117.29	122.70
24	3	308	CLA	C4A-NA-C1A	4.00	108.51	106.68
24	A	823	CLA	C4A-NA-C1A	4.00	108.51	106.68
24	A	856	CLA	C4A-NA-C1A	4.00	108.51	106.68
24	3	306	CLA	C4A-NA-C1A	4.00	108.50	106.68
24	k	308	CLA	C4A-NA-C1A	4.00	108.50	106.68
30	t	314	LMG	O7-C10-C11	4.00	120.13	111.48
24	c	605	CLA	C4A-NA-C1A	4.00	108.50	106.68
24	h	608	CLA	C4A-NA-C1A	3.99	108.50	106.68
26	h	616	DD6	C3-C2-C1	-3.98	121.69	127.28
26	5	609	DD6	C9-C10-C11	-3.98	121.69	127.28
24	h	612	CLA	C4A-NA-C1A	3.98	108.50	106.68
26	7	616	DD6	C14-C13-C11	-3.98	119.36	125.53
25	A	843	BCR	C7-C8-C9	-3.98	120.35	126.23
24	7	603	CLA	C4A-NA-C1A	3.97	108.49	106.68
25	L	206	BCR	C7-C8-C9	-3.97	120.36	126.23
25	B	841	BCR	C7-C8-C9	-3.97	120.36	126.23
25	L	206	BCR	C16-C17-C18	-3.97	121.72	127.28
25	9	316	BCR	C24-C23-C22	-3.96	120.37	126.23
25	4	618	BCR	C11-C10-C9	-3.96	121.72	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	614	DD6	C15-C14-C13	-3.96	117.62	125.99
25	I	101	BCR	C37-C22-C23	3.96	124.14	118.09
26	8	210	DD6	C9-C10-C11	-3.96	121.72	127.28
26	J	102	DD6	C4-C5-C6	-3.96	121.72	127.28
25	t	312	BCR	C11-C10-C9	-3.96	121.72	127.28
25	I	101	BCR	C20-C21-C22	-3.96	121.73	127.28
25	t	312	BCR	C7-C8-C9	-3.96	120.38	126.23
25	L	206	BCR	C20-C21-C22	-3.96	121.73	127.28
25	J	104	BCR	C16-C17-C18	-3.95	121.74	127.28
24	4	613	CLA	C4A-NA-C1A	3.95	108.48	106.68
26	6	616	DD6	C4-C5-C6	-3.95	121.74	127.28
24	A	836	CLA	C4A-NA-C1A	3.94	108.48	106.68
25	R	102	BCR	C36-C18-C19	3.94	124.11	118.09
24	6	605	CLA	C4A-NA-C1A	3.94	108.48	106.68
25	R	102	BCR	C28-C27-C26	-3.94	107.04	114.06
24	A	818	CLA	C4A-NA-C1A	3.93	108.47	106.68
30	A	855	LMG	O7-C10-C11	3.93	119.98	111.48
26	4	617	DD6	C9-C10-C11	-3.93	121.77	127.28
24	B	811	CLA	C4A-NA-C1A	3.93	108.47	106.68
28	A	849	LHG	O7-C7-C8	3.92	119.97	111.48
26	6	614	DD6	C3-C2-C1	-3.92	121.78	127.28
25	A	843	BCR	C20-C21-C22	-3.92	121.78	127.28
25	R	101	BCR	C37-C22-C23	3.92	124.07	118.09
26	5	609	DD6	C15-C14-C13	-3.91	117.72	125.99
25	A	859	BCR	C37-C22-C23	3.91	124.06	118.09
25	9	316	BCR	C28-C27-C26	-3.91	107.09	114.06
26	t	313	DD6	C4-C5-C6	-3.91	121.80	127.28
24	B	828	CLA	C4A-NA-C1A	3.91	108.46	106.68
26	9	314	DD6	C24-C1-C2	3.90	125.15	119.01
24	h	602	CLA	C6-C5-C3	3.90	122.97	113.47
24	B	824	CLA	C4-C3-C5	3.90	121.99	115.23
26	6	617	DD6	C9-C10-C11	-3.89	121.82	127.28
25	k	316	BCR	C7-C8-C9	-3.89	120.48	126.23
25	B	843	BCR	C20-C21-C22	-3.89	121.82	127.28
24	1	317	CLA	C4A-NA-C1A	3.89	108.45	106.68
25	I	101	BCR	C16-C17-C18	-3.89	121.83	127.28
25	B	840	BCR	C7-C8-C9	-3.88	120.49	126.23
30	2	214	LMG	O7-C10-C11	3.88	119.88	111.48
25	c	615	BCR	C3-C4-C5	-3.88	107.14	114.06
26	c	614	DD6	C25-C26-C27	-3.88	115.77	126.61
24	7	602	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
25	J	101	BCR	C37-C22-C23	3.87	124.00	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	BCR	C33-C5-C6	-3.86	120.27	124.48
24	t	305	CLA	C4A-NA-C1A	3.86	108.44	106.68
24	A	822	CLA	C4A-NA-C1A	3.86	108.44	106.68
25	t	312	BCR	C33-C5-C6	-3.85	120.28	124.48
25	A	859	BCR	C16-C17-C18	-3.85	121.88	127.28
25	A	846	BCR	C27-C26-C25	-3.85	117.50	122.70
25	I	102	BCR	C20-C21-C22	-3.84	121.89	127.28
24	k	309	CLA	C4A-NA-C1A	3.84	108.43	106.68
25	B	843	BCR	C33-C5-C4	3.83	121.77	113.60
26	4	614	DD6	C15-C14-C13	-3.83	117.89	125.99
25	J	101	BCR	C16-C17-C18	-3.83	121.91	127.28
28	8	213	LHG	C5-O7-C7	-3.83	108.64	117.80
24	B	836	CLA	C4A-NA-C1A	3.83	108.42	106.68
26	h	616	DD6	C15-C14-C13	-3.82	117.91	125.99
26	3	312	DD6	O1-C15-C14	-3.82	105.93	116.88
24	B	832	CLA	C4A-NA-C1A	3.81	108.42	106.68
26	c	614	DD6	O1-C20-C21	3.81	119.31	115.05
25	2	211	BCR	C38-C26-C25	-3.80	120.33	124.48
25	I	101	BCR	C36-C18-C19	3.80	123.89	118.09
25	A	843	BCR	C37-C22-C23	3.79	123.88	118.09
26	4	616	DD6	C15-C14-C13	-3.79	117.98	125.99
26	7	618	DD6	C9-C10-C11	-3.79	121.96	127.28
25	L	206	BCR	C37-C22-C23	3.79	123.87	118.09
25	1	310	BCR	C15-C14-C13	-3.78	121.97	127.28
25	R	101	BCR	C38-C26-C25	-3.78	120.36	124.48
24	7	612	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
25	1	314	BCR	C24-C23-C22	-3.78	120.64	126.23
26	6	613	DD6	C4-C5-C6	-3.78	121.97	127.28
24	3	304	CLA	CMB-C2B-C1B	-3.78	119.66	125.42
28	2	215	LHG	O7-C7-C8	3.78	119.65	111.48
24	t	303	CLA	C4A-NA-C1A	3.78	108.40	106.68
24	7	606	CLA	O2D-CGD-O1D	-3.78	116.50	123.85
25	2	211	BCR	C11-C10-C9	-3.77	121.99	127.28
25	2	211	BCR	C21-C20-C19	-3.77	112.29	123.20
26	4	615	DD6	C14-C13-C11	-3.76	119.69	125.53
25	F	204	BCR	C16-C17-C18	-3.76	122.00	127.28
25	A	846	BCR	C4-C5-C6	-3.76	117.62	122.70
24	A	802	CLA	C4A-NA-C1A	3.76	108.39	106.68
25	9	316	BCR	C33-C5-C6	-3.76	120.39	124.48
25	A	846	BCR	C20-C21-C22	-3.75	122.01	127.28
26	1	313	DD6	C15-C14-C13	-3.75	118.06	125.99
24	k	308	CLA	CMB-C2B-C1B	-3.75	119.71	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	840	BCR	C36-C18-C19	3.74	123.80	118.09
26	6	613	DD6	C9-C10-C11	-3.73	122.04	127.28
25	B	843	BCR	C4-C5-C6	-3.73	117.66	122.70
25	B	841	BCR	C11-C10-C9	-3.73	122.04	127.28
25	F	204	BCR	C38-C26-C25	-3.73	120.41	124.48
24	6	606	CLA	C4A-NA-C1A	3.73	108.38	106.68
24	h	603	CLA	C4A-NA-C1A	3.73	108.38	106.68
25	t	312	BCR	C15-C14-C13	-3.73	122.04	127.28
24	B	804	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
28	4	619	LHG	O7-C7-C8	3.72	119.54	111.48
24	A	830	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
24	t	309	CLA	C4A-NA-C1A	3.72	108.37	106.68
25	I	102	BCR	C16-C17-C18	-3.71	122.07	127.28
24	1	302	CLA	C4A-NA-C1A	3.71	108.37	106.68
24	A	811	CLA	C4A-NA-C1A	3.71	108.37	106.68
26	h	615	DD6	C14-C13-C11	-3.71	119.77	125.53
26	2	212	DD6	C15-C14-C13	-3.71	118.15	125.99
25	A	859	BCR	C7-C8-C9	-3.71	120.75	126.23
26	7	616	DD6	C4-C5-C6	-3.70	122.08	127.28
26	6	614	DD6	C4-C5-C6	-3.70	122.08	127.28
28	A	852	LHG	O7-C7-C8	3.70	119.49	111.48
26	k	313	DD6	C4-C5-C6	-3.70	122.09	127.28
24	A	826	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
26	6	615	DD6	C14-C13-C11	-3.70	119.79	125.53
24	3	305	CLA	C4A-NA-C1A	3.70	108.36	106.68
26	t	313	DD6	C9-C10-C11	-3.69	122.10	127.28
25	I	101	BCR	C1-C6-C5	-3.69	117.59	122.64
25	B	840	BCR	C30-C25-C26	-3.69	117.60	122.64
24	k	308	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
25	R	101	BCR	C16-C17-C18	-3.68	122.12	127.28
26	3	311	DD6	C9-C10-C11	-3.67	122.13	127.28
24	6	603	CLA	C4A-NA-C1A	3.67	108.35	106.68
25	R	101	BCR	C20-C21-C22	-3.67	122.14	127.28
25	A	846	BCR	C16-C17-C18	-3.66	122.14	127.28
26	8	212	DD6	C9-C10-C11	-3.66	122.14	127.28
25	B	841	BCR	C36-C18-C19	3.66	123.68	118.09
26	k	313	DD6	C14-C13-C11	-3.66	119.85	125.53
26	4	616	DD6	O1-C20-C19	-3.66	110.06	113.49
24	B	814	CLA	C4A-NA-C1A	3.66	108.35	106.68
24	k	306	CLA	C4A-NA-C1A	3.66	108.35	106.68
26	t	313	DD6	C15-C14-C13	-3.66	118.26	125.99
24	4	612	CLA	C4A-NA-C1A	3.66	108.35	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	302	CLA	C4A-NA-C1A	3.65	108.35	106.68
24	B	829	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
25	J	104	BCR	C36-C18-C19	3.64	123.66	118.09
25	1	314	BCR	C15-C14-C13	-3.64	122.17	127.28
25	J	104	BCR	C7-C8-C9	-3.64	120.85	126.23
24	B	810	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
26	c	614	DD6	C21-C20-C15	-3.63	116.33	122.30
24	2	209	CLA	C4A-NA-C1A	3.63	108.33	106.68
26	2	210	DD6	C15-C14-C13	-3.62	118.33	125.99
25	9	316	BCR	C38-C26-C25	-3.62	120.54	124.48
26	7	615	DD6	C14-C13-C11	-3.62	119.92	125.53
25	M	101	BCR	C7-C8-C9	-3.61	120.89	126.23
24	2	201	CLA	C4A-NA-C1A	3.61	108.33	106.68
25	A	859	BCR	C24-C23-C22	-3.61	120.89	126.23
25	F	204	BCR	C20-C21-C22	-3.61	122.21	127.28
25	A	859	BCR	C36-C18-C19	3.61	123.60	118.09
25	A	845	BCR	C38-C26-C25	-3.61	120.55	124.48
28	8	213	LHG	O8-C23-C24	3.61	122.84	111.83
24	3	307	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
28	L	201	LHG	O7-C7-C8	3.60	119.26	111.48
24	A	860	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
25	B	849	BCR	C36-C18-C19	3.59	123.57	118.09
24	A	813	CLA	C4A-NA-C1A	3.59	108.32	106.68
25	B	843	BCR	C33-C5-C6	-3.58	120.57	124.48
25	R	101	BCR	C36-C18-C19	3.58	123.56	118.09
25	L	206	BCR	C38-C26-C27	3.58	121.23	113.60
24	4	601	CLA	C4A-NA-C1A	3.58	108.31	106.68
26	c	614	DD6	C25-C24-C1	-3.58	116.55	126.36
24	B	824	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
25	I	101	BCR	C7-C8-C9	-3.58	120.94	126.23
24	5	604	CLA	C4A-NA-C1A	3.57	108.31	106.68
24	A	829	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
24	B	823	CLA	C4A-NA-C1A	3.57	108.31	106.68
24	k	303	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
24	B	821	CLA	C4A-NA-C1A	3.57	108.31	106.68
26	h	615	DD6	C9-C10-C11	-3.57	122.28	127.28
26	9	315	DD6	C14-C13-C11	-3.56	120.00	125.53
24	B	818	CLA	C4A-NA-C1A	3.56	108.30	106.68
26	2	210	DD6	C4-C5-C6	-3.56	122.28	127.28
26	9	317	DD6	C25-C24-C1	-3.56	116.60	126.36
24	9	306	CLA	C4A-NA-C1A	3.56	108.30	106.68
25	J	104	BCR	C20-C21-C22	-3.56	122.29	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	206	BCR	C36-C18-C19	3.55	123.52	118.09
25	k	316	BCR	C16-C17-C18	-3.55	122.29	127.28
26	k	313	DD6	C9-C10-C11	-3.55	122.29	127.28
26	c	613	DD6	C9-C10-C11	-3.55	122.30	127.28
24	A	816	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
25	B	849	BCR	C20-C21-C22	-3.54	122.32	127.28
26	l	311	DD6	C15-C14-C13	-3.53	118.52	125.99
25	c	615	BCR	C20-C19-C18	-3.53	116.67	126.36
25	F	204	BCR	C33-C5-C6	-3.53	120.63	124.48
26	5	608	DD6	C9-C10-C11	-3.53	122.33	127.28
25	R	102	BCR	C31-C1-C6	-3.53	104.72	110.24
24	A	833	CLA	C4A-NA-C1A	3.52	108.29	106.68
24	L	204	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
24	B	827	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
24	7	606	CLA	O2D-CGD-CBD	3.52	117.38	111.23
25	J	101	BCR	C20-C21-C22	-3.52	122.34	127.28
25	M	101	BCR	C28-C27-C26	-3.51	107.79	114.06
26	4	614	DD6	C9-C10-C11	-3.51	122.35	127.28
25	L	202	BCR	C36-C18-C19	3.51	123.45	118.09
24	B	817	CLA	C4A-NA-C1A	3.51	108.28	106.68
24	B	834	CLA	C4A-NA-C1A	3.51	108.28	106.68
28	A	841	LHG	O7-C7-C8	3.51	119.07	111.48
26	7	613	DD6	C25-C26-C27	-3.51	116.81	126.61
25	B	842	BCR	C33-C5-C6	-3.50	120.67	124.48
25	B	841	BCR	C3-C4-C5	-3.49	107.83	114.06
25	2	211	BCR	C33-C5-C6	-3.49	120.67	124.48
25	1	310	BCR	C20-C21-C22	-3.49	122.39	127.28
24	B	826	CLA	C4A-NA-C1A	3.49	108.27	106.68
25	R	102	BCR	C20-C21-C22	-3.48	122.39	127.28
26	8	210	DD6	C4-C5-C6	-3.48	122.39	127.28
25	I	102	BCR	C1-C6-C7	3.47	125.07	115.65
26	4	617	DD6	C4-C3-C2	-3.47	116.42	123.52
24	A	802	CLA	CMB-C2B-C1B	-3.47	120.14	125.42
25	L	202	BCR	C7-C8-C9	-3.46	121.12	126.23
25	k	316	BCR	C15-C16-C17	-3.46	116.44	123.52
26	6	616	DD6	C21-C20-C15	-3.45	116.62	122.30
26	8	210	DD6	C13-C11-C10	3.45	124.44	119.01
26	t	311	DD6	C4-C5-C6	-3.45	122.44	127.28
24	B	815	CLA	C4A-NA-C1A	3.45	108.25	106.68
26	3	311	DD6	C4-C5-C6	-3.45	122.44	127.28
25	I	101	BCR	C27-C26-C25	-3.45	118.04	122.70
25	A	843	BCR	C36-C18-C19	3.45	123.36	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	310	BCR	C11-C10-C9	-3.45	122.44	127.28
26	4	615	DD6	C9-C10-C11	-3.44	122.45	127.28
25	2	211	BCR	C7-C8-C9	-3.44	121.14	126.23
25	k	316	BCR	C28-C27-C26	-3.44	107.92	114.06
24	h	606	CLA	C4A-NA-C1A	3.44	108.25	106.68
24	6	607	CLA	C4A-NA-C1A	3.43	108.25	106.68
26	8	211	DD6	C9-C10-C11	-3.43	122.47	127.28
26	k	315	DD6	C10-C9-C8	-3.43	113.26	123.20
25	4	618	BCR	C3-C4-C5	-3.43	107.94	114.06
25	B	843	BCR	C11-C12-C13	-3.42	116.97	126.36
25	I	101	BCR	C33-C5-C4	3.42	120.89	113.60
25	F	204	BCR	C24-C23-C22	-3.42	121.17	126.23
25	J	101	BCR	C15-C16-C17	-3.42	116.53	123.52
28	A	842	LHG	C10-C9-C8	-3.41	100.60	113.13
25	R	102	BCR	C11-C10-C9	-3.41	122.50	127.28
24	B	808	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
26	7	618	DD6	C14-C13-C11	-3.41	120.25	125.53
30	2	214	LMG	C7-O1-C1	-3.40	106.50	113.80
24	1	304	CLA	C4A-NA-C1A	3.40	108.23	106.68
26	t	311	DD6	C15-C14-C13	-3.39	118.82	125.99
25	B	849	BCR	C16-C15-C14	-3.39	116.58	123.52
25	R	101	BCR	C30-C25-C26	-3.39	118.00	122.64
25	B	841	BCR	C20-C21-C22	-3.39	122.53	127.28
24	4	604	CLA	C4A-NA-C1A	3.38	108.22	106.68
30	t	314	LMG	C8-O7-C10	-3.38	109.71	117.80
26	h	613	DD6	C4-C5-C6	-3.38	122.54	127.28
24	A	857	CLA	C1-C2-C3	-3.38	120.67	126.20
27	3	314	LMT	O1'-C1'-C2'	3.37	113.39	108.27
25	A	844	BCR	C38-C26-C25	-3.37	120.81	124.48
24	k	303	CLA	C4-C3-C5	3.37	121.08	115.23
24	2	206	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
24	h	602	CLA	C1-O2A-CGA	3.37	124.81	116.65
26	7	616	DD6	C25-C26-C27	-3.37	117.20	126.61
24	4	612	CLA	CMB-C2B-C1B	-3.37	120.30	125.42
24	t	301	CLA	CMB-C2B-C1B	-3.36	120.30	125.42
24	A	803	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
25	1	310	BCR	C16-C15-C14	-3.36	116.65	123.52
26	9	317	DD6	C10-C9-C8	-3.35	113.49	123.20
26	R	105	DD6	C12-C11-C13	3.35	123.20	118.09
25	A	845	BCR	C28-C27-C26	-3.35	108.09	114.06
24	A	836	CLA	O2D-CGD-O1D	-3.35	117.34	123.85
26	2	210	DD6	C14-C13-C11	-3.33	120.36	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	807	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
25	B	849	BCR	C29-C30-C25	3.33	115.28	110.44
25	L	202	BCR	C33-C5-C6	-3.33	120.85	124.48
25	B	849	BCR	C7-C8-C9	-3.33	121.31	126.23
24	7	606	CLA	C4A-NA-C1A	3.33	108.20	106.68
26	9	317	DD6	C12-C11-C13	3.32	123.17	118.09
25	B	843	BCR	C1-C6-C5	-3.32	118.09	122.64
24	h	611	CLA	CAA-C2A-C3A	-3.32	108.62	116.23
26	6	614	DD6	C15-C14-C13	-3.32	118.98	125.99
26	7	613	DD6	C25-C24-C1	-3.32	117.27	126.36
24	A	805	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
25	B	843	BCR	C8-C7-C6	-3.31	118.16	127.00
28	A	842	LHG	C6-C5-C4	-3.31	104.08	111.78
24	L	203	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
24	9	306	CLA	CHB-C4A-NA	3.30	129.17	124.40
26	9	314	DD6	C14-C13-C11	-3.30	120.41	125.53
24	1	306	CLA	C4A-NA-C1A	3.30	108.18	106.68
26	A	848	DD6	C25-C26-C27	-3.30	117.39	126.61
24	k	303	CLA	O2D-CGD-CBD	3.29	116.99	111.23
24	c	608	CLA	C4A-NA-C1A	3.29	108.18	106.68
24	A	840	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
26	7	618	DD6	O1-C15-C14	-3.29	107.45	116.88
26	3	313	DD6	C25-C26-C27	-3.29	117.41	126.61
25	J	101	BCR	C11-C12-C13	-3.28	117.36	126.36
26	1	313	DD6	C4-C5-C6	-3.28	122.67	127.28
24	A	838	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	1	310	BCR	C23-C24-C25	-3.28	118.24	127.00
25	L	202	BCR	C30-C25-C26	-3.28	118.16	122.64
25	M	101	BCR	C20-C19-C18	-3.28	117.38	126.36
25	B	841	BCR	C16-C17-C18	-3.28	122.68	127.28
25	J	101	BCR	C33-C5-C4	3.27	120.57	113.60
25	k	316	BCR	C33-C5-C6	-3.27	120.92	124.48
26	k	314	DD6	C30-C29-C27	-3.26	165.14	176.23
24	3	303	CLA	C1-C2-C3	-3.26	120.85	126.20
24	A	819	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
25	A	846	BCR	C30-C25-C24	3.26	124.48	115.65
25	I	102	BCR	C27-C26-C25	-3.25	118.31	122.70
24	A	833	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
25	2	211	BCR	C15-C16-C17	-3.25	116.87	123.52
26	4	615	DD6	C4-C5-C6	-3.25	122.73	127.28
24	7	607	CLA	C4A-NA-C1A	3.24	108.16	106.68
26	8	211	DD6	O1-C20-C19	-3.24	110.45	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	212	DD6	C4-C5-C6	-3.24	122.73	127.28
24	A	835	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
25	4	618	BCR	C33-C5-C6	-3.24	120.95	124.48
24	B	834	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
24	L	205	CLA	C4A-NA-C1A	3.24	108.16	106.68
25	A	843	BCR	C38-C26-C27	3.23	120.49	113.60
24	B	804	CLA	C3B-C4B-NB	-3.23	107.65	110.53
24	9	307	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
25	c	615	BCR	C23-C22-C21	3.23	124.08	119.01
26	7	618	DD6	O1-C20-C19	-3.22	110.47	113.49
24	B	835	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
25	1	310	BCR	C8-C7-C6	-3.22	118.41	127.00
25	c	615	BCR	C16-C15-C14	-3.22	116.94	123.52
25	B	843	BCR	C15-C16-C17	-3.21	116.96	123.52
24	A	804	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
25	4	618	BCR	C20-C19-C18	-3.20	117.58	126.36
26	h	615	DD6	C10-C9-C8	-3.20	113.92	123.20
26	6	617	DD6	C14-C13-C11	-3.20	120.56	125.53
25	I	101	BCR	C24-C23-C22	-3.20	121.50	126.23
25	A	845	BCR	C20-C21-C22	-3.20	122.79	127.28
24	k	310	CLA	O2D-CGD-CBD	3.20	116.82	111.23
24	t	303	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
25	2	211	BCR	C16-C17-C18	-3.19	122.80	127.28
25	I	101	BCR	C38-C26-C27	3.19	120.41	113.60
25	A	843	BCR	C33-C5-C4	3.19	120.40	113.60
25	2	211	BCR	C23-C24-C25	-3.19	118.47	127.00
24	B	823	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	1	314	BCR	C20-C21-C22	-3.19	122.81	127.28
28	3	315	LHG	O7-C7-C8	3.18	118.37	111.48
25	F	204	BCR	C3-C4-C5	-3.18	108.38	114.06
25	I	102	BCR	C8-C9-C10	-3.18	114.01	119.01
24	B	805	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	B	838	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	h	610	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
25	1	314	BCR	C30-C25-C26	-3.18	118.30	122.64
25	c	615	BCR	C15-C14-C13	-3.17	122.83	127.28
24	A	837	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
24	4	602	CLA	C4-C3-C5	3.17	120.73	115.23
25	c	615	BCR	C30-C25-C24	3.17	124.24	115.65
26	t	313	DD6	C10-C9-C8	-3.17	114.03	123.20
26	9	317	DD6	C4-C3-C2	-3.16	117.05	123.52
25	7	617	BCR	C15-C16-C17	-3.16	117.05	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	822	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
26	t	311	DD6	C9-C10-C11	-3.16	122.85	127.28
26	4	614	DD6	C34-C35-C36	-3.16	104.31	112.18
25	4	618	BCR	C7-C8-C9	-3.16	121.56	126.23
26	4	614	DD6	C25-C26-C27	-3.15	117.79	126.61
25	M	101	BCR	C10-C11-C12	-3.15	114.07	123.20
24	3	302	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
26	5	609	DD6	C4-C5-C6	-3.14	122.87	127.28
24	B	847	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
25	B	840	BCR	C1-C6-C5	-3.14	118.34	122.64
26	h	613	DD6	C9-C10-C11	-3.14	122.88	127.28
24	B	846	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	1	310	BCR	C27-C26-C25	-3.13	118.47	122.70
25	L	202	BCR	C27-C26-C25	-3.13	118.47	122.70
24	7	604	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	R	101	BCR	C33-C5-C6	-3.13	121.07	124.48
24	A	822	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	8	202	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	A	824	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	B	817	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	7	606	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
24	6	605	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	A	832	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	B	842	BCR	C38-C26-C25	-3.12	121.08	124.48
24	B	815	CLA	C4-C3-C5	3.12	120.64	115.23
25	4	618	BCR	C27-C26-C25	-3.11	118.50	122.70
24	B	818	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
24	3	304	CLA	CMB-C2B-C3B	3.11	133.87	126.55
24	B	813	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
26	h	615	DD6	C7-C6-C8	3.11	122.84	118.09
25	I	102	BCR	C15-C16-C17	-3.11	117.16	123.52
24	B	836	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
24	8	203	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
24	A	818	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	7	613	DD6	C9-C10-C11	-3.10	122.94	127.28
25	1	310	BCR	C38-C26-C27	3.10	120.20	113.60
26	J	102	DD6	C15-C14-C13	-3.10	119.45	125.99
29	9	312	A1L1G	C17-C20-C25	-3.10	117.21	122.30
25	J	104	BCR	C39-C30-C25	-3.09	105.39	110.24
25	1	314	BCR	C3-C4-C5	-3.09	108.54	114.06
24	3	301	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
24	B	803	CLA	O2D-CGD-O1D	-3.09	117.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	602	CLA	CMB-C2B-C1B	-3.09	120.71	125.42
24	A	811	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	B	807	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	3	304	CLA	C4A-NA-C1A	3.09	108.09	106.68
24	A	834	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
26	3	312	DD6	O1-C20-C19	-3.08	110.60	113.49
25	R	102	BCR	C8-C9-C10	3.08	123.86	119.01
26	k	313	DD6	C19-C18-C17	3.08	116.55	110.79
24	J	103	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	B	830	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
26	9	313	DD6	O1-C20-C19	-3.07	110.61	113.49
25	A	846	BCR	C33-C5-C4	3.07	120.14	113.60
25	I	102	BCR	C1-C6-C5	-3.07	118.44	122.64
26	3	312	DD6	C19-C18-C17	3.07	116.53	110.79
24	R	103	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
25	t	312	BCR	C16-C17-C18	-3.06	122.99	127.28
25	A	844	BCR	C7-C8-C9	-3.06	121.71	126.23
24	A	825	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	7	605	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
25	R	101	BCR	C38-C26-C27	3.06	120.11	113.60
24	1	317	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
24	3	304	CLA	CAA-C2A-C3A	-3.06	104.74	113.00
24	2	209	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
25	J	104	BCR	C29-C30-C25	3.05	114.87	110.44
24	k	308	CLA	CMB-C2B-C3B	3.05	133.73	126.55
24	B	833	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	5	602	CLA	C4A-NA-C1A	3.05	108.07	106.68
26	R	105	DD6	C12-C11-C10	-3.05	117.87	122.82
24	B	821	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	A	817	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
25	R	102	BCR	C16-C17-C18	-3.04	123.01	127.28
25	7	617	BCR	C7-C8-C9	-3.04	121.73	126.23
24	h	605	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
24	c	606	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
24	A	815	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
24	A	823	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
24	k	304	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	R	101	BCR	C28-C27-C26	-3.04	108.64	114.06
24	h	611	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	1	304	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
26	3	313	DD6	C10-C9-C8	-3.03	114.41	123.20
24	L	204	CLA	O2D-CGD-CBD	3.03	116.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	841	BCR	C15-C16-C17	-3.02	117.33	123.52
24	k	306	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	2	211	BCR	C38-C26-C27	3.02	120.04	113.60
24	7	607	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	1	305	CLA	C2A-C1A-CHA	3.02	129.11	123.87
25	7	617	BCR	C3-C4-C5	-3.02	108.67	114.06
28	3	315	LHG	O8-C23-C24	3.02	121.04	111.83
26	A	848	DD6	C4-C3-C2	-3.02	117.34	123.52
24	4	606	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	c	607	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	7	617	BCR	C10-C11-C12	-3.01	114.47	123.20
25	R	101	BCR	C1-C6-C5	-3.01	118.52	122.64
26	c	614	DD6	C34-C35-C36	-3.01	104.68	112.18
24	A	856	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
24	B	837	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
24	k	307	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
24	B	804	CLA	C1-O2A-CGA	3.01	123.93	116.65
24	1	305	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
24	B	826	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	R	102	BCR	C1-C6-C5	-3.00	118.53	122.64
24	A	833	CLA	C4-C3-C5	3.00	120.44	115.23
27	3	314	LMT	C1B-O1B-C4'	-3.00	110.87	117.98
26	9	314	DD6	C-C1-C2	-3.00	117.96	122.82
26	R	105	DD6	C26-C25-C24	-3.00	114.51	123.20
25	L	202	BCR	C20-C21-C22	-3.00	123.08	127.28
24	c	602	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
26	5	609	DD6	C19-C18-C17	3.00	116.39	110.79
25	B	840	BCR	C4-C5-C6	-2.99	118.66	122.70
24	h	606	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
25	B	849	BCR	C12-C13-C14	-2.99	114.30	119.01
24	c	609	CLA	O2A-CGA-O1A	-2.99	116.15	123.63
24	B	814	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
24	t	303	CLA	C4-C3-C5	2.99	120.42	115.23
24	t	309	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
25	4	618	BCR	C38-C26-C27	2.99	119.97	113.60
26	k	315	DD6	C7-C6-C8	2.99	122.65	118.09
24	B	812	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	B	813	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	t	303	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
26	A	848	DD6	C25-C24-C1	-2.98	118.19	126.36
26	1	313	DD6	C10-C9-C8	-2.98	114.56	123.20
25	L	202	BCR	C1-C6-C7	2.98	123.73	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	819	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	1	314	BCR	C16-C15-C14	-2.98	117.42	123.52
25	2	211	BCR	C8-C7-C6	-2.98	119.04	127.00
24	B	811	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	8	204	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
26	1	311	DD6	C4-C5-C6	-2.97	123.11	127.28
24	A	847	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
24	A	820	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
24	2	201	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
26	3	313	DD6	C21-C20-C19	-2.97	110.90	114.24
24	7	608	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
26	7	618	DD6	C25-C26-C27	-2.97	118.30	126.61
24	4	602	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	t	310	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	9	303	CLA	CHB-C4A-NA	2.97	128.69	124.40
25	J	104	BCR	C30-C25-C26	-2.97	118.58	122.64
24	2	204	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
25	R	101	BCR	C7-C8-C9	-2.97	121.85	126.23
24	B	825	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
25	2	211	BCR	C33-C5-C4	2.96	119.92	113.60
24	4	604	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	6	607	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	3	309	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	c	608	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	L	202	BCR	C34-C9-C10	-2.96	118.03	122.82
24	h	612	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	6	604	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	L	202	BCR	C11-C10-C9	-2.96	123.13	127.28
24	A	810	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
24	h	607	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	R	104	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	1	305	CLA	CHB-C4A-NA	2.95	128.66	124.40
28	A	849	LHG	O8-C23-C24	2.95	120.84	111.83
29	7	614	A1L1G	O15-C20-C21	-2.95	110.72	113.49
24	A	816	CLA	O2D-CGD-CBD	2.95	116.39	111.23
25	A	846	BCR	C15-C16-C17	-2.95	117.48	123.52
25	7	617	BCR	C28-C27-C26	-2.95	108.80	114.06
25	1	310	BCR	C3-C4-C5	-2.95	108.80	114.06
25	A	845	BCR	C38-C26-C27	2.95	119.88	113.60
24	B	828	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	A	846	BCR	C11-C10-C9	-2.95	123.14	127.28
28	L	201	LHG	O8-C23-C24	2.95	120.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	604	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
25	4	618	BCR	C8-C7-C6	-2.94	119.14	127.00
24	5	607	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
24	2	206	CLA	O2D-CGD-CBD	2.94	116.37	111.23
24	A	830	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	B	801	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	B	815	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	t	307	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
25	A	844	BCR	C8-C7-C6	-2.93	119.16	127.00
24	9	304	CLA	CHB-C4A-NA	2.93	128.63	124.40
24	7	601	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	A	860	CLA	C1-C2-C3	-2.93	121.39	126.20
24	5	604	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
31	B	839	PQN	C11-C3-C4	-2.93	115.49	118.58
26	9	314	DD6	O1-C20-C19	-2.93	110.75	113.49
24	B	824	CLA	O2D-CGD-CBD	2.93	116.35	111.23
24	4	609	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	c	604	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
25	A	843	BCR	C30-C25-C26	-2.92	118.64	122.64
25	I	102	BCR	C30-C25-C24	2.92	123.58	115.65
25	I	102	BCR	C33-C5-C4	2.92	119.83	113.60
25	1	310	BCR	C38-C26-C25	-2.92	121.30	124.48
24	9	311	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
24	1	306	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	4	616	DD6	C10-C9-C8	-2.92	114.74	123.20
24	A	821	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	c	605	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	B	820	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	A	806	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	A	829	CLA	O2D-CGD-CBD	2.92	116.33	111.23
24	A	828	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
24	B	832	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
24	B	848	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
24	5	602	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
24	4	613	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	F	202	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
25	J	104	BCR	C16-C15-C14	-2.91	117.57	123.52
24	k	303	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
24	2	208	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
24	A	827	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	611	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
26	8	212	DD6	C12-C11-C13	2.90	122.52	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	808	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	9	304	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	4	603	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
24	2	202	CLA	C4-C3-C5	2.90	120.26	115.23
25	A	843	BCR	C16-C15-C14	-2.90	117.59	123.52
24	5	606	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	A	814	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	J	101	BCR	C24-C23-C22	-2.89	121.95	126.23
24	A	812	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	k	314	DD6	O1-C20-C19	-2.89	110.78	113.49
25	I	102	BCR	C7-C8-C9	-2.89	121.96	126.23
25	L	202	BCR	C16-C17-C18	-2.89	123.22	127.28
24	A	802	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	7	617	BCR	C30-C25-C26	-2.89	118.69	122.64
24	7	603	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	9	305	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	B	804	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
24	1	305	CLA	CAA-CBA-CGA	-2.89	104.79	112.49
24	4	605	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	A	857	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	F	203	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	B	831	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	2	203	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	B	816	CLA	CHB-C4A-NA	2.88	128.56	124.40
26	6	616	DD6	O1-C20-C19	-2.88	110.79	113.49
29	k	312	A1L1G	C43-C44-C42	-2.88	118.15	122.82
26	k	313	DD6	O1-C15-C14	-2.88	108.63	116.88
29	9	312	A1L1G	C43-C44-C42	-2.88	118.15	122.82
25	A	843	BCR	C4-C5-C6	-2.88	118.82	122.70
25	1	310	BCR	C33-C5-C4	2.87	119.72	113.60
24	1	303	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	5	605	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	6	608	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	A	831	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
26	k	315	DD6	C8-C6-C5	-2.87	114.50	119.01
24	9	310	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	9	315	DD6	C25-C24-C1	-2.87	118.50	126.36
25	I	101	BCR	C38-C26-C25	-2.87	121.36	124.48
24	3	305	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	7	617	BCR	C24-C23-C22	-2.87	122.00	126.23
25	L	202	BCR	C38-C26-C27	2.87	119.71	113.60
24	B	809	CLA	O2D-CGD-O1D	-2.86	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	603	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	A	845	BCR	C11-C12-C13	-2.86	118.52	126.36
24	5	602	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	9	306	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	9	316	BCR	C33-C5-C4	2.86	119.69	113.60
24	B	808	CLA	O2A-CGA-O1A	-2.86	116.49	123.63
24	4	610	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
24	A	853	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
25	7	617	BCR	C16-C17-C18	-2.85	123.28	127.28
26	J	102	DD6	C10-C9-C8	-2.85	114.93	123.20
24	3	306	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
24	t	301	CLA	CMB-C2B-C3B	2.85	133.26	126.55
24	k	309	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	2	211	BCR	C3-C4-C5	-2.85	108.97	114.06
24	7	610	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	h	608	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	A	802	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	t	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
24	A	813	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
24	h	601	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	7	608	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	B	803	CLA	CHB-C4A-NA	2.84	128.50	124.40
24	k	308	CLA	O2D-CGD-CBD	2.84	116.20	111.23
28	1	318	LHG	O8-C23-C24	2.84	120.50	111.83
24	B	814	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	7	613	DD6	C10-C9-C8	-2.84	114.97	123.20
26	5	609	DD6	C14-C13-C11	-2.84	121.12	125.53
24	B	831	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	6	615	DD6	C4-C3-C2	-2.84	117.71	123.52
25	R	102	BCR	C33-C5-C6	2.84	127.58	124.48
24	2	207	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
24	A	809	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
24	B	829	CLA	C1-C2-C3	-2.83	121.56	126.20
24	3	303	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	6	617	DD6	O1-C20-C21	-2.83	111.89	115.05
24	B	838	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	1	301	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	3	308	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	A	813	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	B	842	BCR	C3-C4-C5	-2.82	109.02	114.06
24	1	308	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	B	842	BCR	C33-C5-C4	2.82	119.61	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	208	CLA	CHB-C4A-NA	2.82	128.47	124.40
26	k	313	DD6	C26-C25-C24	-2.82	115.03	123.20
24	8	208	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	4	611	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	2	202	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	8	205	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	B	829	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
24	B	830	CLA	C4A-NA-C1A	2.82	107.96	106.68
24	B	806	CLA	C3B-C4B-NB	-2.82	108.02	110.53
24	A	857	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	7	617	BCR	C38-C26-C25	-2.81	121.42	124.48
25	J	104	BCR	C2-C1-C6	2.81	114.52	110.44
24	7	609	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	A	848	DD6	O1-C15-C14	-2.81	108.83	116.88
24	8	206	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	k	312	A1L1G	O15-C20-C17	-2.81	111.91	115.05
24	2	202	CLA	C4A-NA-C1A	2.81	107.96	106.68
24	6	606	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
24	c	603	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	5	601	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	8	201	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	B	810	CLA	C4A-NA-C1A	2.80	107.96	106.68
24	k	302	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	t	305	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	M	101	BCR	C16-C15-C14	-2.79	117.81	123.52
26	9	317	DD6	C21-C20-C15	-2.79	117.71	122.30
26	7	615	DD6	C25-C26-C27	-2.79	118.81	126.61
25	9	316	BCR	C3-C4-C5	-2.79	109.08	114.06
25	B	841	BCR	C28-C27-C26	-2.79	109.08	114.06
24	4	608	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	B	811	CLA	C1-C2-C3	-2.79	121.63	126.20
26	R	105	DD6	O1-C15-C14	-2.79	108.89	116.88
26	6	617	DD6	C4-C5-C6	-2.79	123.37	127.28
24	4	612	CLA	CMB-C2B-C3B	2.79	133.10	126.55
25	7	617	BCR	C8-C7-C6	-2.78	119.56	127.00
25	7	617	BCR	C21-C20-C19	-2.78	115.13	123.20
24	2	205	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
24	B	803	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	1	307	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
25	B	841	BCR	C8-C7-C6	-2.78	119.57	127.00
24	B	827	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	8	209	CLA	O2D-CGD-O1D	-2.78	118.44	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	615	DD6	C26-C25-C24	-2.78	115.14	123.20
24	A	802	CLA	CMB-C2B-C3B	2.78	133.08	126.55
26	c	612	DD6	O1-C20-C21	-2.78	111.95	115.05
24	A	857	CLA	O2A-CGA-O1A	-2.78	116.69	123.63
24	t	306	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
25	4	618	BCR	C38-C26-C25	-2.77	121.46	124.48
24	2	205	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	F	201	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	B	806	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
27	1	316	LMT	C1B-O1B-C4'	-2.77	111.42	117.98
24	A	802	CLA	C1-C2-C3	-2.77	121.66	126.20
25	4	618	BCR	C33-C5-C4	2.77	119.49	113.60
28	I	103	LHG	C5-O7-C7	-2.76	111.18	117.80
25	B	840	BCR	C11-C10-C9	-2.76	123.40	127.28
24	t	302	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	4	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
24	c	609	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	k	301	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
26	2	212	DD6	C14-C13-C11	-2.75	121.26	125.53
24	B	821	CLA	C1-C2-C3	-2.75	121.69	126.20
24	6	609	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	B	841	BCR	C33-C5-C4	2.75	119.45	113.60
26	9	314	DD6	C28-C27-C26	-2.75	118.85	124.18
24	B	833	CLA	C4-C3-C5	2.74	119.99	115.23
24	L	205	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	h	613	DD6	C10-C9-C8	-2.74	115.26	123.20
24	A	860	CLA	CHB-C4A-NA	2.74	128.35	124.40
26	t	311	DD6	C30-C29-C27	-2.74	166.92	176.23
24	c	610	CLA	C4A-NA-C1A	2.74	107.93	106.68
24	3	307	CLA	O2D-CGD-CBD	2.74	116.02	111.23
24	6	610	CLA	C4A-NA-C1A	2.74	107.93	106.68
24	B	808	CLA	C1-C2-C3	-2.73	121.72	126.20
26	4	617	DD6	O1-C20-C21	-2.73	111.99	115.05
24	A	830	CLA	C1D-ND-C4D	2.73	108.23	106.31
25	B	849	BCR	C30-C25-C26	-2.73	118.90	122.64
24	6	603	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
26	4	616	DD6	C25-C26-C27	-2.73	118.97	126.61
24	8	207	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	4	618	BCR	C16-C15-C14	-2.73	117.93	123.52
24	7	604	CLA	CMB-C2B-C1B	-2.73	121.27	125.42
26	t	313	DD6	C14-C13-C11	-2.73	121.30	125.53
24	c	603	CLA	C3B-C4B-NB	-2.73	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	602	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
24	9	309	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	4	607	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
28	I	103	LHG	O8-C23-C24	2.72	120.14	111.83
25	I	101	BCR	C16-C15-C14	-2.72	117.95	123.52
24	B	810	CLA	C1-C2-C3	-2.72	121.74	126.20
29	2	213	A1L1G	O15-C20-C17	-2.72	112.01	115.05
24	7	602	CLA	C1-C2-C3	-2.72	122.36	126.76
24	1	306	CLA	C1-C2-C3	-2.72	122.36	126.76
26	k	313	DD6	C10-C9-C8	-2.72	115.33	123.20
25	c	615	BCR	C37-C22-C21	-2.72	118.42	122.82
24	9	302	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
24	8	203	CLA	C1-C2-C3	-2.71	122.37	126.76
24	5	602	CLA	C1-C2-C3	-2.71	121.75	126.20
25	7	617	BCR	C33-C5-C4	2.71	119.38	113.60
24	B	808	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	B	830	CLA	C4-C3-C5	2.71	119.93	115.23
25	J	104	BCR	C38-C26-C25	2.71	127.44	124.48
25	1	310	BCR	C7-C8-C9	-2.71	122.23	126.23
24	c	601	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	4	617	DD6	C3-C4-C5	2.71	129.06	123.52
24	5	607	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	I	102	BCR	C29-C30-C25	2.70	114.37	110.44
24	B	811	CLA	C4-C3-C5	2.70	119.92	115.23
26	5	608	DD6	C14-C13-C11	-2.70	121.34	125.53
24	h	609	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	6	610	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	9	311	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	7	616	DD6	C25-C24-C1	-2.70	118.97	126.36
24	L	203	CLA	C1-C2-C3	-2.70	121.78	126.20
24	t	301	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	B	813	CLA	CHB-C4A-NA	2.70	128.29	124.40
26	7	613	DD6	C34-C35-C36	-2.69	105.48	112.18
25	B	840	BCR	C27-C26-C25	-2.69	119.07	122.70
26	k	314	DD6	O1-C15-C14	-2.69	109.17	116.88
25	R	102	BCR	C15-C16-C17	-2.69	118.02	123.52
24	k	311	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
24	1	302	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
30	A	855	LMG	O8-C28-C29	2.68	120.02	111.83
25	A	859	BCR	C16-C15-C14	-2.68	118.03	123.52
26	4	617	DD6	C15-C14-C13	-2.68	120.32	125.99
26	c	613	DD6	C25-C24-C1	-2.68	119.00	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	305	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
24	t	304	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	9	302	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
24	A	817	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	B	837	CLA	C4-C3-C5	2.68	119.88	115.23
29	2	213	A1L1G	C37-C36-C35	2.68	129.00	123.52
26	8	212	DD6	C10-C9-C8	-2.68	115.44	123.20
24	6	612	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
24	9	308	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
24	A	826	CLA	O2D-CGD-CBD	2.68	115.91	111.23
25	F	204	BCR	C28-C27-C26	-2.68	109.28	114.06
24	9	301	CLA	CHB-C4A-NA	2.68	128.26	124.40
26	k	314	DD6	C14-C13-C11	-2.67	121.39	125.53
25	A	859	BCR	C30-C25-C26	-2.67	118.99	122.64
24	k	310	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	6	602	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
25	R	101	BCR	C33-C5-C4	2.67	119.28	113.60
24	7	611	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
25	L	206	BCR	C38-C26-C25	-2.66	121.58	124.48
27	A	851	LMT	C2'-C3'-C4'	2.66	115.73	109.68
25	2	211	BCR	C10-C11-C12	-2.66	115.48	123.20
25	A	846	BCR	C38-C26-C27	2.66	119.28	113.60
25	c	615	BCR	C7-C6-C5	-2.66	115.42	121.56
24	9	307	CLA	CHB-C4A-NA	2.66	128.24	124.40
28	J	105	LHG	C5-O7-C7	-2.66	111.43	117.80
24	4	608	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
24	h	602	CLA	CMB-C2B-C3B	2.65	132.79	126.55
24	3	304	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
26	h	616	DD6	C3-C4-C5	2.65	128.94	123.52
26	t	313	DD6	C25-C24-C1	-2.65	119.10	126.36
26	3	313	DD6	C7-C6-C8	2.65	122.13	118.09
28	3	315	LHG	C5-O7-C7	-2.64	111.48	117.80
24	5	602	CLA	CHB-C4A-NA	2.64	128.20	124.40
24	B	847	CLA	C3B-C4B-NB	-2.64	108.18	110.53
25	A	844	BCR	C28-C27-C26	-2.64	109.36	114.06
25	L	202	BCR	C38-C26-C25	-2.63	121.61	124.48
26	c	614	DD6	C14-C13-C11	-2.63	121.45	125.53
24	7	603	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
26	t	313	DD6	C7-C6-C8	2.63	122.10	118.09
24	7	608	CLA	CMB-C2B-C3B	2.63	132.73	126.55
24	B	832	CLA	C3B-C4B-NB	-2.63	108.19	110.53
24	6	609	CLA	O2D-CGD-O1D	-2.63	118.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	618	DD6	C3-C4-C5	2.63	128.89	123.52
25	R	101	BCR	C24-C23-C22	-2.63	122.35	126.23
26	1	311	DD6	C41-C32-C31	2.63	115.23	110.52
24	7	612	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	6	616	DD6	C22-C16-C17	-2.62	104.36	108.97
25	M	101	BCR	C38-C26-C25	-2.62	121.62	124.48
24	9	302	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	k	307	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	9	313	DD6	C19-C18-C17	2.61	115.68	110.79
24	B	810	CLA	CAA-C2A-C1A	-2.61	103.41	111.97
24	9	301	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
24	F	202	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	7	607	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
24	t	303	CLA	CMB-C2B-C3B	2.61	132.69	126.55
24	7	602	CLA	CAC-C3C-C2C	-2.61	122.77	127.56
24	c	610	CLA	O2D-CGD-O1D	-2.61	118.17	124.08
26	c	614	DD6	O1-C15-C14	-2.61	109.41	116.88
24	k	303	CLA	CAC-C3C-C4C	2.60	128.18	124.79
24	R	104	CLA	CHB-C4A-NA	2.60	128.16	124.40
24	5	602	CLA	CMB-C2B-C1B	-2.60	121.45	125.42
24	A	801	CLA	C4A-NA-C1A	2.60	107.87	106.68
24	k	302	CLA	C3B-C4B-NB	-2.60	108.21	110.53
26	3	312	DD6	C4-C3-C2	-2.60	118.19	123.52
25	B	843	BCR	C7-C8-C9	-2.60	122.39	126.23
25	J	104	BCR	C12-C13-C14	-2.60	114.92	119.01
24	1	306	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
25	I	102	BCR	C15-C14-C13	-2.60	123.64	127.28
26	k	315	DD6	C25-C24-C1	-2.60	119.24	126.36
25	c	615	BCR	C24-C25-C26	-2.60	115.57	121.56
25	B	842	BCR	C1-C6-C5	-2.60	119.09	122.64
25	F	204	BCR	C11-C12-C13	-2.59	119.25	126.36
26	9	317	DD6	C13-C11-C10	-2.59	114.93	119.01
25	M	101	BCR	C11-C10-C9	-2.59	123.65	127.28
25	k	316	BCR	C2-C1-C6	2.59	114.20	110.44
24	A	853	CLA	C1-C2-C3	-2.59	121.96	126.20
24	2	201	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
24	7	602	CLA	CBC-CAC-C3C	2.59	119.44	112.42
24	A	837	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	h	615	DD6	C8-C6-C5	-2.59	114.94	119.01
25	B	841	BCR	C11-C12-C13	-2.59	119.27	126.36
24	B	804	CLA	CMB-C2B-C3B	2.59	132.63	126.55
26	h	616	DD6	C25-C26-C27	-2.59	119.38	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	601	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
26	6	615	DD6	O1-C20-C21	-2.58	112.17	115.05
25	7	617	BCR	C38-C26-C27	2.58	119.09	113.60
25	A	843	BCR	C29-C30-C25	2.58	114.18	110.44
24	4	603	CLA	C3B-C4B-NB	-2.57	108.23	110.53
26	9	315	DD6	C21-C20-C19	-2.57	111.35	114.24
25	k	316	BCR	C11-C12-C13	-2.57	119.31	126.36
25	k	316	BCR	C23-C24-C25	-2.57	120.13	127.00
25	B	841	BCR	C24-C23-C22	-2.57	122.43	126.23
24	h	603	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
24	B	811	CLA	C3B-C4B-NB	-2.57	108.24	110.53
24	9	302	CLA	CHB-C4A-NA	2.57	128.11	124.40
25	R	101	BCR	C23-C24-C25	-2.57	120.14	127.00
24	B	808	CLA	O2D-CGD-CBD	2.57	115.72	111.23
26	6	617	DD6	C25-C26-C27	-2.57	119.44	126.61
24	B	804	CLA	C4D-CHA-C1A	2.57	124.30	121.24
26	9	317	DD6	O1-C15-C14	-2.57	109.53	116.88
24	9	308	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	k	303	CLA	C4A-NA-C1A	2.56	107.85	106.68
24	A	803	CLA	O2D-CGD-CBD	2.56	115.71	111.23
24	h	603	CLA	O2D-CGD-O1D	-2.56	118.26	124.08
24	A	820	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
25	2	211	BCR	C29-C30-C25	2.56	114.16	110.44
26	6	616	DD6	O1-C20-C21	2.56	117.91	115.05
25	1	314	BCR	C28-C27-C26	-2.56	109.50	114.06
25	I	101	BCR	C28-C27-C26	-2.56	109.50	114.06
26	4	615	DD6	O1-C15-C14	-2.55	109.56	116.88
25	L	206	BCR	C33-C5-C6	-2.55	121.70	124.48
25	9	316	BCR	C16-C15-C14	-2.55	118.29	123.52
25	B	841	BCR	C30-C25-C26	-2.55	119.15	122.64
24	7	602	CLA	O2D-CGD-CBD	2.55	115.69	111.23
24	8	203	CLA	O2D-CGD-CBD	2.55	115.69	111.23
24	h	611	CLA	CHB-C4A-NA	2.55	128.08	124.40
24	6	611	CLA	O2D-CGD-O1D	-2.55	118.29	124.08
24	4	601	CLA	O2D-CGD-O1D	-2.55	118.30	124.08
26	9	313	DD6	C10-C9-C8	-2.55	115.82	123.20
26	7	616	DD6	C28-C27-C26	-2.55	119.23	124.18
24	9	303	CLA	C3B-C4B-NB	-2.55	108.26	110.53
24	A	860	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
25	A	846	BCR	C3-C4-C5	-2.55	109.52	114.06
24	A	840	CLA	C1-C2-C3	-2.54	122.03	126.20
26	9	315	DD6	C25-C26-C27	-2.54	119.50	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	610	CLA	C1D-ND-C4D	-2.54	104.53	106.31
26	h	615	DD6	C9-C8-C6	2.54	133.33	126.36
26	c	612	DD6	C12-C11-C10	-2.54	118.70	122.82
26	c	613	DD6	C10-C9-C8	-2.54	115.84	123.20
26	4	617	DD6	C14-C13-C11	-2.54	121.59	125.53
28	A	841	LHG	O8-C23-C24	2.53	119.56	111.83
26	k	313	DD6	O1-C20-C19	-2.53	111.12	113.49
25	A	844	BCR	C3-C4-C5	-2.53	109.54	114.06
25	A	843	BCR	C11-C10-C9	-2.53	123.73	127.28
26	5	609	DD6	C10-C9-C8	-2.53	115.88	123.20
24	B	831	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
25	A	844	BCR	C34-C9-C8	2.53	121.95	118.09
26	9	317	DD6	C19-C18-C17	2.52	115.51	110.79
24	A	822	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	J	103	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	1	306	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
29	7	614	A1L1G	C2-C45-C1	-2.52	174.69	177.66
25	B	843	BCR	C2-C1-C6	-2.52	106.78	110.44
24	8	208	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
24	2	201	CLA	CMB-C2B-C3B	2.52	132.47	126.55
26	8	210	DD6	C25-C24-C1	-2.52	119.47	126.36
27	h	617	LMT	C1'-O5'-C5'	-2.52	108.81	113.72
25	A	844	BCR	C16-C15-C14	-2.51	118.37	123.52
24	B	829	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	B	816	CLA	C1-C2-C3	-2.51	122.08	126.20
28	2	215	LHG	O8-C23-C24	2.51	119.50	111.83
24	1	309	CLA	O2D-CGD-O1D	-2.51	118.38	124.08
25	L	202	BCR	C1-C6-C5	-2.51	119.20	122.64
25	B	840	BCR	C33-C5-C4	2.51	118.94	113.60
26	6	613	DD6	C10-C9-C8	-2.51	115.93	123.20
25	I	101	BCR	C15-C16-C17	-2.51	118.39	123.52
24	3	305	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	B	802	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
25	2	211	BCR	C36-C18-C19	2.51	121.92	118.09
24	A	853	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
26	R	105	DD6	C15-C14-C13	2.50	131.28	125.99
26	t	313	DD6	C26-C25-C24	-2.50	115.95	123.20
25	k	316	BCR	C38-C26-C27	2.50	118.93	113.60
30	2	214	LMG	C8-O7-C10	-2.50	111.81	117.80
24	B	812	CLA	C3B-C4B-NB	-2.50	108.30	110.53
24	2	204	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	6	611	CLA	CMB-C2B-C1B	-2.50	121.61	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	305	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
24	F	203	CLA	CHB-C4A-NA	2.50	128.00	124.40
26	6	615	DD6	C33-C32-C31	2.50	114.41	109.49
24	c	601	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	B	810	CLA	CMB-C2B-C3B	2.50	130.16	123.53
25	k	316	BCR	C20-C19-C18	-2.50	119.52	126.36
31	A	839	PQN	C11-C3-C4	-2.49	115.95	118.58
25	B	843	BCR	C16-C17-C18	-2.49	123.78	127.28
24	1	303	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	B	848	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	A	802	CLA	CHB-C4A-NA	2.49	127.99	124.40
25	I	102	BCR	C31-C1-C6	2.49	114.14	110.24
24	4	602	CLA	CHB-C4A-NA	2.48	127.99	124.40
25	B	840	BCR	C24-C23-C22	-2.48	122.56	126.23
25	B	840	BCR	C36-C18-C17	-2.48	118.79	122.82
26	7	613	DD6	C7-C6-C8	2.48	121.88	118.09
24	A	847	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
24	B	822	CLA	C4-C3-C2	-2.48	117.26	123.63
26	c	613	DD6	C25-C26-C27	-2.48	119.68	126.61
25	4	618	BCR	C30-C25-C26	-2.48	119.25	122.64
24	A	830	CLA	C2A-C1A-CHA	2.48	128.16	123.87
25	A	844	BCR	C21-C20-C19	-2.48	116.02	123.20
25	A	846	BCR	C29-C30-C25	2.48	114.04	110.44
24	L	203	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	B	825	CLA	C3B-C4B-NB	-2.48	108.32	110.53
26	6	616	DD6	C-C1-C2	-2.48	118.81	122.82
24	B	835	CLA	C3B-C4B-NB	-2.47	108.32	110.53
26	2	212	DD6	C25-C26-C27	-2.47	119.69	126.61
24	B	810	CLA	O2D-CGD-CBD	2.47	115.56	111.23
24	9	311	CLA	CMB-C2B-C3B	2.47	132.36	126.55
29	3	310	A1L1G	C43-C44-C42	-2.47	118.81	122.82
24	A	804	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	B	817	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
24	4	610	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	9	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	k	312	A1L1G	C36-C37-C38	2.47	128.56	123.52
26	4	616	DD6	C9-C10-C11	-2.46	123.82	127.28
24	1	306	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	B	822	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
25	A	846	BCR	C24-C25-C26	-2.46	115.89	121.56
24	B	838	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
26	3	311	DD6	C10-C9-C8	-2.46	116.07	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	313	DD6	C25-C24-C1	-2.46	119.62	126.36
24	A	840	CLA	O2D-CGD-CBD	2.46	115.53	111.23
25	I	102	BCR	C19-C18-C17	-2.46	115.14	119.01
26	6	614	DD6	C9-C10-C11	-2.46	123.83	127.28
24	h	603	CLA	C3B-C4B-NB	-2.46	108.34	110.53
24	A	818	CLA	CMB-C2B-C1B	-2.45	121.68	125.42
24	L	203	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	A	845	BCR	C23-C24-C25	-2.45	120.45	127.00
24	5	604	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	2	211	BCR	C4-C5-C6	-2.45	119.39	122.70
26	9	317	DD6	C25-C26-C27	-2.45	119.76	126.61
24	4	611	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	1	310	BCR	C35-C13-C12	2.45	121.83	118.09
24	A	813	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	L	206	BCR	C30-C25-C24	2.44	122.28	115.65
25	1	314	BCR	C33-C5-C4	2.44	118.81	113.60
26	5	608	DD6	C15-C14-C13	-2.44	120.83	125.99
25	A	844	BCR	C33-C5-C4	2.44	118.80	113.60
26	1	311	DD6	C28-C27-C26	-2.44	119.44	124.18
26	h	614	DD6	C10-C9-C8	-2.44	116.13	123.20
26	4	616	DD6	C25-C24-C1	-2.44	119.67	126.36
24	c	601	CLA	CBA-CAA-C2A	-2.44	109.00	114.05
24	A	803	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	7	618	DD6	C25-C24-C1	-2.44	119.68	126.36
25	L	206	BCR	C16-C15-C14	-2.44	118.53	123.52
25	I	101	BCR	C8-C9-C10	-2.44	115.17	119.01
25	1	310	BCR	C24-C23-C22	-2.44	122.63	126.23
26	6	615	DD6	C7-C6-C8	2.43	121.80	118.09
24	A	860	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
24	B	820	CLA	C1-C2-C3	-2.43	122.22	126.20
24	k	308	CLA	C1D-ND-C4D	-2.43	104.61	106.31
24	B	802	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	B	826	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	A	843	BCR	C2-C1-C6	2.42	113.96	110.44
24	6	602	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	B	829	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	L	202	BCR	C15-C16-C17	-2.42	118.56	123.52
26	A	848	DD6	C12-C11-C13	2.42	121.79	118.09
24	A	812	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	A	820	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	B	841	BCR	C19-C18-C17	-2.42	115.20	119.01
26	9	314	DD6	C15-C14-C13	-2.42	120.87	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	615	BCR	C38-C26-C27	2.42	118.76	113.60
26	9	313	DD6	O1-C15-C14	-2.42	109.94	116.88
24	A	834	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	4	614	DD6	C25-C24-C1	-2.42	119.73	126.36
26	8	210	DD6	C25-C26-C27	-2.42	119.85	126.61
26	k	315	DD6	C3-C4-C5	-2.42	118.57	123.52
24	A	807	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	J	101	BCR	C30-C25-C24	2.42	122.20	115.65
24	3	302	CLA	C3B-C4B-NB	-2.42	108.37	110.53
28	B	844	LHG	C5-O7-C7	-2.42	112.02	117.80
29	9	312	A1L1G	C3-C6-C1	2.41	111.56	109.21
26	4	616	DD6	C4-C3-C2	-2.41	118.58	123.52
25	L	202	BCR	C23-C24-C25	-2.41	120.55	127.00
24	c	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	3	305	CLA	C1-C2-C3	-2.41	122.25	126.20
24	B	822	CLA	C5-C3-C2	2.41	126.58	121.17
24	1	305	CLA	O1A-CGA-CBA	2.41	130.73	123.09
24	A	812	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	J	105	LHG	O8-C23-C24	2.41	119.18	111.83
26	1	313	DD6	C7-C6-C8	2.41	121.76	118.09
25	A	845	BCR	C30-C25-C26	-2.40	119.35	122.64
25	B	840	BCR	C28-C27-C26	-2.40	109.77	114.06
25	7	617	BCR	C27-C26-C25	-2.40	119.45	122.70
24	3	306	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
24	A	816	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
26	3	311	DD6	C25-C26-C27	-2.40	119.89	126.61
24	t	301	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	A	860	CLA	O2D-CGD-CBD	2.40	115.43	111.23
25	R	101	BCR	C3-C4-C5	-2.40	109.77	114.06
28	A	852	LHG	O8-C23-C24	2.40	119.16	111.83
25	B	849	BCR	C10-C11-C12	-2.40	116.24	123.20
26	7	615	DD6	C10-C9-C8	-2.40	116.25	123.20
24	8	204	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	F	204	BCR	C38-C26-C27	2.40	118.71	113.60
25	J	101	BCR	C37-C22-C21	-2.40	118.93	122.82
24	A	808	CLA	CAA-CBA-CGA	-2.40	106.40	113.21
24	A	830	CLA	O2D-CGD-CBD	2.40	115.42	111.23
25	9	316	BCR	C23-C24-C25	-2.39	120.60	127.00
24	7	607	CLA	CMB-C2B-C3B	2.39	132.18	126.55
24	5	602	CLA	CMB-C2B-C3B	2.39	132.18	126.55
24	2	202	CLA	C1-C2-C3	-2.39	122.28	126.20
26	h	616	DD6	C4-C3-C2	-2.39	118.62	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	608	CLA	C3B-C4B-NB	-2.39	108.39	110.53
24	A	826	CLA	C1-C2-C3	-2.39	122.28	126.20
24	9	301	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
26	J	102	DD6	C25-C24-C1	-2.39	119.80	126.36
25	B	843	BCR	C3-C4-C5	-2.39	109.79	114.06
26	1	311	DD6	C10-C9-C8	-2.39	116.27	123.20
24	4	604	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
24	9	306	CLA	C2A-C1A-CHA	2.39	128.01	123.87
24	B	824	CLA	C1-C2-C3	-2.39	122.28	126.20
25	4	618	BCR	C1-C6-C5	-2.39	119.37	122.64
26	8	210	DD6	C7-C6-C5	-2.39	118.95	122.82
25	B	849	BCR	C2-C1-C6	2.39	113.91	110.44
25	B	840	BCR	C3-C4-C5	-2.39	109.80	114.06
25	R	101	BCR	C27-C26-C25	-2.39	119.48	122.70
24	9	301	CLA	CMB-C2B-C3B	2.39	132.16	126.55
25	B	849	BCR	C4-C5-C6	-2.39	119.48	122.70
25	I	102	BCR	C24-C25-C26	-2.39	116.06	121.56
24	5	605	CLA	CHB-C4A-NA	2.39	127.84	124.40
25	F	204	BCR	C15-C16-C17	-2.38	118.64	123.52
24	A	807	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	7	617	BCR	C37-C22-C23	2.38	121.73	118.09
24	A	801	CLA	C4D-C3D-CAD	-2.38	105.52	108.11
24	B	804	CLA	CHB-C1B-NB	2.38	127.62	124.05
24	A	835	CLA	C3B-C4B-NB	-2.38	108.41	110.53
24	A	838	CLA	C3B-C4B-NB	-2.38	108.41	110.53
26	R	105	DD6	C19-C18-C17	2.38	115.24	110.79
24	A	835	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	A	828	CLA	C3B-C4B-NB	-2.38	108.41	110.53
24	7	612	CLA	O1D-CGD-CBD	2.38	129.21	124.52
25	A	846	BCR	C23-C22-C21	-2.38	115.27	119.01
25	B	840	BCR	C38-C26-C27	2.37	118.66	113.60
27	A	851	LMT	C1B-O1B-C4'	-2.37	112.35	117.98
25	J	101	BCR	C28-C27-C26	-2.37	109.82	114.06
25	B	840	BCR	C15-C16-C17	-2.37	118.66	123.52
30	2	214	LMG	O8-C28-C29	2.37	119.07	111.83
24	B	829	CLA	O2D-CGD-CBD	2.37	115.38	111.23
26	8	211	DD6	C10-C9-C8	-2.37	116.33	123.20
26	h	613	DD6	C25-C26-C27	-2.37	119.98	126.61
25	B	841	BCR	C21-C20-C19	-2.37	116.34	123.20
24	k	311	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
26	5	608	DD6	C25-C24-C1	-2.37	119.87	126.36
25	R	102	BCR	C38-C26-C27	2.37	118.64	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	BCR	C23-C24-C25	-2.36	120.68	127.00
25	A	844	BCR	C10-C11-C12	-2.36	116.35	123.20
24	A	813	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	A	853	CLA	CMB-C2B-C3B	2.36	132.11	126.55
25	M	101	BCR	C3-C4-C5	-2.36	109.85	114.06
24	B	833	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	1	311	DD6	C25-C26-C27	-2.36	120.01	126.61
26	7	615	DD6	C4-C3-C2	-2.36	118.69	123.52
25	c	615	BCR	C1-C6-C7	2.36	122.05	115.65
25	4	618	BCR	C4-C5-C6	-2.36	119.52	122.70
24	7	603	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
27	A	851	LMT	O3'-C3'-C2'	-2.36	104.82	110.38
24	A	831	CLA	C3B-C4B-NB	-2.36	108.43	110.53
24	B	829	CLA	CMB-C2B-C3B	2.36	132.09	126.55
24	k	302	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	1	313	DD6	C12-C11-C13	2.36	121.69	118.09
27	1	315	LMT	O1B-C4'-C3'	2.36	113.22	107.23
24	A	838	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
26	k	313	DD6	C4-C3-C2	-2.35	118.70	123.52
24	h	603	CLA	CMB-C2B-C3B	2.35	132.09	126.55
24	B	818	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
25	A	843	BCR	C38-C26-C25	-2.35	121.92	124.48
25	B	841	BCR	C32-C1-C6	-2.35	106.56	110.24
25	A	846	BCR	C24-C23-C22	-2.35	122.76	126.23
25	t	312	BCR	C33-C5-C4	2.35	118.61	113.60
24	A	805	CLA	C3B-C4B-NB	-2.35	108.43	110.53
24	A	837	CLA	O2D-CGD-CBD	2.35	115.34	111.23
24	B	810	CLA	CAB-C3B-C2B	2.35	129.78	123.53
25	A	844	BCR	C15-C16-C17	-2.35	118.71	123.52
26	J	102	DD6	C25-C26-C27	-2.35	120.04	126.61
24	B	822	CLA	CHB-C4A-NA	2.35	127.79	124.40
26	k	315	DD6	O1-C20-C21	-2.35	112.42	115.05
25	9	316	BCR	C38-C26-C27	2.35	118.60	113.60
24	9	302	CLA	CMB-C2B-C3B	2.35	132.07	126.55
25	R	102	BCR	C4-C5-C6	-2.35	119.53	122.70
26	3	313	DD6	C4-C5-C6	-2.35	123.99	127.28
25	B	840	BCR	C37-C22-C21	-2.34	119.02	122.82
24	k	303	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	B	812	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	c	612	DD6	C40-C32-C31	-2.34	106.32	110.52
24	1	304	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	c	608	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	102	BCR	C10-C11-C12	-2.34	116.42	123.20
25	R	101	BCR	C4-C5-C6	-2.34	119.54	122.70
25	A	846	BCR	C15-C14-C13	-2.34	124.00	127.28
24	B	801	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	B	802	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
24	3	308	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	B	803	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	9	313	DD6	C4-C3-C2	-2.34	118.74	123.52
25	A	843	BCR	C36-C18-C17	-2.34	119.03	122.82
24	k	305	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	7	617	BCR	C11-C10-C9	-2.34	124.00	127.28
24	A	827	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
24	A	817	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	A	824	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
28	A	841	LHG	C5-O7-C7	-2.33	112.21	117.80
24	A	816	CLA	CHB-C4A-NA	2.33	127.77	124.40
24	k	309	CLA	CHB-C4A-NA	2.33	127.77	124.40
26	4	616	DD6	C12-C11-C13	2.33	121.65	118.09
24	B	804	CLA	CHA-C1A-NA	-2.33	121.11	126.39
24	A	847	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
24	t	306	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	B	814	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
24	A	834	CLA	O2D-CGD-CBD	2.33	115.31	111.23
26	6	617	DD6	C10-C9-C8	-2.33	116.44	123.20
29	9	312	A1L1G	C28-C39-C38	-2.33	119.04	122.82
26	k	315	DD6	C26-C25-C24	-2.33	116.45	123.20
24	8	208	CLA	CMB-C2B-C3B	2.33	132.03	126.55
24	A	811	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	B	849	BCR	C24-C23-C22	-2.33	122.79	126.23
26	9	314	DD6	C12-C11-C10	-2.33	119.04	122.82
25	J	104	BCR	C23-C22-C21	-2.33	115.35	119.01
26	1	313	DD6	C9-C10-C11	-2.33	124.01	127.28
24	L	203	CLA	O2D-CGD-CBD	2.33	115.30	111.23
25	2	211	BCR	C16-C15-C14	-2.33	118.76	123.52
26	4	614	DD6	C14-C13-C11	-2.33	121.92	125.53
25	2	211	BCR	C37-C22-C23	2.33	121.64	118.09
24	A	856	CLA	CMB-C2B-C3B	2.33	132.02	126.55
25	R	102	BCR	C7-C6-C5	2.32	126.91	121.56
24	L	204	CLA	C3B-C4B-NB	-2.32	108.45	110.53
24	2	206	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	2	201	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	7	609	CLA	CHB-C4A-NA	2.32	127.75	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	311	DD6	C25-C24-C1	-2.32	120.00	126.36
24	2	206	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	t	305	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	A	845	BCR	C27-C26-C25	-2.32	119.57	122.70
25	R	101	BCR	C16-C15-C14	-2.32	118.77	123.52
24	h	611	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
24	7	601	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	J	104	BCR	C23-C24-C25	-2.32	120.81	127.00
26	A	848	DD6	O1-C20-C19	-2.32	111.32	113.49
24	A	803	CLA	CHB-C4A-NA	2.32	127.74	124.40
24	6	609	CLA	CHB-C4A-NA	2.32	127.74	124.40
24	A	830	CLA	C4D-CHA-C1A	2.31	124.00	121.24
26	7	613	DD6	C12-C11-C13	2.31	121.62	118.09
26	7	618	DD6	C7-C6-C5	-2.31	119.07	122.82
24	A	822	CLA	C1-C2-C3	-2.31	122.41	126.20
25	9	316	BCR	C11-C12-C13	-2.31	120.02	126.36
24	1	302	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	B	818	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	k	314	DD6	C26-C25-C24	-2.31	116.50	123.20
24	A	802	CLA	CHB-C1B-NB	2.31	127.52	124.05
26	3	312	DD6	C26-C25-C24	-2.31	116.50	123.20
24	5	605	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	9	303	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
25	R	102	BCR	C19-C18-C17	-2.31	115.38	119.01
25	c	615	BCR	C33-C5-C4	2.31	118.52	113.60
24	A	836	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	B	817	CLA	C3B-C4B-NB	-2.31	108.47	110.53
24	1	317	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
26	c	612	DD6	C25-C24-C1	-2.31	120.04	126.36
24	B	810	CLA	CHB-C4A-NA	2.31	127.73	124.40
24	7	606	CLA	CMB-C2B-C3B	2.31	131.97	126.55
25	B	840	BCR	C15-C14-C13	-2.30	124.05	127.28
24	A	817	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
25	A	846	BCR	C19-C18-C17	-2.30	115.39	119.01
26	R	105	DD6	C4-C3-C2	-2.30	118.81	123.52
24	A	801	CLA	C3B-C4B-NB	-2.30	108.47	110.53
24	3	304	CLA	CHB-C1B-C2B	-2.30	120.75	127.43
25	B	840	BCR	C16-C15-C14	-2.30	118.82	123.52
24	1	304	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	h	610	CLA	C4A-NA-C1A	2.30	107.73	106.68
24	B	808	CLA	CHB-C4A-NA	2.30	127.71	124.40
26	6	613	DD6	C26-C25-C24	-2.30	116.55	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	834	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
24	A	847	CLA	CMB-C2B-C3B	2.29	131.94	126.55
24	2	208	CLA	CHB-C4A-NA	2.29	127.71	124.40
24	3	301	CLA	C3B-C4B-NB	-2.29	108.48	110.53
24	B	830	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	c	609	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	B	818	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
26	k	313	DD6	C7-C6-C8	2.29	121.58	118.09
24	h	606	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	F	204	BCR	C23-C24-C25	-2.29	120.89	127.00
24	A	824	CLA	C1-C2-C3	-2.29	122.45	126.20
26	6	615	DD6	C32-C33-C34	2.29	118.61	113.59
24	c	610	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	I	101	BCR	C10-C11-C12	-2.29	116.58	123.20
24	9	311	CLA	CHB-C4A-NA	2.28	127.70	124.40
24	9	309	CLA	C3B-C4B-NB	-2.28	108.49	110.53
24	B	824	CLA	C3B-C4B-NB	-2.28	108.49	110.53
24	A	825	CLA	CHB-C4A-NA	2.28	127.70	124.40
26	1	311	DD6	C7-C6-C8	2.28	121.58	118.09
26	c	614	DD6	C28-C27-C26	-2.28	119.75	124.18
26	h	615	DD6	C25-C24-C1	-2.28	120.10	126.36
25	A	846	BCR	C12-C13-C14	-2.28	115.42	119.01
25	B	849	BCR	C8-C9-C10	-2.28	115.42	119.01
24	k	306	CLA	C3B-C4B-NB	-2.28	108.49	110.53
24	7	604	CLA	CMB-C2B-C3B	2.28	131.92	126.55
24	k	306	CLA	CHB-C4A-NA	2.28	127.69	124.40
24	L	204	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	A	811	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	2	211	BCR	C27-C26-C25	-2.28	119.62	122.70
26	5	608	DD6	C10-C9-C8	-2.28	116.59	123.20
26	4	617	DD6	C26-C25-C24	-2.28	116.59	123.20
24	A	805	CLA	O2D-CGD-CBD	2.28	115.22	111.23
24	L	205	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
24	A	813	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
24	A	857	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
24	A	832	CLA	O2D-CGD-CBD	2.28	115.21	111.23
26	3	313	DD6	C9-C8-C6	2.28	132.60	126.36
26	h	615	DD6	C26-C25-C24	-2.27	116.61	123.20
24	3	308	CLA	C3B-C4B-NB	-2.27	108.50	110.53
26	7	618	DD6	C33-C32-C31	2.27	113.96	109.49
24	A	819	CLA	CHB-C4A-NA	2.27	127.68	124.40
25	I	101	BCR	C31-C1-C6	-2.27	106.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	313	DD6	C-C1-C2	-2.27	119.14	122.82
24	6	611	CLA	CMB-C2B-C3B	2.27	131.89	126.55
25	2	211	BCR	C1-C6-C5	-2.27	119.54	122.64
26	t	313	DD6	C4-C3-C2	-2.27	118.88	123.52
26	5	609	DD6	C34-C35-C36	-2.27	106.53	112.18
25	1	310	BCR	C10-C11-C12	-2.27	116.63	123.20
24	6	607	CLA	CHB-C4A-NA	2.27	127.67	124.40
24	c	607	CLA	CHB-C4A-NA	2.27	127.67	124.40
24	7	609	CLA	C3B-C4B-NB	-2.27	108.51	110.53
26	7	618	DD6	C28-C27-C26	-2.27	119.78	124.18
24	9	304	CLA	CBA-CAA-C2A	-2.27	107.05	113.79
26	4	614	DD6	C10-C9-C8	-2.27	116.63	123.20
24	h	607	CLA	C3B-C4B-NB	-2.27	108.51	110.53
24	1	317	CLA	CHB-C4A-NA	2.26	127.67	124.40
26	7	615	DD6	C25-C24-C1	-2.26	120.15	126.36
24	A	803	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
24	8	202	CLA	CHB-C4A-NA	2.26	127.67	124.40
24	A	821	CLA	CHB-C4A-NA	2.26	127.67	124.40
26	8	212	DD6	C7-C6-C8	2.26	121.55	118.09
25	B	842	BCR	C23-C22-C21	2.26	122.57	119.01
24	h	602	CLA	CHB-C4A-NA	2.26	127.67	124.40
28	2	215	LHG	C5-O7-C7	-2.26	112.38	117.80
24	3	302	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	A	846	BCR	C16-C15-C14	-2.26	118.89	123.52
24	6	605	CLA	C3B-C4B-NB	-2.26	108.51	110.53
24	A	827	CLA	CMB-C2B-C3B	2.26	131.87	126.55
24	9	307	CLA	O2D-CGD-CBD	2.26	115.18	111.23
25	A	859	BCR	C8-C7-C6	-2.26	120.96	127.00
24	4	606	CLA	C3B-C4B-NB	-2.26	108.51	110.53
26	8	211	DD6	O1-C15-C14	-2.26	110.41	116.88
24	8	202	CLA	C3B-C4B-NB	-2.26	108.52	110.53
24	B	836	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
26	4	614	DD6	C4-C3-C2	-2.26	118.90	123.52
24	3	308	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
24	B	815	CLA	CHB-C4A-NA	2.26	127.66	124.40
24	F	201	CLA	C1-C2-C3	-2.26	122.50	126.20
24	2	207	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	6	612	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	A	827	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	t	308	CLA	C4A-NA-C1A	2.25	107.71	106.68
25	A	845	BCR	C4-C5-C6	-2.25	122.33	124.48
24	B	829	CLA	C2A-C1A-CHA	2.25	127.78	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	830	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
26	A	848	DD6	C10-C9-C8	-2.25	116.68	123.20
24	A	804	CLA	CHB-C4A-NA	2.25	127.64	124.40
24	B	809	CLA	C3B-C4B-NB	-2.25	108.52	110.53
26	J	102	DD6	C9-C10-C11	-2.25	124.12	127.28
24	k	311	CLA	CMB-C2B-C3B	2.25	131.83	126.55
25	J	104	BCR	C1-C6-C5	-2.25	119.57	122.64
30	t	314	LMG	O8-C28-C29	2.25	118.68	111.83
24	A	856	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
24	B	814	CLA	C1-C2-C3	-2.24	123.13	126.76
29	7	614	A1L1G	C28-C39-C38	-2.24	119.18	122.82
27	A	851	LMT	C1'-O5'-C5'	-2.24	109.34	113.72
26	3	311	DD6	C7-C6-C8	2.24	121.52	118.09
25	R	101	BCR	C15-C16-C17	-2.24	118.93	123.52
24	k	301	CLA	CHB-C4A-NA	2.24	127.64	124.40
25	B	841	BCR	C23-C22-C21	-2.24	115.48	119.01
24	6	611	CLA	CHB-C4A-NA	2.24	127.64	124.40
24	9	304	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	B	811	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
24	A	832	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	B	817	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
28	4	619	LHG	O8-C23-C24	2.24	118.66	111.83
25	7	617	BCR	C20-C21-C22	-2.24	124.14	127.28
24	A	801	CLA	C2A-C1A-CHA	2.24	127.75	123.87
25	I	102	BCR	C24-C23-C22	-2.24	122.92	126.23
25	9	316	BCR	C8-C7-C6	-2.24	121.02	127.00
24	6	607	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	A	840	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	6	615	DD6	C25-C26-C27	-2.24	120.36	126.61
25	L	206	BCR	C11-C10-C9	-2.24	124.14	127.28
25	1	310	BCR	C21-C20-C19	-2.24	116.72	123.20
24	9	301	CLA	C3B-C4B-NB	-2.23	108.53	110.53
24	1	303	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	B	807	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	h	612	CLA	C3B-C4B-NB	-2.23	108.54	110.53
26	8	212	DD6	C25-C26-C27	-2.23	120.38	126.61
24	B	821	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
25	1	314	BCR	C34-C9-C10	-2.23	119.21	122.82
24	B	828	CLA	C1-C2-C3	-2.23	123.16	126.76
26	c	612	DD6	C33-C32-C31	2.23	113.88	109.49
25	1	314	BCR	C27-C26-C25	-2.23	119.70	122.70
24	4	607	CLA	C3B-C4B-NB	-2.23	108.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	817	CLA	CHB-C4A-NA	2.23	127.61	124.40
26	3	311	DD6	C25-C24-C1	-2.23	120.26	126.36
24	h	605	CLA	CHB-C4A-NA	2.23	127.61	124.40
24	A	827	CLA	C3B-C4B-NB	-2.22	108.55	110.53
24	J	103	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	c	601	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	t	304	CLA	CHB-C4A-NA	2.22	127.61	124.40
25	I	102	BCR	C7-C6-C5	-2.22	116.44	121.56
26	h	614	DD6	C26-C25-C24	-2.22	116.76	123.20
25	1	310	BCR	C30-C25-C26	-2.22	119.60	122.64
26	8	211	DD6	C12-C11-C13	2.22	121.48	118.09
25	7	617	BCR	C34-C9-C8	2.22	121.48	118.09
24	h	601	CLA	CHB-C4A-NA	2.22	127.60	124.40
26	6	615	DD6	C-C1-C24	2.22	121.48	118.09
25	B	842	BCR	C4-C5-C6	-2.22	119.71	122.70
24	R	103	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	8	209	CLA	CHD-C1D-ND	-2.22	121.68	124.80
24	B	805	CLA	CHB-C4A-NA	2.21	127.60	124.40
26	4	616	DD6	O1-C15-C14	-2.21	110.54	116.88
24	A	860	CLA	C16-C15-C13	-2.21	108.61	115.97
26	J	102	DD6	C7-C6-C8	2.21	121.47	118.09
24	h	604	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	B	837	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	6	617	DD6	C25-C24-C1	-2.21	120.30	126.36
25	I	102	BCR	C37-C22-C21	-2.21	119.23	122.82
24	B	836	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	8	205	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	k	310	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	A	846	BCR	C30-C25-C26	-2.21	119.61	122.64
24	A	824	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	3	303	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
24	A	810	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	B	842	BCR	C37-C22-C21	-2.21	119.24	122.82
26	J	102	DD6	C12-C11-C13	2.21	121.46	118.09
24	B	801	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	8	203	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	t	305	CLA	CMB-C2B-C3B	2.21	131.74	126.55
26	k	315	DD6	C12-C11-C10	-2.21	119.24	122.82
26	4	615	DD6	C10-C9-C8	-2.21	116.81	123.20
24	3	309	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	k	310	CLA	C3B-C4B-NB	-2.21	108.56	110.53
26	3	312	DD6	C10-C9-C8	-2.21	116.81	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	838	CLA	CHB-C4A-NA	2.21	127.58	124.40
25	L	202	BCR	C8-C7-C6	-2.21	121.10	127.00
24	6	602	CLA	O2D-CGD-CBD	2.21	115.09	111.23
24	B	823	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	A	860	CLA	CMB-C2B-C3B	2.20	131.74	126.55
26	6	613	DD6	C12-C11-C13	2.20	121.46	118.09
24	8	202	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	B	818	CLA	O2D-CGD-CBD	2.20	115.08	111.23
24	B	805	CLA	C3B-C4B-NB	-2.20	108.56	110.53
24	B	806	CLA	CHB-C4A-NA	2.20	127.58	124.40
24	B	846	CLA	CHB-C4A-NA	2.20	127.58	124.40
24	B	835	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
24	A	825	CLA	O2D-CGD-CBD	2.20	115.08	111.23
25	L	202	BCR	C23-C22-C21	-2.20	115.55	119.01
25	t	312	BCR	C8-C7-C6	-2.20	121.12	127.00
24	B	833	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
24	B	820	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	6	615	DD6	C10-C9-C8	-2.20	116.82	123.20
28	I	103	LHG	O7-C7-O9	-2.20	118.56	123.70
29	9	312	A1L1G	C36-C37-C38	2.20	128.02	123.52
24	1	302	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	6	609	CLA	C1-C2-C3	-2.20	123.20	126.76
25	I	102	BCR	C12-C13-C14	-2.20	115.55	119.01
24	6	602	CLA	CHB-C4A-NA	2.20	127.57	124.40
26	8	210	DD6	C33-C32-C31	2.20	113.82	109.49
24	A	826	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	A	829	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	k	303	CLA	C4-C3-C2	-2.20	117.98	123.63
24	7	602	CLA	C3B-C4B-NB	-2.20	108.57	110.53
24	B	815	CLA	C1-C2-C3	-2.20	122.60	126.20
24	4	603	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	h	610	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	4	611	CLA	CHB-C4A-NA	2.19	127.57	124.40
26	h	613	DD6	C7-C6-C8	2.19	121.44	118.09
25	k	316	BCR	C33-C5-C4	2.19	118.27	113.60
24	h	605	CLA	C3B-C4B-NB	-2.19	108.57	110.53
24	8	206	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	B	815	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
25	k	316	BCR	C10-C11-C12	-2.19	116.85	123.20
24	4	609	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	6	602	CLA	CHD-C1D-ND	-2.19	121.72	124.80
26	h	613	DD6	C12-C11-C13	2.19	121.44	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	827	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	9	317	DD6	C3-C4-C5	2.19	128.00	123.52
24	B	834	CLA	O2D-CGD-CBD	2.19	115.06	111.23
24	B	821	CLA	CAC-C3C-C4C	2.19	127.64	124.79
24	A	805	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	6	614	DD6	C10-C9-C8	-2.19	116.86	123.20
24	B	816	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	A	814	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	A	820	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	B	815	CLA	C3B-C4B-NB	-2.19	108.58	110.53
24	9	305	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	B	831	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	B	841	BCR	C15-C14-C13	-2.19	124.21	127.28
25	1	314	BCR	C11-C12-C13	-2.19	120.37	126.36
24	B	814	CLA	CMB-C2B-C3B	2.19	131.69	126.55
24	h	610	CLA	C1D-ND-C4D	-2.19	104.78	106.31
25	I	101	BCR	C21-C20-C19	-2.18	116.87	123.20
24	9	310	CLA	CHB-C4A-NA	2.18	127.55	124.40
26	5	609	DD6	C7-C6-C8	2.18	121.42	118.09
25	I	101	BCR	C19-C18-C17	-2.18	115.57	119.01
25	B	841	BCR	C37-C22-C21	-2.18	119.28	122.82
24	3	302	CLA	O2D-CGD-CBD	2.18	115.05	111.23
24	h	605	CLA	O2D-CGD-CBD	2.18	115.05	111.23
24	A	803	CLA	CHD-C1D-ND	-2.18	121.73	124.80
24	6	605	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	A	853	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
24	A	820	CLA	CHB-C4A-NA	2.18	127.55	124.40
24	9	308	CLA	C3B-C4B-NB	-2.18	108.58	110.53
25	R	102	BCR	C37-C22-C21	-2.18	119.28	122.82
24	6	601	CLA	CHB-C4A-NA	2.18	127.55	124.40
24	A	833	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	B	822	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	3	304	CLA	CHB-C1B-NB	2.18	127.32	124.05
24	B	807	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	8	201	CLA	CHB-C4A-NA	2.18	127.54	124.40
24	B	817	CLA	CMB-C2B-C3B	2.18	131.67	126.55
24	A	825	CLA	CHD-C1D-ND	-2.17	121.74	124.80
25	B	843	BCR	C21-C20-C19	-2.17	116.90	123.20
24	B	847	CLA	O2D-CGD-CBD	2.17	115.03	111.23
24	4	607	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	7	603	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	7	611	CLA	CHB-C4A-NA	2.17	127.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	857	CLA	CMB-C2B-C3B	2.17	131.66	126.55
24	3	304	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	7	602	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
24	c	607	CLA	O2D-CGD-CBD	2.17	115.03	111.23
28	1	318	LHG	C9-C8-C7	-2.17	105.74	113.69
24	9	304	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
25	A	845	BCR	C21-C20-C19	-2.17	116.91	123.20
24	c	611	CLA	CMA-C3A-C2A	-2.17	111.25	116.23
24	A	860	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
25	A	859	BCR	C33-C5-C6	-2.17	122.11	124.48
24	t	309	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	I	101	BCR	C12-C13-C14	-2.17	115.60	119.01
24	k	311	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	A	815	CLA	O2D-CGD-CBD	2.17	115.02	111.23
24	A	804	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	4	615	DD6	C7-C6-C8	2.17	121.40	118.09
26	t	313	DD6	C12-C11-C13	2.17	121.40	118.09
25	M	101	BCR	C33-C5-C6	-2.17	122.12	124.48
24	9	309	CLA	C2A-C1A-CHA	2.16	127.62	123.87
24	B	838	CLA	O2D-CGD-CBD	2.16	115.01	111.23
24	h	610	CLA	O2D-CGD-CBD	2.16	115.01	111.23
24	B	821	CLA	O2D-CGD-CBD	2.16	115.01	111.23
24	A	815	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	I	102	BCR	C38-C26-C27	2.16	118.21	113.60
26	h	614	DD6	C4-C3-C2	-2.16	119.09	123.52
24	A	823	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	A	846	BCR	C21-C20-C19	-2.16	116.94	123.20
25	L	206	BCR	C36-C18-C17	-2.16	119.31	122.82
24	7	604	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	c	602	CLA	O2D-CGD-CBD	2.16	115.01	111.23
26	8	212	DD6	C34-C35-C36	-2.16	106.80	112.18
24	A	838	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	8	203	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	7	616	DD6	C-C1-C2	-2.16	119.32	122.82
24	4	606	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	A	836	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	4	617	DD6	C10-C9-C8	-2.16	116.94	123.20
26	k	313	DD6	C-C1-C24	2.16	121.39	118.09
24	A	809	CLA	CHB-C4A-NA	2.16	127.51	124.40
25	B	849	BCR	C37-C22-C21	-2.16	119.32	122.82
24	2	204	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	h	609	CLA	C3B-C4B-NB	-2.16	108.60	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	835	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
25	B	843	BCR	C38-C26-C27	2.16	118.19	113.60
26	9	315	DD6	C4-C5-C6	-2.16	124.25	127.28
24	c	609	CLA	C4-C3-C5	2.16	118.97	115.23
24	2	203	CLA	CHD-C1D-ND	-2.16	121.77	124.80
24	B	809	CLA	CHB-C4A-NA	2.16	127.51	124.40
24	A	824	CLA	CMB-C2B-C3B	2.16	131.62	126.55
24	5	607	CLA	C2B-C1B-NB	2.16	112.56	110.33
24	2	203	CLA	C1-C2-C3	-2.15	123.28	126.76
24	A	820	CLA	CMB-C2B-C3B	2.15	131.62	126.55
24	4	605	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	A	810	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	c	608	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
26	J	102	DD6	O1-C20-C19	-2.15	111.47	113.49
24	5	602	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	A	825	CLA	C3B-C4B-NB	-2.15	108.61	110.53
25	I	102	BCR	C23-C22-C21	-2.15	115.62	119.01
24	3	301	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	t	306	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	A	831	CLA	CHB-C4A-NA	2.15	127.51	124.40
26	3	311	DD6	C12-C11-C13	2.15	121.38	118.09
28	A	842	LHG	O8-C23-C24	2.15	118.40	111.83
26	9	315	DD6	C41-C32-C31	-2.15	106.66	110.52
24	2	205	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	7	606	CLA	CED-O2D-CGD	2.15	120.80	115.92
24	B	825	CLA	CHB-C4A-NA	2.15	127.51	124.40
26	2	212	DD6	C25-C24-C1	-2.15	120.46	126.36
24	A	801	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	B	820	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	B	804	CLA	O1D-CGD-CBD	2.15	128.76	124.52
24	6	608	CLA	CHB-C4A-NA	2.15	127.50	124.40
24	7	606	CLA	C1-C2-C3	-2.15	122.67	126.20
26	1	312	DD6	C12-C11-C13	2.15	121.37	118.09
25	L	202	BCR	C7-C6-C5	-2.15	116.61	121.56
24	B	835	CLA	O2D-CGD-CBD	2.15	114.99	111.23
24	4	611	CLA	CHD-C1D-ND	-2.15	121.78	124.80
26	J	102	DD6	C4-C3-C2	-2.15	119.12	123.52
24	F	203	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	A	833	CLA	CHB-C4A-NA	2.15	127.50	124.40
24	B	820	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
30	t	314	LMG	O7-C10-O9	-2.15	118.69	123.70
24	4	602	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	615	DD6	C33-C32-C31	2.15	113.72	109.49
24	A	818	CLA	O2D-CGD-CBD	2.15	114.98	111.23
24	B	805	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
24	4	613	CLA	CHB-C4A-NA	2.14	127.50	124.40
24	7	603	CLA	CMB-C2B-C3B	2.14	131.59	126.55
24	A	837	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	B	842	BCR	C21-C20-C19	-2.14	116.99	123.20
24	2	201	CLA	C2B-C1B-NB	2.14	112.55	110.33
26	t	311	DD6	C10-C9-C8	-2.14	116.99	123.20
24	A	809	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	8	206	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	B	835	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	A	829	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
24	B	802	CLA	CHC-C4B-NB	2.14	127.26	124.05
24	c	603	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
24	A	818	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
24	B	804	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	B	810	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	A	812	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	k	310	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	A	826	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
24	8	209	CLA	CMA-C3A-C2A	-2.14	111.33	116.23
24	4	608	CLA	CHB-C4A-NA	2.14	127.48	124.40
26	6	616	DD6	C26-C25-C24	-2.14	117.01	123.20
24	7	612	CLA	CHD-C1D-ND	-2.14	121.80	124.80
24	A	856	CLA	CHD-C1D-ND	-2.14	121.80	124.80
24	A	837	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
24	4	608	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	A	830	CLA	C4D-C3D-CAD	-2.14	105.79	108.11
24	c	602	CLA	CHB-C4A-NA	2.14	127.48	124.40
24	A	818	CLA	CHB-C4A-NA	2.14	127.48	124.40
28	A	842	LHG	O7-C7-O9	-2.13	118.72	123.70
24	F	201	CLA	C3B-C4B-NB	-2.13	108.62	110.53
24	3	304	CLA	CHA-C1A-NA	-2.13	121.56	126.39
24	A	819	CLA	O2D-CGD-CBD	2.13	114.96	111.23
25	B	840	BCR	C38-C26-C25	-2.13	122.16	124.48
26	8	210	DD6	O1-C20-C21	-2.13	112.66	115.05
24	B	847	CLA	C1-C2-C3	-2.13	122.70	126.20
24	2	201	CLA	C3A-C2A-C1A	2.13	104.53	101.34
24	B	823	CLA	O2D-CGD-CBD	2.13	114.96	111.23
24	2	202	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	7	602	CLA	CMB-C2B-C3B	2.13	131.57	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	617	DD6	C25-C24-C1	-2.13	120.52	126.36
24	4	605	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	2	206	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	c	602	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	A	826	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	7	615	DD6	C7-C6-C8	2.13	121.34	118.09
24	B	847	CLA	CHB-C4A-NA	2.13	127.47	124.40
27	1	316	LMT	C2'-C3'-C4'	-2.13	104.85	109.68
24	A	807	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	B	811	CLA	CHB-C4A-NA	2.13	127.47	124.40
24	A	821	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	1	307	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	B	810	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
28	8	213	LHG	O7-C7-O9	-2.12	118.75	123.70
24	4	609	CLA	O2D-CGD-CBD	2.12	114.94	111.23
25	J	104	BCR	C40-C30-C25	2.12	113.57	110.24
27	h	617	LMT	O5B-C5B-C4B	2.12	113.52	109.70
24	A	838	CLA	C1-C2-C3	-2.12	122.72	126.20
24	B	827	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	A	835	CLA	O2D-CGD-CBD	2.12	114.93	111.23
24	1	302	CLA	CHC-C4B-NB	2.12	127.22	124.05
25	1	310	BCR	C37-C22-C23	2.12	121.32	118.09
26	7	616	DD6	C12-C11-C10	-2.12	119.39	122.82
26	9	313	DD6	C25-C26-C27	-2.12	120.69	126.61
24	5	603	CLA	C3B-C4B-NB	-2.11	108.64	110.53
24	A	806	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
24	A	805	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
24	1	307	CLA	CHB-C4A-NA	2.11	127.45	124.40
25	B	849	BCR	C38-C26-C27	2.11	118.10	113.60
24	A	834	CLA	CHB-C4A-NA	2.11	127.45	124.40
24	k	303	CLA	CHD-C1D-ND	-2.11	121.83	124.80
24	B	821	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	8	210	DD6	O1-C20-C19	2.11	115.47	113.49
24	A	832	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
24	B	821	CLA	CHB-C4A-NA	2.11	127.44	124.40
24	B	823	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	c	607	CLA	CMB-C2B-C3B	2.11	131.51	126.55
24	2	204	CLA	C1-C2-C3	-2.11	122.74	126.20
26	1	312	DD6	C23-C16-C15	2.11	115.74	110.05
25	A	845	BCR	C16-C15-C14	-2.11	119.20	123.52
25	I	102	BCR	C21-C20-C19	-2.11	117.09	123.20
24	1	304	CLA	CHB-C4A-NA	2.11	127.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	211	DD6	C26-C25-C24	-2.11	117.09	123.20
24	9	304	CLA	CMB-C2B-C3B	2.11	131.51	126.55
26	1	311	DD6	C12-C11-C13	2.11	121.31	118.09
24	2	207	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
24	1	301	CLA	CHD-C1D-ND	-2.11	121.84	124.80
24	B	814	CLA	CHB-C4A-NA	2.11	127.44	124.40
26	k	313	DD6	C30-C29-C27	-2.11	169.07	176.23
26	6	616	DD6	O1-C15-C14	-2.11	110.84	116.88
24	2	207	CLA	CMB-C2B-C3B	2.11	131.50	126.55
24	4	601	CLA	CHB-C4A-NA	2.10	127.44	124.40
24	c	607	CLA	CHC-C4B-NB	2.10	127.21	124.05
24	6	606	CLA	CHB-C4A-NA	2.10	127.44	124.40
25	F	204	BCR	C33-C5-C4	2.10	118.08	113.60
26	t	311	DD6	C25-C26-C27	-2.10	120.73	126.61
24	B	826	CLA	O2D-CGD-CBD	2.10	114.91	111.23
24	B	848	CLA	CHB-C4A-NA	2.10	127.44	124.40
25	L	206	BCR	C15-C16-C17	-2.10	119.22	123.52
24	7	602	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
24	B	838	CLA	C1-C2-C3	-2.10	122.75	126.20
24	A	818	CLA	CMB-C2B-C3B	2.10	131.49	126.55
25	k	316	BCR	C34-C9-C8	2.10	121.30	118.09
25	M	101	BCR	C37-C22-C21	-2.10	119.41	122.82
26	6	614	DD6	C35-C36-C31	2.10	124.87	120.50
26	h	614	DD6	C-C1-C24	2.10	121.30	118.09
24	B	829	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
26	9	313	DD6	C14-C13-C11	-2.10	122.27	125.53
24	5	606	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	h	612	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	k	303	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	A	846	BCR	C33-C5-C6	-2.10	122.19	124.48
24	A	802	CLA	C4D-C3D-CAD	-2.10	105.83	108.11
24	h	611	CLA	CMB-C2B-C3B	2.10	131.48	126.55
26	2	210	DD6	C25-C24-C1	-2.10	120.62	126.36
24	A	823	CLA	C1-C2-C3	-2.10	122.76	126.20
24	c	602	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
24	c	606	CLA	CHD-C1D-ND	-2.10	121.85	124.80
24	4	606	CLA	O2D-CGD-CBD	2.09	114.89	111.23
25	A	859	BCR	C8-C9-C10	-2.09	115.72	119.01
24	9	303	CLA	C2A-C1A-CHA	2.09	127.50	123.87
26	5	609	DD6	C26-C25-C24	-2.09	117.14	123.20
26	1	311	DD6	C9-C8-C6	2.09	132.10	126.36
24	k	308	CLA	CMA-C3A-C2A	-2.09	111.43	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	826	CLA	CHB-C4A-NA	2.09	127.42	124.40
25	A	859	BCR	C3-C4-C5	-2.09	110.33	114.06
24	B	836	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	t	301	CLA	CAA-C2A-C1A	2.09	118.83	111.97
24	A	807	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	B	837	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	R	103	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	k	309	CLA	O2A-CGA-O1A	-2.09	117.95	123.33
25	I	101	BCR	C37-C22-C21	-2.09	119.43	122.82
25	1	314	BCR	C20-C19-C18	-2.09	120.63	126.36
24	A	820	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	F	201	CLA	CHB-C4A-NA	2.09	127.42	124.40
25	A	845	BCR	C3-C4-C5	-2.09	107.79	112.27
25	B	843	BCR	C34-C9-C10	-2.09	119.43	122.82
24	F	202	CLA	CHB-C4A-NA	2.09	127.41	124.40
26	5	608	DD6	C19-C18-C17	2.09	114.69	110.79
24	A	835	CLA	C1-C2-C3	-2.09	122.78	126.20
24	A	832	CLA	C3B-C4B-NB	-2.09	108.67	110.53
24	B	809	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	1	301	CLA	CHB-C4A-NA	2.09	127.41	124.40
24	B	802	CLA	CHB-C4A-NA	2.09	127.41	124.40
29	k	312	A1L1G	C28-C39-C38	-2.09	119.44	122.82
24	A	814	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
24	3	305	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	A	838	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	A	815	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	A	826	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	t	302	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	L	205	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	F	204	BCR	C21-C20-C19	-2.08	117.17	123.20
26	3	313	DD6	C12-C11-C13	2.08	121.27	118.09
26	7	613	DD6	C28-C27-C26	-2.08	120.14	124.18
24	B	816	CLA	C3B-C4B-NB	-2.08	108.67	110.53
24	B	804	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	8	207	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	L	204	CLA	CHB-C4A-NA	2.08	127.40	124.40
26	k	315	DD6	C9-C8-C6	2.08	132.07	126.36
26	h	614	DD6	C7-C6-C8	2.08	121.27	118.09
24	B	823	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
24	A	860	CLA	C3B-C4B-NB	-2.08	108.67	110.53
25	t	312	BCR	C21-C20-C19	-2.08	117.18	123.20
24	t	310	CLA	CHB-C4A-NA	2.08	127.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	805	CLA	CHD-C1D-ND	-2.08	121.88	124.80
25	J	101	BCR	C24-C25-C26	-2.08	116.77	121.56
24	h	607	CLA	CHB-C4A-NA	2.08	127.40	124.40
25	J	104	BCR	C33-C5-C4	2.08	118.02	113.60
24	k	311	CLA	CHD-C1D-ND	-2.08	121.88	124.80
24	8	204	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
25	L	206	BCR	C37-C22-C21	-2.08	119.45	122.82
24	6	612	CLA	C3B-C4B-NB	-2.08	108.68	110.53
24	t	305	CLA	C3B-C4B-NB	-2.08	108.68	110.53
26	6	616	DD6	C15-C14-C13	-2.08	121.61	125.99
24	A	830	CLA	C1-C2-C3	-2.07	122.80	126.20
26	8	210	DD6	C34-C35-C36	-2.07	107.01	112.18
27	A	854	LMT	C1B-O1B-C4'	-2.07	113.06	117.98
24	L	203	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	2	210	DD6	C10-C9-C8	-2.07	117.19	123.20
26	5	608	DD6	C4-C3-C2	-2.07	119.28	123.52
25	B	849	BCR	C21-C20-C19	-2.07	117.20	123.20
24	B	848	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
24	4	608	CLA	CBC-CAC-C3C	2.07	118.03	112.42
25	J	101	BCR	C3-C4-C5	-2.07	110.36	114.06
24	7	610	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	c	608	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	A	851	LMT	C1'-C2'-C3'	2.07	114.36	110.01
24	3	306	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	7	607	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	c	608	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	B	818	CLA	CHB-C4A-NA	2.07	127.38	124.40
25	7	617	BCR	C36-C18-C19	2.07	121.24	118.09
25	B	841	BCR	C12-C13-C14	-2.06	115.76	119.01
24	A	823	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
24	A	832	CLA	CHD-C1D-ND	-2.06	121.90	124.80
24	k	305	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	B	824	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
24	B	804	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
29	2	213	A1L1G	C28-C39-C40	2.06	121.24	118.09
24	A	807	CLA	C1-C2-C3	-2.06	122.82	126.20
24	A	840	CLA	CHB-C4A-NA	2.06	127.38	124.40
25	B	840	BCR	C11-C12-C13	-2.06	120.71	126.36
24	1	309	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	1	310	BCR	C1-C6-C7	2.06	121.24	115.65
24	8	205	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
24	A	823	CLA	CHB-C4A-NA	2.06	127.37	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	316	BCR	C4-C5-C6	-2.06	119.92	122.70
24	5	603	CLA	CHB-C4A-NA	2.06	127.37	124.40
24	A	822	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	A	804	CLA	CHD-C1D-ND	-2.06	121.91	124.80
24	1	308	CLA	CHB-C4A-NA	2.06	127.37	124.40
26	4	616	DD6	C7-C6-C8	2.06	121.23	118.09
28	3	315	LHG	O8-C23-O10	-2.06	118.48	123.63
24	B	828	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	7	607	CLA	CHD-C1D-ND	-2.06	121.91	124.80
26	9	315	DD6	C12-C11-C10	-2.06	119.48	122.82
24	6	601	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
24	7	601	CLA	O2D-CGD-CBD	2.06	114.82	111.23
24	9	305	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
24	h	605	CLA	CHD-C1D-ND	-2.05	121.91	124.80
24	t	308	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	B	846	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
24	2	203	CLA	C3B-C4B-NB	-2.05	108.70	110.53
26	7	613	DD6	C33-C32-C31	2.05	113.54	109.49
24	A	806	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	L	205	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	A	847	CLA	C4-C3-C5	2.05	118.79	115.23
24	2	203	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
24	3	309	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	k	306	CLA	O2D-CGD-CBD	2.05	114.82	111.23
26	4	617	DD6	C12-C11-C13	2.05	121.22	118.09
24	B	830	CLA	C1-C2-C3	-2.05	122.83	126.20
26	1	313	DD6	C25-C24-C1	-2.05	120.73	126.36
24	L	204	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	4	615	DD6	C-C1-C24	2.05	121.22	118.09
25	L	206	BCR	C3-C4-C5	-2.05	110.40	114.06
24	B	807	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
24	h	603	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	7	612	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	h	613	DD6	C25-C24-C1	-2.05	120.74	126.36
24	k	309	CLA	CHD-C1D-ND	-2.05	121.92	124.80
28	B	844	LHG	O7-C7-O9	-2.05	118.92	123.70
24	c	604	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	6	607	CLA	CHD-C1D-ND	-2.05	121.92	124.80
26	9	314	DD6	C4-C3-C2	2.05	127.71	123.52
26	t	311	DD6	C33-C32-C31	2.05	113.52	109.49
24	9	306	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	A	814	CLA	C3B-C4B-NB	-2.05	108.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	305	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
26	9	317	DD6	C28-C27-C26	-2.05	120.21	124.18
24	R	103	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	B	825	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
24	A	821	CLA	CHD-C1D-ND	-2.05	121.92	124.80
26	8	210	DD6	C9-C8-C6	2.05	131.97	126.36
25	B	849	BCR	C23-C22-C21	-2.05	115.79	119.01
24	5	604	CLA	CHB-C4A-NA	2.04	127.35	124.40
24	B	823	CLA	CMB-C2B-C3B	2.04	131.36	126.55
26	c	613	DD6	C12-C11-C13	2.04	121.21	118.09
24	B	821	CLA	CAA-C2A-C3A	-2.04	107.47	113.00
25	I	101	BCR	C23-C24-C25	-2.04	121.54	127.00
24	B	809	CLA	CBA-CAA-C2A	-2.04	107.71	113.79
24	2	209	CLA	CHB-C4A-NA	2.04	127.35	124.40
24	h	608	CLA	C3B-C4B-NB	-2.04	108.71	110.53
24	B	823	CLA	CHB-C4A-NA	2.04	127.35	124.40
24	4	608	CLA	CHD-C1D-ND	-2.04	121.93	124.80
24	B	807	CLA	CHD-C1D-ND	-2.04	121.93	124.80
24	8	201	CLA	CHD-C1D-ND	-2.04	121.93	124.80
24	A	828	CLA	CHB-C4A-NA	2.04	127.34	124.40
24	4	610	CLA	CHD-C1D-ND	-2.04	121.93	124.80
24	A	833	CLA	C3B-C4B-NB	-2.04	108.71	110.53
24	1	305	CLA	O2D-CGD-CBD	2.04	114.79	111.23
25	R	102	BCR	C15-C14-C13	-2.04	124.42	127.28
24	5	606	CLA	CHD-C1D-ND	-2.04	121.93	124.80
24	R	104	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
24	A	826	CLA	CMB-C2B-C3B	2.04	131.34	126.55
26	9	317	DD6	C9-C10-C11	-2.04	124.42	127.28
26	9	315	DD6	C28-C27-C26	-2.04	120.23	124.18
25	B	840	BCR	C33-C5-C6	-2.04	122.26	124.48
24	7	607	CLA	O2A-CGA-O1A	-2.04	118.10	123.33
26	1	312	DD6	C15-C14-C13	-2.04	121.69	125.99
24	A	838	CLA	O2D-CGD-CBD	2.03	114.79	111.23
24	B	833	CLA	C4-C3-C2	-2.03	118.40	123.63
24	3	303	CLA	CHB-C4A-NA	2.03	127.33	124.40
26	c	612	DD6	O1-C20-C19	2.03	115.40	113.49
24	c	611	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	A	810	CLA	CHD-C1D-ND	-2.03	121.94	124.80
24	A	812	CLA	CHD-C1D-ND	-2.03	121.94	124.80
26	5	608	DD6	C12-C11-C13	2.03	121.19	118.09
26	c	613	DD6	C7-C6-C8	2.03	121.19	118.09
26	4	616	DD6	C28-C27-C26	-2.03	120.24	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	818	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	4	602	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	J	101	BCR	C1-C6-C7	2.03	121.16	115.65
24	6	602	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
28	J	105	LHG	O7-C7-O9	-2.03	118.96	123.70
24	6	604	CLA	CHB-C4A-NA	2.03	127.33	124.40
26	k	313	DD6	C21-C20-C15	-2.03	118.97	122.30
24	B	835	CLA	CMB-C2B-C3B	2.03	131.31	126.55
25	k	316	BCR	C8-C7-C6	-2.03	121.59	127.00
25	R	101	BCR	C15-C14-C13	-2.03	124.44	127.28
24	R	104	CLA	CMB-C2B-C3B	2.02	131.31	126.55
24	A	808	CLA	C3B-C4B-NB	-2.02	108.72	110.53
24	k	304	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
26	R	105	DD6	C35-C36-C31	2.02	124.71	120.50
26	h	614	DD6	C9-C10-C11	-2.02	124.44	127.28
24	B	819	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	R	104	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
26	8	210	DD6	C7-C6-C8	2.02	121.18	118.09
24	8	204	CLA	O2D-CGD-CBD	2.02	114.77	111.23
24	B	826	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	B	812	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	3	309	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	I	102	BCR	C2-C1-C6	-2.02	107.50	110.44
24	7	605	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	B	823	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	4	613	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	c	607	CLA	C3B-C4B-NB	-2.02	108.73	110.53
24	4	602	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	7	602	CLA	CGD-CBD-CAD	2.02	117.38	110.85
24	5	601	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	7	603	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
26	9	315	DD6	C-C1-C2	-2.02	119.55	122.82
24	4	607	CLA	O2A-CGA-O1A	-2.02	117.17	123.20
24	A	825	CLA	C1-C2-C3	-2.02	122.89	126.20
26	6	617	DD6	C7-C6-C8	2.02	121.17	118.09
24	h	606	CLA	O2A-CGA-O1A	-2.02	117.18	123.20
24	A	856	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	c	612	DD6	C4-C3-C2	-2.02	119.39	123.52
24	A	817	CLA	O2D-CGD-CBD	2.02	114.76	111.23
28	B	845	LHG	O8-C23-C24	2.02	117.98	111.83
25	A	859	BCR	C37-C22-C21	-2.02	119.55	122.82
24	7	603	CLA	O1D-CGD-CBD	2.02	128.49	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	826	CLA	CHD-C1D-ND	-2.02	121.97	124.80
24	A	803	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
25	9	316	BCR	C20-C19-C18	-2.02	120.84	126.36
24	6	603	CLA	CHB-C4A-NA	2.02	127.31	124.40
26	8	210	DD6	C12-C11-C13	-2.01	115.01	118.09
25	R	102	BCR	C11-C12-C13	-2.01	120.84	126.36
24	8	203	CLA	C3B-C4B-NB	-2.01	108.73	110.53
25	A	843	BCR	C8-C7-C6	-2.01	121.62	127.00
26	8	211	DD6	C34-C35-C36	-2.01	107.17	112.18
24	A	829	CLA	C1-C2-C3	-2.01	122.90	126.20
24	B	833	CLA	CMB-C2B-C3B	2.01	131.28	126.55
24	6	601	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	B	825	CLA	CMB-C2B-C3B	2.01	131.28	126.55
24	A	812	CLA	C1-C2-C3	-2.01	122.90	126.20
26	1	311	DD6	C29-C30-C31	-2.01	170.80	175.48
24	h	609	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	9	309	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
24	7	607	CLA	C3B-C4B-NB	-2.01	108.74	110.53
24	t	305	CLA	CHD-C1D-ND	-2.01	121.98	124.80
26	2	212	DD6	C-C1-C2	-2.01	119.56	122.82
26	6	616	DD6	C23-C16-C15	2.01	115.47	110.05
25	c	615	BCR	C36-C18-C17	-2.01	119.56	122.82
24	B	824	CLA	CHB-C4A-NA	2.01	127.30	124.40
29	2	213	A1L1G	C3-C6-C1	2.01	111.16	109.21
25	A	859	BCR	C10-C11-C12	-2.01	117.39	123.20
26	6	613	DD6	C14-C13-C11	-2.01	122.42	125.53
24	A	806	CLA	C3B-C4B-NB	-2.01	108.74	110.53
29	k	312	A1L1G	C27-C34-C33	2.01	121.15	118.09
24	A	809	CLA	CHD-C1D-ND	-2.00	121.98	124.80
24	F	201	CLA	CHD-C1D-ND	-2.00	121.98	124.80
25	1	314	BCR	C1-C6-C7	2.00	121.09	115.65
24	A	826	CLA	CHD-C1D-ND	-2.00	121.98	124.80
24	B	811	CLA	CHD-C1D-ND	-2.00	121.98	124.80
26	c	612	DD6	C26-C25-C24	-2.00	117.39	123.20
26	9	317	DD6	C34-C35-C36	-2.00	107.19	112.18
24	c	606	CLA	C3B-C4B-NB	-2.00	108.74	110.53
24	A	840	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	4	605	CLA	CHD-C1D-ND	-2.00	121.98	124.80
24	A	834	CLA	CHD-C1D-ND	-2.00	121.98	124.80
24	A	856	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
24	B	805	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	1	309	CLA	CHB-C4A-NA	2.00	127.29	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	302	CLA	O2A-CGA-O1A	-2.00	117.22	123.20
24	A	818	CLA	C7-C6-C5	-2.00	107.93	113.26
24	3	307	CLA	CHB-C4A-NA	2.00	127.29	124.40
24	A	803	CLA	CMB-C2B-C3B	2.00	131.26	126.55
24	R	103	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	R	101	BCR	C21-C20-C19	-2.00	117.40	123.20
24	1	301	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	A	837	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (218) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	301	CLA	ND
24	1	302	CLA	ND
24	1	303	CLA	ND
24	1	304	CLA	ND
24	1	305	CLA	ND
24	1	306	CLA	ND
24	1	307	CLA	ND
24	1	308	CLA	ND
24	1	309	CLA	ND
24	1	317	CLA	ND
24	2	201	CLA	ND
24	2	202	CLA	ND
24	2	203	CLA	ND
24	2	204	CLA	ND
24	2	206	CLA	ND
24	2	207	CLA	ND
24	2	208	CLA	ND
24	2	209	CLA	ND
24	3	302	CLA	ND
24	3	303	CLA	ND
24	3	304	CLA	ND
24	3	305	CLA	ND
24	3	306	CLA	ND
24	3	307	CLA	ND
24	3	308	CLA	ND
24	3	309	CLA	ND
24	4	601	CLA	ND
24	4	602	CLA	ND
24	4	603	CLA	ND
24	4	604	CLA	ND

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Mol	Chain	Res	Type	Atom
24	4	605	CLA	ND
24	4	606	CLA	ND
24	4	607	CLA	ND
24	4	608	CLA	ND
24	4	609	CLA	ND
24	4	610	CLA	ND
24	4	611	CLA	ND
24	4	612	CLA	ND
24	4	613	CLA	ND
24	5	601	CLA	ND
24	5	602	CLA	ND
24	5	603	CLA	ND
24	5	604	CLA	ND
24	5	605	CLA	ND
24	5	606	CLA	ND
24	5	607	CLA	ND
24	6	601	CLA	ND
24	6	602	CLA	ND
24	6	603	CLA	ND
24	6	604	CLA	ND
24	6	606	CLA	ND
24	6	607	CLA	ND
24	6	608	CLA	ND
24	6	609	CLA	ND
24	6	610	CLA	ND
24	6	611	CLA	ND
24	6	612	CLA	ND
24	7	601	CLA	ND
24	7	602	CLA	ND
24	7	603	CLA	ND
24	7	604	CLA	ND
24	7	605	CLA	ND
24	7	606	CLA	ND
24	7	607	CLA	ND
24	7	608	CLA	ND
24	7	609	CLA	ND
24	7	610	CLA	ND
24	7	611	CLA	ND
24	7	612	CLA	ND
24	8	201	CLA	ND
24	8	202	CLA	ND
24	8	203	CLA	ND

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Mol	Chain	Res	Type	Atom
24	8	204	CLA	ND
24	8	205	CLA	ND
24	8	206	CLA	ND
24	8	207	CLA	ND
24	8	208	CLA	ND
24	8	209	CLA	ND
24	9	301	CLA	ND
24	9	302	CLA	ND
24	9	303	CLA	ND
24	9	304	CLA	ND
24	9	306	CLA	ND
24	9	307	CLA	ND
24	9	308	CLA	ND
24	9	309	CLA	ND
24	9	310	CLA	ND
24	9	311	CLA	ND
24	h	601	CLA	ND
24	h	602	CLA	ND
24	h	603	CLA	ND
24	h	604	CLA	ND
24	h	605	CLA	ND
24	h	606	CLA	ND
24	h	607	CLA	ND
24	h	608	CLA	ND
24	h	609	CLA	ND
24	h	610	CLA	ND
24	h	612	CLA	ND
24	c	601	CLA	ND
24	c	602	CLA	ND
24	c	603	CLA	ND
24	c	604	CLA	ND
24	c	605	CLA	ND
24	c	606	CLA	ND
24	c	607	CLA	ND
24	c	608	CLA	ND
24	c	609	CLA	ND
24	c	610	CLA	ND
24	c	611	CLA	ND
24	t	301	CLA	ND
24	t	302	CLA	ND
24	t	303	CLA	ND
24	t	304	CLA	ND

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Mol	Chain	Res	Type	Atom
24	t	305	CLA	ND
24	t	306	CLA	ND
24	t	307	CLA	ND
24	t	308	CLA	ND
24	t	309	CLA	ND
24	t	310	CLA	ND
24	k	301	CLA	ND
24	k	302	CLA	ND
24	k	304	CLA	ND
24	k	305	CLA	ND
24	k	306	CLA	ND
24	k	307	CLA	ND
24	k	308	CLA	ND
24	k	309	CLA	ND
24	k	310	CLA	ND
24	k	311	CLA	ND
24	A	801	CLA	ND
24	A	802	CLA	ND
24	A	804	CLA	ND
24	A	805	CLA	ND
24	A	806	CLA	ND
24	A	807	CLA	ND
24	A	808	CLA	ND
24	A	809	CLA	ND
24	A	810	CLA	ND
24	A	811	CLA	ND
24	A	812	CLA	ND
24	A	813	CLA	ND
24	A	814	CLA	ND
24	A	815	CLA	ND
24	A	816	CLA	ND
24	A	817	CLA	ND
24	A	818	CLA	ND
24	A	819	CLA	ND
24	A	820	CLA	ND
24	A	821	CLA	ND
24	A	822	CLA	ND
24	A	823	CLA	ND
24	A	824	CLA	ND
24	A	825	CLA	ND
24	A	826	CLA	ND
24	A	827	CLA	ND

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Mol	Chain	Res	Type	Atom
24	A	828	CLA	ND
24	A	829	CLA	ND
24	A	831	CLA	ND
24	A	833	CLA	ND
24	A	834	CLA	ND
24	A	835	CLA	ND
24	A	836	CLA	ND
24	A	837	CLA	ND
24	A	838	CLA	ND
24	A	840	CLA	ND
24	A	847	CLA	ND
24	A	853	CLA	ND
24	A	857	CLA	ND
24	A	860	CLA	ND
24	B	801	CLA	ND
24	B	802	CLA	ND
24	B	803	CLA	ND
24	B	804	CLA	ND
24	B	805	CLA	ND
24	B	806	CLA	ND
24	B	808	CLA	ND
24	B	809	CLA	ND
24	B	810	CLA	ND
24	B	811	CLA	ND
24	B	812	CLA	ND
24	B	813	CLA	ND
24	B	814	CLA	ND
24	B	815	CLA	ND
24	B	816	CLA	ND
24	B	817	CLA	ND
24	B	818	CLA	ND
24	B	819	CLA	ND
24	B	820	CLA	ND
24	B	821	CLA	ND
24	B	822	CLA	ND
24	B	823	CLA	ND
24	B	824	CLA	ND
24	B	825	CLA	ND
24	B	826	CLA	ND
24	B	827	CLA	ND
24	B	828	CLA	ND
24	B	829	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	830	CLA	ND
24	B	831	CLA	ND
24	B	832	CLA	ND
24	B	833	CLA	ND
24	B	834	CLA	ND
24	B	835	CLA	ND
24	B	836	CLA	ND
24	B	837	CLA	ND
24	B	838	CLA	ND
24	B	846	CLA	ND
24	B	847	CLA	ND
24	B	848	CLA	ND
24	F	201	CLA	ND
24	F	202	CLA	ND
24	F	203	CLA	ND
24	J	103	CLA	ND
24	L	203	CLA	ND
24	L	205	CLA	ND
24	R	103	CLA	ND
24	R	104	CLA	ND

All (2313) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	301	CLA	C1A-C2A-CAA-CBA
24	1	301	CLA	C3A-C2A-CAA-CBA
24	1	301	CLA	CBD-CGD-O2D-CED
24	1	303	CLA	CBD-CGD-O2D-CED
24	1	304	CLA	CAD-CBD-CGD-O1D
24	1	304	CLA	CAD-CBD-CGD-O2D
24	1	305	CLA	CAD-CBD-CGD-O1D
24	1	305	CLA	CAD-CBD-CGD-O2D
24	1	307	CLA	CHA-CBD-CGD-O1D
24	1	307	CLA	CHA-CBD-CGD-O2D
24	1	309	CLA	C1A-C2A-CAA-CBA
24	1	317	CLA	CAD-CBD-CGD-O1D
24	1	317	CLA	CAD-CBD-CGD-O2D
24	2	201	CLA	C1A-C2A-CAA-CBA
24	2	201	CLA	CAD-CBD-CGD-O1D
24	2	201	CLA	CAD-CBD-CGD-O2D
24	2	201	CLA	CBD-CGD-O2D-CED
24	2	202	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	2	204	CLA	C4B-C3B-CAB-CBB
24	2	204	CLA	CHA-CBD-CGD-O1D
24	2	204	CLA	CHA-CBD-CGD-O2D
24	2	205	CLA	CBA-CGA-O2A-C1
24	2	205	CLA	CBD-CGD-O2D-CED
24	2	206	CLA	C3A-C2A-CAA-CBA
24	2	206	CLA	C2B-C3B-CAB-CBB
24	2	206	CLA	C4B-C3B-CAB-CBB
24	2	208	CLA	CBA-CGA-O2A-C1
24	2	208	CLA	CHA-CBD-CGD-O1D
24	2	208	CLA	CHA-CBD-CGD-O2D
24	2	209	CLA	CBD-CGD-O2D-CED
24	2	209	CLA	O1D-CGD-O2D-CED
24	3	303	CLA	CAD-CBD-CGD-O1D
24	3	303	CLA	CAD-CBD-CGD-O2D
24	3	303	CLA	CBD-CGD-O2D-CED
24	3	304	CLA	CBA-CGA-O2A-C1
24	3	305	CLA	CBD-CGD-O2D-CED
24	3	306	CLA	C1A-C2A-CAA-CBA
24	3	308	CLA	C1A-C2A-CAA-CBA
24	3	308	CLA	C3A-C2A-CAA-CBA
24	4	602	CLA	C1A-C2A-CAA-CBA
24	4	602	CLA	C3A-C2A-CAA-CBA
24	4	604	CLA	C3A-C2A-CAA-CBA
24	4	604	CLA	CBD-CGD-O2D-CED
24	4	607	CLA	CBD-CGD-O2D-CED
24	4	608	CLA	O1A-CGA-O2A-C1
24	4	608	CLA	C2B-C3B-CAB-CBB
24	4	608	CLA	C4B-C3B-CAB-CBB
24	4	611	CLA	CBA-CGA-O2A-C1
24	4	612	CLA	CBD-CGD-O2D-CED
24	4	613	CLA	CBA-CGA-O2A-C1
24	4	613	CLA	O1A-CGA-O2A-C1
24	4	613	CLA	C2B-C3B-CAB-CBB
24	4	613	CLA	C4B-C3B-CAB-CBB
24	4	613	CLA	CAD-CBD-CGD-O1D
24	4	613	CLA	CAD-CBD-CGD-O2D
24	5	601	CLA	CBD-CGD-O2D-CED
24	5	601	CLA	O1D-CGD-O2D-CED
24	5	602	CLA	C1A-C2A-CAA-CBA
24	5	602	CLA	C3A-C2A-CAA-CBA
24	5	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	5	605	CLA	C3A-C2A-CAA-CBA
24	5	605	CLA	CBA-CGA-O2A-C1
24	5	605	CLA	C2B-C3B-CAB-CBB
24	5	605	CLA	C4B-C3B-CAB-CBB
24	6	601	CLA	CAD-CBD-CGD-O1D
24	6	601	CLA	CAD-CBD-CGD-O2D
24	6	601	CLA	CBD-CGD-O2D-CED
24	6	603	CLA	CBA-CGA-O2A-C1
24	6	603	CLA	O1A-CGA-O2A-C1
24	6	603	CLA	CHA-CBD-CGD-O1D
24	6	603	CLA	CHA-CBD-CGD-O2D
24	6	605	CLA	C2B-C3B-CAB-CBB
24	6	605	CLA	C4B-C3B-CAB-CBB
24	6	606	CLA	CBD-CGD-O2D-CED
24	6	608	CLA	CHA-CBD-CGD-O1D
24	6	608	CLA	CHA-CBD-CGD-O2D
24	6	608	CLA	CBD-CGD-O2D-CED
24	6	610	CLA	C2B-C3B-CAB-CBB
24	6	610	CLA	C4B-C3B-CAB-CBB
24	6	611	CLA	C1A-C2A-CAA-CBA
24	6	611	CLA	C3A-C2A-CAA-CBA
24	7	601	CLA	C2B-C3B-CAB-CBB
24	7	601	CLA	C4B-C3B-CAB-CBB
24	7	602	CLA	C2C-C3C-CAC-CBC
24	7	602	CLA	C4C-C3C-CAC-CBC
24	7	604	CLA	CBD-CGD-O2D-CED
24	7	605	CLA	CHA-CBD-CGD-O1D
24	7	605	CLA	CHA-CBD-CGD-O2D
24	7	606	CLA	CBD-CGD-O2D-CED
24	7	608	CLA	C1A-C2A-CAA-CBA
24	7	608	CLA	C3A-C2A-CAA-CBA
24	7	609	CLA	CBD-CGD-O2D-CED
24	7	610	CLA	C1A-C2A-CAA-CBA
24	7	610	CLA	C3A-C2A-CAA-CBA
24	7	610	CLA	CBD-CGD-O2D-CED
24	7	611	CLA	C1A-C2A-CAA-CBA
24	7	612	CLA	C1A-C2A-CAA-CBA
24	7	612	CLA	C3A-C2A-CAA-CBA
24	8	201	CLA	C2B-C3B-CAB-CBB
24	8	201	CLA	C4B-C3B-CAB-CBB
24	8	201	CLA	CBD-CGD-O2D-CED
24	8	202	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	8	202	CLA	CHA-CBD-CGD-O2D
24	8	203	CLA	C2B-C3B-CAB-CBB
24	8	203	CLA	C4B-C3B-CAB-CBB
24	8	204	CLA	C1A-C2A-CAA-CBA
24	8	204	CLA	C3A-C2A-CAA-CBA
24	8	205	CLA	C1A-C2A-CAA-CBA
24	8	205	CLA	C3A-C2A-CAA-CBA
24	8	205	CLA	C2B-C3B-CAB-CBB
24	8	205	CLA	C4B-C3B-CAB-CBB
24	8	207	CLA	C1A-C2A-CAA-CBA
24	8	207	CLA	C3A-C2A-CAA-CBA
24	8	209	CLA	C2B-C3B-CAB-CBB
24	8	209	CLA	C4B-C3B-CAB-CBB
24	9	303	CLA	C1A-C2A-CAA-CBA
24	9	303	CLA	C3A-C2A-CAA-CBA
24	9	303	CLA	CBD-CGD-O2D-CED
24	9	304	CLA	CBD-CGD-O2D-CED
24	9	305	CLA	CBD-CGD-O2D-CED
24	9	306	CLA	CAD-CBD-CGD-O2D
24	9	307	CLA	C1A-C2A-CAA-CBA
24	9	308	CLA	CBD-CGD-O2D-CED
24	9	310	CLA	C1A-C2A-CAA-CBA
24	9	310	CLA	C3A-C2A-CAA-CBA
24	9	310	CLA	CBA-CGA-O2A-C1
24	9	310	CLA	C2B-C3B-CAB-CBB
24	9	310	CLA	C4B-C3B-CAB-CBB
24	9	310	CLA	CBD-CGD-O2D-CED
24	9	310	CLA	O1D-CGD-O2D-CED
24	h	604	CLA	CBD-CGD-O2D-CED
24	h	606	CLA	CHA-CBD-CGD-O1D
24	h	606	CLA	CHA-CBD-CGD-O2D
24	h	608	CLA	CBD-CGD-O2D-CED
24	h	609	CLA	CBD-CGD-O2D-CED
24	h	610	CLA	C1A-C2A-CAA-CBA
24	h	612	CLA	CHA-CBD-CGD-O1D
24	h	612	CLA	CHA-CBD-CGD-O2D
24	c	601	CLA	CAD-CBD-CGD-O2D
24	c	601	CLA	CBD-CGD-O2D-CED
24	c	603	CLA	CBA-CGA-O2A-C1
24	c	603	CLA	CBD-CGD-O2D-CED
24	c	605	CLA	CBA-CGA-O2A-C1
24	c	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	c	608	CLA	C1A-C2A-CAA-CBA
24	c	609	CLA	C1A-C2A-CAA-CBA
24	c	609	CLA	CBA-CGA-O2A-C1
24	c	609	CLA	O1A-CGA-O2A-C1
24	c	610	CLA	C1A-C2A-CAA-CBA
24	c	610	CLA	C3A-C2A-CAA-CBA
24	t	301	CLA	C1A-C2A-CAA-CBA
24	t	301	CLA	C3A-C2A-CAA-CBA
24	t	302	CLA	C1A-C2A-CAA-CBA
24	t	302	CLA	C3A-C2A-CAA-CBA
24	t	302	CLA	CAD-CBD-CGD-O1D
24	t	302	CLA	CAD-CBD-CGD-O2D
24	t	302	CLA	CBD-CGD-O2D-CED
24	t	303	CLA	C4-C3-C5-C6
24	t	303	CLA	C11-C12-C13-C14
24	t	305	CLA	CBA-CGA-O2A-C1
24	t	305	CLA	CBD-CGD-O2D-CED
24	t	306	CLA	C1A-C2A-CAA-CBA
24	t	306	CLA	C3A-C2A-CAA-CBA
24	t	306	CLA	CBD-CGD-O2D-CED
24	t	307	CLA	C3A-C2A-CAA-CBA
24	t	308	CLA	C1A-C2A-CAA-CBA
24	t	308	CLA	C3A-C2A-CAA-CBA
24	t	308	CLA	CBD-CGD-O2D-CED
24	k	302	CLA	C3A-C2A-CAA-CBA
24	k	302	CLA	CBA-CGA-O2A-C1
24	k	302	CLA	CBD-CGD-O2D-CED
24	k	304	CLA	C1A-C2A-CAA-CBA
24	k	304	CLA	C3A-C2A-CAA-CBA
24	k	305	CLA	C1A-C2A-CAA-CBA
24	k	305	CLA	CBD-CGD-O2D-CED
24	k	307	CLA	CBA-CGA-O2A-C1
24	k	308	CLA	CAD-CBD-CGD-O1D
24	k	308	CLA	CAD-CBD-CGD-O2D
24	k	309	CLA	C1A-C2A-CAA-CBA
24	k	309	CLA	C3A-C2A-CAA-CBA
24	k	309	CLA	CBD-CGD-O2D-CED
24	k	310	CLA	CBD-CGD-O2D-CED
24	A	801	CLA	C4B-C3B-CAB-CBB
24	A	803	CLA	C3A-C2A-CAA-CBA
24	A	807	CLA	C3A-C2A-CAA-CBA
24	A	807	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	A	807	CLA	CHA-CBD-CGD-O2D
24	A	809	CLA	C1A-C2A-CAA-CBA
24	A	809	CLA	C3A-C2A-CAA-CBA
24	A	809	CLA	CBD-CGD-O2D-CED
24	A	810	CLA	C2B-C3B-CAB-CBB
24	A	810	CLA	C4B-C3B-CAB-CBB
24	A	811	CLA	C3A-C2A-CAA-CBA
24	A	812	CLA	C4B-C3B-CAB-CBB
24	A	812	CLA	C11-C10-C8-C9
24	A	813	CLA	C1A-C2A-CAA-CBA
24	A	814	CLA	CBD-CGD-O2D-CED
24	A	817	CLA	C1A-C2A-CAA-CBA
24	A	817	CLA	C3A-C2A-CAA-CBA
24	A	818	CLA	C1A-C2A-CAA-CBA
24	A	818	CLA	C3A-C2A-CAA-CBA
24	A	820	CLA	CBD-CGD-O2D-CED
24	A	822	CLA	CAD-CBD-CGD-O1D
24	A	822	CLA	CAD-CBD-CGD-O2D
24	A	823	CLA	C1A-C2A-CAA-CBA
24	A	823	CLA	C3A-C2A-CAA-CBA
24	A	823	CLA	C2B-C3B-CAB-CBB
24	A	823	CLA	C4B-C3B-CAB-CBB
24	A	824	CLA	C11-C12-C13-C14
24	A	829	CLA	CHA-CBD-CGD-O1D
24	A	829	CLA	CHA-CBD-CGD-O2D
24	A	830	CLA	C1A-C2A-CAA-CBA
24	A	830	CLA	C3A-C2A-CAA-CBA
24	A	831	CLA	C1A-C2A-CAA-CBA
24	A	832	CLA	C2B-C3B-CAB-CBB
24	A	832	CLA	C4B-C3B-CAB-CBB
24	A	833	CLA	CHA-CBD-CGD-O1D
24	A	833	CLA	CHA-CBD-CGD-O2D
24	A	833	CLA	C2-C3-C5-C6
24	A	833	CLA	C4-C3-C5-C6
24	A	835	CLA	CHA-CBD-CGD-O1D
24	A	835	CLA	CHA-CBD-CGD-O2D
24	A	836	CLA	C4B-C3B-CAB-CBB
24	A	838	CLA	CAD-CBD-CGD-O1D
24	A	838	CLA	CAD-CBD-CGD-O2D
24	A	840	CLA	CAD-CBD-CGD-O1D
24	A	840	CLA	CAD-CBD-CGD-O2D
24	A	860	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	860	CLA	C11-C12-C13-C14
24	B	802	CLA	C2B-C3B-CAB-CBB
24	B	802	CLA	C4B-C3B-CAB-CBB
24	B	802	CLA	CBD-CGD-O2D-CED
24	B	803	CLA	CBD-CGD-O2D-CED
24	B	804	CLA	C1A-C2A-CAA-CBA
24	B	804	CLA	C3A-C2A-CAA-CBA
24	B	804	CLA	CAD-CBD-CGD-O1D
24	B	804	CLA	CAD-CBD-CGD-O2D
24	B	805	CLA	C3A-C2A-CAA-CBA
24	B	808	CLA	CHA-CBD-CGD-O1D
24	B	808	CLA	CHA-CBD-CGD-O2D
24	B	809	CLA	CBD-CGD-O2D-CED
24	B	813	CLA	C1A-C2A-CAA-CBA
24	B	815	CLA	CAD-CBD-CGD-O1D
24	B	815	CLA	CAD-CBD-CGD-O2D
24	B	816	CLA	CHA-CBD-CGD-O1D
24	B	816	CLA	CHA-CBD-CGD-O2D
24	B	817	CLA	CAD-CBD-CGD-O2D
24	B	820	CLA	CAD-CBD-CGD-O1D
24	B	820	CLA	CAD-CBD-CGD-O2D
24	B	821	CLA	C3A-C2A-CAA-CBA
24	B	822	CLA	CHA-CBD-CGD-O1D
24	B	822	CLA	CHA-CBD-CGD-O2D
24	B	826	CLA	C1A-C2A-CAA-CBA
24	B	826	CLA	C3A-C2A-CAA-CBA
24	B	827	CLA	CHA-CBD-CGD-O1D
24	B	827	CLA	CHA-CBD-CGD-O2D
24	B	828	CLA	C3A-C2A-CAA-CBA
24	B	829	CLA	C1A-C2A-CAA-CBA
24	B	830	CLA	C1A-C2A-CAA-CBA
24	B	830	CLA	C3A-C2A-CAA-CBA
24	B	830	CLA	C2B-C3B-CAB-CBB
24	B	830	CLA	C4B-C3B-CAB-CBB
24	B	830	CLA	C4-C3-C5-C6
24	B	835	CLA	C1A-C2A-CAA-CBA
24	B	835	CLA	CAD-CBD-CGD-O1D
24	B	835	CLA	CAD-CBD-CGD-O2D
24	B	836	CLA	C1A-C2A-CAA-CBA
24	B	836	CLA	C11-C10-C8-C9
24	B	837	CLA	CAD-CBD-CGD-O1D
24	B	837	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	846	CLA	C3A-C2A-CAA-CBA
24	B	846	CLA	C2B-C3B-CAB-CBB
24	B	846	CLA	C4B-C3B-CAB-CBB
24	F	201	CLA	C1A-C2A-CAA-CBA
24	F	203	CLA	C1A-C2A-CAA-CBA
24	F	203	CLA	C3A-C2A-CAA-CBA
24	F	203	CLA	CBD-CGD-O2D-CED
24	J	103	CLA	C1A-C2A-CAA-CBA
24	J	103	CLA	C3A-C2A-CAA-CBA
24	J	103	CLA	CAD-CBD-CGD-O1D
24	J	103	CLA	CAD-CBD-CGD-O2D
24	L	203	CLA	CHA-CBD-CGD-O1D
24	L	203	CLA	CHA-CBD-CGD-O2D
25	1	310	BCR	C21-C22-C23-C24
25	1	310	BCR	C37-C22-C23-C24
25	1	314	BCR	C5-C6-C7-C8
25	1	314	BCR	C21-C22-C23-C24
25	1	314	BCR	C23-C24-C25-C26
25	1	314	BCR	C23-C24-C25-C30
25	7	617	BCR	C21-C22-C23-C24
25	7	617	BCR	C37-C22-C23-C24
25	9	316	BCR	C7-C8-C9-C34
25	c	615	BCR	C1-C6-C7-C8
25	c	615	BCR	C5-C6-C7-C8
25	c	615	BCR	C7-C8-C9-C10
25	c	615	BCR	C7-C8-C9-C34
25	c	615	BCR	C17-C18-C19-C20
25	t	312	BCR	C23-C24-C25-C26
25	t	312	BCR	C23-C24-C25-C30
25	A	844	BCR	C17-C18-C19-C20
25	A	846	BCR	C5-C6-C7-C8
25	A	859	BCR	C23-C24-C25-C26
25	A	859	BCR	C23-C24-C25-C30
25	B	840	BCR	C5-C6-C7-C8
25	B	840	BCR	C23-C24-C25-C26
25	B	841	BCR	C23-C24-C25-C26
25	B	843	BCR	C21-C22-C23-C24
25	B	849	BCR	C23-C24-C25-C26
25	I	101	BCR	C5-C6-C7-C8
25	I	101	BCR	C23-C24-C25-C26
25	J	101	BCR	C5-C6-C7-C8
25	J	104	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	J	104	BCR	C5-C6-C7-C8
25	L	206	BCR	C23-C24-C25-C26
25	L	206	BCR	C23-C24-C25-C30
25	M	101	BCR	C17-C18-C19-C20
25	M	101	BCR	C36-C18-C19-C20
25	M	101	BCR	C21-C22-C23-C24
25	M	101	BCR	C37-C22-C23-C24
25	R	101	BCR	C5-C6-C7-C8
25	R	102	BCR	C5-C6-C7-C8
26	2	212	DD6	C11-C13-C14-C15
26	3	313	DD6	C13-C14-C15-C20
26	4	616	DD6	C13-C14-C15-O1
26	4	617	DD6	C11-C13-C14-C15
26	5	608	DD6	C9-C10-C11-C12
26	5	608	DD6	C11-C13-C14-C15
26	5	609	DD6	C11-C13-C14-C15
26	6	615	DD6	C11-C13-C14-C15
26	6	616	DD6	C13-C14-C15-O1
26	6	617	DD6	C11-C13-C14-C15
26	7	615	DD6	C9-C10-C11-C12
26	7	615	DD6	C11-C13-C14-C15
26	7	616	DD6	C11-C13-C14-C15
26	7	616	DD6	C13-C14-C15-O1
26	8	211	DD6	C11-C13-C14-C15
26	9	315	DD6	C13-C14-C15-C20
26	9	315	DD6	C13-C14-C15-O1
26	9	317	DD6	C13-C14-C15-O1
26	h	614	DD6	C11-C13-C14-C15
26	h	615	DD6	C11-C13-C14-C15
26	h	616	DD6	C11-C13-C14-C15
26	t	311	DD6	C11-C13-C14-C15
26	k	313	DD6	C13-C14-C15-C16
26	k	314	DD6	C13-C14-C15-C20
26	k	314	DD6	C13-C14-C15-O1
26	J	102	DD6	C13-C14-C15-O1
26	R	105	DD6	C11-C13-C14-C15
26	R	105	DD6	C13-C14-C15-C20
26	R	105	DD6	C13-C14-C15-O1
27	1	316	LMT	O5'-C1'-O1'-C1
27	3	314	LMT	O5'-C1'-O1'-C1
27	3	314	LMT	C2-C1-O1'-C1'
28	1	318	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	1	318	LHG	C3-O3-P-O4
28	1	318	LHG	C3-O3-P-O5
28	1	318	LHG	C3-O3-P-O6
28	1	318	LHG	C4-O6-P-O4
28	2	215	LHG	C3-O3-P-O5
28	3	315	LHG	C3-O3-P-O5
28	3	315	LHG	C3-O3-P-O6
28	3	315	LHG	C4-O6-P-O3
28	3	315	LHG	C4-O6-P-O4
28	3	315	LHG	C4-O6-P-O5
28	4	619	LHG	C4-O6-P-O3
28	4	619	LHG	C4-O6-P-O4
28	8	213	LHG	C3-O3-P-O6
28	8	213	LHG	C4-O6-P-O4
28	A	841	LHG	C3-O3-P-O6
28	A	842	LHG	C3-O3-P-O4
28	A	842	LHG	C3-O3-P-O6
28	A	842	LHG	C4-O6-P-O3
28	A	842	LHG	C4-O6-P-O4
28	A	842	LHG	O6-C4-C5-O7
28	A	849	LHG	C3-O3-P-O6
28	A	849	LHG	C4-O6-P-O4
28	A	852	LHG	C4-O6-P-O3
28	A	852	LHG	C4-O6-P-O4
28	B	844	LHG	C3-O3-P-O5
28	B	844	LHG	C3-O3-P-O6
28	B	844	LHG	C4-O6-P-O5
28	B	845	LHG	C3-O3-P-O4
28	B	845	LHG	C3-O3-P-O6
28	B	845	LHG	C4-O6-P-O3
28	B	845	LHG	C4-O6-P-O5
28	I	103	LHG	C3-O3-P-O4
28	I	103	LHG	C3-O3-P-O6
28	J	105	LHG	C3-O3-P-O4
28	J	105	LHG	C3-O3-P-O6
28	J	105	LHG	O9-C7-O7-C5
28	J	105	LHG	C8-C7-O7-C5
28	L	201	LHG	C3-O3-P-O4
28	L	201	LHG	C3-O3-P-O6
28	L	201	LHG	C4-O6-P-O5
28	L	201	LHG	C8-C7-O7-C5
29	2	213	A1L1G	O13-C26-C30-C29

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Mol	Chain	Res	Type	Atoms
29	2	213	A1L1G	O13-C26-C30-C31
29	2	213	A1L1G	C26-C30-C31-C32
29	2	213	A1L1G	C29-C30-C31-C32
29	2	213	A1L1G	C27-C34-C35-C36
29	2	213	A1L1G	C33-C34-C35-C36
29	2	213	A1L1G	C35-C36-C37-C38
29	2	213	A1L1G	C37-C38-C39-C28
29	2	213	A1L1G	C37-C38-C39-C40
29	2	213	A1L1G	C38-C39-C40-C41
29	3	310	A1L1G	C45-C2-C44-C43
29	3	310	A1L1G	C29-C14-C25-O15
29	3	310	A1L1G	C14-C29-C30-C26
29	3	310	A1L1G	C26-C30-C31-C32
29	3	310	A1L1G	C32-C33-C34-C27
29	3	310	A1L1G	C32-C33-C34-C35
29	3	310	A1L1G	C27-C34-C35-C36
29	3	310	A1L1G	C33-C34-C35-C36
29	3	310	A1L1G	C35-C36-C37-C38
29	3	310	A1L1G	C37-C38-C39-C28
29	7	614	A1L1G	C45-C2-C44-C42
29	7	614	A1L1G	C37-C38-C39-C28
29	7	614	A1L1G	C37-C38-C39-C40
29	7	614	A1L1G	C40-C41-C42-C44
29	7	614	A1L1G	C41-C42-C44-C2
29	7	614	A1L1G	C41-C42-C44-C43
29	9	312	A1L1G	O13-C26-C30-C29
29	9	312	A1L1G	C26-C30-C31-C32
29	9	312	A1L1G	C29-C30-C31-C32
29	9	312	A1L1G	C27-C34-C35-C36
29	9	312	A1L1G	C33-C34-C35-C36
29	k	312	A1L1G	C29-C14-C25-C20
29	k	312	A1L1G	C27-C34-C35-C36
29	k	312	A1L1G	C33-C34-C35-C36
30	2	214	LMG	C11-C10-O7-C8
30	t	314	LMG	O9-C10-O7-C8
30	t	314	LMG	C11-C10-O7-C8
30	A	855	LMG	O6-C1-O1-C7
24	2	202	CLA	O1D-CGD-O2D-CED
24	2	205	CLA	O1D-CGD-O2D-CED
24	4	610	CLA	O1D-CGD-O2D-CED
24	4	611	CLA	O1D-CGD-O2D-CED
24	4	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	604	CLA	O1D-CGD-O2D-CED
24	7	606	CLA	O1D-CGD-O2D-CED
24	7	609	CLA	O1D-CGD-O2D-CED
24	9	301	CLA	O1D-CGD-O2D-CED
24	9	311	CLA	O1D-CGD-O2D-CED
24	t	306	CLA	O1D-CGD-O2D-CED
24	k	302	CLA	O1D-CGD-O2D-CED
24	B	832	CLA	C4C-C3C-CAC-CBC
24	1	301	CLA	O1D-CGD-O2D-CED
24	2	201	CLA	O1D-CGD-O2D-CED
24	3	303	CLA	O1D-CGD-O2D-CED
24	4	607	CLA	O1D-CGD-O2D-CED
24	6	601	CLA	O1D-CGD-O2D-CED
24	6	606	CLA	O1D-CGD-O2D-CED
24	8	201	CLA	O1D-CGD-O2D-CED
24	8	208	CLA	O1D-CGD-O2D-CED
24	9	303	CLA	O1D-CGD-O2D-CED
24	h	608	CLA	O1D-CGD-O2D-CED
24	h	609	CLA	O1D-CGD-O2D-CED
24	k	309	CLA	O1D-CGD-O2D-CED
24	k	310	CLA	O1D-CGD-O2D-CED
24	B	802	CLA	O1D-CGD-O2D-CED
24	B	803	CLA	O1D-CGD-O2D-CED
24	L	205	CLA	O1D-CGD-O2D-CED
24	1	304	CLA	CBD-CGD-O2D-CED
24	1	305	CLA	CBD-CGD-O2D-CED
24	4	602	CLA	CBD-CGD-O2D-CED
24	4	608	CLA	CBD-CGD-O2D-CED
24	4	610	CLA	CBD-CGD-O2D-CED
24	4	611	CLA	CBD-CGD-O2D-CED
24	5	602	CLA	CBD-CGD-O2D-CED
24	5	605	CLA	CBD-CGD-O2D-CED
24	6	604	CLA	CBD-CGD-O2D-CED
24	7	602	CLA	CBD-CGD-O2D-CED
24	7	611	CLA	CBD-CGD-O2D-CED
24	8	207	CLA	CBD-CGD-O2D-CED
24	8	208	CLA	CBD-CGD-O2D-CED
24	8	209	CLA	CBD-CGD-O2D-CED
24	9	301	CLA	CBD-CGD-O2D-CED
24	9	311	CLA	CBD-CGD-O2D-CED
24	h	601	CLA	CBD-CGD-O2D-CED
24	h	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	t	307	CLA	CBD-CGD-O2D-CED
24	k	301	CLA	CBD-CGD-O2D-CED
24	k	304	CLA	CBD-CGD-O2D-CED
24	k	311	CLA	CBD-CGD-O2D-CED
24	A	810	CLA	CBD-CGD-O2D-CED
24	A	813	CLA	CBD-CGD-O2D-CED
24	A	847	CLA	CBD-CGD-O2D-CED
24	B	813	CLA	CBD-CGD-O2D-CED
24	B	820	CLA	CBD-CGD-O2D-CED
24	B	846	CLA	CBD-CGD-O2D-CED
24	B	848	CLA	CBD-CGD-O2D-CED
24	F	201	CLA	CBD-CGD-O2D-CED
24	J	103	CLA	CBD-CGD-O2D-CED
24	L	205	CLA	CBD-CGD-O2D-CED
24	A	803	CLA	O1A-CGA-O2A-C1
24	A	804	CLA	O1A-CGA-O2A-C1
28	B	845	LHG	O10-C23-O8-C6
24	2	205	CLA	O1A-CGA-O2A-C1
24	2	208	CLA	O1A-CGA-O2A-C1
24	3	304	CLA	O1A-CGA-O2A-C1
24	5	605	CLA	O1A-CGA-O2A-C1
24	9	307	CLA	O1A-CGA-O2A-C1
24	9	310	CLA	O1A-CGA-O2A-C1
24	h	605	CLA	O1A-CGA-O2A-C1
24	c	603	CLA	O1A-CGA-O2A-C1
24	c	606	CLA	O1A-CGA-O2A-C1
24	t	305	CLA	O1A-CGA-O2A-C1
24	k	307	CLA	O1A-CGA-O2A-C1
24	1	303	CLA	O1D-CGD-O2D-CED
24	6	608	CLA	O1D-CGD-O2D-CED
24	c	601	CLA	O1D-CGD-O2D-CED
24	t	305	CLA	O1D-CGD-O2D-CED
27	A	854	LMT	O5B-C1B-O1B-C4'
24	9	304	CLA	CBA-CGA-O2A-C1
24	9	307	CLA	CBA-CGA-O2A-C1
24	h	605	CLA	CBA-CGA-O2A-C1
24	A	811	CLA	CBA-CGA-O2A-C1
24	B	832	CLA	C2C-C3C-CAC-CBC
24	1	305	CLA	O1D-CGD-O2D-CED
24	4	602	CLA	O1D-CGD-O2D-CED
24	F	201	CLA	O1D-CGD-O2D-CED
24	J	103	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	B	845	LHG	C24-C23-O8-C6
24	7	608	CLA	CBD-CGD-O2D-CED
24	B	817	CLA	CBD-CGD-O2D-CED
27	h	617	LMT	O5B-C1B-O1B-C4'
24	1	301	CLA	O1A-CGA-O2A-C1
24	6	602	CLA	O1A-CGA-O2A-C1
24	8	203	CLA	O1A-CGA-O2A-C1
24	c	608	CLA	O1A-CGA-O2A-C1
24	A	801	CLA	O1A-CGA-O2A-C1
24	A	831	CLA	O1A-CGA-O2A-C1
24	B	801	CLA	O1A-CGA-O2A-C1
24	B	821	CLA	O1A-CGA-O2A-C1
24	R	103	CLA	O1A-CGA-O2A-C1
24	4	611	CLA	O1A-CGA-O2A-C1
24	c	605	CLA	O1A-CGA-O2A-C1
24	k	302	CLA	O1A-CGA-O2A-C1
24	5	603	CLA	O1D-CGD-O2D-CED
24	9	304	CLA	O1D-CGD-O2D-CED
24	9	308	CLA	O1D-CGD-O2D-CED
24	t	302	CLA	O1D-CGD-O2D-CED
24	k	305	CLA	O1D-CGD-O2D-CED
24	3	305	CLA	O1D-CGD-O2D-CED
24	4	604	CLA	O1D-CGD-O2D-CED
24	7	610	CLA	O1D-CGD-O2D-CED
24	c	603	CLA	O1D-CGD-O2D-CED
24	t	308	CLA	O1D-CGD-O2D-CED
24	A	809	CLA	O1D-CGD-O2D-CED
24	A	820	CLA	O1D-CGD-O2D-CED
24	c	609	CLA	CBD-CGD-O2D-CED
28	A	841	LHG	O9-C7-O7-C5
28	L	201	LHG	O9-C7-O7-C5
30	2	214	LMG	O9-C10-O7-C8
24	4	609	CLA	CBA-CGA-O2A-C1
24	4	605	CLA	O1A-CGA-O2A-C1
24	4	612	CLA	O1A-CGA-O2A-C1
24	9	308	CLA	O1A-CGA-O2A-C1
24	h	608	CLA	O1A-CGA-O2A-C1
24	h	609	CLA	O1A-CGA-O2A-C1
24	c	607	CLA	O1A-CGA-O2A-C1
24	L	205	CLA	O1A-CGA-O2A-C1
24	h	602	CLA	C3-C5-C6-C7
24	A	806	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	A	822	CLA	C3-C5-C6-C7
24	A	832	CLA	C3-C5-C6-C7
24	A	847	CLA	C3-C5-C6-C7
24	B	837	CLA	C3-C5-C6-C7
24	B	848	CLA	C3-C5-C6-C7
24	h	602	CLA	O1D-CGD-O2D-CED
24	4	608	CLA	CBA-CGA-O2A-C1
24	c	608	CLA	CBA-CGA-O2A-C1
24	A	801	CLA	CBA-CGA-O2A-C1
24	A	803	CLA	CBA-CGA-O2A-C1
24	A	804	CLA	CBA-CGA-O2A-C1
24	A	818	CLA	CBA-CGA-O2A-C1
24	B	801	CLA	CBA-CGA-O2A-C1
24	B	831	CLA	CBA-CGA-O2A-C1
24	B	846	CLA	CBA-CGA-O2A-C1
24	R	103	CLA	CBA-CGA-O2A-C1
24	1	302	CLA	CBD-CGD-O2D-CED
24	1	308	CLA	CBD-CGD-O2D-CED
24	1	317	CLA	CBD-CGD-O2D-CED
24	3	301	CLA	CBD-CGD-O2D-CED
24	3	304	CLA	CBD-CGD-O2D-CED
24	6	610	CLA	CBD-CGD-O2D-CED
24	8	204	CLA	CBD-CGD-O2D-CED
24	8	206	CLA	CBD-CGD-O2D-CED
24	9	302	CLA	CBD-CGD-O2D-CED
24	9	307	CLA	CBD-CGD-O2D-CED
24	c	602	CLA	CBD-CGD-O2D-CED
24	c	605	CLA	CBD-CGD-O2D-CED
24	c	606	CLA	CBD-CGD-O2D-CED
24	c	611	CLA	CBD-CGD-O2D-CED
24	k	306	CLA	CBD-CGD-O2D-CED
24	A	808	CLA	CBD-CGD-O2D-CED
24	A	822	CLA	CBD-CGD-O2D-CED
24	A	828	CLA	CBD-CGD-O2D-CED
24	A	831	CLA	CBD-CGD-O2D-CED
24	B	815	CLA	CBD-CGD-O2D-CED
24	B	828	CLA	CBD-CGD-O2D-CED
24	B	837	CLA	CBD-CGD-O2D-CED
24	R	104	CLA	CBD-CGD-O2D-CED
28	A	841	LHG	C8-C7-O7-C5
24	4	608	CLA	O1D-CGD-O2D-CED
24	7	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	9	305	CLA	O1D-CGD-O2D-CED
24	h	604	CLA	O1D-CGD-O2D-CED
24	k	304	CLA	O1D-CGD-O2D-CED
24	B	809	CLA	O1D-CGD-O2D-CED
24	F	203	CLA	O1D-CGD-O2D-CED
24	7	605	CLA	O1A-CGA-O2A-C1
24	8	206	CLA	O1A-CGA-O2A-C1
24	k	304	CLA	O1A-CGA-O2A-C1
24	A	814	CLA	O1D-CGD-O2D-CED
24	2	202	CLA	C4-C3-C5-C6
24	4	602	CLA	C4-C3-C5-C6
24	B	833	CLA	C4-C3-C5-C6
24	2	202	CLA	C2-C3-C5-C6
24	4	602	CLA	C2-C3-C5-C6
24	t	303	CLA	C2-C3-C5-C6
24	B	830	CLA	C2-C3-C5-C6
24	B	833	CLA	C2-C3-C5-C6
24	4	605	CLA	CBA-CGA-O2A-C1
24	6	605	CLA	CBA-CGA-O2A-C1
24	6	606	CLA	CBA-CGA-O2A-C1
24	7	605	CLA	CBA-CGA-O2A-C1
24	7	612	CLA	CBA-CGA-O2A-C1
24	8	206	CLA	CBA-CGA-O2A-C1
24	9	308	CLA	CBA-CGA-O2A-C1
24	c	607	CLA	CBA-CGA-O2A-C1
24	k	304	CLA	CBA-CGA-O2A-C1
24	A	801	CLA	CBD-CGD-O2D-CED
24	h	601	CLA	O1D-CGD-O2D-CED
24	B	820	CLA	O1D-CGD-O2D-CED
24	A	838	CLA	C2A-CAA-CBA-CGA
24	A	823	CLA	O1A-CGA-O2A-C1
24	A	823	CLA	C3-C5-C6-C7
24	B	806	CLA	C3-C5-C6-C7
24	B	817	CLA	C3-C5-C6-C7
24	1	301	CLA	CBA-CGA-O2A-C1
24	6	602	CLA	CBA-CGA-O2A-C1
24	8	203	CLA	CBA-CGA-O2A-C1
24	A	822	CLA	CBA-CGA-O2A-C1
24	A	831	CLA	CBA-CGA-O2A-C1
24	A	853	CLA	CBA-CGA-O2A-C1
24	B	816	CLA	CBA-CGA-O2A-C1
24	B	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	828	CLA	CBA-CGA-O2A-C1
24	B	830	CLA	CBA-CGA-O2A-C1
28	J	105	LHG	C24-C23-O8-C6
24	4	609	CLA	O1A-CGA-O2A-C1
24	7	612	CLA	O1A-CGA-O2A-C1
24	A	818	CLA	O1A-CGA-O2A-C1
24	A	820	CLA	O1A-CGA-O2A-C1
24	A	822	CLA	O1A-CGA-O2A-C1
24	A	853	CLA	O1A-CGA-O2A-C1
24	B	828	CLA	O1A-CGA-O2A-C1
24	B	830	CLA	O1A-CGA-O2A-C1
24	B	831	CLA	O1A-CGA-O2A-C1
24	B	846	CLA	O1A-CGA-O2A-C1
24	B	848	CLA	O1A-CGA-O2A-C1
24	L	203	CLA	O1A-CGA-O2A-C1
28	J	105	LHG	O10-C23-O8-C6
28	I	103	LHG	O9-C7-O7-C5
24	4	612	CLA	CBA-CGA-O2A-C1
24	h	608	CLA	CBA-CGA-O2A-C1
24	h	609	CLA	CBA-CGA-O2A-C1
24	L	205	CLA	CBA-CGA-O2A-C1
27	1	315	LMT	C3'-C4'-O1B-C1B
24	6	606	CLA	O1A-CGA-O2A-C1
24	9	304	CLA	O1A-CGA-O2A-C1
24	A	811	CLA	O1A-CGA-O2A-C1
27	A	851	LMT	O5B-C5B-C6B-O6B
24	1	304	CLA	O1D-CGD-O2D-CED
24	k	301	CLA	O1D-CGD-O2D-CED
24	A	810	CLA	O1D-CGD-O2D-CED
24	A	829	CLA	C3-C5-C6-C7
24	6	602	CLA	CBD-CGD-O2D-CED
24	6	609	CLA	CBD-CGD-O2D-CED
24	8	203	CLA	CBD-CGD-O2D-CED
24	h	607	CLA	CBD-CGD-O2D-CED
24	t	304	CLA	CBD-CGD-O2D-CED
24	A	837	CLA	CBD-CGD-O2D-CED
24	B	806	CLA	CBD-CGD-O2D-CED
24	5	605	CLA	O1D-CGD-O2D-CED
24	8	207	CLA	O1D-CGD-O2D-CED
24	t	307	CLA	O1D-CGD-O2D-CED
24	k	311	CLA	O1D-CGD-O2D-CED
24	A	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	847	CLA	O1D-CGD-O2D-CED
27	A	854	LMT	O5B-C5B-C6B-O6B
24	B	848	CLA	O1D-CGD-O2D-CED
27	1	316	LMT	O5B-C5B-C6B-O6B
27	A	850	LMT	O5B-C5B-C6B-O6B
27	A	850	LMT	O5'-C5'-C6'-O6'
24	2	203	CLA	CBD-CGD-O2D-CED
24	A	834	CLA	CBD-CGD-O2D-CED
28	I	103	LHG	C8-C7-O7-C5
24	2	207	CLA	CBA-CGA-O2A-C1
24	3	308	CLA	CBA-CGA-O2A-C1
24	6	607	CLA	CBA-CGA-O2A-C1
24	9	309	CLA	CBA-CGA-O2A-C1
27	A	854	LMT	C4B-C5B-C6B-O6B
24	5	602	CLA	O1D-CGD-O2D-CED
24	7	611	CLA	O1D-CGD-O2D-CED
24	B	846	CLA	O1D-CGD-O2D-CED
24	A	816	CLA	C3-C5-C6-C7
24	6	603	CLA	CBD-CGD-O2D-CED
24	k	308	CLA	CBD-CGD-O2D-CED
24	A	835	CLA	CBD-CGD-O2D-CED
24	B	835	CLA	CBD-CGD-O2D-CED
24	7	602	CLA	O1D-CGD-O2D-CED
24	B	813	CLA	O1D-CGD-O2D-CED
24	A	805	CLA	CBA-CGA-O2A-C1
24	A	820	CLA	CBA-CGA-O2A-C1
24	A	823	CLA	CBA-CGA-O2A-C1
24	B	848	CLA	CBA-CGA-O2A-C1
24	L	203	CLA	CBA-CGA-O2A-C1
24	A	830	CLA	C4-C3-C5-C6
24	B	824	CLA	C4-C3-C5-C6
24	A	830	CLA	C2-C3-C5-C6
24	B	824	CLA	C2-C3-C5-C6
24	B	816	CLA	O1A-CGA-O2A-C1
27	3	314	LMT	O5'-C5'-C6'-O6'
24	h	605	CLA	CBD-CGD-O2D-CED
24	h	610	CLA	CBD-CGD-O2D-CED
24	B	826	CLA	C2A-CAA-CBA-CGA
28	3	315	LHG	C12-C13-C14-C15
24	8	209	CLA	O1D-CGD-O2D-CED
24	B	817	CLA	O1D-CGD-O2D-CED
30	2	214	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	A	850	LMT	C4'-C5'-C6'-O6'
27	h	617	LMT	C2B-C1B-O1B-C4'
24	6	609	CLA	CBA-CGA-O2A-C1
24	A	836	CLA	CBA-CGA-O2A-C1
24	F	203	CLA	CBA-CGA-O2A-C1
28	2	215	LHG	C24-C23-O8-C6
24	4	609	CLA	CBD-CGD-O2D-CED
24	5	606	CLA	CBD-CGD-O2D-CED
24	8	202	CLA	CBD-CGD-O2D-CED
24	A	812	CLA	CBD-CGD-O2D-CED
24	A	838	CLA	CBD-CGD-O2D-CED
24	B	818	CLA	CBD-CGD-O2D-CED
24	B	821	CLA	CBD-CGD-O2D-CED
24	B	822	CLA	CBD-CGD-O2D-CED
24	B	826	CLA	CBD-CGD-O2D-CED
24	B	834	CLA	CBD-CGD-O2D-CED
24	7	611	CLA	CBA-CGA-O2A-C1
27	A	851	LMT	C4B-C5B-C6B-O6B
24	8	205	CLA	CBD-CGD-O2D-CED
24	A	819	CLA	CBD-CGD-O2D-CED
24	6	605	CLA	O1A-CGA-O2A-C1
24	B	808	CLA	C3-C5-C6-C7
24	B	809	CLA	C3-C5-C6-C7
24	7	608	CLA	O1D-CGD-O2D-CED
24	c	609	CLA	O1D-CGD-O2D-CED
24	6	609	CLA	O1A-CGA-O2A-C1
24	A	805	CLA	O1A-CGA-O2A-C1
24	A	836	CLA	O1A-CGA-O2A-C1
28	2	215	LHG	O10-C23-O8-C6
28	3	315	LHG	C1-C2-C3-O3
28	8	213	LHG	C1-C2-C3-O3
28	L	201	LHG	C1-C2-C3-O3
24	7	602	CLA	CBA-CGA-O2A-C1
24	A	807	CLA	CBA-CGA-O2A-C1
24	A	810	CLA	CBA-CGA-O2A-C1
24	A	812	CLA	CBA-CGA-O2A-C1
24	A	814	CLA	CBA-CGA-O2A-C1
24	A	816	CLA	CBA-CGA-O2A-C1
24	A	840	CLA	CBA-CGA-O2A-C1
24	A	847	CLA	CBA-CGA-O2A-C1
24	B	811	CLA	CBA-CGA-O2A-C1
24	B	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	823	CLA	CBA-CGA-O2A-C1
24	B	838	CLA	CBA-CGA-O2A-C1
28	A	852	LHG	C24-C23-O8-C6
24	t	302	CLA	CBA-CGA-O2A-C1
24	A	832	CLA	CBD-CGD-O2D-CED
24	B	812	CLA	CBD-CGD-O2D-CED
27	1	315	LMT	C4'-C5'-C6'-O6'
24	1	302	CLA	O1D-CGD-O2D-CED
24	1	317	CLA	O1D-CGD-O2D-CED
24	c	606	CLA	O1D-CGD-O2D-CED
24	A	822	CLA	O1D-CGD-O2D-CED
27	A	850	LMT	C4B-C5B-C6B-O6B
24	F	201	CLA	C3-C5-C6-C7
24	1	301	CLA	C11-C10-C8-C9
24	2	204	CLA	C11-C10-C8-C9
24	3	301	CLA	C11-C10-C8-C9
24	3	301	CLA	C14-C13-C15-C16
24	7	606	CLA	C6-C7-C8-C9
24	c	609	CLA	C11-C10-C8-C9
24	A	816	CLA	C11-C12-C13-C14
24	A	817	CLA	C11-C10-C8-C9
24	A	829	CLA	C6-C7-C8-C9
24	A	857	CLA	C14-C13-C15-C16
24	B	803	CLA	C14-C13-C15-C16
24	B	818	CLA	C11-C10-C8-C9
24	B	823	CLA	C11-C12-C13-C14
24	B	827	CLA	C6-C7-C8-C9
24	B	831	CLA	C11-C12-C13-C14
24	B	836	CLA	C11-C12-C13-C14
24	F	201	CLA	C6-C7-C8-C9
24	A	808	CLA	O1D-CGD-O2D-CED
24	2	207	CLA	O1A-CGA-O2A-C1
24	4	607	CLA	CBA-CGA-O2A-C1
24	9	301	CLA	CBA-CGA-O2A-C1
28	B	844	LHG	O2-C2-C3-O3
28	L	201	LHG	O2-C2-C3-O3
24	3	304	CLA	O1D-CGD-O2D-CED
24	B	837	CLA	O1D-CGD-O2D-CED
24	A	812	CLA	O1A-CGA-O2A-C1
29	3	310	A1L1G	C14-C29-C30-C31
29	7	614	A1L1G	C14-C29-C30-C31
24	c	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	314	BCR	C37-C22-C23-C24
25	c	615	BCR	C36-C18-C19-C20
25	c	615	BCR	C37-C22-C23-C24
25	t	312	BCR	C7-C8-C9-C34
25	t	312	BCR	C37-C22-C23-C24
25	A	844	BCR	C36-C18-C19-C20
25	A	845	BCR	C7-C8-C9-C34
25	B	843	BCR	C7-C8-C9-C34
25	B	843	BCR	C37-C22-C23-C24
25	R	102	BCR	C7-C8-C9-C34
26	6	616	DD6	C12-C11-C13-C14
29	2	213	A1L1G	C32-C33-C34-C27
29	2	213	A1L1G	C28-C39-C40-C41
29	9	312	A1L1G	C28-C39-C40-C41
25	9	316	BCR	C7-C8-C9-C10
25	c	615	BCR	C21-C22-C23-C24
25	t	312	BCR	C7-C8-C9-C10
25	A	845	BCR	C7-C8-C9-C10
25	B	843	BCR	C7-C8-C9-C10
25	R	102	BCR	C7-C8-C9-C10
26	6	616	DD6	C10-C11-C13-C14
29	9	312	A1L1G	C38-C39-C40-C41
24	k	307	CLA	C2A-CAA-CBA-CGA
24	B	820	CLA	C2A-CAA-CBA-CGA
24	6	610	CLA	O1D-CGD-O2D-CED
24	7	602	CLA	O1A-CGA-O2A-C1
24	A	810	CLA	O1A-CGA-O2A-C1
24	A	816	CLA	O1A-CGA-O2A-C1
24	B	811	CLA	O1A-CGA-O2A-C1
24	B	812	CLA	O1A-CGA-O2A-C1
24	B	838	CLA	O1A-CGA-O2A-C1
27	1	315	LMT	O5'-C5'-C6'-O6'
27	1	316	LMT	C4B-C5B-C6B-O6B
28	3	315	LHG	C8-C7-O7-C5
24	4	604	CLA	CBA-CGA-O2A-C1
24	A	828	CLA	O1D-CGD-O2D-CED
24	3	301	CLA	O1D-CGD-O2D-CED
24	8	206	CLA	O1D-CGD-O2D-CED
24	9	307	CLA	O1D-CGD-O2D-CED
24	A	831	CLA	O1D-CGD-O2D-CED
24	B	828	CLA	O1D-CGD-O2D-CED
24	R	104	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	4	613	CLA	CBD-CGD-O2D-CED
24	B	834	CLA	C5-C6-C7-C8
24	L	204	CLA	C8-C10-C11-C12
24	R	103	CLA	C8-C10-C11-C12
28	A	849	LHG	C7-C8-C9-C10
24	k	306	CLA	O1D-CGD-O2D-CED
28	A	852	LHG	O10-C23-O8-C6
24	t	303	CLA	C8-C10-C11-C12
24	6	606	CLA	C2C-C3C-CAC-CBC
24	3	305	CLA	C11-C10-C8-C7
24	4	602	CLA	C6-C7-C8-C10
24	A	818	CLA	C12-C13-C15-C16
24	A	856	CLA	C11-C10-C8-C7
24	B	829	CLA	C11-C10-C8-C7
31	A	839	PQN	C22-C23-C25-C26
31	B	839	PQN	C17-C18-C20-C21
24	1	308	CLA	O1D-CGD-O2D-CED
24	B	810	CLA	CBA-CGA-O2A-C1
28	3	315	LHG	C11-C10-C9-C8
24	B	804	CLA	C5-C6-C7-C8
31	B	839	PQN	C23-C25-C26-C27
29	2	213	A1L1G	C40-C41-C42-C44
29	9	312	A1L1G	C40-C41-C42-C44
24	9	302	CLA	O1D-CGD-O2D-CED
24	c	605	CLA	O1D-CGD-O2D-CED
24	3	301	CLA	C3-C5-C6-C7
24	A	812	CLA	C8-C10-C11-C12
24	R	103	CLA	C10-C11-C12-C13
24	h	610	CLA	C2C-C3C-CAC-CBC
24	A	840	CLA	O1A-CGA-O2A-C1
24	9	309	CLA	O1A-CGA-O2A-C1
24	c	602	CLA	O1D-CGD-O2D-CED
24	B	815	CLA	O1D-CGD-O2D-CED
24	B	812	CLA	C5-C6-C7-C8
31	B	839	PQN	C25-C26-C27-C28
24	2	201	CLA	C2A-CAA-CBA-CGA
24	A	801	CLA	C2A-CAA-CBA-CGA
24	B	801	CLA	C2A-CAA-CBA-CGA
24	B	829	CLA	C2A-CAA-CBA-CGA
24	B	836	CLA	C2A-CAA-CBA-CGA
24	8	204	CLA	O1D-CGD-O2D-CED
24	1	304	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	806	CLA	C5-C6-C7-C8
24	B	812	CLA	C15-C16-C17-C18
28	3	315	LHG	C7-C8-C9-C10
24	A	807	CLA	O1A-CGA-O2A-C1
24	A	814	CLA	O1A-CGA-O2A-C1
24	A	847	CLA	O1A-CGA-O2A-C1
24	B	823	CLA	O1A-CGA-O2A-C1
24	B	801	CLA	C3-C5-C6-C7
24	A	827	CLA	CBD-CGD-O2D-CED
24	B	832	CLA	CBD-CGD-O2D-CED
24	A	810	CLA	C8-C10-C11-C12
24	B	805	CLA	C15-C16-C17-C18
24	B	833	CLA	C5-C6-C7-C8
28	1	318	LHG	C13-C14-C15-C16
28	1	318	LHG	O2-C2-C3-O3
28	3	315	LHG	O2-C2-C3-O3
28	8	213	LHG	O2-C2-C3-O3
24	5	607	CLA	CBD-CGD-O2D-CED
24	t	309	CLA	CBD-CGD-O2D-CED
24	A	815	CLA	CBD-CGD-O2D-CED
24	F	203	CLA	O1A-CGA-O2A-C1
28	8	213	LHG	C23-C24-C25-C26
24	A	807	CLA	C8-C10-C11-C12
24	B	801	CLA	C5-C6-C7-C8
24	B	812	CLA	C8-C10-C11-C12
24	6	607	CLA	O1A-CGA-O2A-C1
24	A	840	CLA	C5-C6-C7-C8
24	L	203	CLA	C2C-C3C-CAC-CBC
24	9	309	CLA	CBD-CGD-O2D-CED
24	6	602	CLA	O1D-CGD-O2D-CED
24	6	609	CLA	O1D-CGD-O2D-CED
24	h	607	CLA	O1D-CGD-O2D-CED
24	t	304	CLA	O1D-CGD-O2D-CED
24	A	837	CLA	O1D-CGD-O2D-CED
24	A	805	CLA	C8-C10-C11-C12
24	B	802	CLA	C13-C15-C16-C17
24	B	827	CLA	C15-C16-C17-C18
24	B	837	CLA	CBA-CGA-O2A-C1
24	c	604	CLA	CBD-CGD-O2D-CED
24	t	301	CLA	CBD-CGD-O2D-CED
24	A	853	CLA	CBD-CGD-O2D-CED
28	2	215	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
24	B	806	CLA	O1D-CGD-O2D-CED
24	9	303	CLA	CBA-CGA-O2A-C1
24	B	819	CLA	CBA-CGA-O2A-C1
24	3	308	CLA	O1A-CGA-O2A-C1
24	1	317	CLA	C3-C5-C6-C7
24	B	831	CLA	C3-C5-C6-C7
24	h	611	CLA	CBD-CGD-O2D-CED
24	A	828	CLA	C13-C15-C16-C17
28	2	215	LHG	O9-C7-O7-C5
28	3	315	LHG	O9-C7-O7-C5
24	B	805	CLA	CBA-CGA-O2A-C1
24	B	822	CLA	CBA-CGA-O2A-C1
24	B	826	CLA	CBA-CGA-O2A-C1
24	1	317	CLA	C10-C11-C12-C13
24	A	806	CLA	C15-C16-C17-C18
24	B	808	CLA	C13-C15-C16-C17
24	B	824	CLA	C5-C6-C7-C8
24	B	834	CLA	C13-C15-C16-C17
24	B	836	CLA	C13-C15-C16-C17
24	B	837	CLA	C10-C11-C12-C13
24	A	836	CLA	CBD-CGD-O2D-CED
24	B	810	CLA	O1A-CGA-O2A-C1
24	A	807	CLA	C15-C16-C17-C18
24	A	813	CLA	C15-C16-C17-C18
24	B	822	CLA	C10-C11-C12-C13
24	B	822	CLA	C13-C15-C16-C17
24	7	606	CLA	C2C-C3C-CAC-CBC
24	2	207	CLA	CBD-CGD-O2D-CED
27	1	315	LMT	O5B-C5B-C6B-O6B
24	3	306	CLA	C15-C16-C17-C18
24	A	807	CLA	C5-C6-C7-C8
24	A	813	CLA	C5-C6-C7-C8
24	B	810	CLA	C5-C6-C7-C8
24	B	831	CLA	C15-C16-C17-C18
24	B	811	CLA	C4-C3-C5-C6
24	B	815	CLA	C4-C3-C5-C6
24	8	203	CLA	O1D-CGD-O2D-CED
24	A	834	CLA	O1D-CGD-O2D-CED
24	A	835	CLA	O1D-CGD-O2D-CED
24	B	835	CLA	O1D-CGD-O2D-CED
27	A	851	LMT	C2'-C1'-O1'-C1
30	A	855	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
24	k	301	CLA	CBA-CGA-O2A-C1
29	2	213	A1L1G	C14-C29-C30-C31
26	4	616	DD6	C9-C10-C11-C12
26	6	615	DD6	C9-C10-C11-C12
26	7	618	DD6	C9-C10-C11-C12
26	8	212	DD6	C9-C10-C11-C12
26	9	313	DD6	C9-C10-C11-C12
26	R	105	DD6	C9-C10-C11-C12
29	2	213	A1L1G	C41-C42-C44-C43
29	3	310	A1L1G	C41-C42-C44-C43
29	7	614	A1L1G	C27-C34-C35-C36
29	9	312	A1L1G	C41-C42-C44-C43
29	k	312	A1L1G	C41-C42-C44-C43
24	L	203	CLA	C4C-C3C-CAC-CBC
24	A	836	CLA	C13-C15-C16-C17
25	1	314	BCR	C7-C8-C9-C34
25	A	845	BCR	C11-C12-C13-C35
24	h	606	CLA	C2C-C3C-CAC-CBC
25	1	314	BCR	C7-C8-C9-C10
25	t	312	BCR	C21-C22-C23-C24
24	B	805	CLA	O1A-CGA-O2A-C1
24	A	804	CLA	C2A-CAA-CBA-CGA
24	A	812	CLA	C2A-CAA-CBA-CGA
24	A	828	CLA	C2A-CAA-CBA-CGA
24	B	813	CLA	C2A-CAA-CBA-CGA
24	k	306	CLA	CBA-CGA-O2A-C1
24	B	823	CLA	C13-C15-C16-C17
28	3	315	LHG	O1-C1-C2-C3
28	8	213	LHG	O1-C1-C2-C3
24	B	817	CLA	O2A-C1-C2-C3
24	7	611	CLA	O1A-CGA-O2A-C1
29	3	310	A1L1G	C29-C30-C31-C32
24	A	803	CLA	C6-C7-C8-C9
24	A	830	CLA	C6-C7-C8-C10
24	2	203	CLA	O1D-CGD-O2D-CED
24	A	812	CLA	C10-C11-C12-C13
26	4	616	DD6	C9-C10-C11-C13
26	5	608	DD6	C9-C10-C11-C13
26	6	615	DD6	C9-C10-C11-C13
26	7	615	DD6	C9-C10-C11-C13
26	7	618	DD6	C9-C10-C11-C13
26	9	313	DD6	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
26	R	105	DD6	C9-C10-C11-C13
29	2	213	A1L1G	C41-C42-C44-C2
29	3	310	A1L1G	C37-C38-C39-C40
29	3	310	A1L1G	C41-C42-C44-C2
29	7	614	A1L1G	C33-C34-C35-C36
29	9	312	A1L1G	C41-C42-C44-C2
29	k	312	A1L1G	C41-C42-C44-C2
27	A	851	LMT	O5'-C1'-O1'-C1
24	h	605	CLA	O1D-CGD-O2D-CED
24	h	610	CLA	O1D-CGD-O2D-CED
24	6	603	CLA	O1D-CGD-O2D-CED
24	k	308	CLA	O1D-CGD-O2D-CED
24	A	801	CLA	O1D-CGD-O2D-CED
24	B	820	CLA	CBA-CGA-O2A-C1
28	4	619	LHG	C24-C23-O8-C6
24	A	823	CLA	C13-C15-C16-C17
24	A	827	CLA	C8-C10-C11-C12
24	B	827	CLA	C13-C15-C16-C17
24	t	310	CLA	CBD-CGD-O2D-CED
24	A	804	CLA	C2-C1-O2A-CGA
24	B	804	CLA	C2-C1-O2A-CGA
24	B	809	CLA	C2-C1-O2A-CGA
24	h	602	CLA	C6-C7-C8-C10
24	A	823	CLA	C16-C17-C18-C19
24	B	820	CLA	C6-C7-C8-C10
24	B	837	CLA	O1A-CGA-O2A-C1
24	2	209	CLA	CBA-CGA-O2A-C1
24	4	603	CLA	CBA-CGA-O2A-C1
24	9	302	CLA	CBA-CGA-O2A-C1
27	A	854	LMT	C2B-C1B-O1B-C4'
24	5	606	CLA	O1D-CGD-O2D-CED
28	A	841	LHG	C24-C25-C26-C27
27	h	617	LMT	C2-C1-O1'-C1'
24	4	609	CLA	O1D-CGD-O2D-CED
24	B	818	CLA	O1D-CGD-O2D-CED
24	B	834	CLA	O1D-CGD-O2D-CED
24	1	308	CLA	C4B-C3B-CAB-CBB
24	3	302	CLA	C4B-C3B-CAB-CBB
24	4	605	CLA	C4B-C3B-CAB-CBB
24	6	609	CLA	C4B-C3B-CAB-CBB
24	6	612	CLA	C4B-C3B-CAB-CBB
24	8	207	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	B	803	CLA	C4B-C3B-CAB-CBB
24	B	821	CLA	C4B-C3B-CAB-CBB
24	B	828	CLA	C4B-C3B-CAB-CBB
24	B	837	CLA	C4B-C3B-CAB-CBB
24	B	838	CLA	C4B-C3B-CAB-CBB
24	L	204	CLA	C4B-C3B-CAB-CBB
28	3	315	LHG	C16-C17-C18-C19
24	4	606	CLA	CBA-CGA-O2A-C1
24	t	310	CLA	CBA-CGA-O2A-C1
24	h	602	CLA	C6-C7-C8-C9
24	A	823	CLA	C16-C17-C18-C20
24	B	804	CLA	C16-C17-C18-C19
24	B	822	CLA	C16-C17-C18-C20
24	B	822	CLA	O1D-CGD-O2D-CED
24	B	822	CLA	O1A-CGA-O2A-C1
24	1	305	CLA	C2A-CAA-CBA-CGA
31	B	839	PQN	C15-C16-C17-C18
28	8	213	LHG	C8-C7-O7-C5
27	A	850	LMT	C1-C2-C3-C4
28	1	318	LHG	C15-C16-C17-C18
24	t	302	CLA	O1A-CGA-O2A-C1
24	1	303	CLA	C3A-C2A-CAA-CBA
24	1	305	CLA	C3A-C2A-CAA-CBA
24	1	308	CLA	C3A-C2A-CAA-CBA
24	2	201	CLA	C3A-C2A-CAA-CBA
24	3	304	CLA	C3A-C2A-CAA-CBA
24	3	306	CLA	C3A-C2A-CAA-CBA
24	4	601	CLA	C3A-C2A-CAA-CBA
24	4	611	CLA	C3A-C2A-CAA-CBA
24	6	607	CLA	C3A-C2A-CAA-CBA
24	6	609	CLA	C3A-C2A-CAA-CBA
24	7	609	CLA	C3A-C2A-CAA-CBA
24	7	611	CLA	C3A-C2A-CAA-CBA
24	8	202	CLA	C3A-C2A-CAA-CBA
24	9	305	CLA	C3A-C2A-CAA-CBA
24	9	307	CLA	C3A-C2A-CAA-CBA
24	9	309	CLA	C3A-C2A-CAA-CBA
24	h	603	CLA	C3A-C2A-CAA-CBA
24	h	612	CLA	C3A-C2A-CAA-CBA
24	c	605	CLA	C3A-C2A-CAA-CBA
24	c	608	CLA	C3A-C2A-CAA-CBA
24	c	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	k	303	CLA	C3A-C2A-CAA-CBA
24	k	303	CLA	C4-C3-C5-C6
24	k	305	CLA	C3A-C2A-CAA-CBA
24	k	311	CLA	C3A-C2A-CAA-CBA
24	A	801	CLA	C3A-C2A-CAA-CBA
24	A	805	CLA	C3A-C2A-CAA-CBA
24	A	831	CLA	C3A-C2A-CAA-CBA
24	B	810	CLA	C3A-C2A-CAA-CBA
24	B	836	CLA	C3A-C2A-CAA-CBA
24	B	848	CLA	C3A-C2A-CAA-CBA
24	F	201	CLA	C3A-C2A-CAA-CBA
24	B	821	CLA	O1D-CGD-O2D-CED
24	B	826	CLA	O1D-CGD-O2D-CED
24	3	305	CLA	C11-C12-C13-C15
24	7	606	CLA	C11-C12-C13-C15
24	B	804	CLA	C16-C17-C18-C20
24	B	822	CLA	C16-C17-C18-C19
24	B	814	CLA	CBA-CGA-O2A-C1
24	7	606	CLA	C3-C5-C6-C7
24	A	813	CLA	C3-C5-C6-C7
24	A	820	CLA	C3-C5-C6-C7
24	B	807	CLA	C3-C5-C6-C7
24	B	830	CLA	C3-C5-C6-C7
28	3	315	LHG	C17-C18-C19-C20
27	3	314	LMT	C4'-C5'-C6'-O6'
27	h	617	LMT	C1-C2-C3-C4
24	A	812	CLA	O1D-CGD-O2D-CED
24	A	838	CLA	O1D-CGD-O2D-CED
28	I	103	LHG	C25-C26-C27-C28
24	B	826	CLA	O1A-CGA-O2A-C1
24	3	302	CLA	C2B-C3B-CAB-CBB
24	4	605	CLA	C2B-C3B-CAB-CBB
24	6	609	CLA	C2B-C3B-CAB-CBB
24	6	612	CLA	C2B-C3B-CAB-CBB
24	8	207	CLA	C2B-C3B-CAB-CBB
24	9	306	CLA	C2B-C3B-CAB-CBB
24	A	801	CLA	C2B-C3B-CAB-CBB
24	A	812	CLA	C2B-C3B-CAB-CBB
24	A	836	CLA	C2B-C3B-CAB-CBB
25	1	314	BCR	C1-C6-C7-C8
25	2	211	BCR	C23-C24-C25-C26
25	2	211	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	c	615	BCR	C23-C24-C25-C26
25	c	615	BCR	C23-C24-C25-C30
25	A	843	BCR	C5-C6-C7-C8
25	A	843	BCR	C23-C24-C25-C26
25	A	846	BCR	C1-C6-C7-C8
25	B	840	BCR	C1-C6-C7-C8
25	B	840	BCR	C23-C24-C25-C30
25	B	841	BCR	C23-C24-C25-C30
25	B	849	BCR	C1-C6-C7-C8
25	B	849	BCR	C5-C6-C7-C8
25	B	849	BCR	C23-C24-C25-C30
25	I	101	BCR	C1-C6-C7-C8
25	I	101	BCR	C23-C24-C25-C30
25	J	101	BCR	C1-C6-C7-C8
25	L	202	BCR	C23-C24-C25-C26
25	L	202	BCR	C23-C24-C25-C30
25	L	206	BCR	C1-C6-C7-C8
25	L	206	BCR	C5-C6-C7-C8
25	R	101	BCR	C1-C6-C7-C8
25	R	101	BCR	C23-C24-C25-C26
25	R	101	BCR	C23-C24-C25-C30
25	R	102	BCR	C1-C6-C7-C8
24	2	208	CLA	CBD-CGD-O2D-CED
24	4	607	CLA	O1A-CGA-O2A-C1
24	8	202	CLA	O1D-CGD-O2D-CED
27	1	316	LMT	C6-C7-C8-C9
27	1	315	LMT	C1-C2-C3-C4
24	5	602	CLA	C2A-CAA-CBA-CGA
24	h	608	CLA	C2A-CAA-CBA-CGA
28	J	105	LHG	C23-C24-C25-C26
24	B	807	CLA	C15-C16-C17-C18
24	B	820	CLA	O1A-CGA-O2A-C1
24	9	301	CLA	O1A-CGA-O2A-C1
27	A	850	LMT	C4-C5-C6-C7
27	h	617	LMT	C4B-C5B-C6B-O6B
28	8	213	LHG	O9-C7-O7-C5
24	k	303	CLA	C2-C3-C5-C6
24	B	811	CLA	C2-C3-C5-C6
24	B	815	CLA	C2-C3-C5-C6
28	8	213	LHG	C11-C12-C13-C14
24	4	608	CLA	C2C-C3C-CAC-CBC
24	c	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	9	305	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	C14-C13-C15-C16
24	A	813	CLA	C10-C11-C12-C13
27	h	617	LMT	O5'-C5'-C6'-O6'
27	3	314	LMT	C2'-C1'-O1'-C1
24	c	602	CLA	C15-C16-C17-C18
27	3	314	LMT	C1-C2-C3-C4
28	B	844	LHG	C8-C7-O7-C5
24	A	826	CLA	C10-C11-C12-C13
24	B	817	CLA	C10-C11-C12-C13
24	4	604	CLA	O1A-CGA-O2A-C1
25	2	211	BCR	C37-C22-C23-C24
28	B	845	LHG	C33-C34-C35-C36
24	6	612	CLA	C2A-CAA-CBA-CGA
24	9	308	CLA	C2A-CAA-CBA-CGA
24	1	304	CLA	C6-C7-C8-C9
24	1	304	CLA	C6-C7-C8-C10
24	7	606	CLA	C11-C12-C13-C14
24	A	806	CLA	C16-C17-C18-C19
24	A	806	CLA	C16-C17-C18-C20
24	A	830	CLA	C6-C7-C8-C9
24	A	856	CLA	CBD-CGD-O2D-CED
28	4	619	LHG	O10-C23-O8-C6
24	B	807	CLA	C5-C6-C7-C8
24	B	814	CLA	O1A-CGA-O2A-C1
28	I	103	LHG	C28-C29-C30-C31
27	h	617	LMT	O5B-C5B-C6B-O6B
24	B	816	CLA	C3-C5-C6-C7
28	B	844	LHG	O7-C5-C6-O8
24	A	832	CLA	O1D-CGD-O2D-CED
28	3	315	LHG	C28-C29-C30-C31
24	A	813	CLA	C13-C15-C16-C17
24	A	819	CLA	O1D-CGD-O2D-CED
27	1	315	LMT	C7-C8-C9-C10
24	c	604	CLA	CBA-CGA-O2A-C1
27	A	850	LMT	C6-C7-C8-C9
24	3	301	CLA	C16-C17-C18-C20
24	A	803	CLA	C6-C7-C8-C10
24	A	825	CLA	C15-C16-C17-C18
28	3	315	LHG	C26-C27-C28-C29
28	B	844	LHG	O9-C7-O7-C5
24	4	605	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	9	307	CLA	C2A-CAA-CBA-CGA
24	B	807	CLA	C2A-CAA-CBA-CGA
24	8	205	CLA	O1D-CGD-O2D-CED
24	A	831	CLA	C15-C16-C17-C18
24	B	806	CLA	C5-C6-C7-C8
28	A	842	LHG	C8-C7-O7-C5
24	3	305	CLA	C11-C12-C13-C14
24	1	305	CLA	C1A-C2A-CAA-CBA
24	2	202	CLA	C1A-C2A-CAA-CBA
24	2	206	CLA	C1A-C2A-CAA-CBA
24	3	304	CLA	C1A-C2A-CAA-CBA
24	3	307	CLA	C1A-C2A-CAA-CBA
24	4	601	CLA	C1A-C2A-CAA-CBA
24	4	604	CLA	C1A-C2A-CAA-CBA
24	4	611	CLA	C1A-C2A-CAA-CBA
24	5	605	CLA	C1A-C2A-CAA-CBA
24	6	607	CLA	C1A-C2A-CAA-CBA
24	6	609	CLA	C1A-C2A-CAA-CBA
24	6	610	CLA	C1A-C2A-CAA-CBA
24	7	609	CLA	C1A-C2A-CAA-CBA
24	8	202	CLA	C1A-C2A-CAA-CBA
24	9	305	CLA	C1A-C2A-CAA-CBA
24	9	309	CLA	C1A-C2A-CAA-CBA
24	h	603	CLA	C1A-C2A-CAA-CBA
24	h	612	CLA	C1A-C2A-CAA-CBA
24	c	605	CLA	C1A-C2A-CAA-CBA
24	t	307	CLA	C1A-C2A-CAA-CBA
24	k	302	CLA	C1A-C2A-CAA-CBA
24	k	303	CLA	C1A-C2A-CAA-CBA
24	k	311	CLA	C1A-C2A-CAA-CBA
24	A	801	CLA	C1A-C2A-CAA-CBA
24	A	803	CLA	C1A-C2A-CAA-CBA
24	A	805	CLA	C1A-C2A-CAA-CBA
24	A	807	CLA	C1A-C2A-CAA-CBA
24	A	810	CLA	C1A-C2A-CAA-CBA
24	A	811	CLA	C1A-C2A-CAA-CBA
24	A	824	CLA	C1A-C2A-CAA-CBA
24	A	853	CLA	C1A-C2A-CAA-CBA
24	B	805	CLA	C1A-C2A-CAA-CBA
24	B	815	CLA	C1A-C2A-CAA-CBA
24	B	818	CLA	C1A-C2A-CAA-CBA
24	B	820	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	821	CLA	C1A-C2A-CAA-CBA
24	B	828	CLA	C1A-C2A-CAA-CBA
24	B	832	CLA	C1A-C2A-CAA-CBA
24	B	846	CLA	C1A-C2A-CAA-CBA
24	B	847	CLA	C1A-C2A-CAA-CBA
24	B	848	CLA	C1A-C2A-CAA-CBA
24	L	204	CLA	C1A-C2A-CAA-CBA
24	R	103	CLA	C1A-C2A-CAA-CBA
24	c	602	CLA	O1A-CGA-O2A-C1
27	1	315	LMT	C3-C4-C5-C6
28	A	842	LHG	O6-C4-C5-C6
24	1	301	CLA	C6-C7-C8-C10
24	1	301	CLA	C11-C10-C8-C7
24	2	204	CLA	C6-C7-C8-C10
24	2	204	CLA	C11-C10-C8-C7
24	7	606	CLA	C6-C7-C8-C10
24	A	805	CLA	C11-C12-C13-C15
24	A	823	CLA	C12-C13-C15-C16
24	A	825	CLA	C11-C10-C8-C7
24	A	827	CLA	C11-C10-C8-C7
24	A	827	CLA	C12-C13-C15-C16
24	A	832	CLA	C6-C7-C8-C10
24	A	857	CLA	C11-C12-C13-C15
24	B	805	CLA	C11-C10-C8-C7
24	B	817	CLA	C6-C7-C8-C10
24	B	818	CLA	C11-C10-C8-C7
24	B	827	CLA	C11-C10-C8-C7
31	A	839	PQN	C17-C18-C20-C21
24	A	807	CLA	C16-C17-C18-C20
24	B	847	CLA	C15-C16-C17-C18
28	3	315	LHG	C27-C28-C29-C30
24	3	301	CLA	C4-C3-C5-C6
24	A	826	CLA	C4-C3-C5-C6
24	A	828	CLA	C2-C3-C5-C6
24	9	303	CLA	O1A-CGA-O2A-C1
28	A	849	LHG	C27-C28-C29-C30
24	A	826	CLA	C15-C16-C17-C18
24	A	807	CLA	C2A-CAA-CBA-CGA
24	B	837	CLA	C2A-CAA-CBA-CGA
24	c	602	CLA	C11-C10-C8-C9
24	A	817	CLA	C14-C13-C15-C16
24	A	824	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	827	CLA	C14-C13-C15-C16
24	A	828	CLA	C14-C13-C15-C16
24	B	801	CLA	C14-C13-C15-C16
24	B	805	CLA	C11-C10-C8-C9
24	B	817	CLA	C6-C7-C8-C9
24	B	827	CLA	C11-C10-C8-C9
24	B	847	CLA	C14-C13-C15-C16
24	L	204	CLA	C11-C12-C13-C14
24	R	103	CLA	C11-C12-C13-C14
28	A	842	LHG	C15-C16-C17-C18
24	5	602	CLA	CBA-CGA-O2A-C1
24	A	832	CLA	CBA-CGA-O2A-C1
24	B	824	CLA	CBA-CGA-O2A-C1
30	2	214	LMG	C29-C28-O8-C9
24	B	812	CLA	O1D-CGD-O2D-CED
24	A	837	CLA	C3-C5-C6-C7
24	B	838	CLA	C15-C16-C17-C18
24	A	829	CLA	CBA-CGA-O2A-C1
24	A	807	CLA	C16-C17-C18-C19
24	B	803	CLA	C2C-C3C-CAC-CBC
24	B	819	CLA	O1A-CGA-O2A-C1
26	h	614	DD6	C9-C10-C11-C12
24	A	828	CLA	C4-C3-C5-C6
24	c	601	CLA	C2C-C3C-CAC-CBC
24	3	301	CLA	C2-C3-C5-C6
24	A	818	CLA	C2-C3-C5-C6
24	A	826	CLA	C2-C3-C5-C6
24	B	802	CLA	C2-C3-C5-C6
24	3	301	CLA	C16-C17-C18-C19
29	2	213	A1L1G	C32-C33-C34-C35
24	1	301	CLA	C8-C10-C11-C12
24	A	832	CLA	O1A-CGA-O2A-C1
24	4	613	CLA	O1D-CGD-O2D-CED
24	A	804	CLA	O2A-C1-C2-C3
24	A	827	CLA	O2A-C1-C2-C3
24	L	204	CLA	C10-C11-C12-C13
25	4	618	BCR	C15-C16-C17-C18
27	1	315	LMT	C5'-C4'-O1B-C1B
24	A	810	CLA	C13-C15-C16-C17
26	8	212	DD6	C9-C10-C11-C13
26	h	614	DD6	C9-C10-C11-C13
24	B	821	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	A	841	LHG	O6-C4-C5-O7
24	A	827	CLA	O1D-CGD-O2D-CED
24	B	832	CLA	O1D-CGD-O2D-CED
24	h	610	CLA	C4C-C3C-CAC-CBC
24	B	837	CLA	C4-C3-C5-C6
24	A	820	CLA	C2-C3-C5-C6
24	B	817	CLA	C16-C17-C18-C20
30	t	314	LMG	O1-C7-C8-O7
28	L	201	LHG	C24-C23-O8-C6
28	A	849	LHG	C33-C34-C35-C36
30	2	214	LMG	C33-C34-C35-C36
24	5	607	CLA	O1D-CGD-O2D-CED
24	A	815	CLA	O1D-CGD-O2D-CED
24	t	302	CLA	C2A-CAA-CBA-CGA
24	B	830	CLA	C10-C11-C12-C13
26	k	315	DD6	C11-C13-C14-C15
24	B	824	CLA	O1A-CGA-O2A-C1
28	3	315	LHG	C24-C23-O8-C6
24	h	604	CLA	CBA-CGA-O2A-C1
29	9	312	A1L1G	C35-C36-C37-C38
27	1	316	LMT	C5-C6-C7-C8
24	9	309	CLA	O1D-CGD-O2D-CED
24	c	604	CLA	O1D-CGD-O2D-CED
24	t	309	CLA	O1D-CGD-O2D-CED
24	k	301	CLA	O1A-CGA-O2A-C1
24	A	805	CLA	C4-C3-C5-C6
24	A	820	CLA	C4-C3-C5-C6
24	B	802	CLA	C4-C3-C5-C6
31	B	839	PQN	C14-C13-C15-C16
24	B	812	CLA	C13-C15-C16-C17
26	3	313	DD6	C27-C29-C30-C31
26	4	614	DD6	C27-C29-C30-C31
26	7	618	DD6	C27-C29-C30-C31
26	h	615	DD6	C27-C29-C30-C31
26	h	616	DD6	C27-C29-C30-C31
26	A	848	DD6	C27-C29-C30-C31
26	J	102	DD6	C27-C29-C30-C31
27	1	315	LMT	C2-C1-O1'-C1'
24	k	306	CLA	O1A-CGA-O2A-C1
24	2	204	CLA	C6-C7-C8-C9
24	c	608	CLA	C11-C10-C8-C9
24	A	805	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	A	818	CLA	C14-C13-C15-C16
24	A	823	CLA	C11-C10-C8-C9
24	A	825	CLA	C11-C10-C8-C9
24	A	832	CLA	C6-C7-C8-C9
24	A	857	CLA	C11-C10-C8-C9
24	A	857	CLA	C11-C12-C13-C14
24	B	803	CLA	C11-C12-C13-C14
31	A	839	PQN	C19-C18-C20-C21
24	h	611	CLA	O1D-CGD-O2D-CED
28	L	201	LHG	C5-C4-O6-P
24	A	829	CLA	O1A-CGA-O2A-C1
24	1	304	CLA	C4B-C3B-CAB-CBB
24	6	602	CLA	C4B-C3B-CAB-CBB
24	7	612	CLA	C4B-C3B-CAB-CBB
24	8	204	CLA	C4B-C3B-CAB-CBB
24	9	306	CLA	C4B-C3B-CAB-CBB
24	h	601	CLA	C4B-C3B-CAB-CBB
24	k	304	CLA	C4B-C3B-CAB-CBB
24	A	819	CLA	C4B-C3B-CAB-CBB
24	B	801	CLA	C4B-C3B-CAB-CBB
24	9	305	CLA	CAA-CBA-CGA-O2A
24	A	840	CLA	C13-C15-C16-C17
24	B	818	CLA	C13-C15-C16-C17
24	7	609	CLA	CBA-CGA-O2A-C1
24	k	303	CLA	C6-C7-C8-C10
24	B	810	CLA	CAA-CBA-CGA-O2A
24	3	306	CLA	C12-C13-C15-C16
24	c	602	CLA	C11-C10-C8-C7
24	c	608	CLA	C11-C10-C8-C7
24	t	303	CLA	C11-C10-C8-C7
24	t	303	CLA	C11-C12-C13-C15
24	A	812	CLA	C11-C10-C8-C7
24	A	816	CLA	C11-C12-C13-C15
24	A	823	CLA	C11-C10-C8-C7
24	A	824	CLA	C11-C10-C8-C7
24	A	824	CLA	C11-C12-C13-C15
24	A	828	CLA	C12-C13-C15-C16
24	A	840	CLA	C12-C13-C15-C16
24	A	857	CLA	C11-C10-C8-C7
24	A	857	CLA	C12-C13-C15-C16
24	A	860	CLA	C11-C10-C8-C7
24	B	801	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	818	CLA	C11-C12-C13-C15
24	B	831	CLA	C11-C12-C13-C15
24	B	836	CLA	C11-C10-C8-C7
24	B	847	CLA	C12-C13-C15-C16
24	L	204	CLA	C11-C12-C13-C15
24	R	103	CLA	C11-C12-C13-C15
24	t	303	CLA	C10-C11-C12-C13
24	5	602	CLA	O1A-CGA-O2A-C1
28	L	201	LHG	C26-C27-C28-C29
24	4	603	CLA	O1A-CGA-O2A-C1
24	9	302	CLA	O1A-CGA-O2A-C1
24	4	608	CLA	C4C-C3C-CAC-CBC
30	2	214	LMG	O10-C28-O8-C9
24	8	206	CLA	C3A-C2A-CAA-CBA
24	h	610	CLA	C3A-C2A-CAA-CBA
24	A	818	CLA	C4-C3-C5-C6
24	A	824	CLA	C3A-C2A-CAA-CBA
24	B	816	CLA	C3A-C2A-CAA-CBA
24	B	825	CLA	C3A-C2A-CAA-CBA
24	B	832	CLA	C3A-C2A-CAA-CBA
24	L	204	CLA	C3A-C2A-CAA-CBA
24	3	301	CLA	C10-C11-C12-C13
24	t	301	CLA	O1D-CGD-O2D-CED
24	2	207	CLA	O1D-CGD-O2D-CED
24	4	602	CLA	CBA-CGA-O2A-C1
29	k	312	A1L1G	C40-C41-C42-C44
24	A	853	CLA	O1D-CGD-O2D-CED
25	A	844	BCR	C7-C8-C9-C34
25	M	101	BCR	C11-C12-C13-C35
28	8	213	LHG	C24-C25-C26-C27
24	t	310	CLA	O1D-CGD-O2D-CED
28	3	315	LHG	C4-C5-C6-O8
28	B	844	LHG	C4-C5-C6-O8
28	I	103	LHG	C4-C5-C6-O8
30	t	314	LMG	O1-C7-C8-C9
24	k	303	CLA	C6-C7-C8-C9
24	B	817	CLA	C16-C17-C18-C19
24	A	838	CLA	C13-C15-C16-C17
30	t	314	LMG	C29-C30-C31-C32
28	B	844	LHG	C10-C11-C12-C13
24	A	847	CLA	C4-C3-C5-C6
24	L	203	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	A	836	CLA	O1D-CGD-O2D-CED
24	B	802	CLA	CBA-CGA-O2A-C1
24	A	805	CLA	C2-C3-C5-C6
24	4	606	CLA	O1A-CGA-O2A-C1
24	A	832	CLA	C16-C17-C18-C19
28	A	842	LHG	O9-C7-O7-C5
24	6	607	CLA	C2B-C3B-CAB-CBB
24	h	608	CLA	C2B-C3B-CAB-CBB
24	B	801	CLA	C2B-C3B-CAB-CBB
24	B	818	CLA	C2B-C3B-CAB-CBB
25	k	316	BCR	C1-C6-C7-C8
25	A	843	BCR	C23-C24-C25-C30
25	A	859	BCR	C5-C6-C7-C8
25	L	202	BCR	C5-C6-C7-C8
25	M	101	BCR	C23-C24-C25-C30
28	1	318	LHG	C28-C29-C30-C31
24	6	606	CLA	C2A-CAA-CBA-CGA
28	I	103	LHG	O7-C5-C6-O8
30	A	855	LMG	O1-C7-C8-O7
24	5	606	CLA	CBA-CGA-O2A-C1
24	c	601	CLA	C2A-CAA-CBA-CGA
24	c	605	CLA	C2C-C3C-CAC-CBC
24	B	847	CLA	C13-C15-C16-C17
24	L	203	CLA	C2-C3-C5-C6
31	B	839	PQN	C12-C13-C15-C16
24	A	817	CLA	C2C-C3C-CAC-CBC
27	A	854	LMT	C1-C2-C3-C4
27	1	315	LMT	C5-C6-C7-C8
24	1	301	CLA	C6-C7-C8-C9
24	1	317	CLA	C14-C13-C15-C16
24	3	306	CLA	C14-C13-C15-C16
24	7	606	CLA	C11-C10-C8-C9
24	A	816	CLA	C14-C13-C15-C16
24	A	827	CLA	C11-C10-C8-C9
24	A	840	CLA	C14-C13-C15-C16
24	B	802	CLA	C11-C10-C8-C9
24	B	818	CLA	C11-C12-C13-C14
24	B	823	CLA	C6-C7-C8-C9
30	2	214	LMG	C30-C31-C32-C33
28	A	842	LHG	C25-C26-C27-C28
24	2	209	CLA	O1A-CGA-O2A-C1
24	B	820	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	A	850	LMT	C3-C4-C5-C6
24	2	208	CLA	O1D-CGD-O2D-CED
28	A	849	LHG	O1-C1-C2-O2
24	A	828	CLA	C3-C5-C6-C7
24	4	609	CLA	CAA-CBA-CGA-O2A
24	5	602	CLA	C6-C7-C8-C10
24	A	832	CLA	C16-C17-C18-C20
26	8	210	DD6	C4-C5-C6-C7
26	9	314	DD6	C9-C10-C11-C12
24	A	856	CLA	C3-C5-C6-C7
24	B	827	CLA	C3-C5-C6-C7
24	B	827	CLA	CBA-CGA-O2A-C1
28	8	213	LHG	O6-C4-C5-C6
24	A	856	CLA	O1D-CGD-O2D-CED
24	A	826	CLA	C16-C17-C18-C20
24	k	303	CLA	C2C-C3C-CAC-CBC
24	c	609	CLA	C11-C10-C8-C7
24	A	812	CLA	C12-C13-C15-C16
24	B	801	CLA	C11-C10-C8-C7
24	B	802	CLA	C11-C10-C8-C7
24	B	809	CLA	C11-C12-C13-C15
24	B	812	CLA	C12-C13-C15-C16
24	B	823	CLA	C6-C7-C8-C10
24	4	607	CLA	CAA-CBA-CGA-O2A
28	A	849	LHG	C26-C27-C28-C29
24	B	838	CLA	C13-C15-C16-C17
25	A	845	BCR	C11-C12-C13-C14
24	k	303	CLA	CBA-CGA-O2A-C1
24	t	310	CLA	O1A-CGA-O2A-C1
24	4	602	CLA	O1A-CGA-O2A-C1
31	B	839	PQN	C18-C20-C21-C22
24	B	847	CLA	C2A-CAA-CBA-CGA
28	A	852	LHG	C30-C31-C32-C33
24	B	808	CLA	C4-C3-C5-C6
24	9	301	CLA	CAA-CBA-CGA-O2A
24	B	826	CLA	C8-C10-C11-C12
24	B	831	CLA	C5-C6-C7-C8
24	B	814	CLA	O2A-C1-C2-C3
24	B	831	CLA	O2A-C1-C2-C3
24	B	837	CLA	O2A-C1-C2-C3
28	3	315	LHG	C18-C19-C20-C21
24	A	853	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	3	315	LHG	O10-C23-O8-C6
26	8	210	DD6	C4-C5-C6-C8
28	8	213	LHG	O6-C4-C5-O7
30	t	314	LMG	C7-C8-C9-O8
30	A	855	LMG	O1-C7-C8-C9
28	L	201	LHG	O10-C23-O8-C6
24	A	856	CLA	C4-C3-C5-C6
24	B	808	CLA	C2-C3-C5-C6
29	9	312	A1L1G	C45-C2-C44-C43
28	3	315	LHG	O7-C5-C6-O8
28	A	841	LHG	O7-C5-C6-O8
24	t	303	CLA	C11-C10-C8-C9
24	A	810	CLA	C11-C12-C13-C14
24	B	829	CLA	C14-C13-C15-C16
27	A	854	LMT	C11-C10-C9-C8
30	2	214	LMG	C35-C36-C37-C38
30	A	855	LMG	C14-C15-C16-C17
24	k	303	CLA	O1A-CGA-O2A-C1
24	A	808	CLA	O1A-CGA-O2A-C1
24	B	802	CLA	O1A-CGA-O2A-C1
28	4	619	LHG	C10-C11-C12-C13
24	B	827	CLA	O1A-CGA-O2A-C1
24	t	308	CLA	CAA-CBA-CGA-O2A
24	2	204	CLA	C2-C1-O2A-CGA
24	B	831	CLA	C2-C1-O2A-CGA
25	M	101	BCR	C13-C14-C15-C16
24	A	817	CLA	CBA-CGA-O2A-C1
24	A	817	CLA	CBD-CGD-O2D-CED
25	A	845	BCR	C5-C6-C7-C8
24	t	309	CLA	C2A-CAA-CBA-CGA
24	3	308	CLA	CBD-CGD-O2D-CED
27	3	314	LMT	C5'-C4'-O1B-C1B
28	B	845	LHG	C31-C32-C33-C34
26	6	615	DD6	C27-C29-C30-C31
26	8	211	DD6	C27-C29-C30-C31
26	c	614	DD6	C27-C29-C30-C31
26	k	315	DD6	C27-C29-C30-C31
28	8	213	LHG	O1-C1-C2-O2
24	B	822	CLA	C3-C5-C6-C7
25	t	312	BCR	C36-C18-C19-C20
24	1	302	CLA	C1A-C2A-CAA-CBA
24	1	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	1	303	CLA	C4B-C3B-CAB-CBB
24	1	308	CLA	C1A-C2A-CAA-CBA
24	4	601	CLA	C4B-C3B-CAB-CBB
24	6	607	CLA	C4B-C3B-CAB-CBB
24	8	206	CLA	C1A-C2A-CAA-CBA
24	9	303	CLA	C4B-C3B-CAB-CBB
24	h	607	CLA	C4B-C3B-CAB-CBB
24	h	608	CLA	C4B-C3B-CAB-CBB
24	h	610	CLA	C4B-C3B-CAB-CBB
24	k	307	CLA	C4B-C3B-CAB-CBB
24	A	817	CLA	C4B-C3B-CAB-CBB
24	B	808	CLA	C4B-C3B-CAB-CBB
24	B	810	CLA	C1A-C2A-CAA-CBA
24	B	816	CLA	C1A-C2A-CAA-CBA
24	B	816	CLA	C4B-C3B-CAB-CBB
24	B	818	CLA	C4B-C3B-CAB-CBB
24	B	819	CLA	C4B-C3B-CAB-CBB
24	B	825	CLA	C1A-C2A-CAA-CBA
24	B	832	CLA	C4B-C3B-CAB-CBB
24	B	836	CLA	C4B-C3B-CAB-CBB
24	L	203	CLA	C4B-C3B-CAB-CBB
24	A	808	CLA	CBA-CGA-O2A-C1
24	h	606	CLA	C4C-C3C-CAC-CBC
28	A	849	LHG	C28-C29-C30-C31
24	A	822	CLA	C6-C7-C8-C10
24	9	305	CLA	O1A-CGA-O2A-C1
24	6	604	CLA	C2A-CAA-CBA-CGA
24	A	847	CLA	C2A-CAA-CBA-CGA
27	1	315	LMT	C4B-C5B-C6B-O6B
24	c	608	CLA	C12-C13-C15-C16
24	A	802	CLA	C11-C10-C8-C7
24	B	802	CLA	C6-C7-C8-C10
24	B	803	CLA	C12-C13-C15-C16
24	B	806	CLA	C12-C13-C15-C16
24	B	836	CLA	C11-C12-C13-C15
24	A	826	CLA	C16-C17-C18-C19
24	c	604	CLA	O1A-CGA-O2A-C1
28	A	841	LHG	C13-C14-C15-C16
24	A	817	CLA	O1A-CGA-O2A-C1
24	A	860	CLA	C15-C16-C17-C18
28	B	844	LHG	C5-C4-O6-P
24	B	837	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	6	606	CLA	C4C-C3C-CAC-CBC
24	c	606	CLA	C2A-CAA-CBA-CGA
24	A	816	CLA	C2A-CAA-CBA-CGA
24	A	812	CLA	C14-C13-C15-C16
24	B	801	CLA	C11-C10-C8-C9
24	B	802	CLA	C6-C7-C8-C9
24	B	812	CLA	C14-C13-C15-C16
27	3	314	LMT	C3-C4-C5-C6
24	B	836	CLA	C8-C10-C11-C12
29	2	213	A1L1G	C30-C31-C32-C33
29	7	614	A1L1G	C30-C31-C32-C33
24	h	607	CLA	CBA-CGA-O2A-C1
24	c	608	CLA	C13-C15-C16-C17
24	A	822	CLA	C5-C6-C7-C8
24	6	611	CLA	CAD-CBD-CGD-O1D
24	A	821	CLA	C1-C2-C3-C4
29	3	310	A1L1G	C45-C2-C44-C42
24	2	204	CLA	C5-C6-C7-C8
24	3	308	CLA	O1D-CGD-O2D-CED
28	J	105	LHG	O7-C5-C6-O8
24	A	857	CLA	C8-C10-C11-C12
24	2	203	CLA	CAD-CBD-CGD-O2D
24	4	605	CLA	CAD-CBD-CGD-O2D
24	5	604	CLA	CAD-CBD-CGD-O2D
24	7	607	CLA	CAD-CBD-CGD-O2D
24	c	604	CLA	CAD-CBD-CGD-O2D
24	c	606	CLA	CAD-CBD-CGD-O2D
24	A	801	CLA	CAD-CBD-CGD-O2D
24	A	811	CLA	CAD-CBD-CGD-O2D
24	A	813	CLA	CAD-CBD-CGD-O2D
24	A	831	CLA	CAD-CBD-CGD-O2D
24	A	847	CLA	CAD-CBD-CGD-O2D
24	B	813	CLA	CAD-CBD-CGD-O2D
24	B	834	CLA	CAD-CBD-CGD-O2D
24	F	202	CLA	CAD-CBD-CGD-O2D
29	9	312	A1L1G	O13-C26-C30-C31
24	B	824	CLA	C13-C15-C16-C17
24	A	817	CLA	O1D-CGD-O2D-CED
24	R	104	CLA	C2A-CAA-CBA-CGA
24	A	810	CLA	C10-C11-C12-C13
24	B	834	CLA	C15-C16-C17-C18
24	L	204	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	B	844	LHG	C15-C16-C17-C18
24	B	802	CLA	C8-C10-C11-C12
28	3	315	LHG	C19-C20-C21-C22
24	1	306	CLA	CAD-CBD-CGD-O1D
24	2	203	CLA	CAD-CBD-CGD-O1D
24	2	207	CLA	CHA-CBD-CGD-O2D
24	3	302	CLA	CHA-CBD-CGD-O1D
24	3	302	CLA	CHA-CBD-CGD-O2D
24	4	605	CLA	CAD-CBD-CGD-O1D
24	5	601	CLA	CAD-CBD-CGD-O1D
24	5	604	CLA	CAD-CBD-CGD-O1D
24	5	606	CLA	CHA-CBD-CGD-O1D
24	5	606	CLA	CHA-CBD-CGD-O2D
24	6	610	CLA	CHA-CBD-CGD-O1D
24	7	607	CLA	CAD-CBD-CGD-O1D
24	8	208	CLA	CHA-CBD-CGD-O1D
24	8	208	CLA	CHA-CBD-CGD-O2D
24	9	301	CLA	CHA-CBD-CGD-O1D
24	9	301	CLA	CHA-CBD-CGD-O2D
24	9	303	CLA	CHA-CBD-CGD-O1D
24	9	305	CLA	CHA-CBD-CGD-O1D
24	9	305	CLA	CHA-CBD-CGD-O2D
24	9	306	CLA	CAD-CBD-CGD-O1D
24	9	309	CLA	CHA-CBD-CGD-O1D
24	9	309	CLA	CHA-CBD-CGD-O2D
24	c	601	CLA	CAD-CBD-CGD-O1D
24	c	604	CLA	CAD-CBD-CGD-O1D
24	c	606	CLA	CAD-CBD-CGD-O1D
24	t	310	CLA	CHA-CBD-CGD-O1D
24	t	310	CLA	CHA-CBD-CGD-O2D
24	k	304	CLA	CHA-CBD-CGD-O1D
24	k	304	CLA	CHA-CBD-CGD-O2D
24	k	307	CLA	CHA-CBD-CGD-O1D
24	k	307	CLA	CHA-CBD-CGD-O2D
24	A	805	CLA	CHA-CBD-CGD-O1D
24	A	805	CLA	CHA-CBD-CGD-O2D
24	A	811	CLA	CAD-CBD-CGD-O1D
24	A	813	CLA	CAD-CBD-CGD-O1D
24	A	816	CLA	CHA-CBD-CGD-O1D
24	A	816	CLA	CHA-CBD-CGD-O2D
24	A	817	CLA	CHA-CBD-CGD-O1D
24	A	821	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	A	821	CLA	CHA-CBD-CGD-O2D
24	A	824	CLA	CHA-CBD-CGD-O1D
24	A	824	CLA	CHA-CBD-CGD-O2D
24	A	825	CLA	CHA-CBD-CGD-O1D
24	A	830	CLA	CHA-CBD-CGD-O1D
24	A	830	CLA	CHA-CBD-CGD-O2D
24	A	831	CLA	CAD-CBD-CGD-O1D
24	A	847	CLA	CAD-CBD-CGD-O1D
24	A	860	CLA	CHA-CBD-CGD-O1D
24	A	860	CLA	CHA-CBD-CGD-O2D
24	B	813	CLA	CAD-CBD-CGD-O1D
24	B	814	CLA	CHA-CBD-CGD-O1D
24	B	814	CLA	CHA-CBD-CGD-O2D
24	B	817	CLA	CAD-CBD-CGD-O1D
24	B	830	CLA	CHA-CBD-CGD-O1D
24	B	830	CLA	CHA-CBD-CGD-O2D
24	B	834	CLA	CAD-CBD-CGD-O1D
24	B	846	CLA	CHA-CBD-CGD-O1D
24	B	846	CLA	CHA-CBD-CGD-O2D
24	F	201	CLA	CHA-CBD-CGD-O1D
24	F	202	CLA	CAD-CBD-CGD-O1D
25	A	844	BCR	C9-C10-C11-C12
25	B	842	BCR	C19-C20-C21-C22
28	1	318	LHG	C4-O6-P-O3
28	1	318	LHG	C4-O6-P-O5
28	2	215	LHG	C4-O6-P-O5
28	3	315	LHG	C3-O3-P-O4
28	8	213	LHG	C3-O3-P-O5
28	8	213	LHG	C4-O6-P-O3
28	A	841	LHG	C3-O3-P-O5
28	A	849	LHG	C3-O3-P-O5
28	A	849	LHG	C4-O6-P-O3
28	A	849	LHG	C4-O6-P-O5
28	B	844	LHG	C3-O3-P-O4
28	B	845	LHG	C4-O6-P-O4
28	J	105	LHG	C4-O6-P-O5
24	A	831	CLA	C16-C17-C18-C20
27	3	314	LMT	C3'-C4'-O1B-C1B
24	B	807	CLA	C4-C3-C5-C6
24	1	308	CLA	C2B-C3B-CAB-CBB
24	2	204	CLA	C2B-C3B-CAB-CBB
24	6	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	h	609	CLA	C2B-C3B-CAB-CBB
24	h	610	CLA	C2B-C3B-CAB-CBB
24	k	307	CLA	C2B-C3B-CAB-CBB
24	A	822	CLA	C2B-C3B-CAB-CBB
24	B	803	CLA	C2B-C3B-CAB-CBB
24	B	808	CLA	C2B-C3B-CAB-CBB
24	B	821	CLA	C2B-C3B-CAB-CBB
24	B	828	CLA	C2B-C3B-CAB-CBB
24	B	836	CLA	C2B-C3B-CAB-CBB
24	B	837	CLA	C2B-C3B-CAB-CBB
24	B	838	CLA	C2B-C3B-CAB-CBB
24	L	204	CLA	C2B-C3B-CAB-CBB
24	A	856	CLA	C2-C3-C5-C6
25	2	211	BCR	C21-C22-C23-C24
24	A	824	CLA	CBD-CGD-O2D-CED
28	A	852	LHG	C28-C29-C30-C31
24	A	805	CLA	C3-C5-C6-C7
24	B	831	CLA	C8-C10-C11-C12
28	A	841	LHG	C7-C8-C9-C10
24	A	847	CLA	C2-C3-C5-C6
24	3	306	CLA	CBD-CGD-O2D-CED
24	5	602	CLA	C6-C7-C8-C9
24	A	801	CLA	C16-C17-C18-C20
24	A	831	CLA	C16-C17-C18-C19
24	4	602	CLA	C6-C7-C8-C9
24	A	807	CLA	C14-C13-C15-C16
24	A	836	CLA	C11-C10-C8-C9
24	A	838	CLA	C14-C13-C15-C16
24	B	801	CLA	C11-C12-C13-C14
24	B	809	CLA	C11-C12-C13-C14
24	B	816	CLA	C6-C7-C8-C9
24	A	833	CLA	C11-C12-C13-C15
24	A	836	CLA	C11-C10-C8-C7
24	A	838	CLA	C12-C13-C15-C16
24	B	807	CLA	C12-C13-C15-C16
24	B	817	CLA	C12-C13-C15-C16
24	F	201	CLA	C6-C7-C8-C10
24	A	822	CLA	C6-C7-C8-C9
27	1	316	LMT	C4'-C5'-C6'-O6'
24	h	606	CLA	CAA-CBA-CGA-O2A
24	B	803	CLA	C10-C11-C12-C13
24	k	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A	817	CLA	CAA-CBA-CGA-O2A
24	A	820	CLA	C2A-CAA-CBA-CGA
24	A	827	CLA	O1A-CGA-O2A-C1
24	B	822	CLA	C4-C3-C5-C6
24	7	606	CLA	C4C-C3C-CAC-CBC
24	t	302	CLA	CAA-CBA-CGA-O2A
24	B	834	CLA	C16-C17-C18-C20
24	B	802	CLA	C3-C5-C6-C7
24	A	811	CLA	CAA-CBA-CGA-O2A
24	7	612	CLA	C2A-CAA-CBA-CGA
24	h	604	CLA	C2A-CAA-CBA-CGA
24	A	856	CLA	C2A-CAA-CBA-CGA
24	B	817	CLA	C2A-CAA-CBA-CGA
24	L	203	CLA	C2A-CAA-CBA-CGA
24	A	823	CLA	O1D-CGD-O2D-CED
27	A	854	LMT	C7-C8-C9-C10
24	h	604	CLA	O1A-CGA-O2A-C1
24	L	205	CLA	C2C-C3C-CAC-CBC
26	4	615	DD6	C27-C29-C30-C31
26	4	616	DD6	C27-C29-C30-C31
26	6	613	DD6	C27-C29-C30-C31
26	6	616	DD6	C27-C29-C30-C31
26	h	613	DD6	C27-C29-C30-C31
27	A	850	LMT	C2-C1-O1'-C1'
24	2	202	CLA	C6-C7-C8-C10
24	7	606	CLA	CAA-CBA-CGA-O2A
24	7	609	CLA	O1A-CGA-O2A-C1
24	B	806	CLA	C14-C13-C15-C16
24	A	827	CLA	CBA-CGA-O2A-C1
24	7	610	CLA	C4B-C3B-CAB-CBB
24	h	609	CLA	C4B-C3B-CAB-CBB
24	c	603	CLA	C4B-C3B-CAB-CBB
24	A	830	CLA	C4B-C3B-CAB-CBB
24	A	823	CLA	CBD-CGD-O2D-CED
24	B	818	CLA	C5-C6-C7-C8
24	A	853	CLA	C6-C7-C8-C10
24	B	815	CLA	C6-C7-C8-C9
24	A	824	CLA	O1D-CGD-O2D-CED
24	A	816	CLA	C8-C10-C11-C12
24	B	804	CLA	C10-C11-C12-C13
24	B	817	CLA	C13-C15-C16-C17
24	9	305	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	1	318	LHG	O6-C4-C5-O7
27	1	316	LMT	C5'-C4'-O1B-C1B
28	A	841	LHG	O6-C4-C5-C6
24	5	607	CLA	CAA-CBA-CGA-O2A
28	1	318	LHG	C11-C12-C13-C14
25	k	316	BCR	C19-C20-C21-C22
24	A	801	CLA	C16-C17-C18-C19
24	t	303	CLA	C6-C7-C8-C10
24	A	831	CLA	C11-C10-C8-C7
28	8	213	LHG	C9-C10-C11-C12
28	I	103	LHG	C24-C23-O8-C6
27	1	315	LMT	C6-C7-C8-C9
24	c	608	CLA	C10-C11-C12-C13
28	4	619	LHG	O7-C5-C6-O8
24	7	601	CLA	C3A-C2A-CAA-CBA
24	B	829	CLA	C3A-C2A-CAA-CBA
24	B	835	CLA	C3A-C2A-CAA-CBA
24	B	847	CLA	C3A-C2A-CAA-CBA
24	B	802	CLA	CAA-CBA-CGA-O2A
25	B	842	BCR	C20-C21-C22-C37
25	F	204	BCR	C35-C13-C14-C15
25	L	202	BCR	C11-C10-C9-C34
26	8	211	DD6	C9-C10-C11-C12
26	t	311	DD6	C9-C10-C11-C12
29	7	614	A1L1G	C14-C29-C30-C26
29	2	213	A1L1G	C34-C35-C36-C37
24	B	818	CLA	C15-C16-C17-C18
24	B	836	CLA	C5-C6-C7-C8
24	5	607	CLA	CAA-CBA-CGA-O1A
27	A	850	LMT	C9-C10-C11-C12
25	A	844	BCR	C7-C8-C9-C10
24	B	807	CLA	C2-C3-C5-C6
24	A	808	CLA	C8-C10-C11-C12
24	B	833	CLA	C8-C10-C11-C12
31	A	839	PQN	C23-C25-C26-C27
28	A	841	LHG	O2-C2-C3-O3
27	A	854	LMT	C3-C4-C5-C6
27	1	316	LMT	O5'-C5'-C6'-O6'
24	9	305	CLA	CAA-CBA-CGA-O1A
24	3	307	CLA	CAA-CBA-CGA-O1A
24	3	301	CLA	C6-C7-C8-C9
24	t	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	820	CLA	C11-C10-C8-C9
24	A	823	CLA	C11-C12-C13-C14
24	B	827	CLA	C11-C12-C13-C14
24	B	837	CLA	C6-C7-C8-C9
31	A	839	PQN	C24-C23-C25-C26
24	A	824	CLA	C16-C17-C18-C19
24	B	803	CLA	C15-C16-C17-C18
24	1	307	CLA	CAA-CBA-CGA-O2A
28	4	619	LHG	C6-C5-O7-C7
28	L	201	LHG	C6-C5-O7-C7
24	A	816	CLA	C15-C16-C17-C18
24	t	306	CLA	CAA-CBA-CGA-O2A
24	2	204	CLA	C2A-CAA-CBA-CGA
24	7	604	CLA	C2A-CAA-CBA-CGA
24	c	604	CLA	C2A-CAA-CBA-CGA
24	t	306	CLA	C2A-CAA-CBA-CGA
24	7	601	CLA	C1A-C2A-CAA-CBA
24	A	856	CLA	C1A-C2A-CAA-CBA
24	B	812	CLA	C1A-C2A-CAA-CBA
25	B	842	BCR	C20-C21-C22-C23
25	F	204	BCR	C12-C13-C14-C15
25	L	202	BCR	C11-C10-C9-C8
24	A	804	CLA	C15-C16-C17-C18
24	1	303	CLA	C2B-C3B-CAB-CBB
24	4	601	CLA	C2B-C3B-CAB-CBB
24	7	612	CLA	C2B-C3B-CAB-CBB
24	8	204	CLA	C2B-C3B-CAB-CBB
24	9	303	CLA	C2B-C3B-CAB-CBB
24	h	601	CLA	C2B-C3B-CAB-CBB
24	h	607	CLA	C2B-C3B-CAB-CBB
24	t	310	CLA	C2B-C3B-CAB-CBB
24	A	817	CLA	C2B-C3B-CAB-CBB
24	A	830	CLA	C2B-C3B-CAB-CBB
24	A	835	CLA	C2B-C3B-CAB-CBB
24	B	816	CLA	C2B-C3B-CAB-CBB
24	B	819	CLA	C2B-C3B-CAB-CBB
24	B	832	CLA	C2B-C3B-CAB-CBB
24	J	103	CLA	C2B-C3B-CAB-CBB
24	L	203	CLA	C2B-C3B-CAB-CBB
25	k	316	BCR	C5-C6-C7-C8
25	A	843	BCR	C1-C6-C7-C8
25	M	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	3	307	CLA	CAA-CBA-CGA-O2A
28	A	841	LHG	C11-C12-C13-C14
24	5	603	CLA	CAA-CBA-CGA-O1A
24	h	602	CLA	C4-C3-C5-C6
28	1	318	LHG	O6-C4-C5-C6
28	A	841	LHG	C29-C30-C31-C32
24	A	821	CLA	O2A-C1-C2-C3
24	5	606	CLA	O1A-CGA-O2A-C1
24	1	317	CLA	C11-C12-C13-C15
24	3	301	CLA	C12-C13-C15-C16
24	A	807	CLA	C12-C13-C15-C16
24	A	810	CLA	C11-C12-C13-C15
24	A	816	CLA	C12-C13-C15-C16
24	A	829	CLA	C6-C7-C8-C10
24	A	840	CLA	C6-C7-C8-C10
24	B	801	CLA	C11-C12-C13-C15
24	B	831	CLA	C11-C10-C8-C7
24	B	838	CLA	C11-C12-C13-C15
24	3	303	CLA	C2A-CAA-CBA-CGA
24	k	303	CLA	C2A-CAA-CBA-CGA
24	1	307	CLA	CAA-CBA-CGA-O1A
24	t	306	CLA	CAA-CBA-CGA-O1A
24	c	602	CLA	C3-C5-C6-C7
25	1	310	BCR	C11-C12-C13-C35
24	h	612	CLA	CAA-CBA-CGA-O2A
24	B	831	CLA	C4-C3-C5-C6
24	B	806	CLA	C8-C10-C11-C12
24	A	837	CLA	C2-C3-C5-C6
24	A	832	CLA	C5-C6-C7-C8
24	9	311	CLA	CAA-CBA-CGA-O2A
24	A	812	CLA	C16-C17-C18-C19
24	B	847	CLA	CBA-CGA-O2A-C1
24	B	847	CLA	O1A-CGA-O2A-C1
28	A	841	LHG	C28-C29-C30-C31
24	5	603	CLA	CAA-CBA-CGA-O2A
24	B	806	CLA	C11-C12-C13-C14
24	B	825	CLA	C6-C7-C8-C10
24	B	834	CLA	C16-C17-C18-C19
28	A	841	LHG	C10-C11-C12-C13
24	4	601	CLA	C2C-C3C-CAC-CBC
24	A	837	CLA	C4-C3-C5-C6
24	B	816	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	825	CLA	C4-C3-C5-C6
28	2	215	LHG	C2-C3-O3-P
28	B	844	LHG	C2-C3-O3-P
28	A	841	LHG	C12-C13-C14-C15
24	B	810	CLA	CAA-CBA-CGA-O1A
24	B	831	CLA	C2-C3-C5-C6
24	1	317	CLA	C16-C17-C18-C19
24	B	825	CLA	C3-C5-C6-C7
24	8	208	CLA	CAA-CBA-CGA-O2A
28	1	318	LHG	C10-C11-C12-C13
28	A	841	LHG	C4-C5-C6-O8
28	J	105	LHG	C4-C5-C6-O8
24	7	608	CLA	CAA-CBA-CGA-O2A
24	7	601	CLA	C2A-CAA-CBA-CGA
24	h	612	CLA	C2A-CAA-CBA-CGA
24	t	303	CLA	C16-C17-C18-C20
24	h	601	CLA	CAA-CBA-CGA-O2A
26	1	313	DD6	C27-C29-C30-C31
26	2	210	DD6	C27-C29-C30-C31
26	3	311	DD6	C27-C29-C30-C31
28	3	315	LHG	O1-C1-C2-O2
24	6	601	CLA	CAA-CBA-CGA-O2A
24	1	317	CLA	CAA-CBA-CGA-O2A
24	5	602	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	C2-C3-C5-C6
24	B	805	CLA	C16-C17-C18-C19
24	1	309	CLA	C4B-C3B-CAB-CBB
24	5	604	CLA	C4B-C3B-CAB-CBB
24	9	304	CLA	C4B-C3B-CAB-CBB
24	c	608	CLA	C4B-C3B-CAB-CBB
24	J	103	CLA	C4B-C3B-CAB-CBB
24	3	305	CLA	O1A-CGA-O2A-C1
24	1	306	CLA	CAA-CBA-CGA-O2A
24	4	604	CLA	CAA-CBA-CGA-O2A
24	t	309	CLA	CAA-CBA-CGA-O2A
24	B	805	CLA	C16-C17-C18-C20
26	9	315	DD6	C9-C10-C11-C12
24	7	610	CLA	CAA-CBA-CGA-O1A
24	A	836	CLA	C5-C6-C7-C8
24	9	311	CLA	CAA-CBA-CGA-O1A
24	A	823	CLA	C15-C16-C17-C18
24	B	812	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	3	306	CLA	O1D-CGD-O2D-CED
24	3	302	CLA	CAA-CBA-CGA-O2A
24	7	603	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	C13-C15-C16-C17
24	c	602	CLA	C14-C13-C15-C16
24	c	609	CLA	C6-C7-C8-C9
24	A	826	CLA	C11-C12-C13-C14
24	A	836	CLA	C11-C12-C13-C14
31	B	839	PQN	C24-C23-C25-C26
28	I	103	LHG	O10-C23-O8-C6
24	B	829	CLA	CAA-CBA-CGA-O2A
24	h	612	CLA	CAA-CBA-CGA-O1A
24	A	815	CLA	CAA-CBA-CGA-O2A
24	6	602	CLA	C2A-CAA-CBA-CGA
24	8	203	CLA	C2A-CAA-CBA-CGA
24	A	822	CLA	C2A-CAA-CBA-CGA
24	F	203	CLA	C2A-CAA-CBA-CGA
24	B	812	CLA	C2-C1-O2A-CGA
24	R	103	CLA	C2-C1-O2A-CGA
24	A	824	CLA	C16-C17-C18-C20
24	c	605	CLA	C4C-C3C-CAC-CBC
24	1	309	CLA	C3A-C2A-CAA-CBA
24	A	804	CLA	C3A-C2A-CAA-CBA
24	A	814	CLA	C3A-C2A-CAA-CBA
24	B	812	CLA	C3A-C2A-CAA-CBA
24	R	103	CLA	C3A-C2A-CAA-CBA
24	B	825	CLA	C2-C3-C5-C6
24	F	201	CLA	C15-C16-C17-C18
24	7	603	CLA	CAA-CBA-CGA-O1A
24	h	601	CLA	CAA-CBA-CGA-O1A
24	1	306	CLA	O1D-CGD-O2D-CED
24	9	306	CLA	CAA-CBA-CGA-O2A
24	k	302	CLA	CAA-CBA-CGA-O2A
24	c	608	CLA	O2A-C1-C2-C3
24	6	601	CLA	CAA-CBA-CGA-O1A
24	B	816	CLA	CAA-CBA-CGA-O2A
26	8	210	DD6	C11-C10-C9-C8
24	3	305	CLA	CBA-CGA-O2A-C1
24	8	208	CLA	CAA-CBA-CGA-O1A
24	8	202	CLA	C2A-CAA-CBA-CGA
24	t	310	CLA	C2A-CAA-CBA-CGA
24	8	207	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	A	828	CLA	C8-C10-C11-C12
26	3	312	DD6	C13-C14-C15-O1
26	9	314	DD6	C9-C10-C11-C13
26	h	615	DD6	C13-C14-C15-O1
26	c	612	DD6	C13-C14-C15-O1
29	k	312	A1L1G	C29-C14-C25-O15
24	F	202	CLA	CBA-CGA-O2A-C1
24	3	302	CLA	CAA-CBA-CGA-O1A
24	7	608	CLA	CAA-CBA-CGA-O1A
28	A	852	LHG	C5-C4-O6-P
24	h	607	CLA	O1A-CGA-O2A-C1
24	7	601	CLA	CAA-CBA-CGA-O2A
25	A	844	BCR	C19-C20-C21-C22
29	7	614	A1L1G	C45-C2-C44-C43
24	7	604	CLA	CAA-CBA-CGA-O1A
24	k	307	CLA	CAA-CBA-CGA-O2A
28	A	841	LHG	C14-C15-C16-C17
24	B	833	CLA	O1A-CGA-O2A-C1
24	8	207	CLA	CAA-CBA-CGA-O1A
24	A	815	CLA	CAA-CBA-CGA-O1A
24	c	608	CLA	C14-C13-C15-C16
24	A	802	CLA	C11-C10-C8-C9
24	A	823	CLA	C6-C7-C8-C9
24	A	812	CLA	C16-C17-C18-C20
24	B	808	CLA	C16-C17-C18-C19
24	A	801	CLA	CAA-CBA-CGA-O2A
24	A	807	CLA	CAA-CBA-CGA-O2A
24	7	604	CLA	CAA-CBA-CGA-O2A
24	k	305	CLA	CAA-CBA-CGA-O2A
24	A	847	CLA	C6-C7-C8-C9
24	A	831	CLA	C2A-CAA-CBA-CGA
24	B	825	CLA	C2A-CAA-CBA-CGA
24	A	801	CLA	C12-C13-C15-C16
24	A	804	CLA	C11-C10-C8-C7
24	A	860	CLA	C11-C12-C13-C15
24	B	806	CLA	C11-C12-C13-C15
31	B	839	PQN	C22-C23-C25-C26
24	1	304	CLA	C2B-C3B-CAB-CBB
24	5	604	CLA	C2B-C3B-CAB-CBB
24	7	610	CLA	C2B-C3B-CAB-CBB
24	t	307	CLA	C2B-C3B-CAB-CBB
24	k	304	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	k	308	CLA	C2B-C3B-CAB-CBB
24	A	819	CLA	C2B-C3B-CAB-CBB
25	A	859	BCR	C1-C6-C7-C8
24	B	828	CLA	CAA-CBA-CGA-O2A
28	I	103	LHG	C27-C28-C29-C30
24	1	317	CLA	C2-C1-O2A-CGA
24	4	602	CLA	C2-C1-O2A-CGA
24	4	609	CLA	CAA-CBA-CGA-O1A
26	6	613	DD6	C11-C13-C14-C15
26	6	614	DD6	C11-C13-C14-C15
26	9	317	DD6	C11-C13-C14-C15
24	A	806	CLA	CAA-CBA-CGA-O2A
28	A	852	LHG	C25-C26-C27-C28
24	B	825	CLA	C6-C7-C8-C9
24	c	602	CLA	C10-C11-C12-C13
24	A	824	CLA	C2-C3-C5-C6
24	9	306	CLA	C2A-CAA-CBA-CGA
24	B	802	CLA	C2A-CAA-CBA-CGA
24	B	847	CLA	C2C-C3C-CAC-CBC
24	6	603	CLA	CAA-CBA-CGA-O2A
24	7	602	CLA	CAA-CBA-CGA-O2A
24	B	847	CLA	CAA-CBA-CGA-O2A
24	7	610	CLA	CAA-CBA-CGA-O2A
24	6	602	CLA	C2-C1-O2A-CGA
24	c	605	CLA	CAA-CBA-CGA-O2A
24	B	804	CLA	CAA-CBA-CGA-O2A
24	7	601	CLA	CAA-CBA-CGA-O1A
24	L	204	CLA	C3-C5-C6-C7
24	A	836	CLA	C2A-CAA-CBA-CGA
24	B	831	CLA	C2A-CAA-CBA-CGA
24	t	307	CLA	CAA-CBA-CGA-O2A
26	9	313	DD6	C27-C29-C30-C31
26	h	614	DD6	C27-C29-C30-C31
27	A	854	LMT	C2-C1-O1'-C1'
28	A	849	LHG	C10-C11-C12-C13
24	A	818	CLA	C6-C7-C8-C9
24	B	831	CLA	C11-C10-C8-C9
24	7	612	CLA	CAA-CBA-CGA-O2A
24	9	309	CLA	CAA-CBA-CGA-O2A
28	L	201	LHG	O8-C23-C24-C25
24	3	301	CLA	C5-C6-C7-C8
24	1	317	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	5	601	CLA	C4B-C3B-CAB-CBB
24	9	304	CLA	C1A-C2A-CAA-CBA
24	9	308	CLA	C1A-C2A-CAA-CBA
24	h	601	CLA	C1A-C2A-CAA-CBA
24	h	612	CLA	C4B-C3B-CAB-CBB
24	c	609	CLA	C4B-C3B-CAB-CBB
24	t	310	CLA	C4B-C3B-CAB-CBB
24	A	804	CLA	C1A-C2A-CAA-CBA
24	A	808	CLA	C4B-C3B-CAB-CBB
24	A	814	CLA	C1A-C2A-CAA-CBA
24	A	815	CLA	C4B-C3B-CAB-CBB
24	A	822	CLA	C4B-C3B-CAB-CBB
24	A	826	CLA	C1A-C2A-CAA-CBA
24	A	834	CLA	C4B-C3B-CAB-CBB
24	A	835	CLA	C1A-C2A-CAA-CBA
24	B	809	CLA	C1A-C2A-CAA-CBA
24	A	824	CLA	C4-C3-C5-C6
24	B	831	CLA	CAA-CBA-CGA-O2A
24	B	848	CLA	CAA-CBA-CGA-O2A
24	B	822	CLA	C2-C3-C5-C6
25	t	312	BCR	C17-C18-C19-C20
25	L	202	BCR	C7-C8-C9-C10
25	M	101	BCR	C11-C12-C13-C14
26	R	105	DD6	C10-C11-C13-C14
27	A	854	LMT	C5'-C4'-O1B-C1B
24	h	603	CLA	CAA-CBA-CGA-O2A
24	B	821	CLA	CAA-CBA-CGA-O2A
24	t	304	CLA	C2A-CAA-CBA-CGA
24	A	860	CLA	C2A-CAA-CBA-CGA
24	4	607	CLA	CAA-CBA-CGA-O1A
24	B	832	CLA	CAA-CBA-CGA-O2A
24	A	804	CLA	CAA-CBA-CGA-O2A
24	A	808	CLA	CAA-CBA-CGA-O2A
24	A	824	CLA	C13-C15-C16-C17
24	B	831	CLA	C13-C15-C16-C17
24	3	306	CLA	C13-C15-C16-C17
24	A	808	CLA	C2-C1-O2A-CGA
24	B	801	CLA	C2-C1-O2A-CGA
24	B	828	CLA	C2-C1-O2A-CGA
24	3	301	CLA	C11-C10-C8-C7
24	c	602	CLA	C12-C13-C15-C16
24	A	818	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	805	CLA	C11-C12-C13-C15
24	B	827	CLA	C6-C7-C8-C10
24	F	201	CLA	C11-C10-C8-C7
24	F	201	CLA	C11-C12-C13-C15
24	B	836	CLA	C16-C17-C18-C20
24	B	801	CLA	C8-C10-C11-C12
28	I	103	LHG	C29-C30-C31-C32
24	k	311	CLA	CAA-CBA-CGA-O2A
24	A	832	CLA	CAA-CBA-CGA-O2A
24	9	301	CLA	CAA-CBA-CGA-O1A
24	A	807	CLA	CAA-CBA-CGA-O1A
24	1	304	CLA	C2A-CAA-CBA-CGA
24	t	303	CLA	C2A-CAA-CBA-CGA
24	k	302	CLA	C2C-C3C-CAC-CBC
28	A	849	LHG	O7-C7-C8-C9
27	A	854	LMT	C3'-C4'-O1B-C1B
24	7	602	CLA	C3A-C2A-CAA-CBA
24	9	308	CLA	C3A-C2A-CAA-CBA
24	A	856	CLA	C3A-C2A-CAA-CBA
24	B	813	CLA	C3A-C2A-CAA-CBA
24	t	308	CLA	CAA-CBA-CGA-O1A
24	A	806	CLA	CAA-CBA-CGA-O1A
24	B	808	CLA	C16-C17-C18-C20
29	k	312	A1L1G	C14-C29-C30-C31
24	4	613	CLA	CAA-CBA-CGA-O2A
28	B	844	LHG	C27-C28-C29-C30
26	8	211	DD6	C9-C10-C11-C13
24	7	602	CLA	CAA-CBA-CGA-O1A
24	B	828	CLA	CAA-CBA-CGA-O1A
24	B	847	CLA	CAA-CBA-CGA-O1A
24	5	606	CLA	CAA-CBA-CGA-O2A
24	8	202	CLA	CAA-CBA-CGA-O2A
24	A	837	CLA	CAA-CBA-CGA-O2A
24	8	205	CLA	CAA-CBA-CGA-O2A
27	1	316	LMT	C3'-C4'-O1B-C1B
24	k	307	CLA	CAA-CBA-CGA-O1A
24	2	204	CLA	C11-C12-C13-C14
24	A	817	CLA	C2A-CAA-CBA-CGA
24	c	608	CLA	C6-C7-C8-C9
24	A	818	CLA	C11-C12-C13-C14
24	A	840	CLA	C6-C7-C8-C9
24	A	856	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	812	CLA	C11-C10-C8-C9
24	B	817	CLA	C14-C13-C15-C16
24	6	603	CLA	CAA-CBA-CGA-O1A
24	1	302	CLA	CAA-CBA-CGA-O2A
24	A	801	CLA	C8-C10-C11-C12
24	A	806	CLA	C8-C10-C11-C12
26	3	313	DD6	C13-C14-C15-C16
26	6	616	DD6	C13-C14-C15-C16
26	k	315	DD6	C13-C14-C15-C16
26	J	102	DD6	C13-C14-C15-C16
24	L	204	CLA	O1A-CGA-O2A-C1
24	h	603	CLA	CAA-CBA-CGA-O1A
24	k	305	CLA	CAA-CBA-CGA-O1A
24	7	606	CLA	C10-C11-C12-C13
24	3	308	CLA	CAA-CBA-CGA-O2A
24	1	306	CLA	CBD-CGD-O2D-CED
27	A	851	LMT	C3'-C4'-O1B-C1B
24	7	612	CLA	CAA-CBA-CGA-O1A
24	9	309	CLA	CAA-CBA-CGA-O1A
24	t	307	CLA	CAA-CBA-CGA-O1A
24	A	801	CLA	CAA-CBA-CGA-O1A
24	c	602	CLA	C13-C15-C16-C17
28	J	105	LHG	O8-C23-C24-C25
24	B	846	CLA	C2A-CAA-CBA-CGA
24	c	605	CLA	CAA-CBA-CGA-O1A
24	B	831	CLA	CAA-CBA-CGA-O1A
24	B	848	CLA	CAA-CBA-CGA-O1A
24	3	301	CLA	CAA-CBA-CGA-O2A
28	J	105	LHG	C9-C10-C11-C12
24	A	838	CLA	C16-C17-C18-C20
24	1	302	CLA	CAD-CBD-CGD-O2D
24	7	602	CLA	CAD-CBD-CGD-O2D
24	8	207	CLA	CAD-CBD-CGD-O2D
24	9	304	CLA	CAD-CBD-CGD-O2D
24	9	308	CLA	CAD-CBD-CGD-O2D
24	h	609	CLA	CAD-CBD-CGD-O2D
24	c	607	CLA	CAD-CBD-CGD-O2D
24	t	304	CLA	CAD-CBD-CGD-O2D
24	A	823	CLA	CAD-CBD-CGD-O2D
24	B	809	CLA	CAD-CBD-CGD-O2D
24	B	831	CLA	CAD-CBD-CGD-O2D
24	B	832	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	836	CLA	CAD-CBD-CGD-O2D
29	3	310	A1L1G	O13-C26-C30-C31
24	t	303	CLA	CAA-CBA-CGA-O2A
24	B	809	CLA	CAA-CBA-CGA-O2A
24	B	832	CLA	CAA-CBA-CGA-O1A
24	A	804	CLA	CAA-CBA-CGA-O1A
24	B	812	CLA	C10-C11-C12-C13
24	A	814	CLA	C2-C1-O2A-CGA
24	B	804	CLA	CAA-CBA-CGA-O1A
28	L	201	LHG	O10-C23-C24-C25
24	t	304	CLA	CAA-CBA-CGA-O2A
24	1	302	CLA	CAA-CBA-CGA-O1A
30	2	214	LMG	C38-C39-C40-C41
24	k	311	CLA	CAA-CBA-CGA-O1A
24	A	832	CLA	CAA-CBA-CGA-O1A
24	t	303	CLA	C5-C6-C7-C8
24	A	823	CLA	C6-C7-C8-C10
24	6	610	CLA	CAA-CBA-CGA-O2A
24	c	603	CLA	CAA-CBA-CGA-O2A
24	B	804	CLA	C8-C10-C11-C12
24	8	205	CLA	CAA-CBA-CGA-O1A
24	5	606	CLA	CAA-CBA-CGA-O1A
24	1	304	CLA	C3-C5-C6-C7
24	9	303	CLA	CAA-CBA-CGA-O2A
24	F	202	CLA	CAA-CBA-CGA-O2A
24	B	833	CLA	CBA-CGA-O2A-C1
24	3	308	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

205 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	615	DD6	1	0
27	h	617	LMT	1	0
24	4	608	CLA	4	0
24	A	817	CLA	2	0
25	F	204	BCR	2	0
24	1	307	CLA	2	0
24	2	209	CLA	4	0
24	9	303	CLA	1	0
25	A	845	BCR	1	0
24	c	607	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	824	CLA	2	0
24	B	838	CLA	2	0
24	t	306	CLA	1	0
24	8	204	CLA	2	0
27	1	316	LMT	2	0
27	A	851	LMT	1	0
24	8	209	CLA	1	0
24	7	611	CLA	2	0
24	9	302	CLA	2	0
24	5	604	CLA	2	0
24	B	821	CLA	1	0
24	B	834	CLA	2	0
24	B	804	CLA	6	0
24	8	203	CLA	2	0
24	3	308	CLA	2	0
24	c	601	CLA	2	0
24	6	607	CLA	2	0
24	4	607	CLA	4	0
24	A	840	CLA	1	0
26	2	212	DD6	1	0
25	M	101	BCR	2	0
24	9	301	CLA	8	0
24	L	204	CLA	1	0
24	B	808	CLA	2	0
28	1	318	LHG	2	0
24	4	611	CLA	10	0
24	B	835	CLA	1	0
26	9	317	DD6	1	0
25	k	316	BCR	2	0
26	9	315	DD6	3	0
25	B	843	BCR	5	0
26	c	613	DD6	1	0
24	2	204	CLA	1	0
25	B	849	BCR	1	0
24	5	605	CLA	2	0
24	1	304	CLA	3	0
24	B	803	CLA	4	0
24	8	206	CLA	2	0
24	A	830	CLA	6	0
28	J	105	LHG	1	0
25	A	859	BCR	1	0
24	9	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	k	313	DD6	1	0
24	B	829	CLA	4	0
26	8	211	DD6	1	0
24	2	206	CLA	2	0
24	B	817	CLA	2	0
24	B	823	CLA	1	0
24	t	307	CLA	2	0
24	h	612	CLA	2	0
24	4	613	CLA	2	0
25	I	101	BCR	1	0
26	6	613	DD6	1	0
24	B	827	CLA	1	0
28	L	201	LHG	4	0
24	t	308	CLA	1	0
24	A	824	CLA	1	0
24	A	838	CLA	1	0
24	B	807	CLA	1	0
24	B	828	CLA	1	0
24	A	818	CLA	3	0
24	B	802	CLA	2	0
25	I	102	BCR	2	0
24	2	202	CLA	1	0
24	7	602	CLA	9	0
24	A	814	CLA	1	0
24	B	822	CLA	1	0
26	1	311	DD6	5	0
24	c	602	CLA	2	0
24	A	819	CLA	1	0
26	5	608	DD6	2	0
24	k	301	CLA	4	0
24	h	608	CLA	2	0
24	4	612	CLA	2	0
24	B	806	CLA	1	0
24	B	832	CLA	3	0
24	A	835	CLA	1	0
24	5	607	CLA	2	0
24	A	847	CLA	1	0
24	t	305	CLA	3	0
24	6	611	CLA	1	0
26	9	313	DD6	2	0
24	B	812	CLA	3	0
25	J	101	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	614	DD6	1	0
24	k	308	CLA	2	0
24	A	805	CLA	1	0
24	4	602	CLA	3	0
24	B	810	CLA	1	0
24	B	833	CLA	2	0
27	A	854	LMT	3	0
26	4	615	DD6	1	0
24	1	303	CLA	1	0
25	1	310	BCR	4	0
31	A	839	PQN	1	0
25	A	844	BCR	3	0
24	A	801	CLA	1	0
26	7	618	DD6	1	0
24	B	848	CLA	1	0
29	9	312	A1L1G	1	0
24	7	606	CLA	4	0
24	B	830	CLA	7	0
25	B	842	BCR	2	0
24	6	601	CLA	3	0
24	4	605	CLA	1	0
26	7	613	DD6	1	0
24	F	202	CLA	1	0
24	2	201	CLA	3	0
24	7	612	CLA	2	0
24	1	302	CLA	1	0
25	4	618	BCR	7	0
24	1	305	CLA	4	0
24	6	603	CLA	3	0
28	3	315	LHG	1	0
24	3	304	CLA	5	0
24	3	305	CLA	1	0
24	R	103	CLA	1	0
26	8	212	DD6	1	0
28	A	842	LHG	2	0
24	A	823	CLA	1	0
24	c	603	CLA	1	0
27	3	314	LMT	1	0
24	t	302	CLA	1	0
24	2	205	CLA	1	0
24	2	207	CLA	1	0
24	A	816	CLA	1	0

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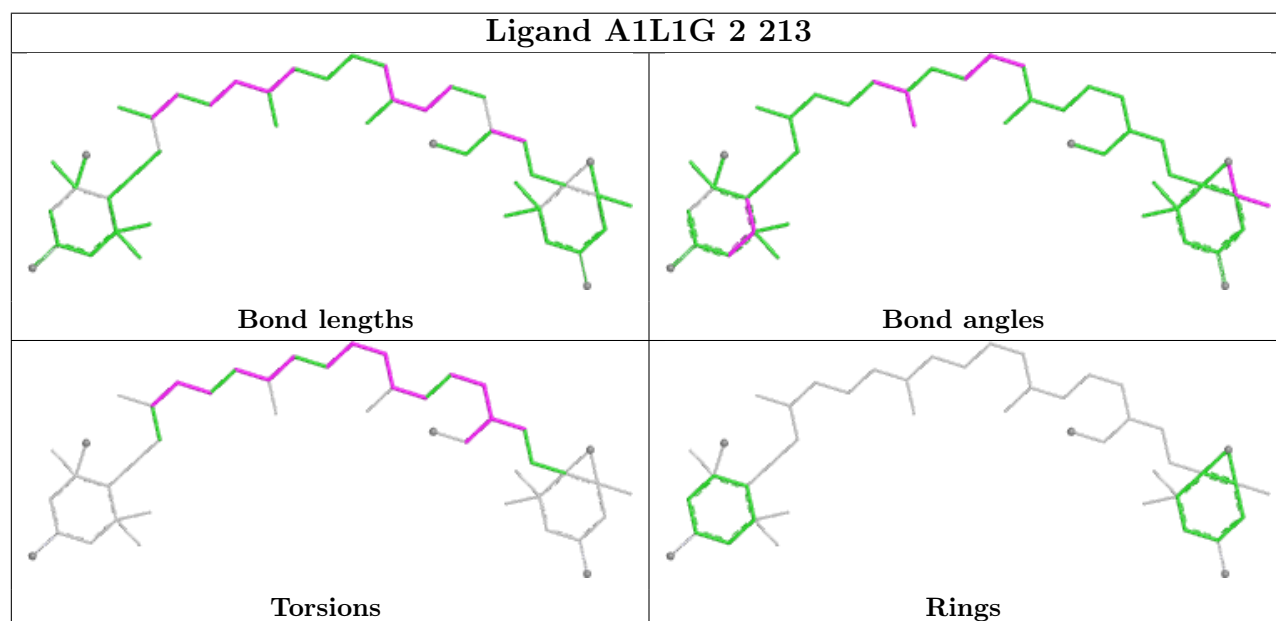
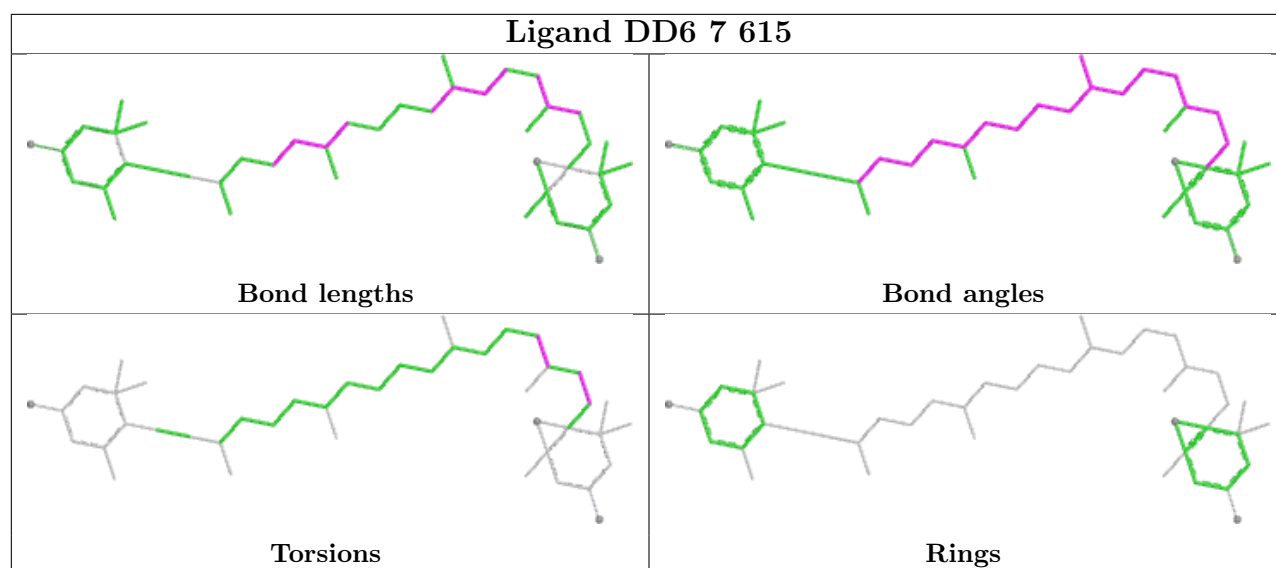
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	606	CLA	1	0
24	B	825	CLA	1	0
26	2	210	DD6	1	0
26	6	615	DD6	1	0
25	B	841	BCR	2	0
26	5	609	DD6	1	0
24	k	304	CLA	2	0
24	9	308	CLA	2	0
24	1	317	CLA	2	0
24	7	610	CLA	2	0
24	6	608	CLA	1	0
24	A	804	CLA	1	0
24	k	309	CLA	1	0
24	c	610	CLA	1	0
26	1	313	DD6	1	0
24	h	610	CLA	1	0
25	A	843	BCR	2	0
24	A	832	CLA	1	0
24	A	853	CLA	2	0
25	t	312	BCR	2	0
24	9	305	CLA	3	0
28	8	213	LHG	1	0
24	7	607	CLA	4	0
24	A	812	CLA	1	0
24	B	846	CLA	1	0
24	L	205	CLA	5	0
24	A	810	CLA	1	0
28	I	103	LHG	1	0
25	R	102	BCR	2	0
24	B	831	CLA	3	0
26	1	312	DD6	1	0
24	7	601	CLA	1	0
25	B	840	BCR	1	0
25	1	314	BCR	3	0
25	9	316	BCR	9	0
24	5	606	CLA	1	0
25	A	846	BCR	2	0
24	B	847	CLA	1	0
25	7	617	BCR	2	0
24	k	305	CLA	1	0
25	c	615	BCR	7	0
24	9	311	CLA	1	0

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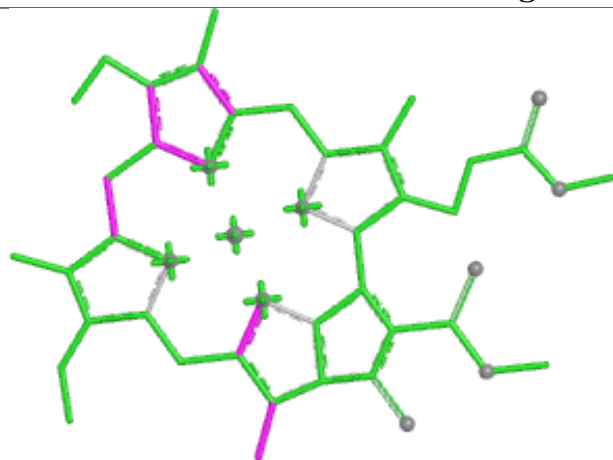
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	3	312	DD6	1	0
24	B	815	CLA	1	0
24	1	306	CLA	1	0
29	3	310	A1L1G	2	0
24	A	829	CLA	2	0
30	2	214	LMG	1	0
24	A	826	CLA	2	0
24	6	606	CLA	1	0
24	8	201	CLA	2	0
24	B	801	CLA	1	0
28	4	619	LHG	1	0
24	A	834	CLA	1	0
25	J	104	BCR	1	0
25	L	202	BCR	2	0
24	4	609	CLA	2	0
24	k	307	CLA	1	0
24	J	103	CLA	1	0
26	c	612	DD6	2	0
24	B	811	CLA	1	0
24	B	805	CLA	3	0
26	h	614	DD6	1	0
26	k	315	DD6	3	0
24	6	602	CLA	2	0
29	k	312	A1L1G	2	0
25	2	211	BCR	4	0
24	A	802	CLA	2	0
24	1	301	CLA	2	0

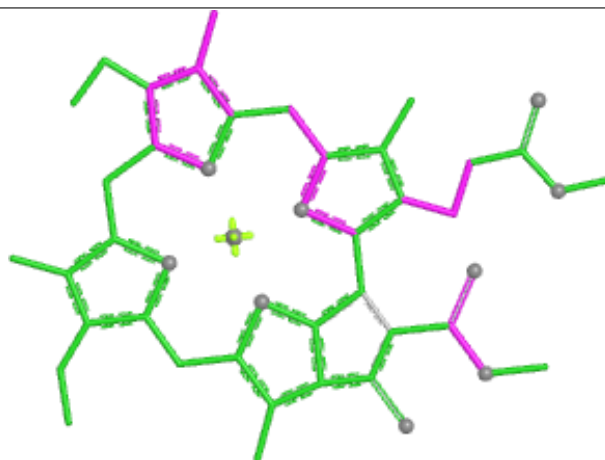
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



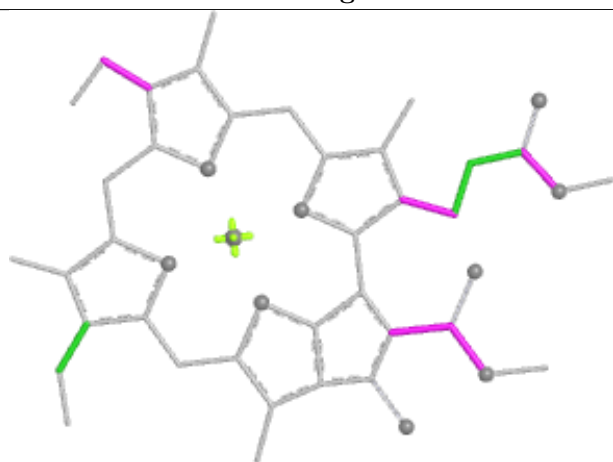
Ligand CLA 9 304



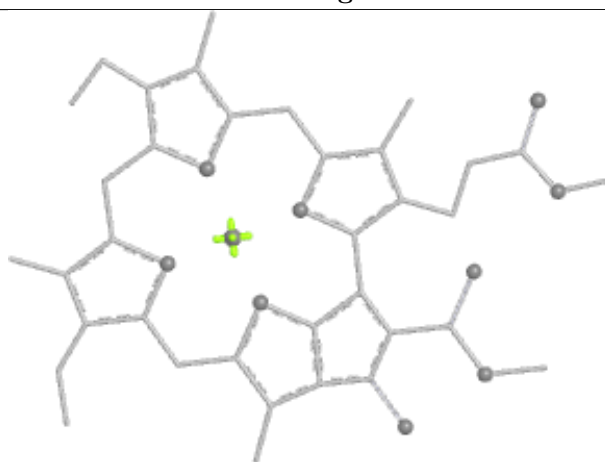
Bond lengths



Bond angles

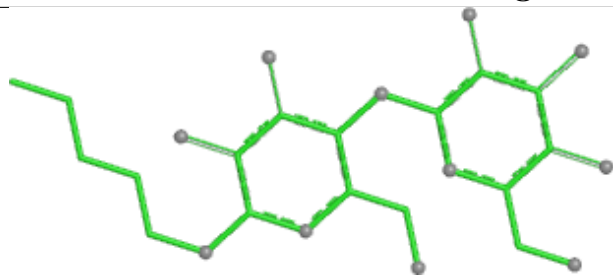


Torsions

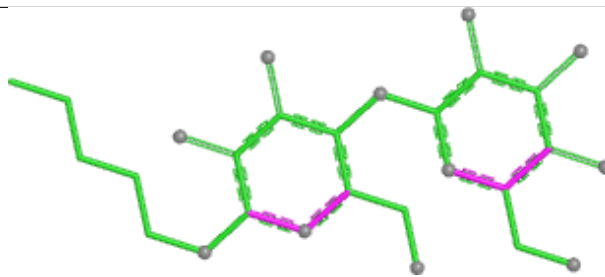


Rings

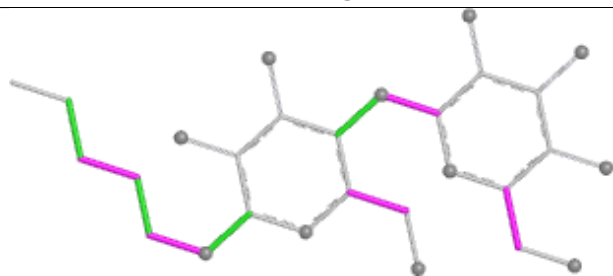
Ligand LMT h 617



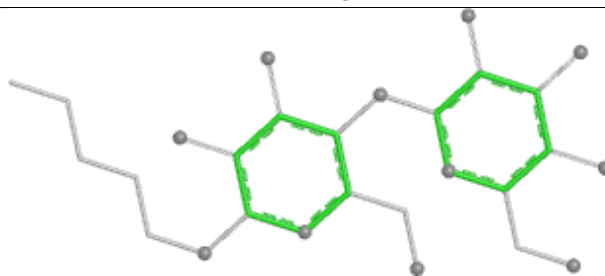
Bond lengths



Bond angles

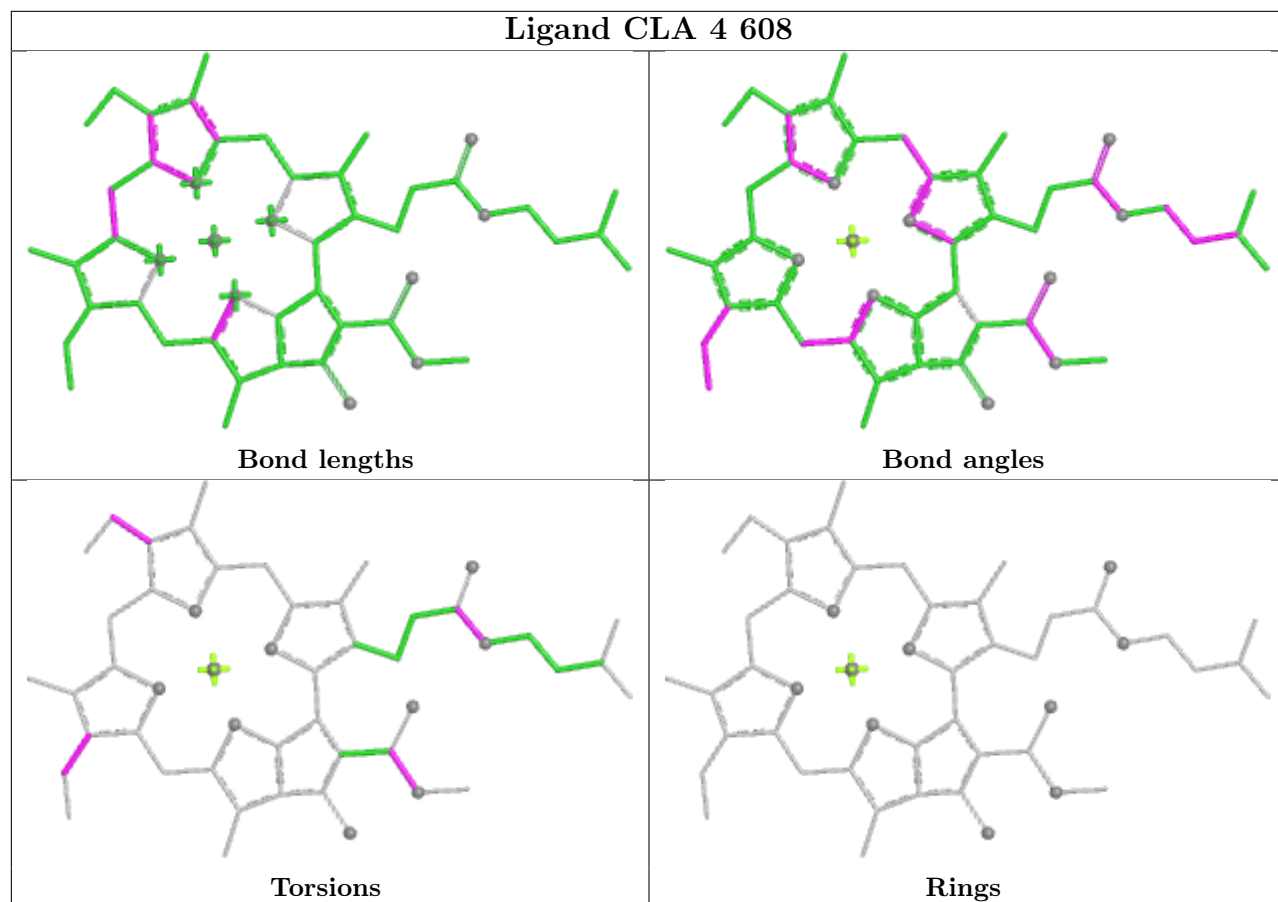


Torsions

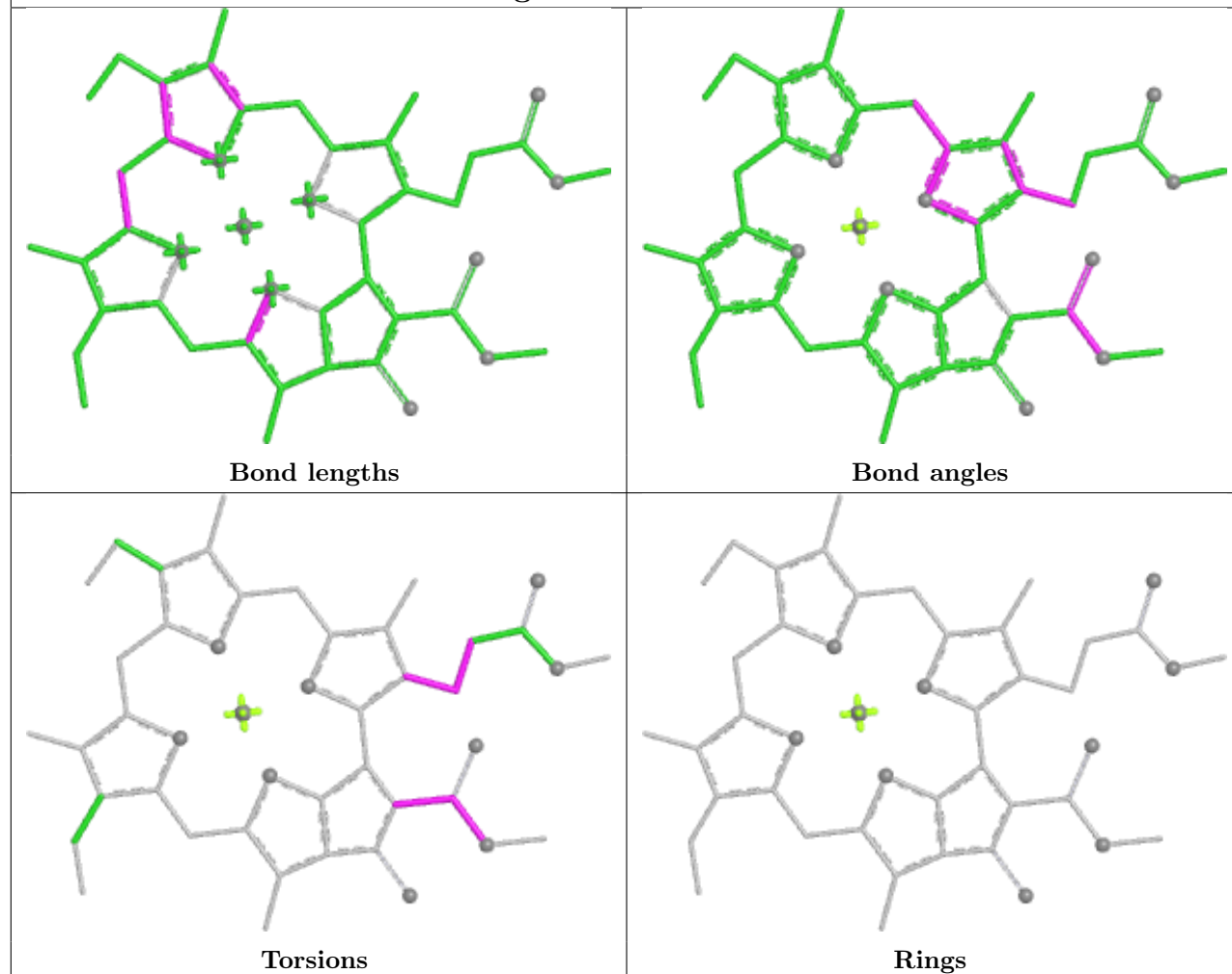


Rings

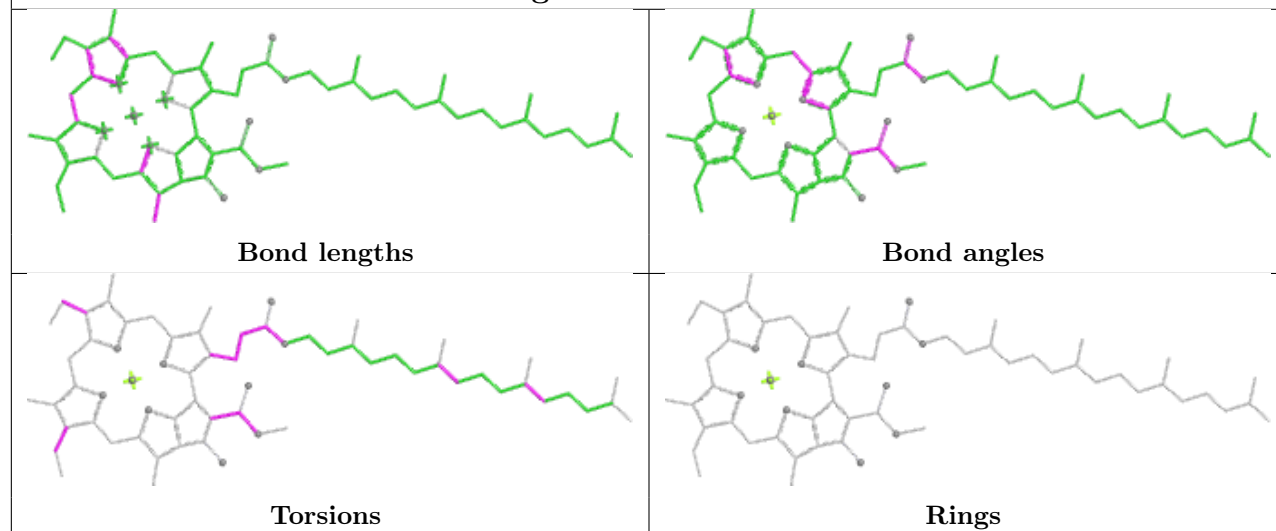
Ligand CLA 4 608

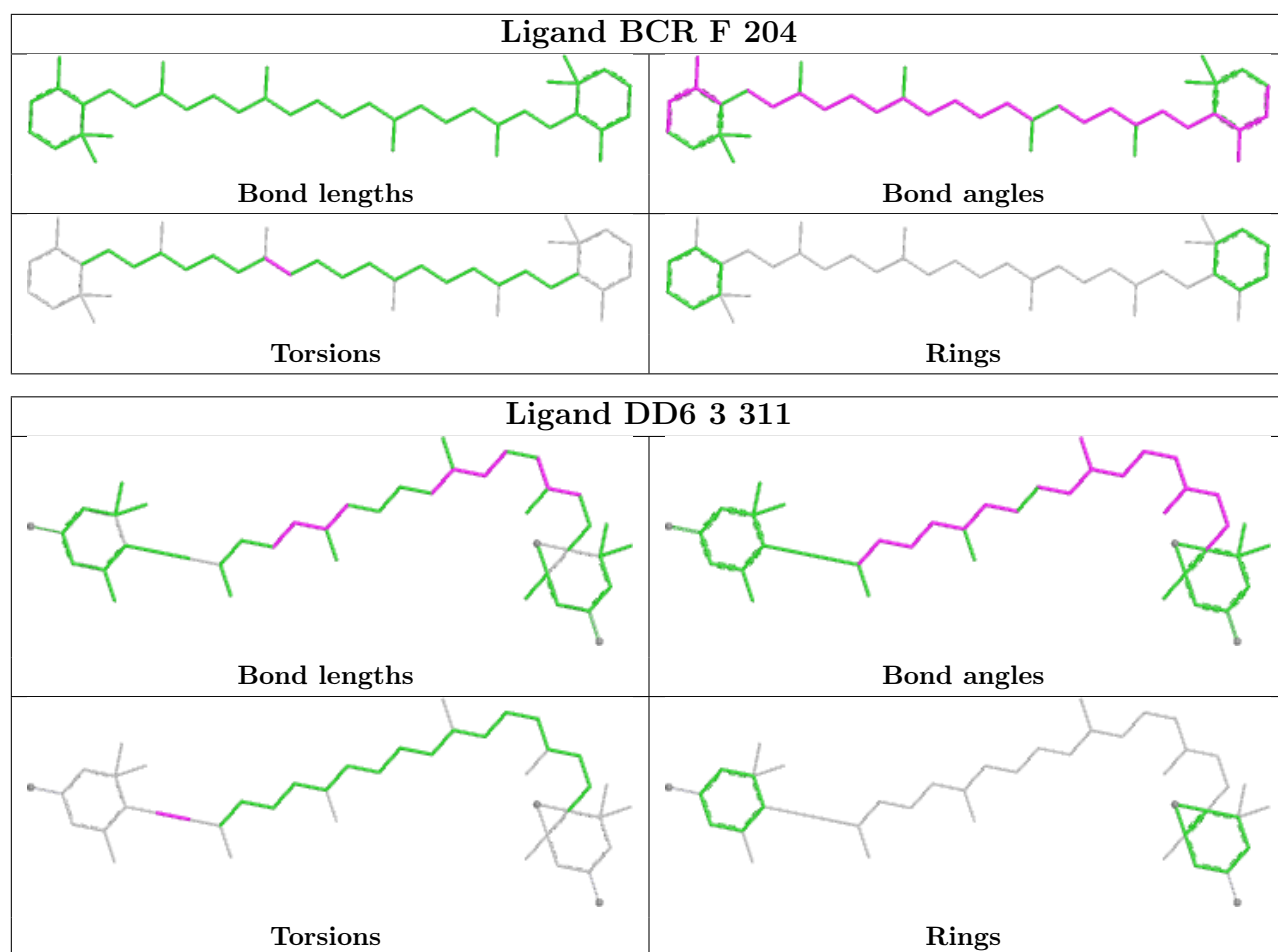


Ligand CLA B 813

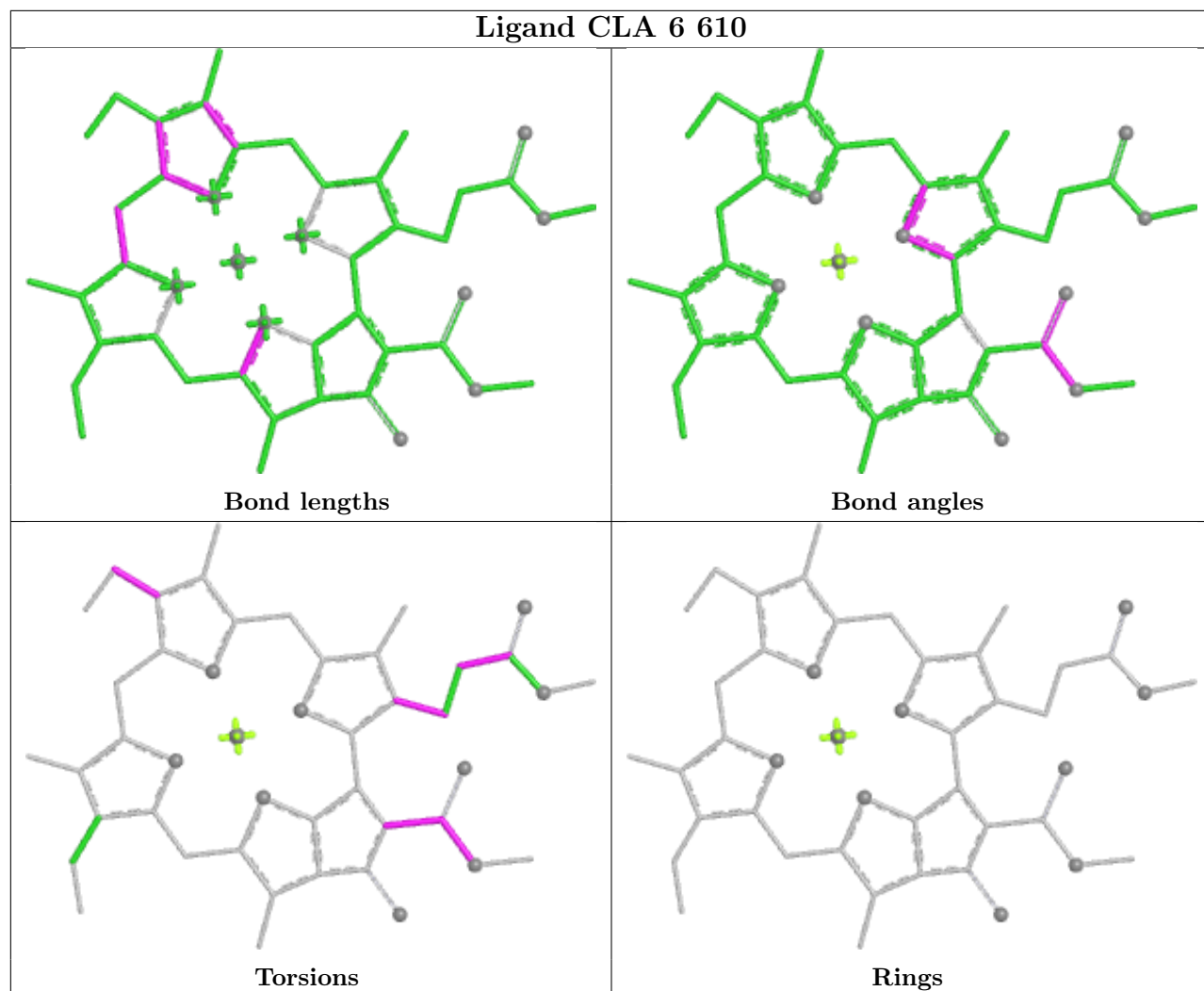


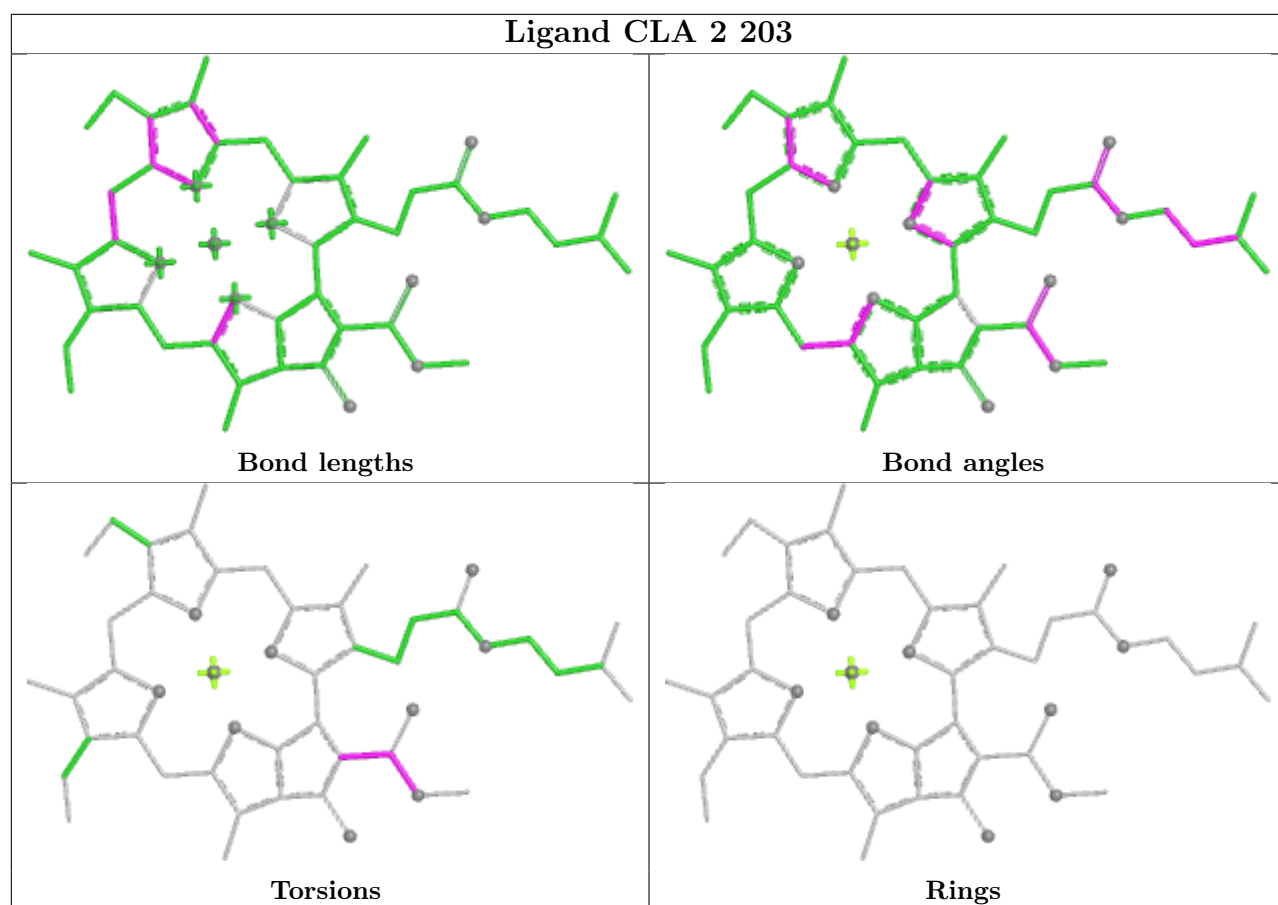
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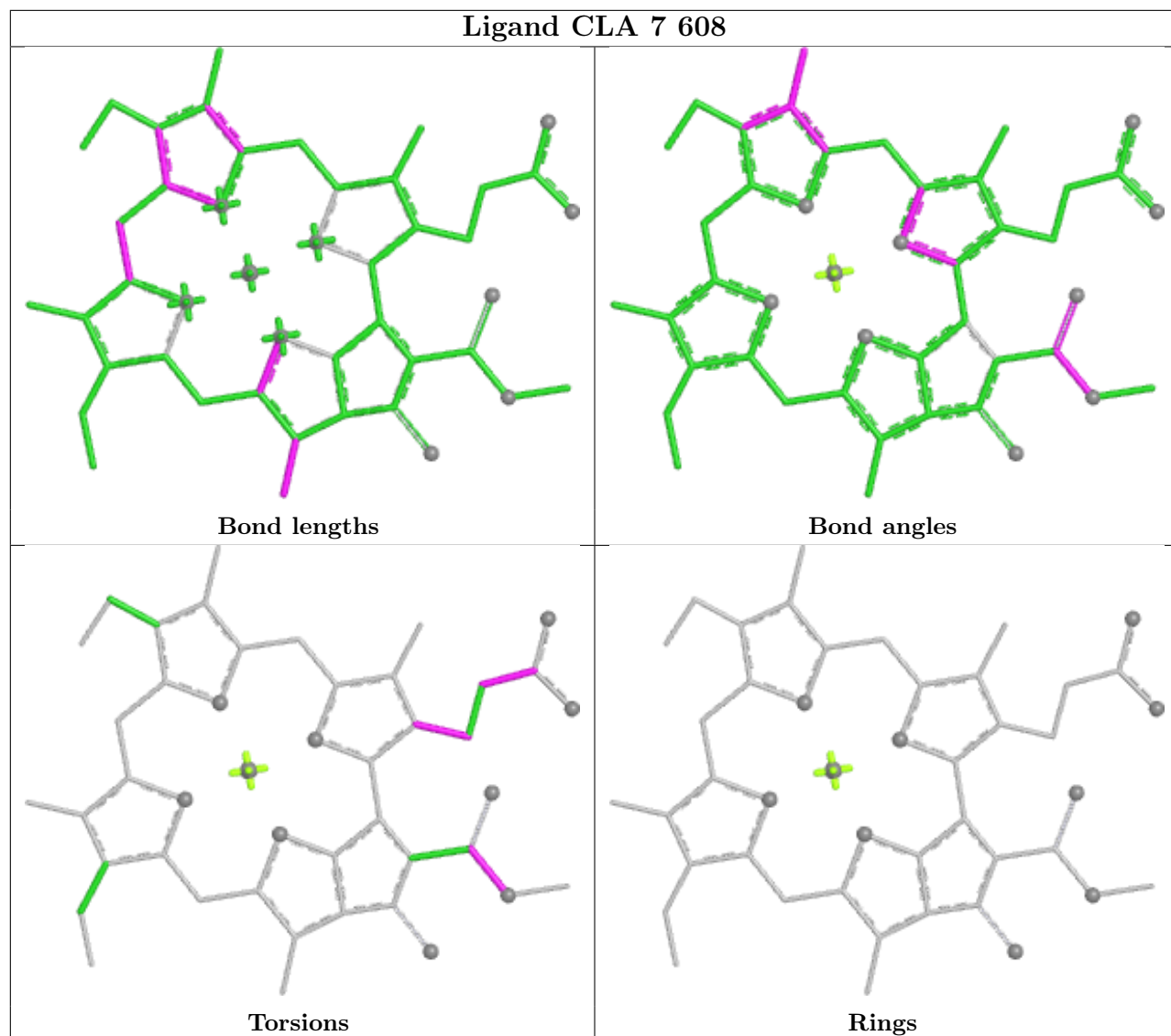


Ligand CLA 6 610

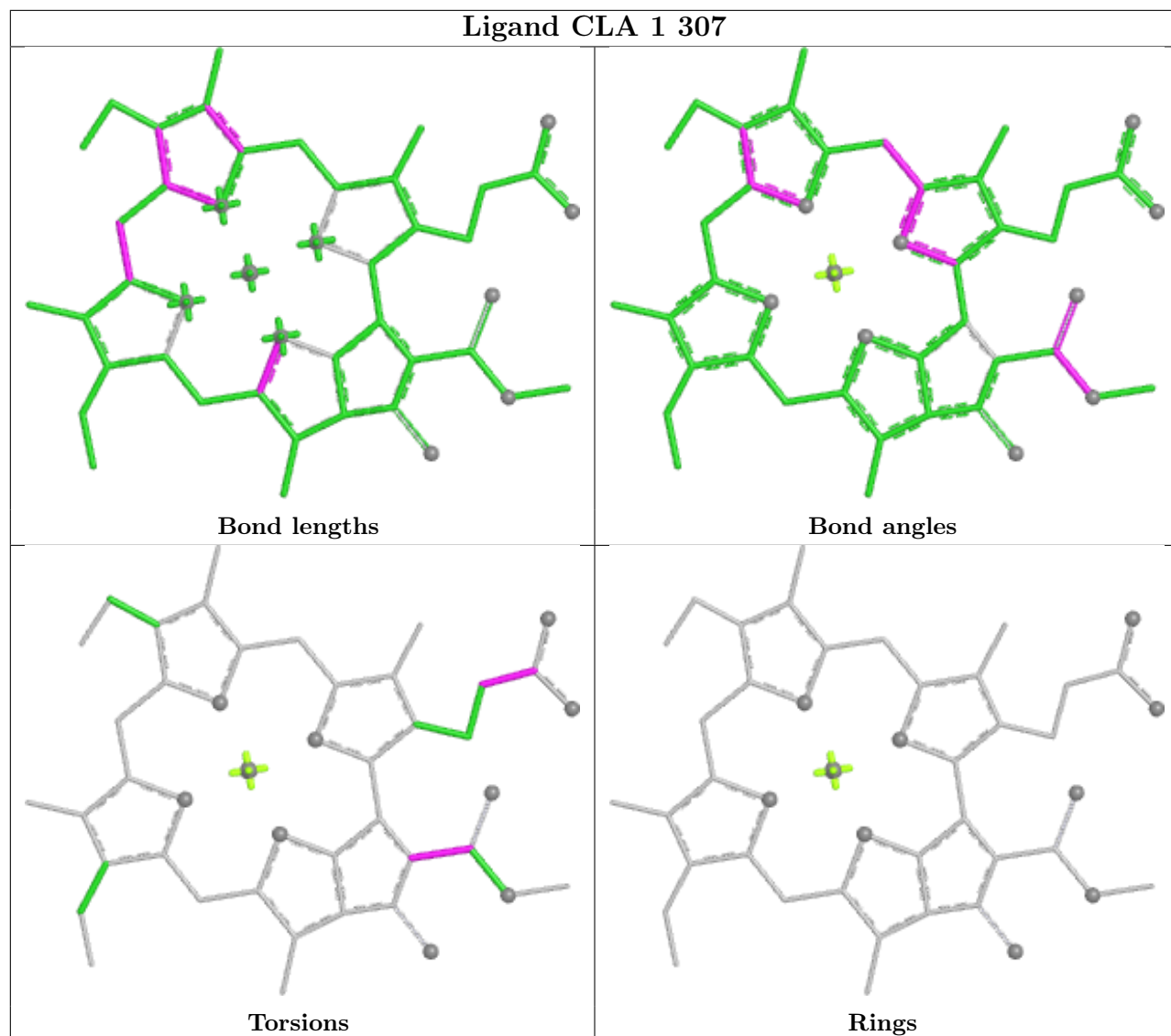




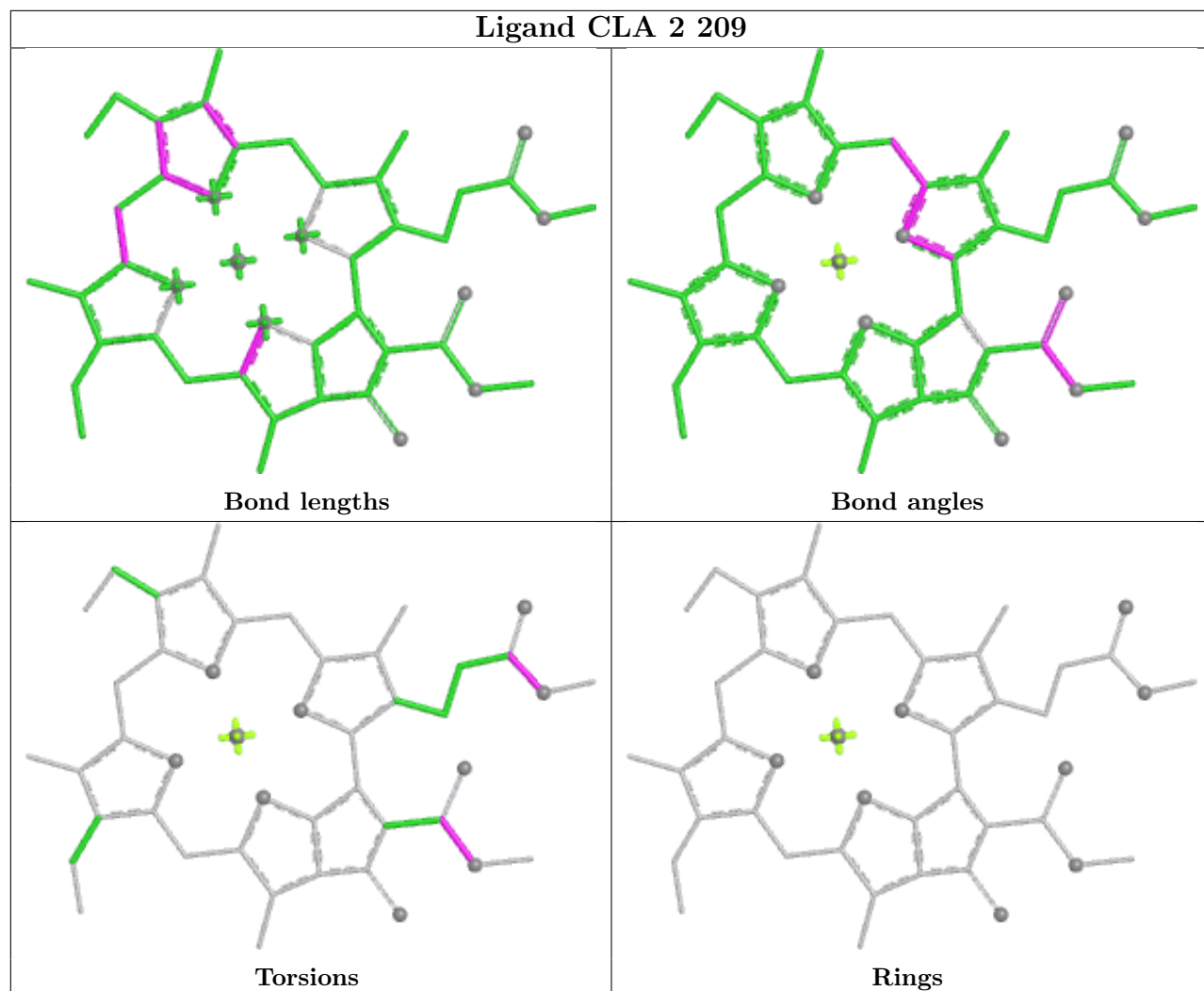
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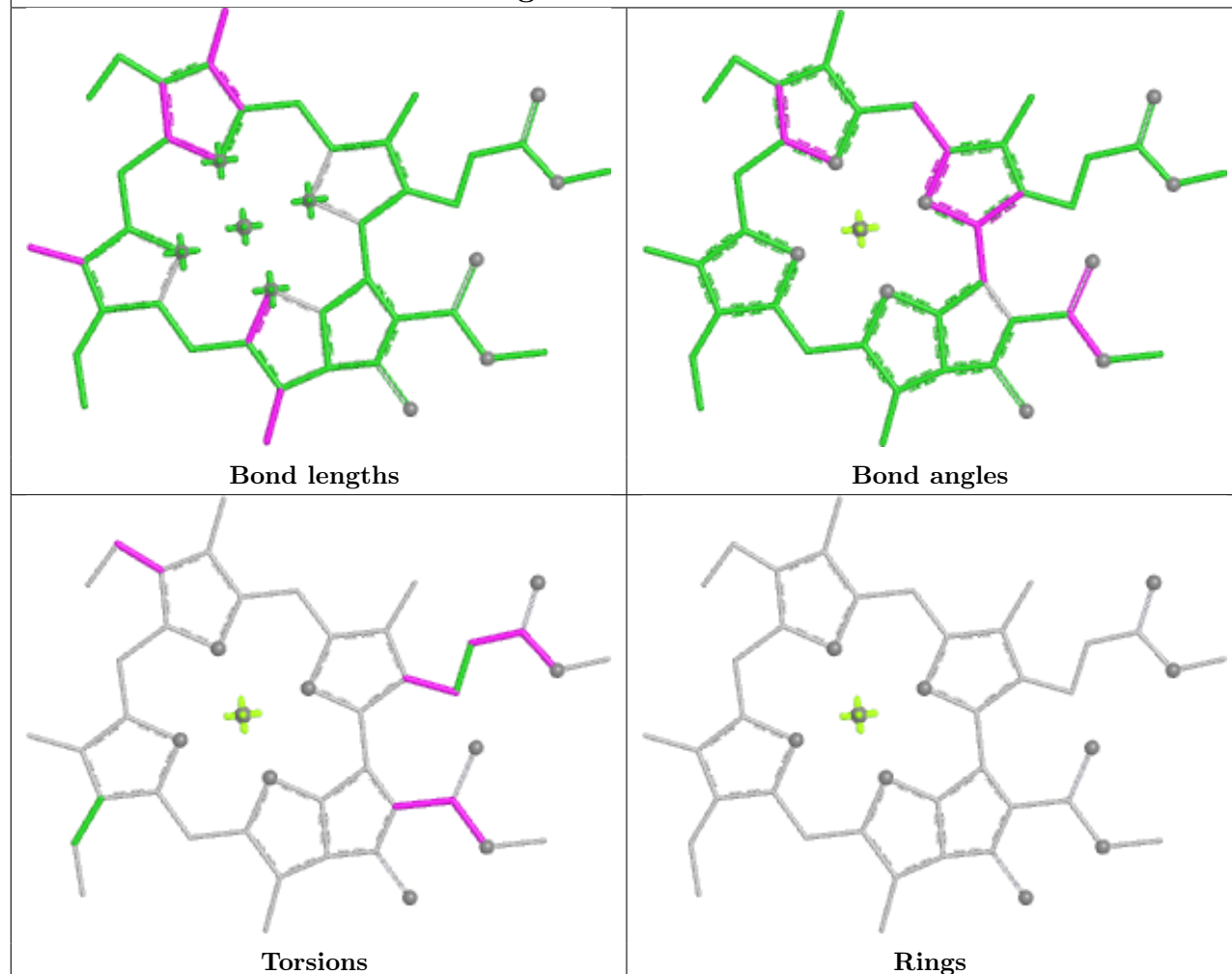
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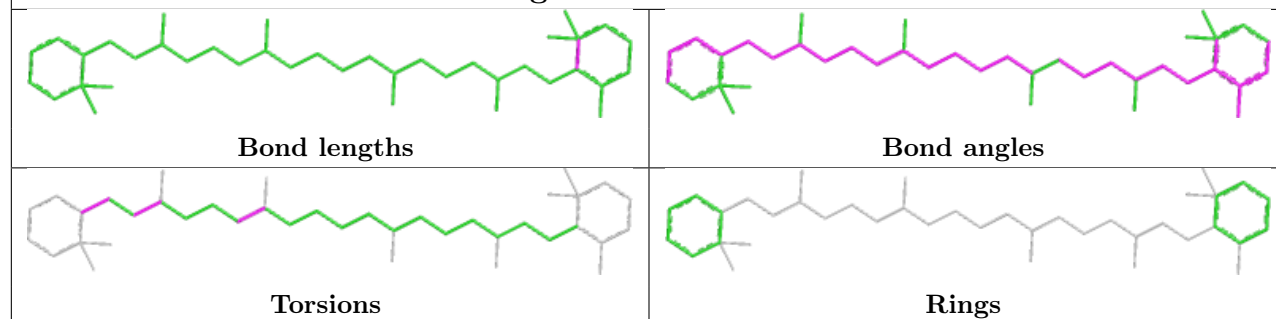
Ligand CLA 2 209



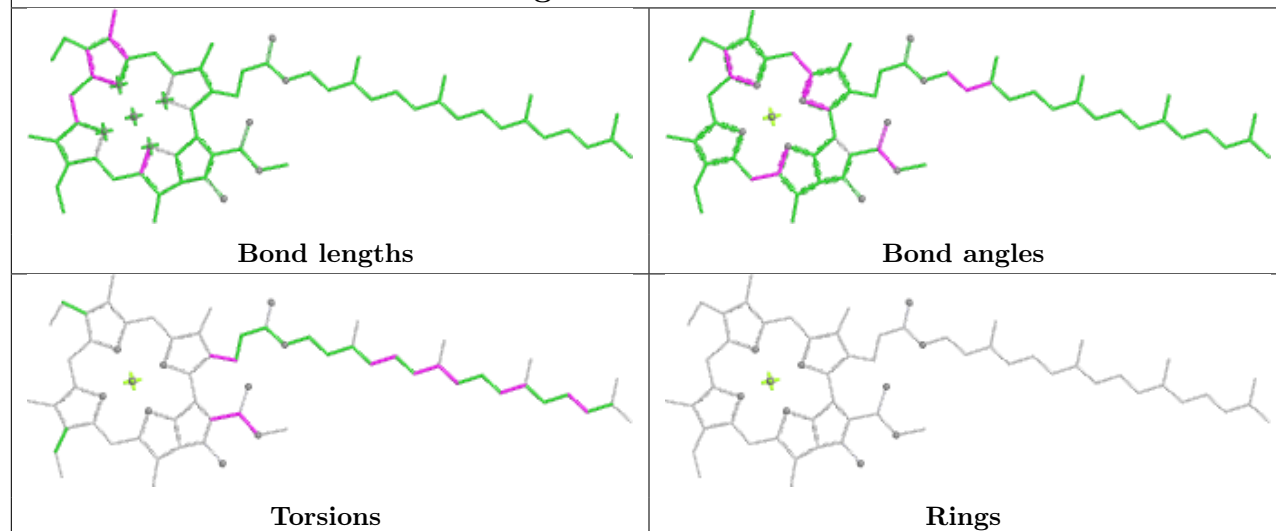
Ligand CLA 9 303



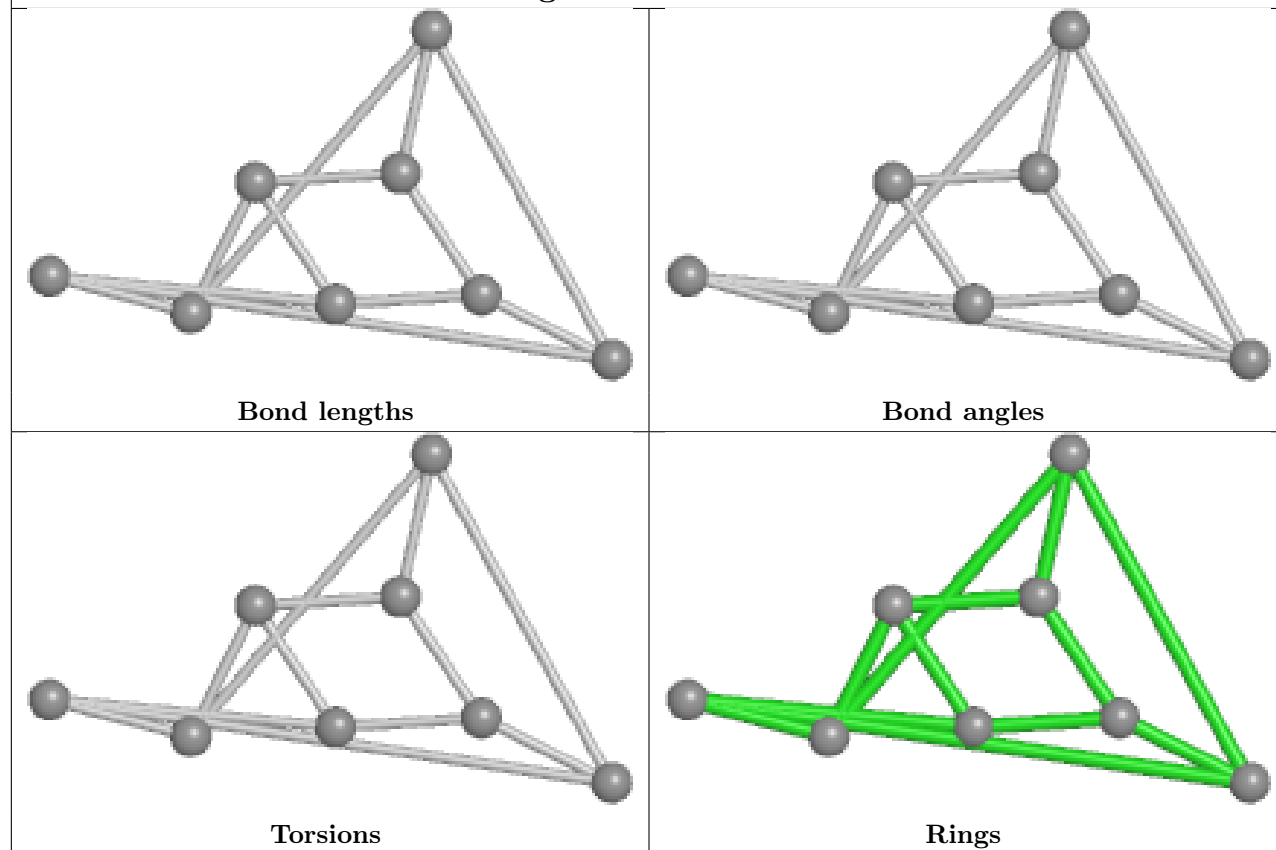
Ligand BCR A 845



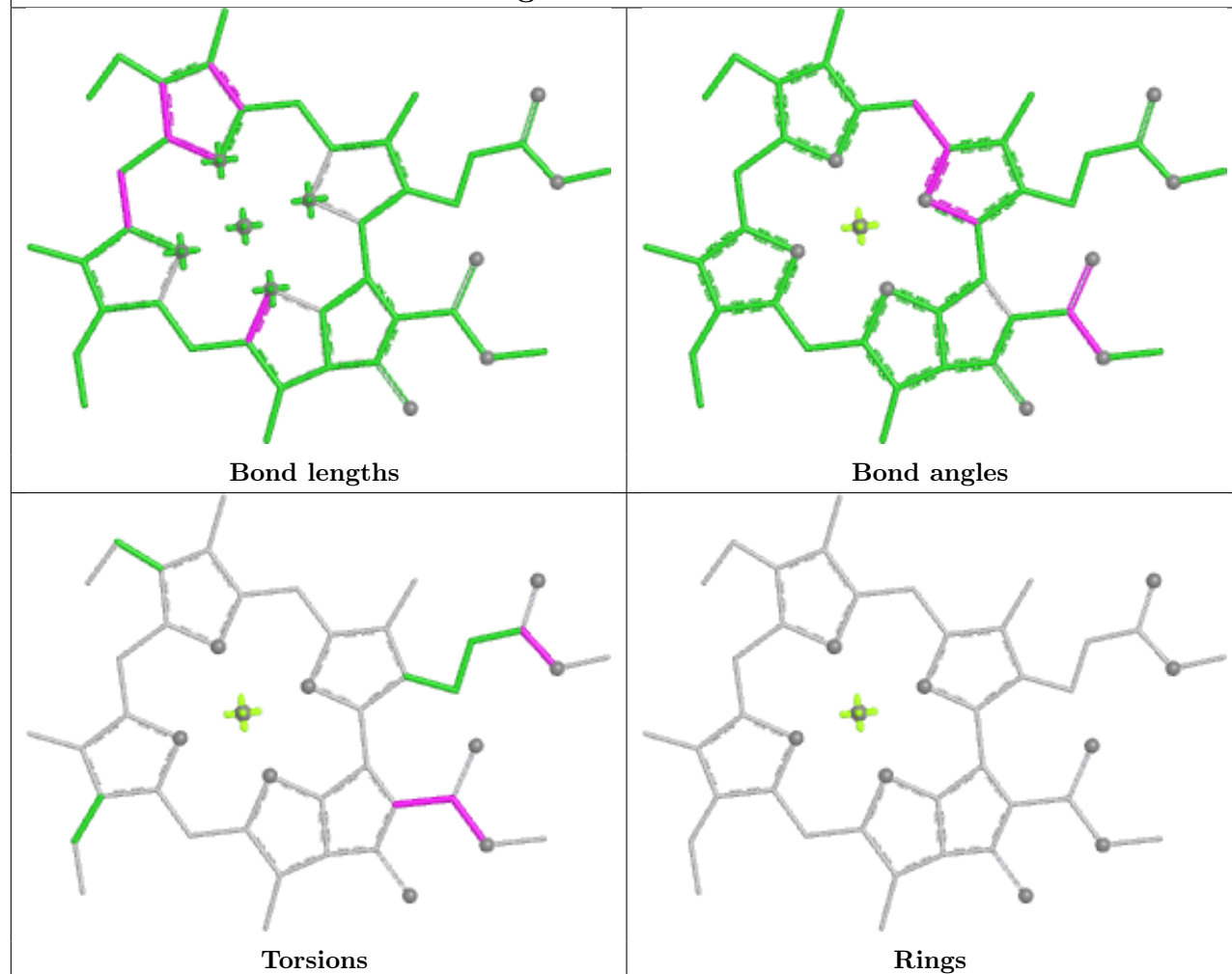
Ligand CLA F 201



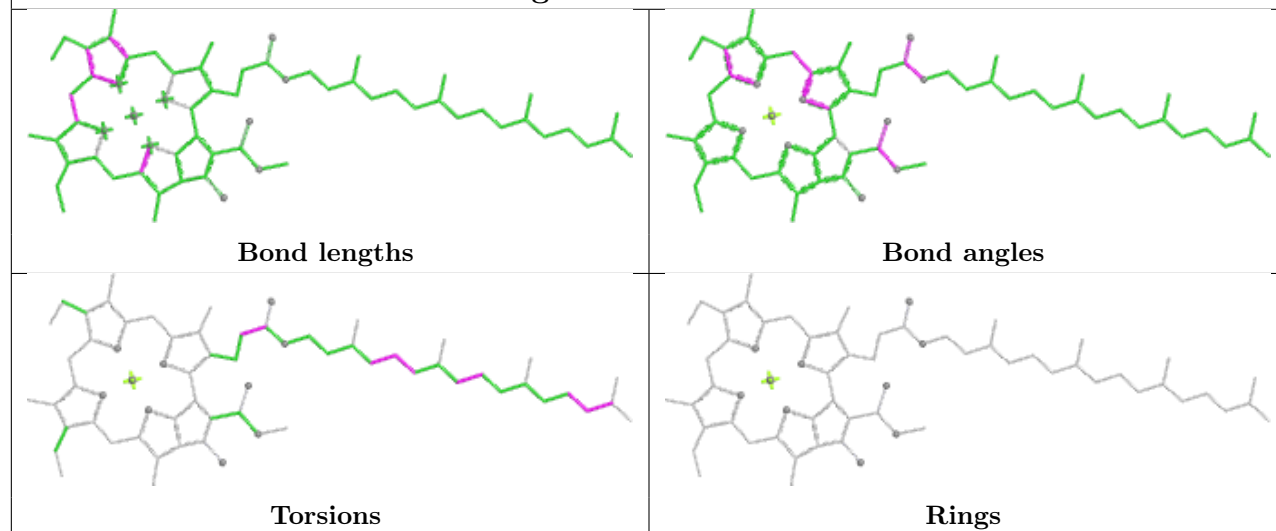
Ligand SF4 A 858

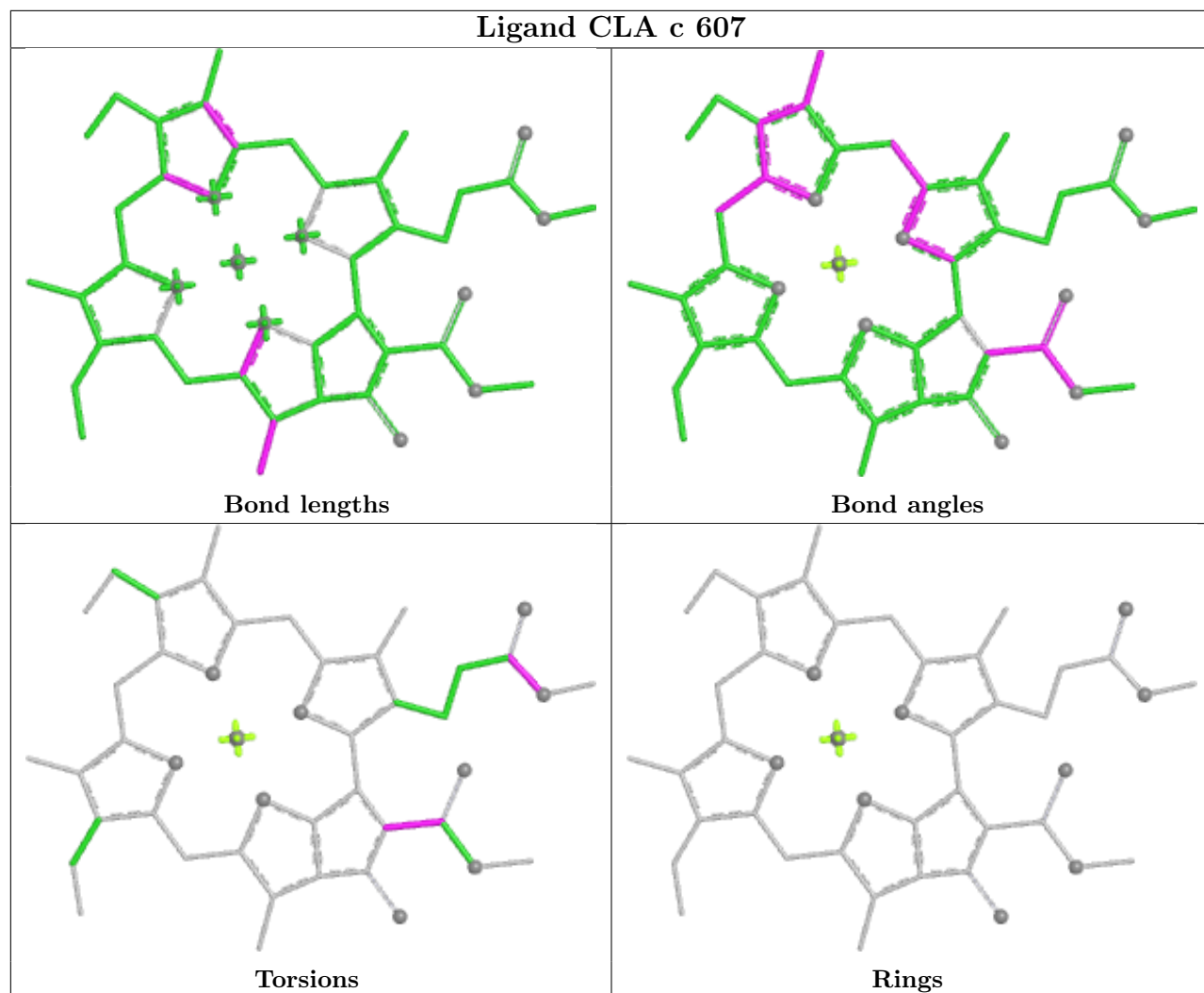


Ligand CLA 2 208

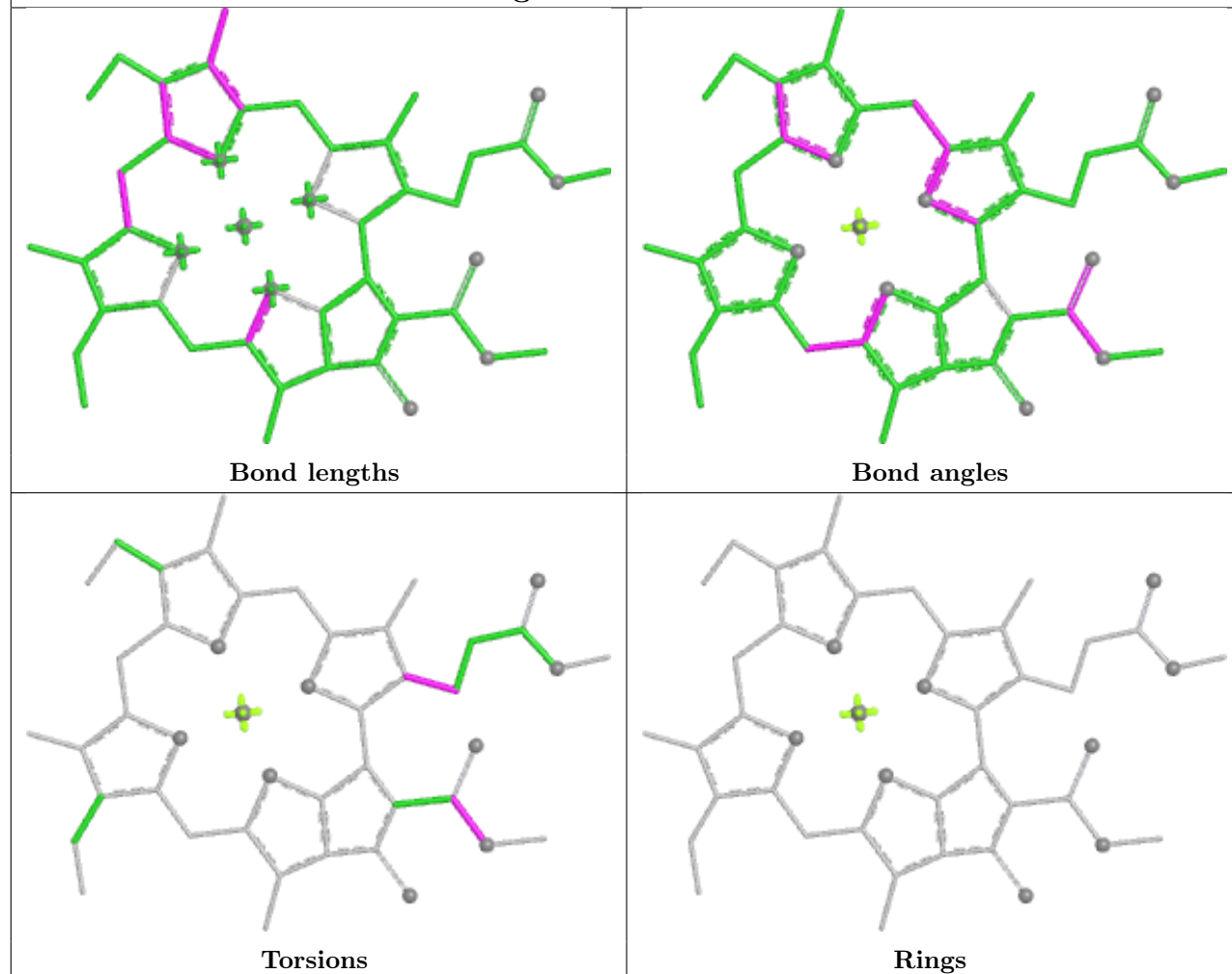


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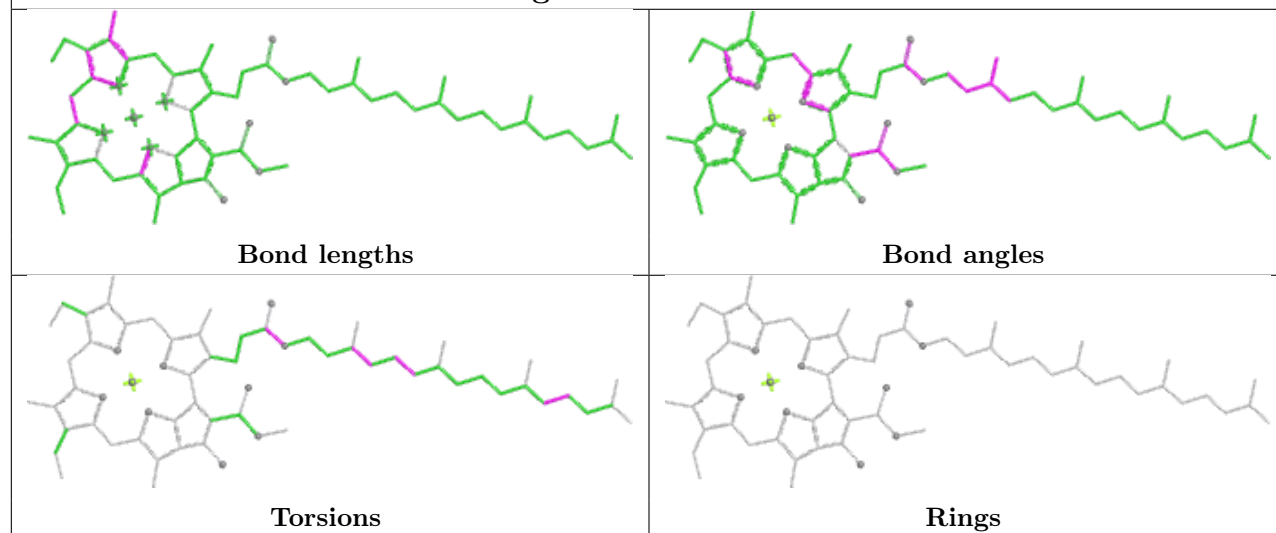




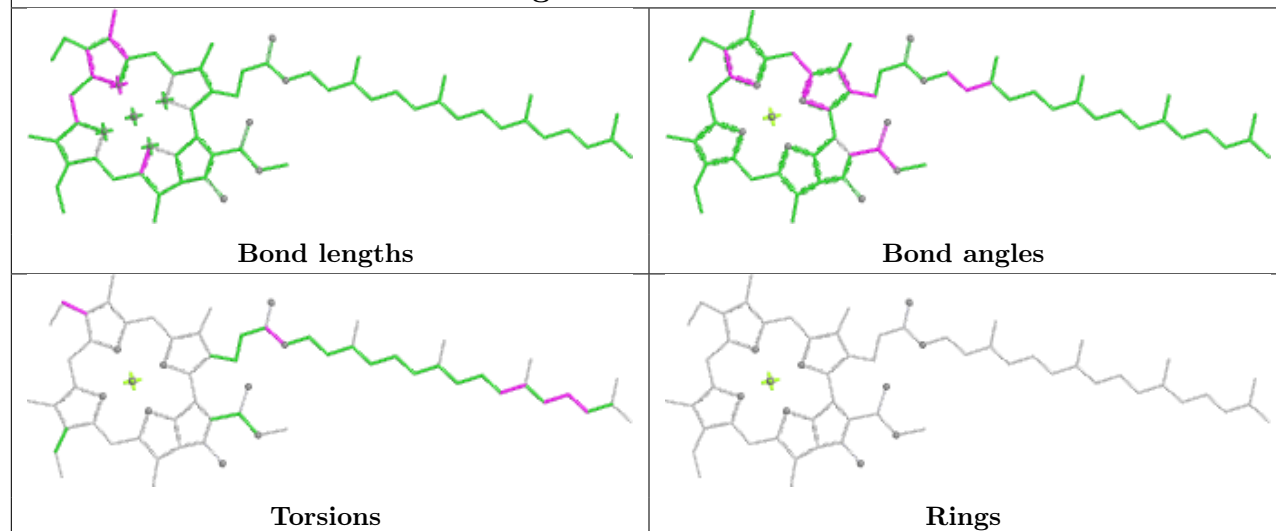
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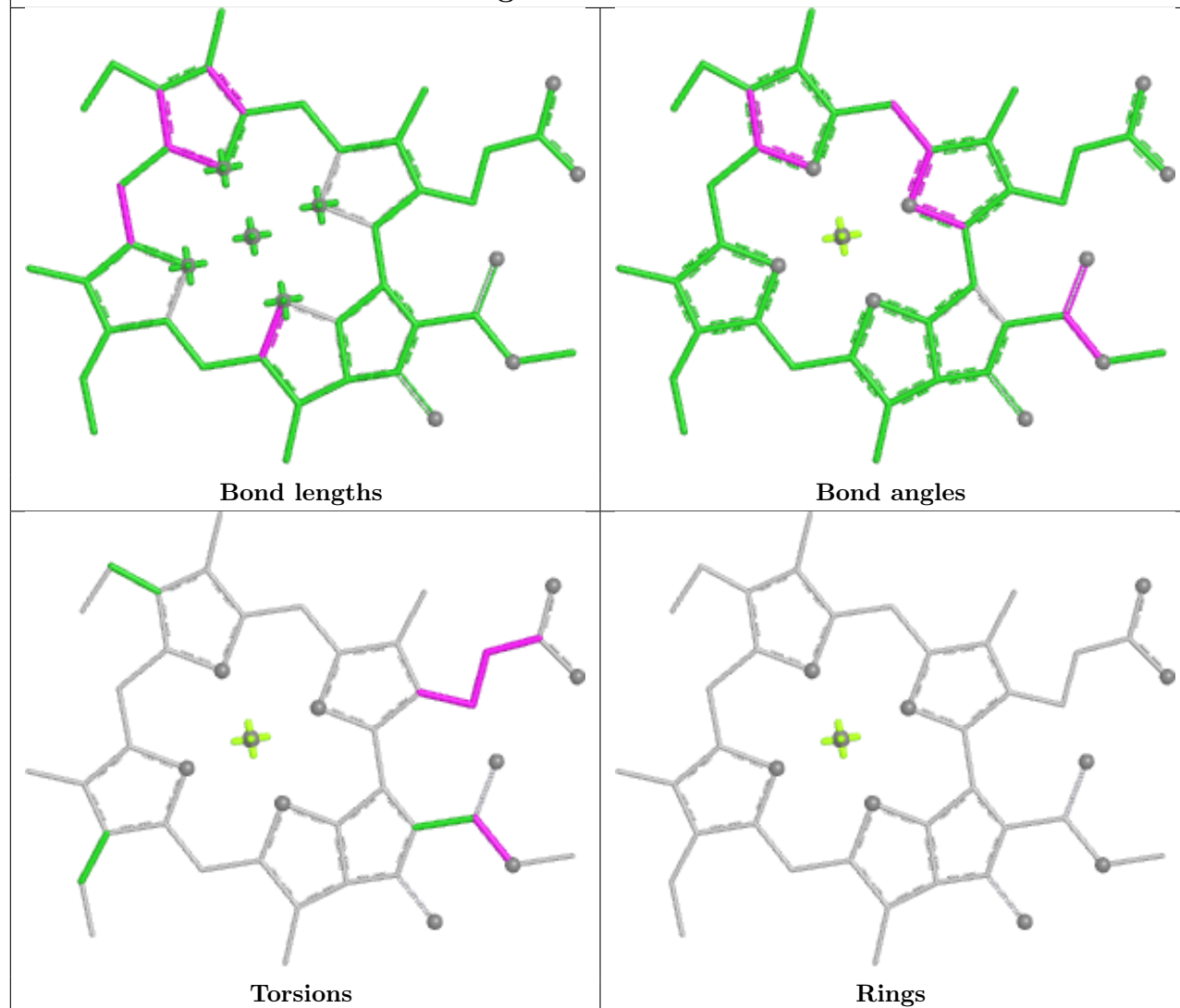
Ligand CLA B 824



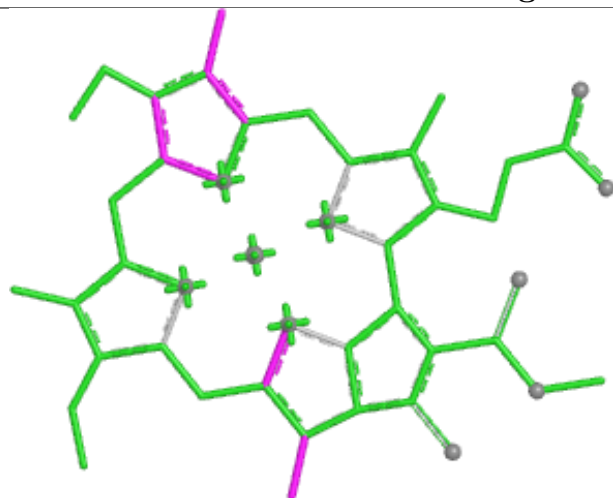
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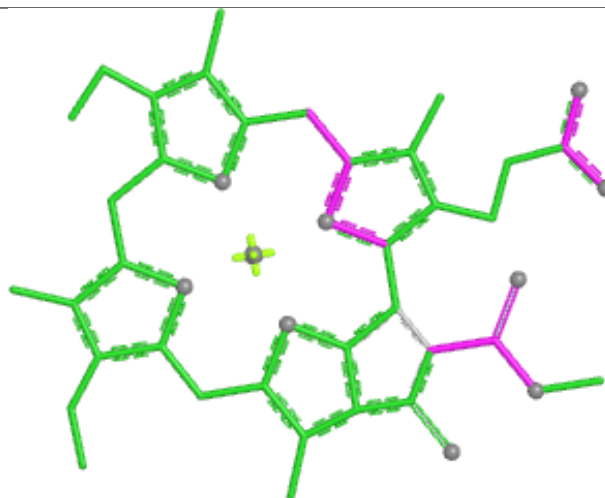
Ligand CLA t 306



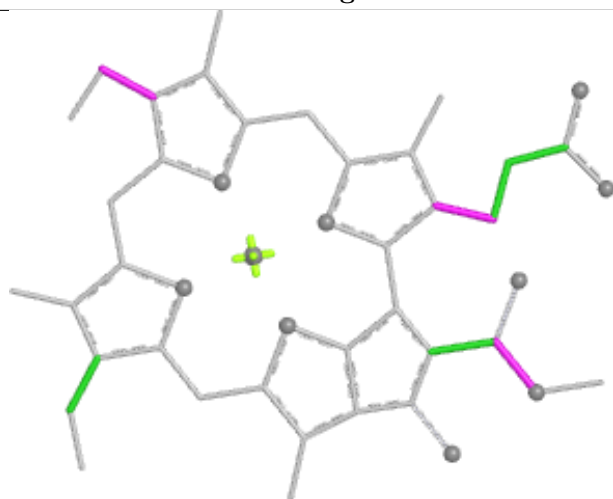
Ligand CLA 8 204



Bond lengths



Bond angles

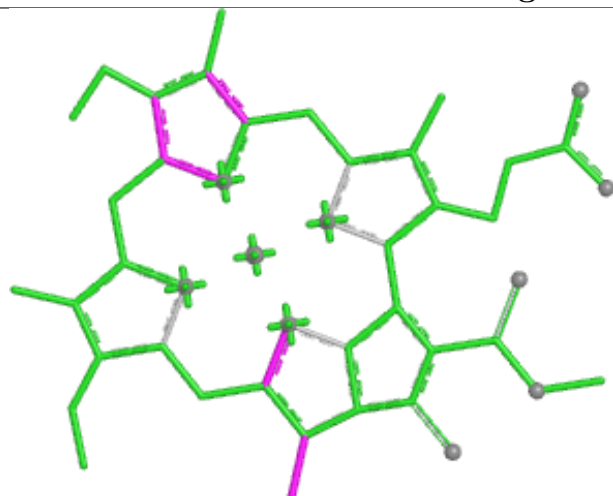


Torsions

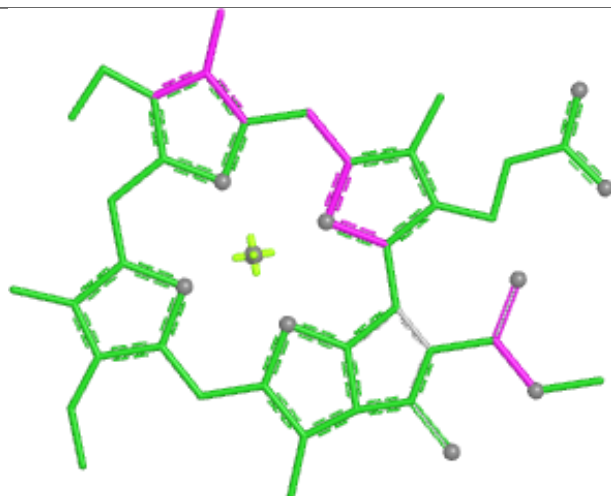


Rings

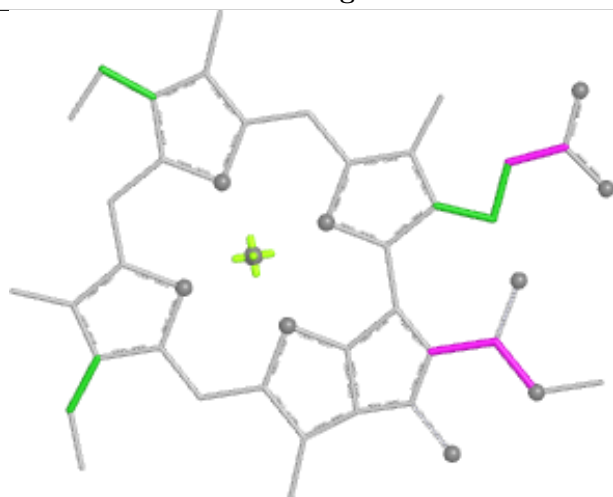
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Bond lengths



Bond angles

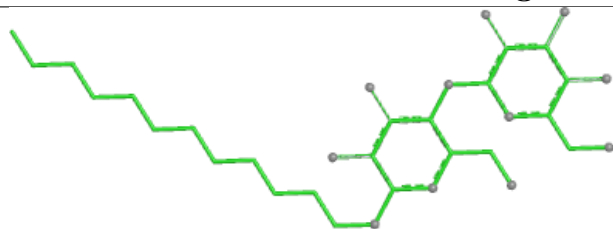


Torsions

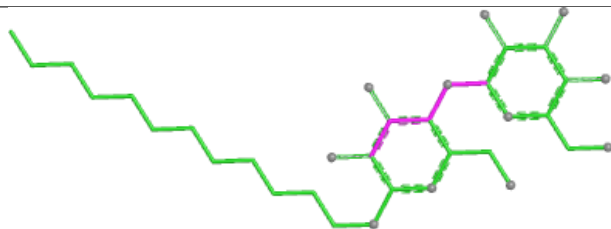


Rings

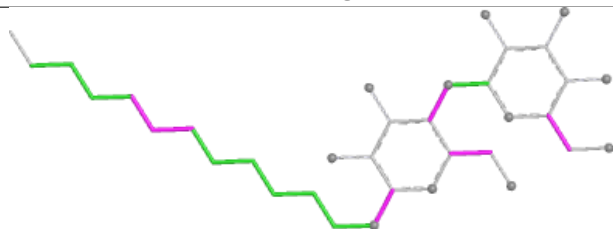
Ligand LMT 1 316



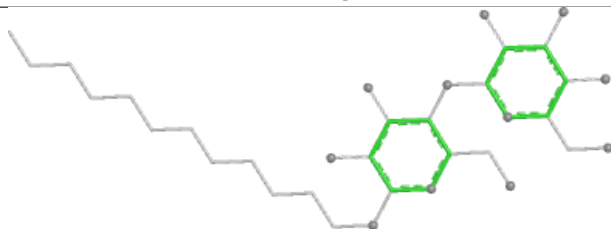
Bond lengths



Bond angles

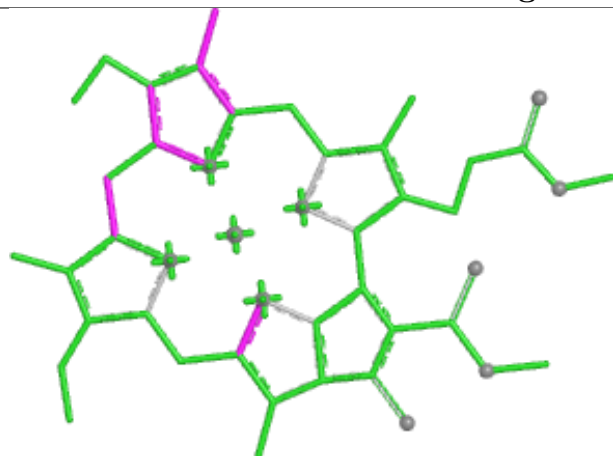


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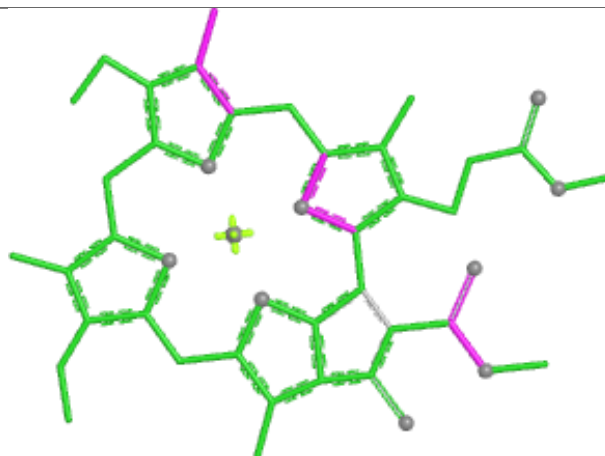


Rings

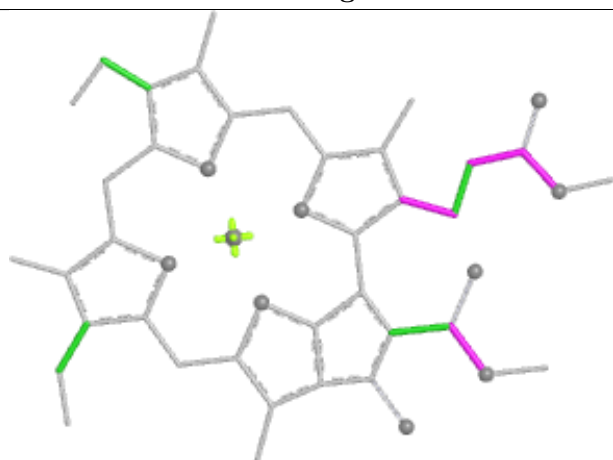
Ligand CLA 4 604



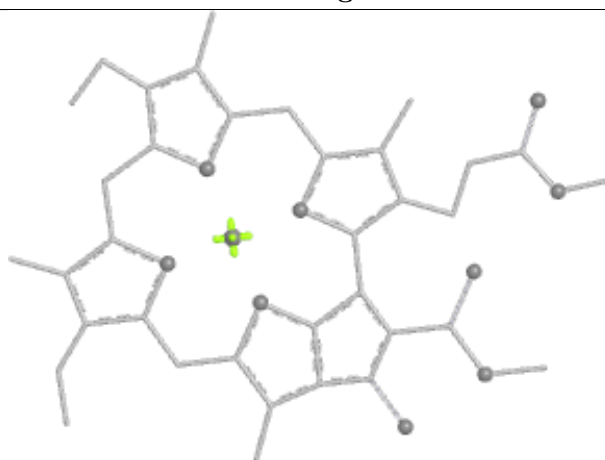
Bond lengths



Bond angles

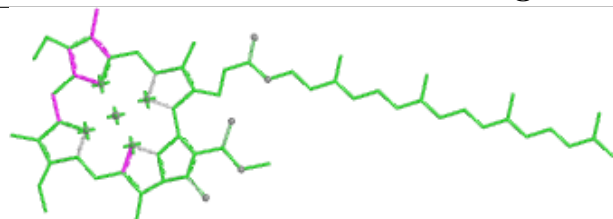


Torsions

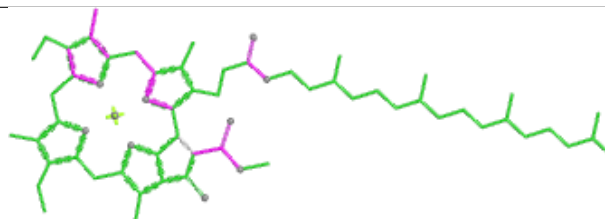


Rings

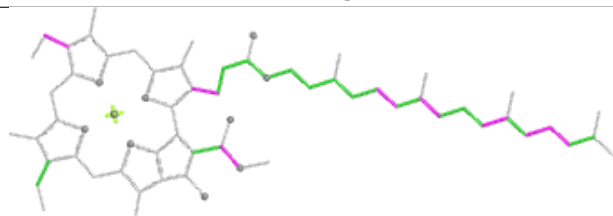
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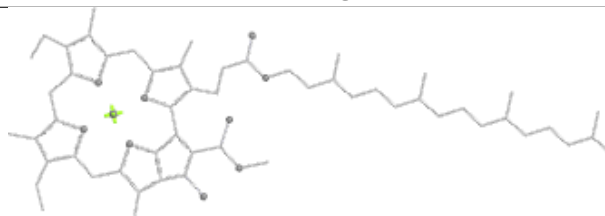
Bond lengths



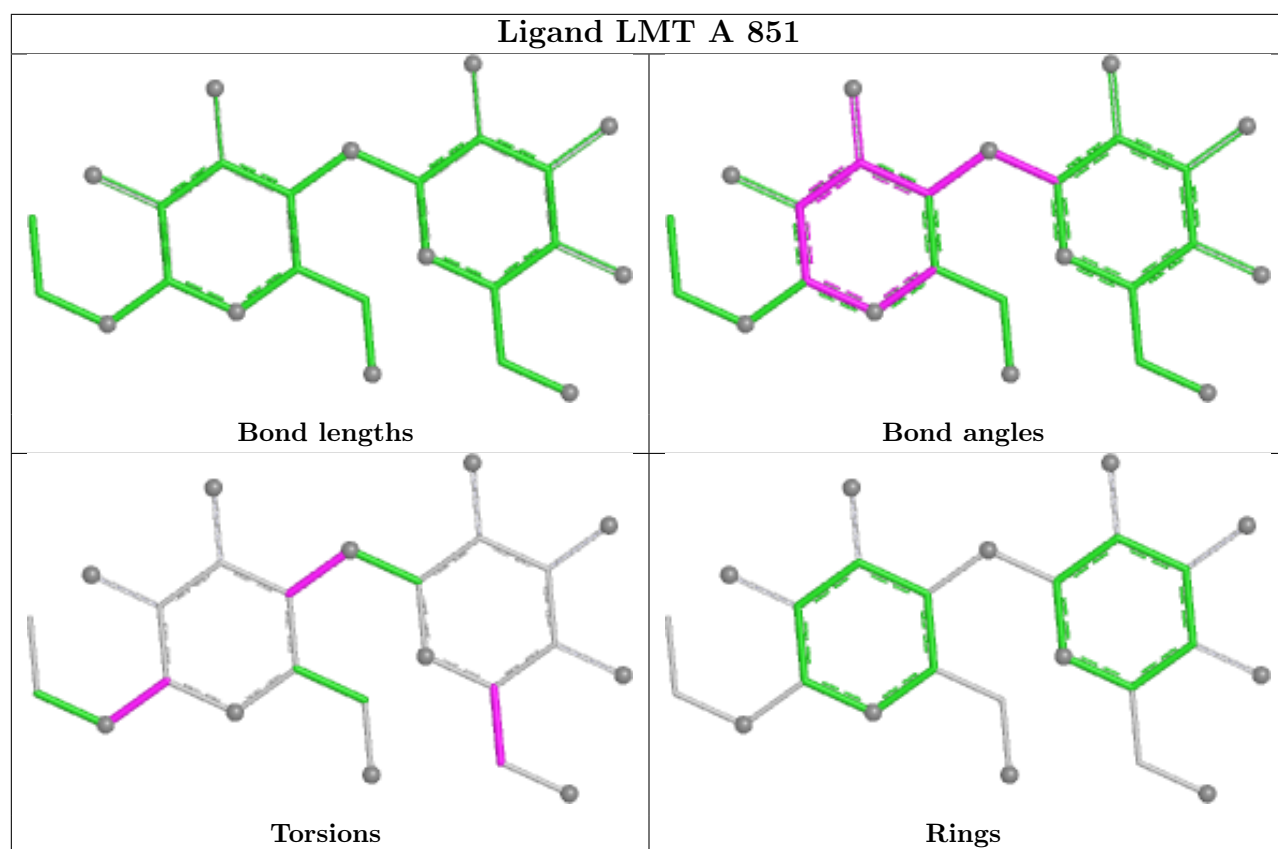
Bond angles



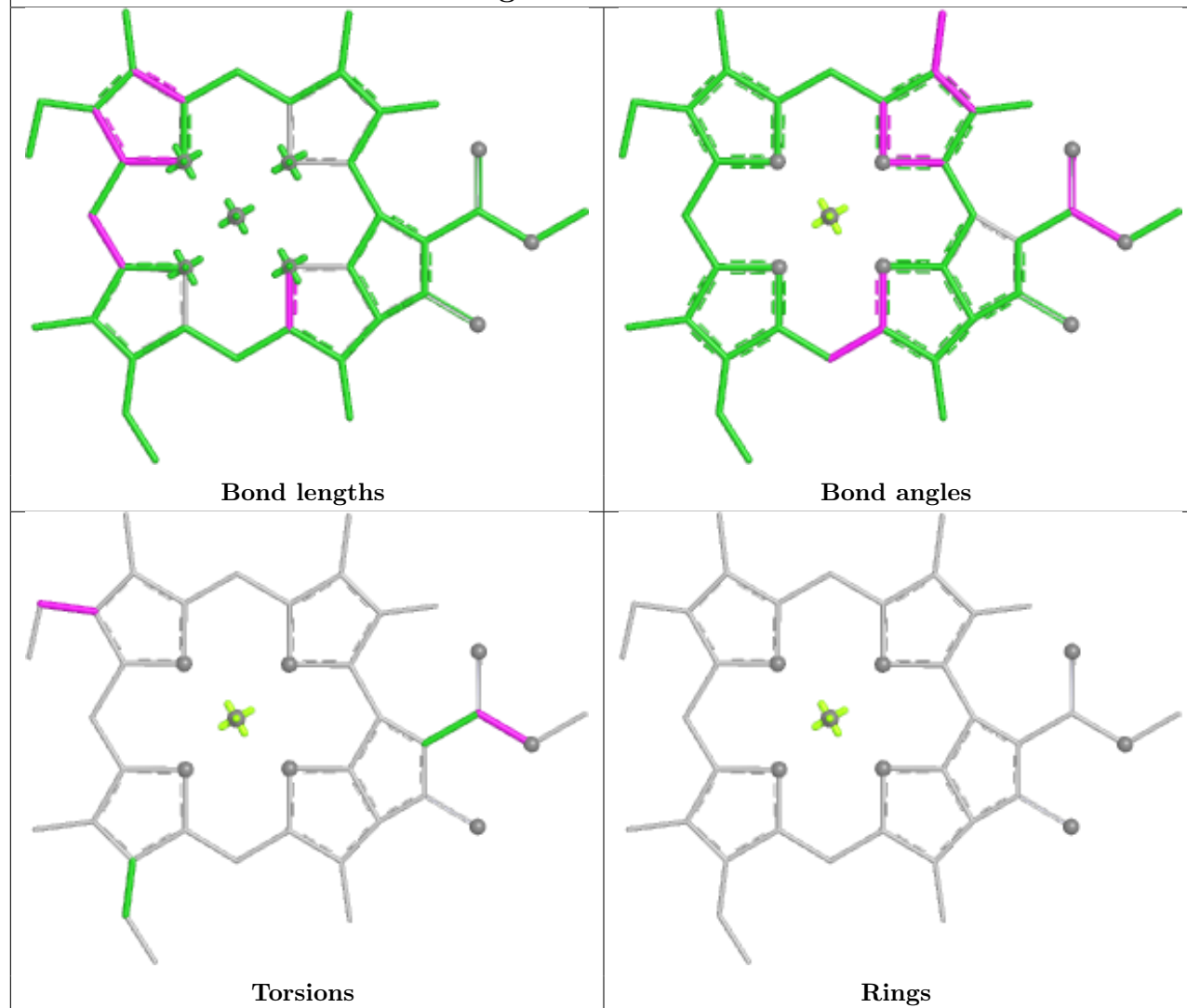
Torsions



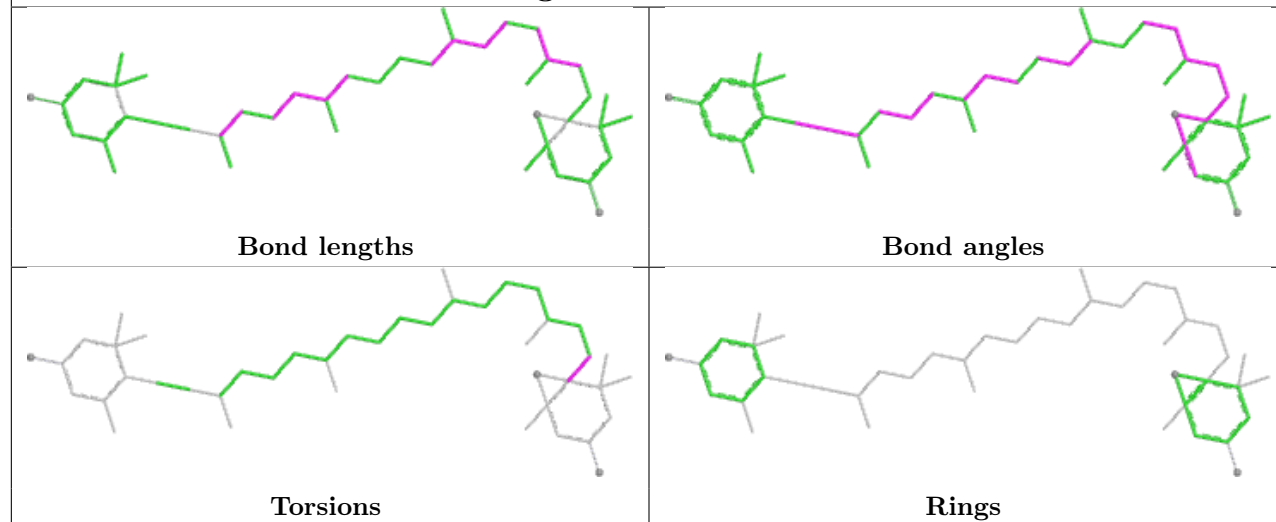
Rings



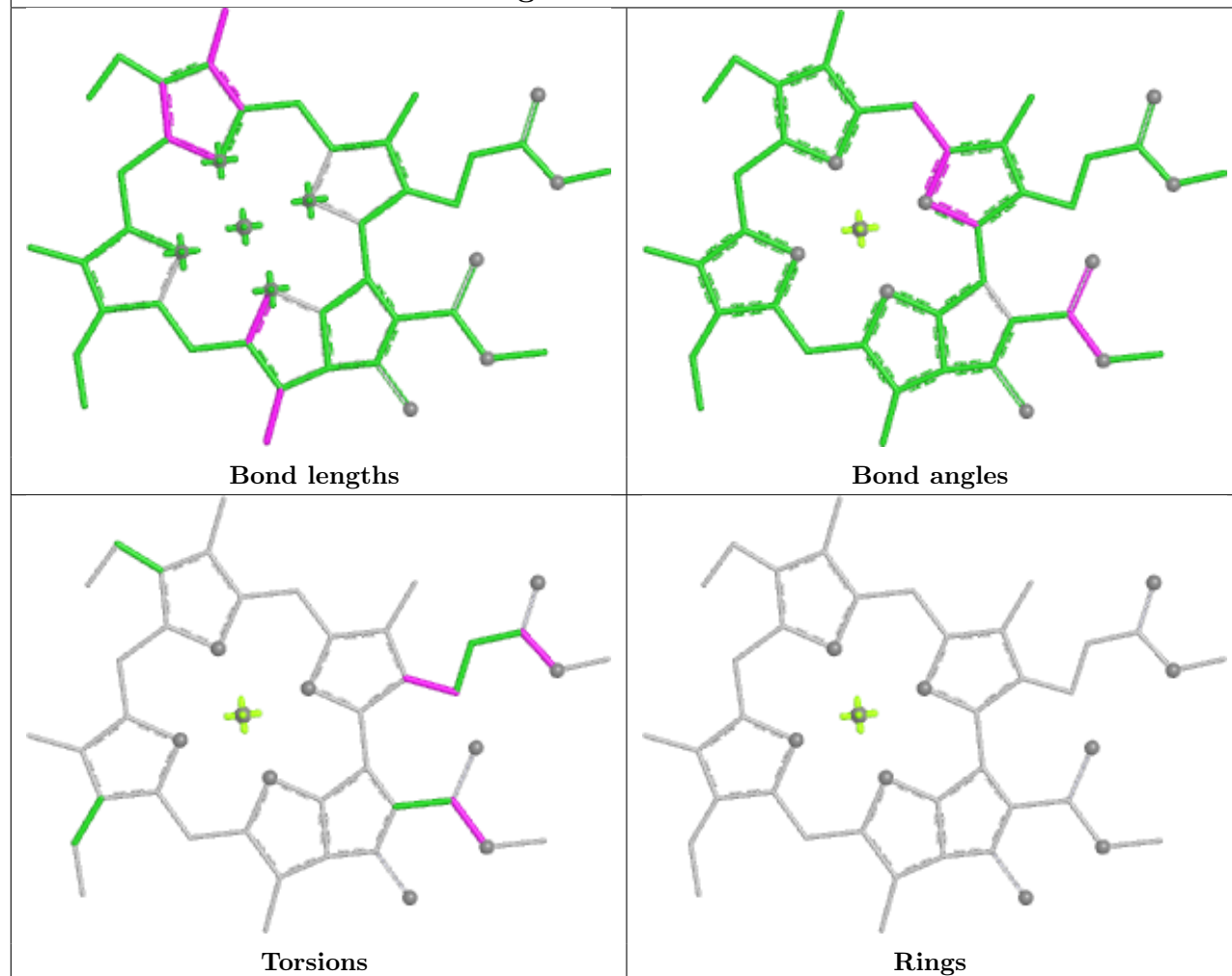
Ligand CLA 8 209



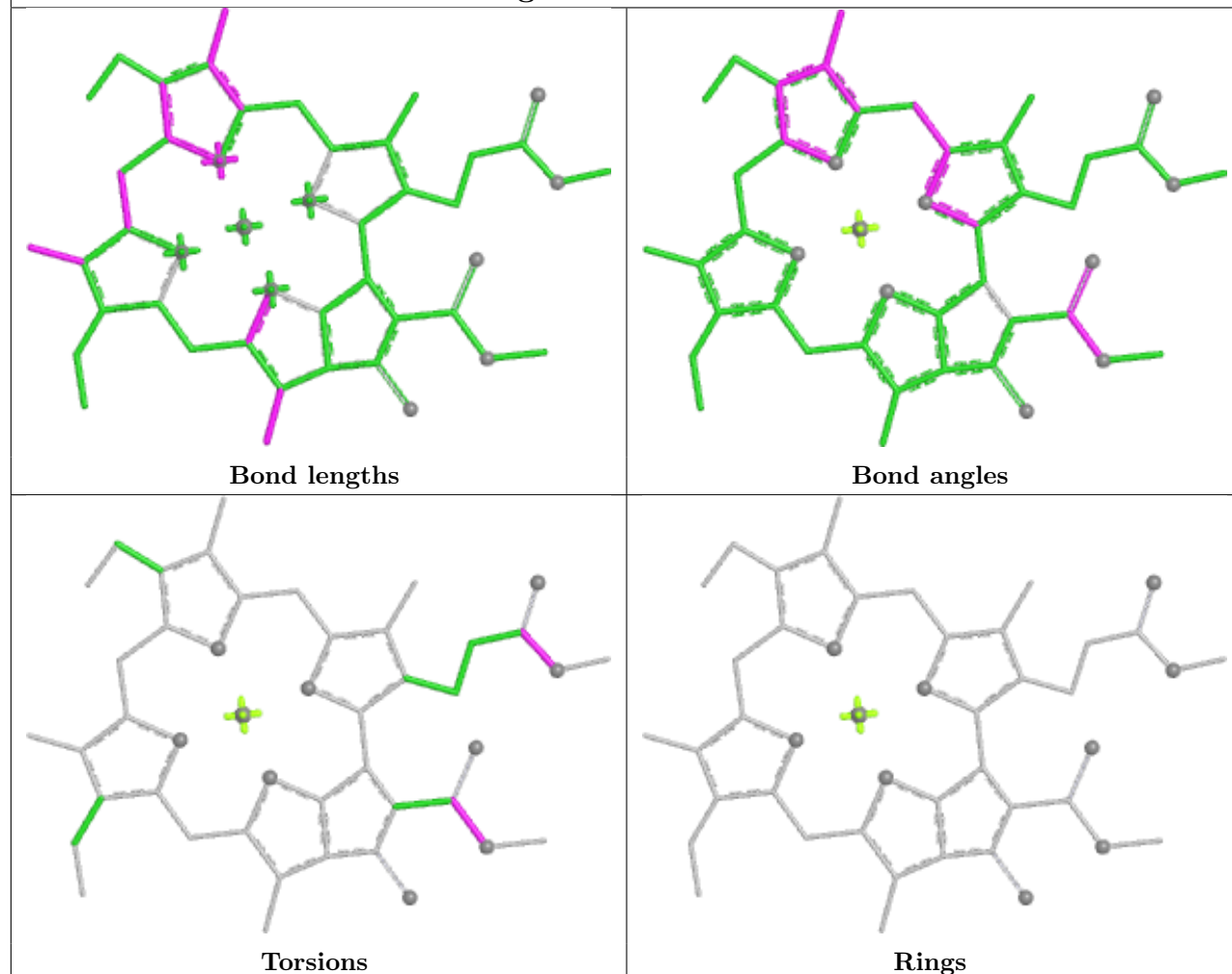
Ligand DD6 k 314



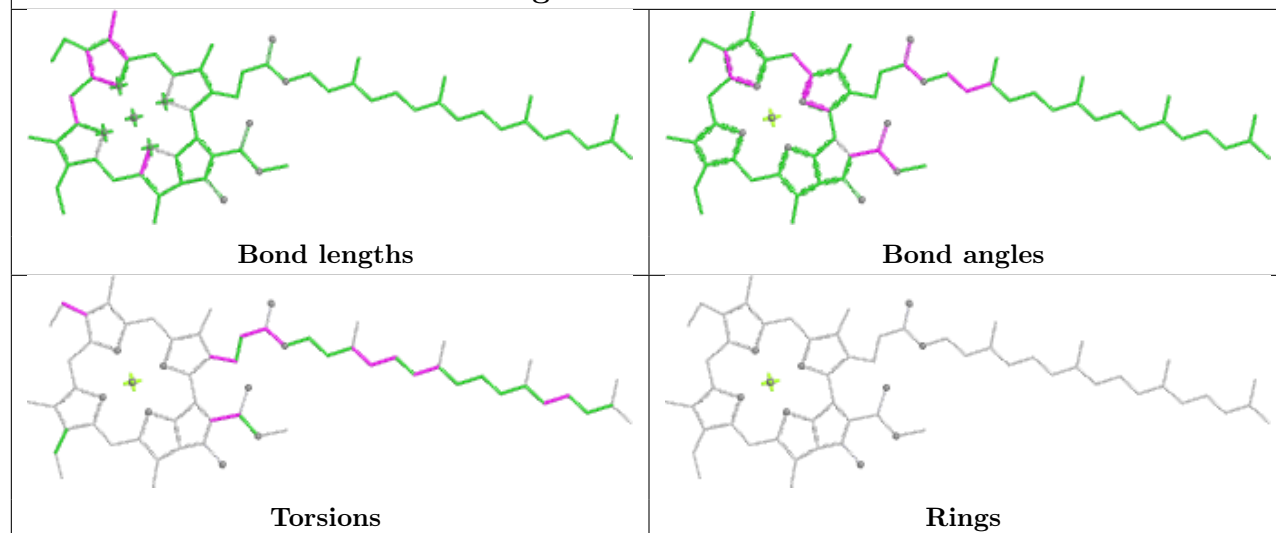
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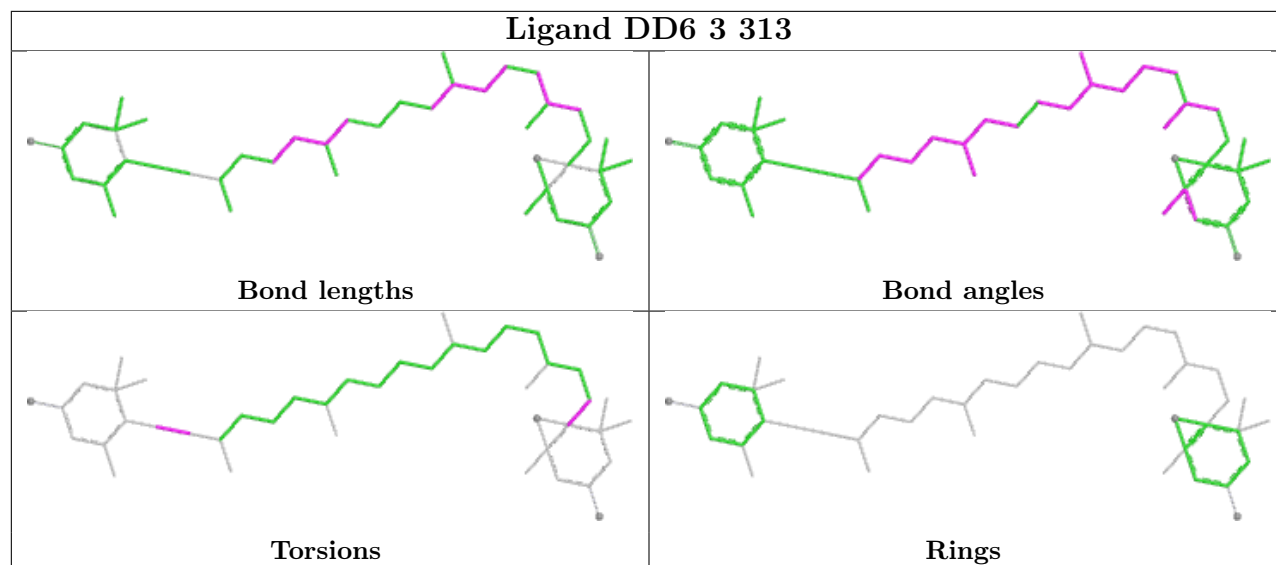
Ligand CLA 9 302



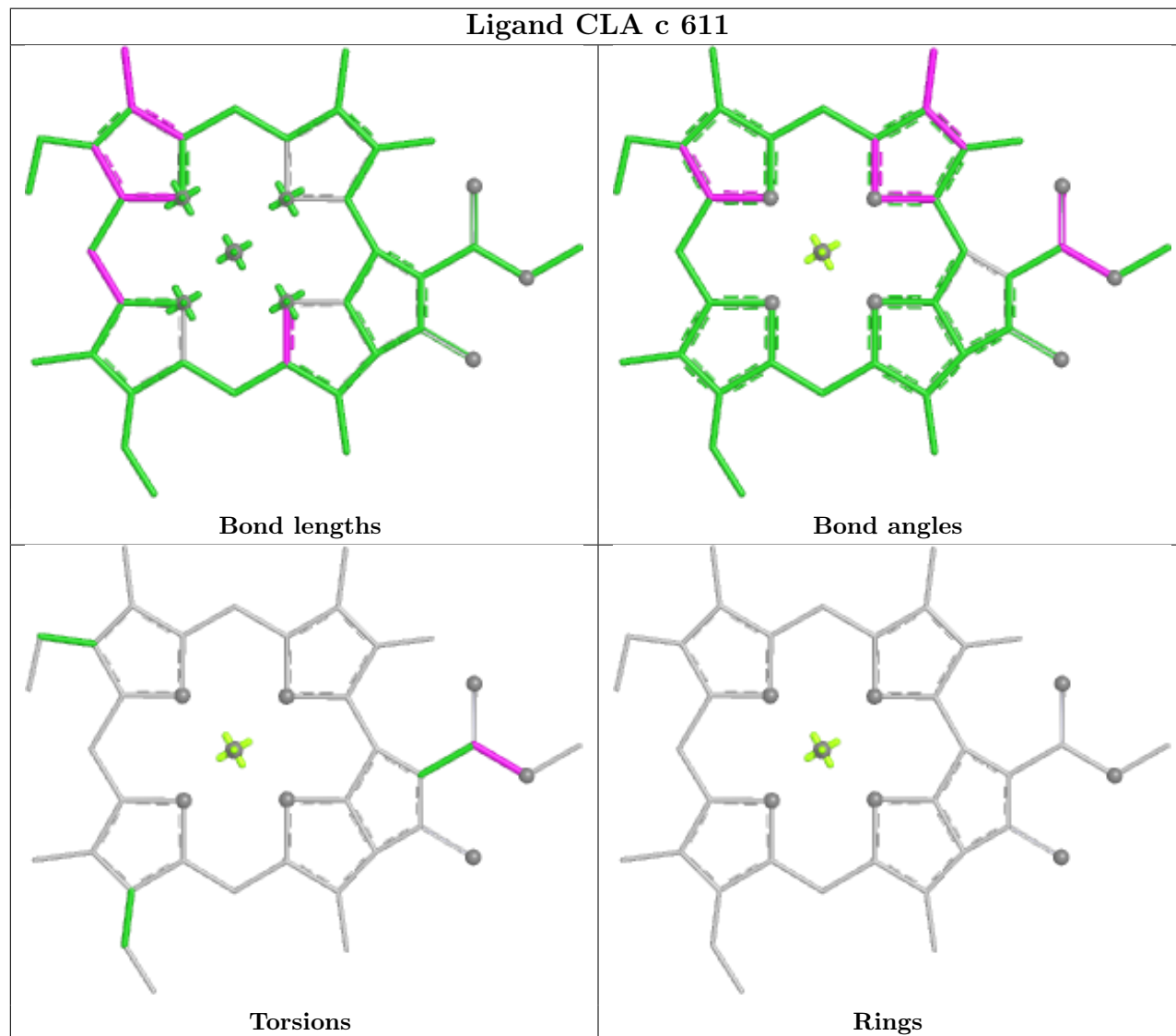
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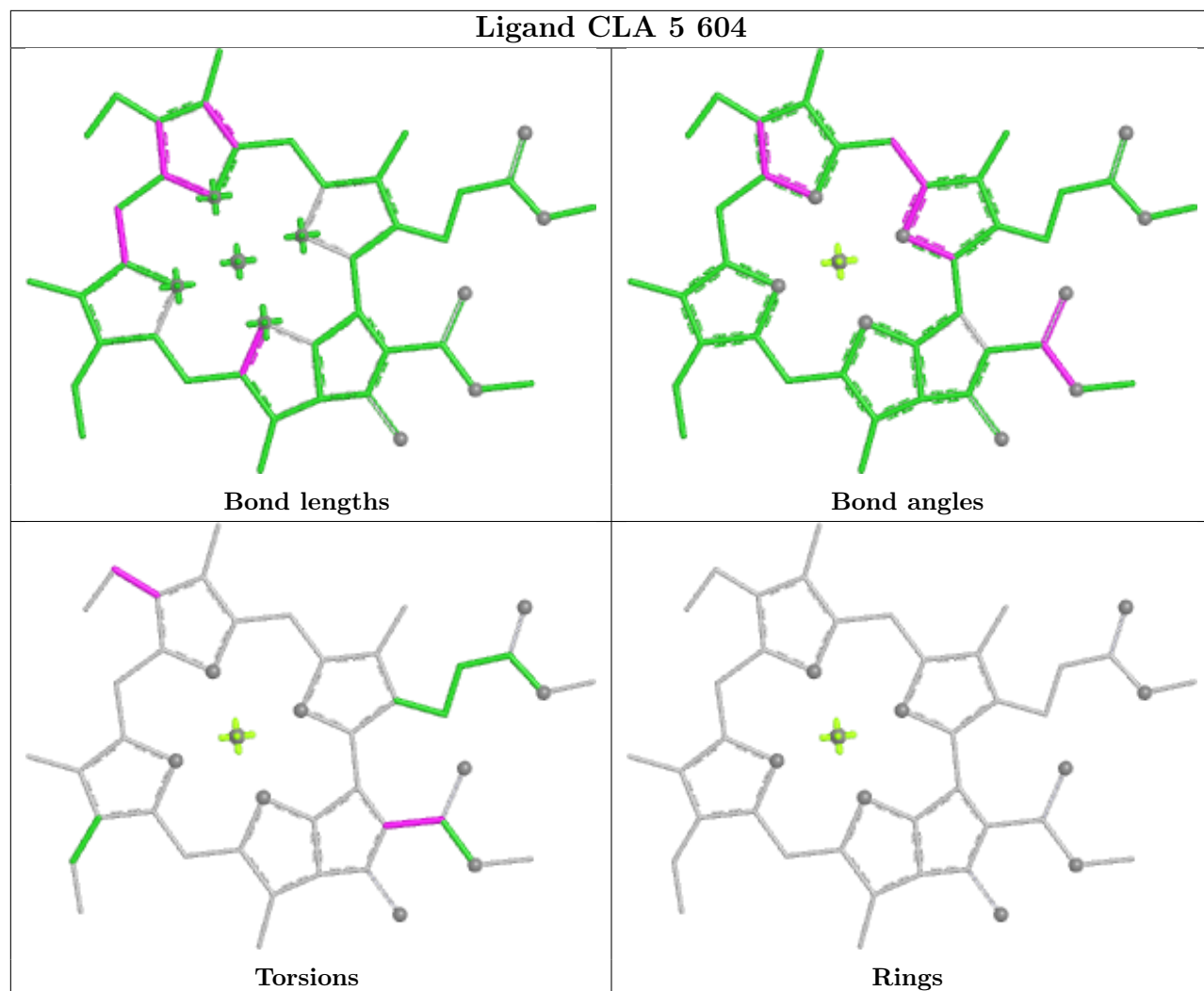
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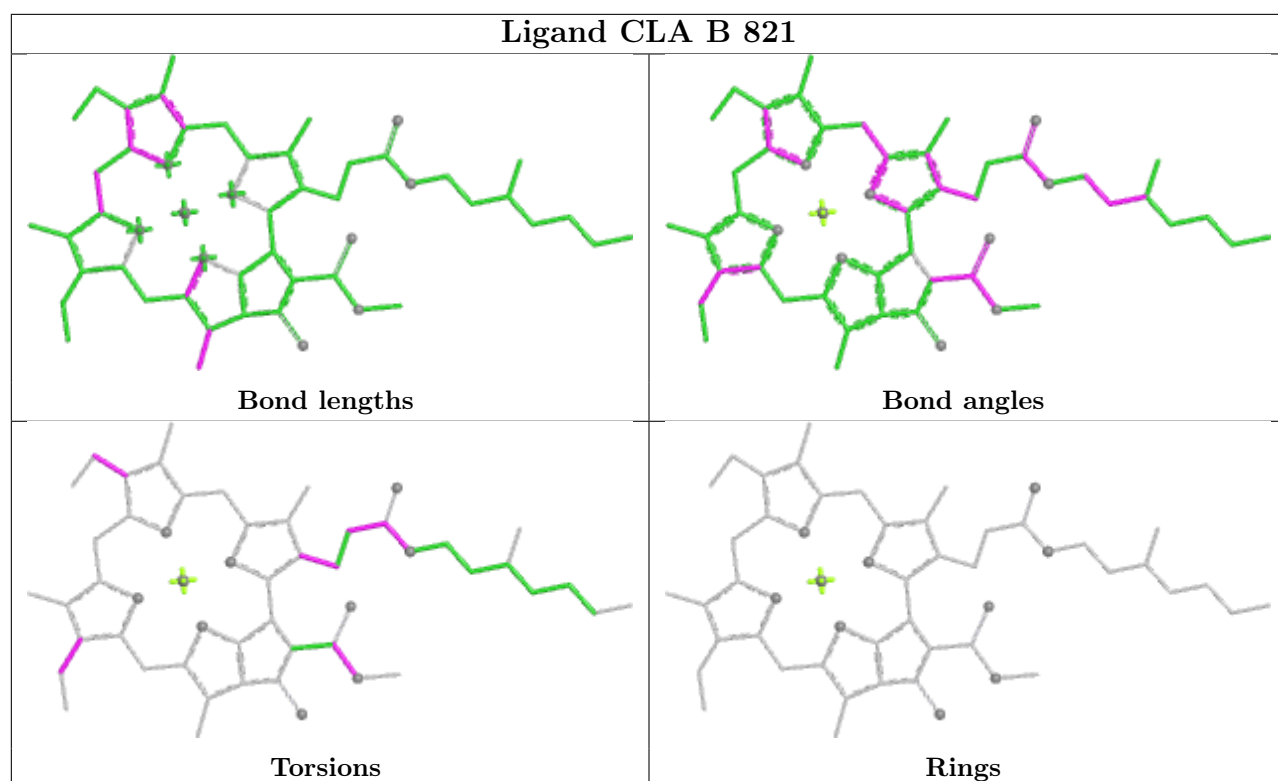


Ligand CLA c 611

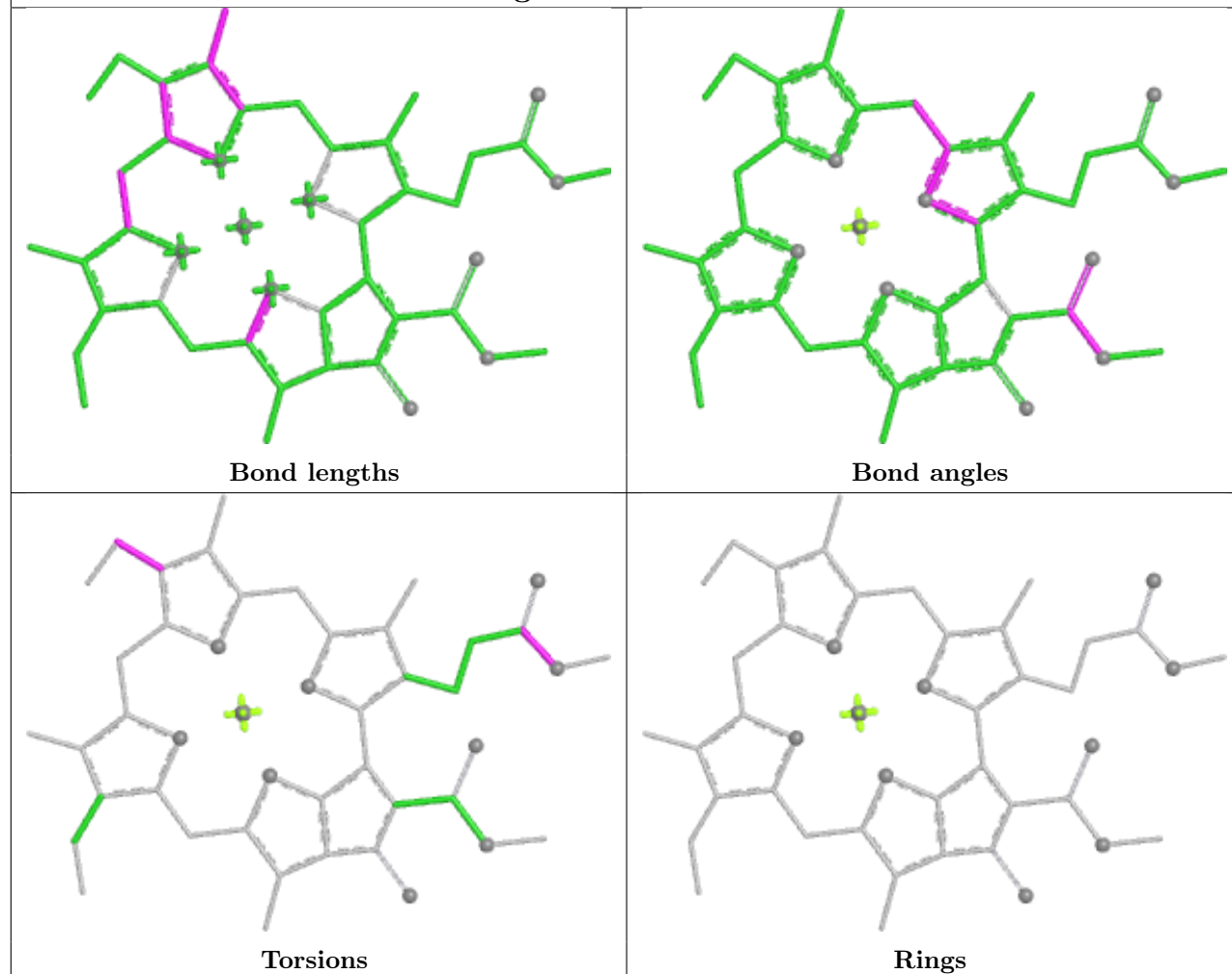


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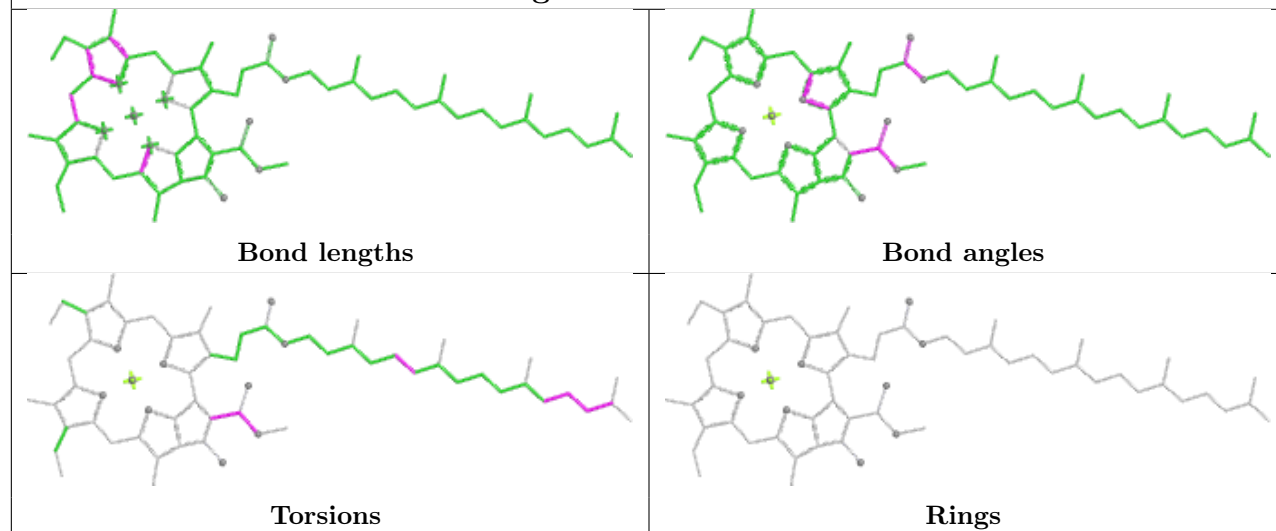




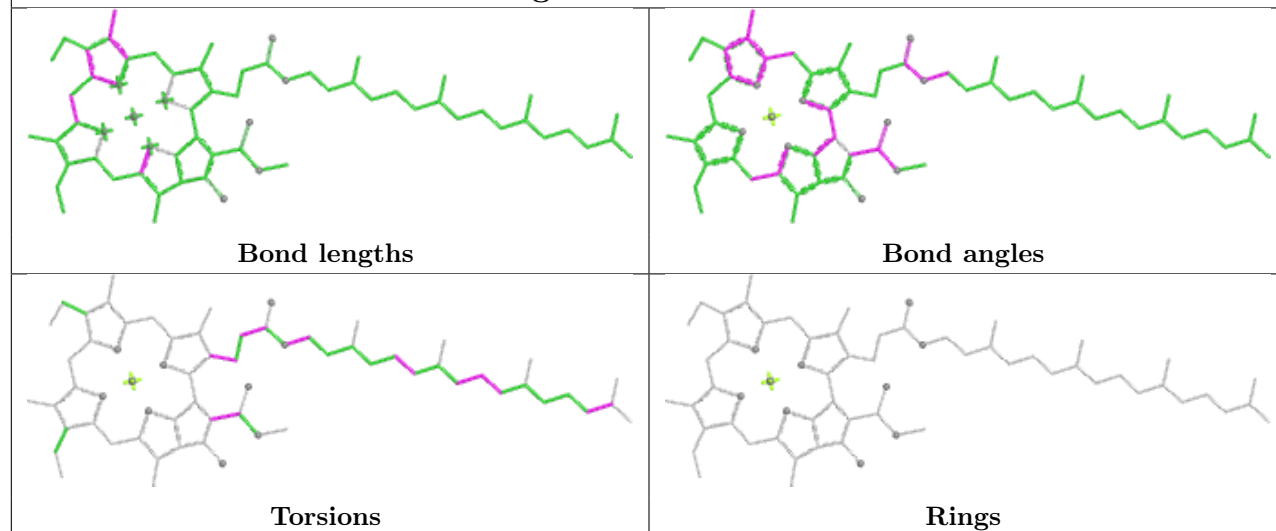
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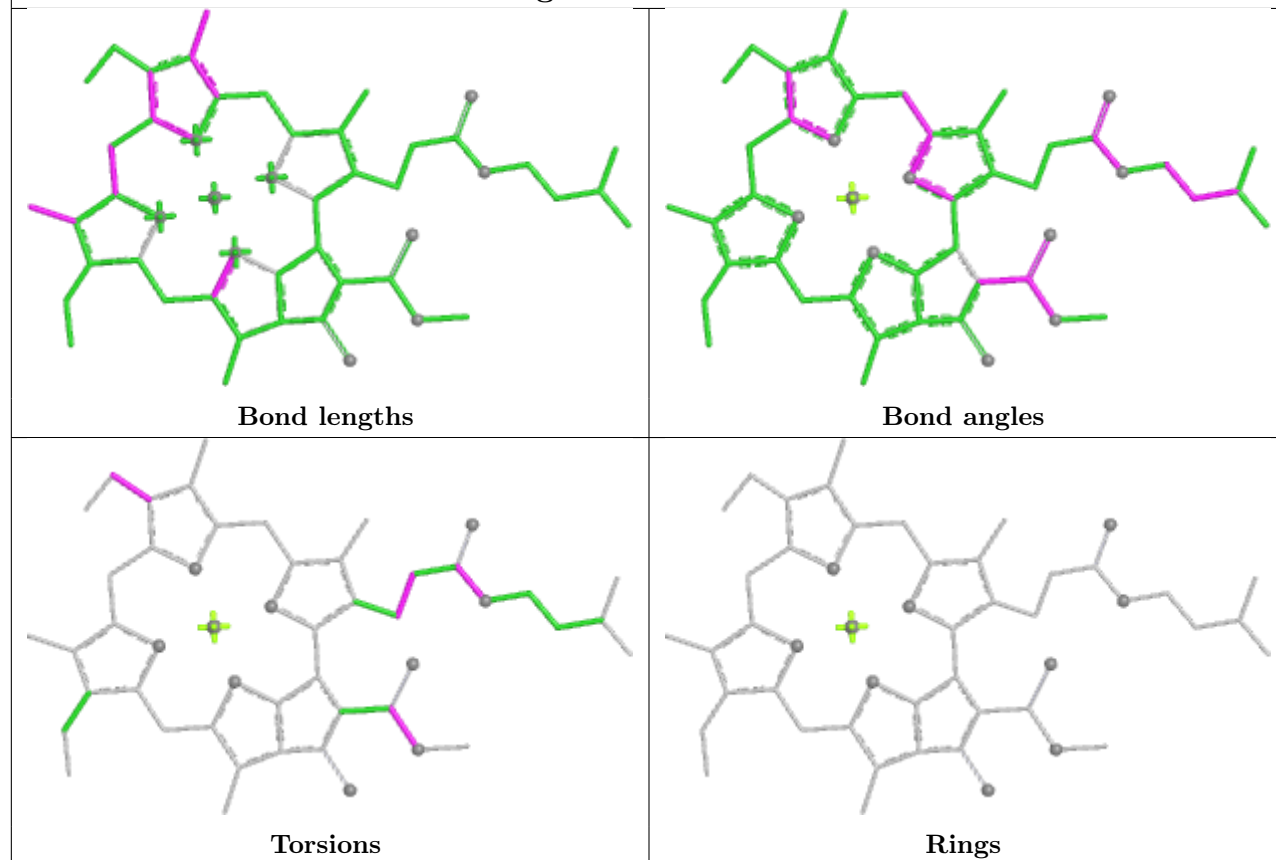
Ligand CLA B 834



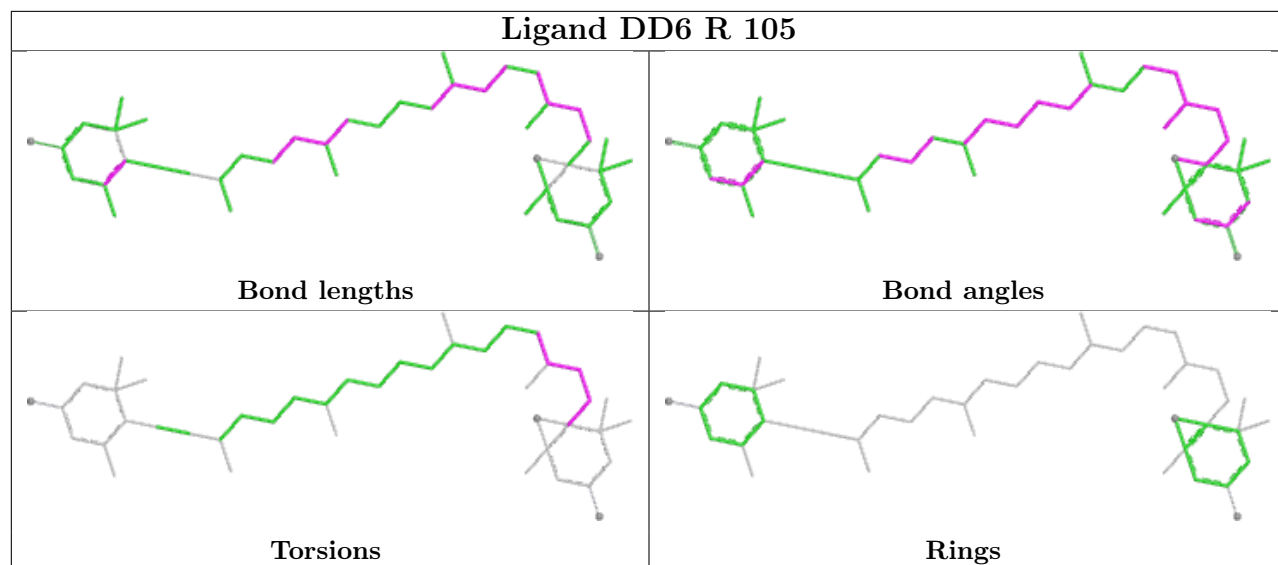
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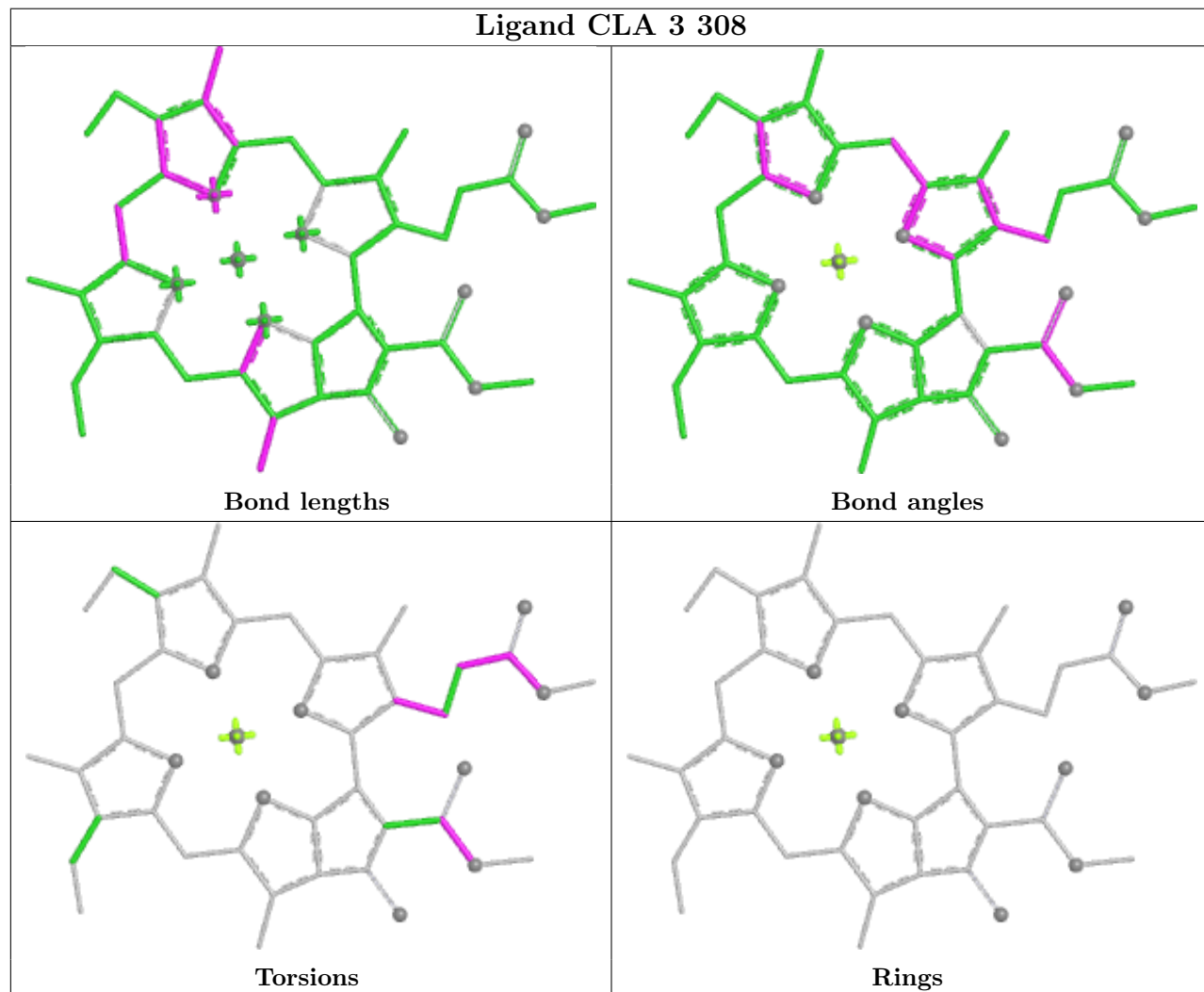
Ligand CLA 8 203



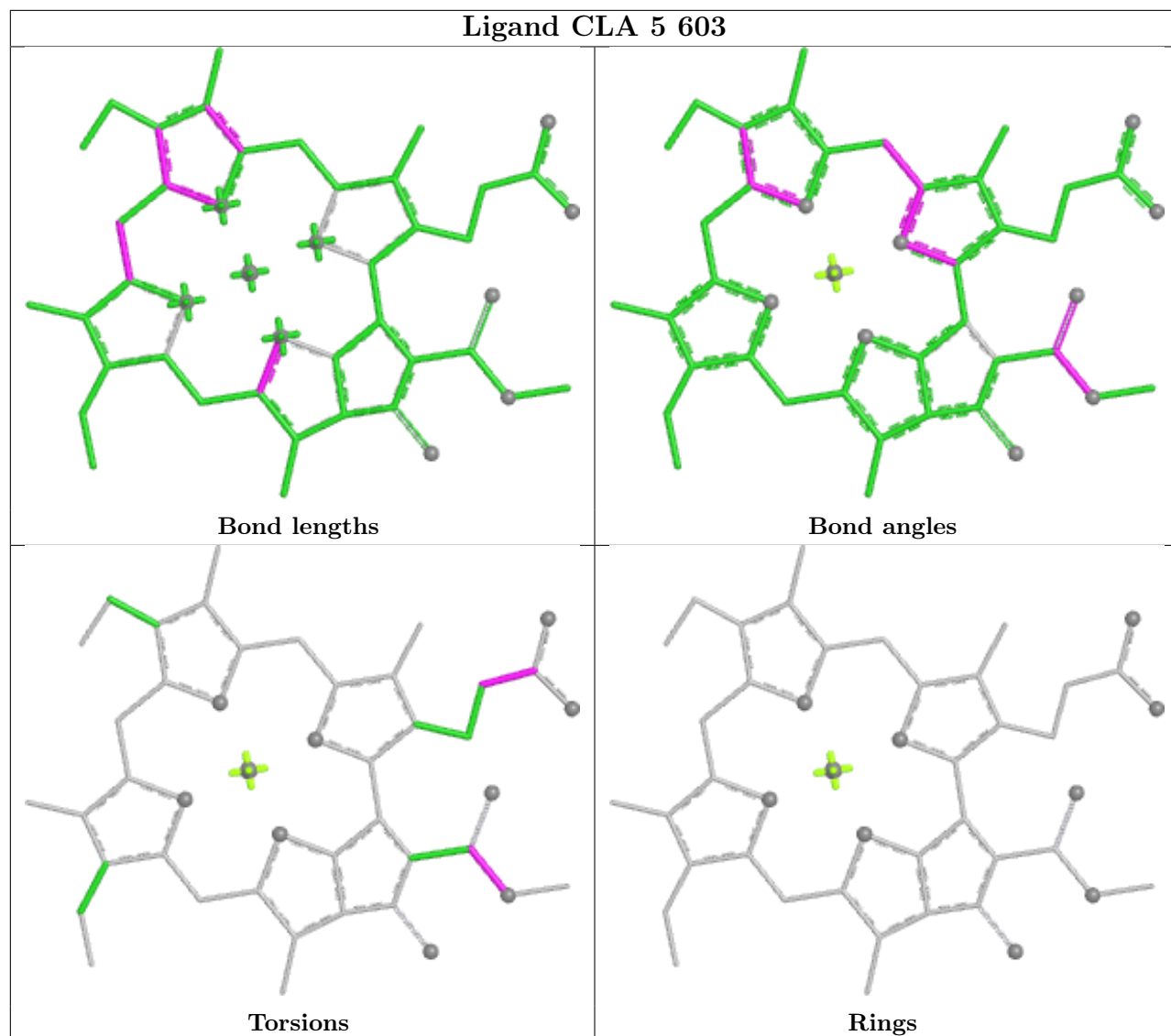
Ligand DD6 R 105



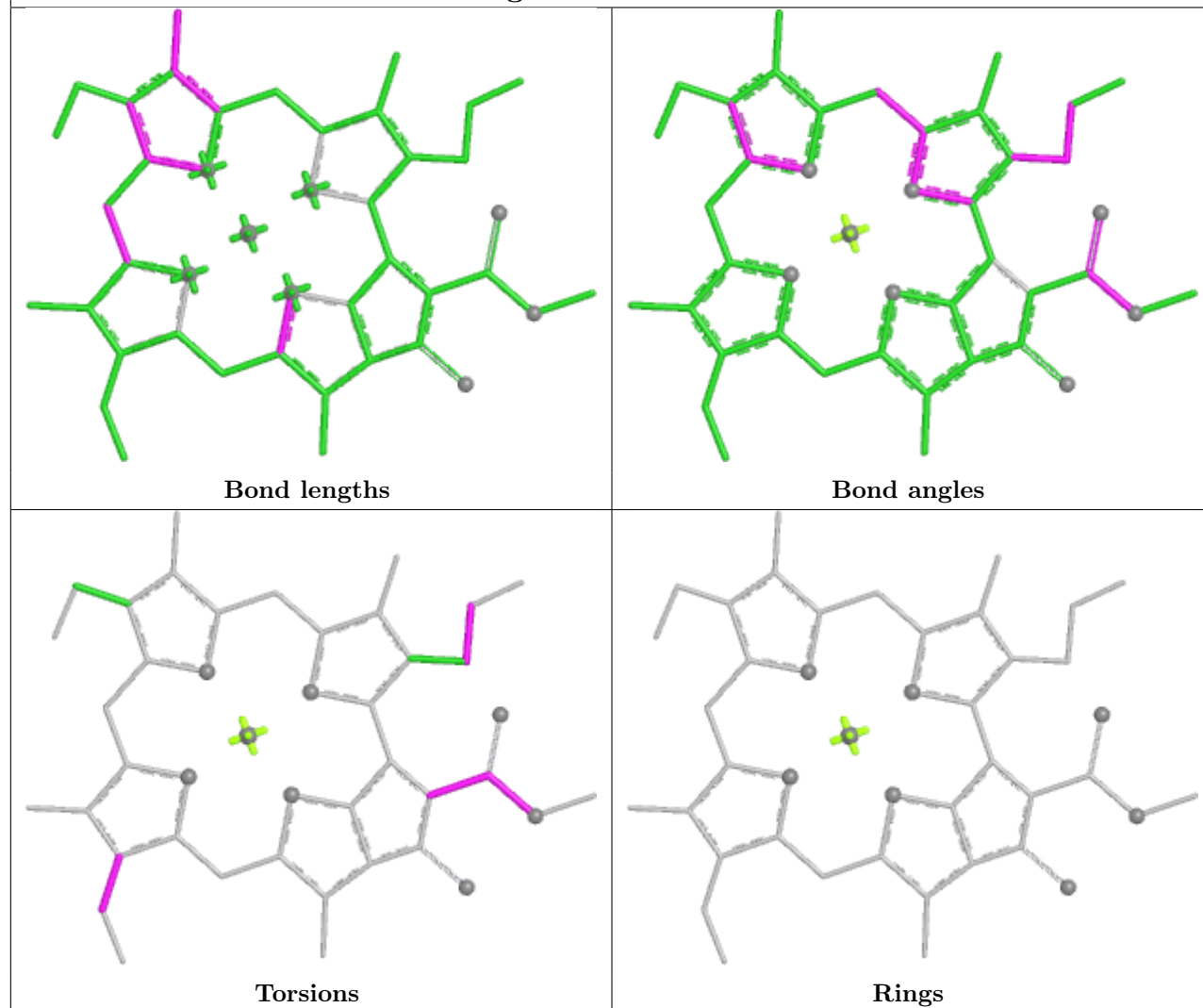
Ligand CLA 3 308



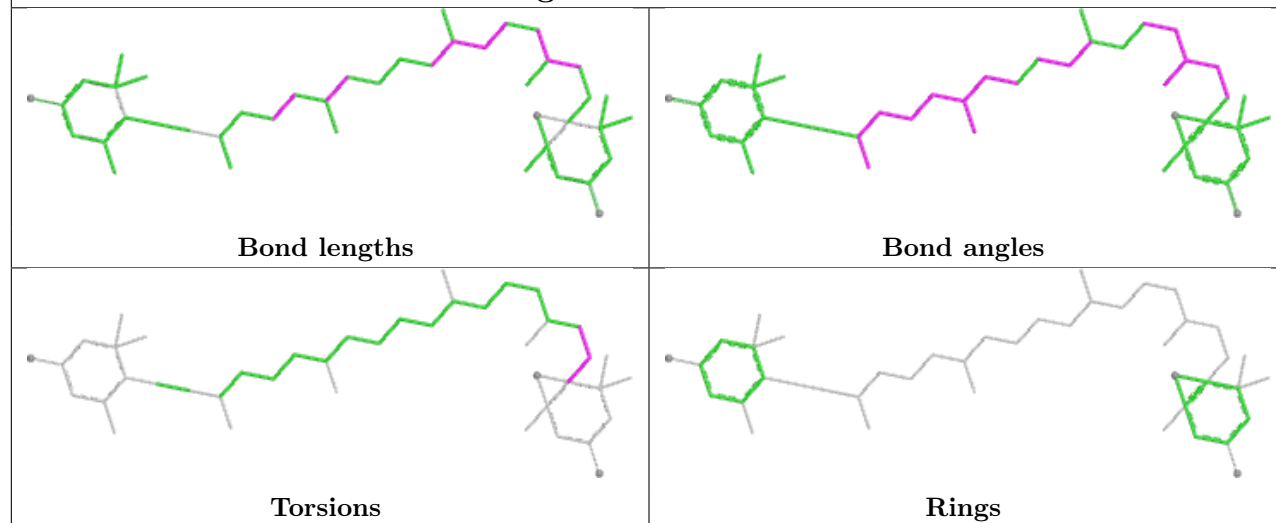
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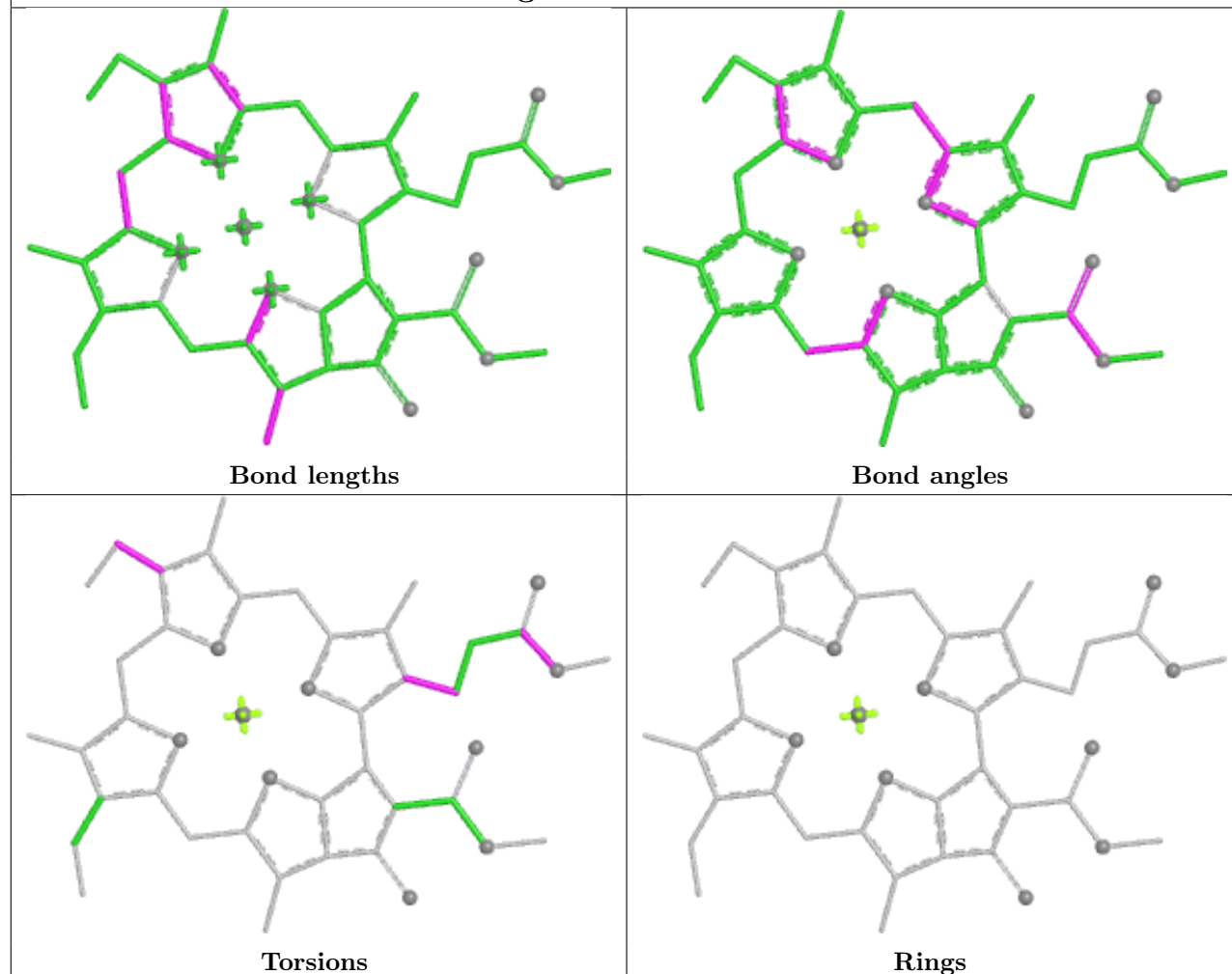
Ligand CLA c 601



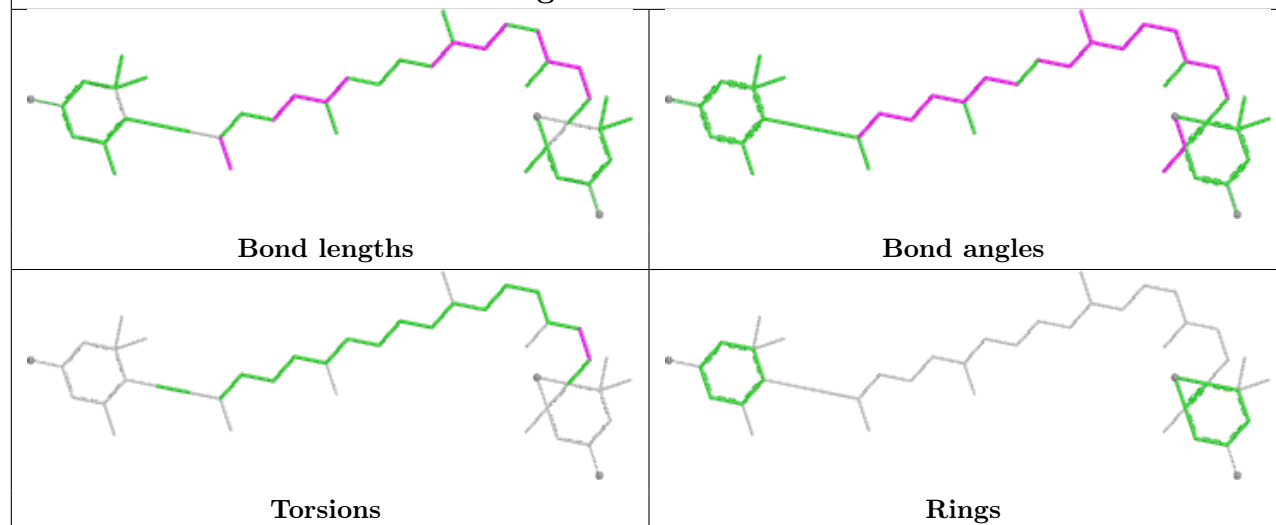
Ligand DD6 7 616



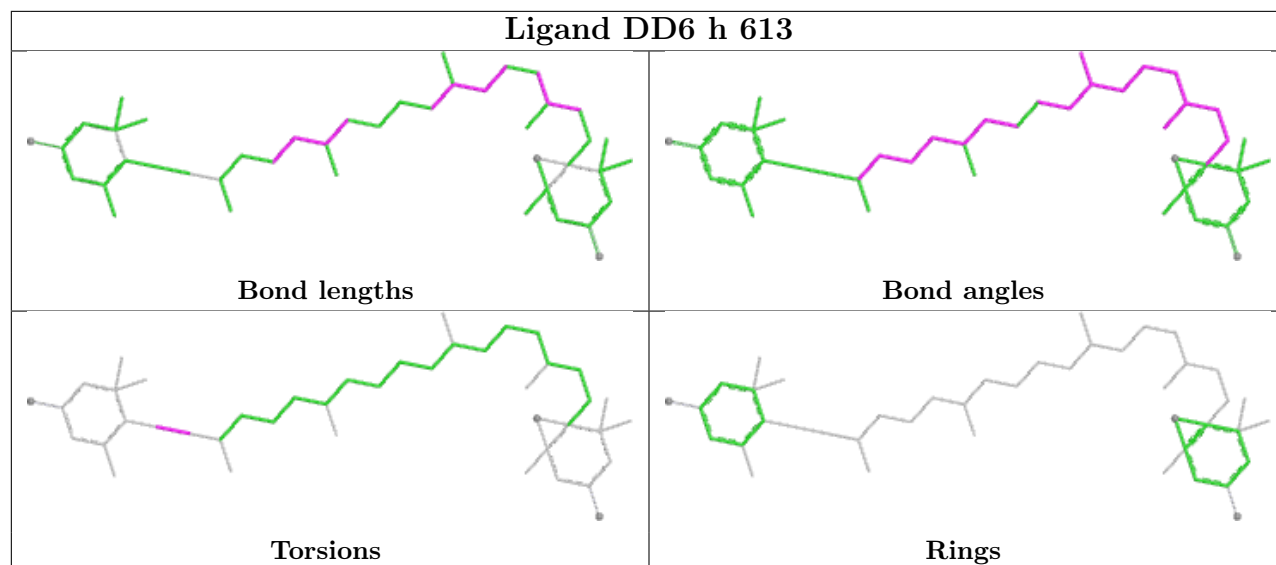
Ligand CLA 6 607



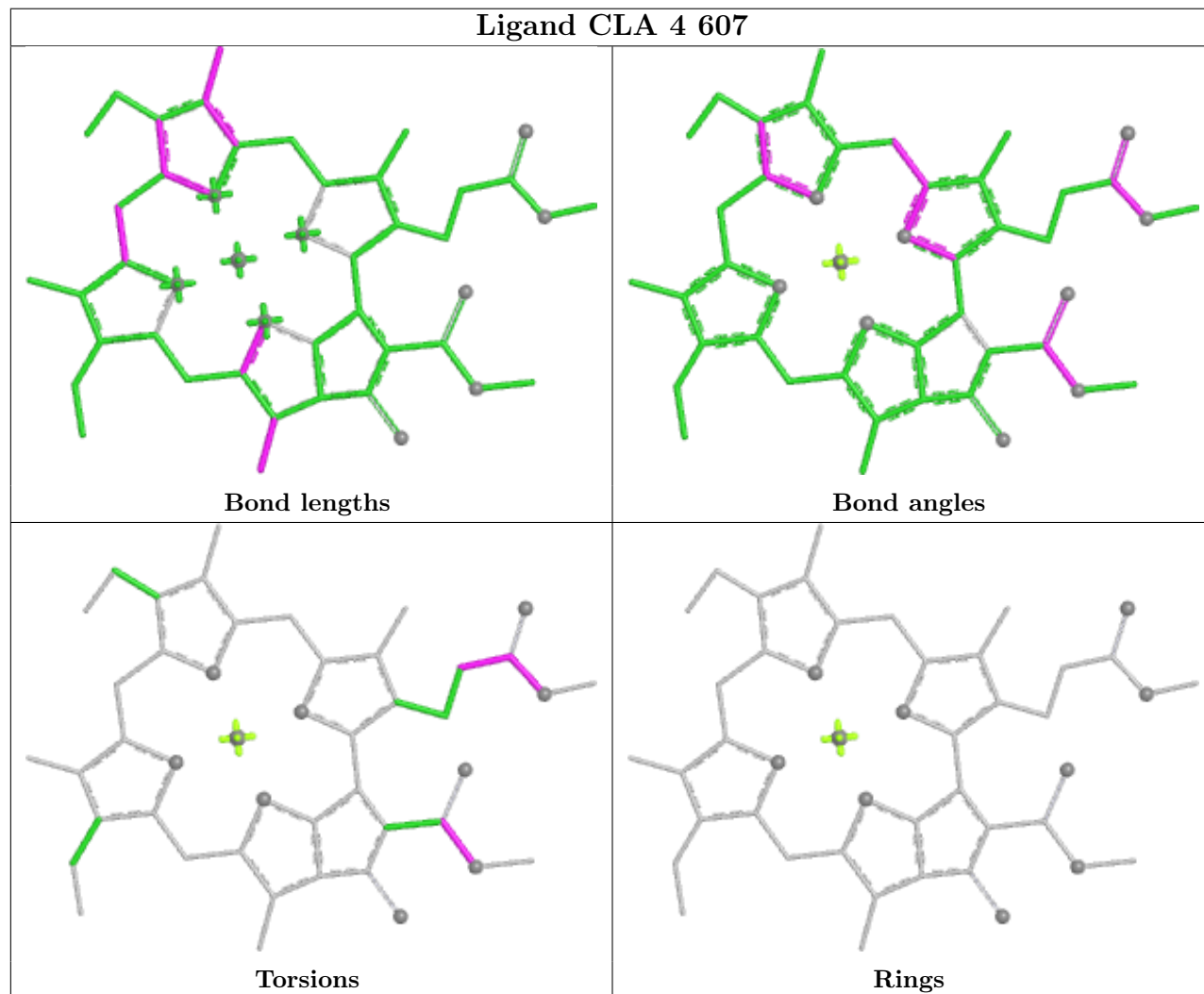
Ligand DD6 6 617

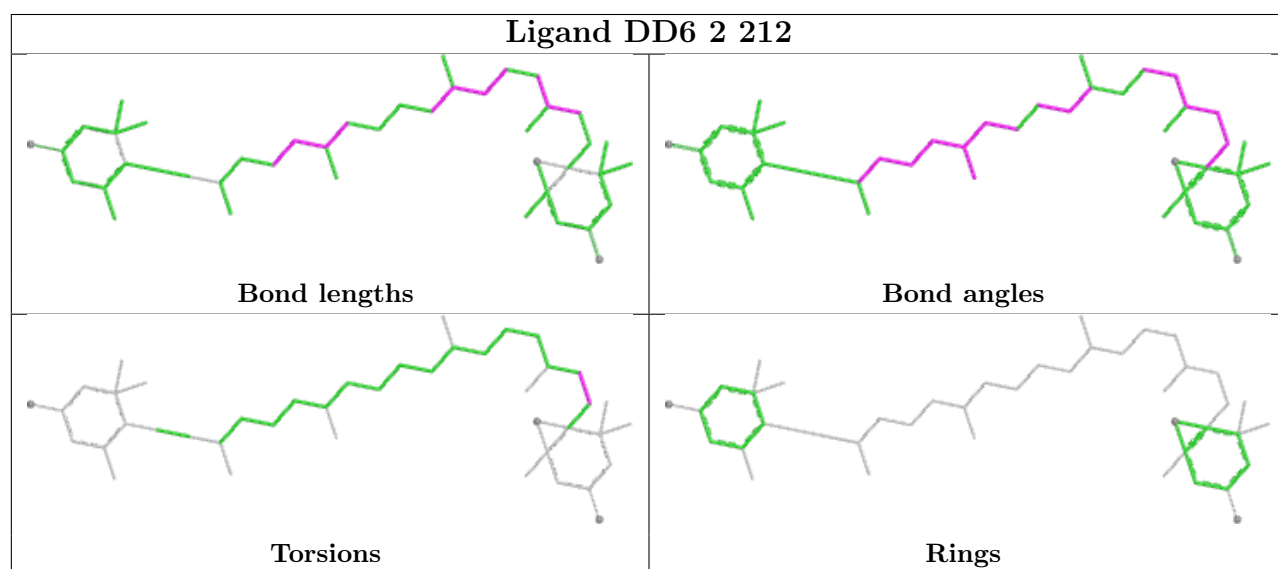
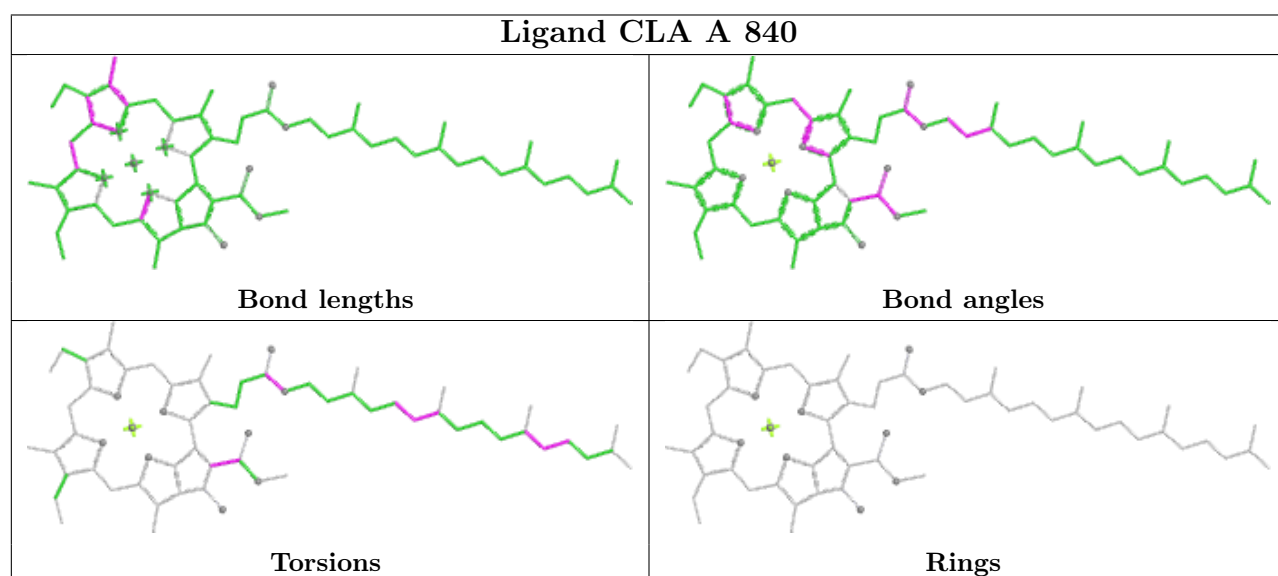
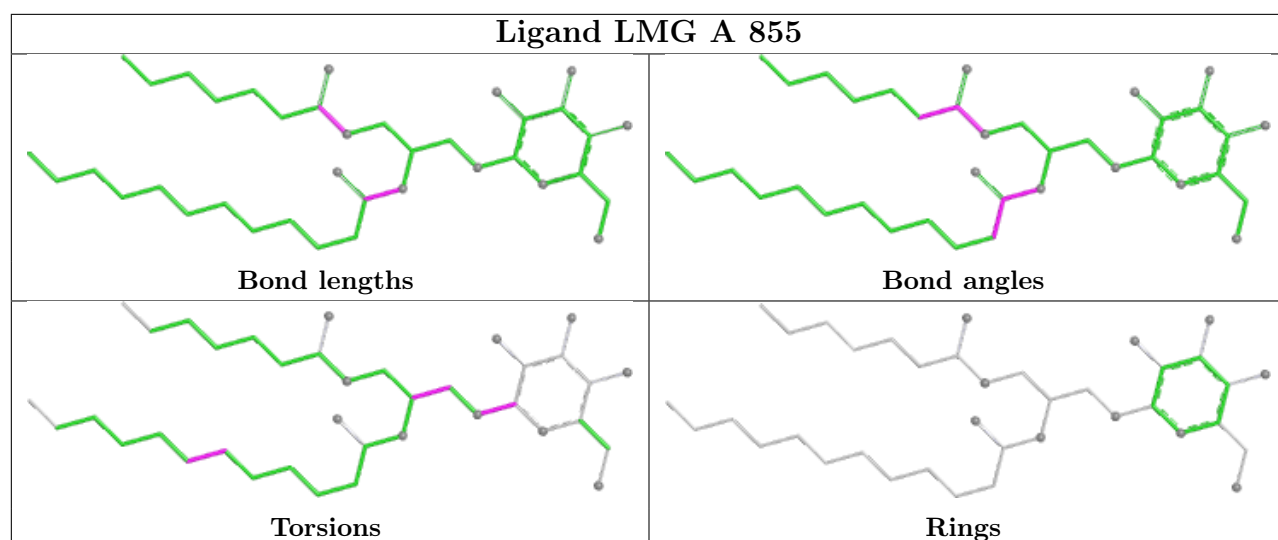


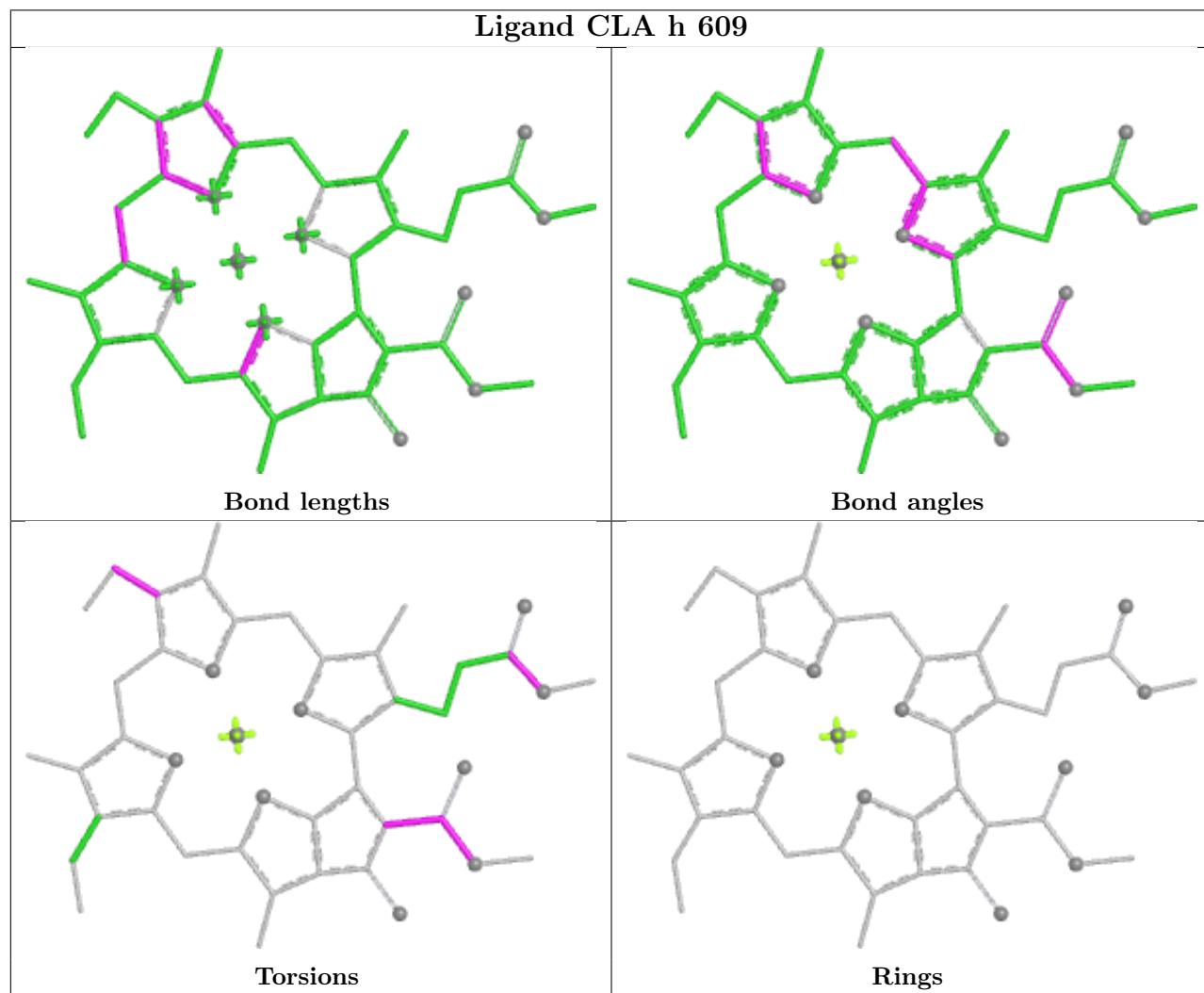
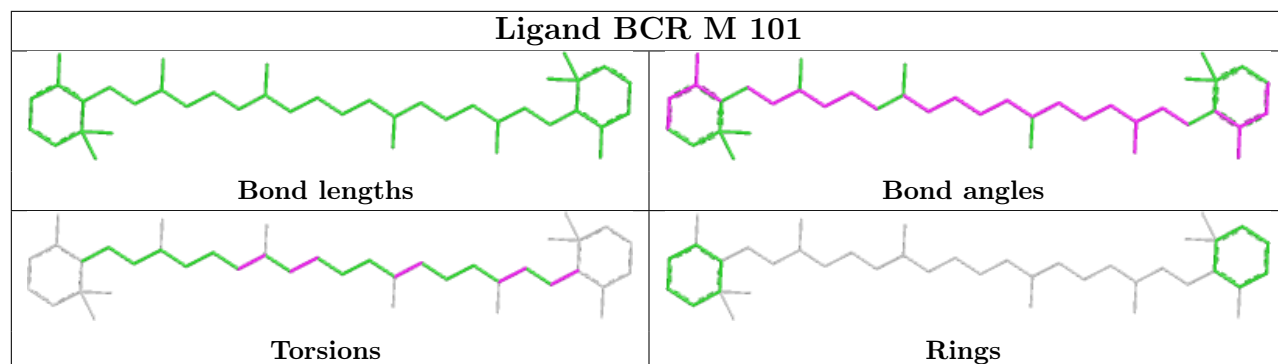
Ligand DD6 h 613



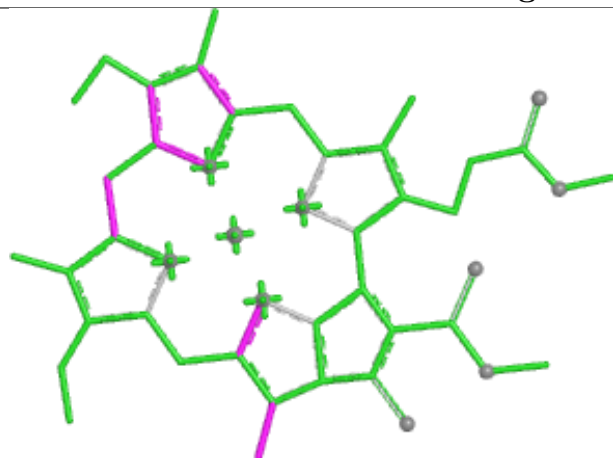
Ligand CLA 4 607



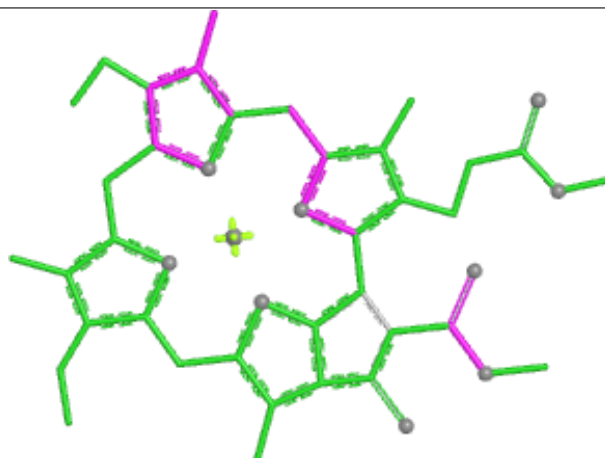




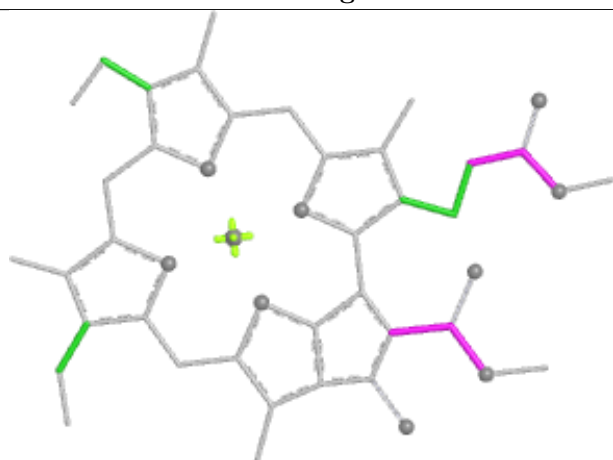
Ligand CLA 9 301



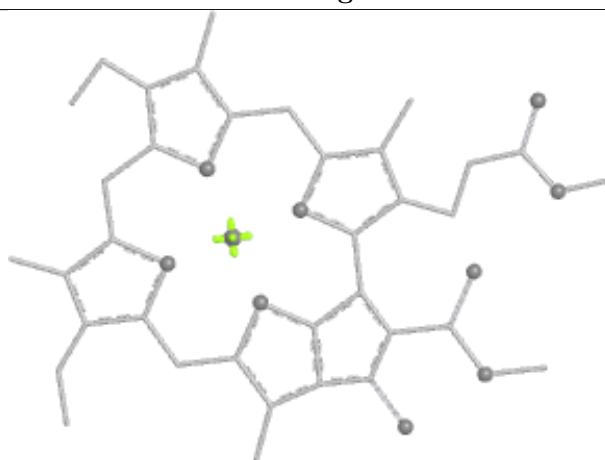
Bond lengths



Bond angles

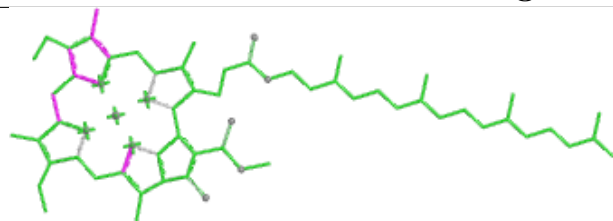


Torsions

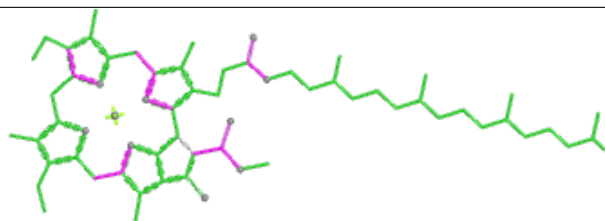


Rings

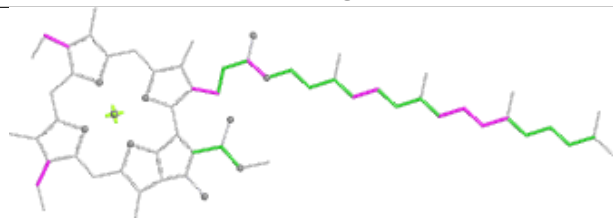
Ligand CLA L 204



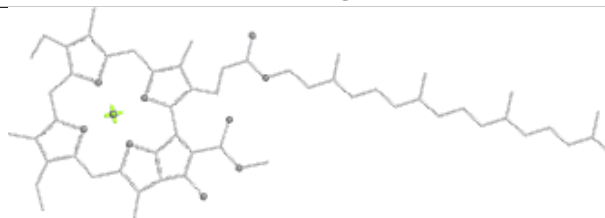
Bond lengths



Bond angles

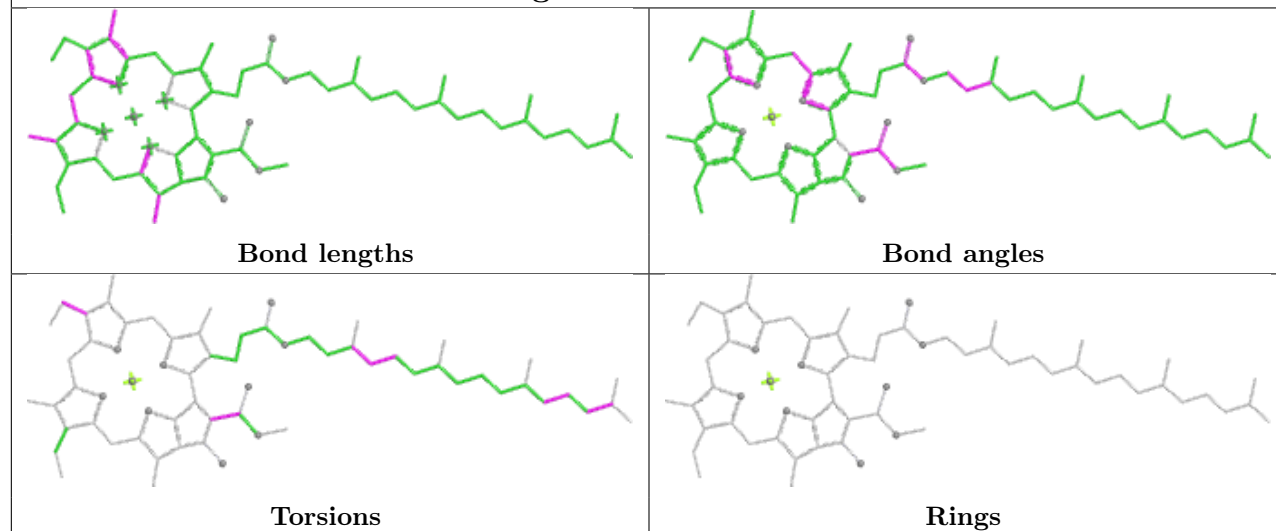


Torsions

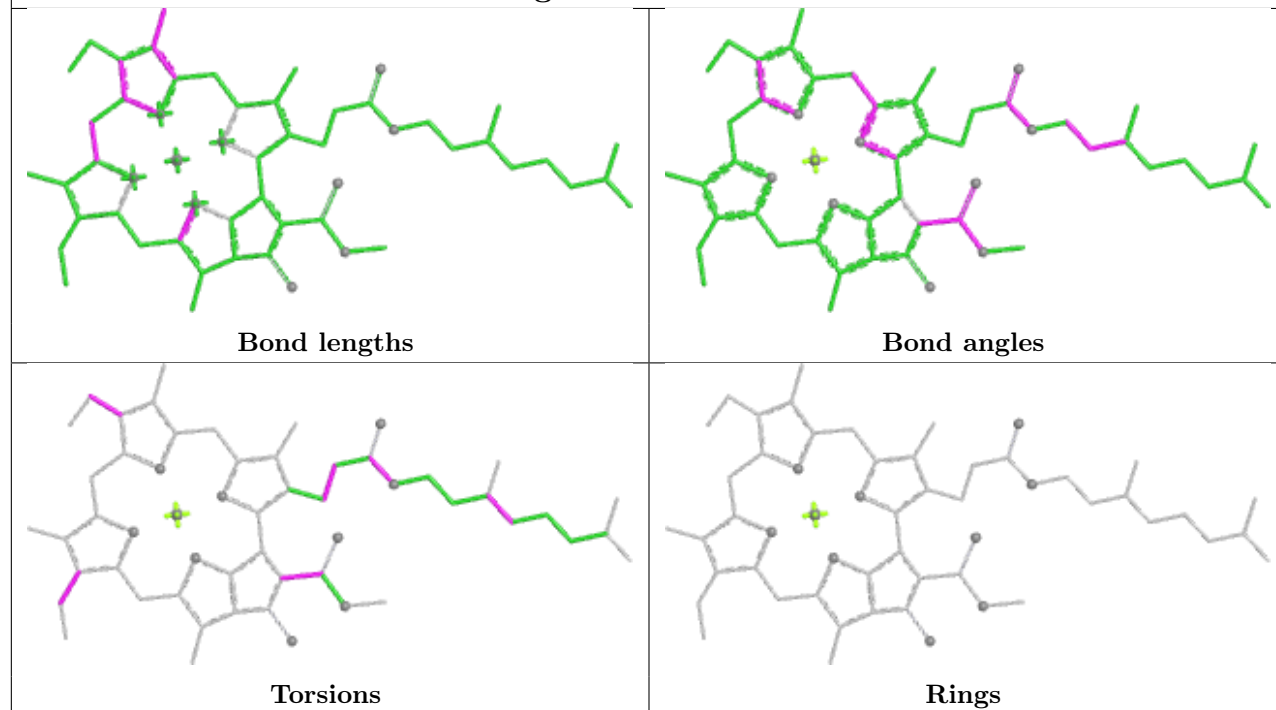


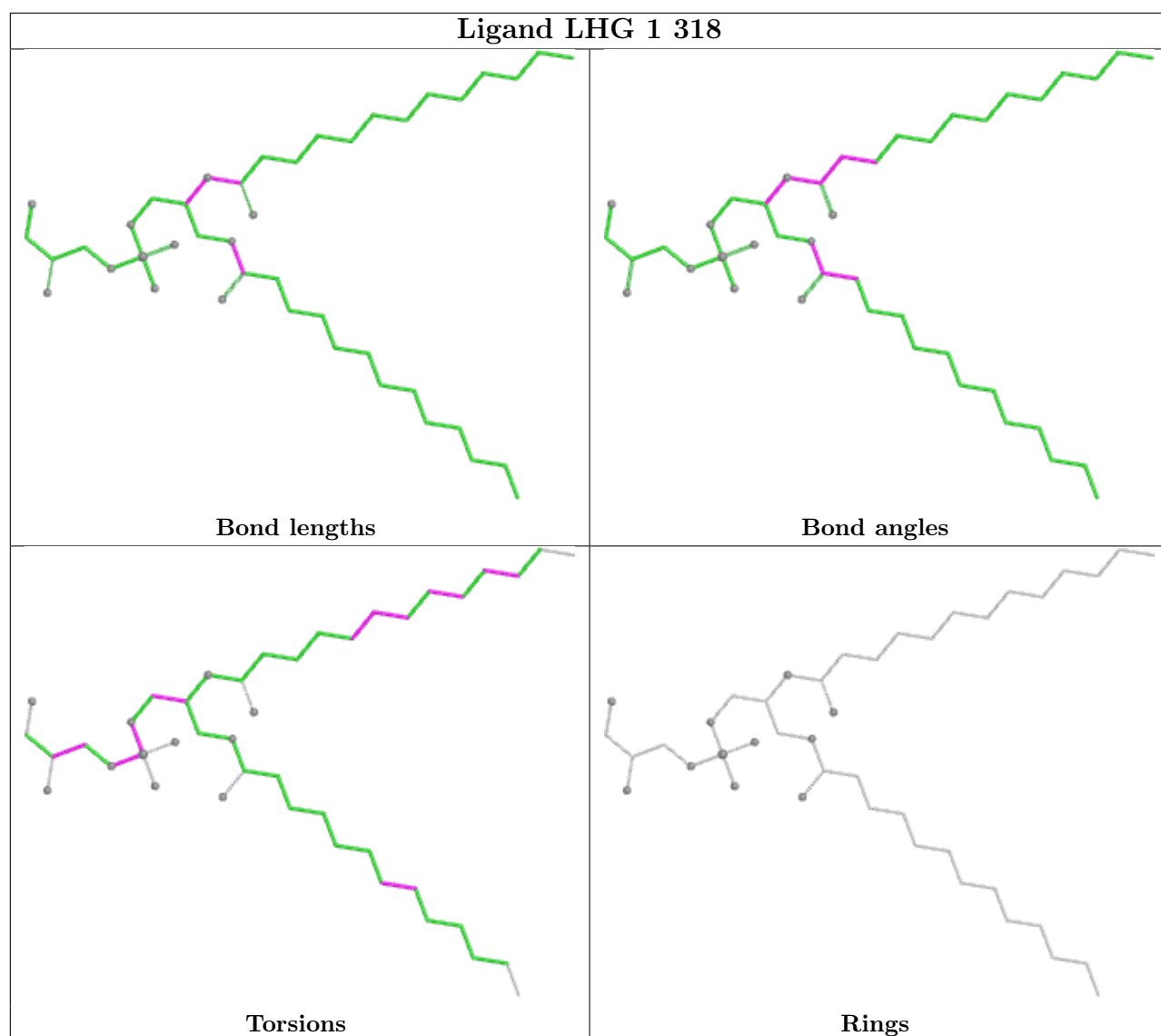
Rings

Ligand CLA B 808

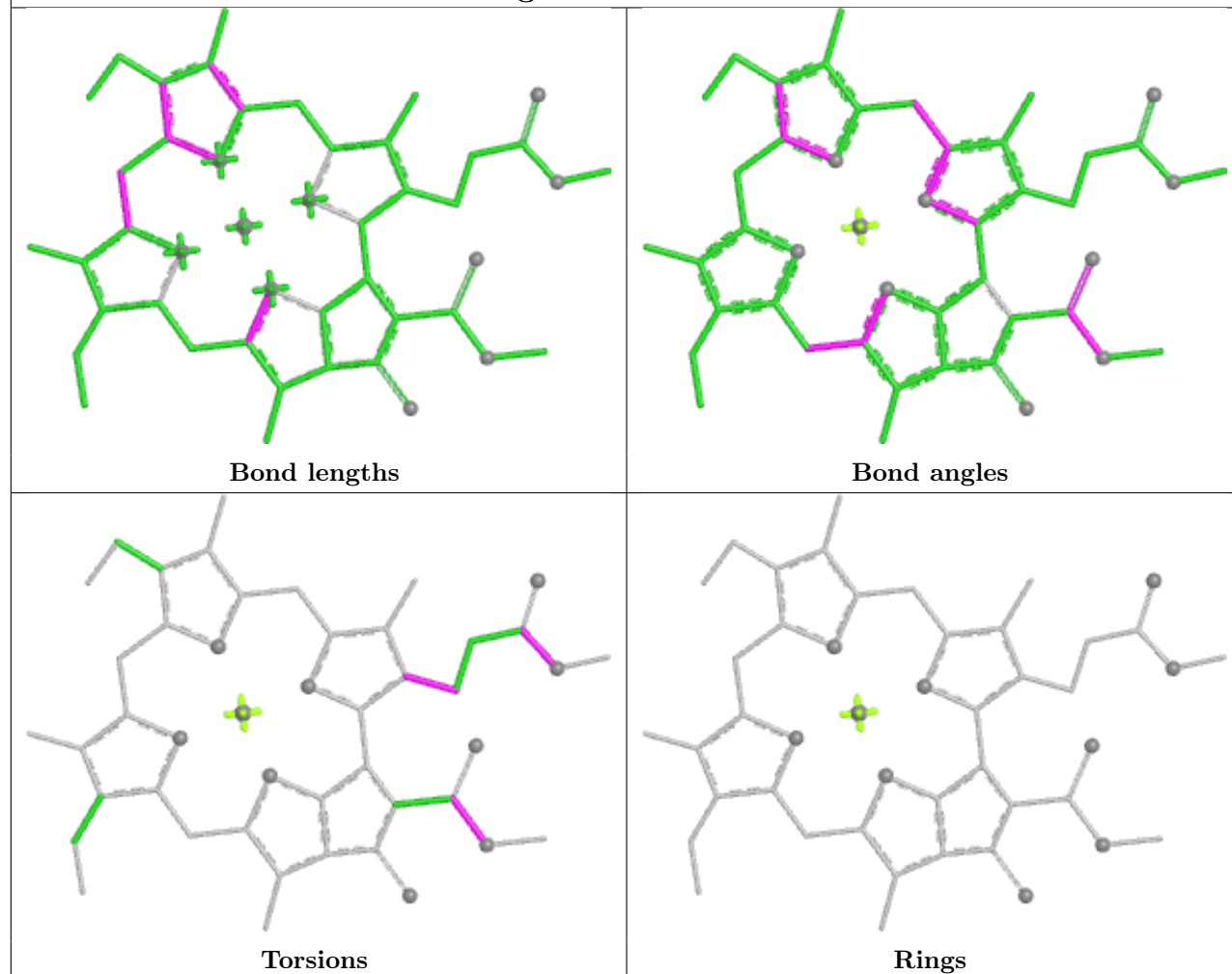


Ligand CLA L 203

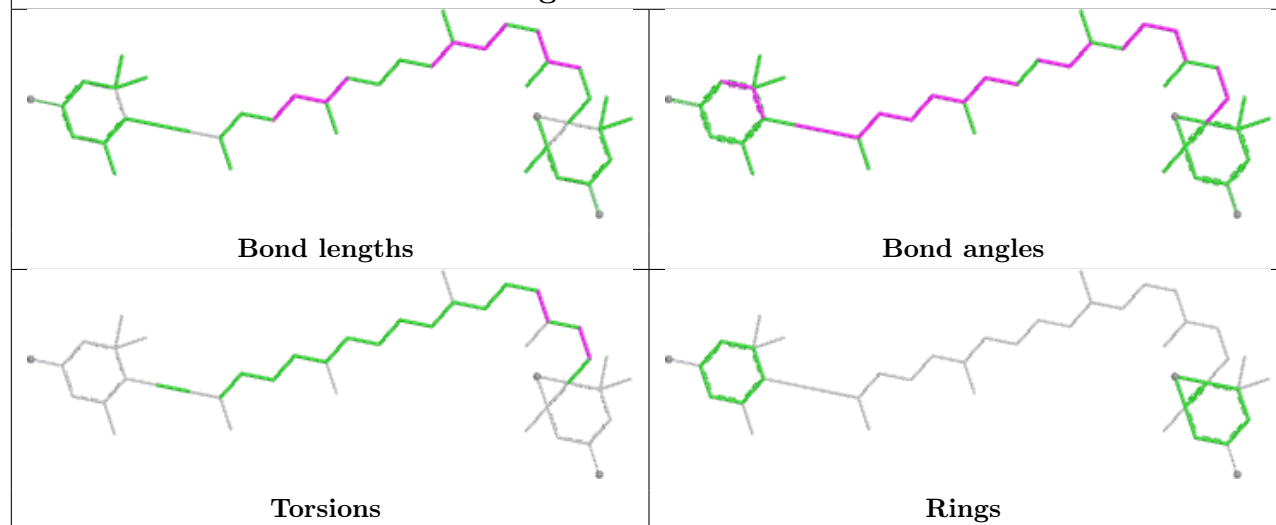




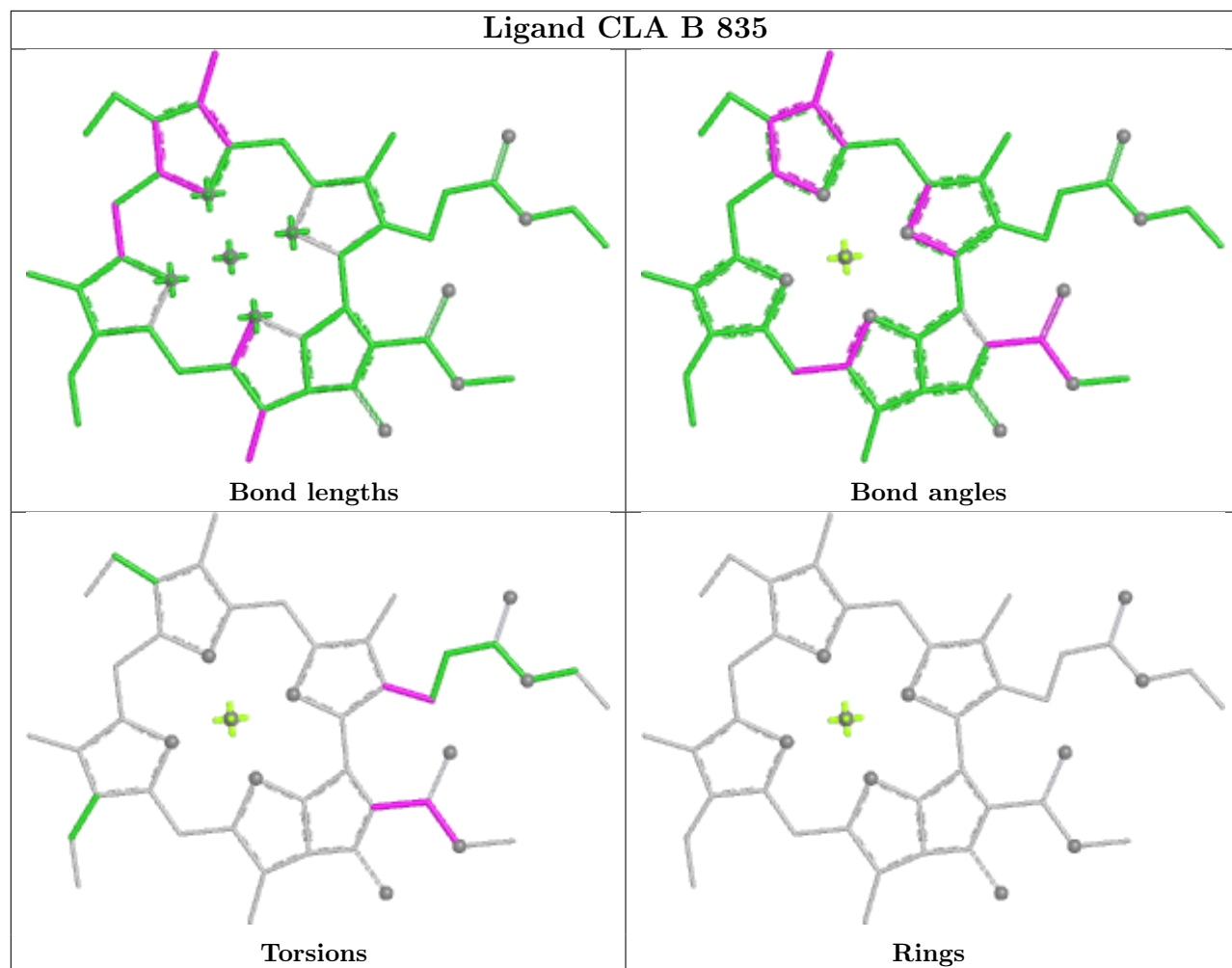
Ligand CLA 4 611



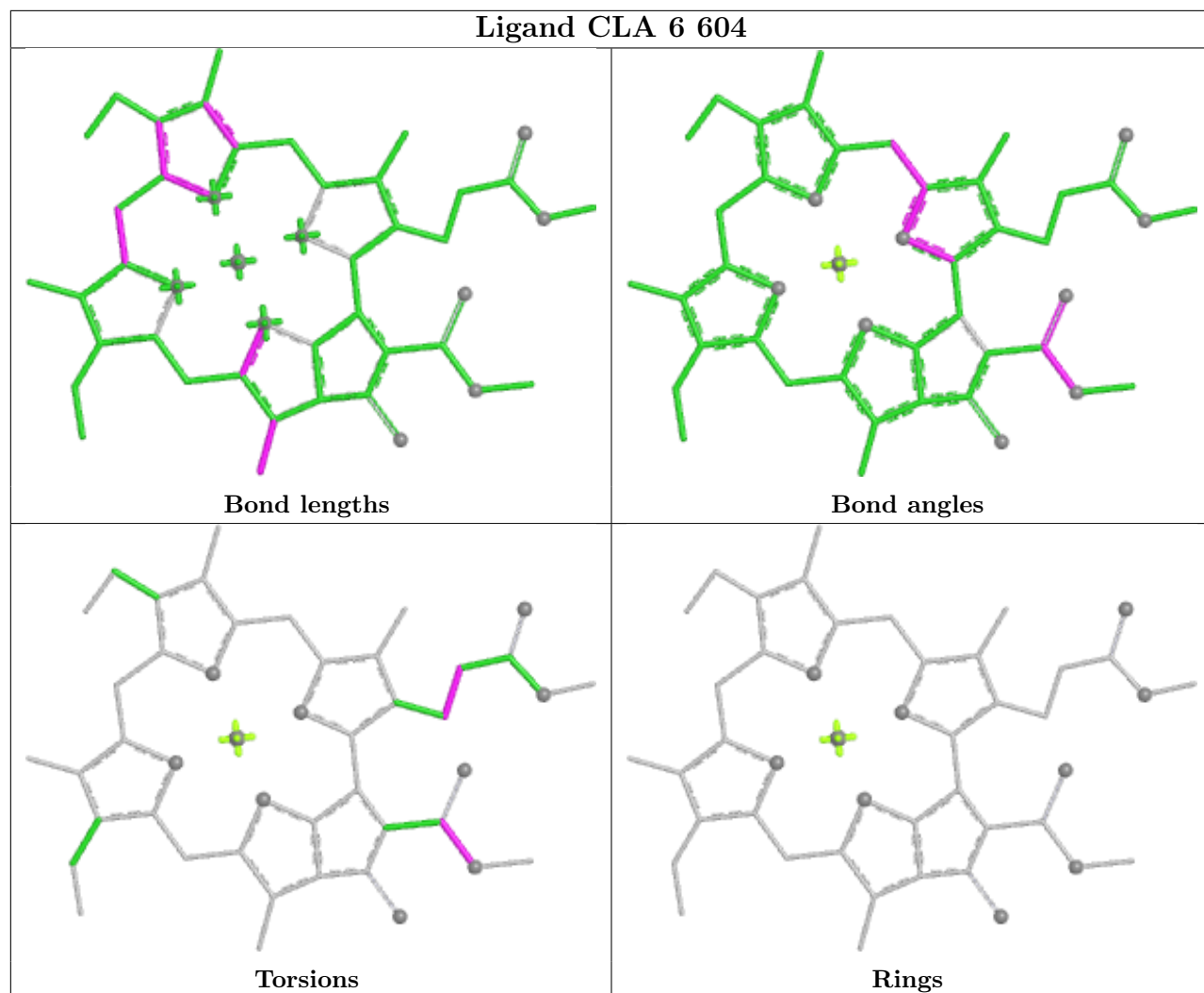
Ligand DD6 t 311



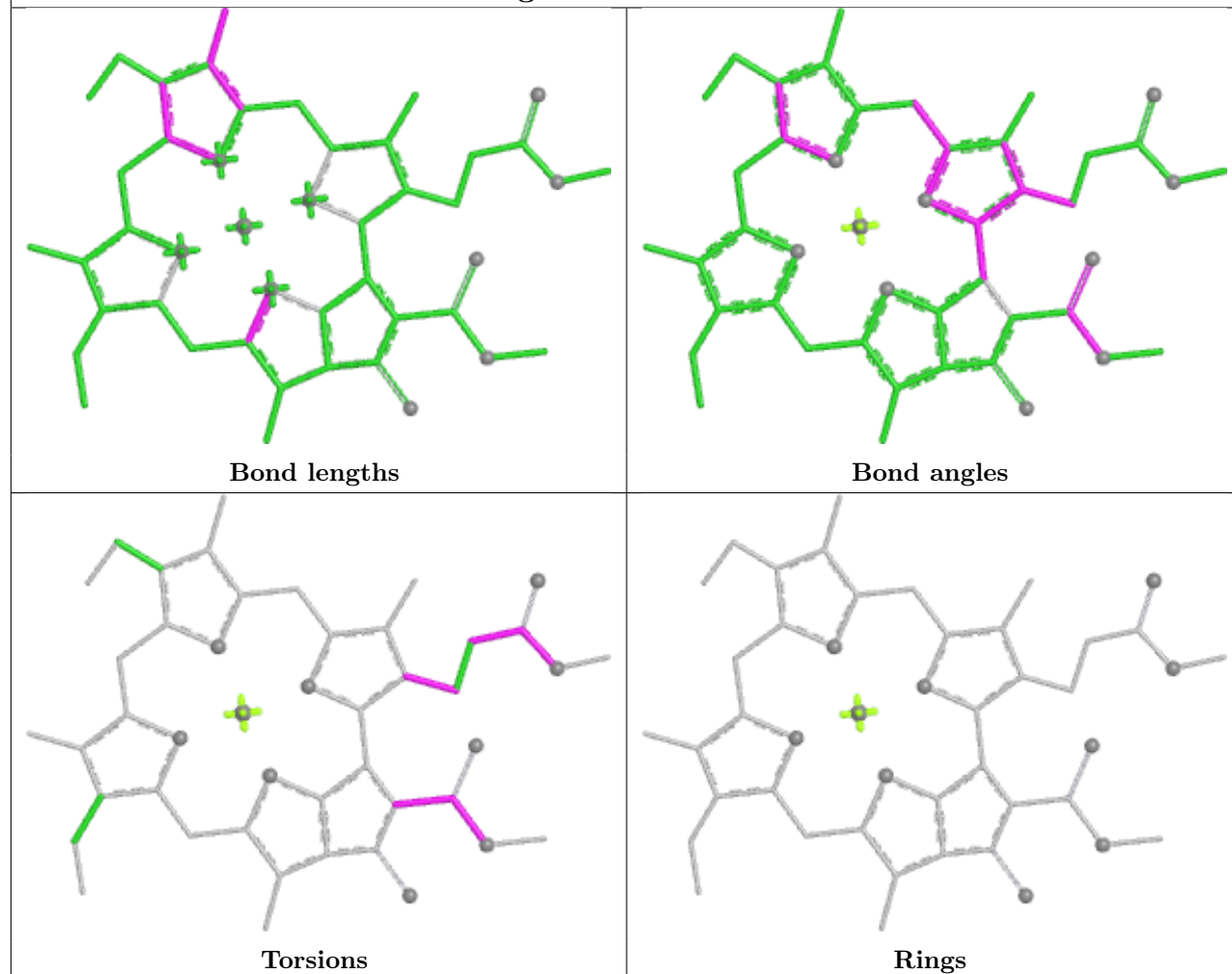
Ligand CLA B 835



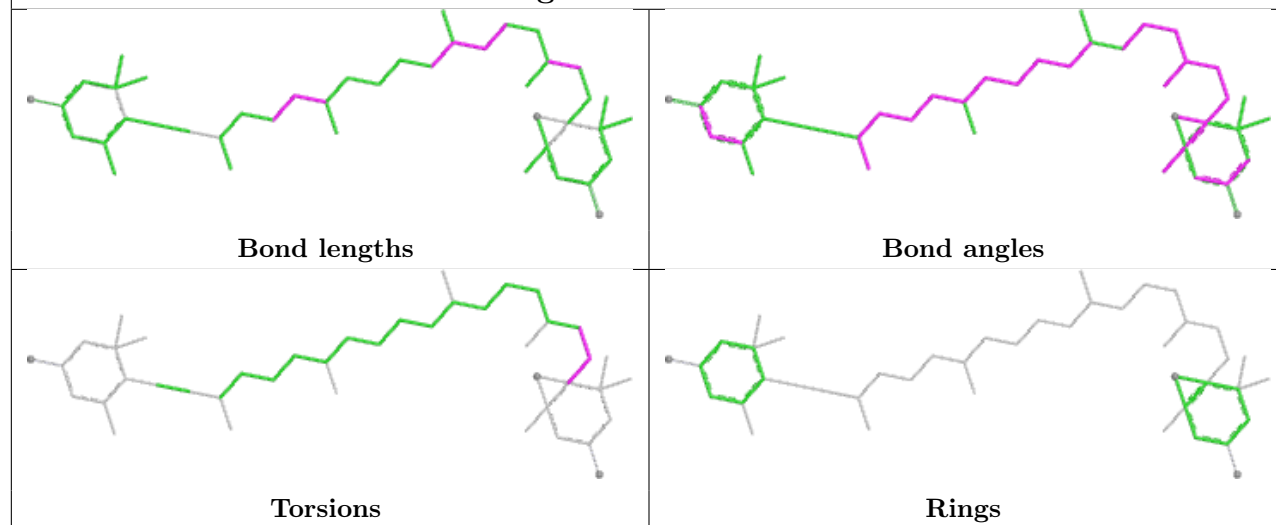
Ligand CLA 6 604



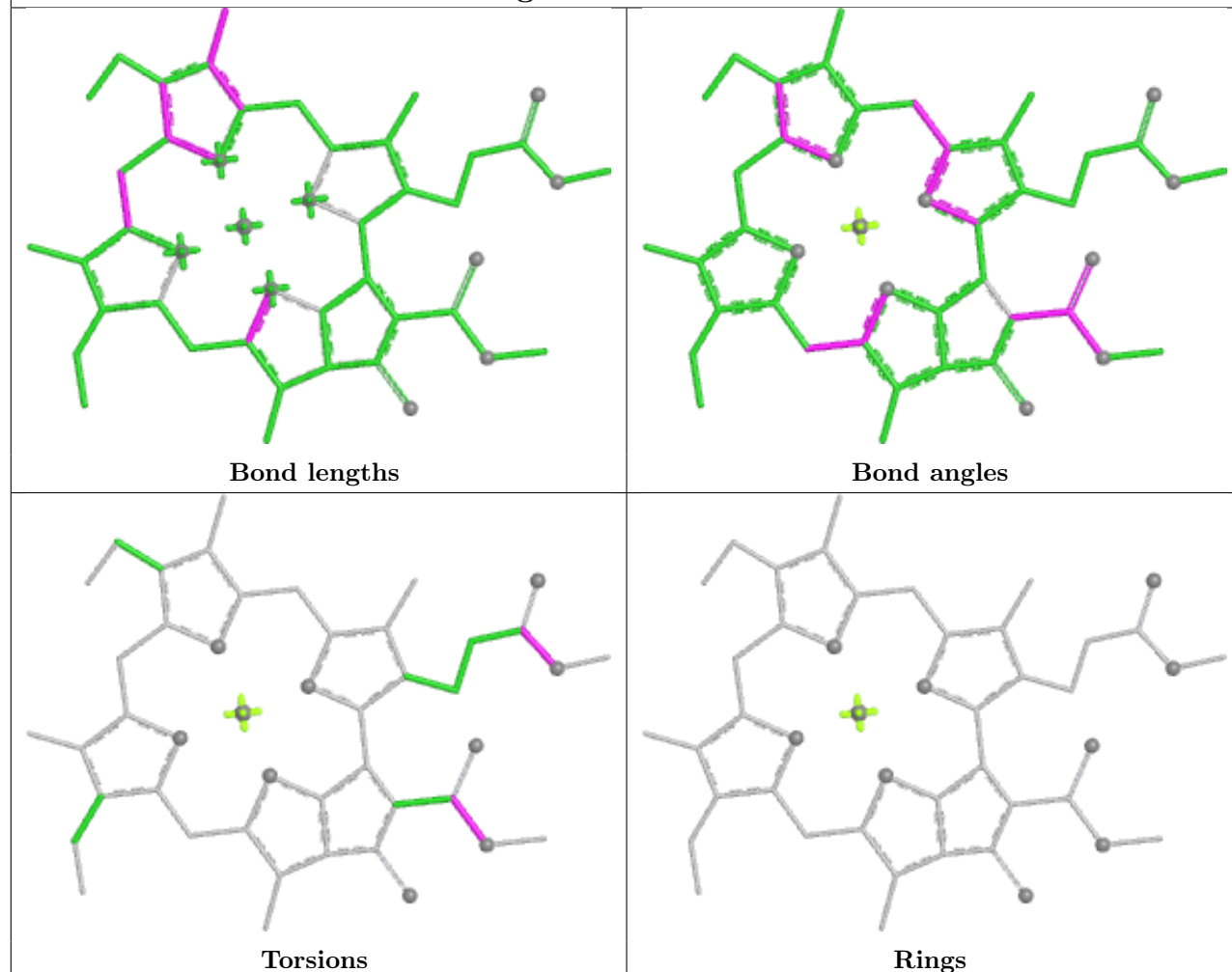
Ligand CLA 9 309



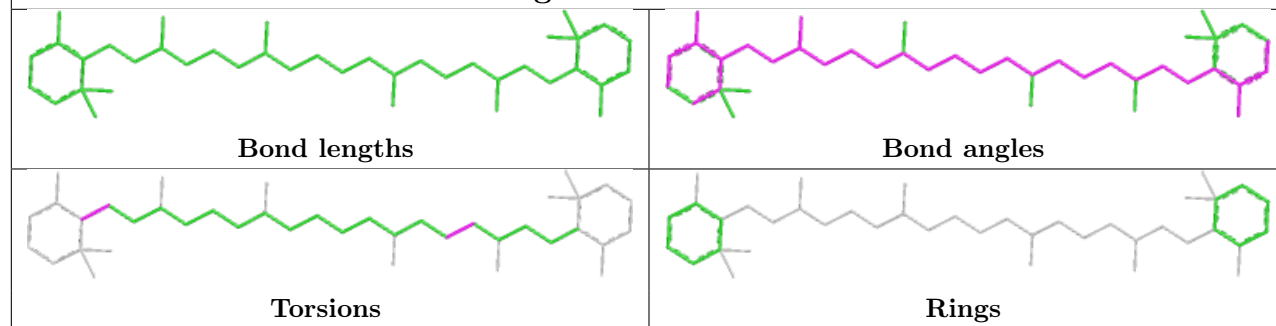
Ligand DD6 9 317

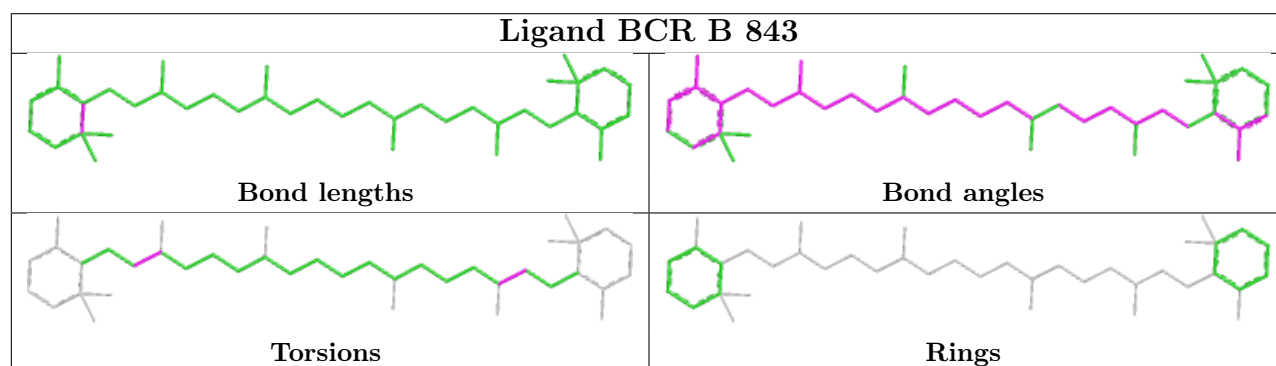
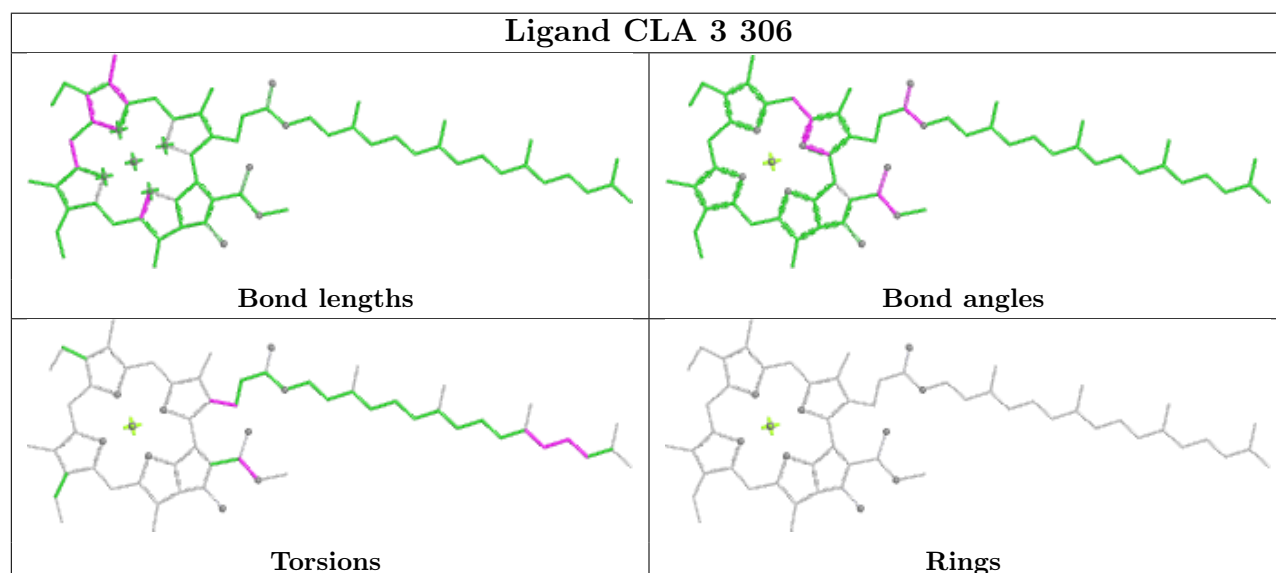
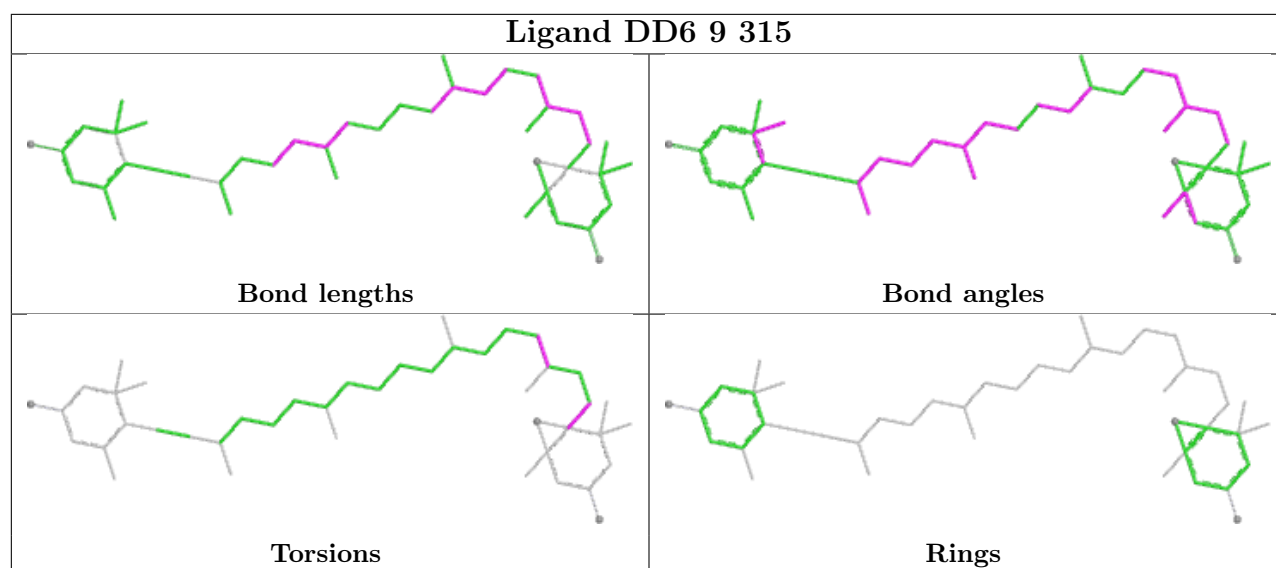


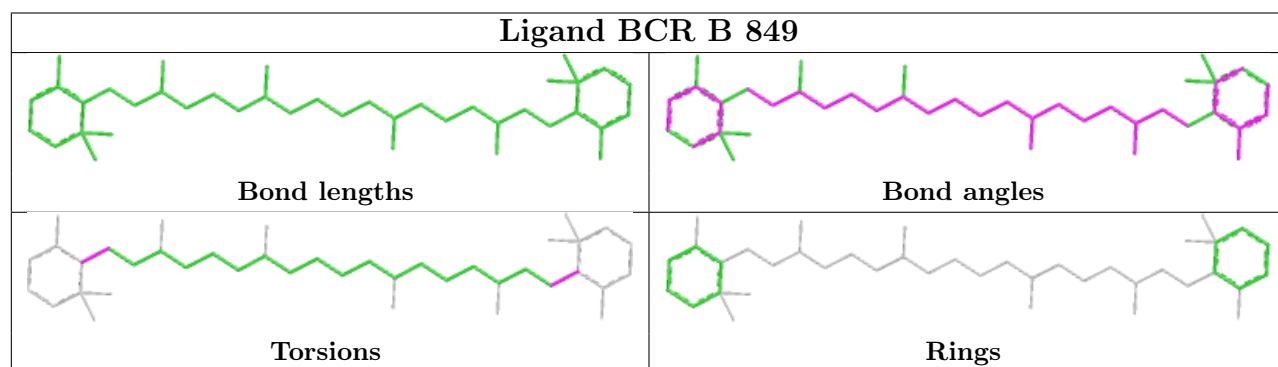
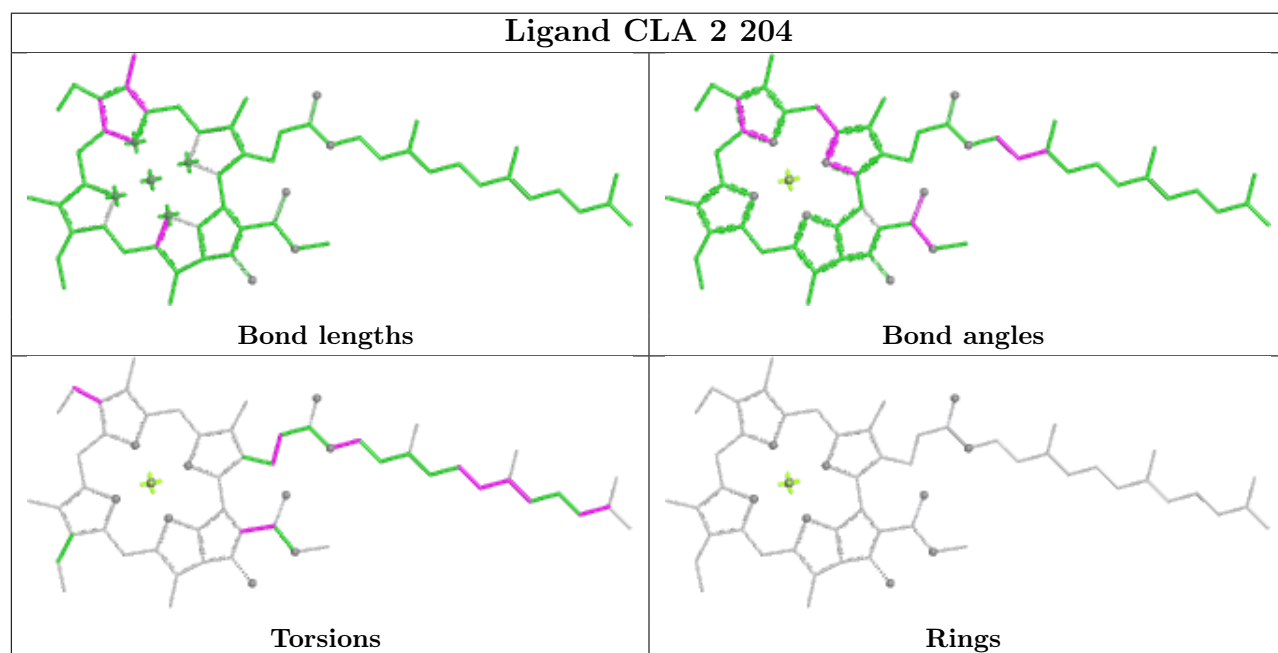
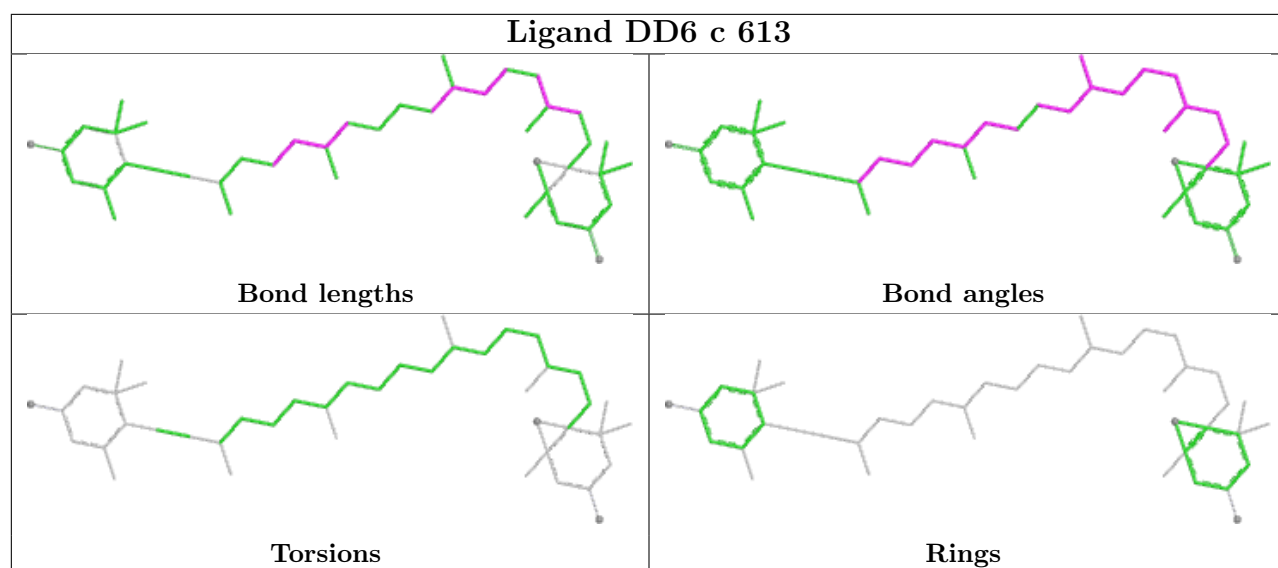
Ligand CLA h 605



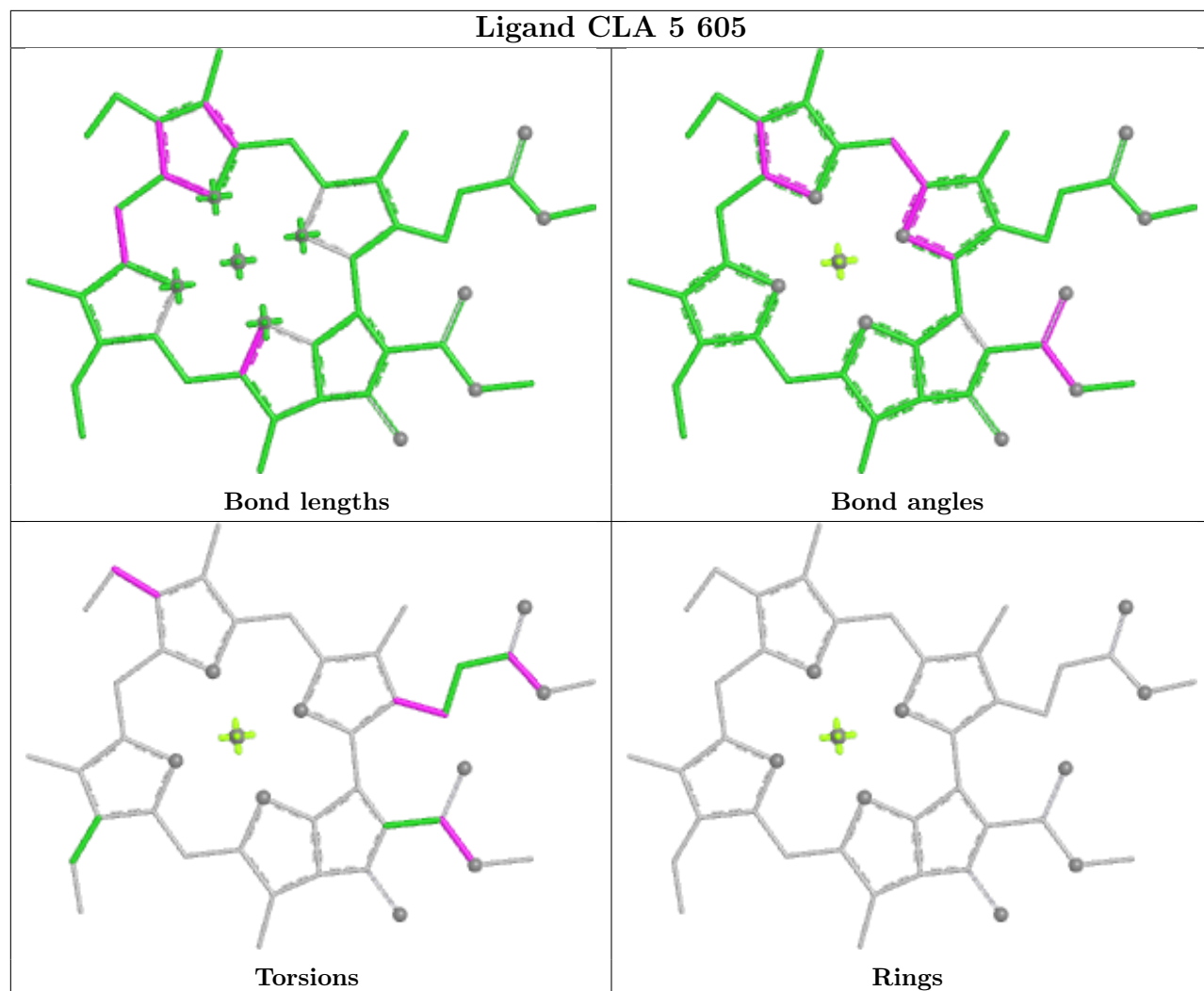
Ligand BCR k 316

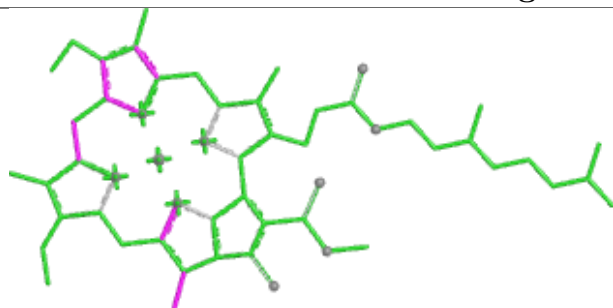




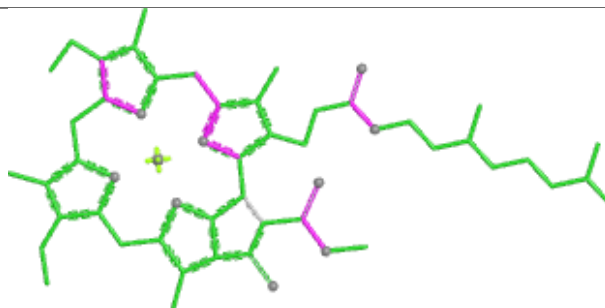


Ligand CLA 5 605

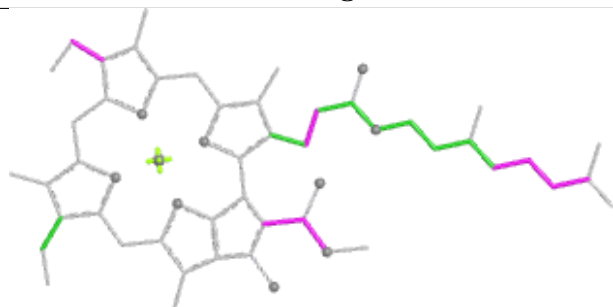


Ligand CLA 1 304

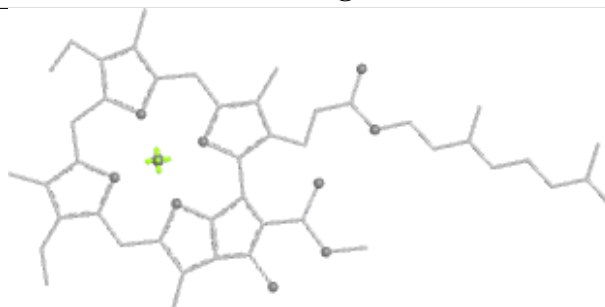
Bond lengths



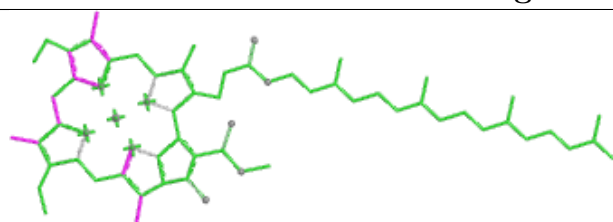
Bond angles



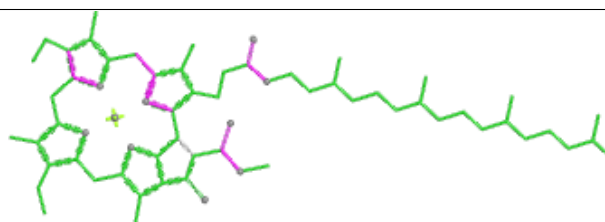
Torsions



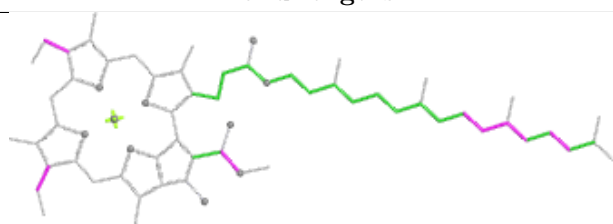
Rings

Ligand CLA B 803

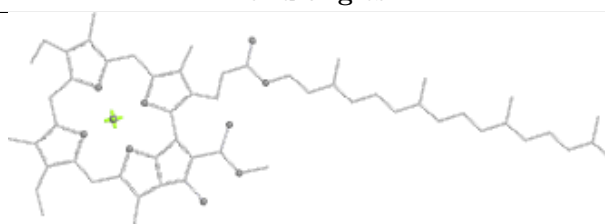
Bond lengths



Bond angles

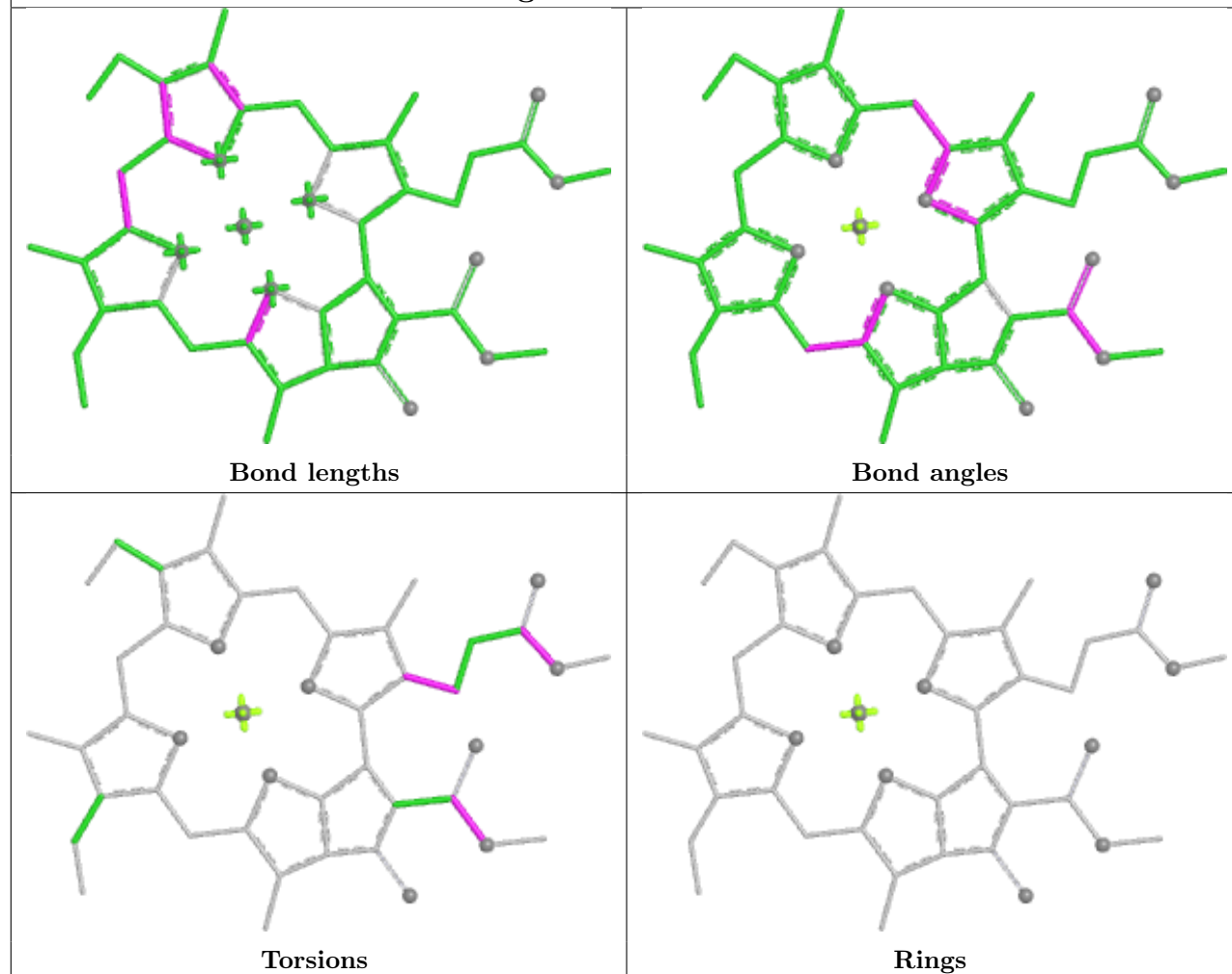


Torsions

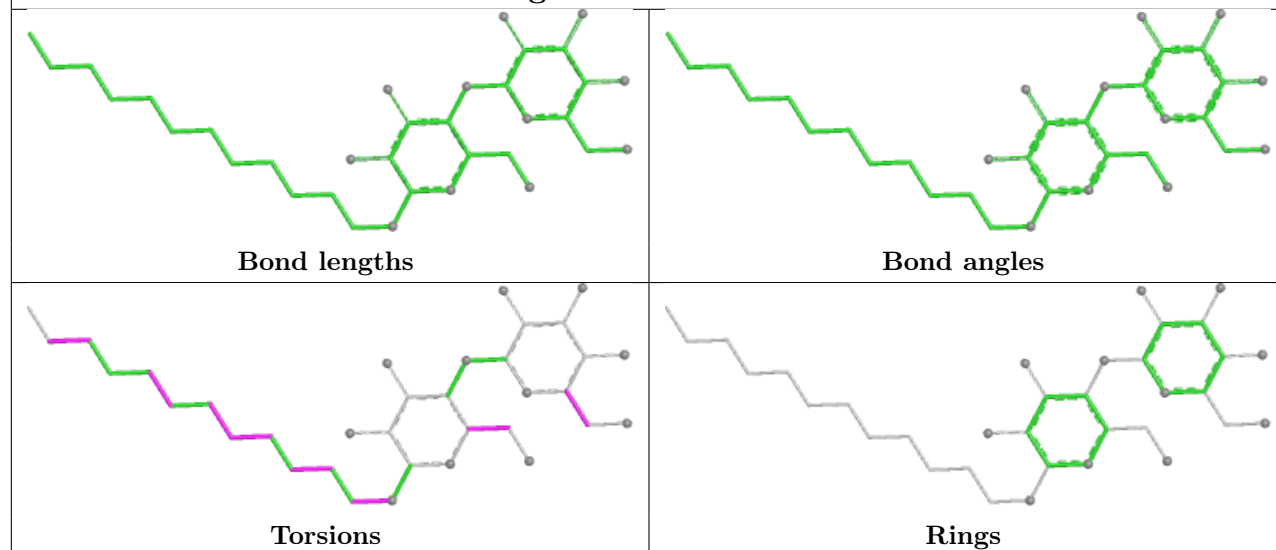


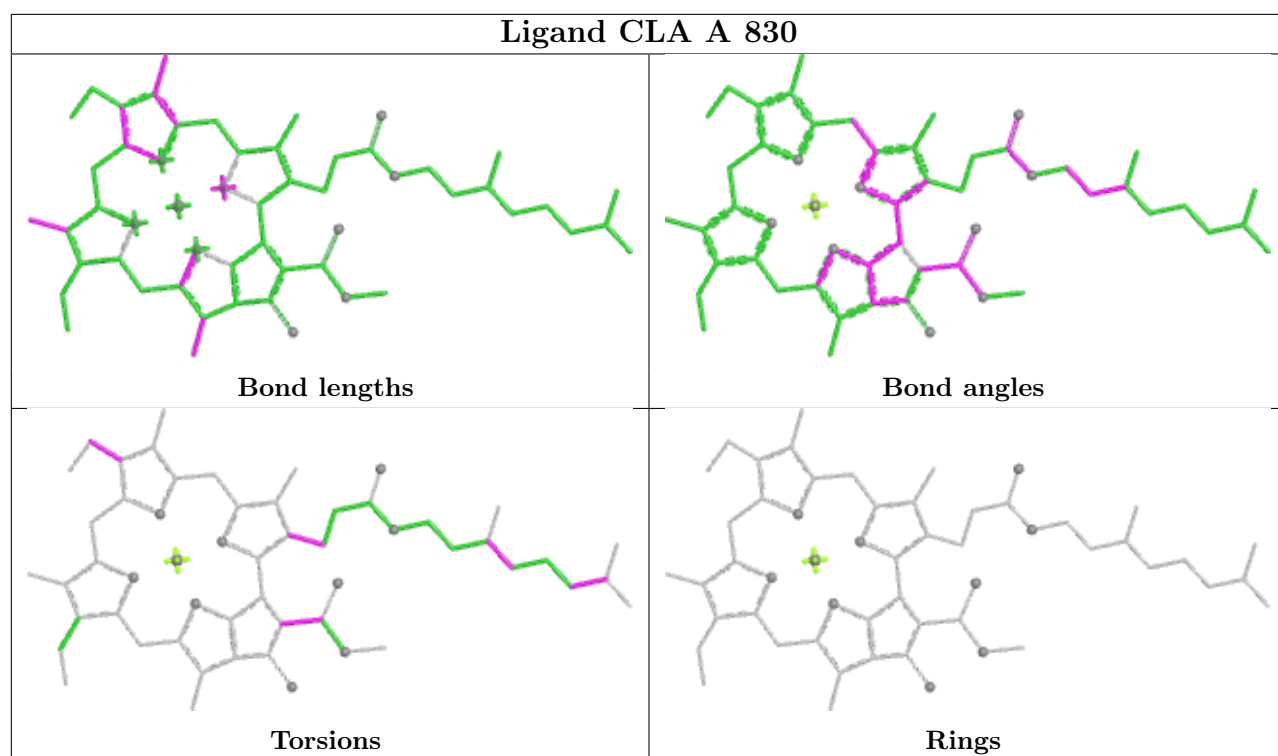
Rings

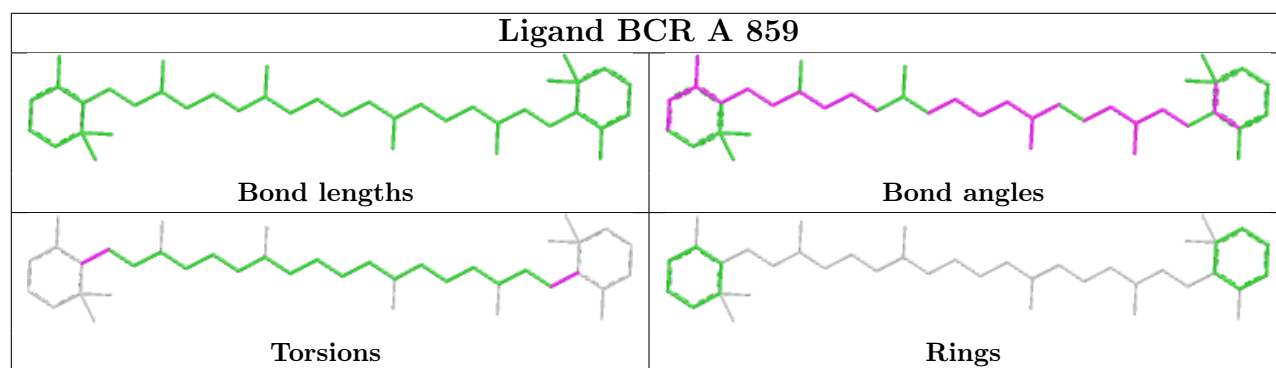
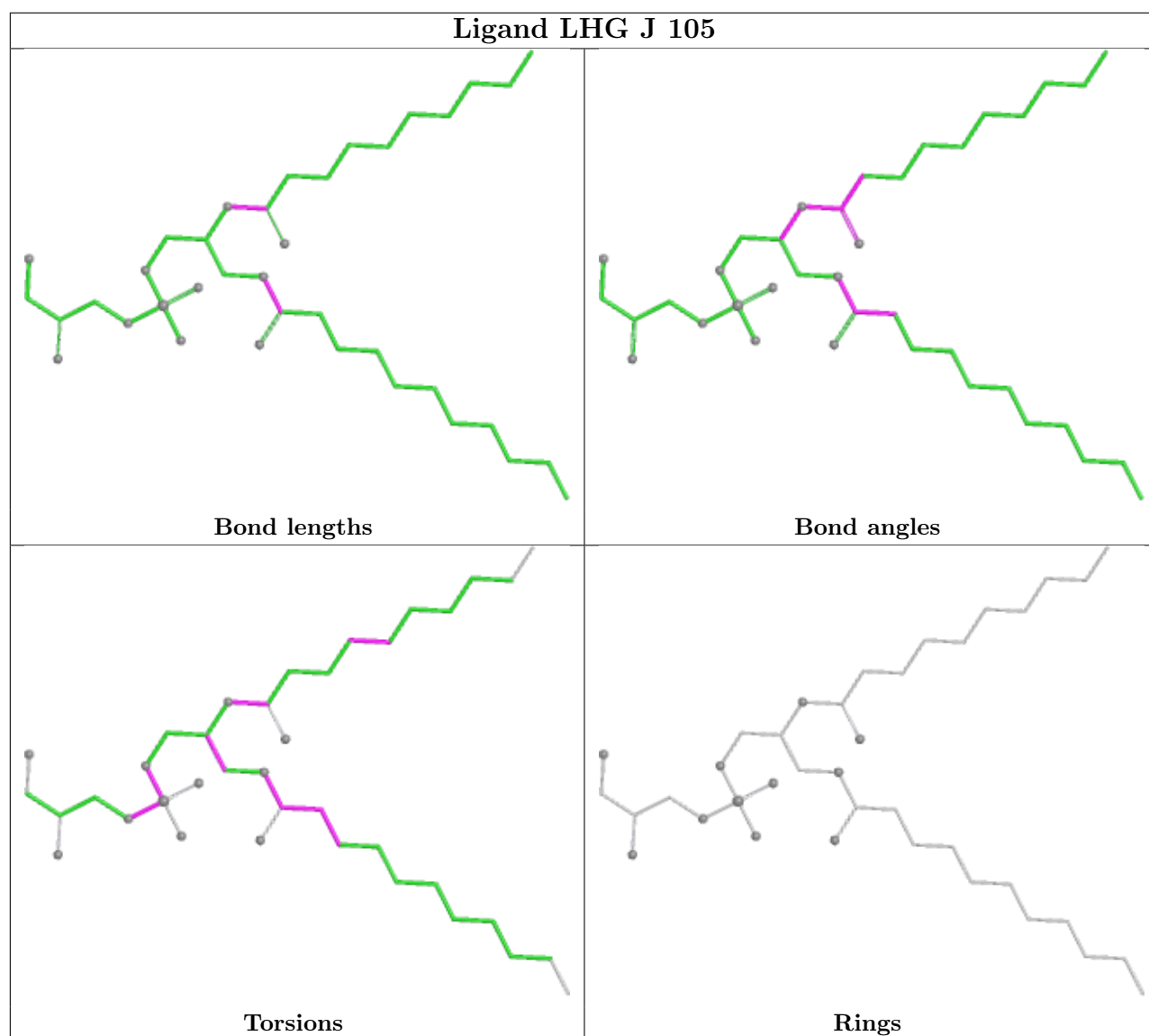
Ligand CLA 8 206



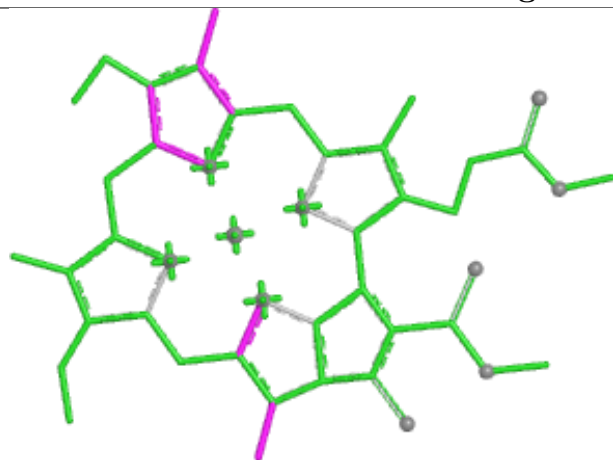
Ligand LMT A 850



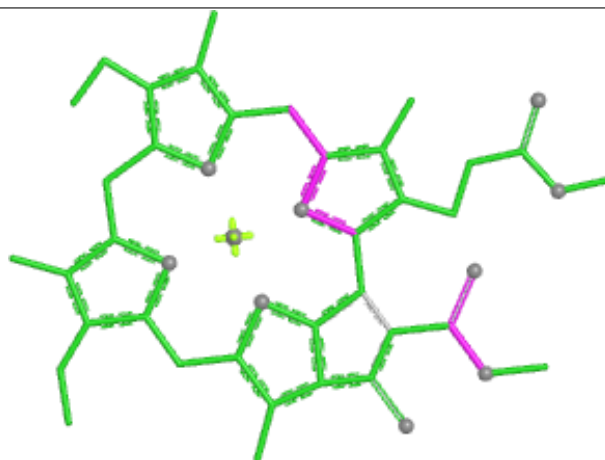




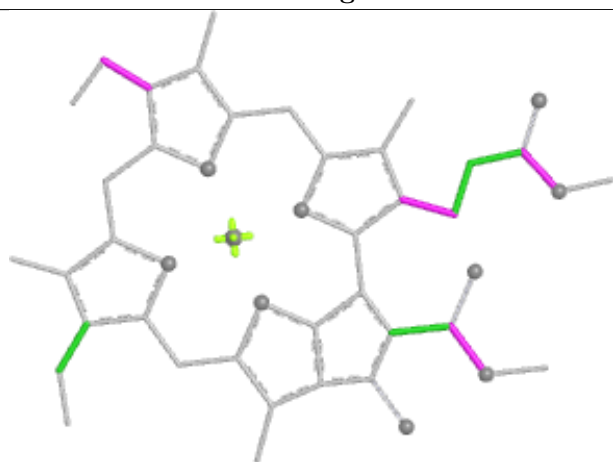
Ligand CLA 9 310



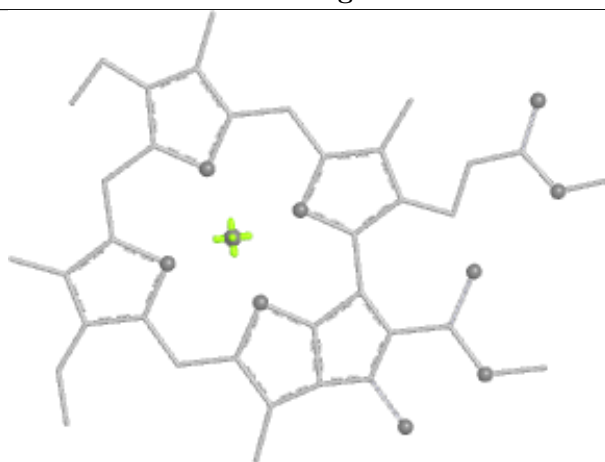
Bond lengths



Bond angles

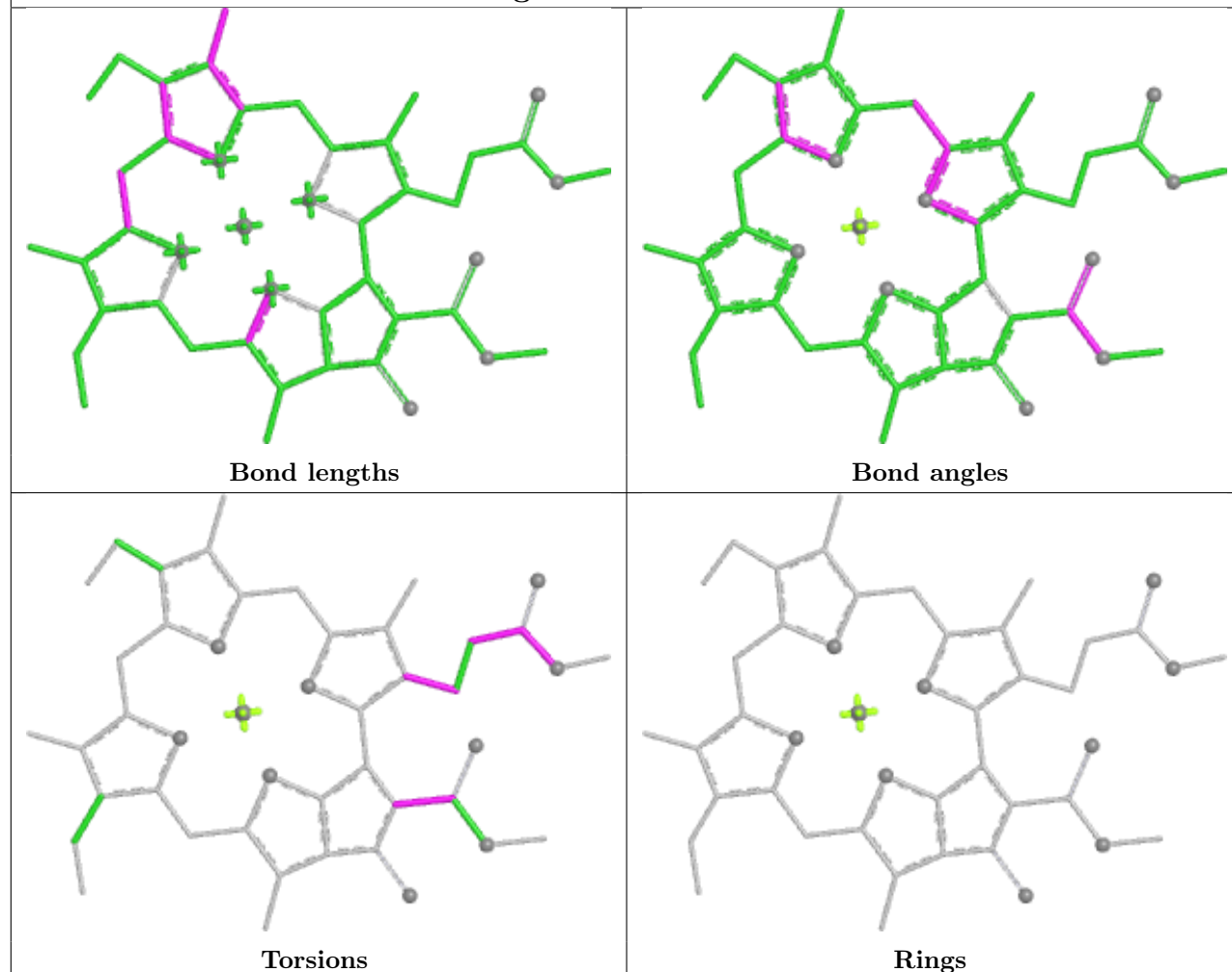


Torsions

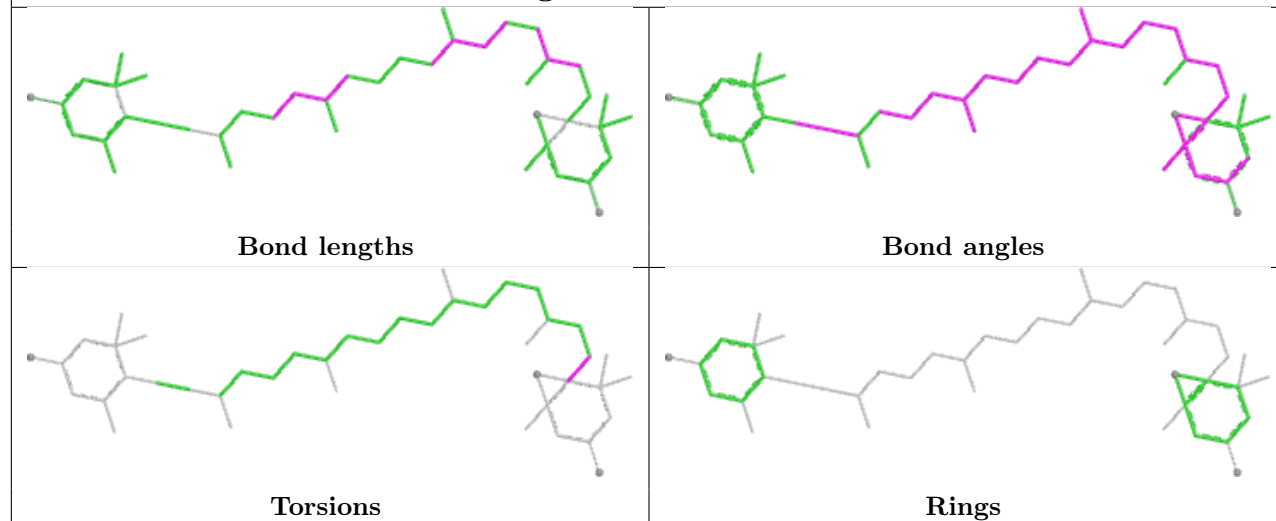


Rings

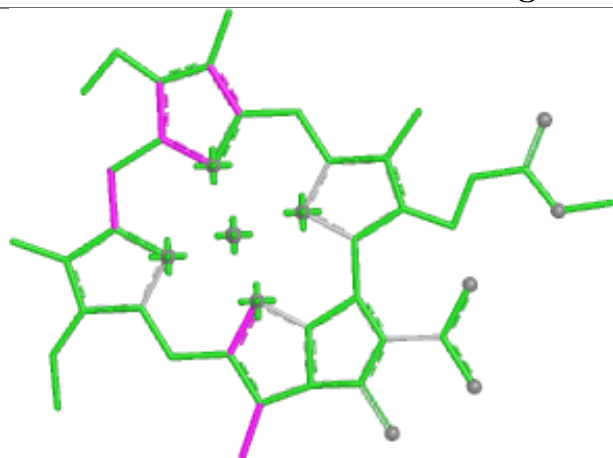
Ligand CLA A 811



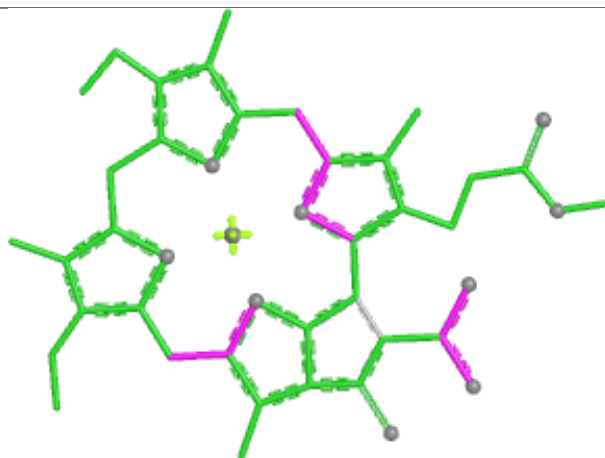
Ligand DD6 k 313



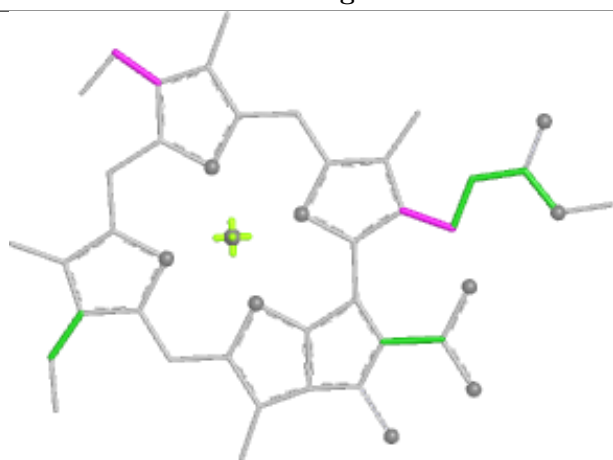
Ligand CLA 1 309



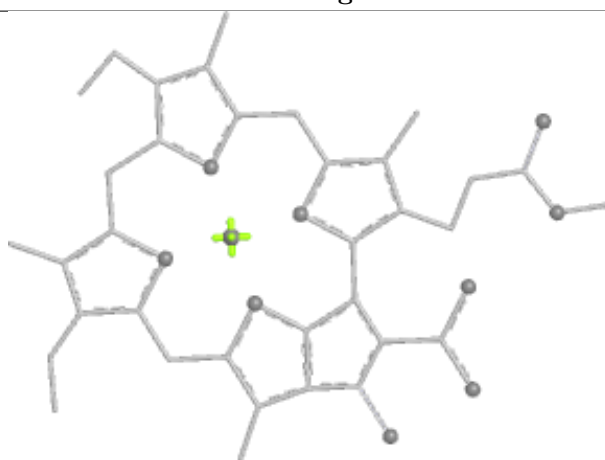
Bond lengths



Bond angles

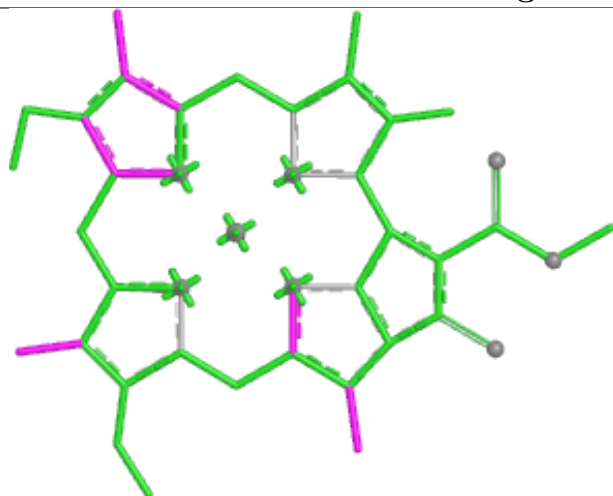


Torsions

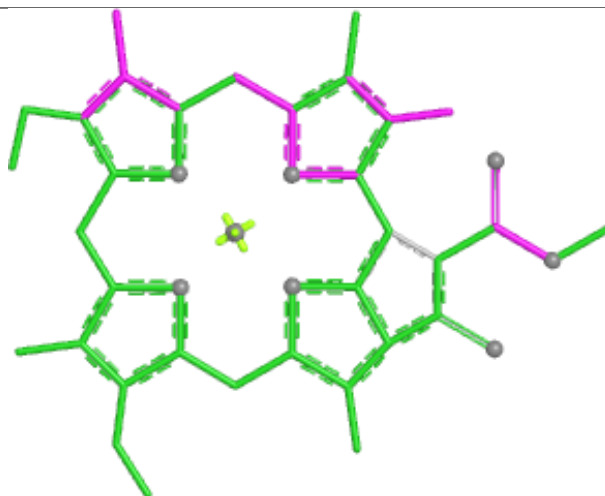


Rings

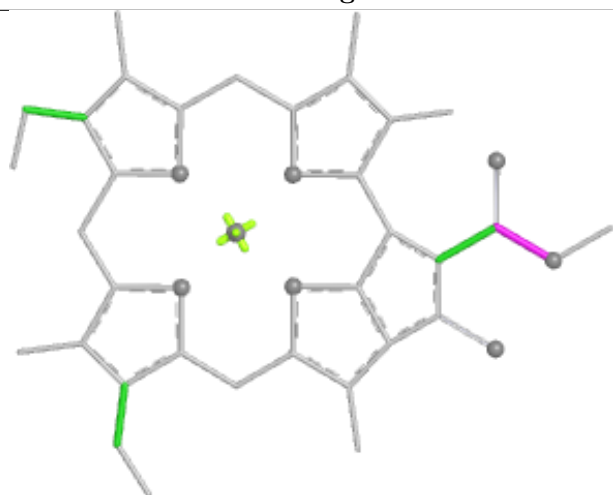
Ligand CLA h 611



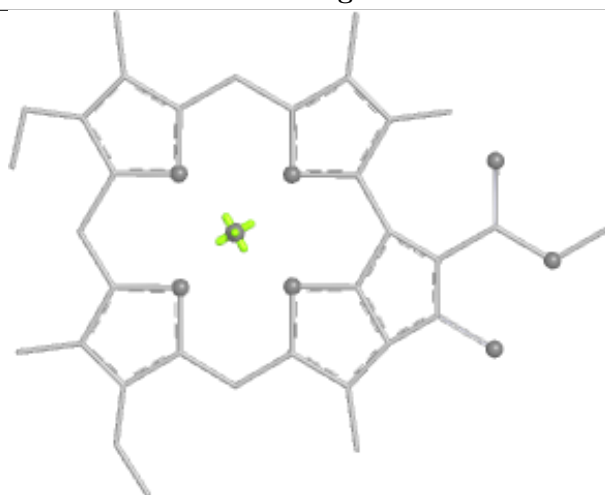
Bond lengths



Bond angles

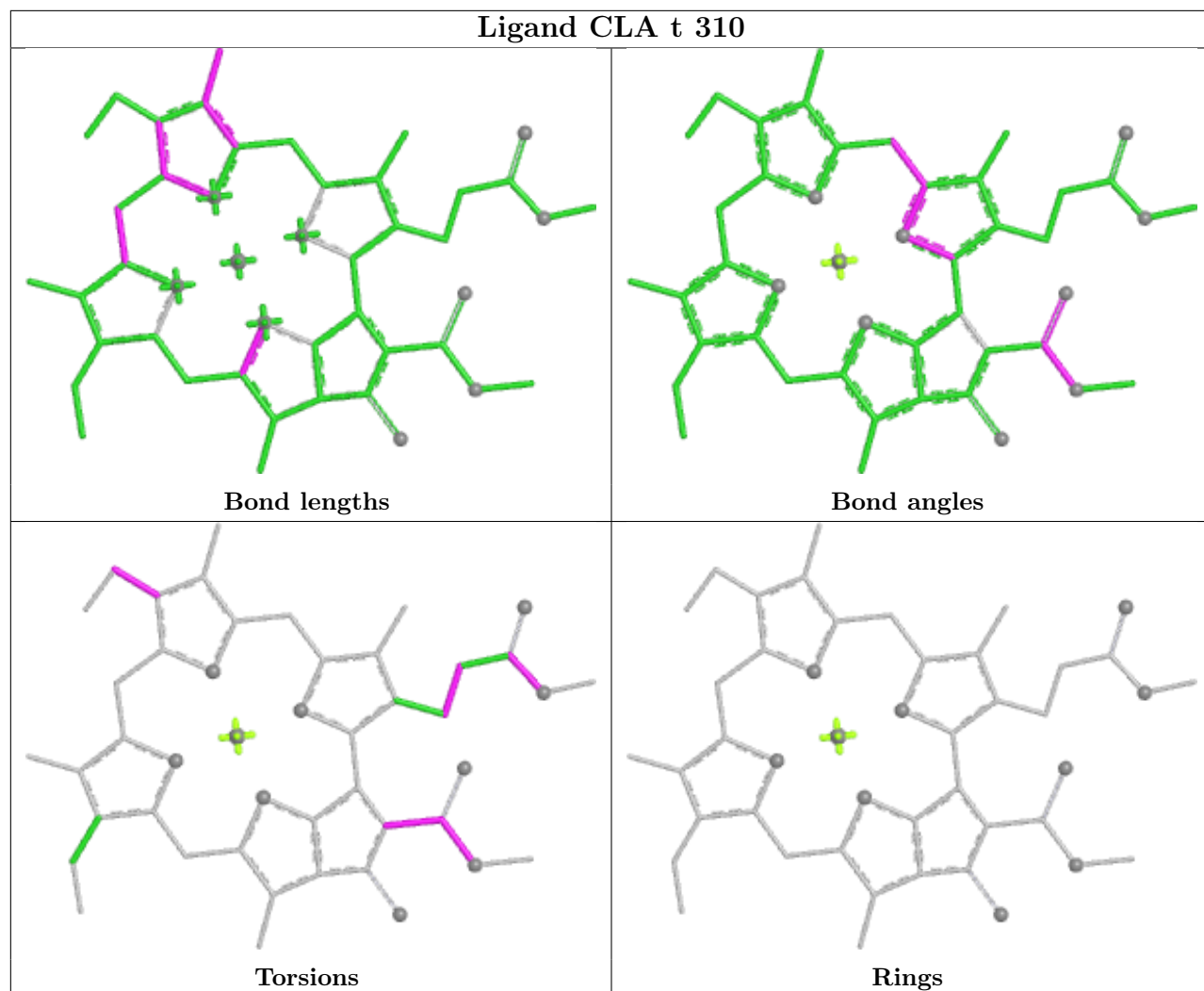


Torsions

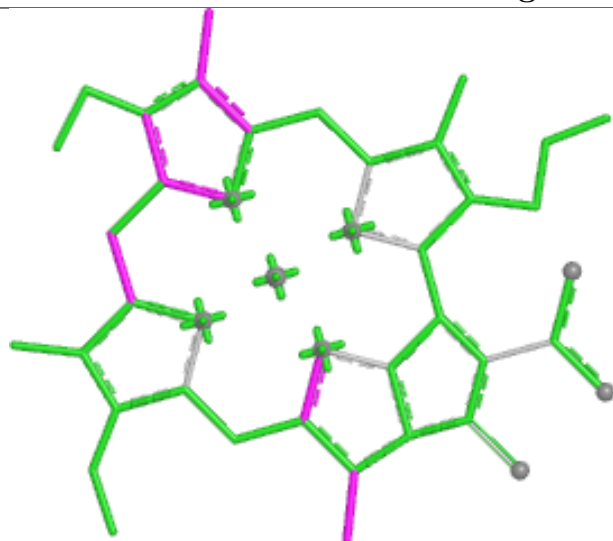


Rings

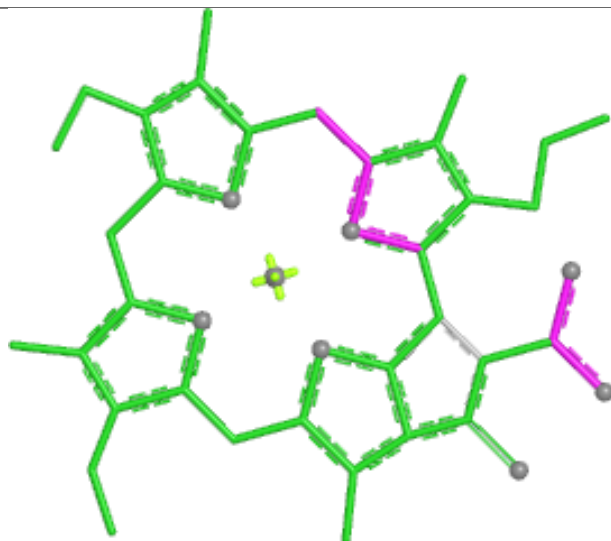
Ligand CLA t 310



Ligand CLA 4 601



Bond lengths



Bond angles

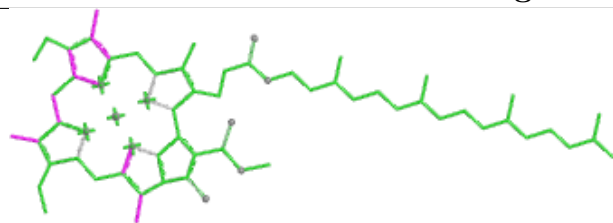


Torsions

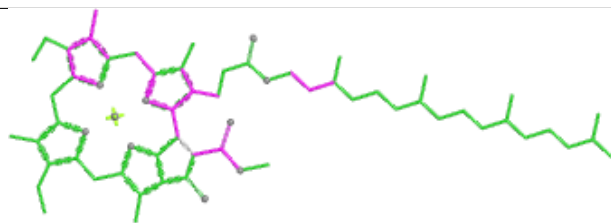


Rings

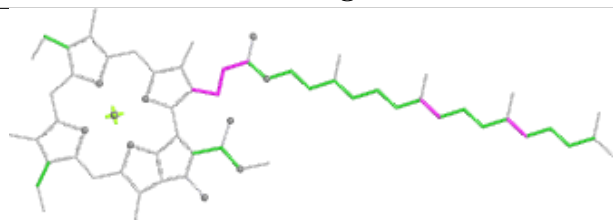
Ligand CLA B 829



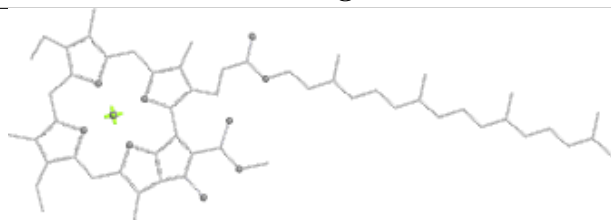
Bond lengths



Bond angles

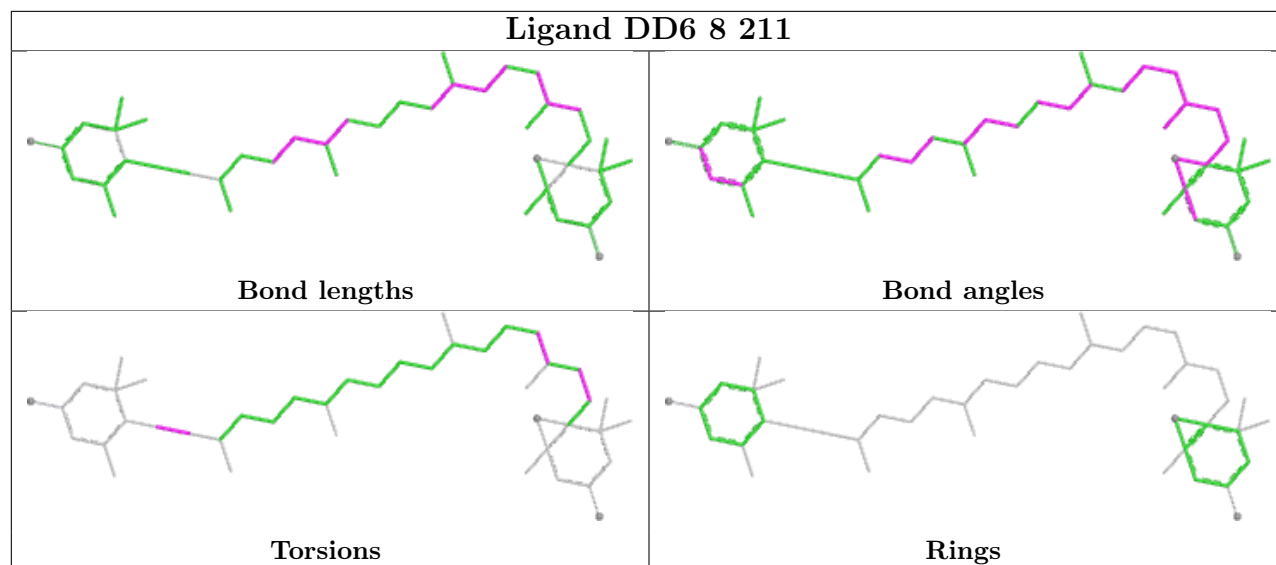


Torsions

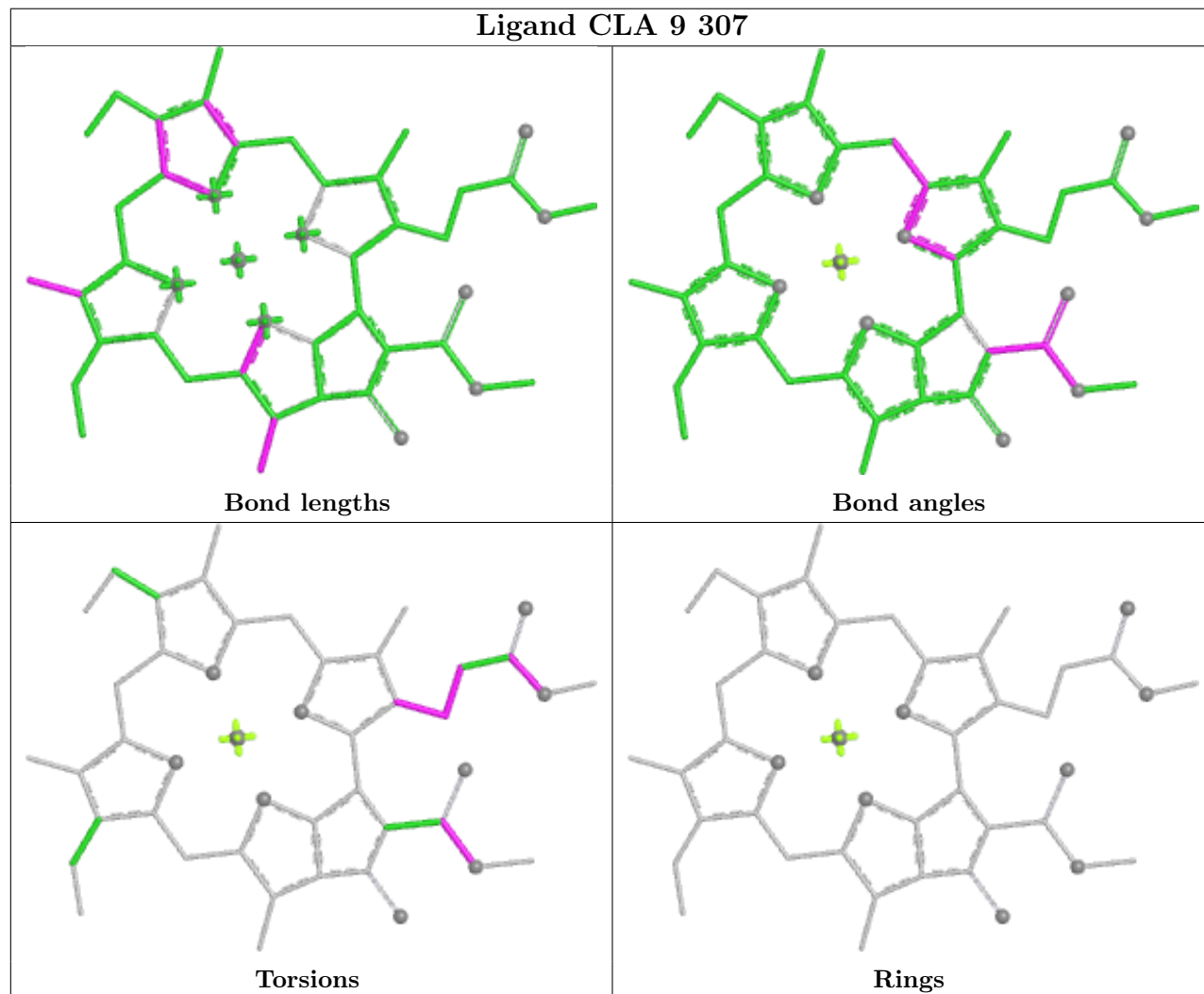


Rings

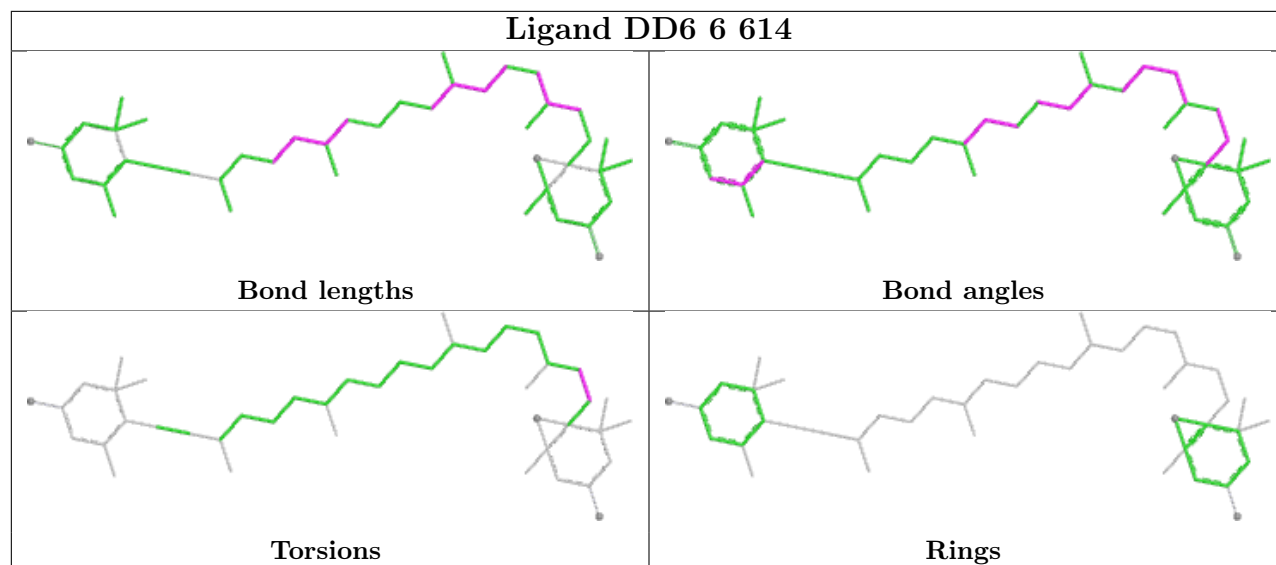
Ligand DD6 8 211



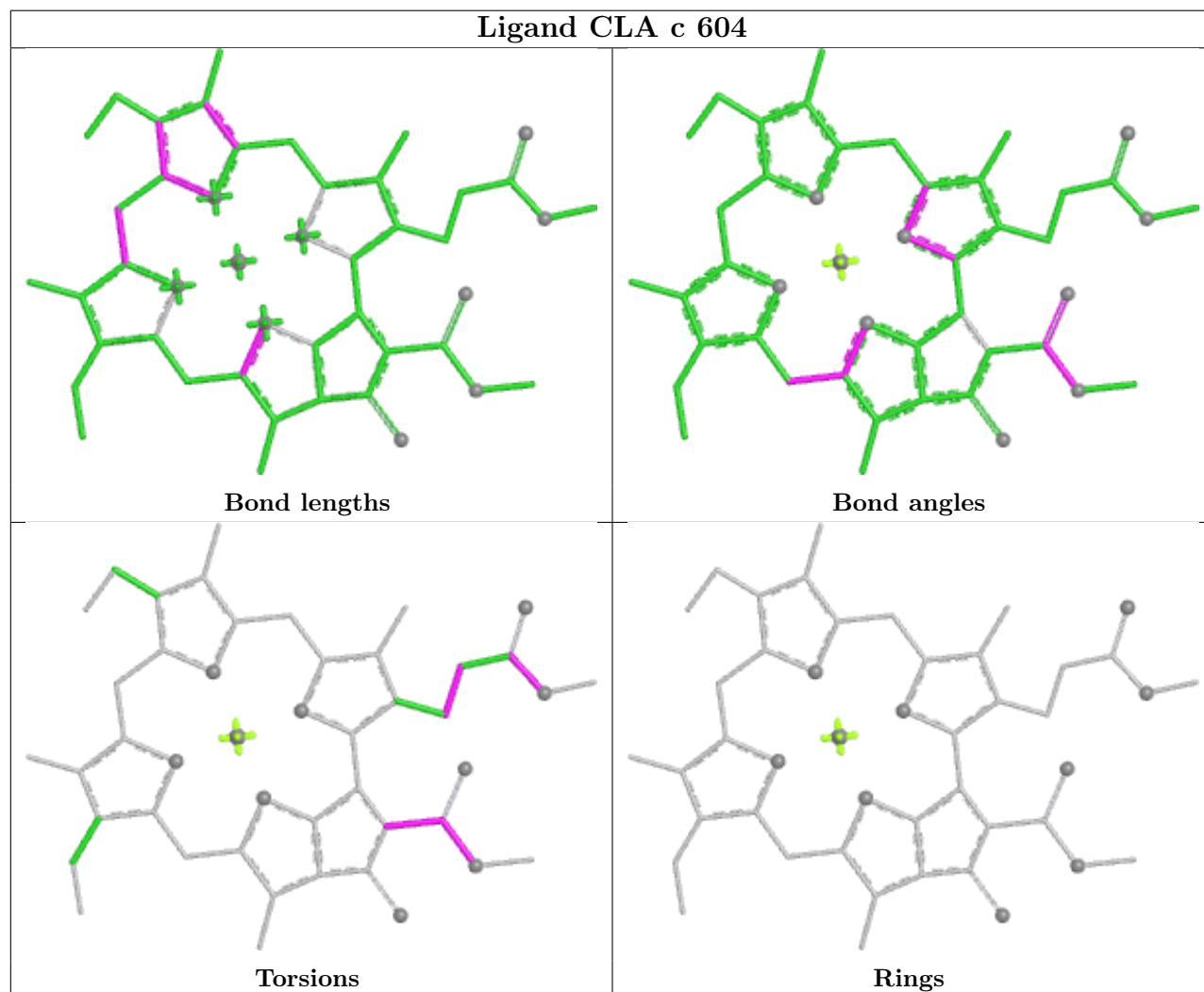
Ligand CLA 9 307



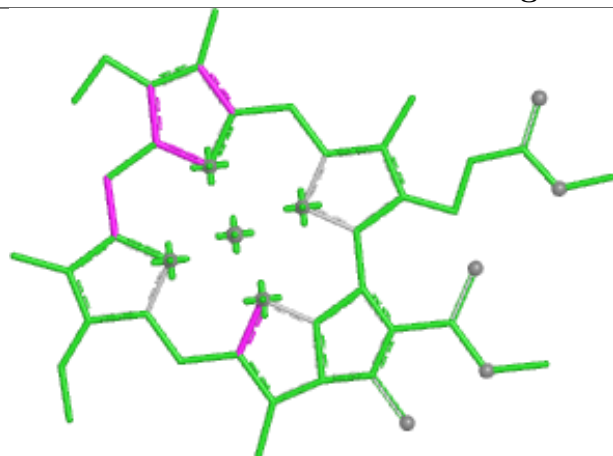
Ligand DD6 6 614



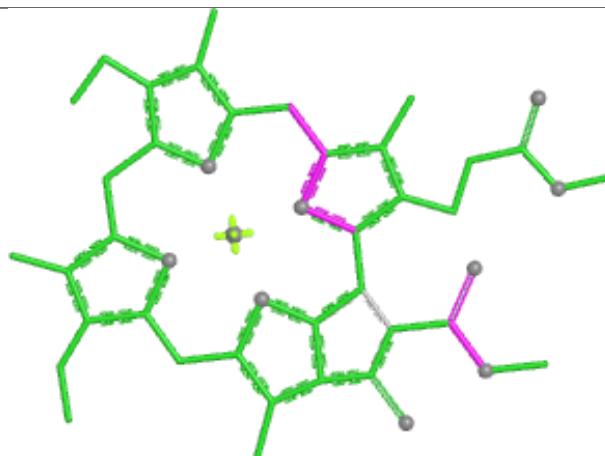
Ligand CLA c 604



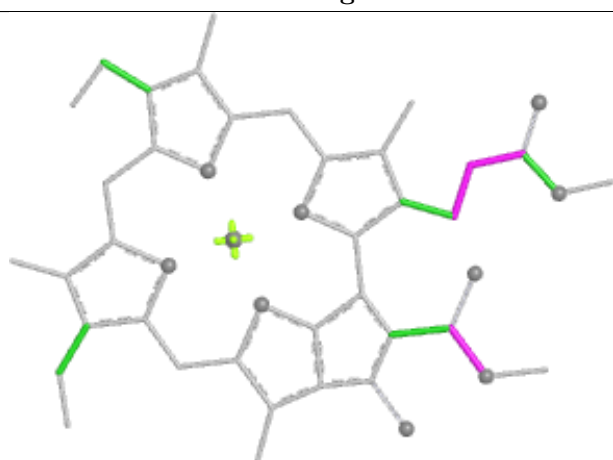
Ligand CLA t 309



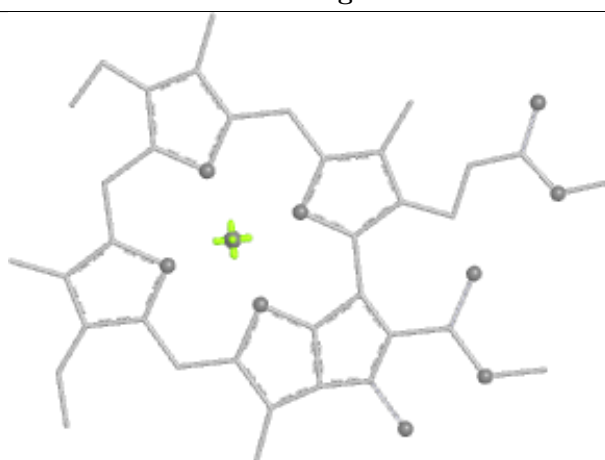
Bond lengths



Bond angles

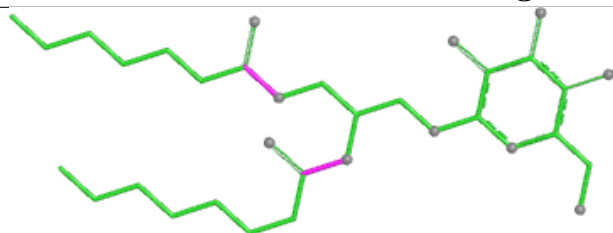


Torsions

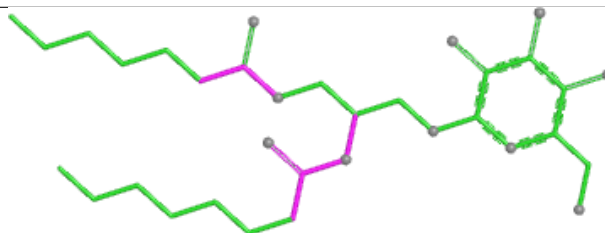


Rings

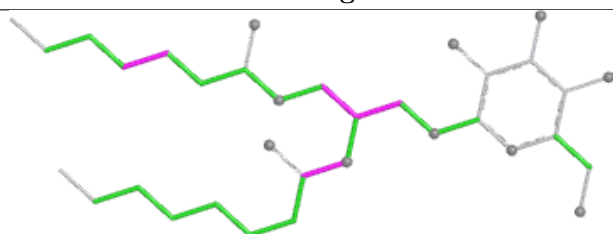
Ligand LMG t 314



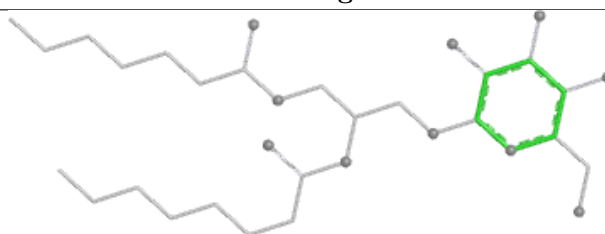
Bond lengths



Bond angles

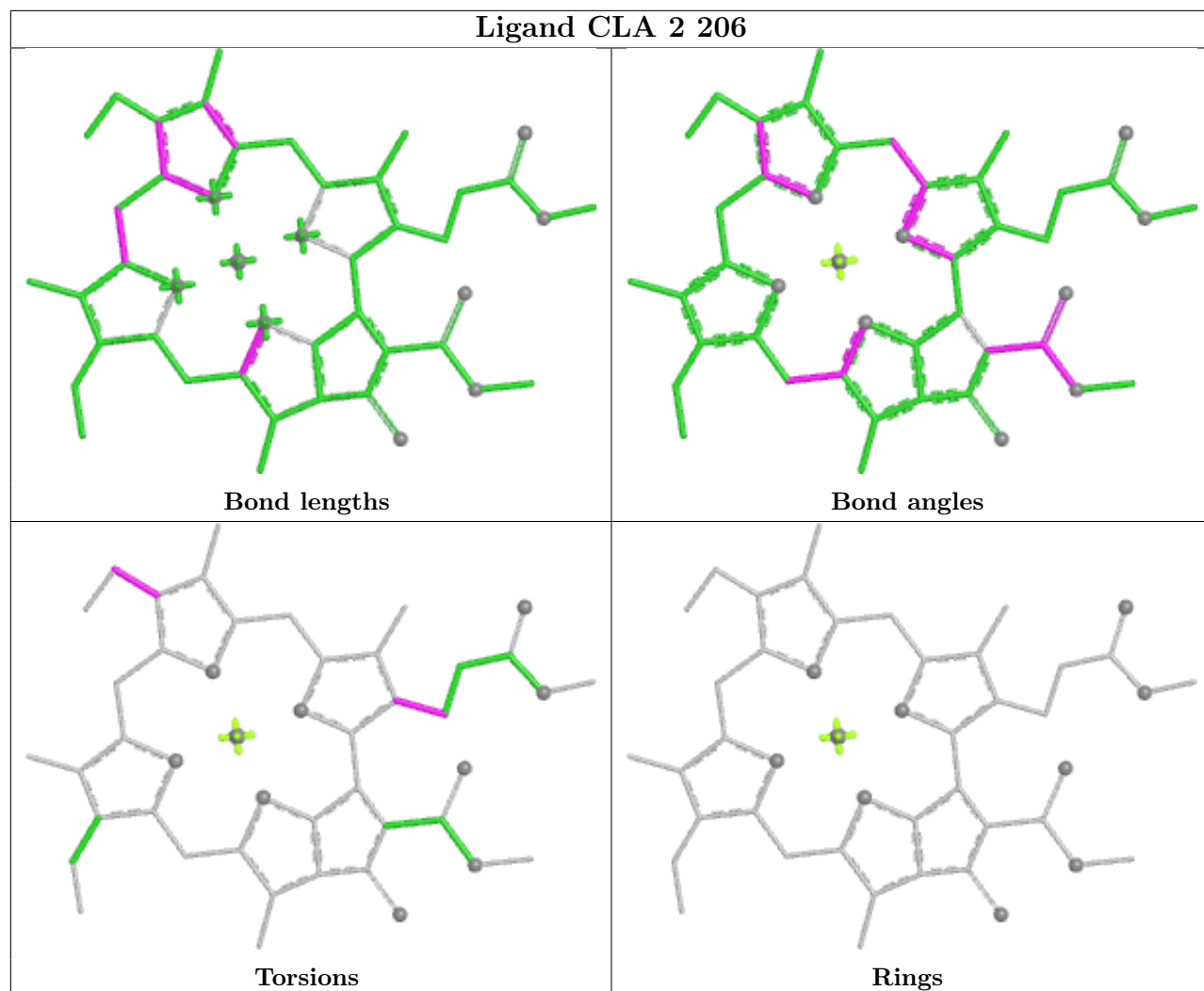


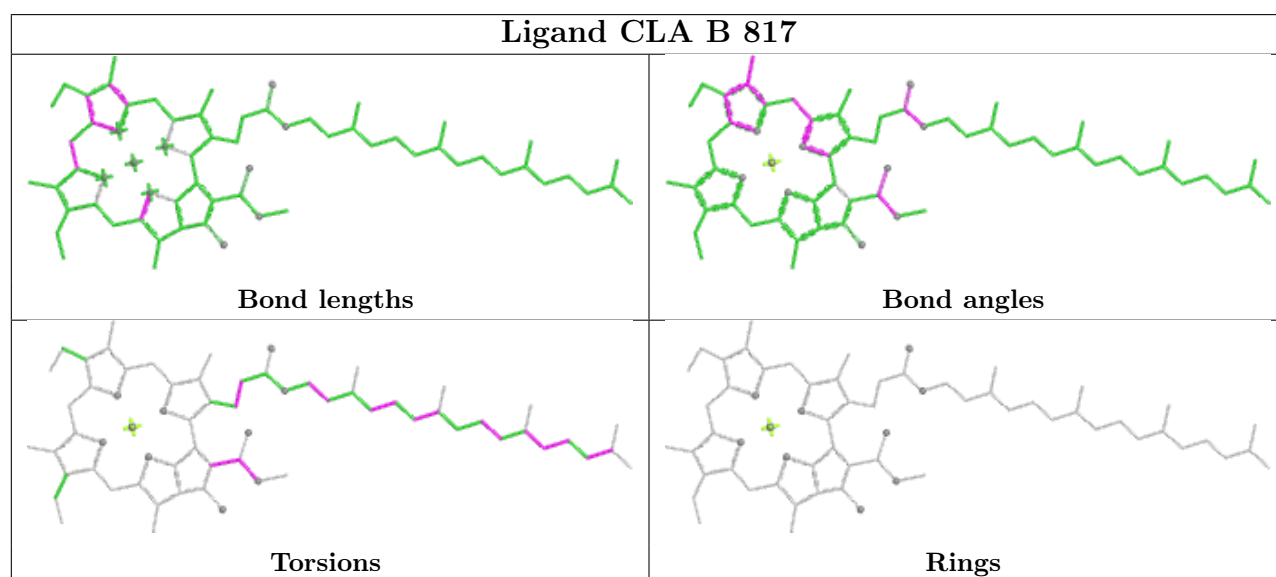
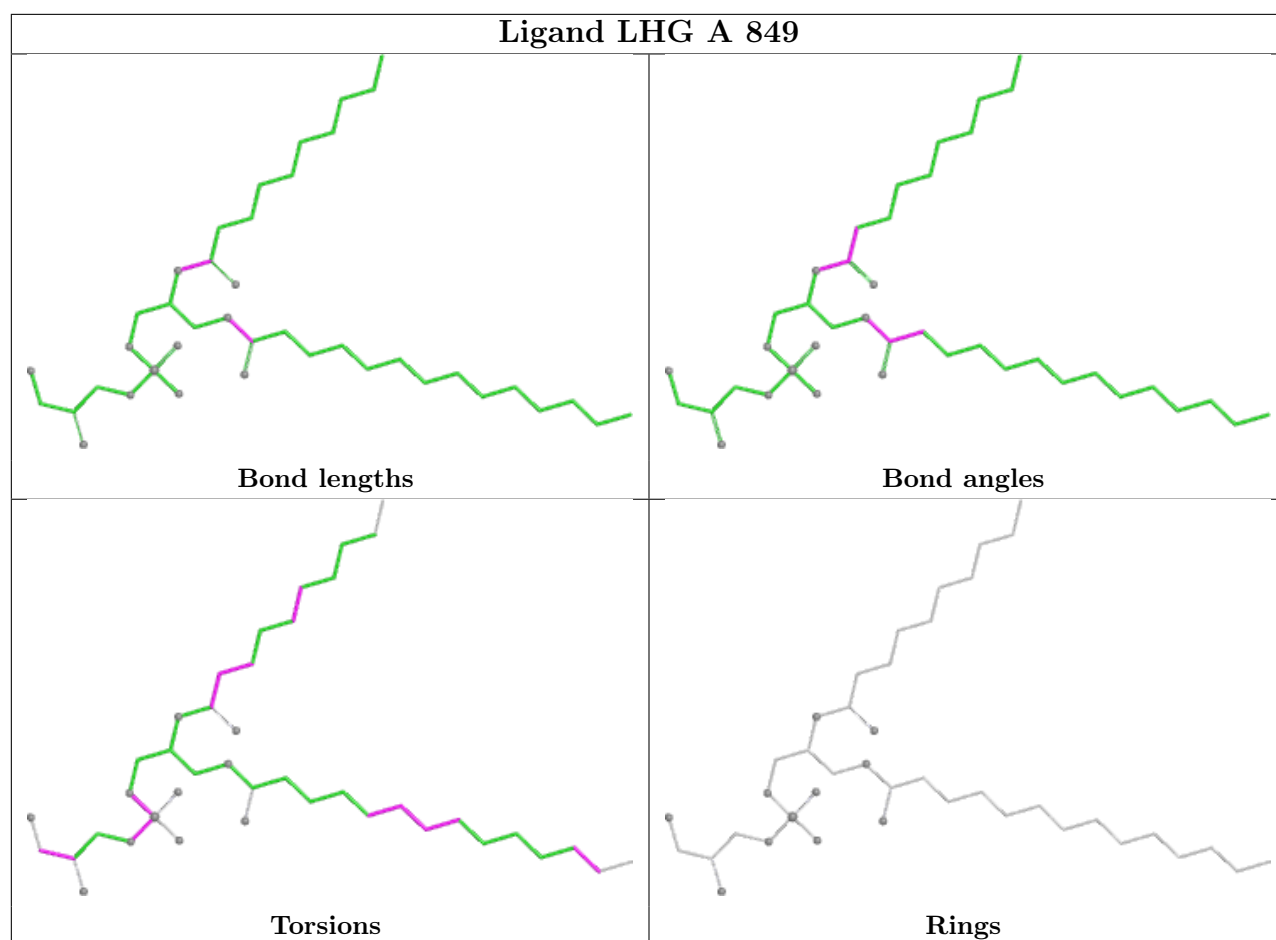
Torsions

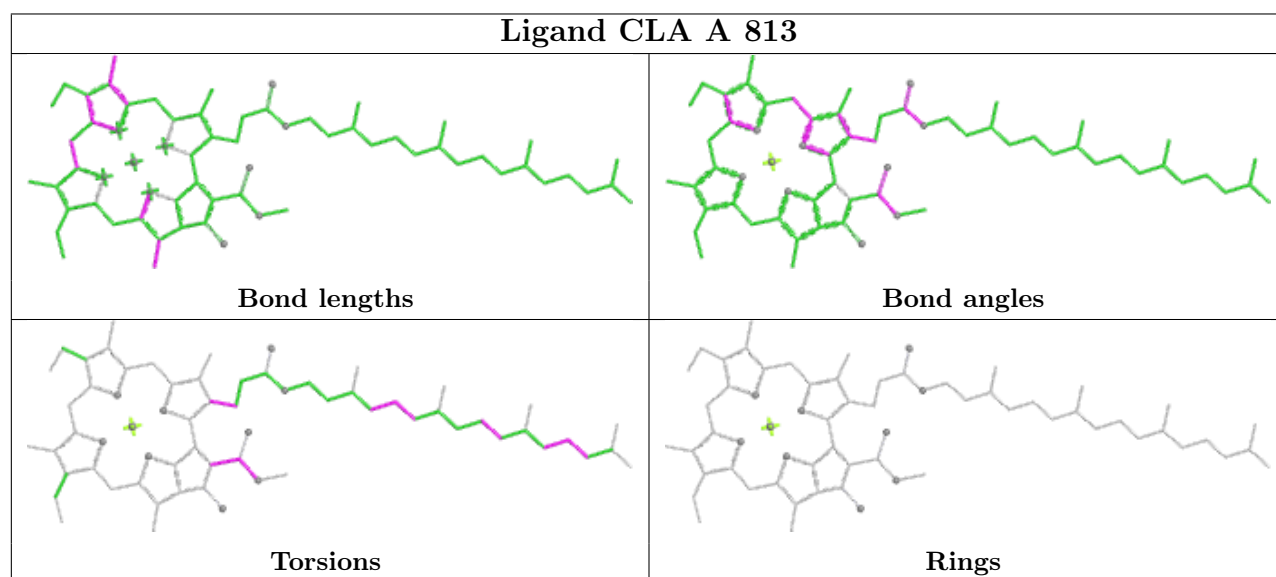
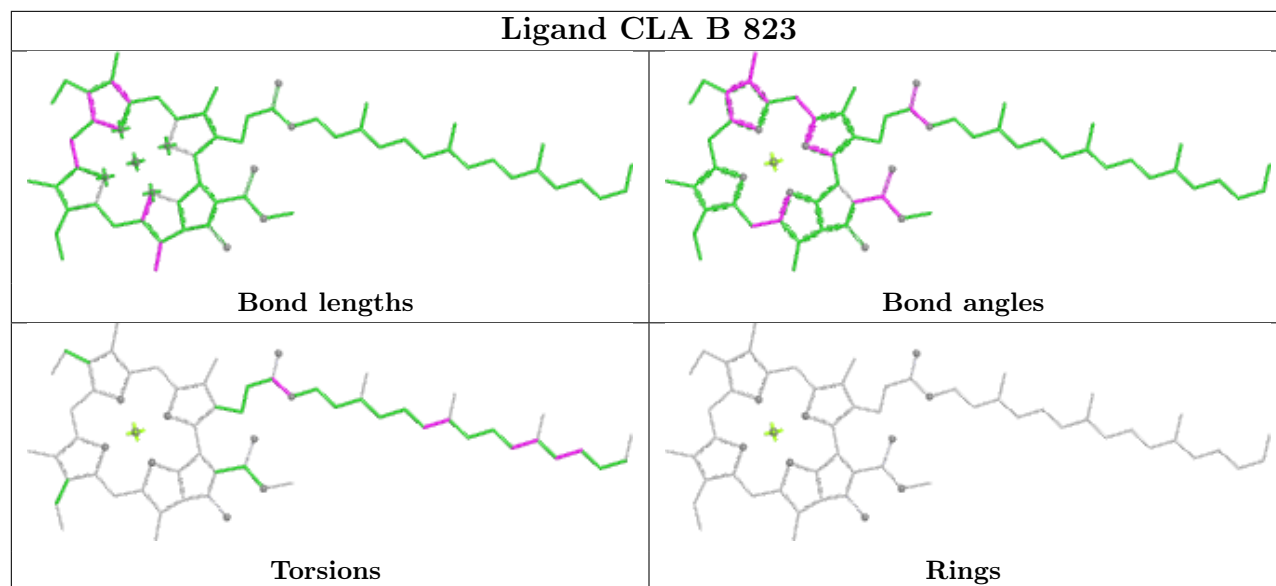


Rings

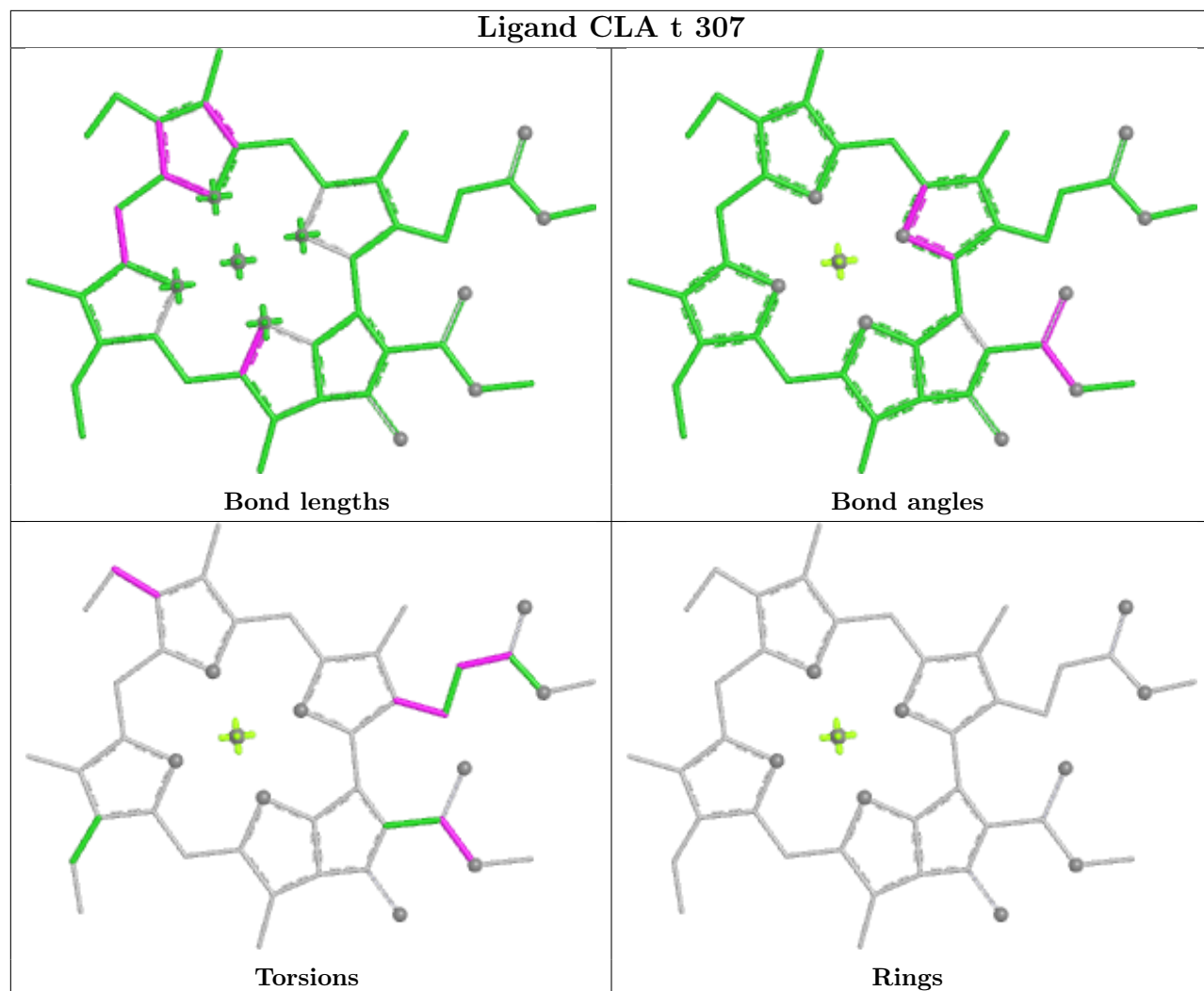
Ligand CLA 2 206



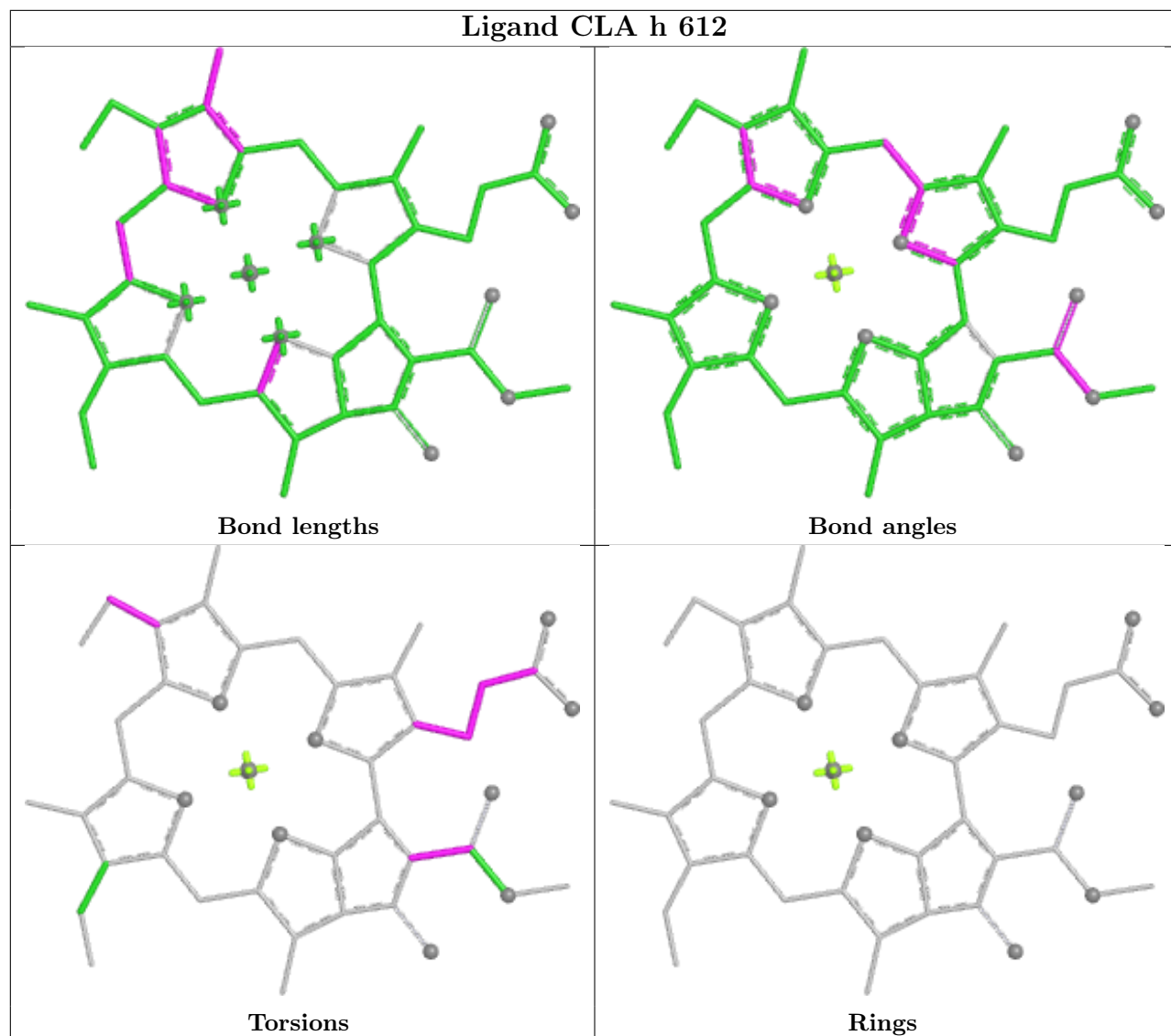




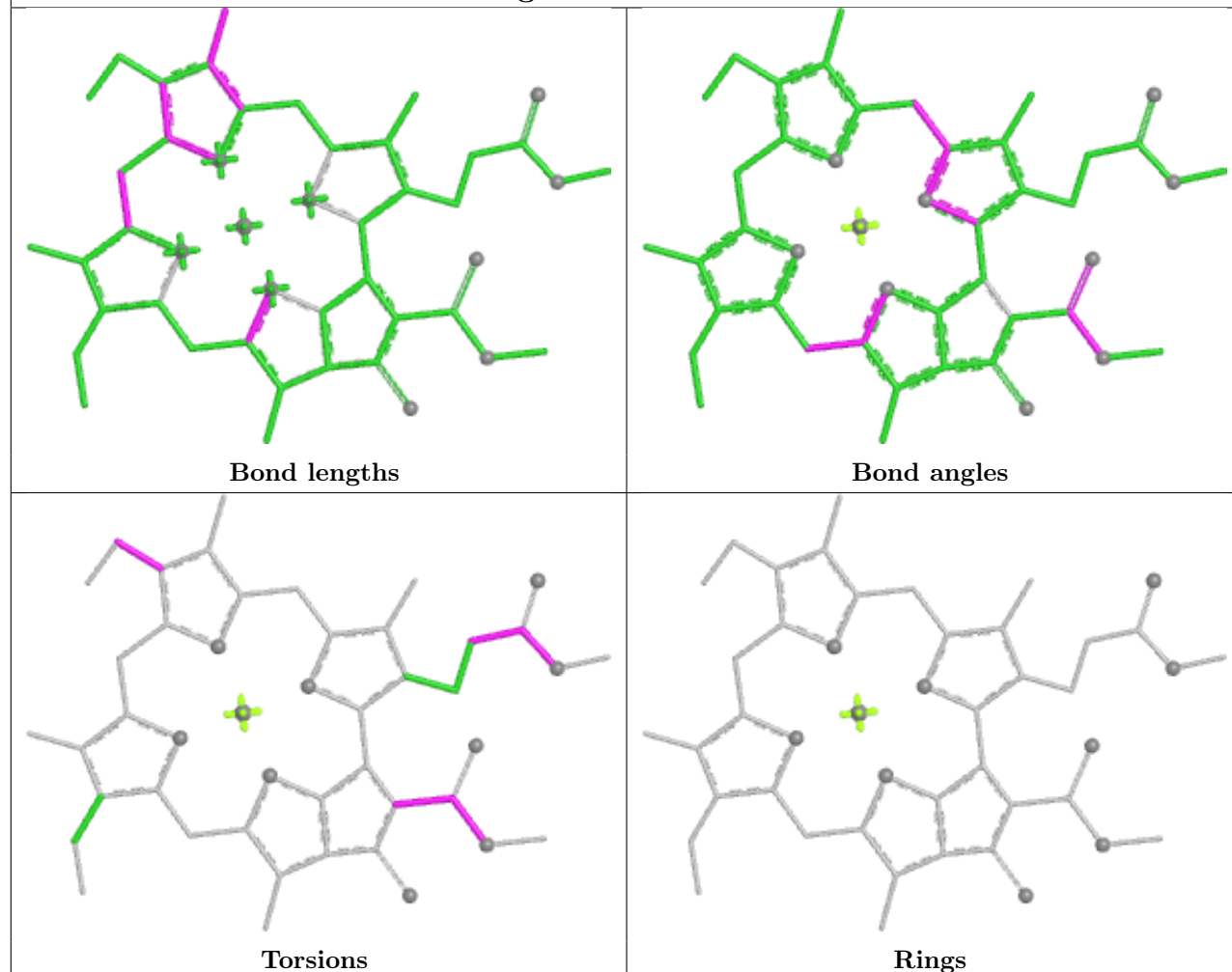
Ligand CLA t 307



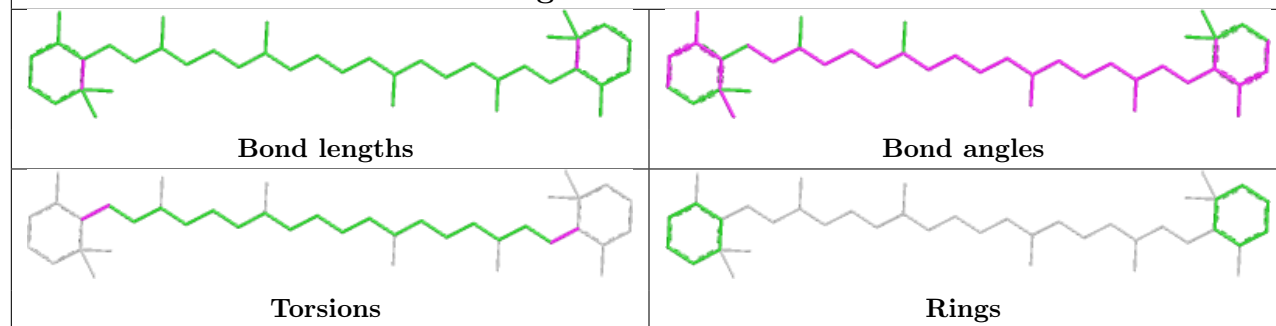
Ligand CLA h 612

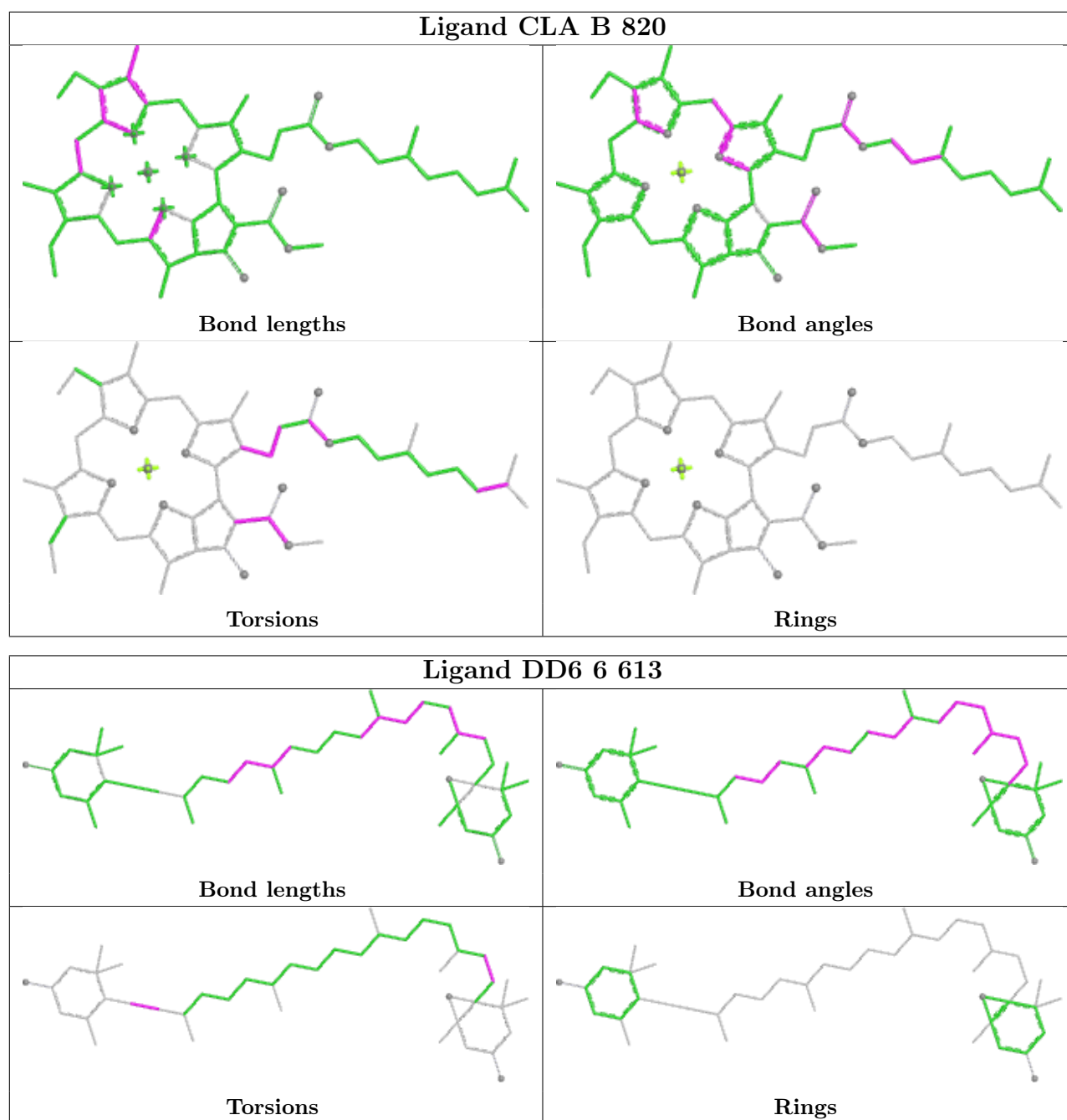


Ligand CLA 4 613

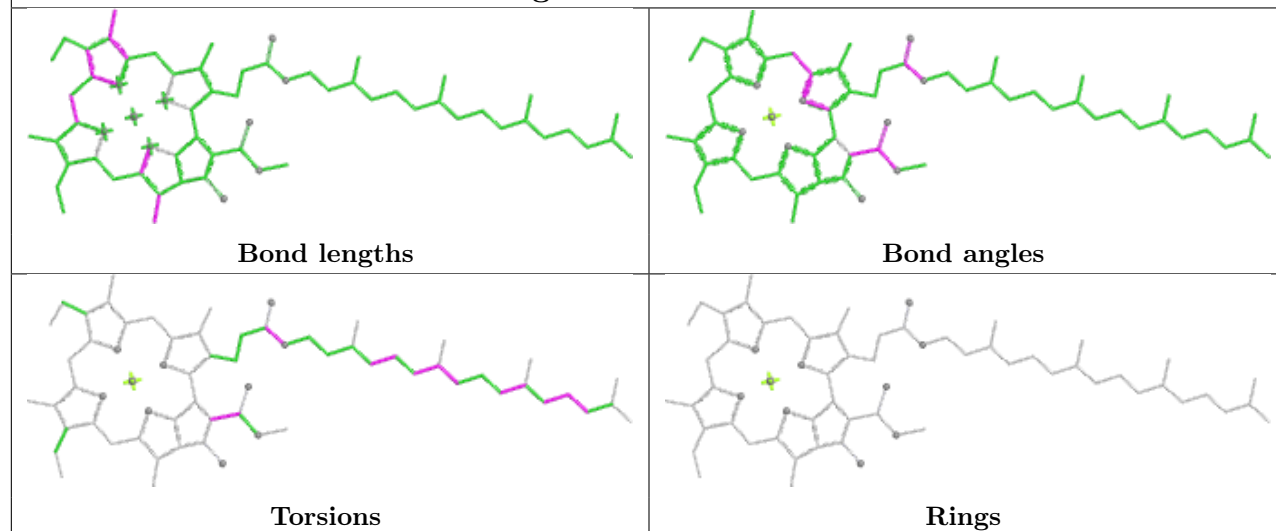


Ligand BCR I 101

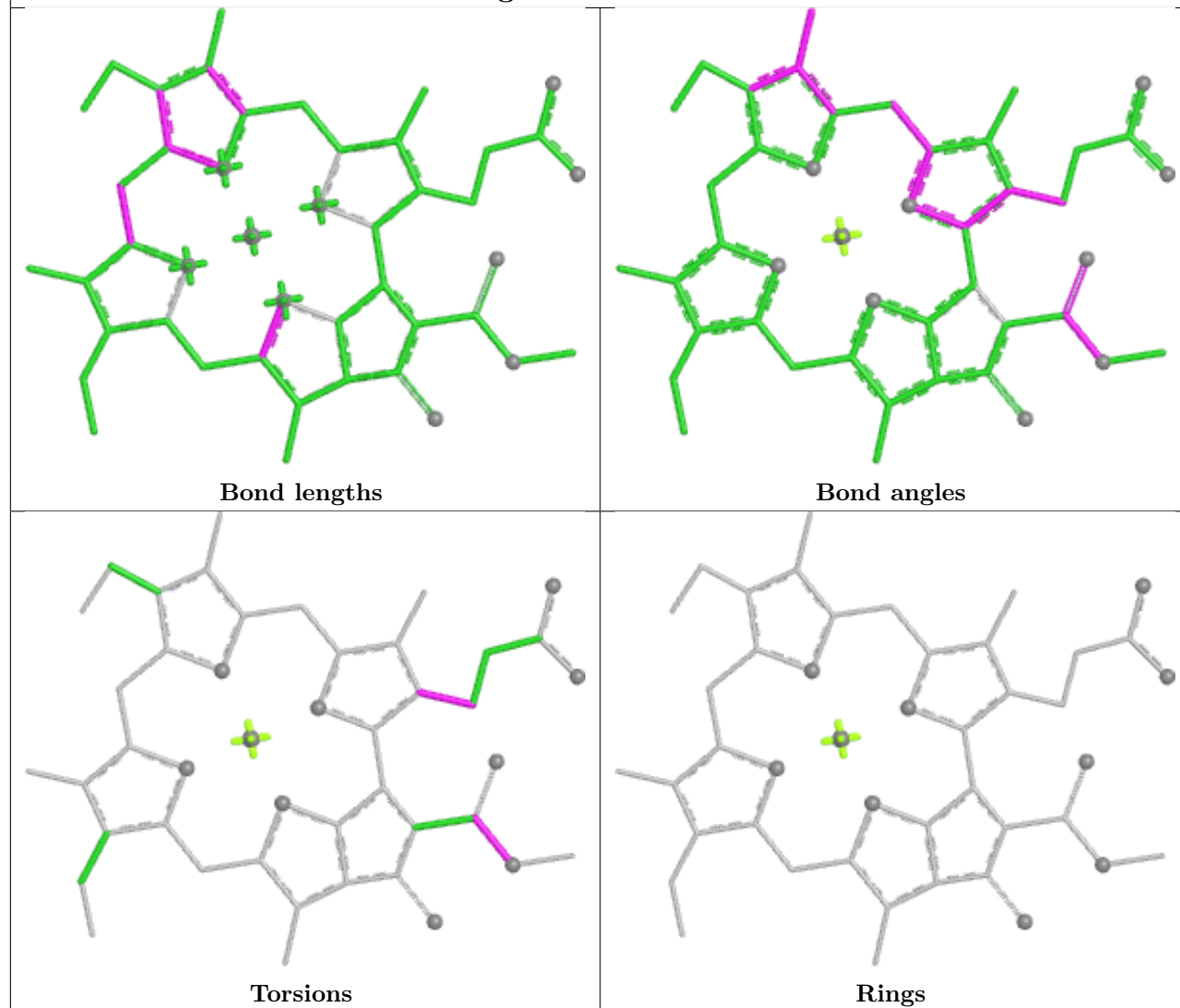


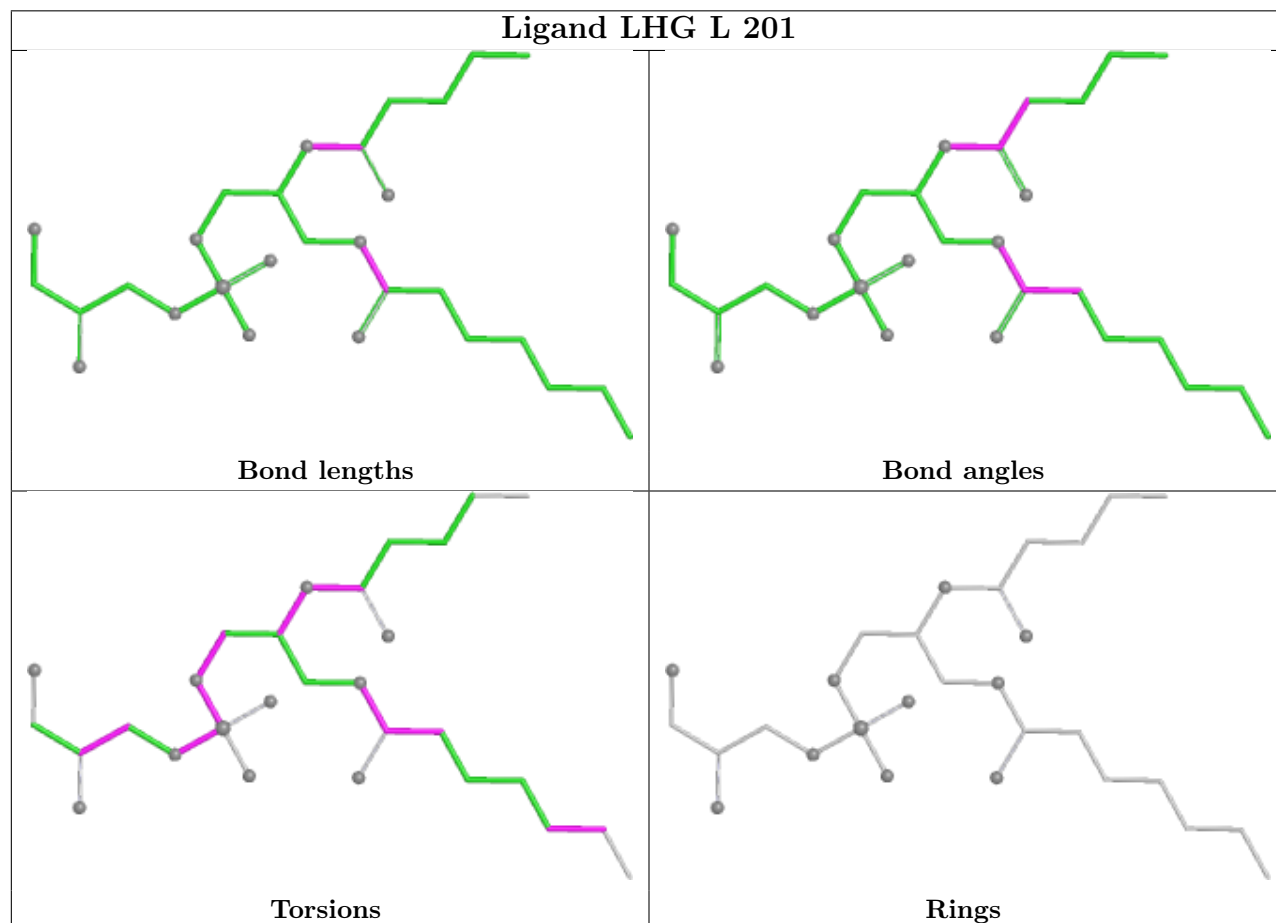
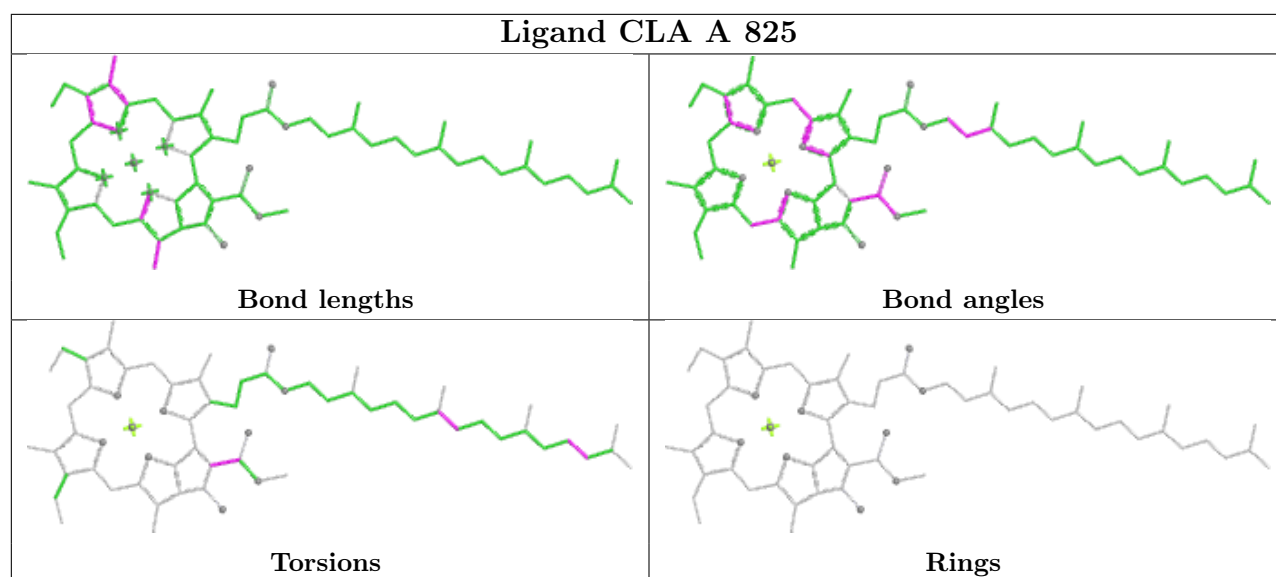


Ligand CLA B 827

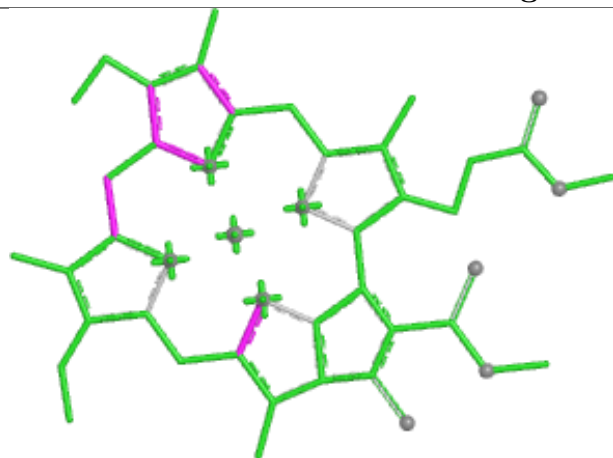


Ligand CLA t 301

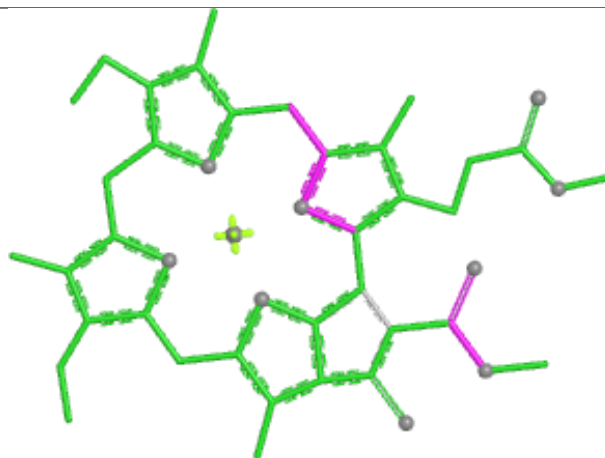




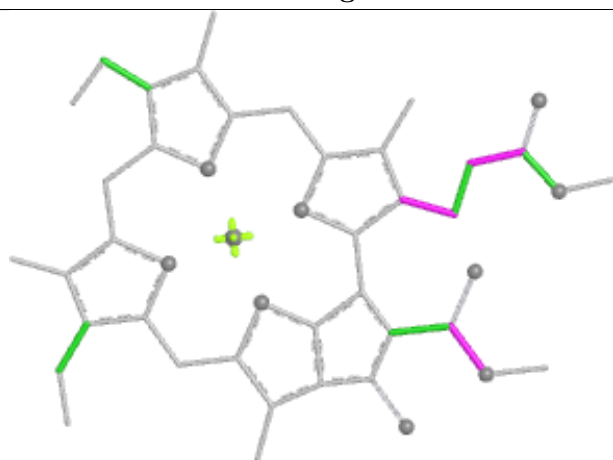
Ligand CLA t 308



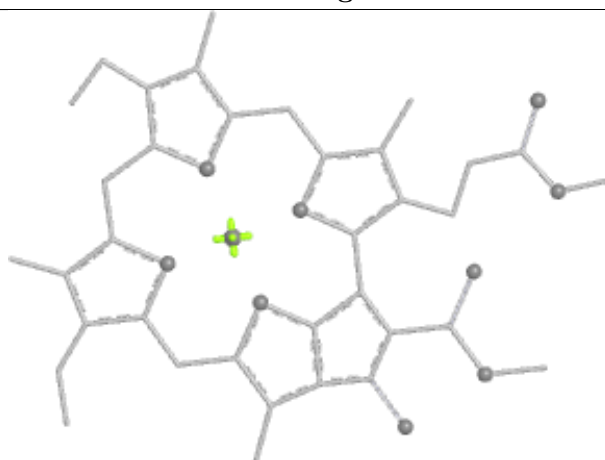
Bond lengths



Bond angles

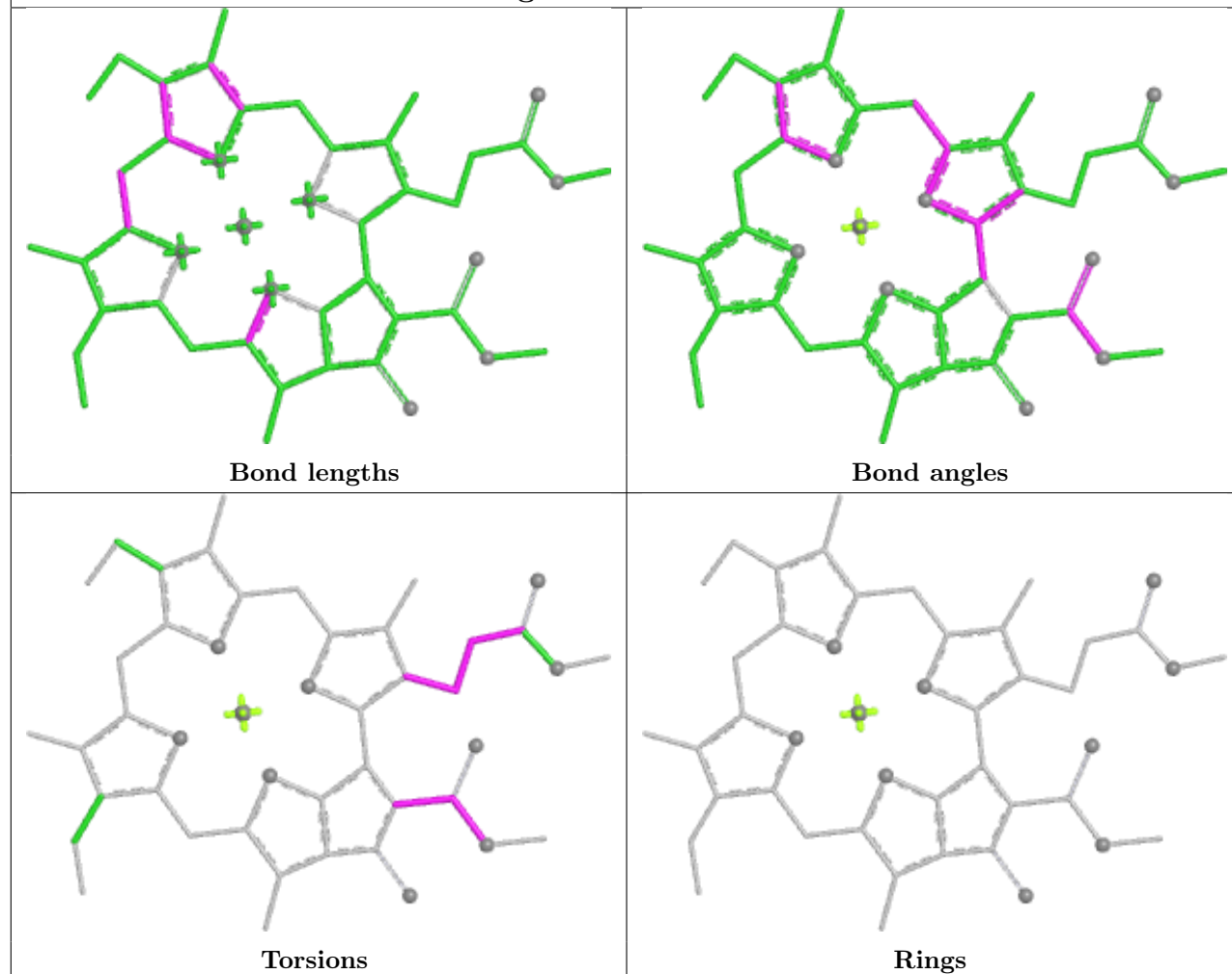


Torsions

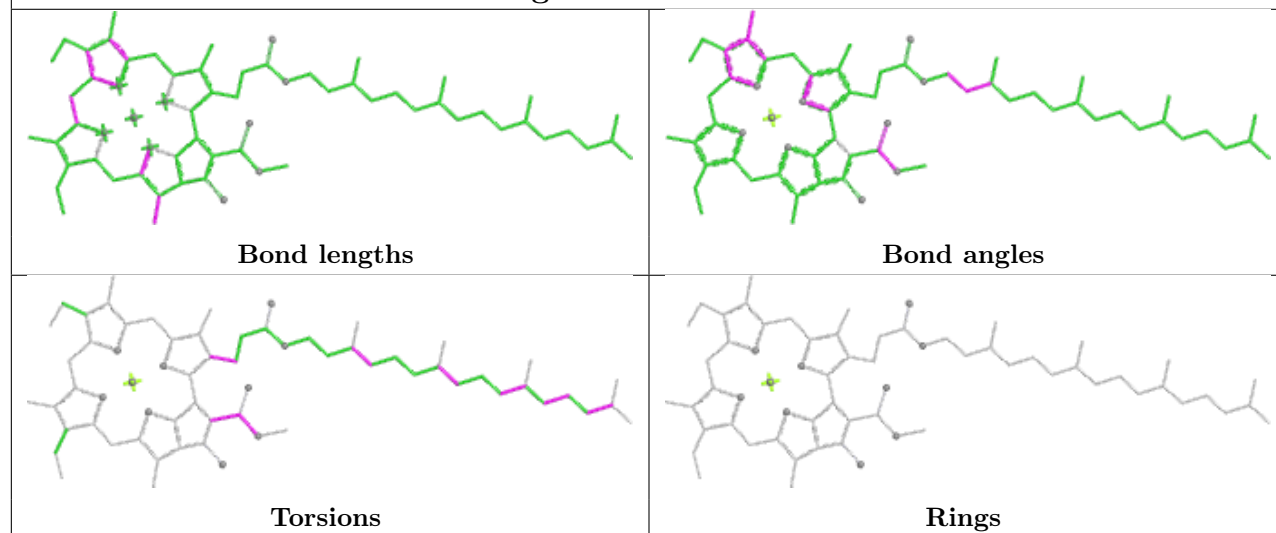


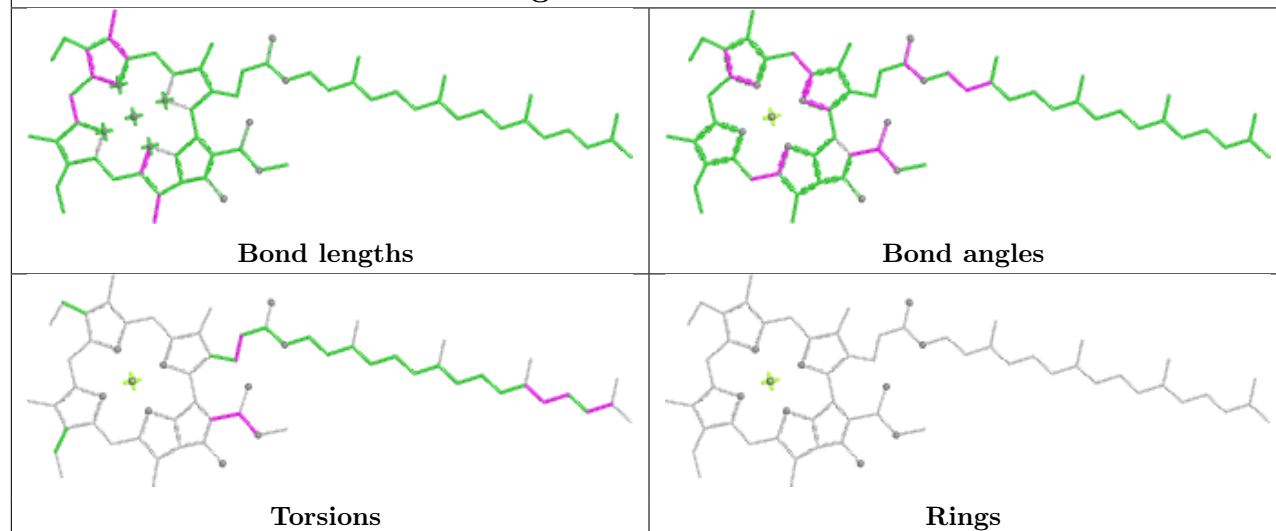
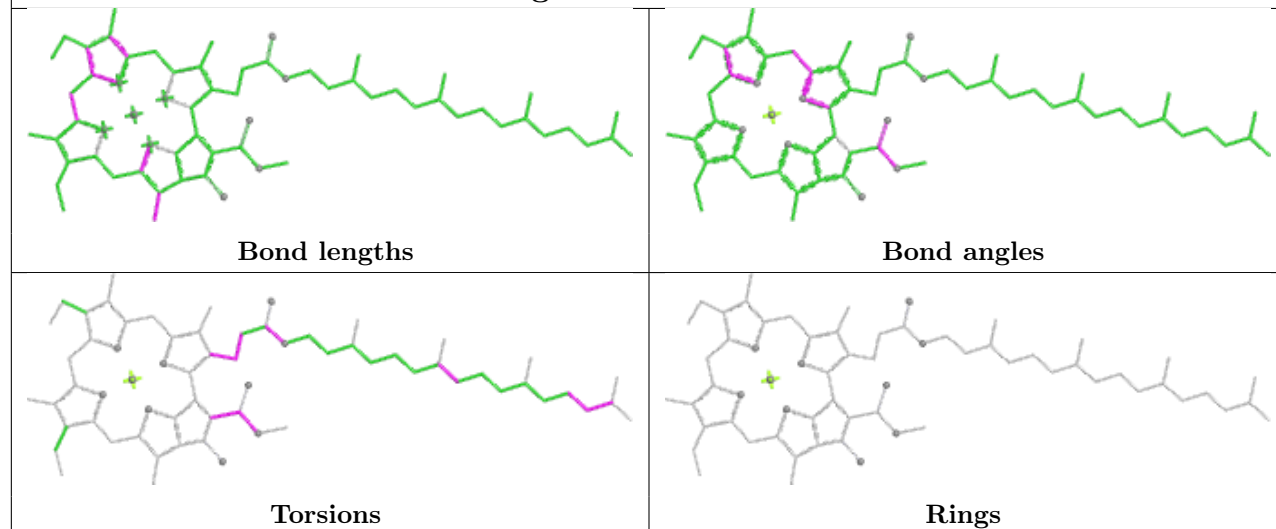
Rings

Ligand CLA 8 202

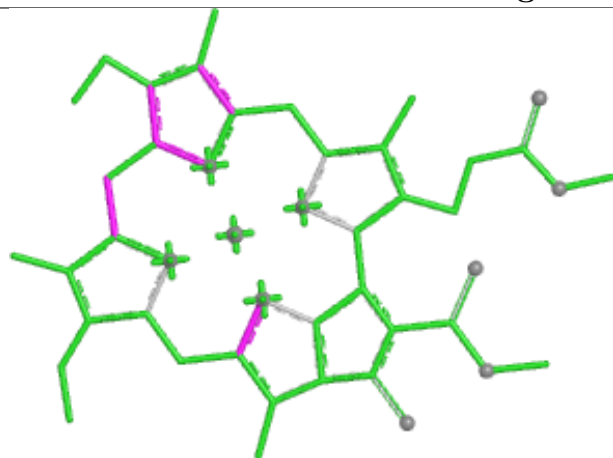


Ligand CLA A 824

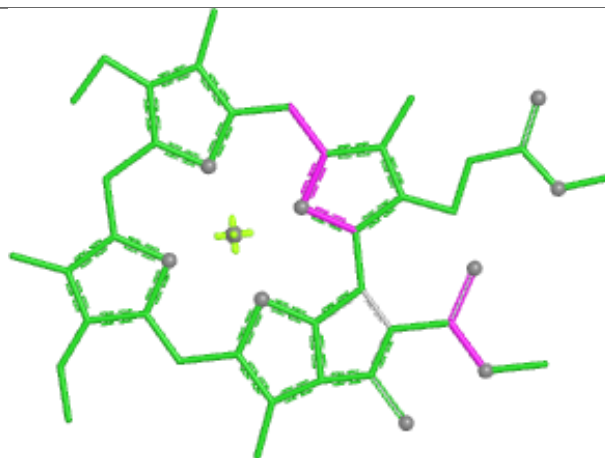


Ligand CLA A 838**Ligand CLA A 831**

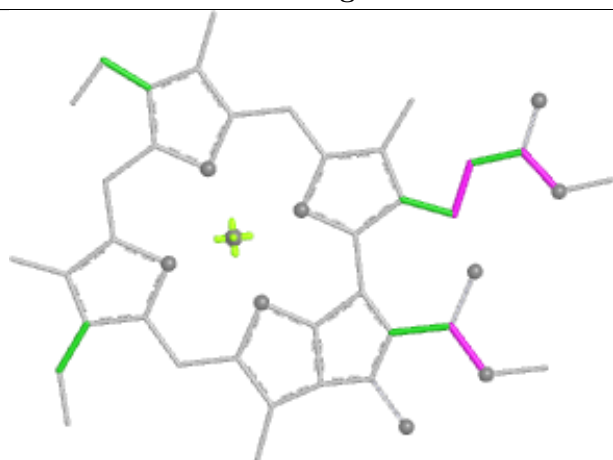
Ligand CLA h 604



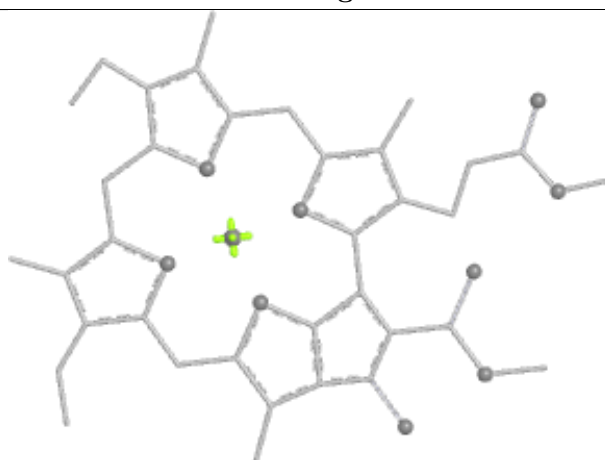
Bond lengths



Bond angles

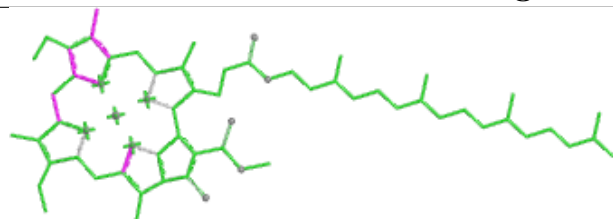


Torsions

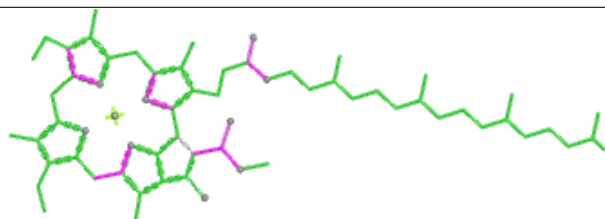


Rings

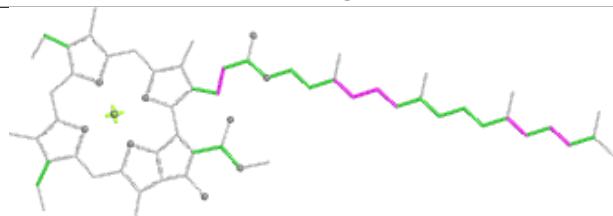
Ligand CLA B 807



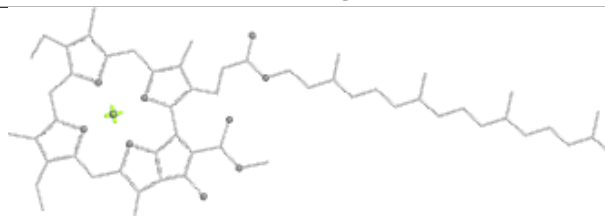
Bond lengths



Bond angles

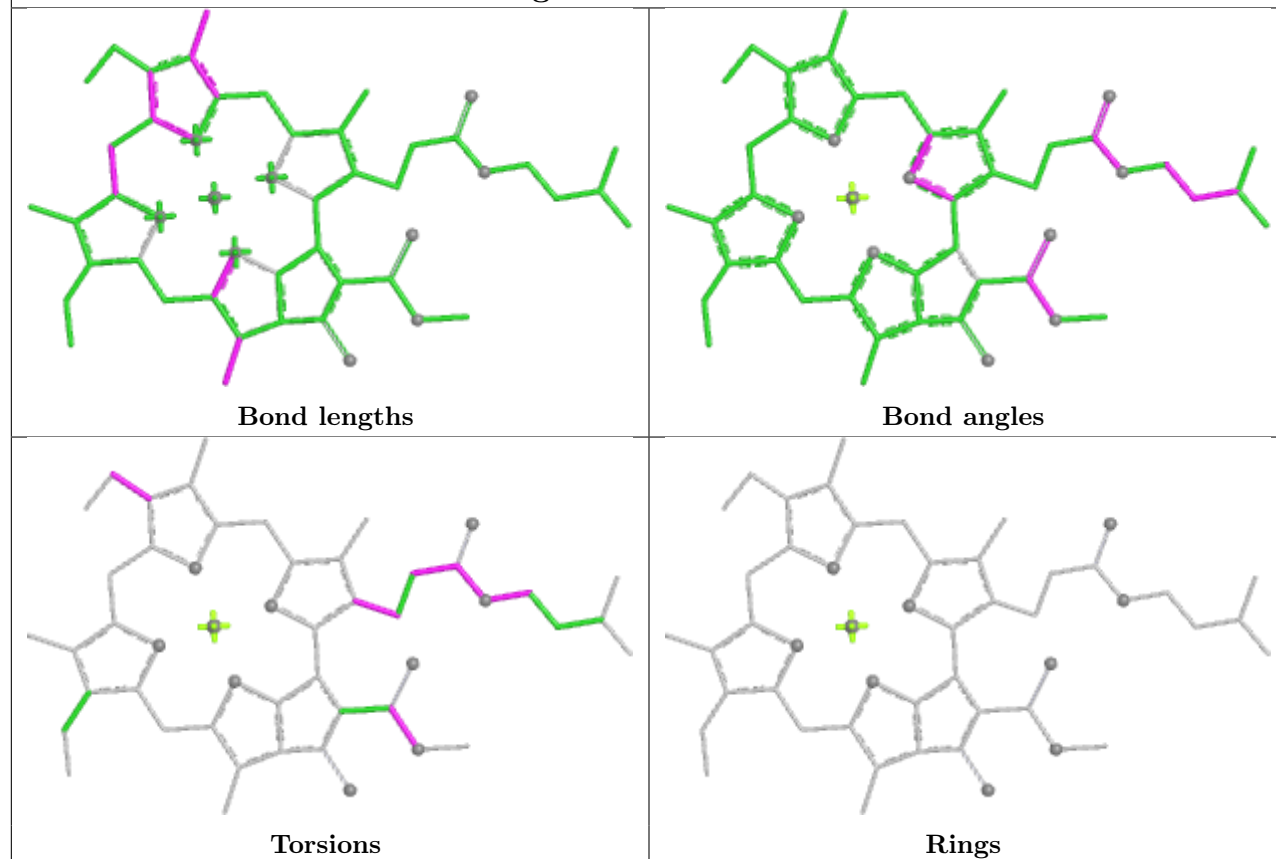


Torsions

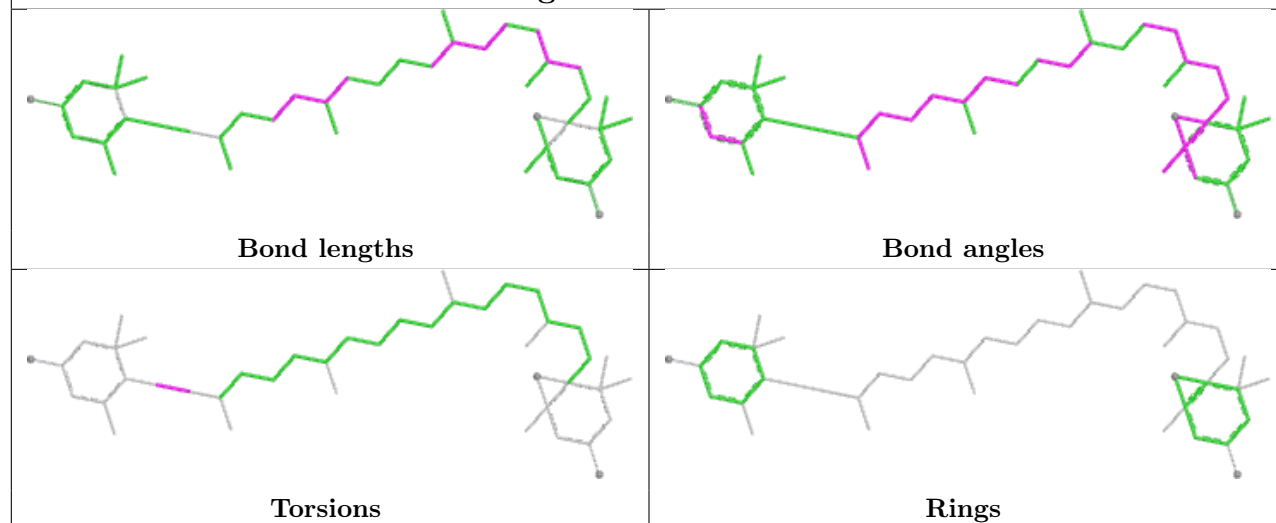


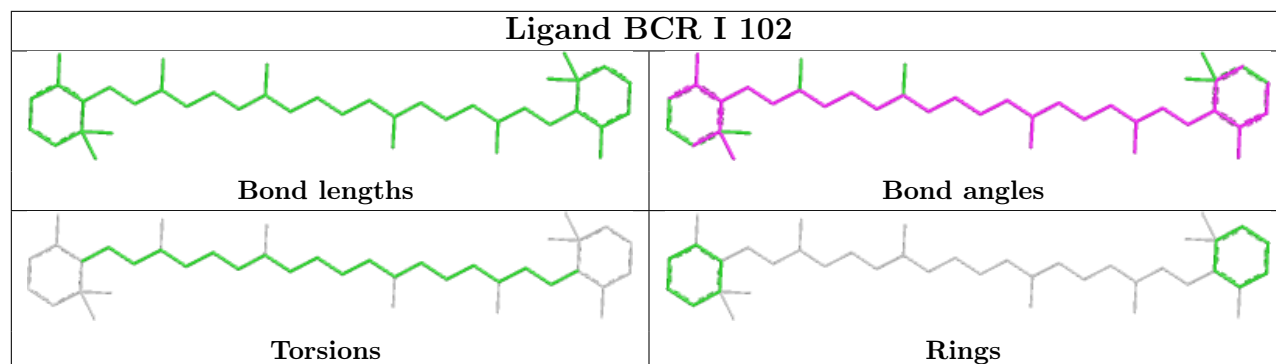
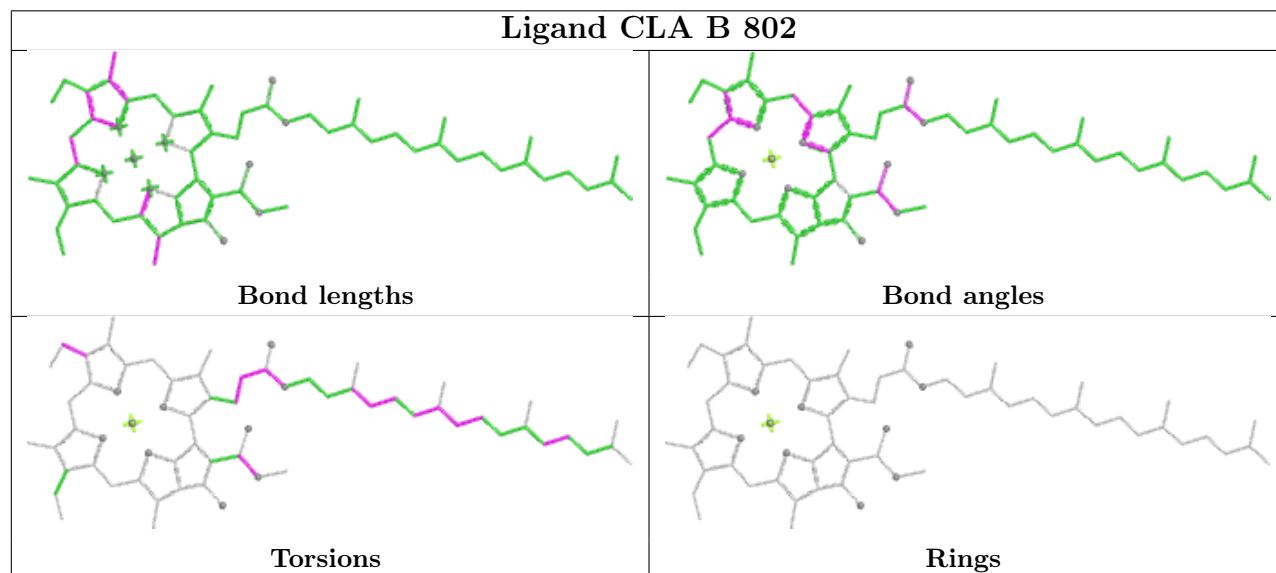
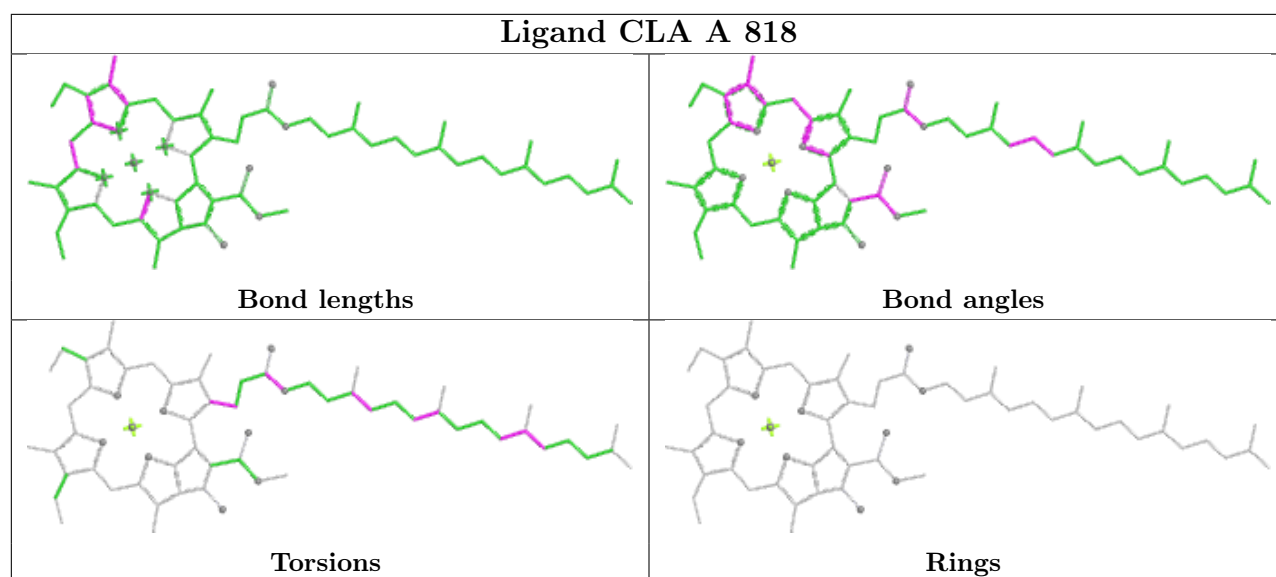
Rings

Ligand CLA B 828

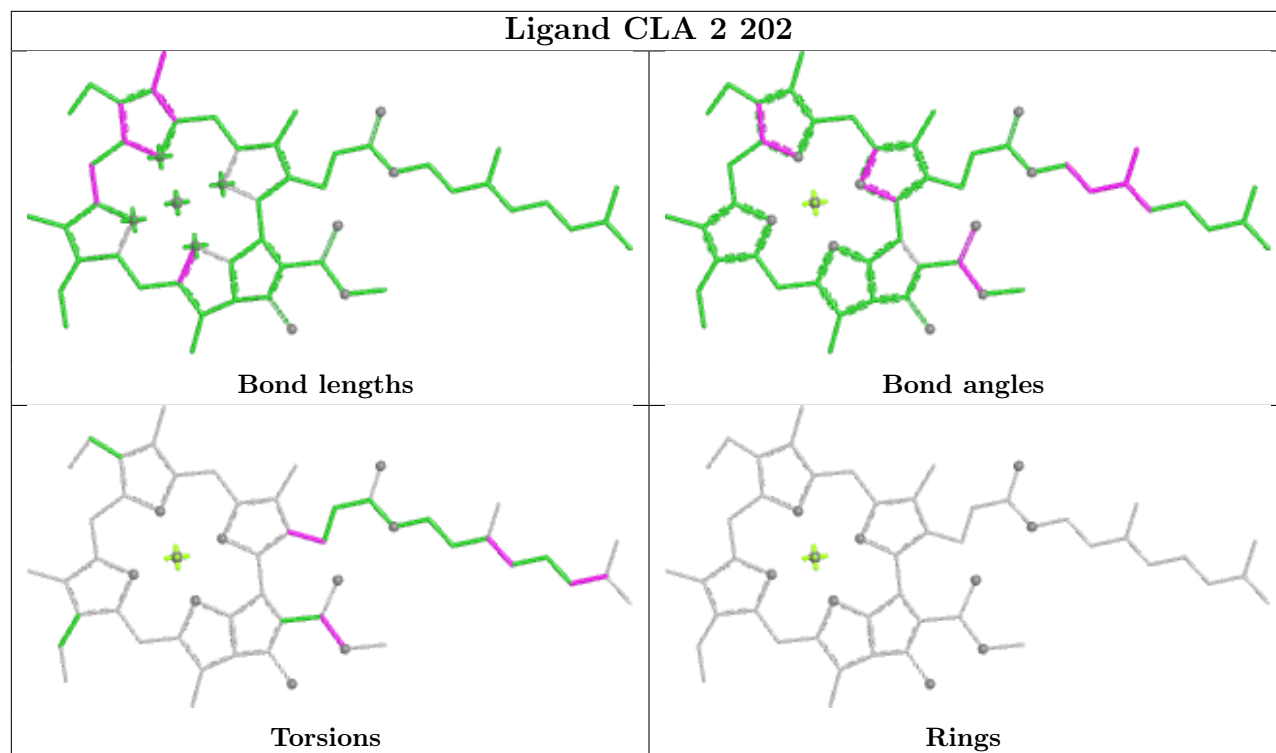


Ligand DD6 c 614

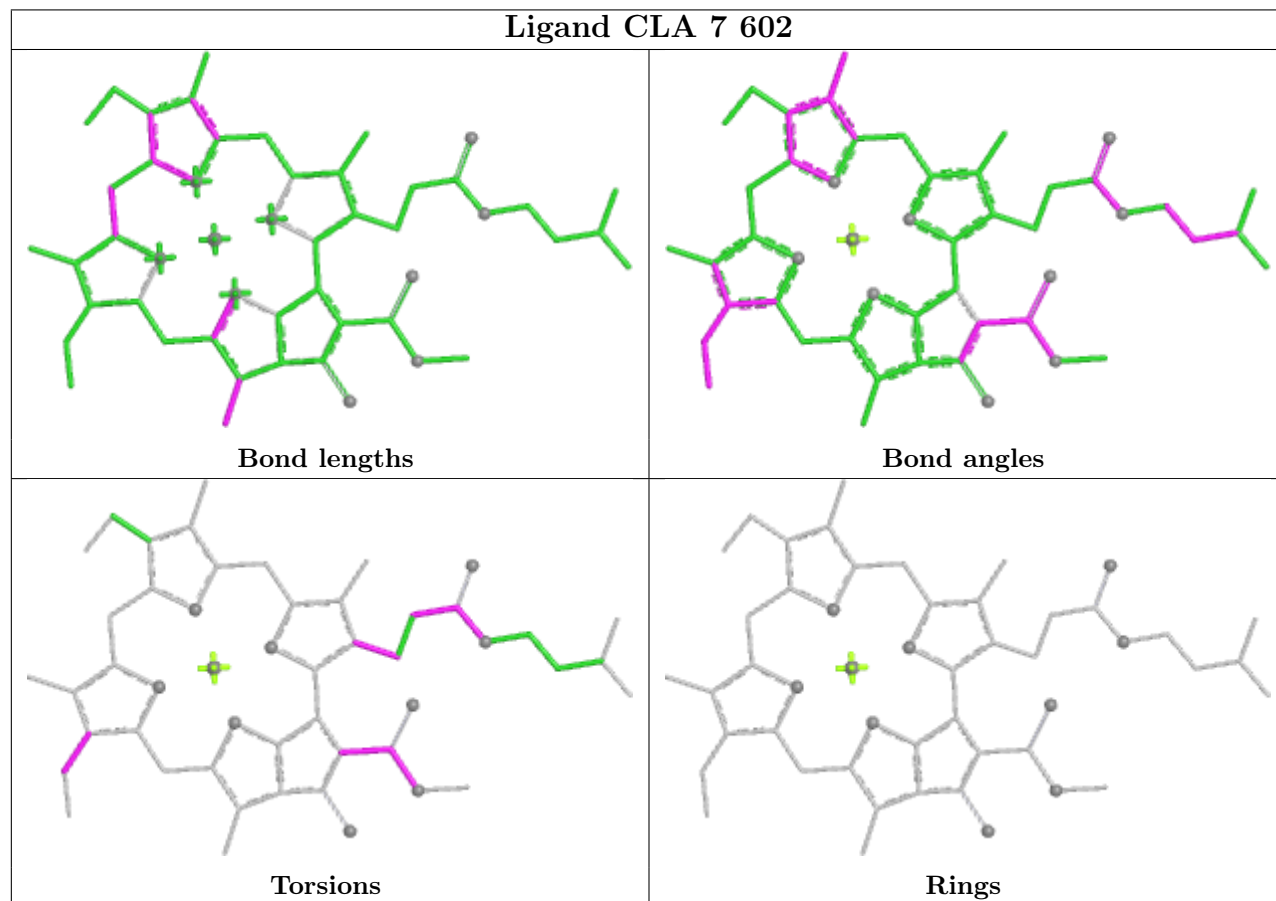




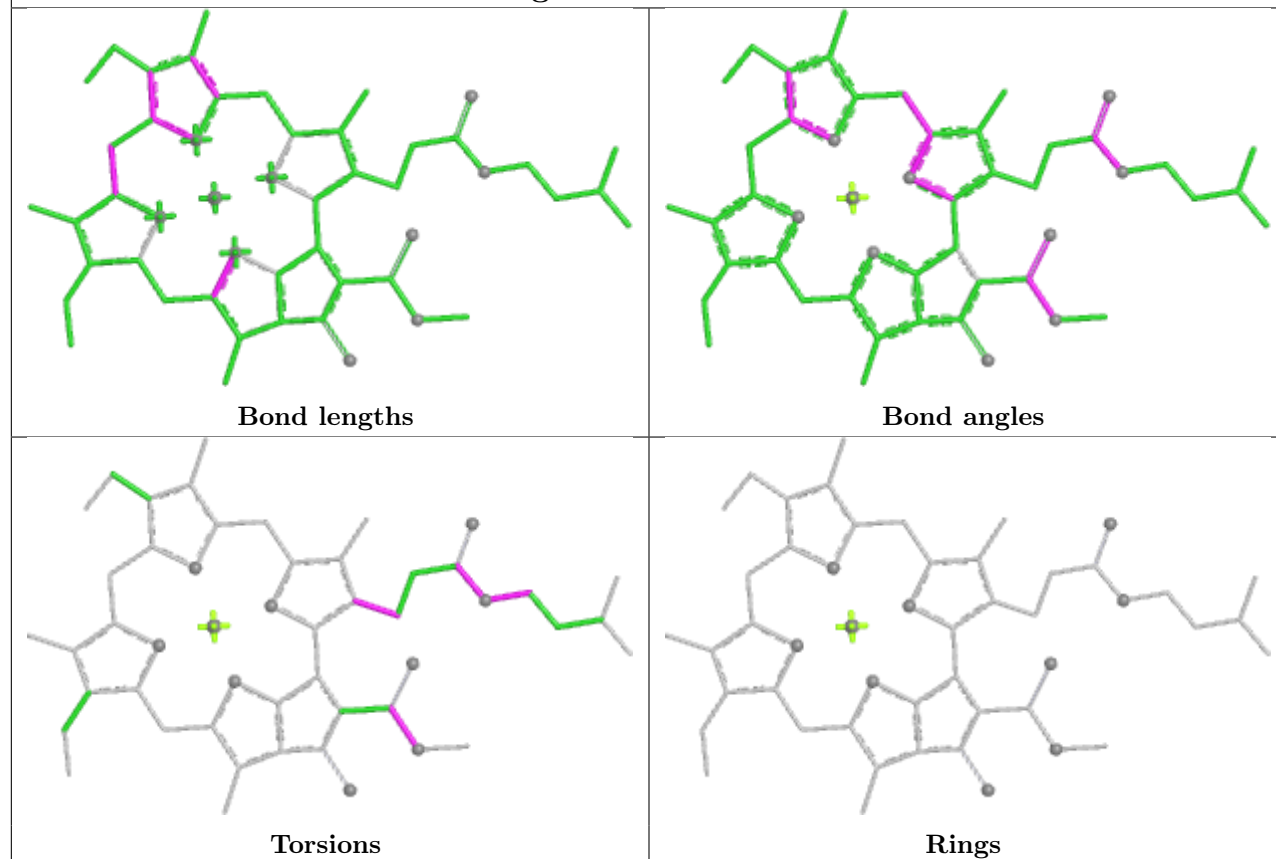
Ligand CLA 2 202



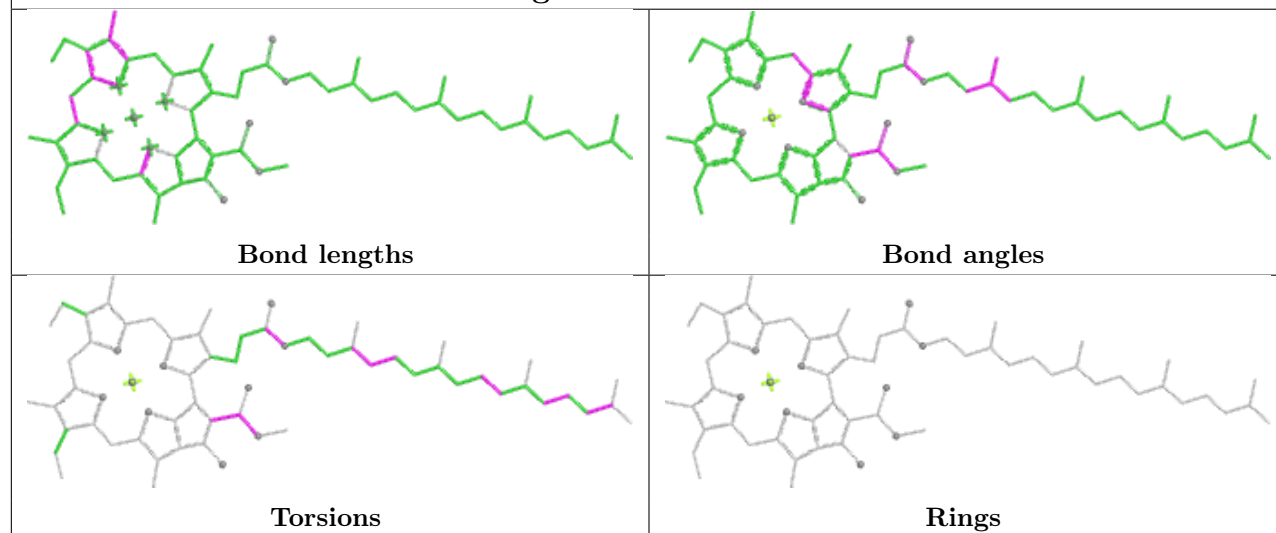
Ligand CLA 7 602

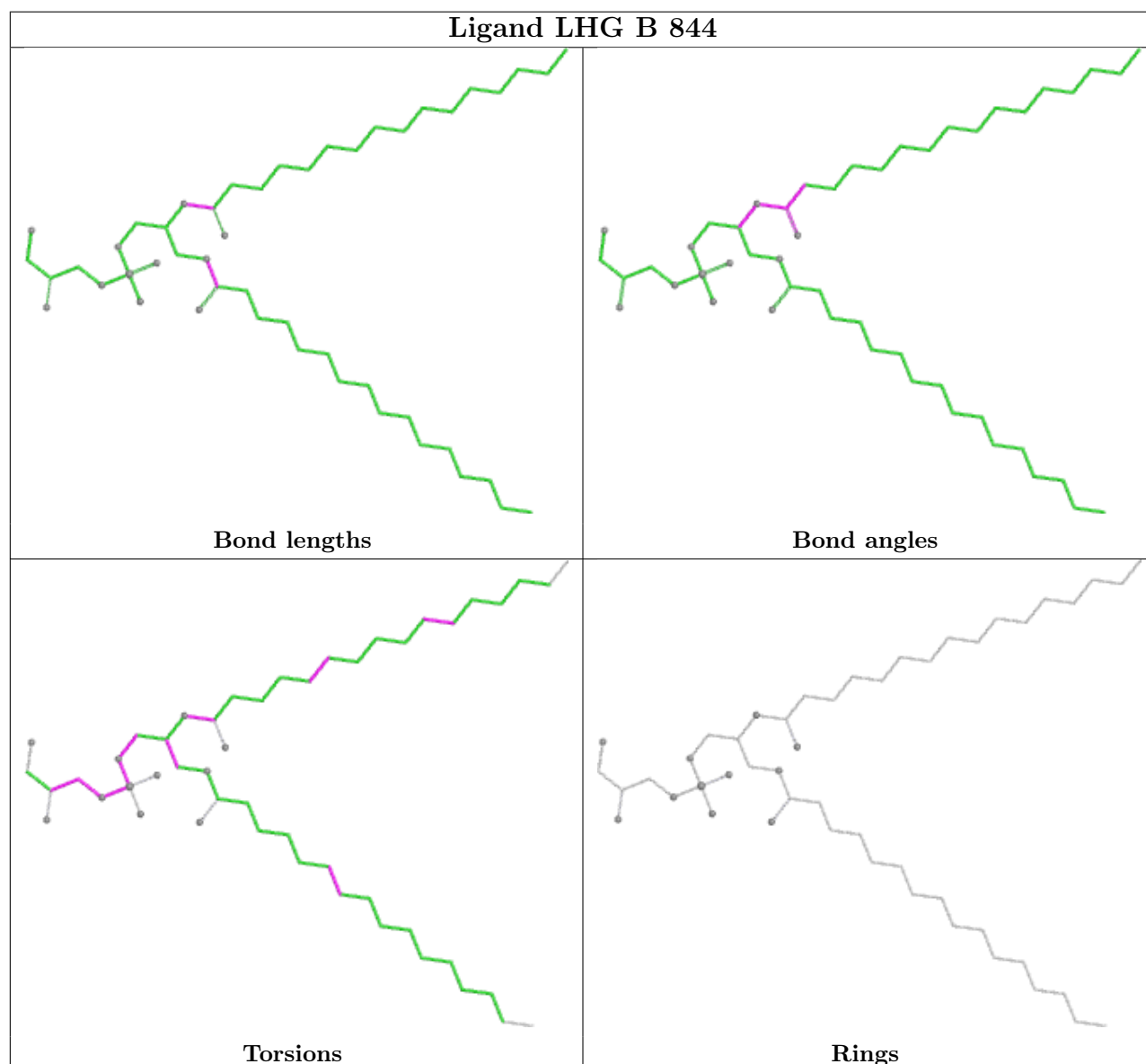
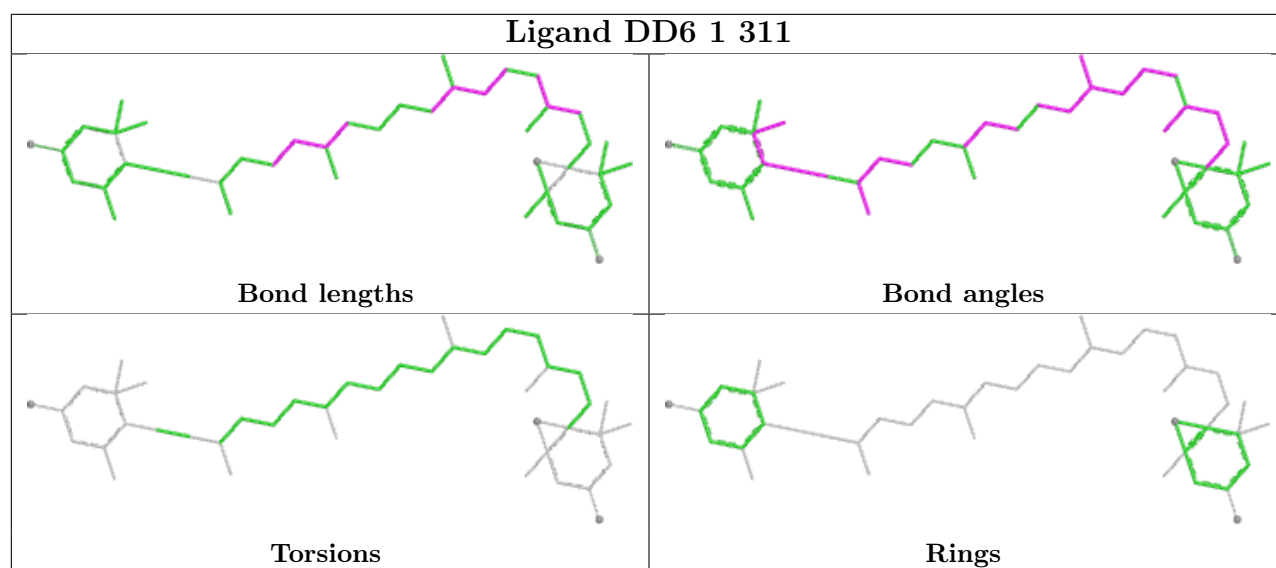


Ligand CLA A 814

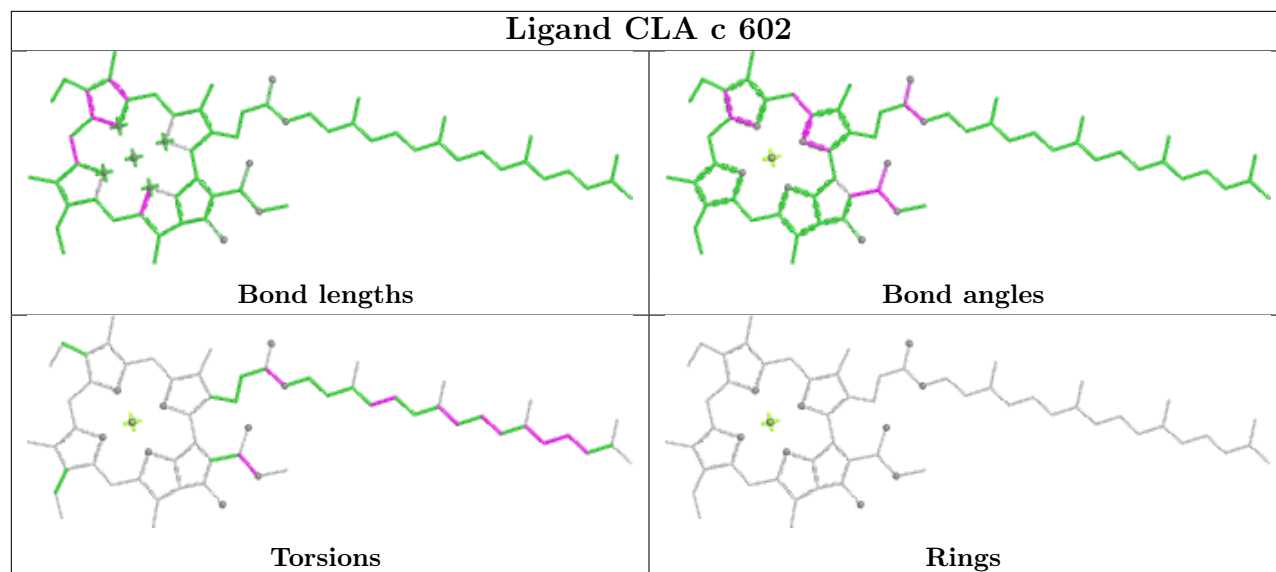


Ligand CLA B 822

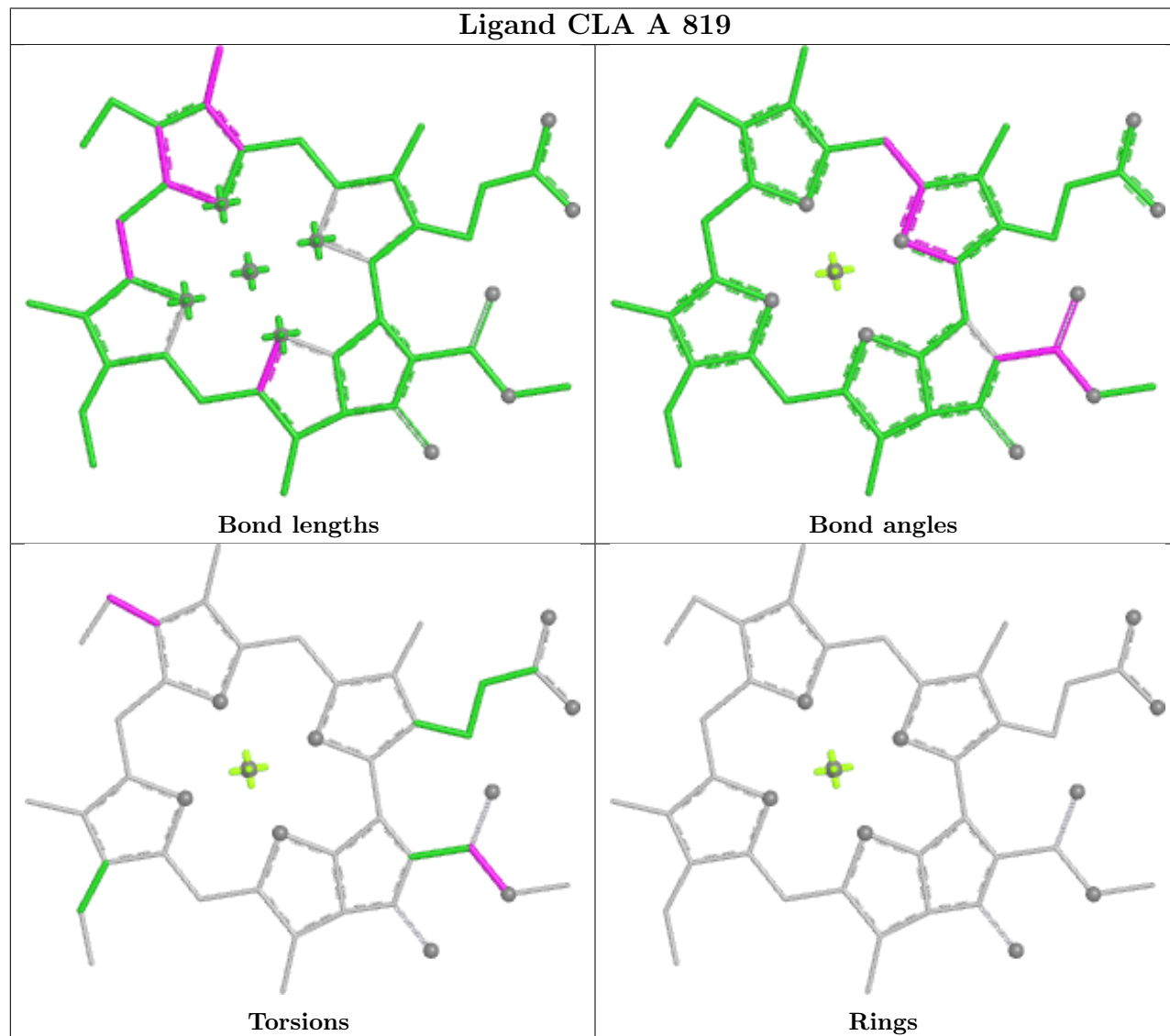




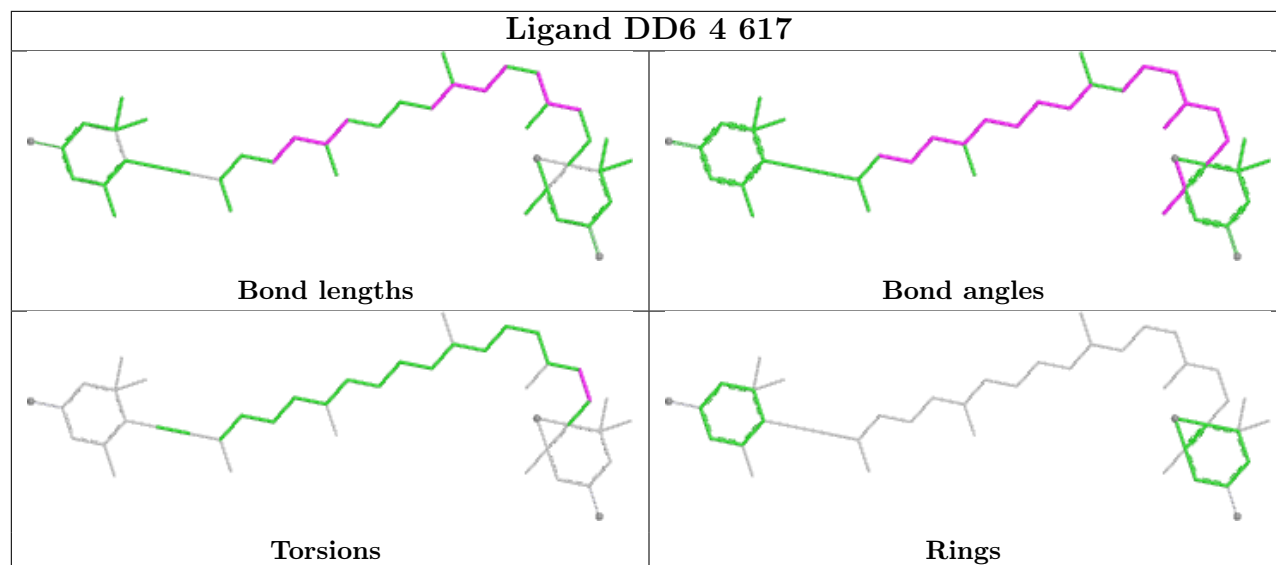
Ligand CLA c 602



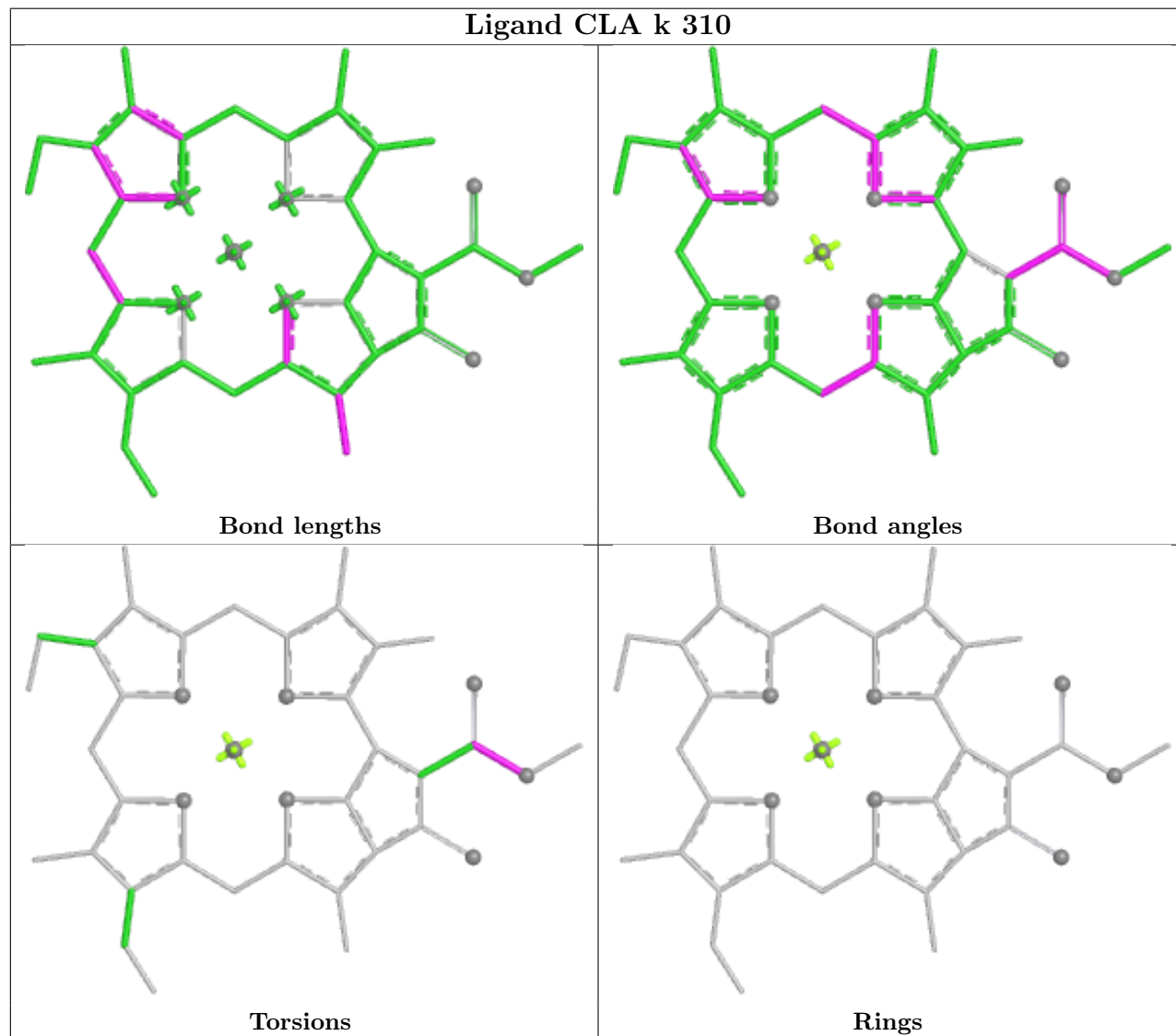
Ligand CLA A 819



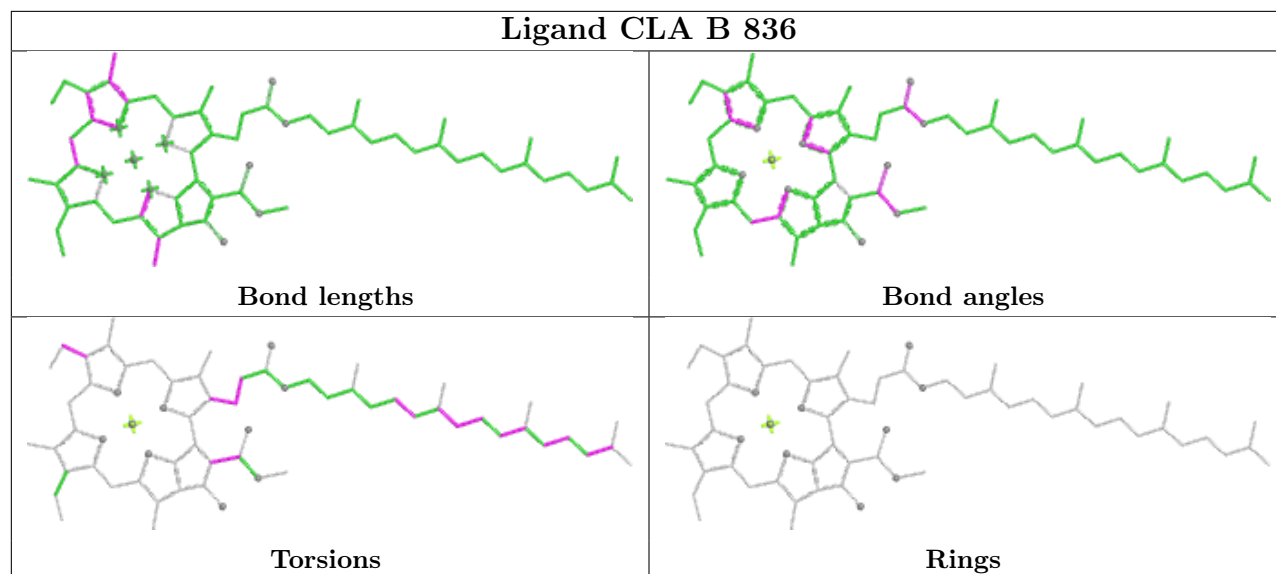
Ligand DD6 4 617



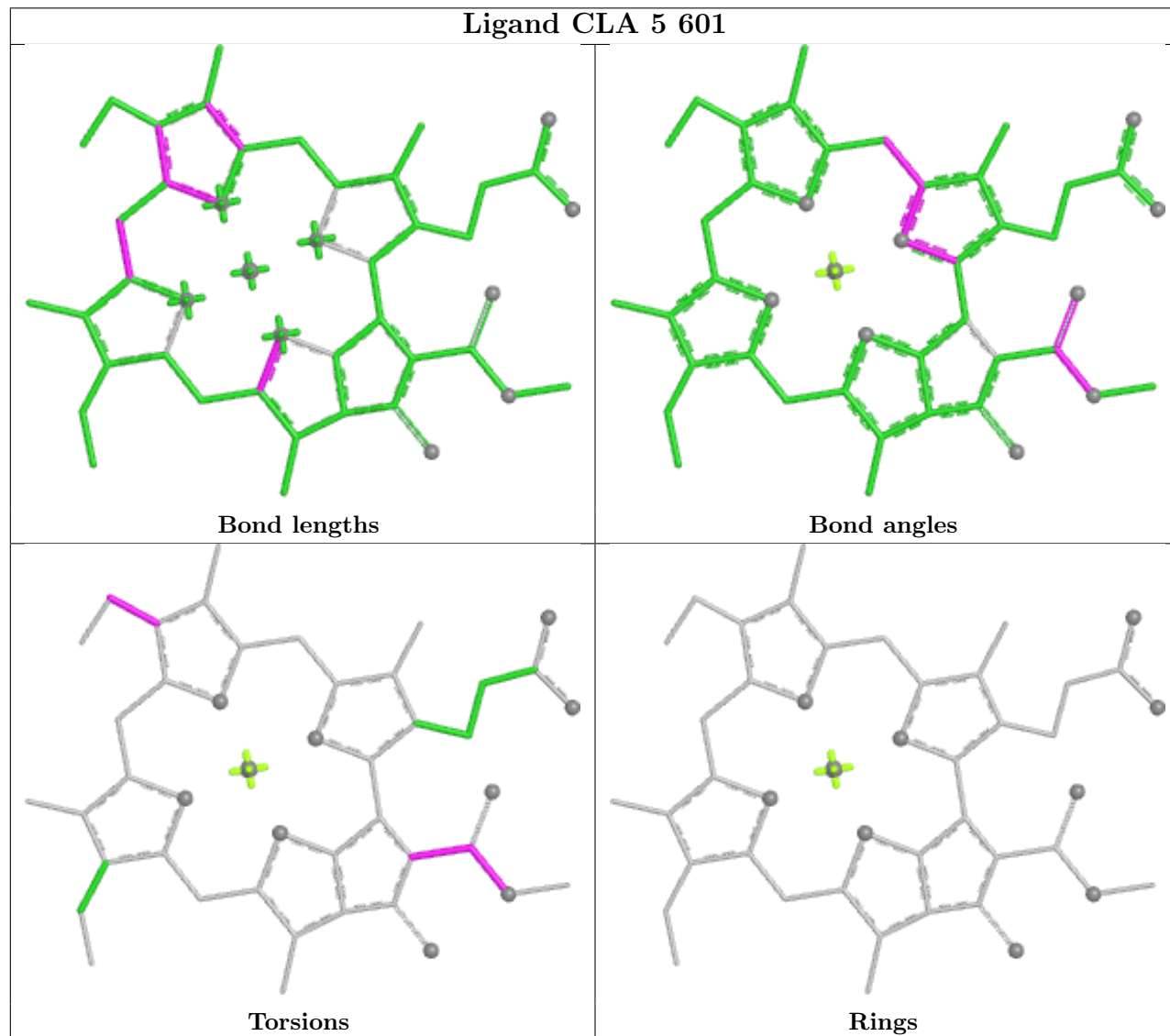
Ligand CLA k 310

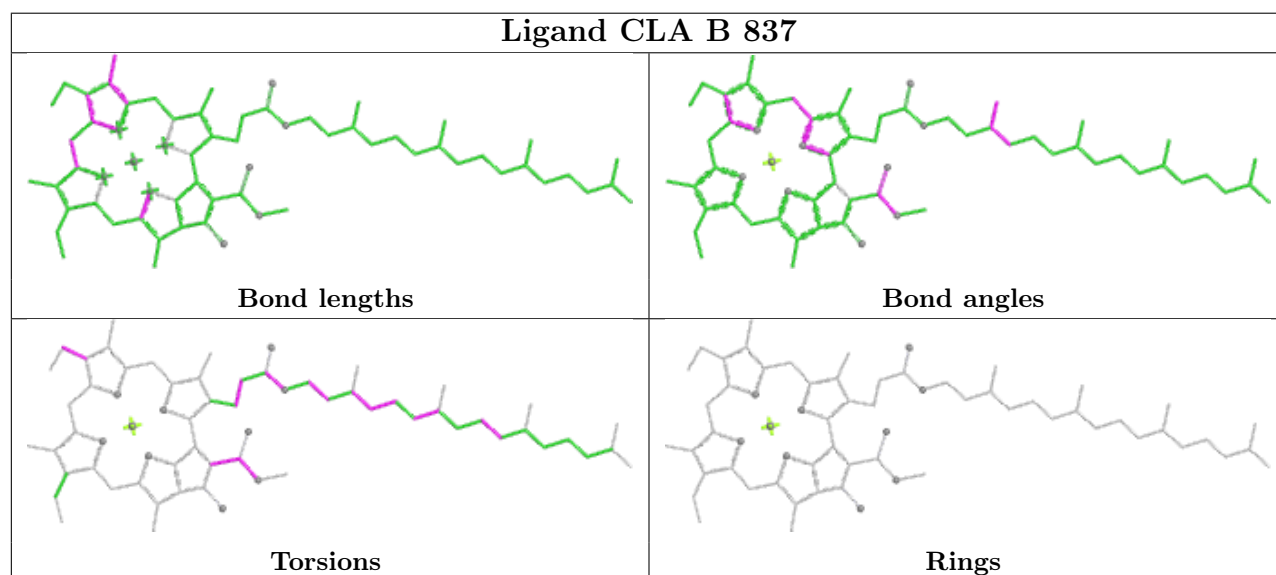
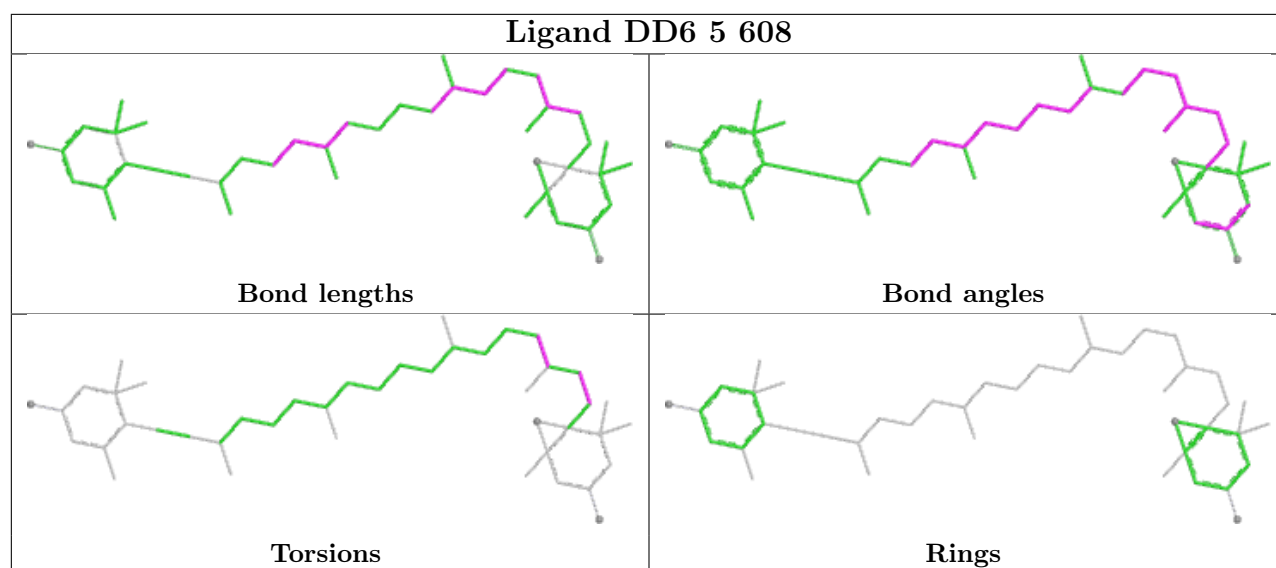


Ligand CLA B 836

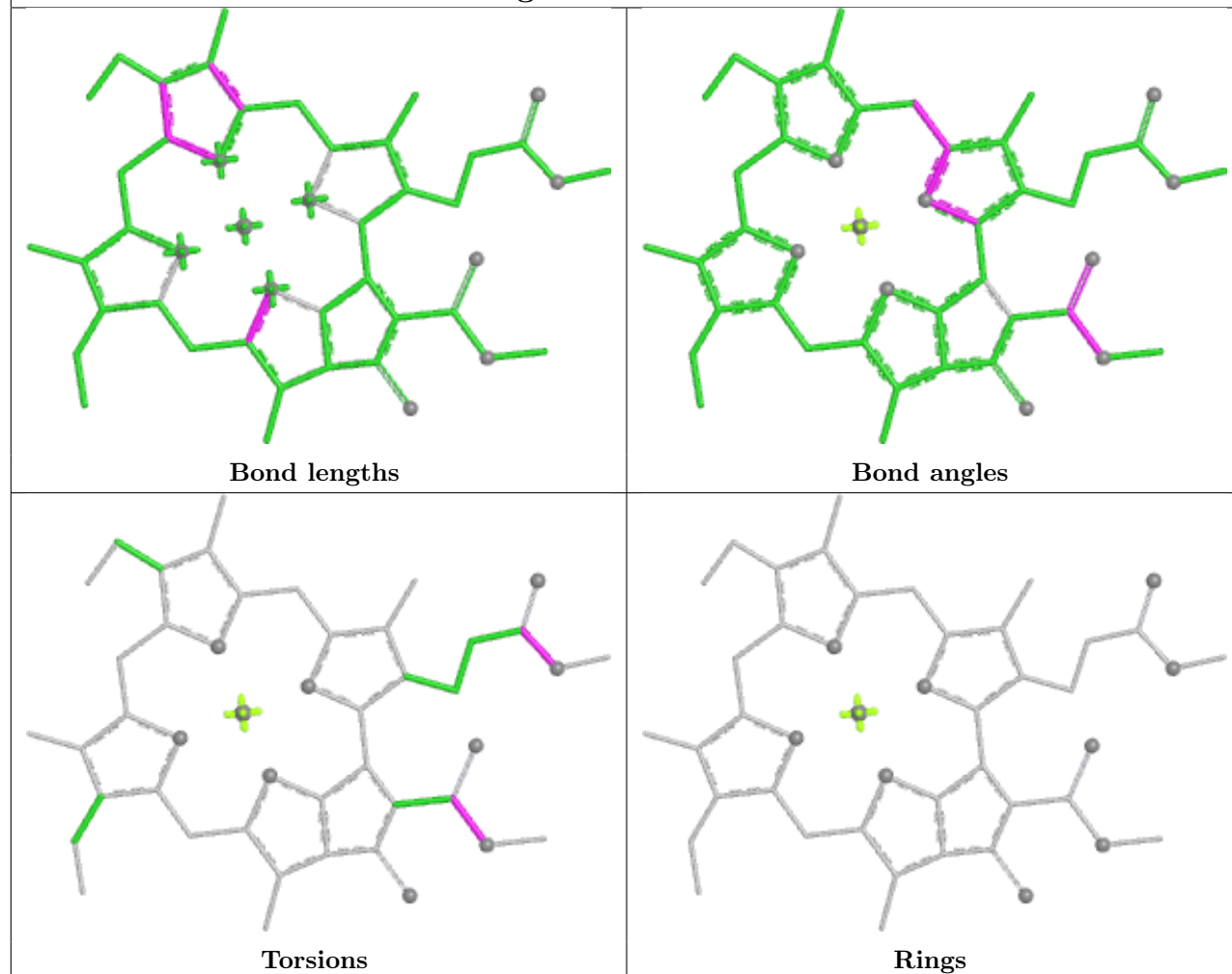


Ligand CLA 5 601

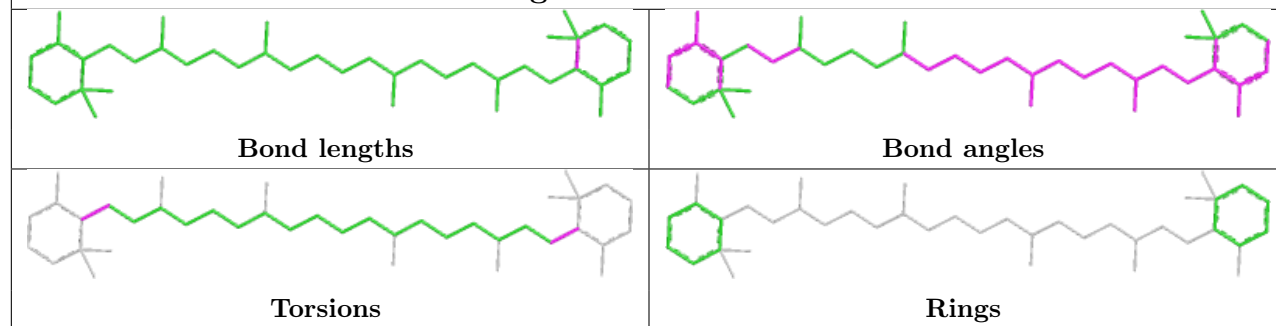




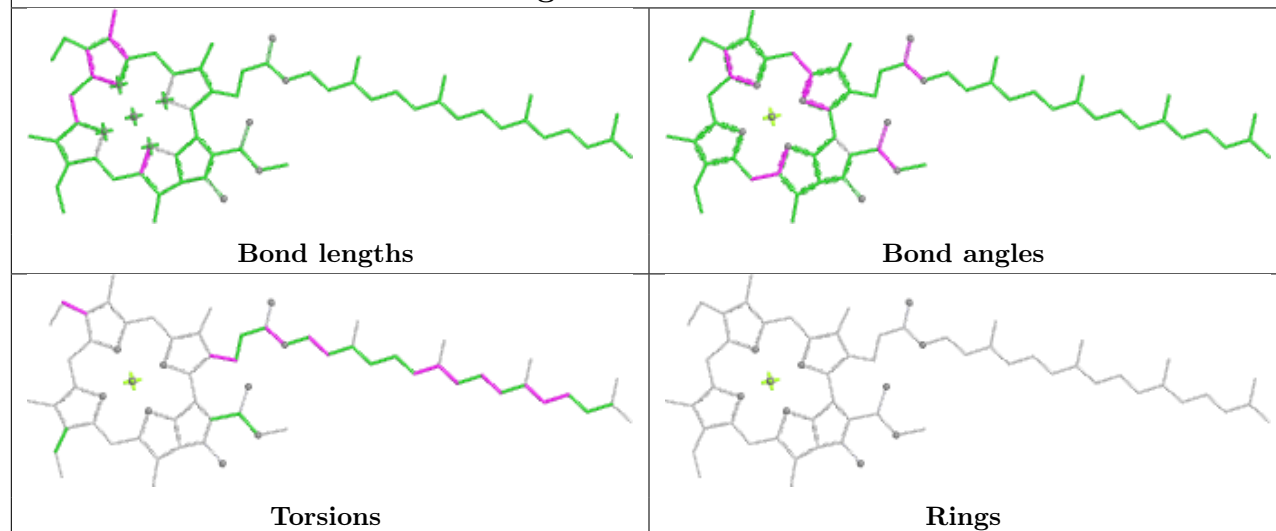
Ligand CLA k 301



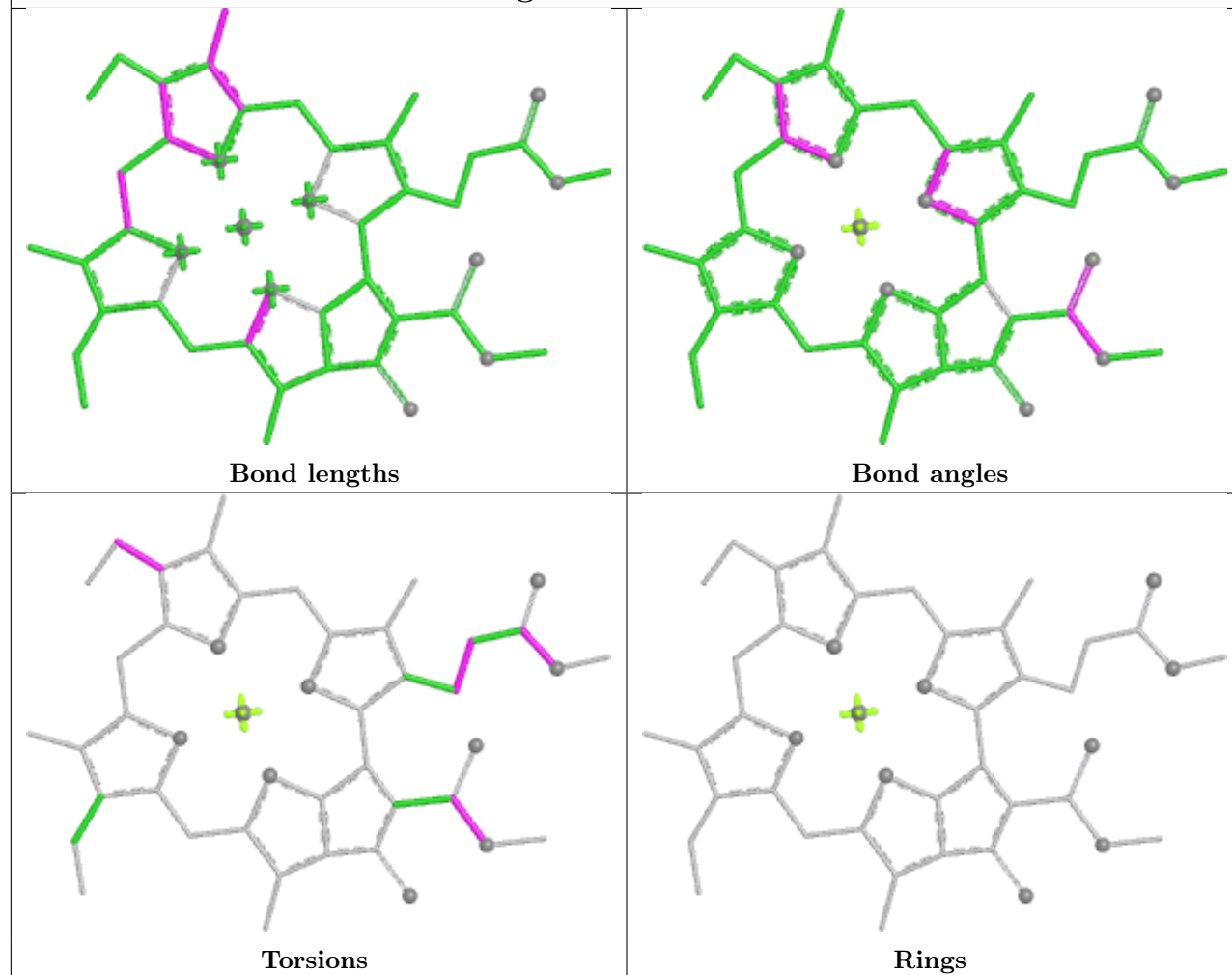
Ligand BCR R 101



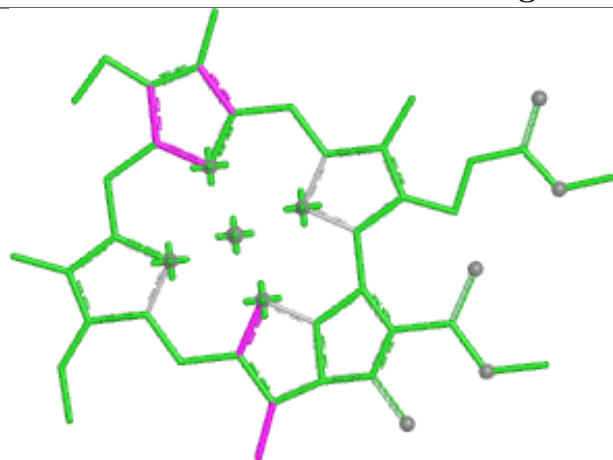
Ligand CLA c 608



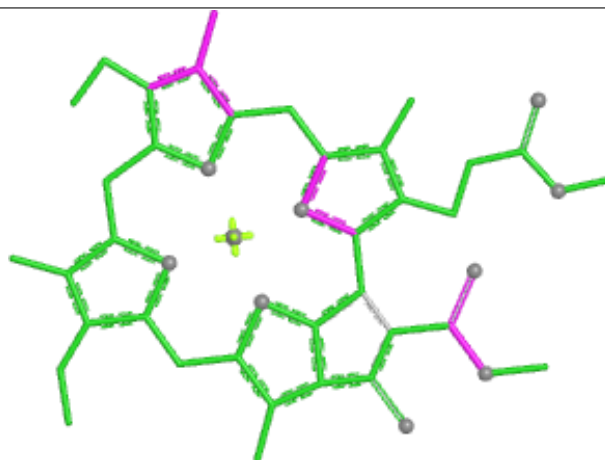
Ligand CLA h 608



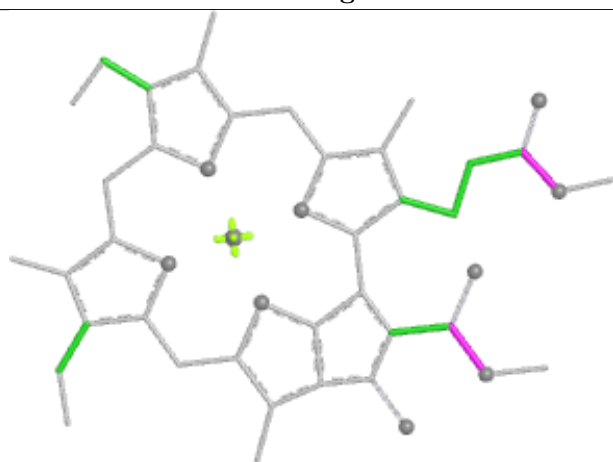
Ligand CLA 4 612



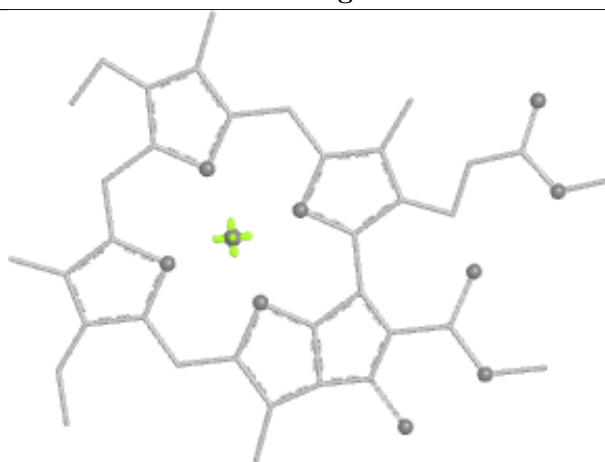
Bond lengths



Bond angles

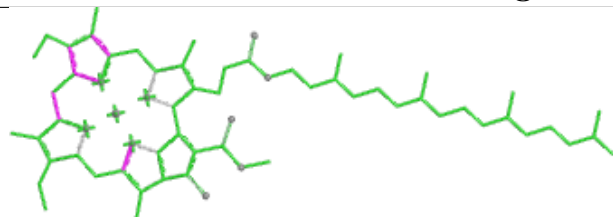


Torsions

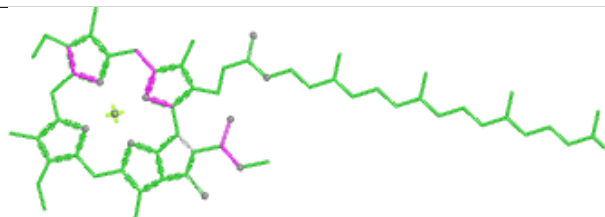


Rings

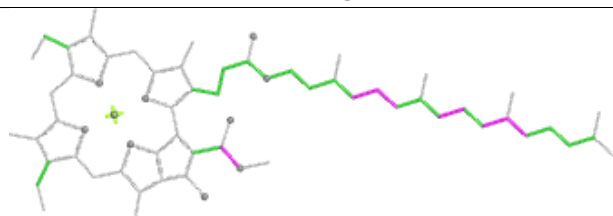
Ligand CLA B 806



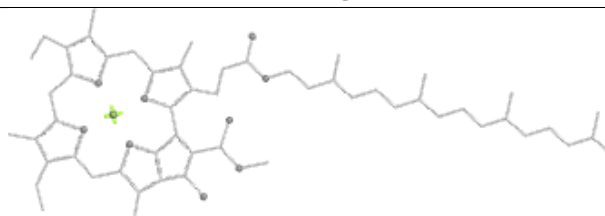
Bond lengths



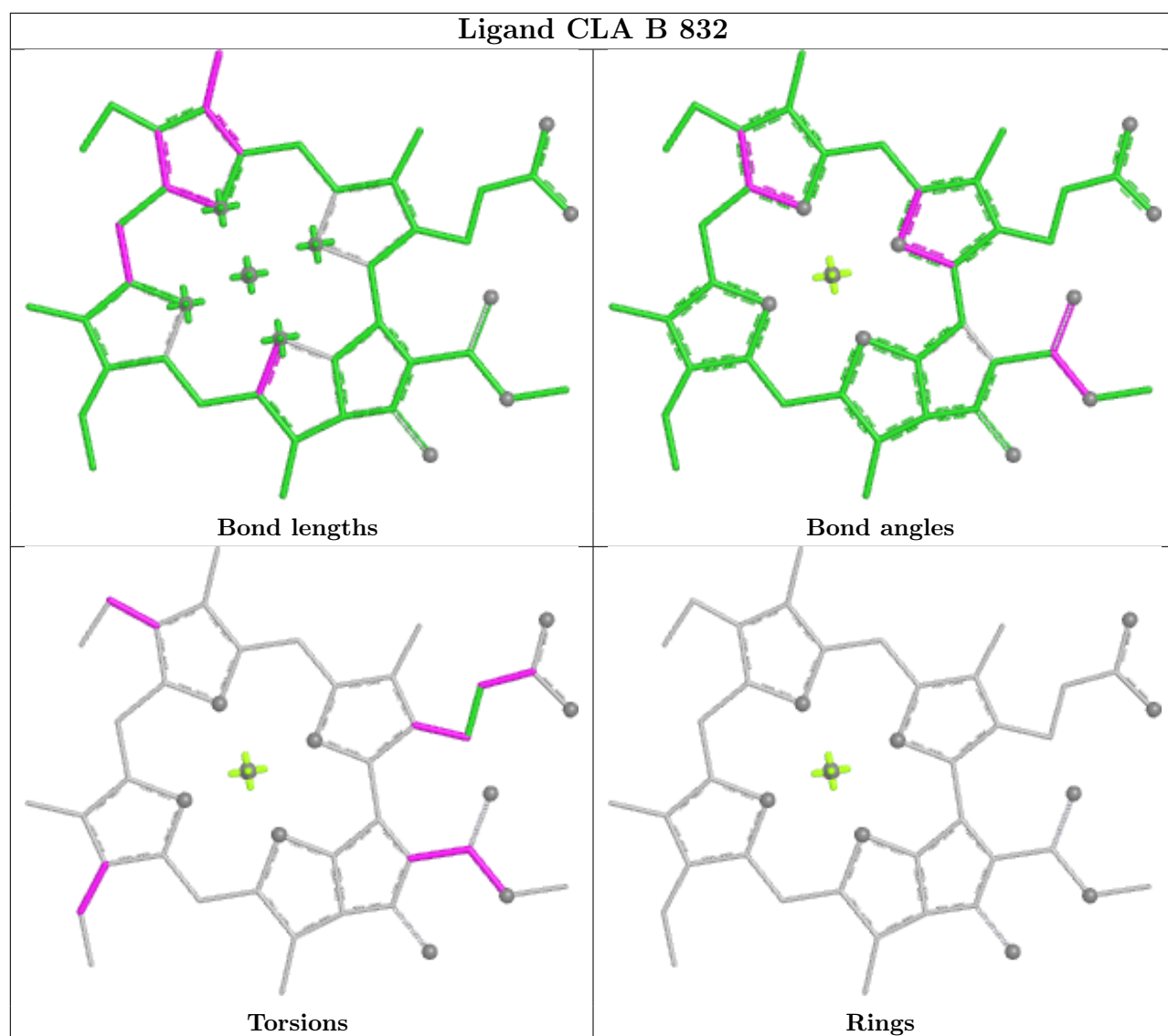
Bond angles



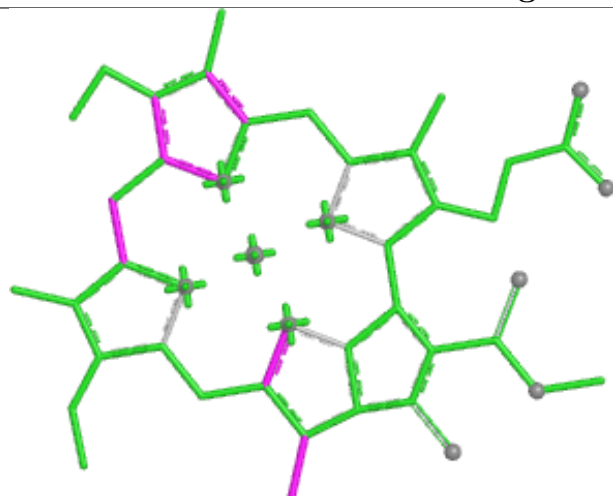
Torsions



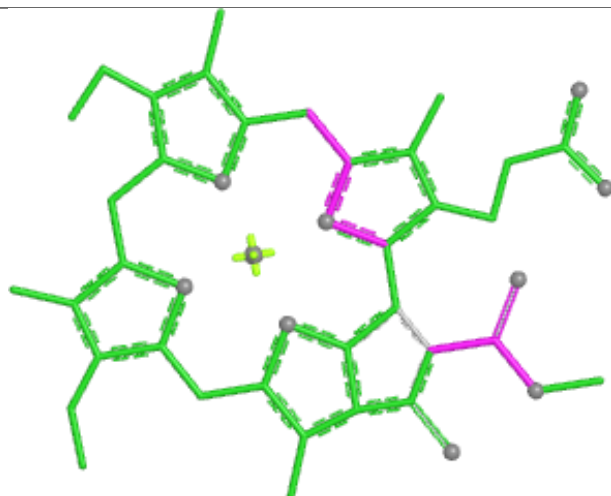
Rings



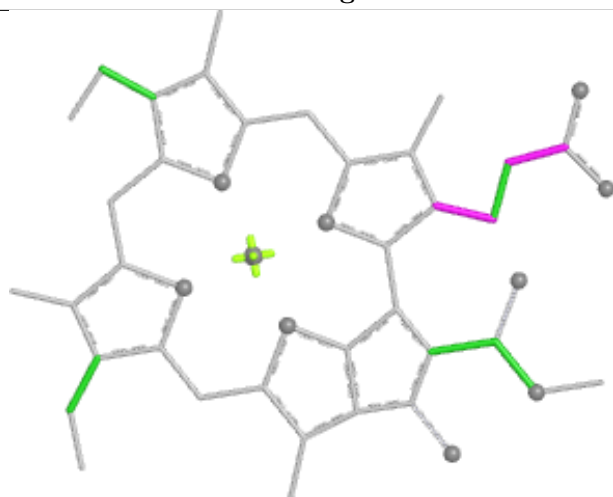
Ligand CLA 3 307



Bond lengths



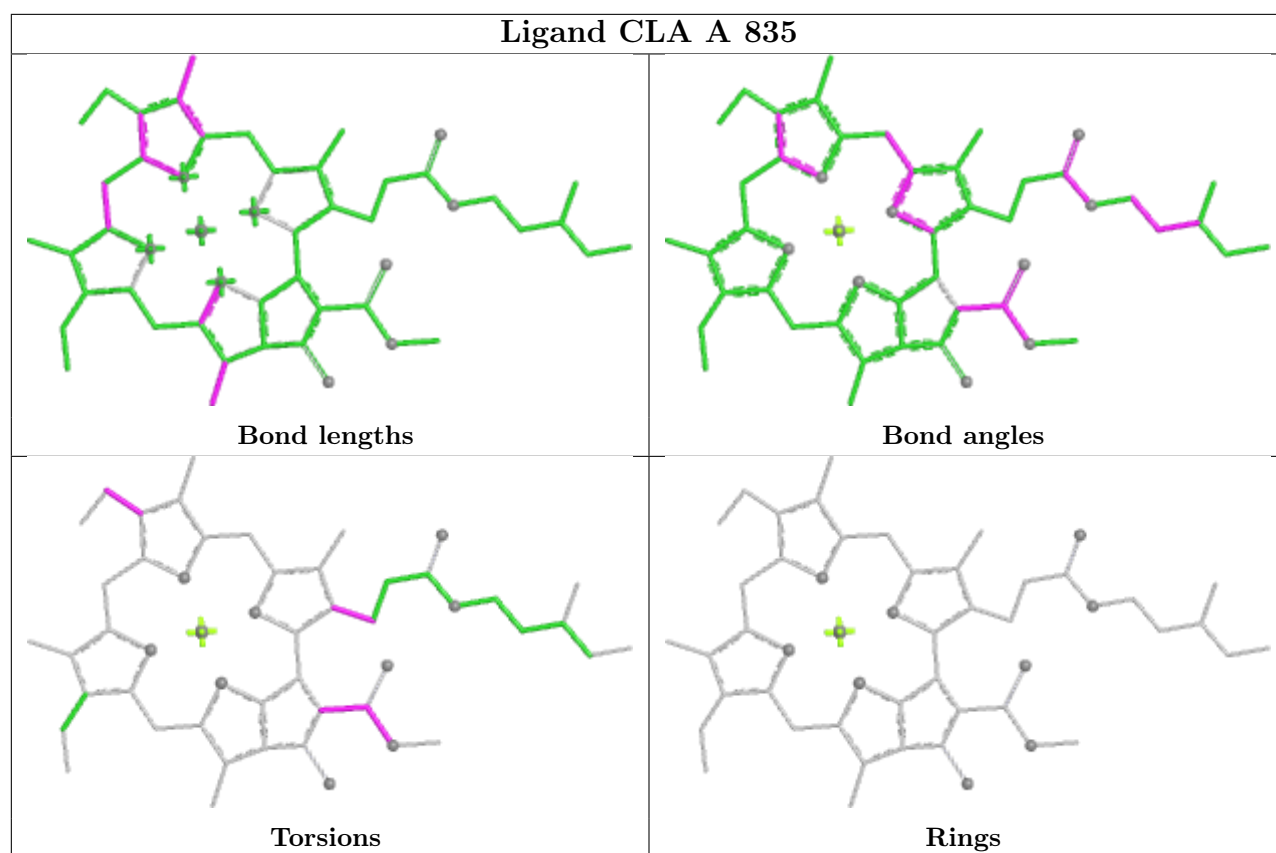
Bond angles



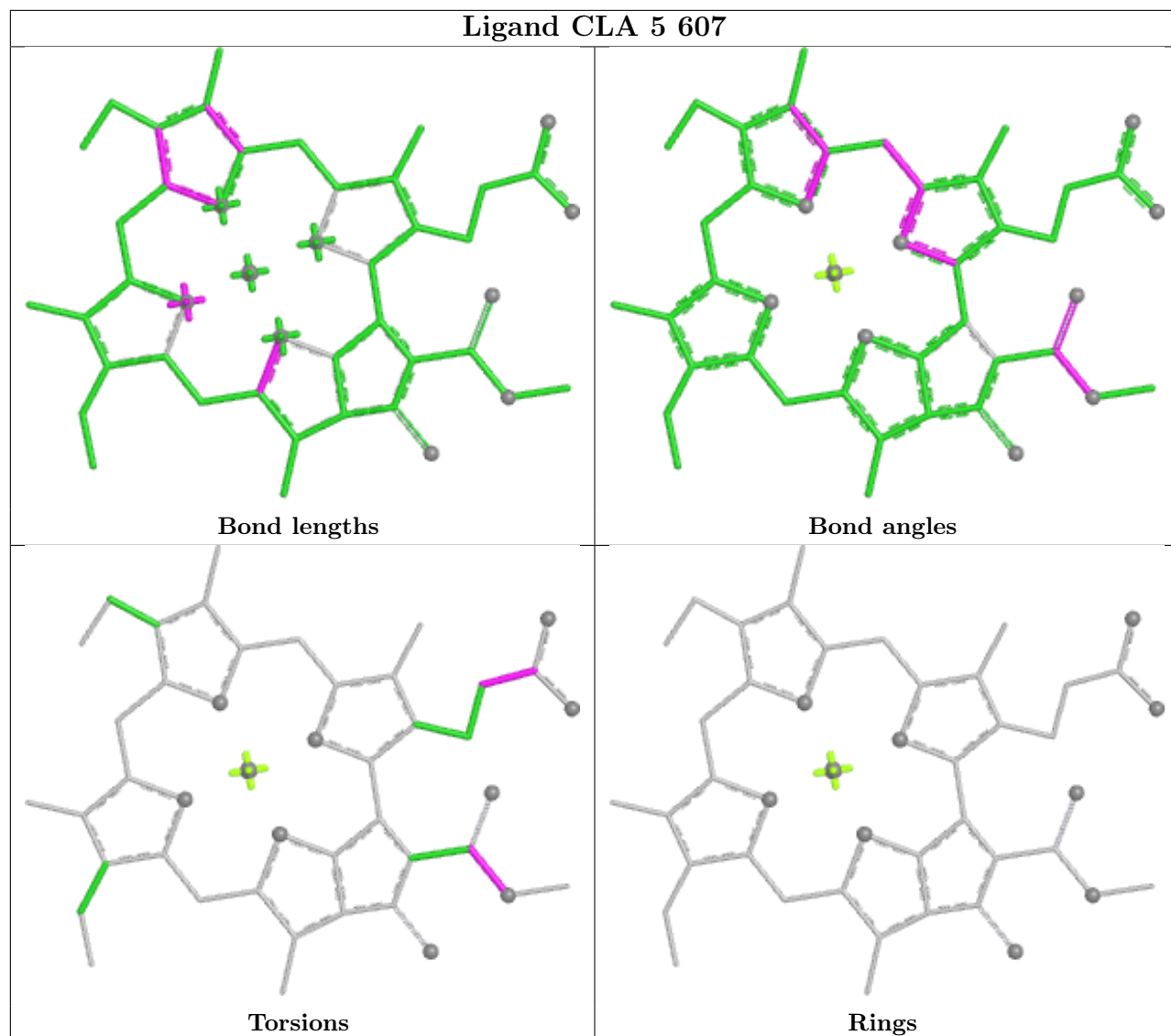
Torsions

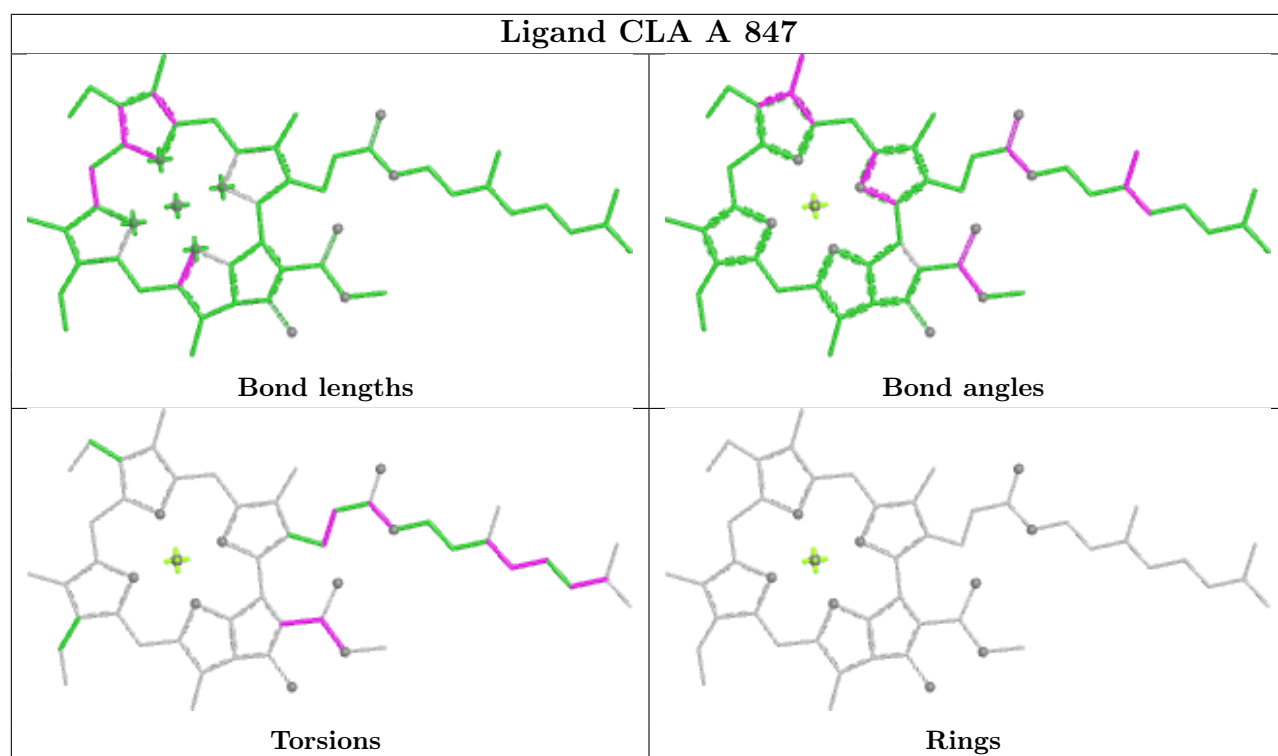


Rings

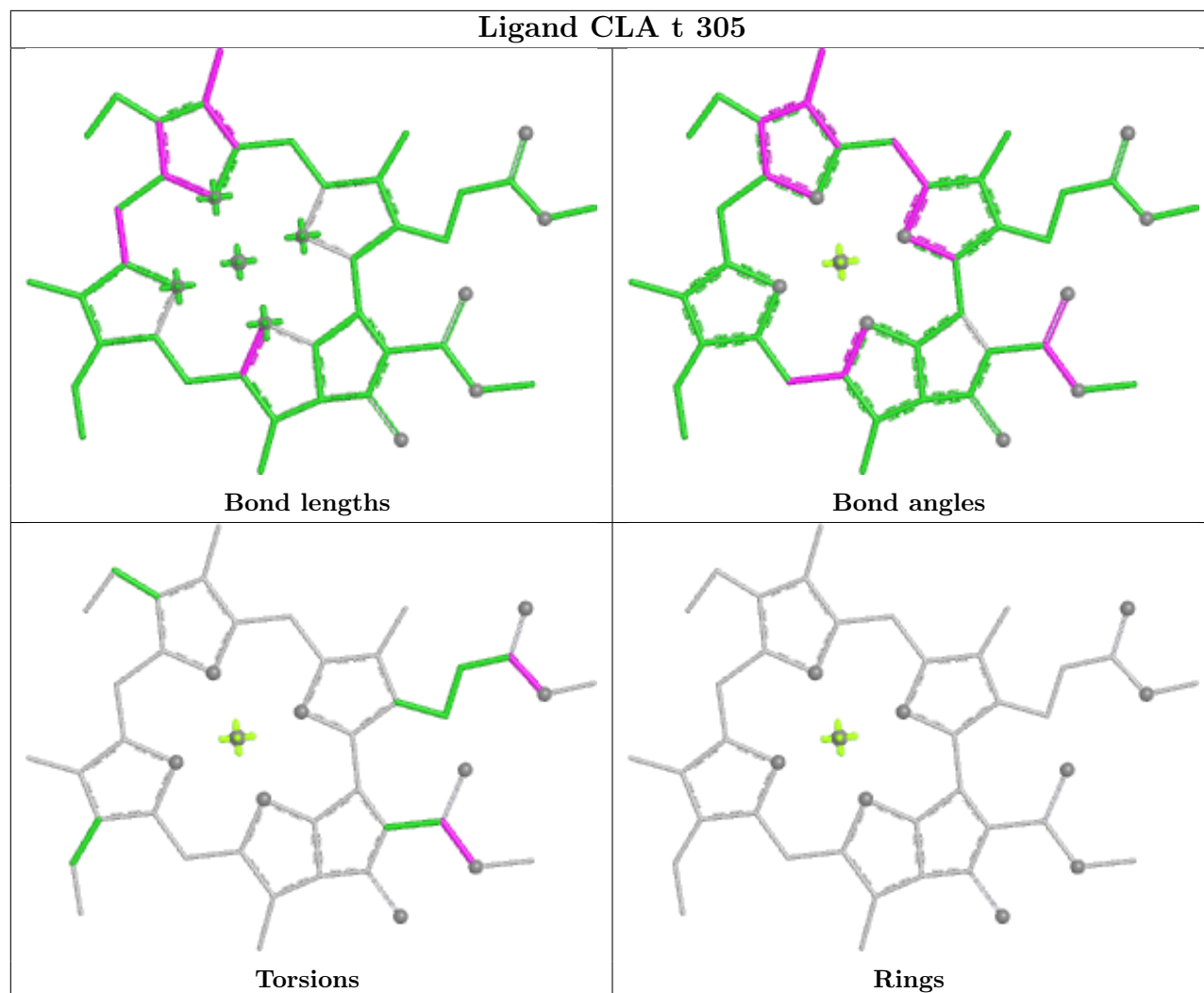


Ligand CLA 5 607

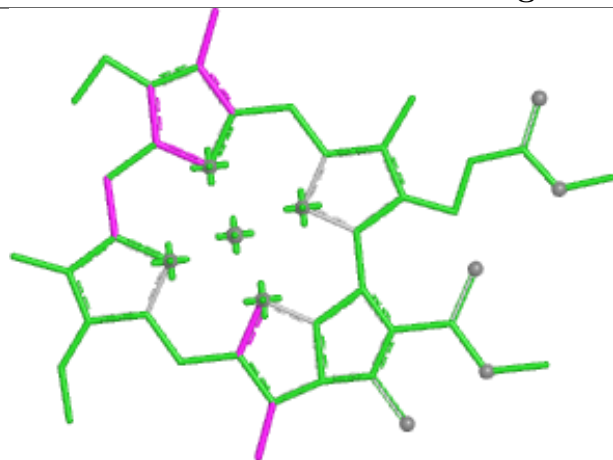




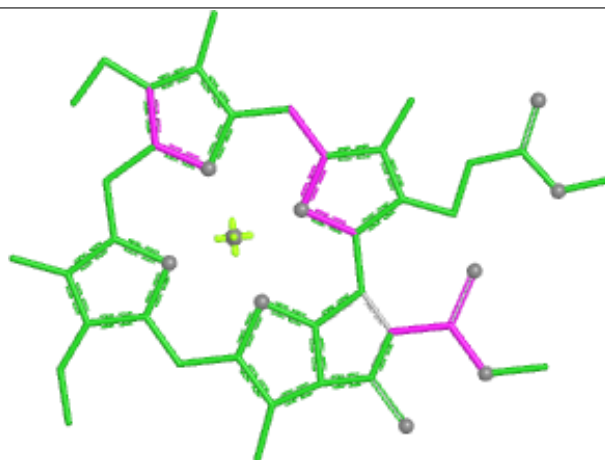
Ligand CLA t 305



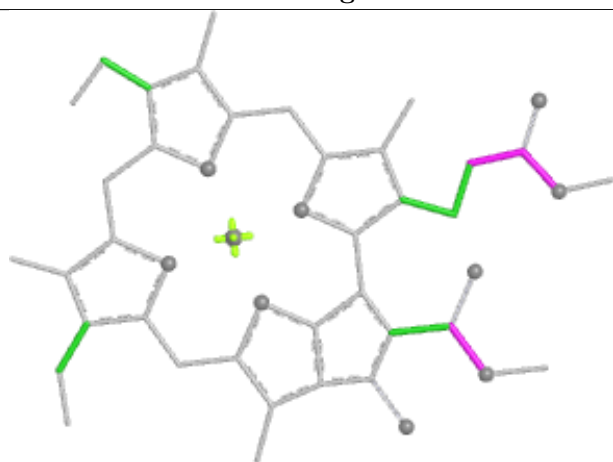
Ligand CLA k 306



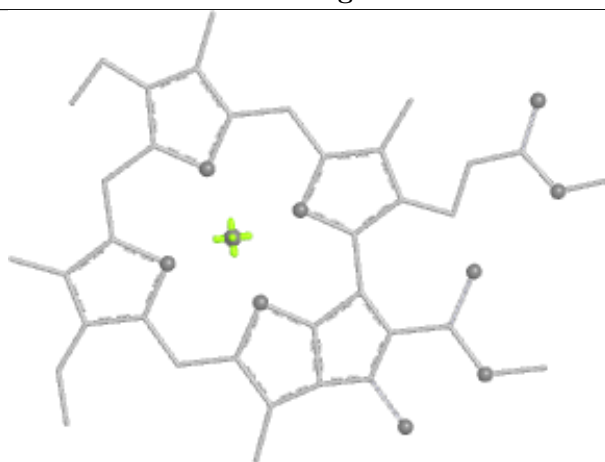
Bond lengths



Bond angles

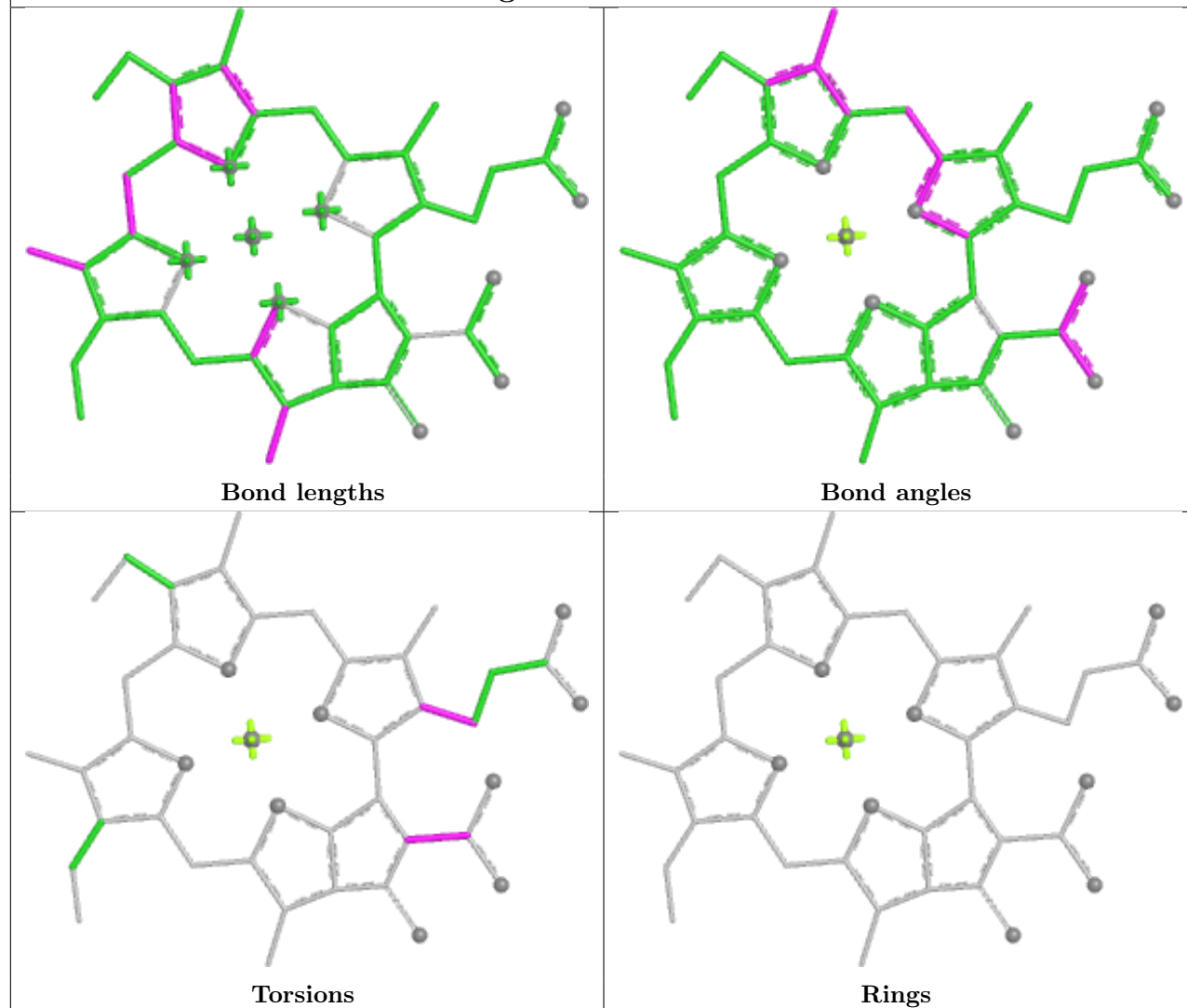


Torsions

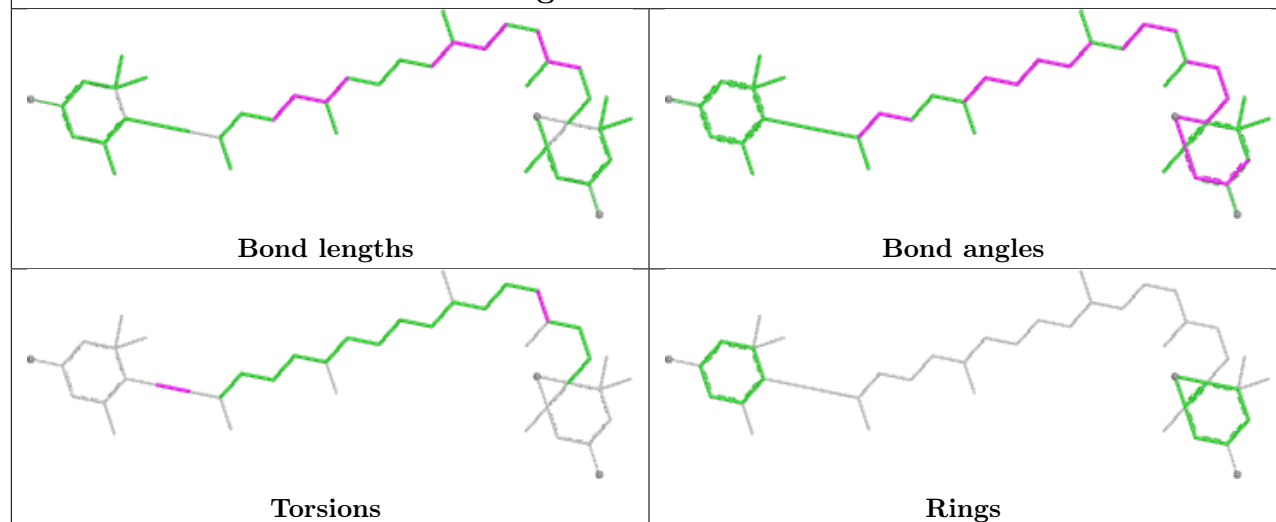


Rings

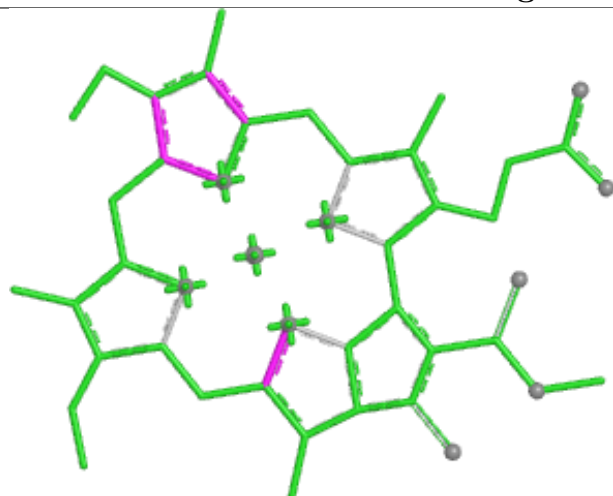
Ligand CLA 6 611



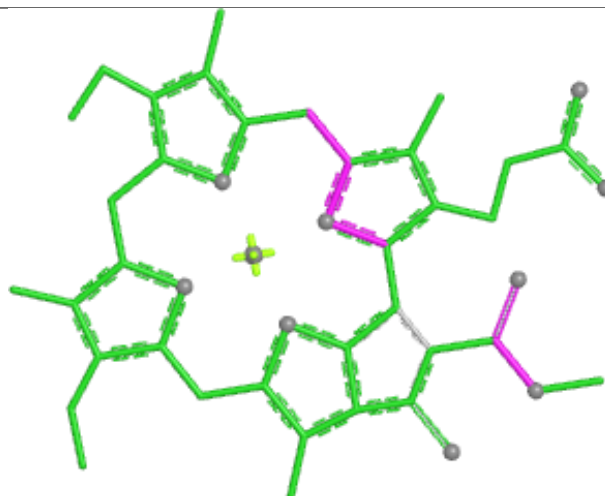
Ligand DD6 9 313



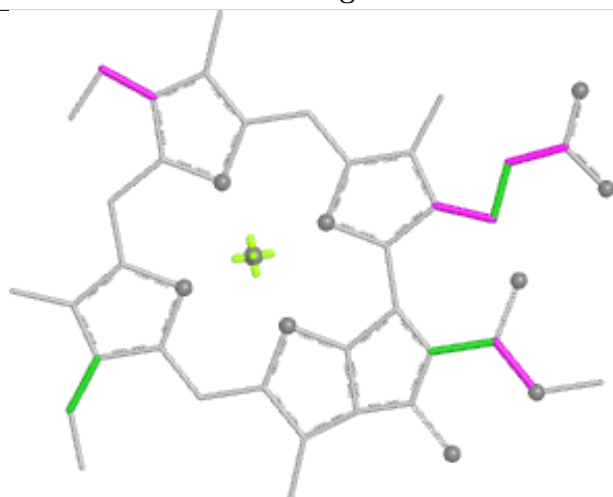
Ligand CLA h 601



Bond lengths



Bond angles

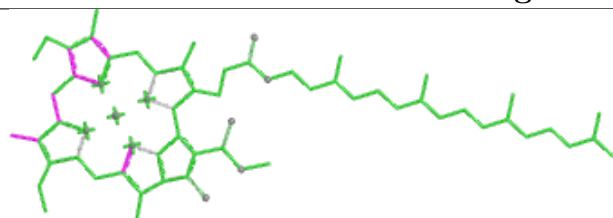


Torsions

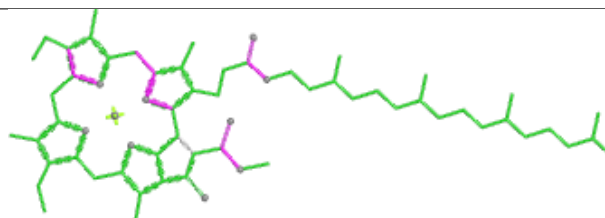


Rings

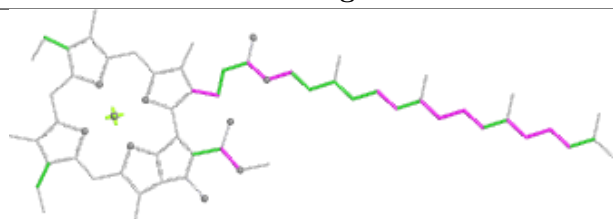
Ligand CLA B 812



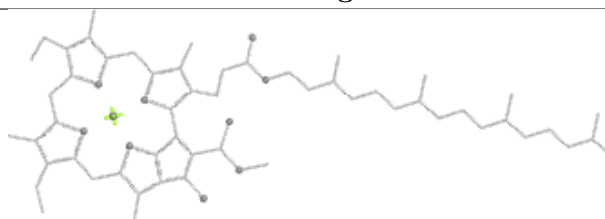
Bond lengths



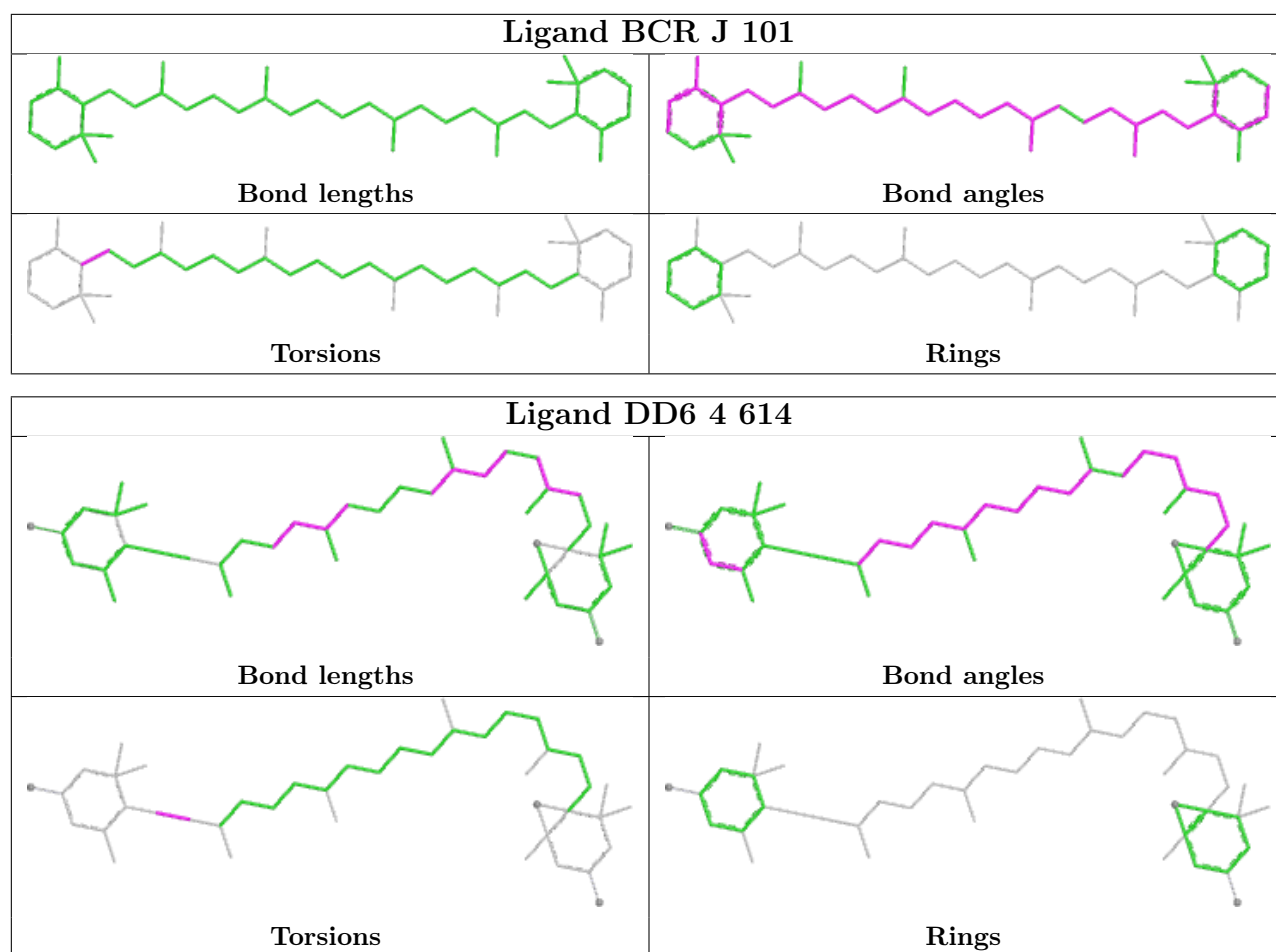
Bond angles

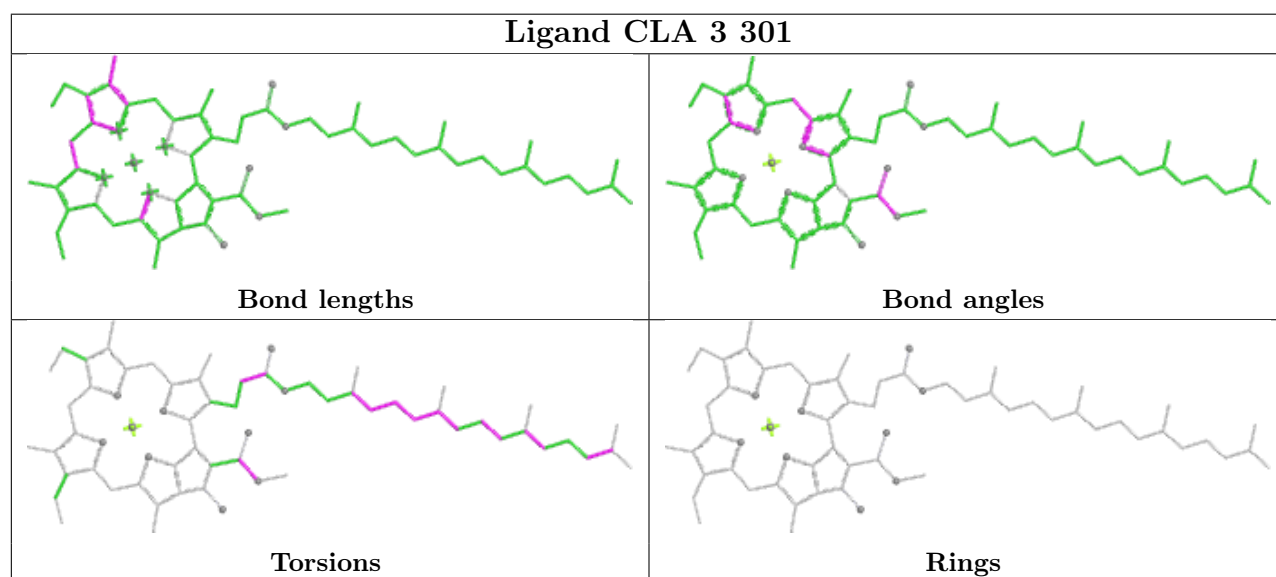
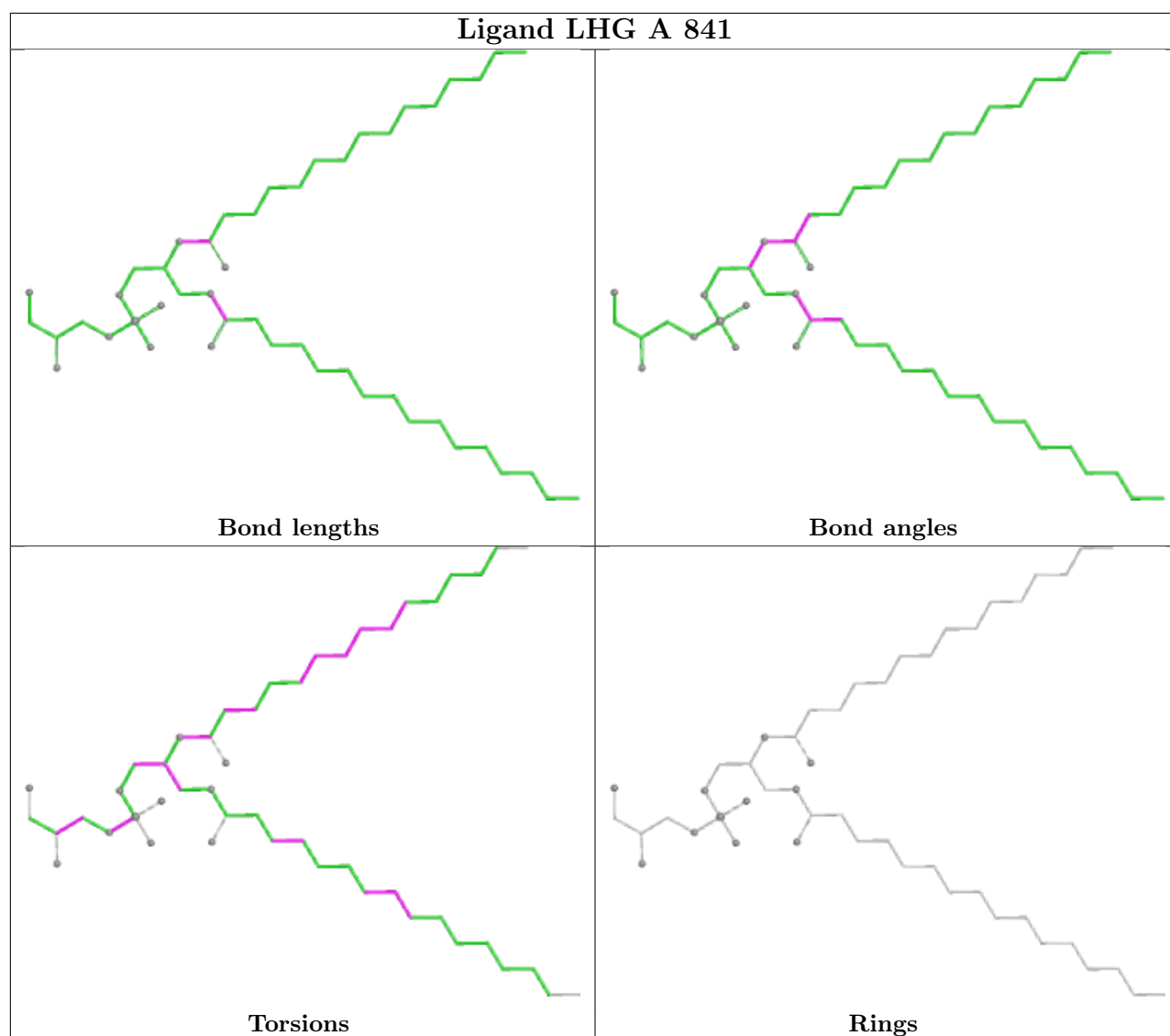


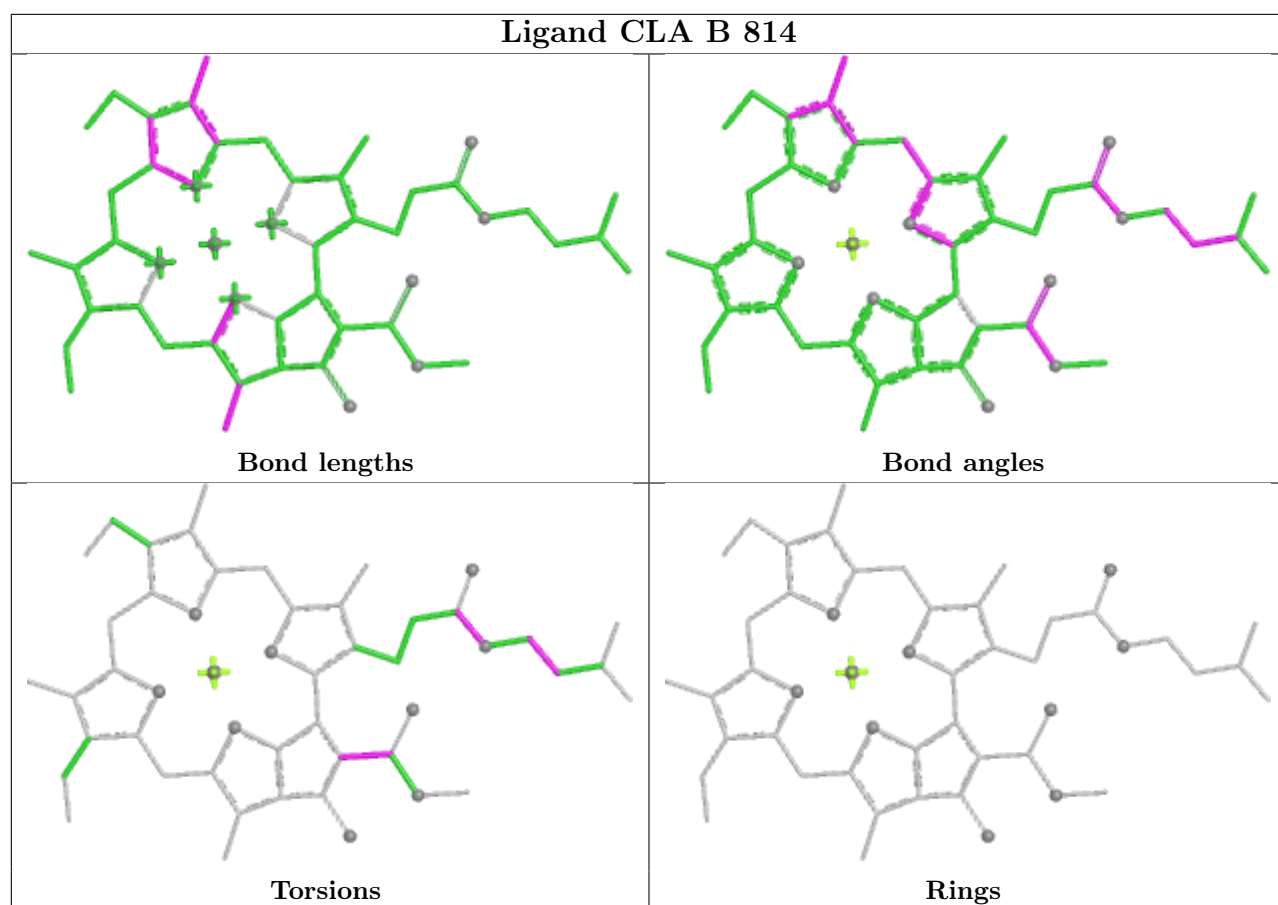
Torsions



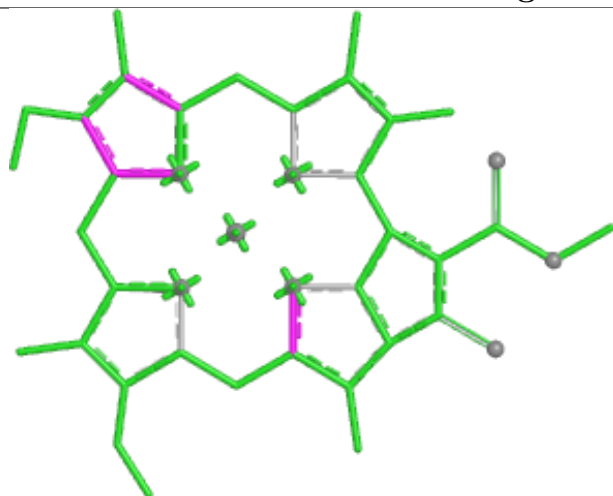
Rings



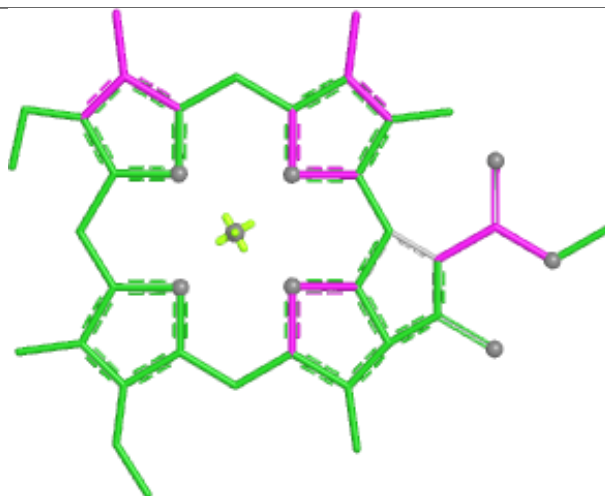




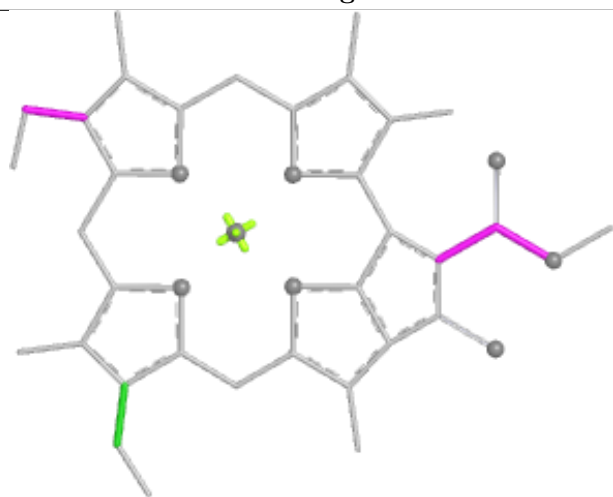
Ligand CLA k 308



Bond lengths



Bond angles

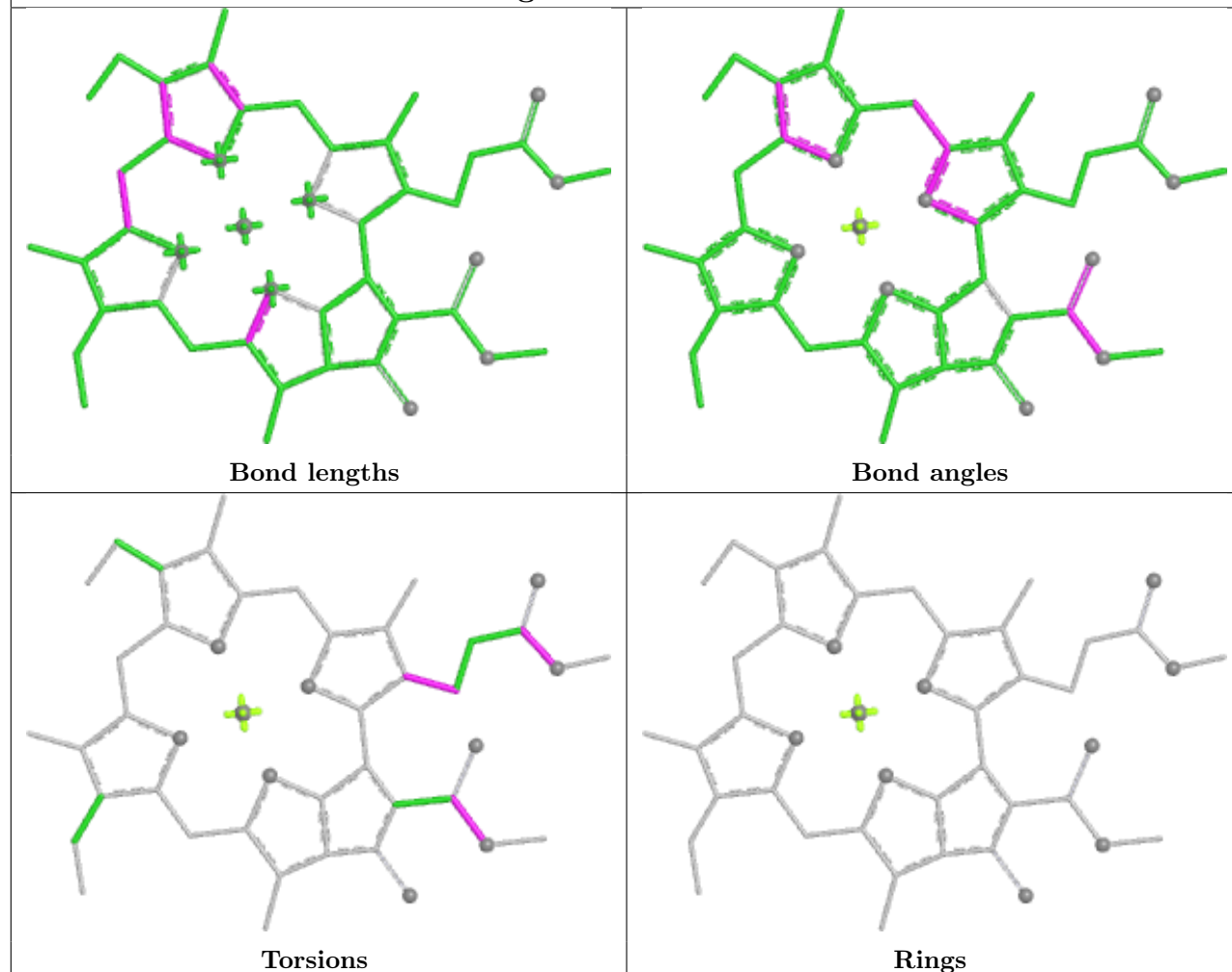


Torsions

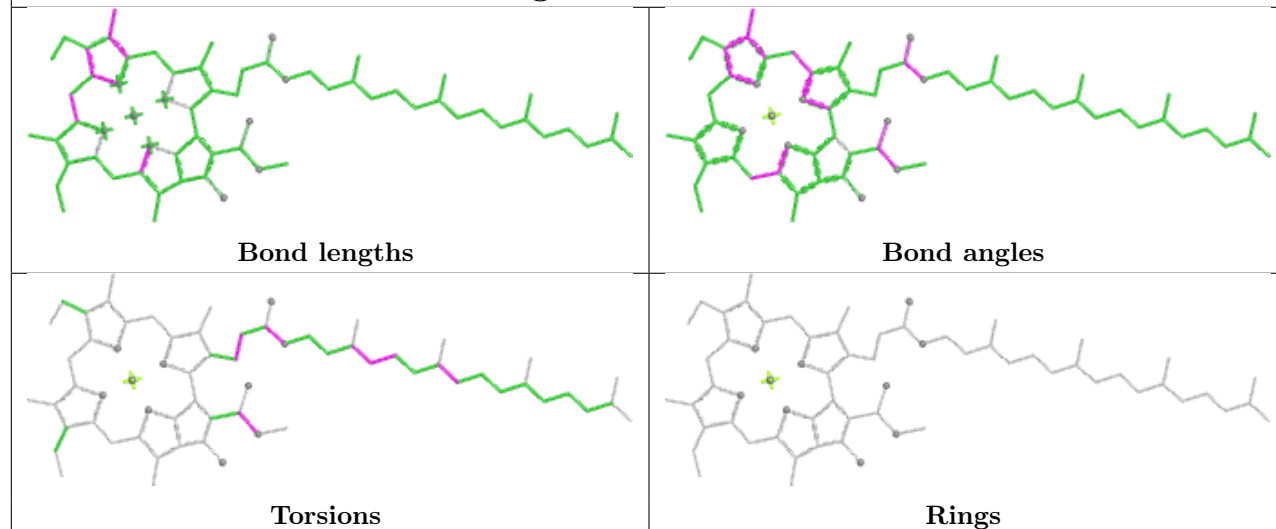


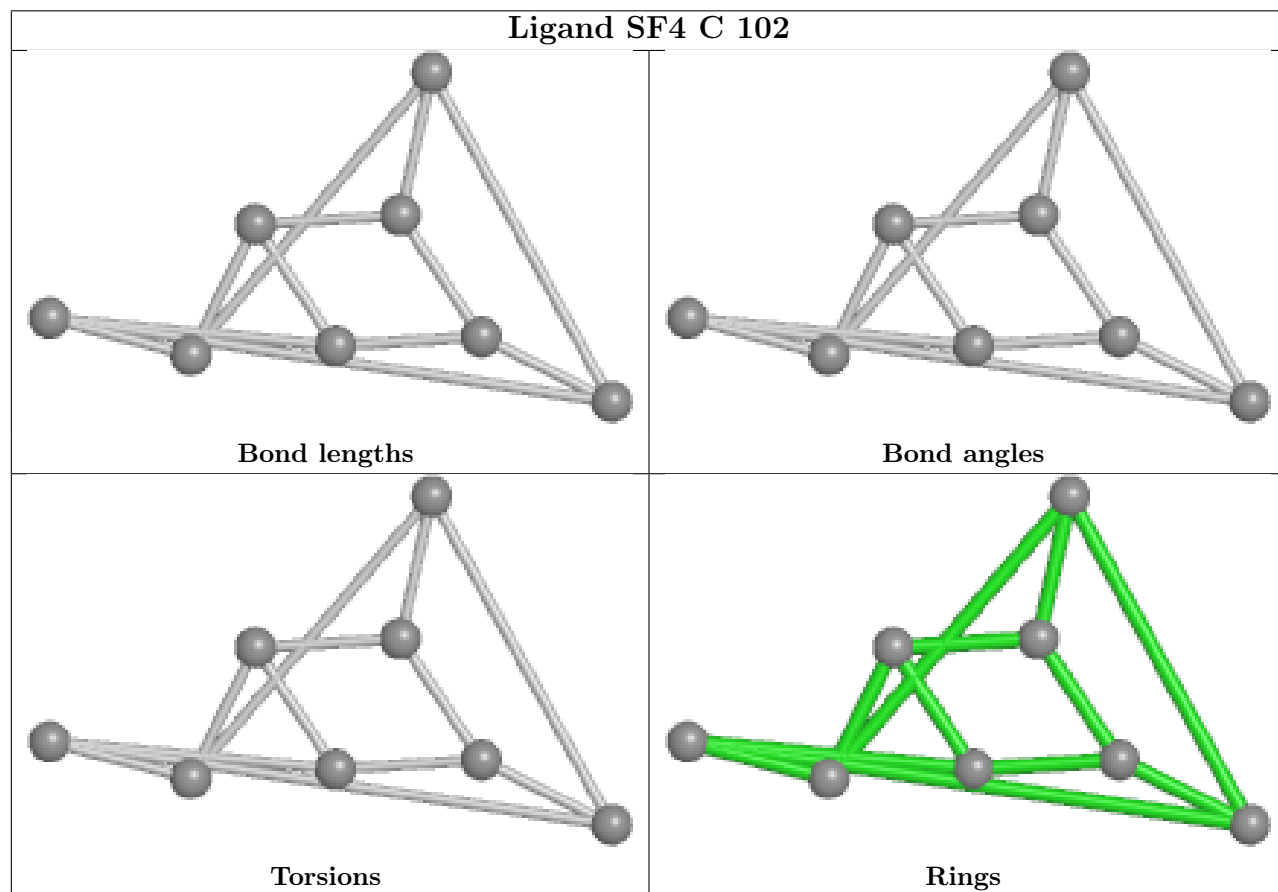
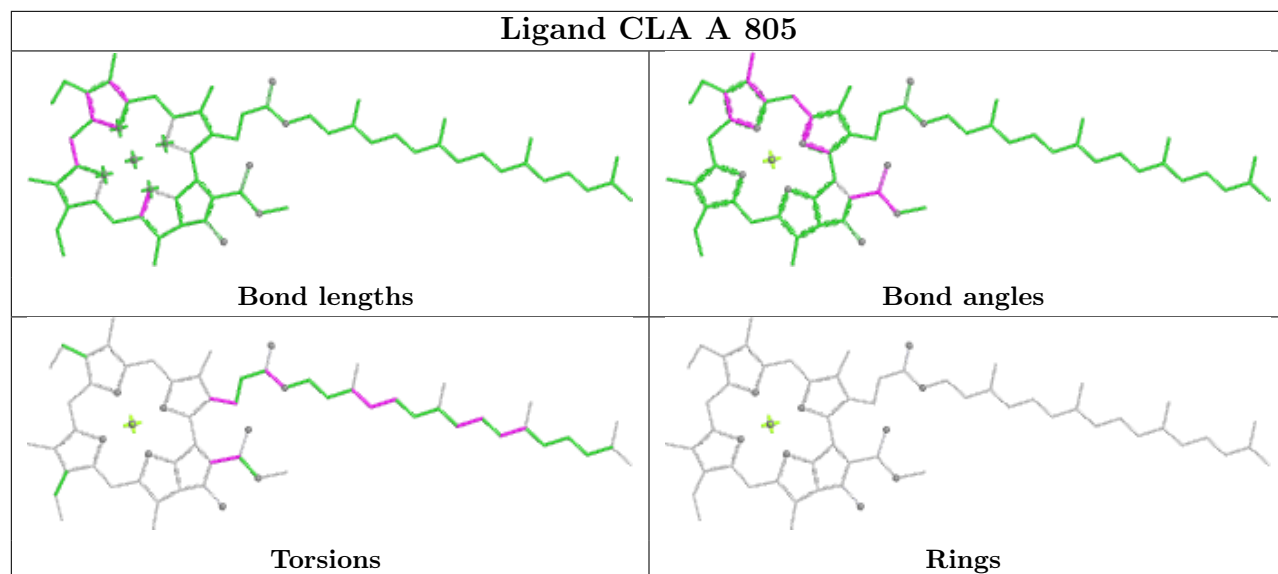
Rings

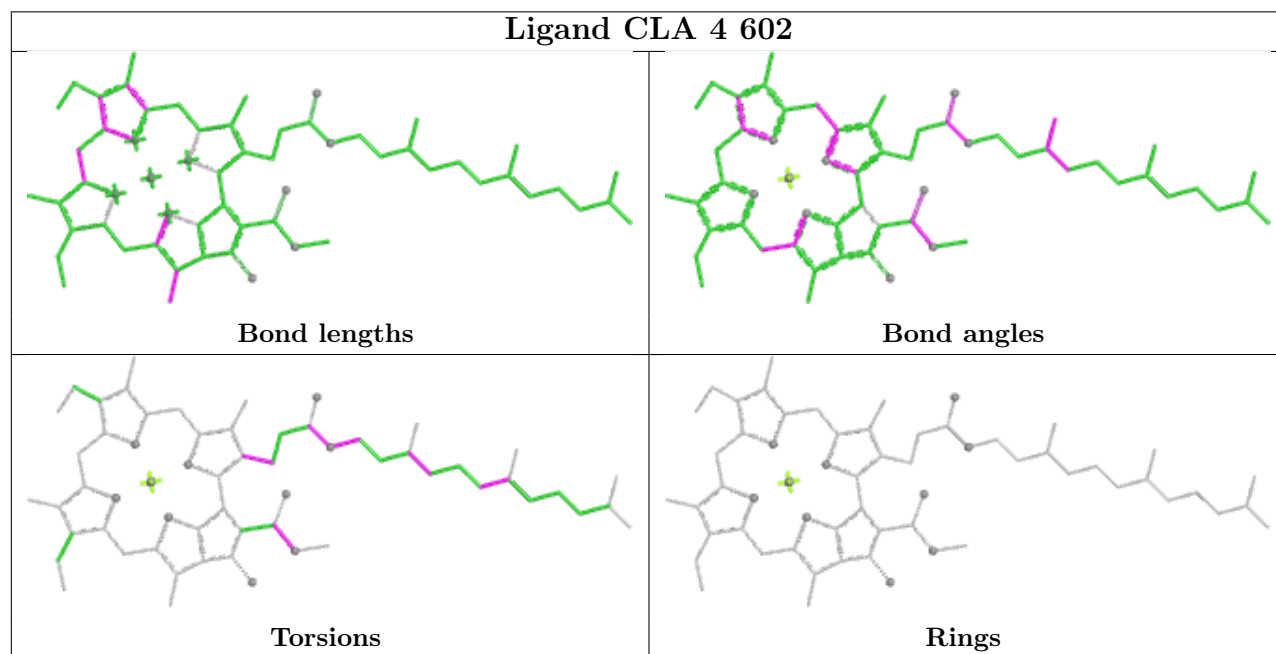
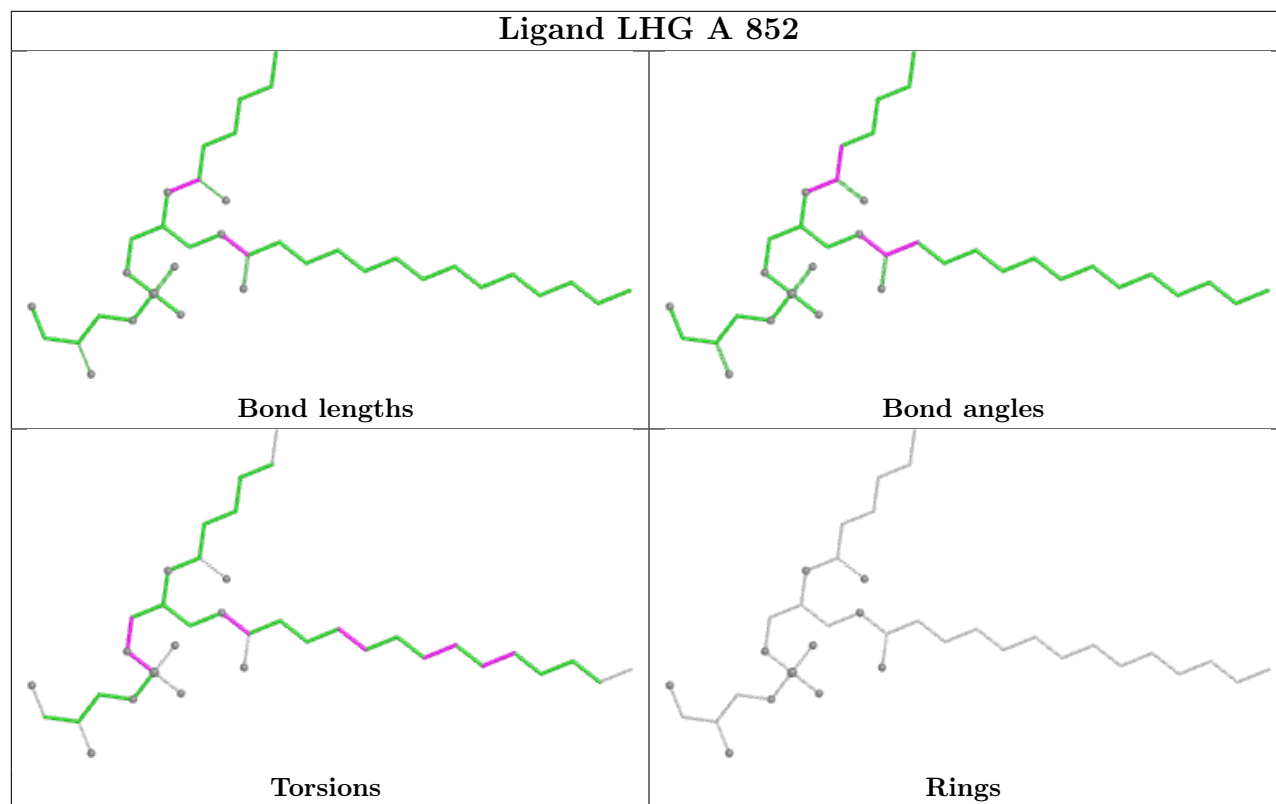
Ligand CLA 7 609



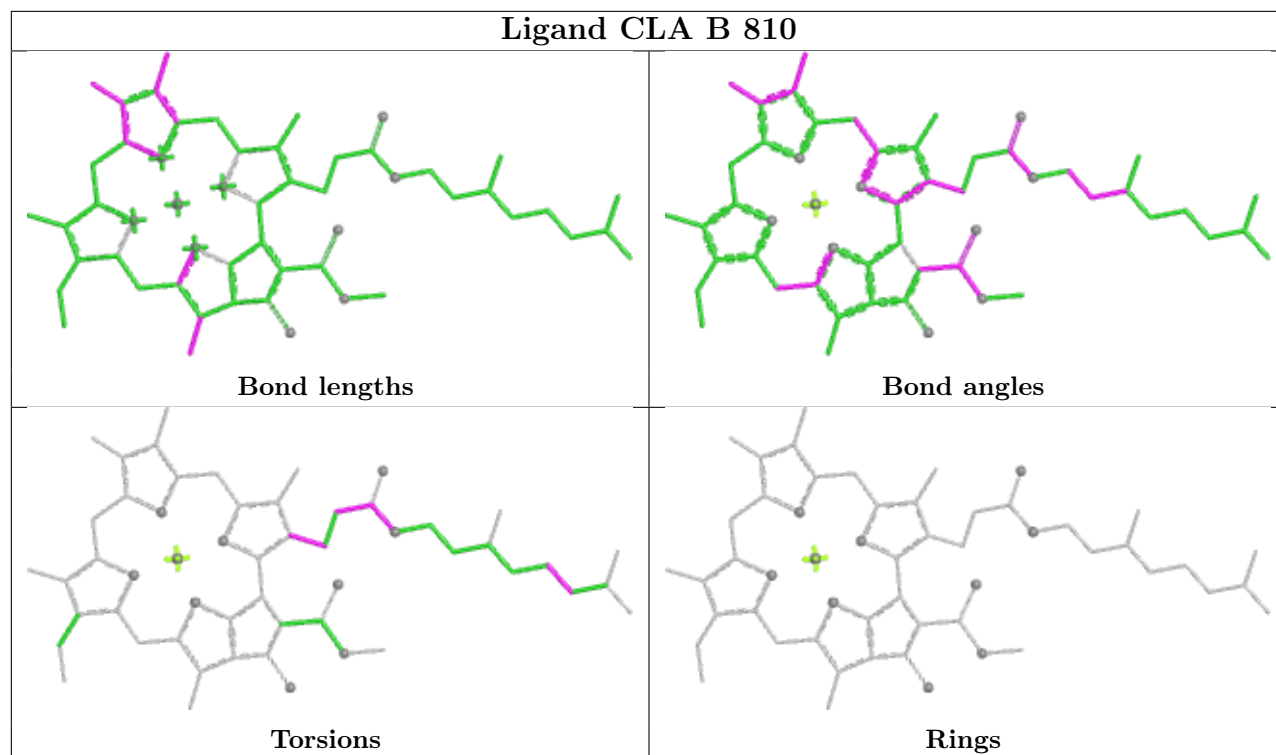
Ligand CLA A 820



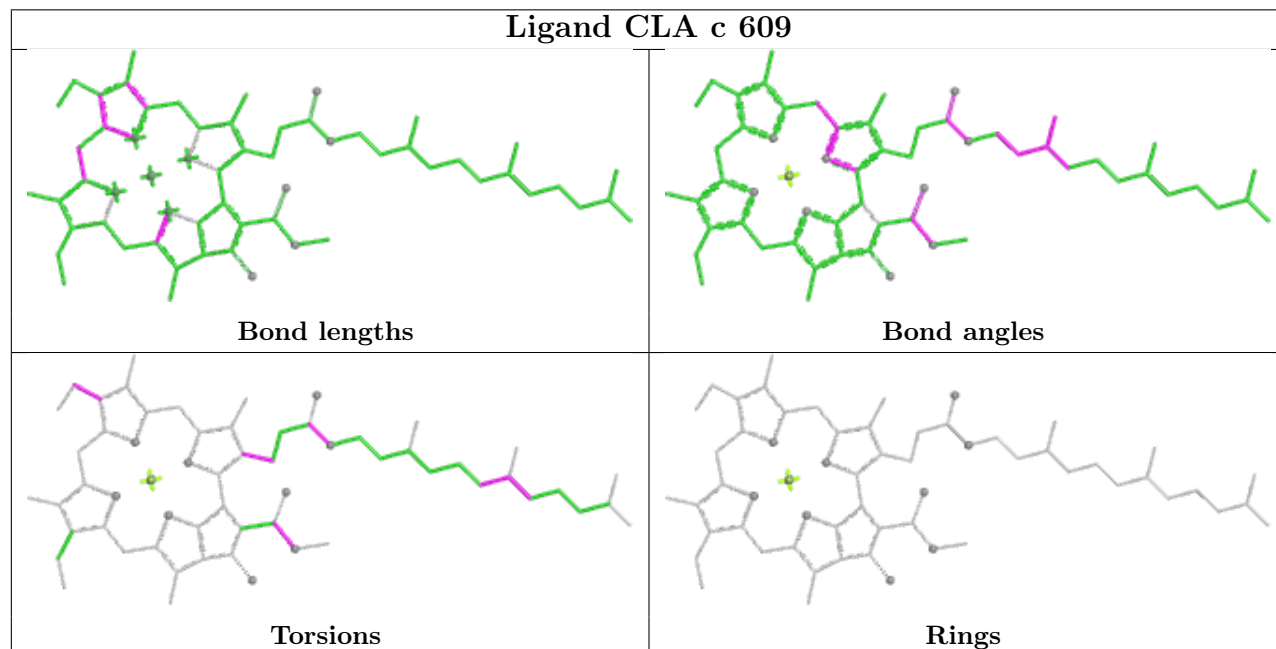


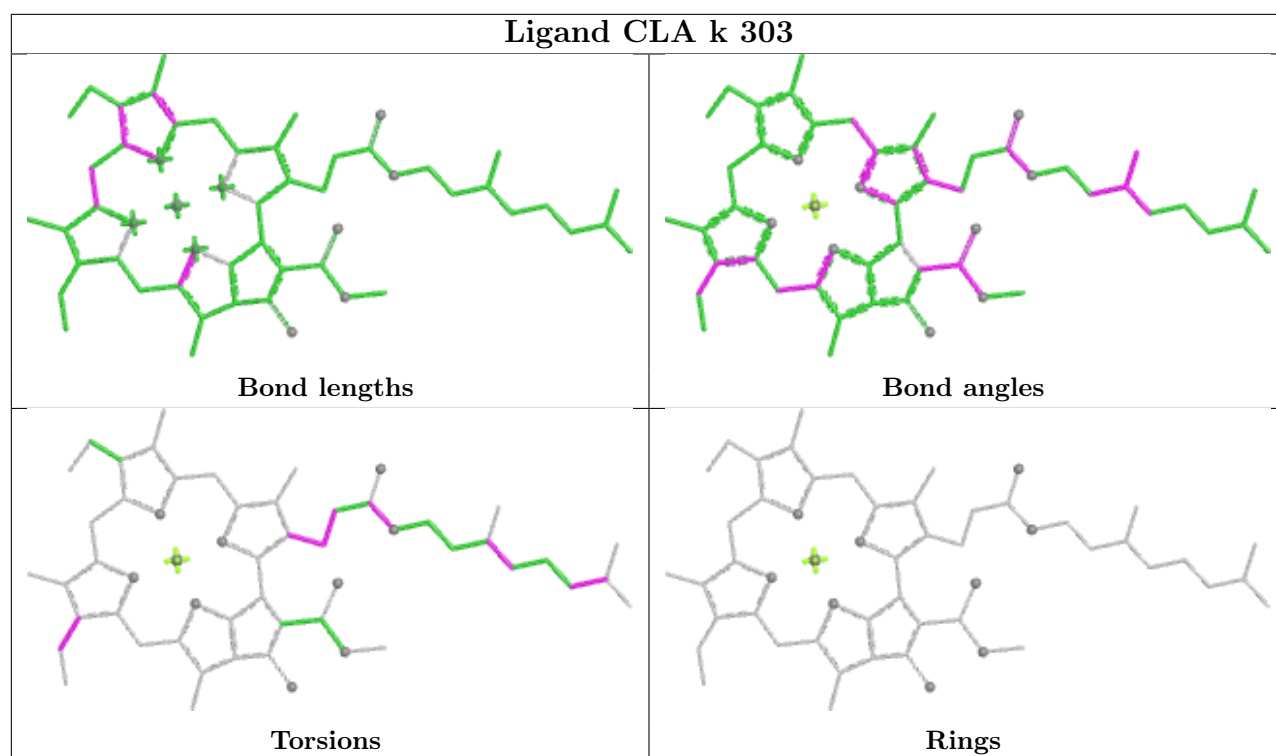


Ligand CLA B 810

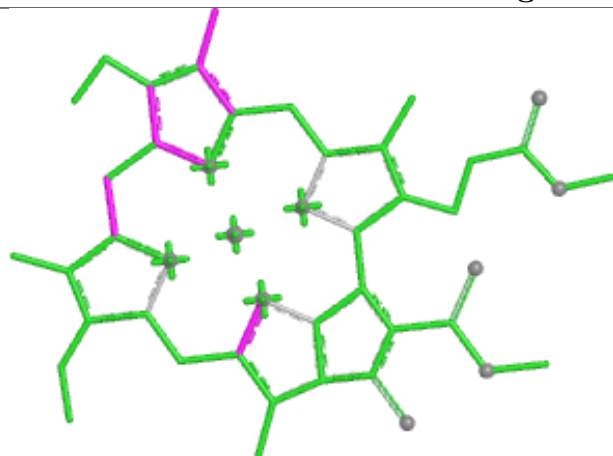


Ligand CLA c 609

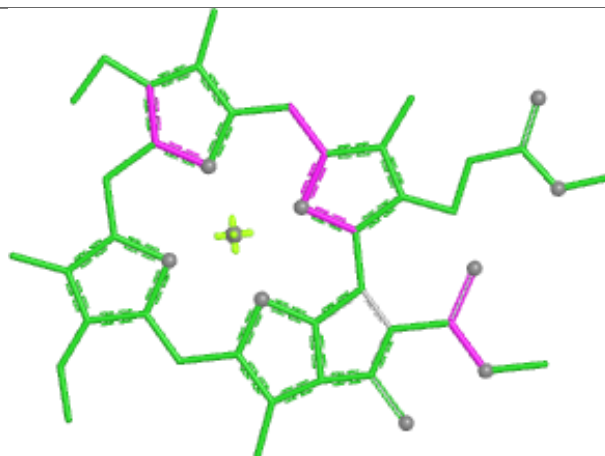




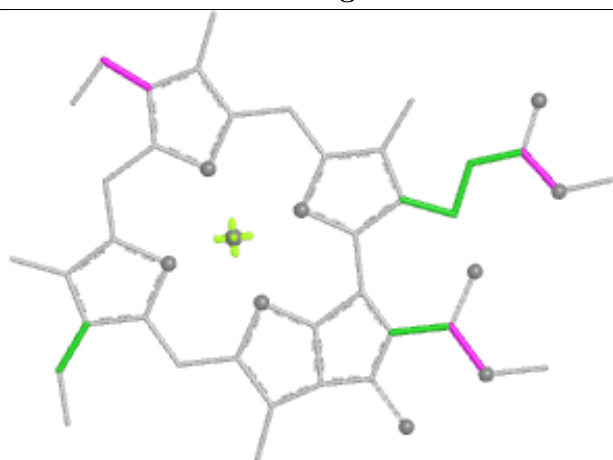
Ligand CLA h 607



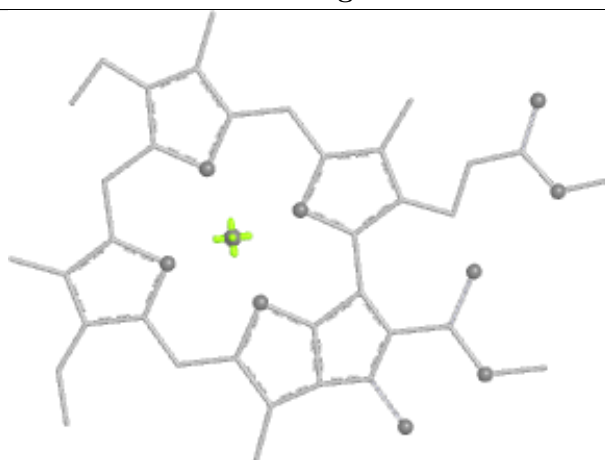
Bond lengths



Bond angles

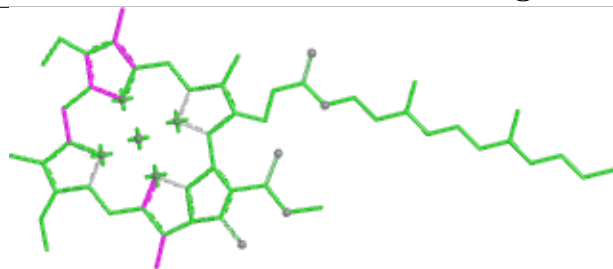


Torsions

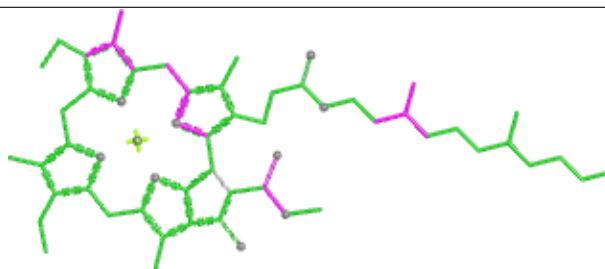


Rings

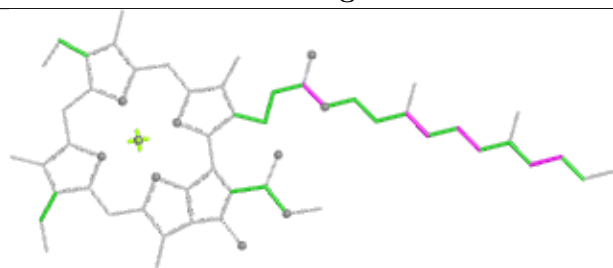
Ligand CLA B 833



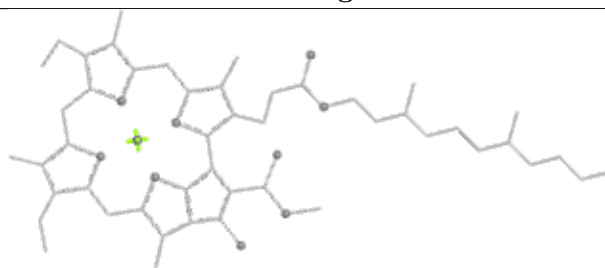
Bond lengths



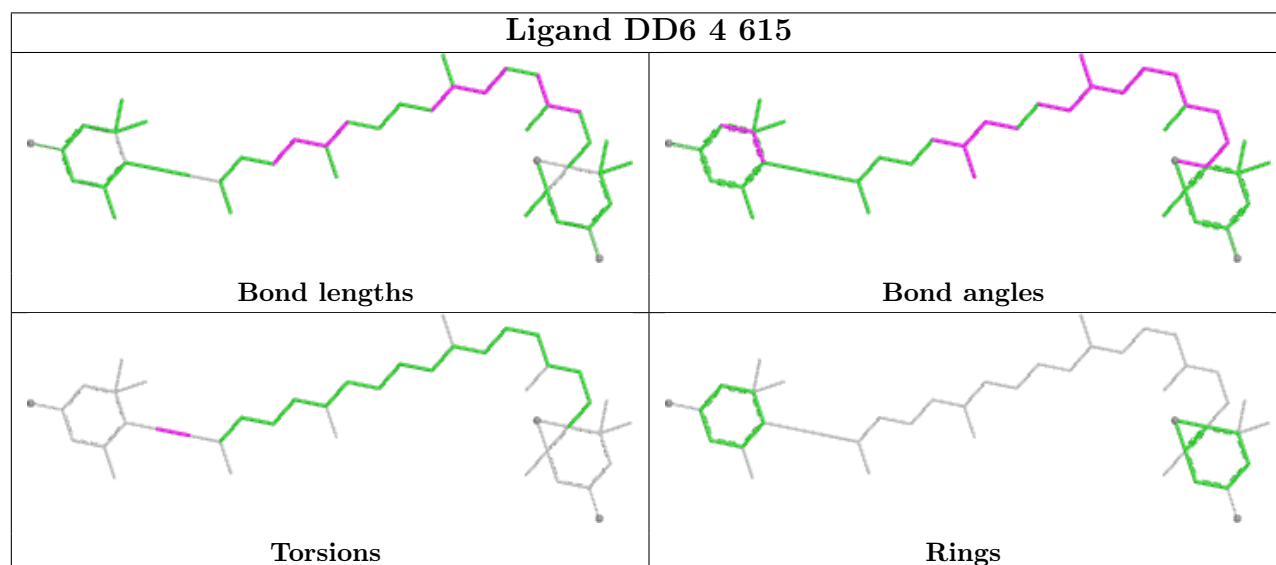
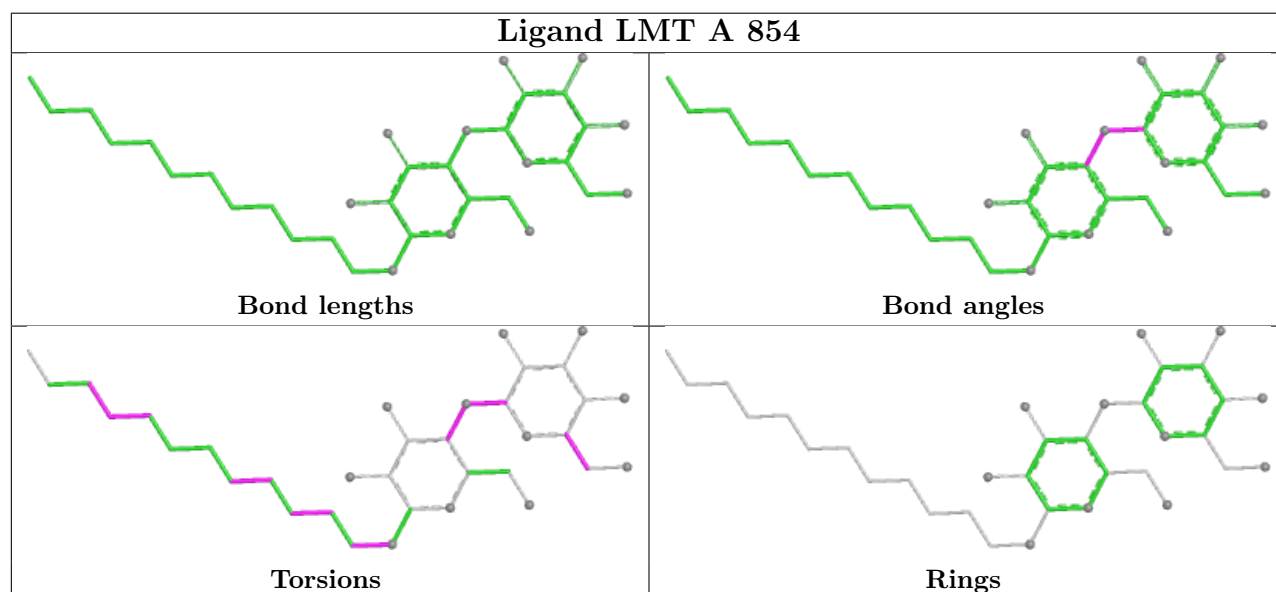
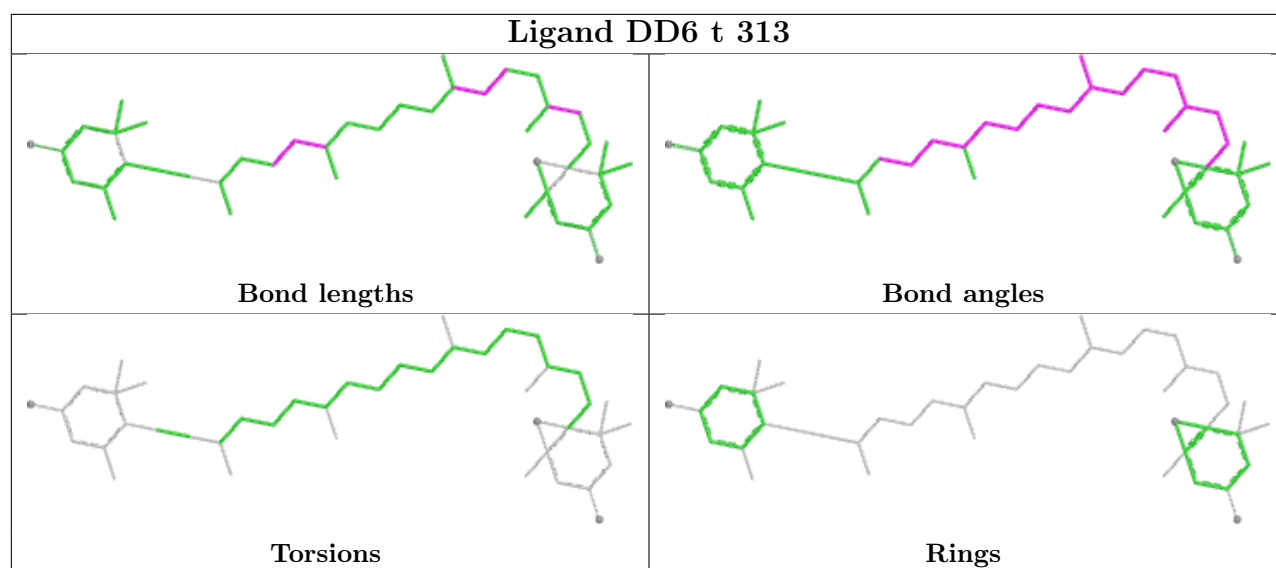
Bond angles



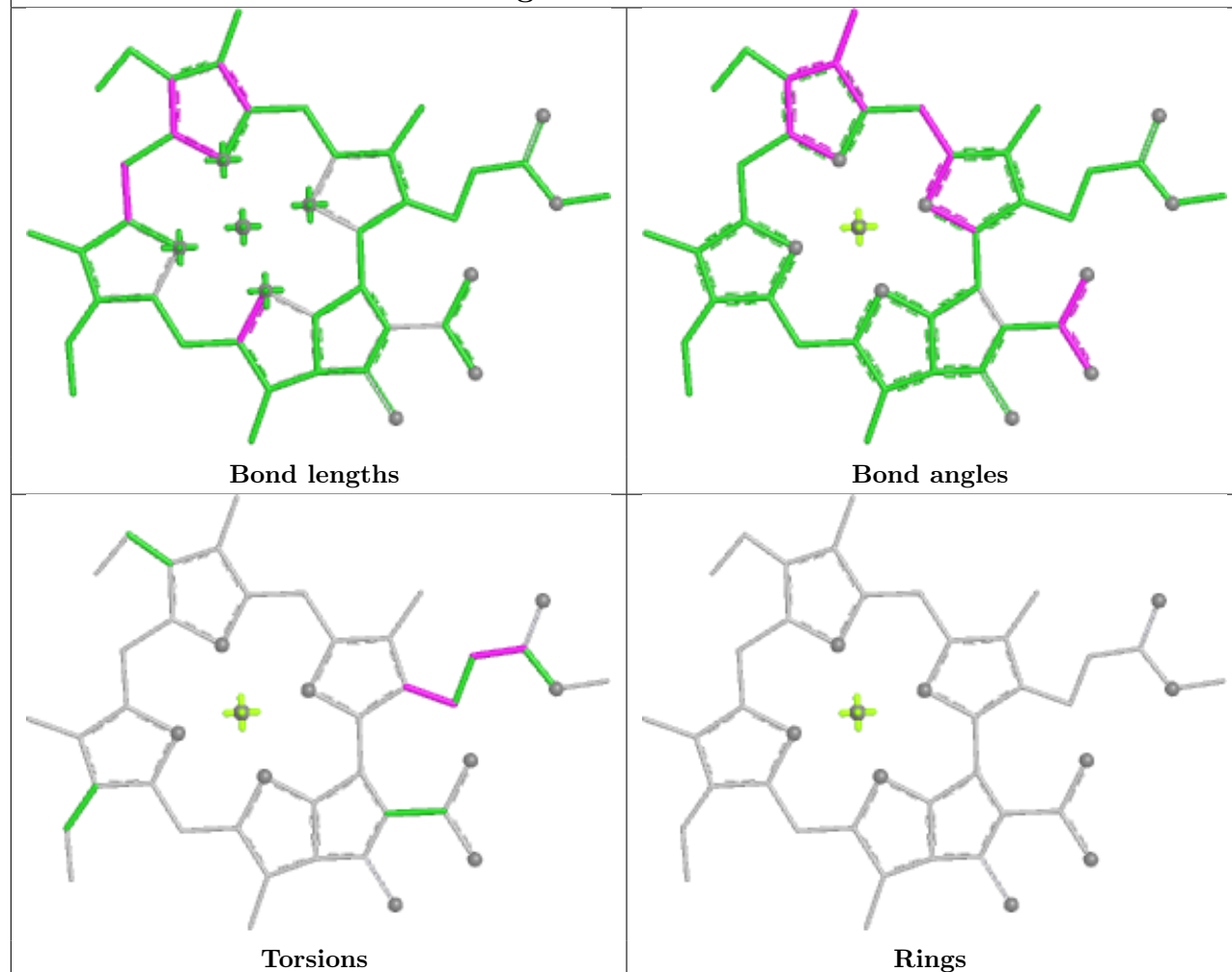
Torsions



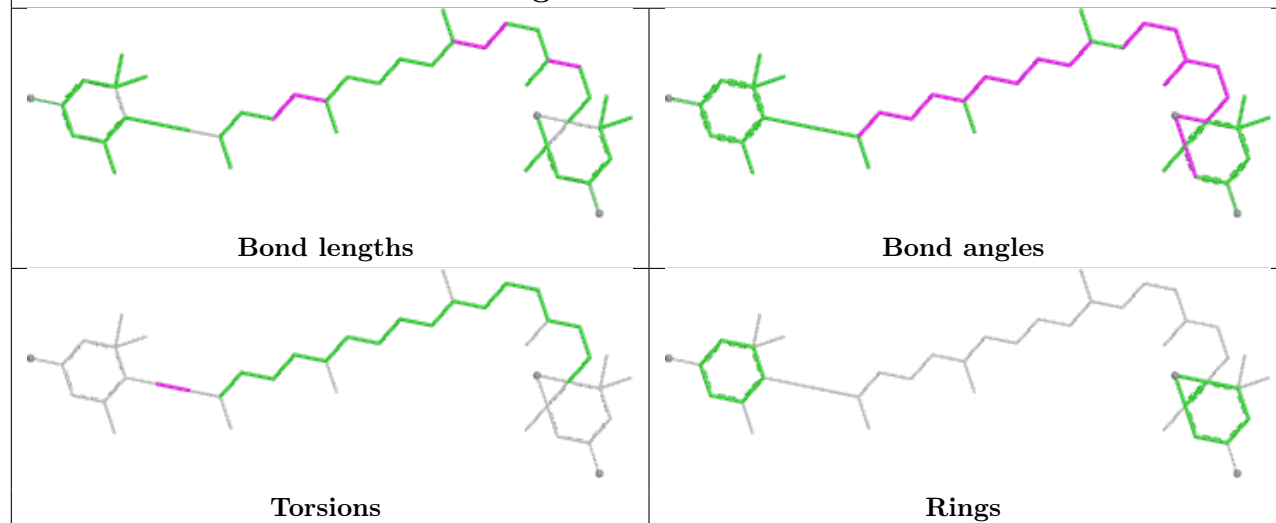
Rings



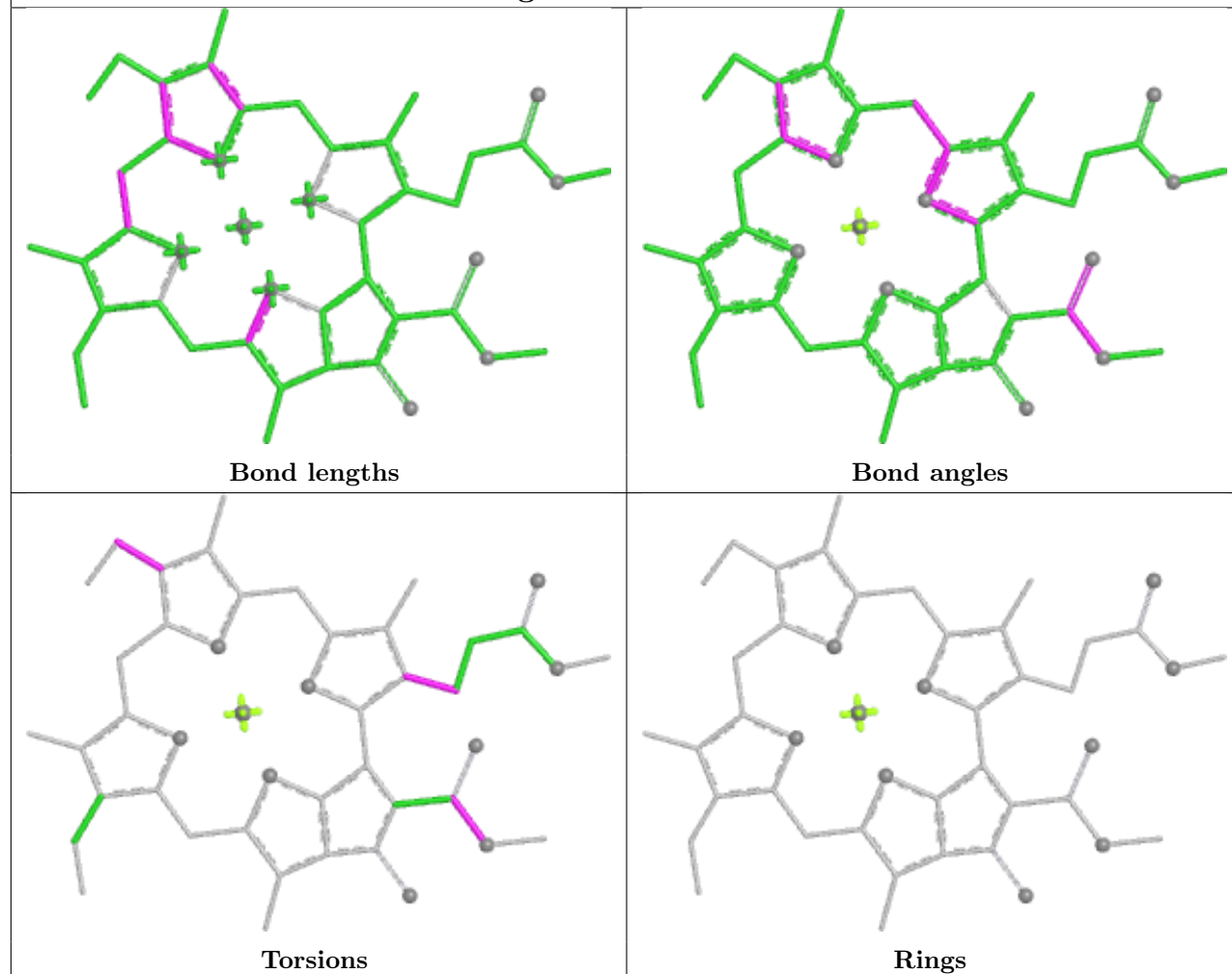
Ligand CLA h 603



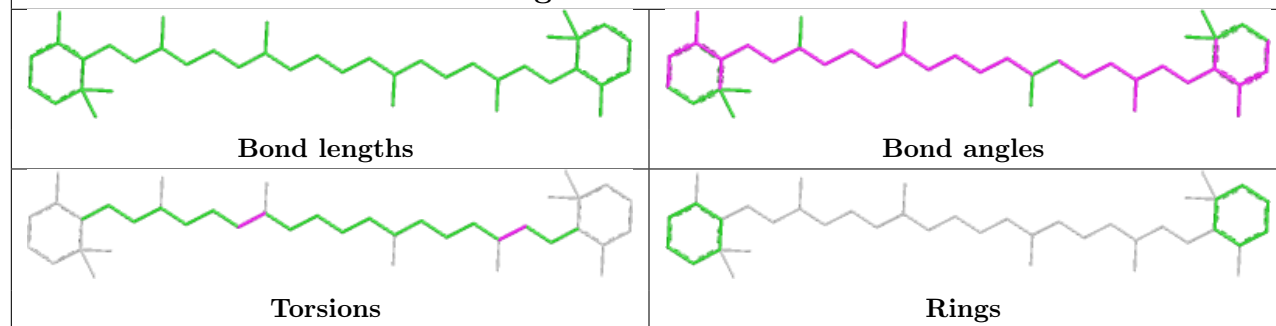
Ligand DD6 A 848

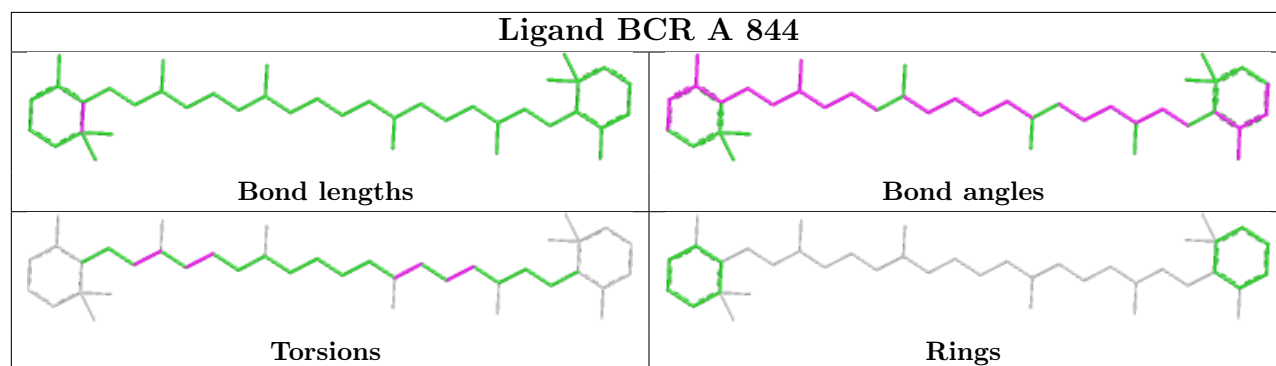
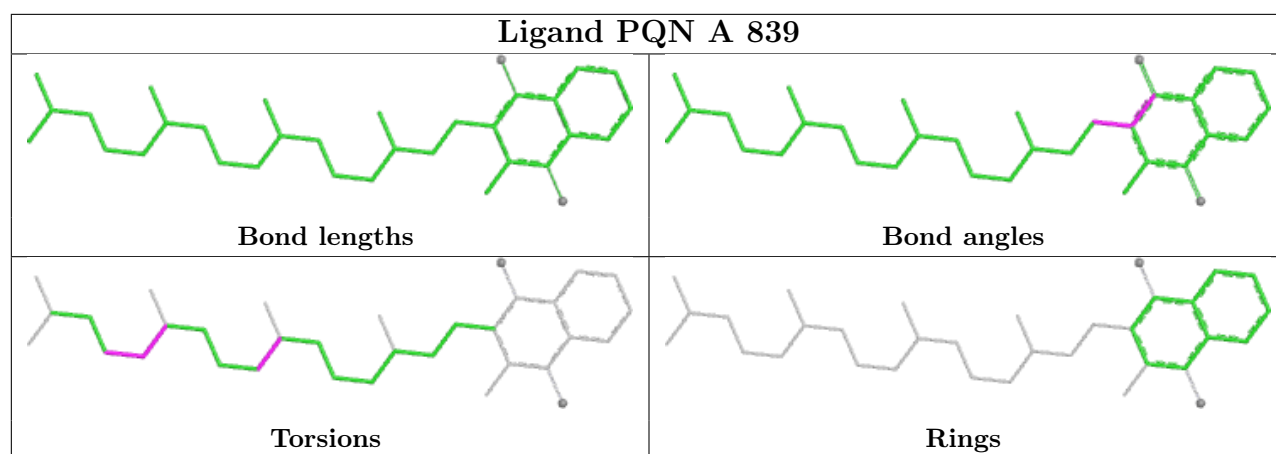


Ligand CLA 1 303

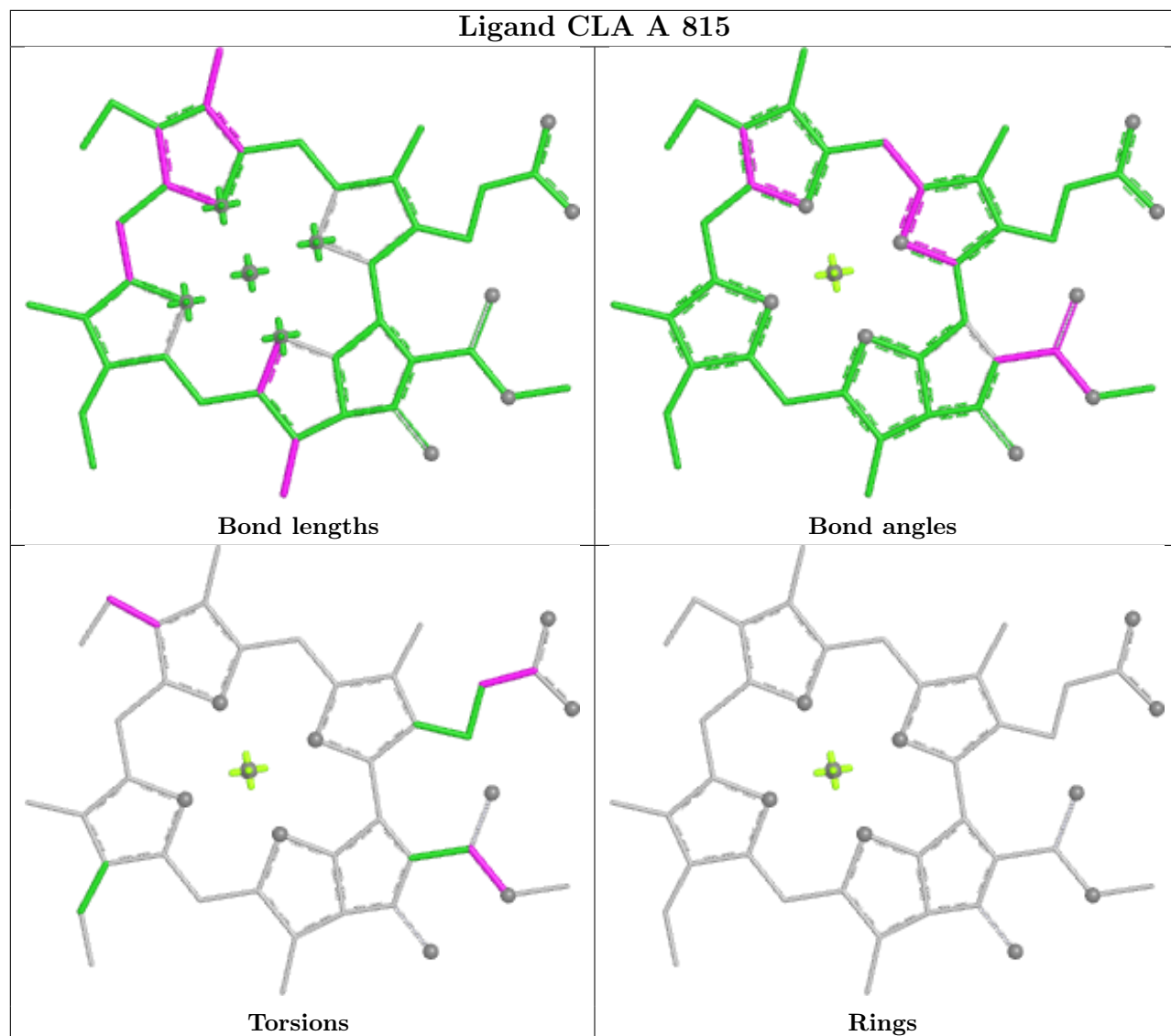


Ligand BCR 1 310

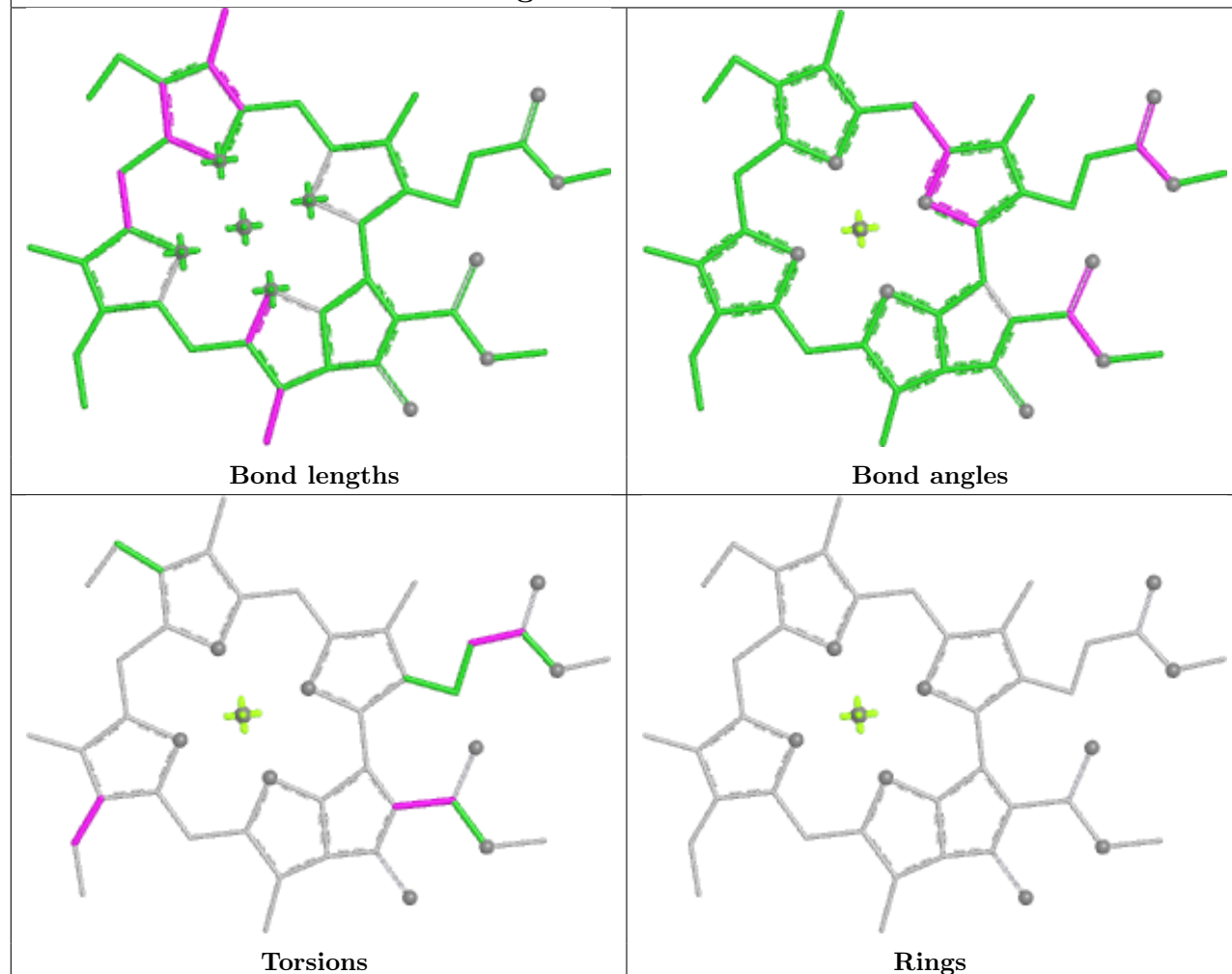




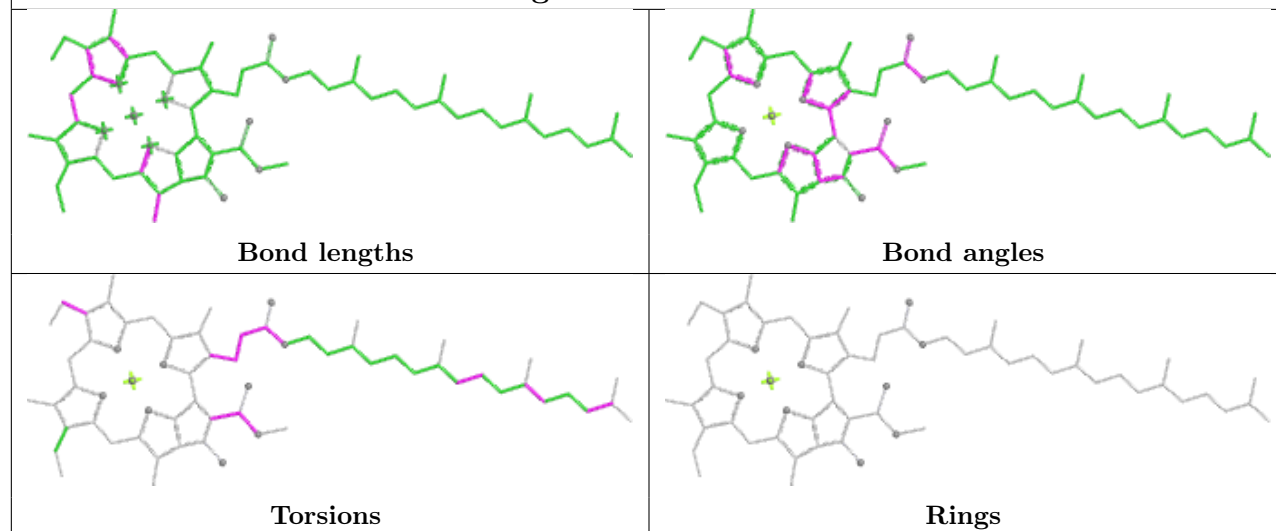
Ligand CLA A 815

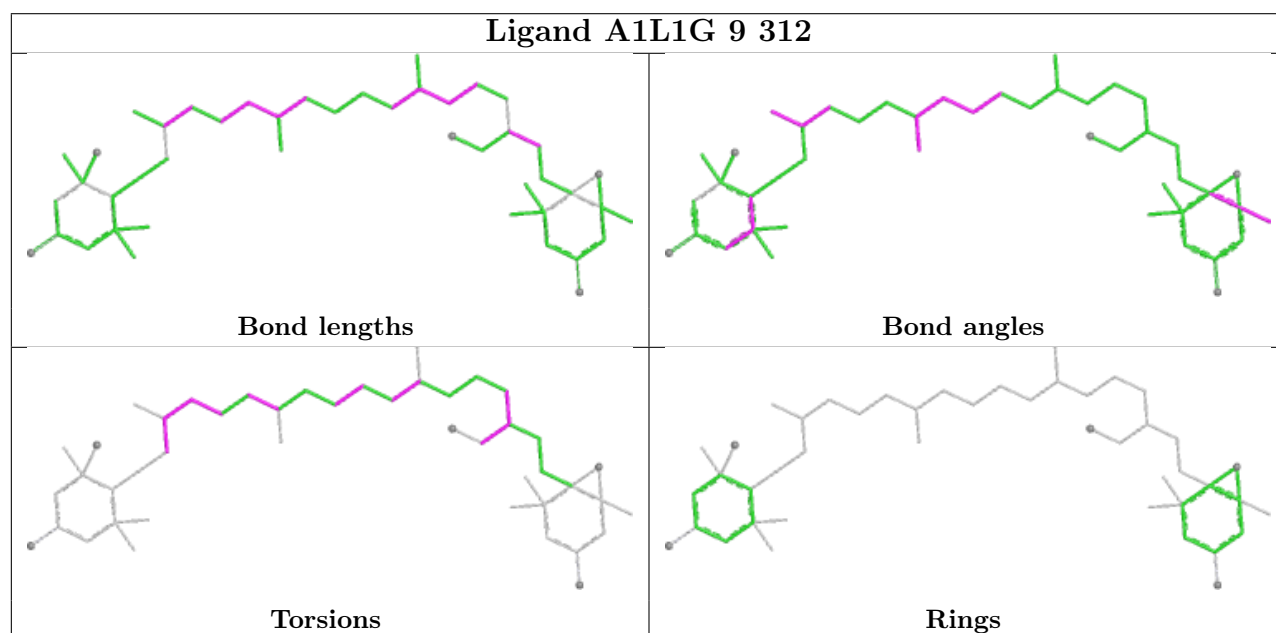
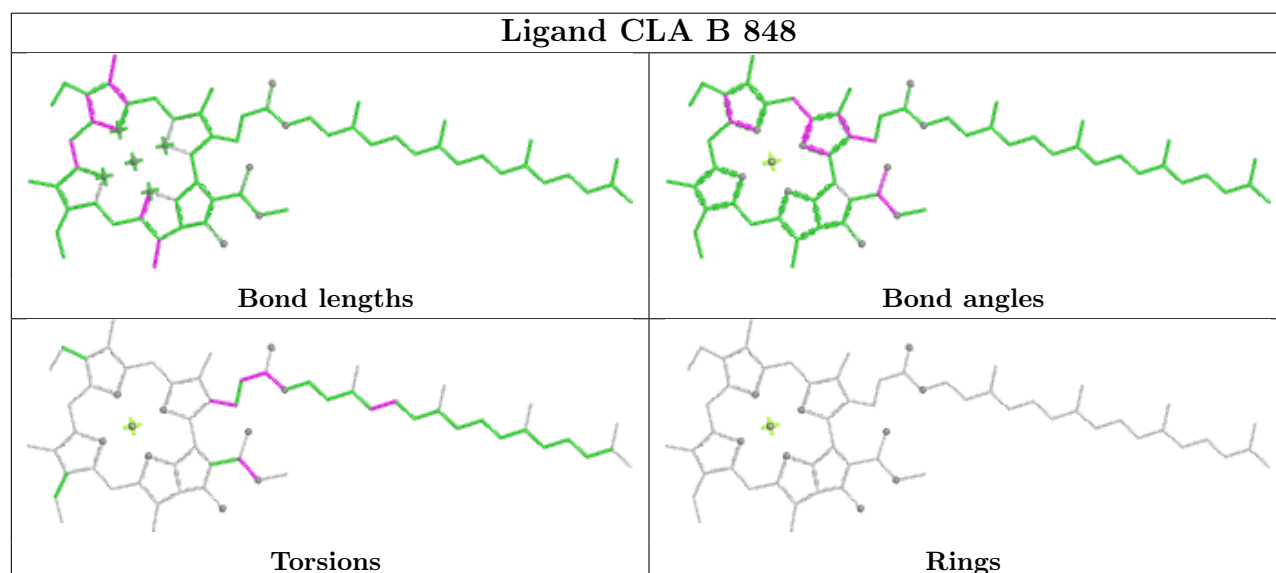
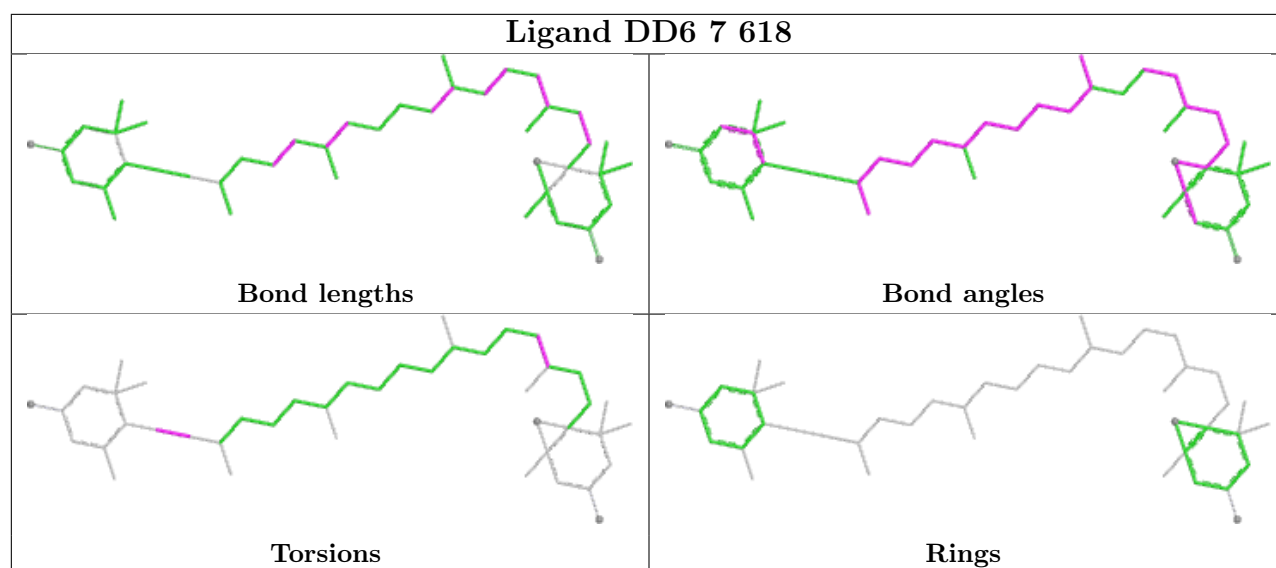


Ligand CLA h 606

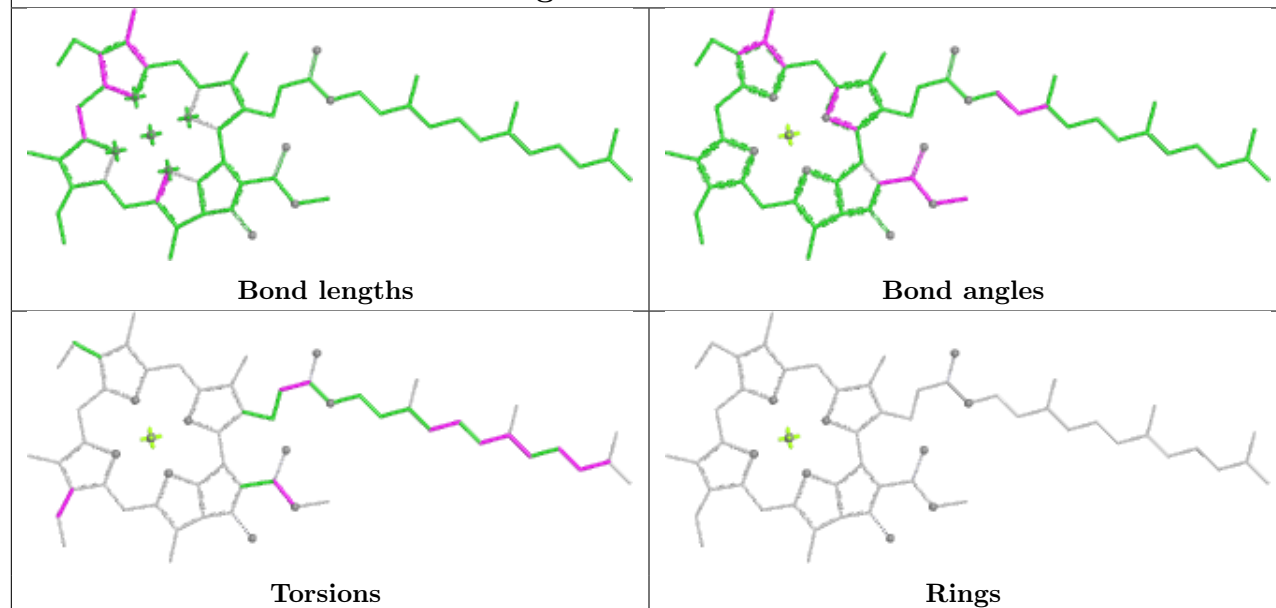


Ligand CLA A 801

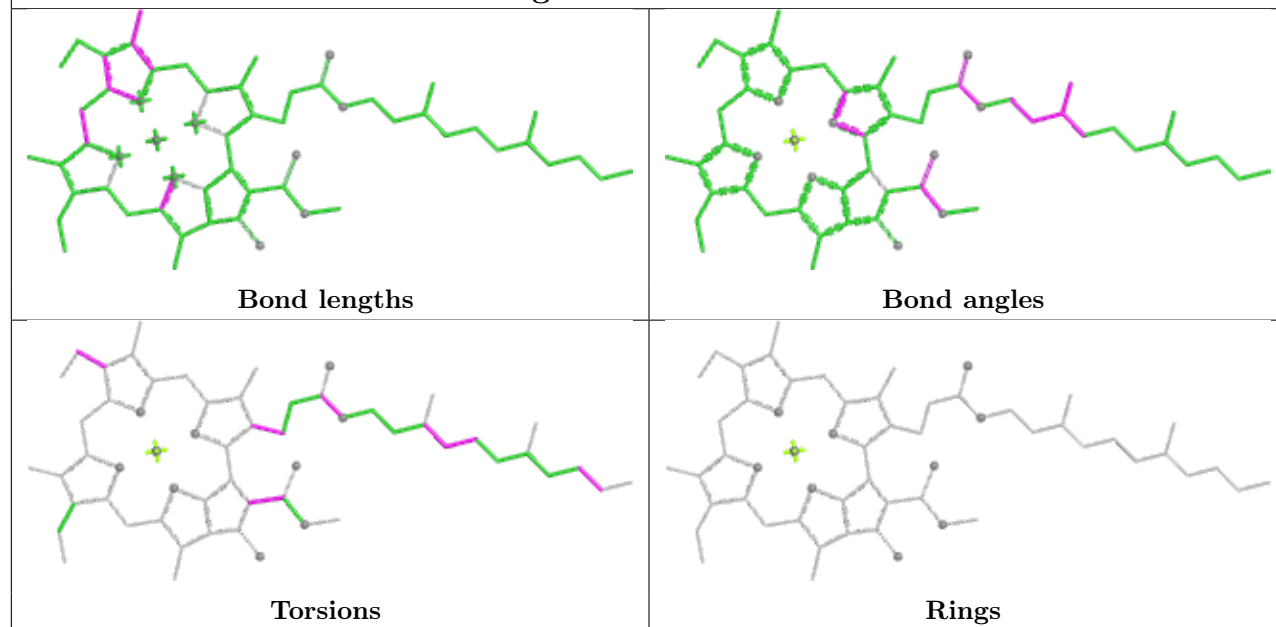




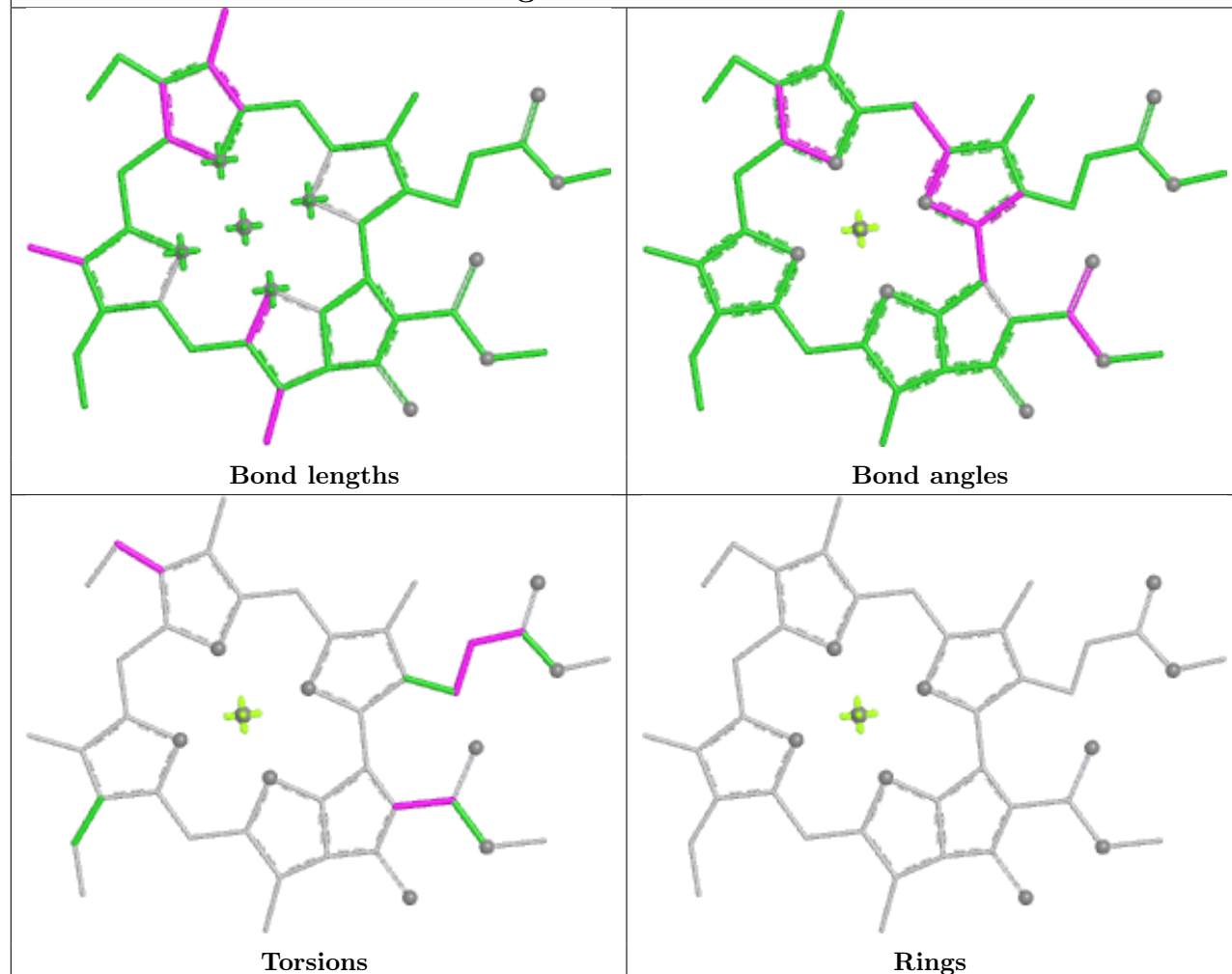
Ligand CLA 7 606



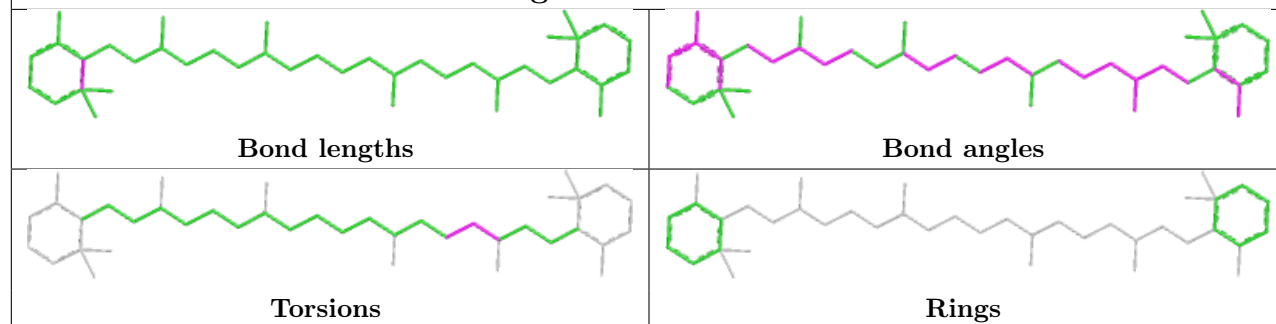
Ligand CLA B 830



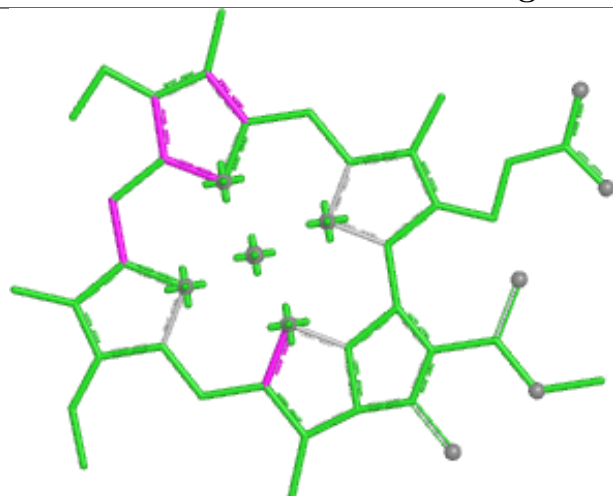
Ligand CLA 9 306



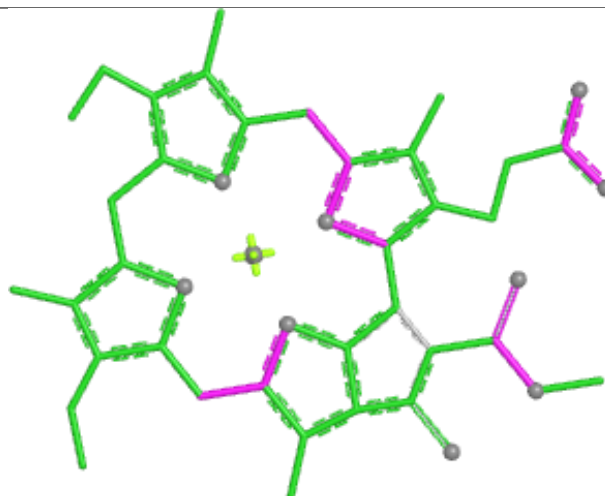
Ligand BCR B 842



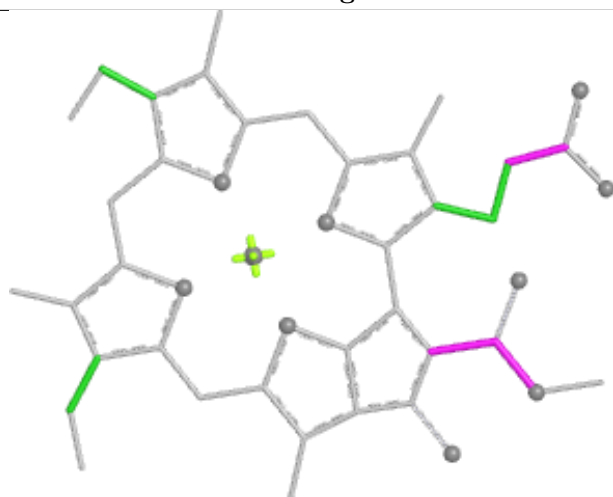
Ligand CLA 6 601



Bond lengths



Bond angles

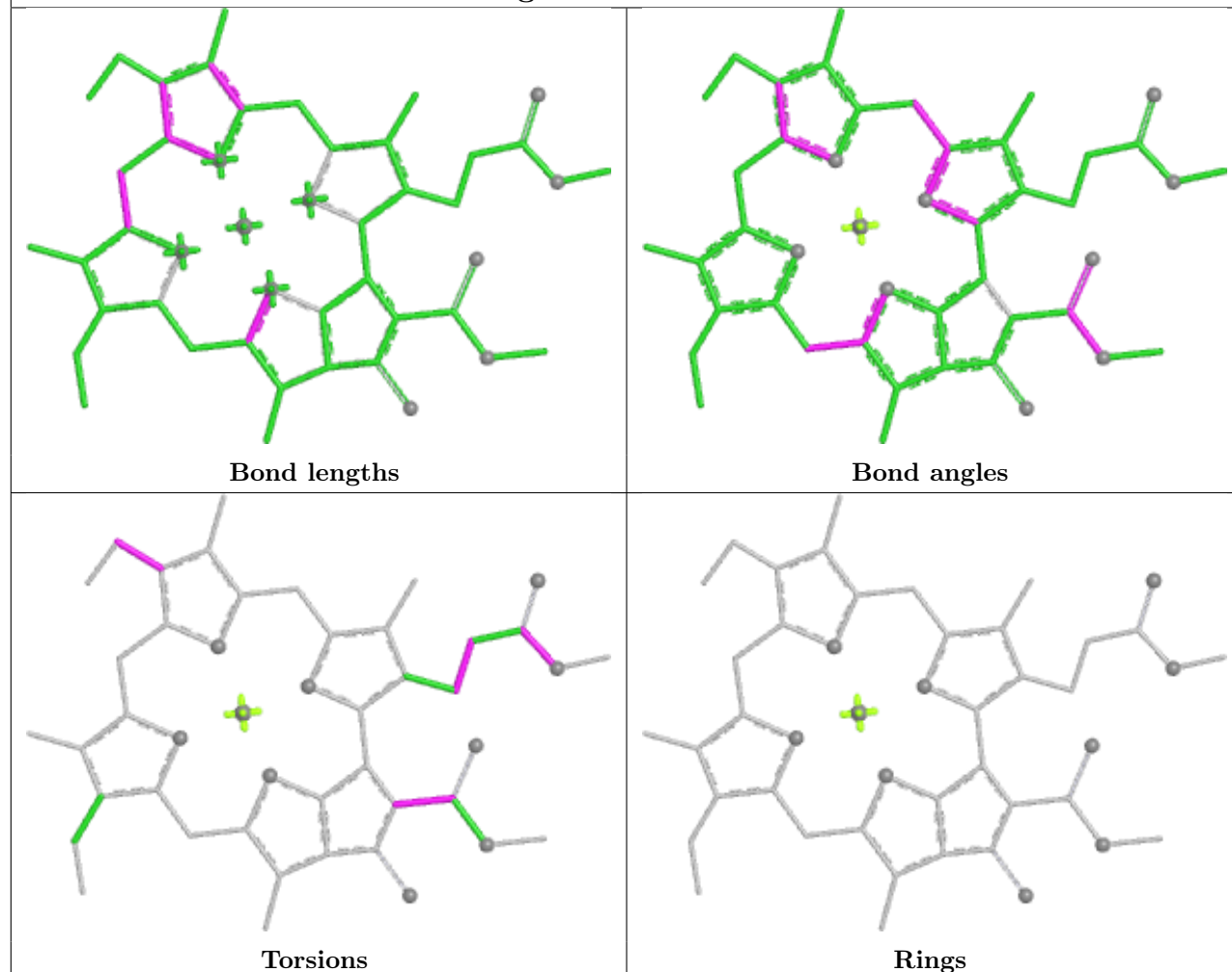


Torsions

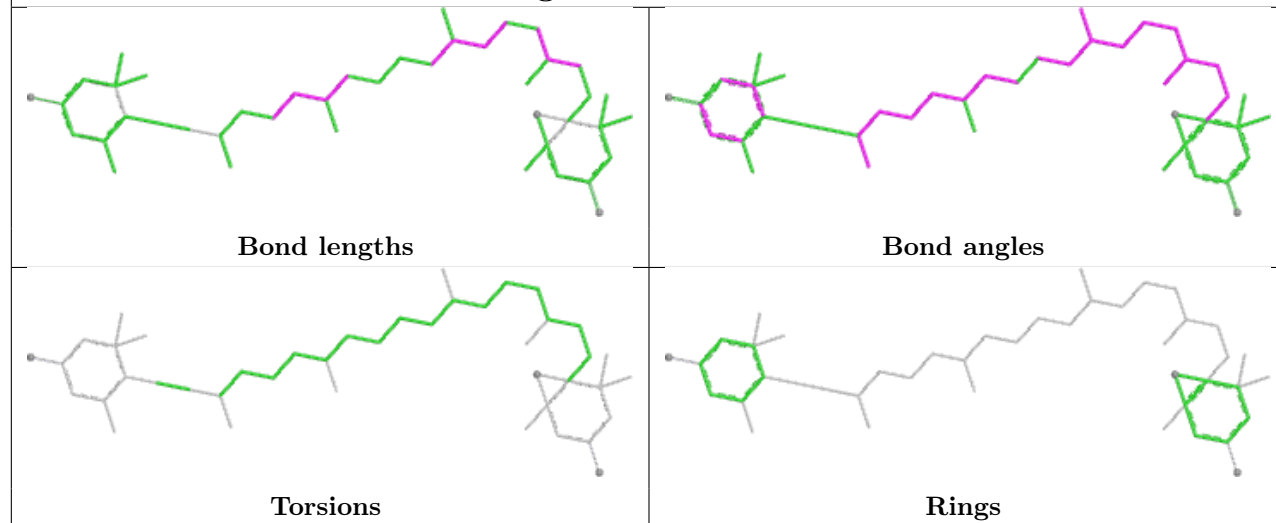


Rings

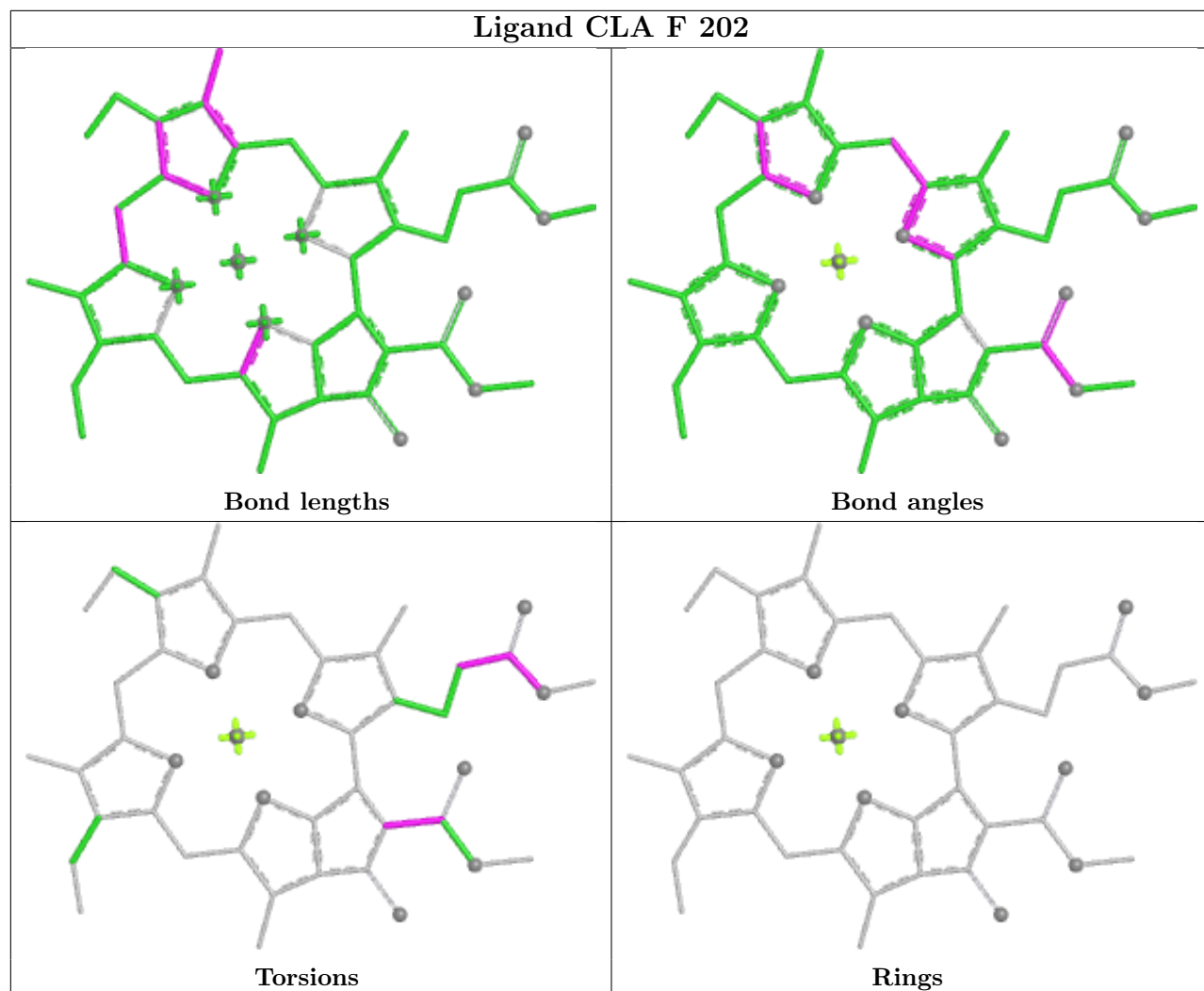
Ligand CLA 4 605



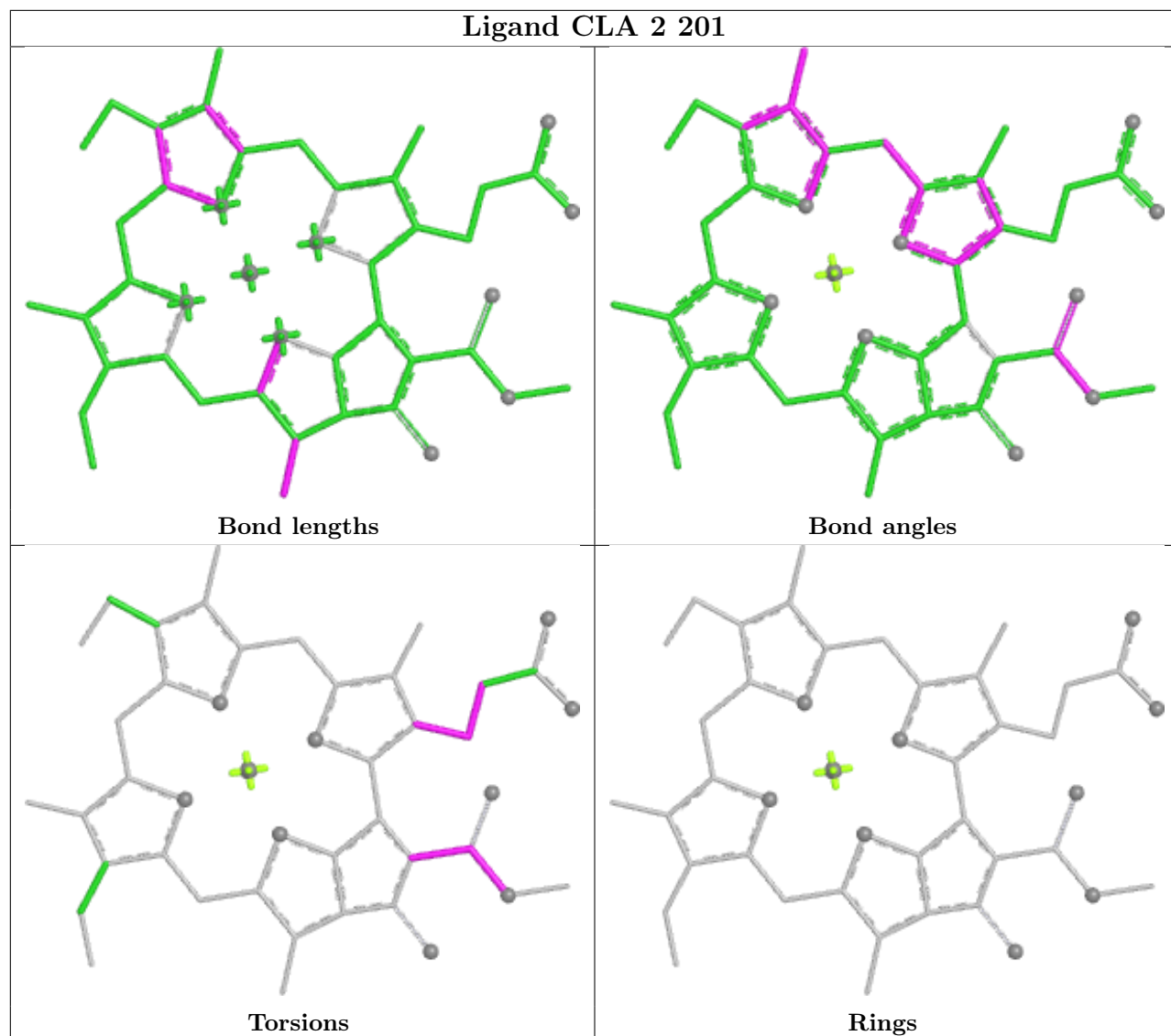
Ligand DD6 7 613



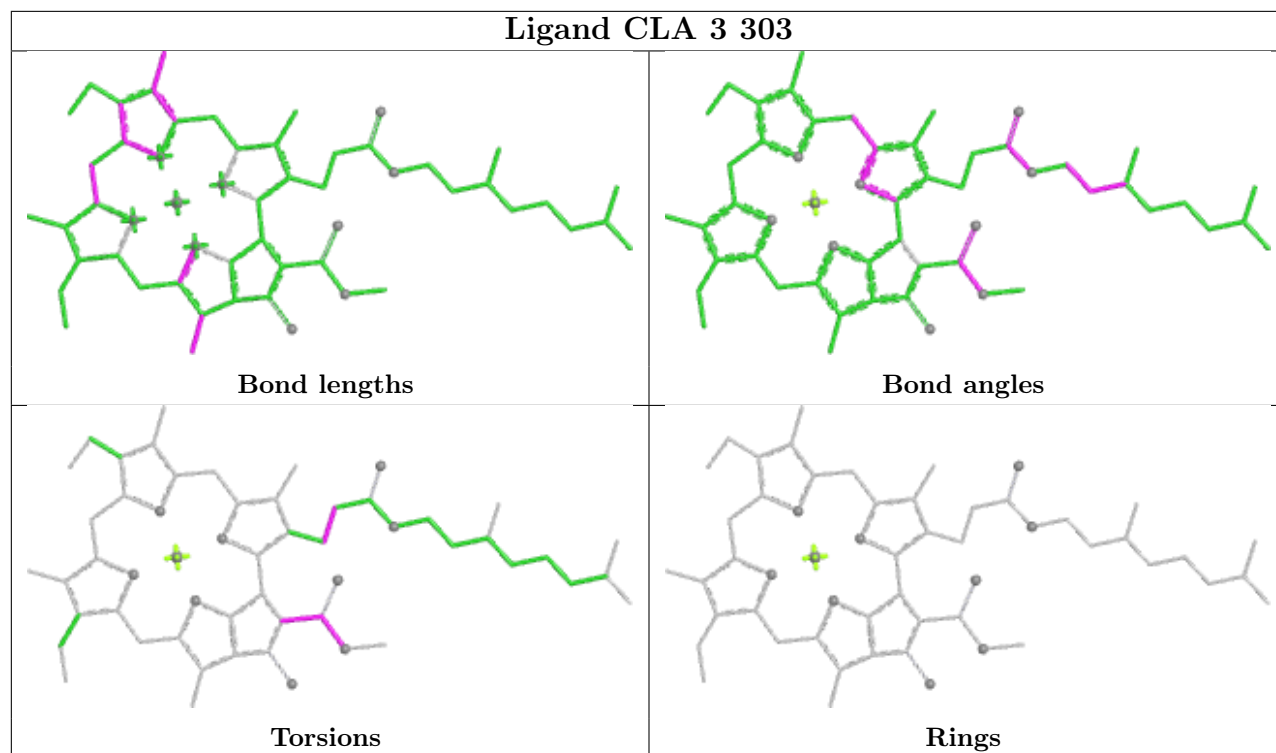
Ligand CLA F 202



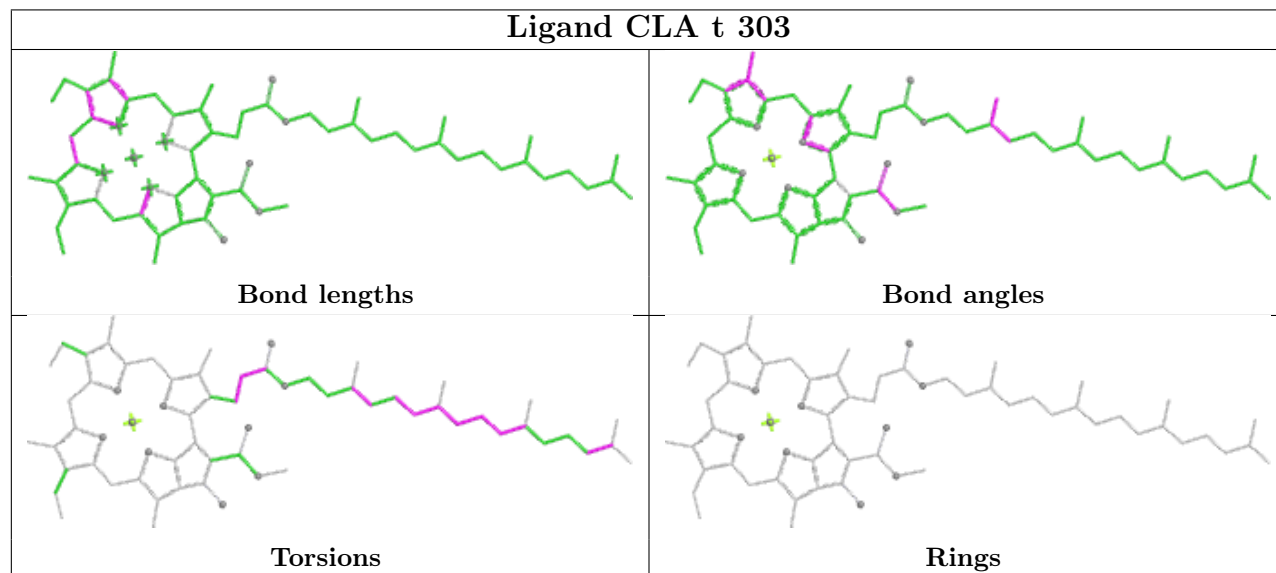
Ligand CLA 2 201



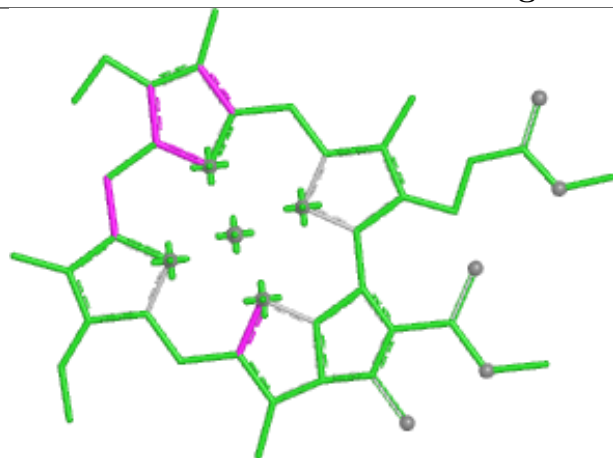
Ligand CLA 3 303



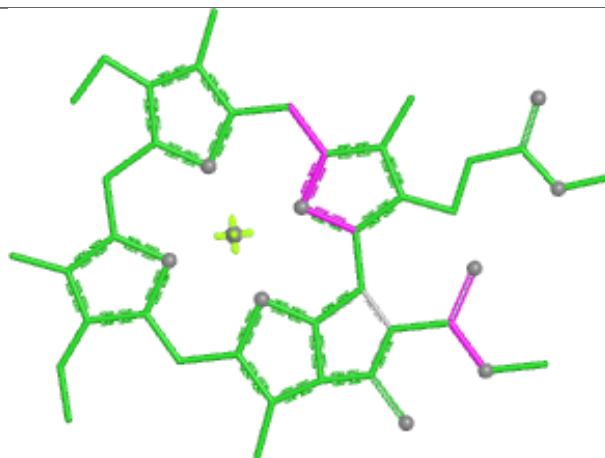
Ligand CLA t 303



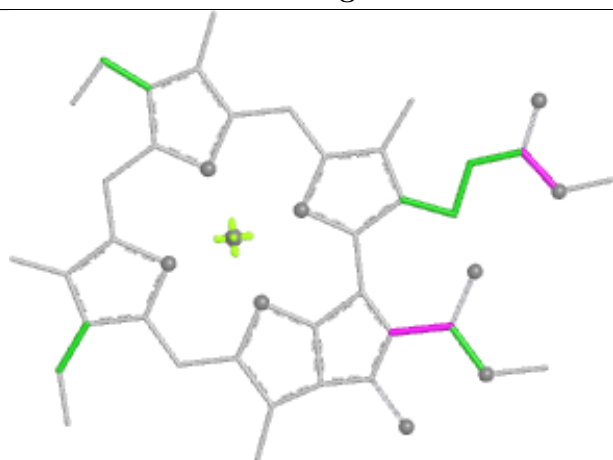
Ligand CLA 7 605



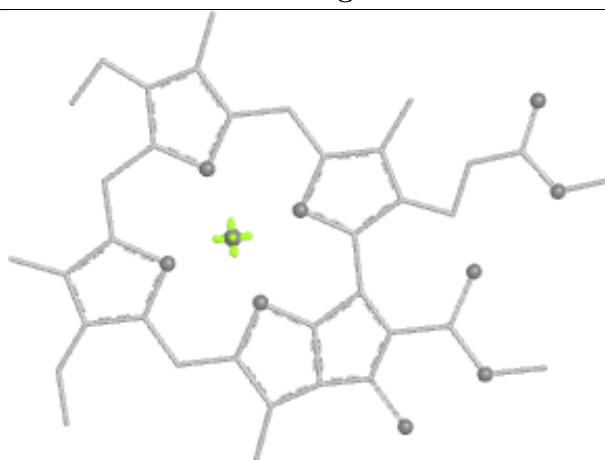
Bond lengths



Bond angles

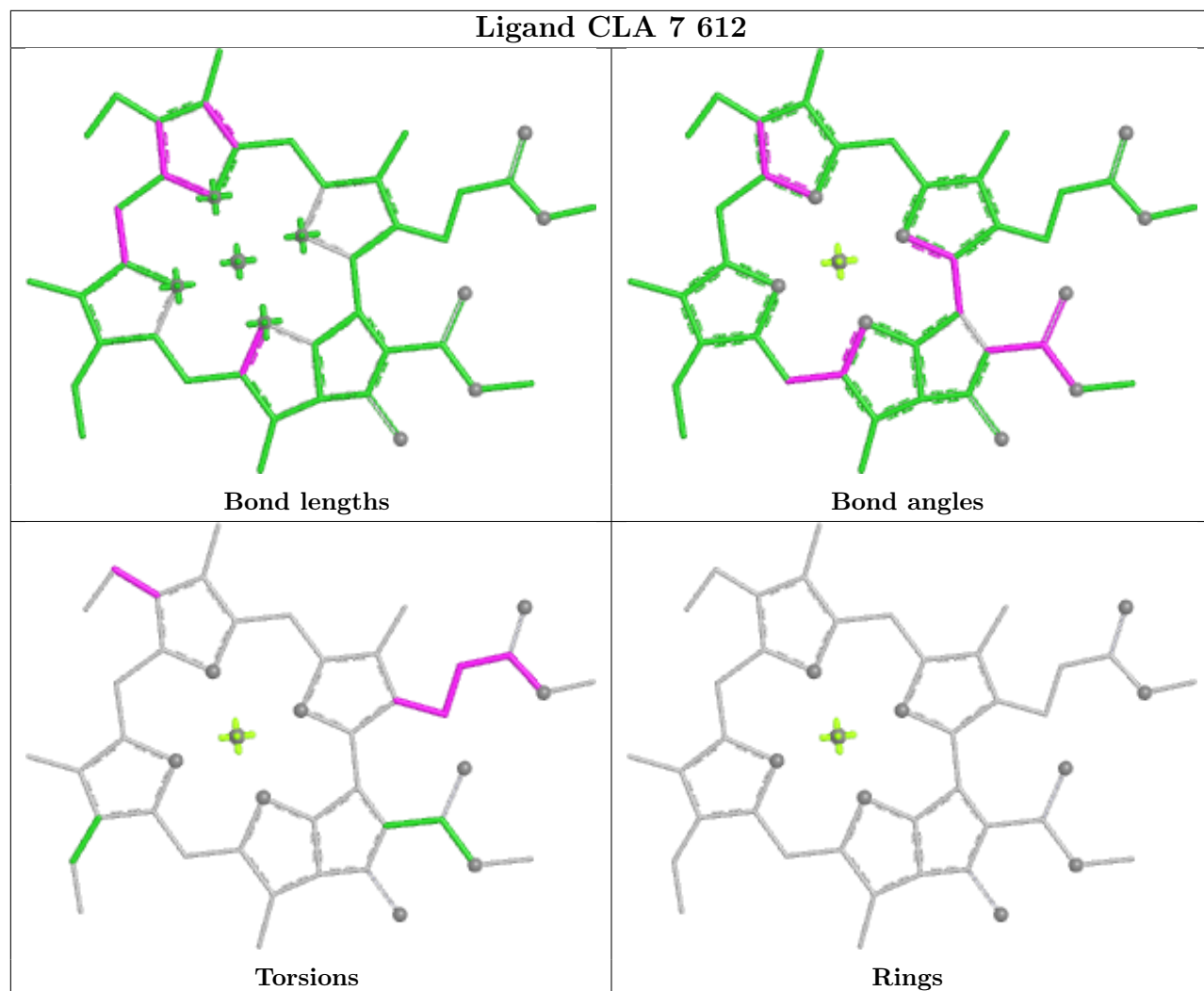


Torsions

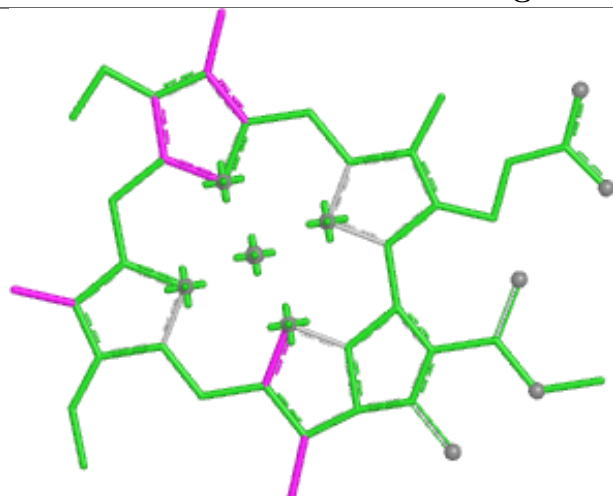


Rings

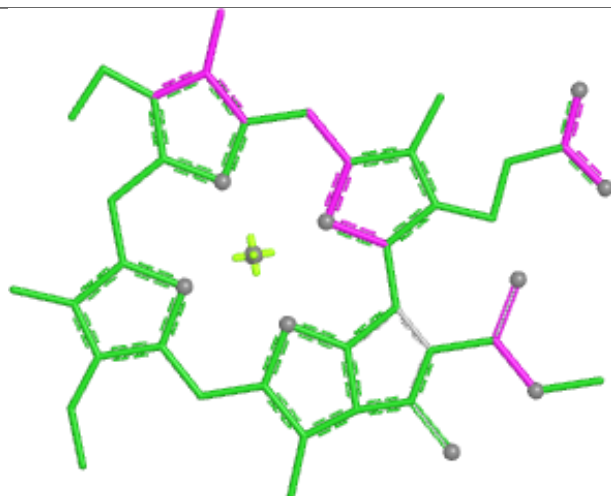
Ligand CLA 7 612



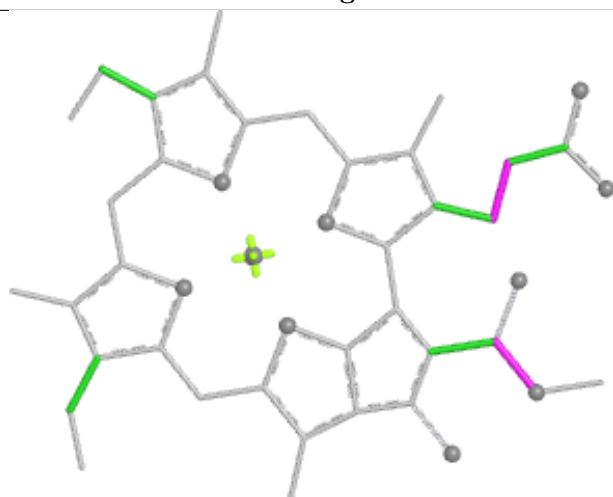
Ligand CLA R 104



Bond lengths



Bond angles

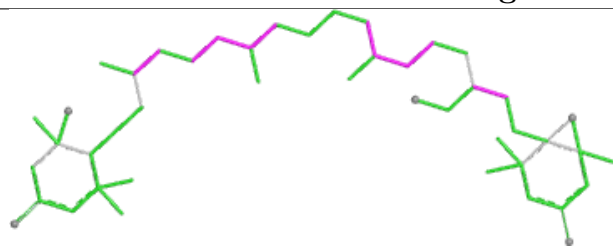


Torsions

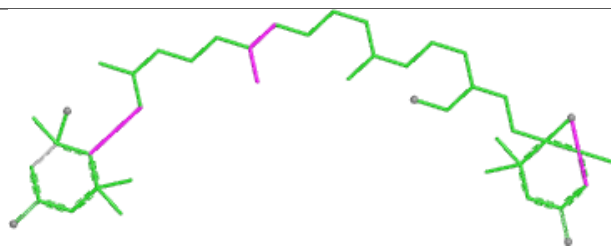


Rings

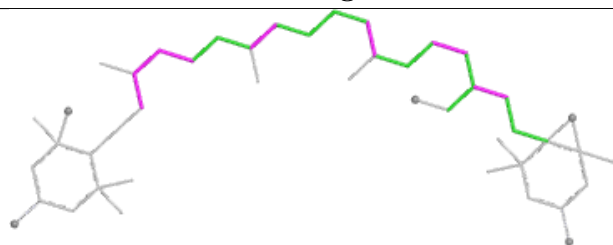
Ligand A1L1G 7 614



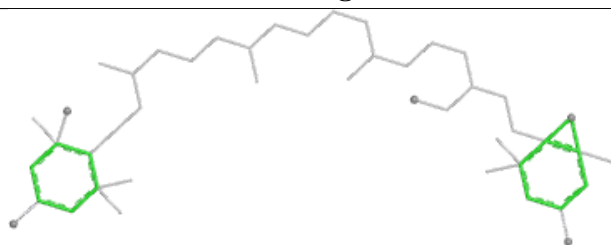
Bond lengths



Bond angles

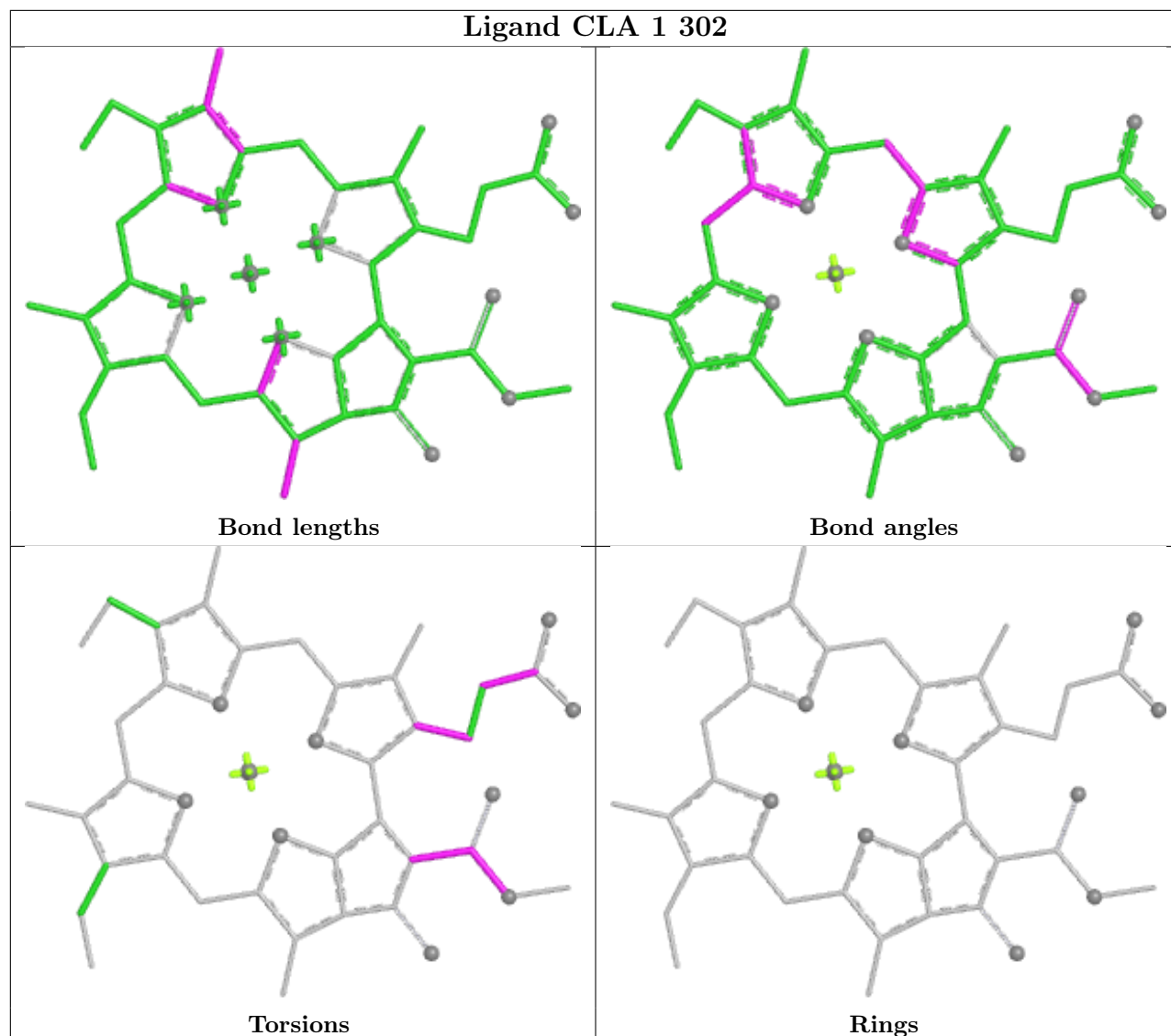


Torsions

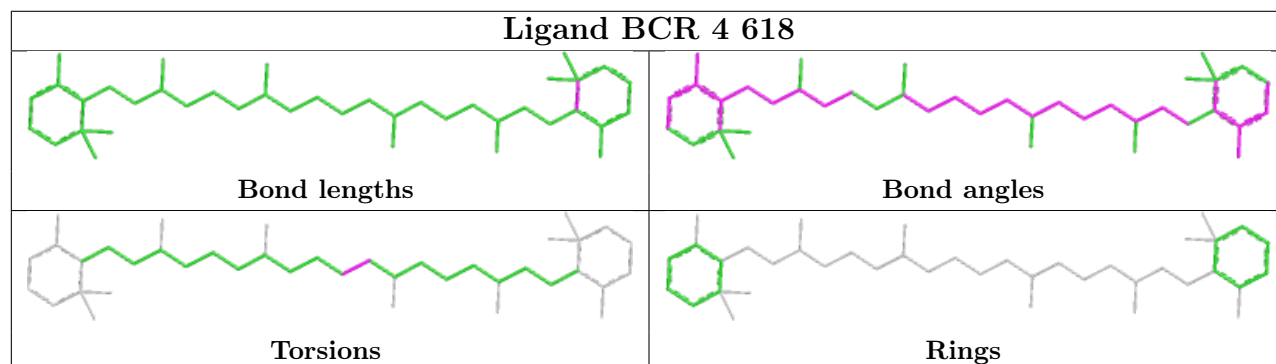


Rings

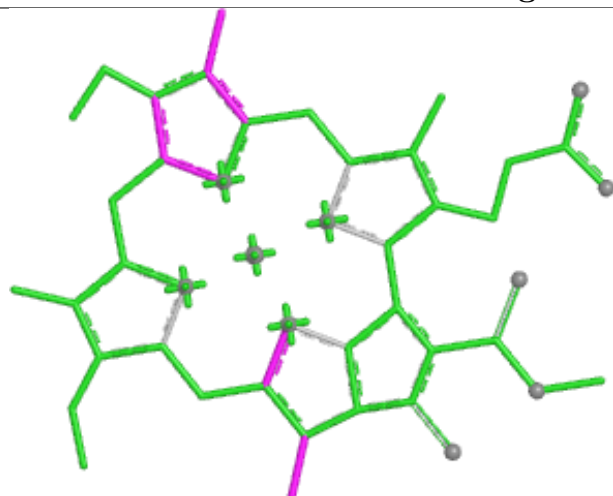
Ligand CLA 1 302



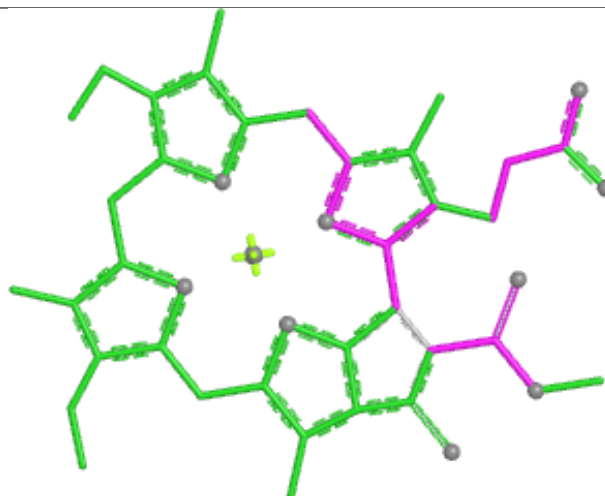
Ligand BCR 4 618



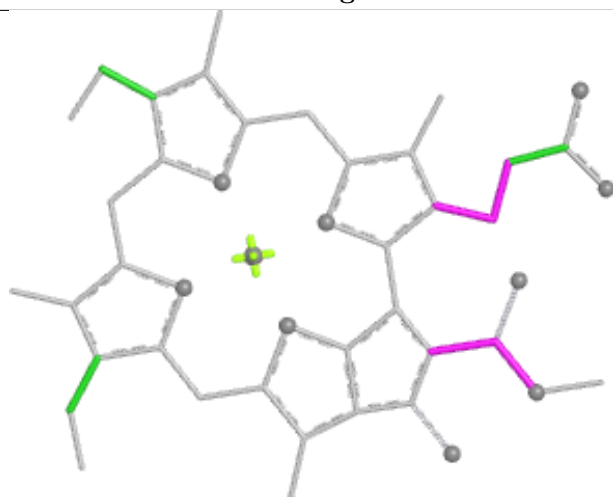
Ligand CLA 1 305



Bond lengths



Bond angles

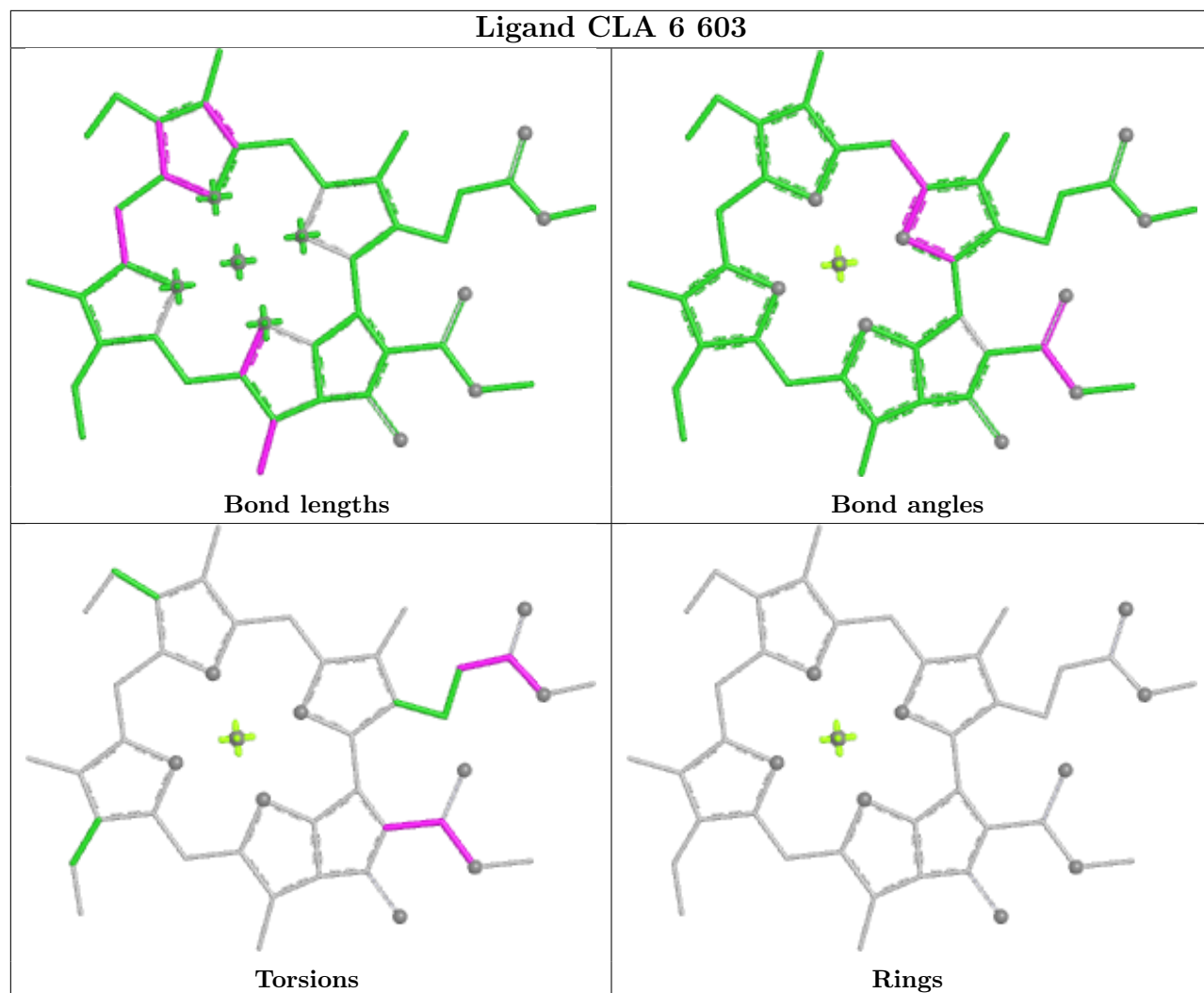


Torsions

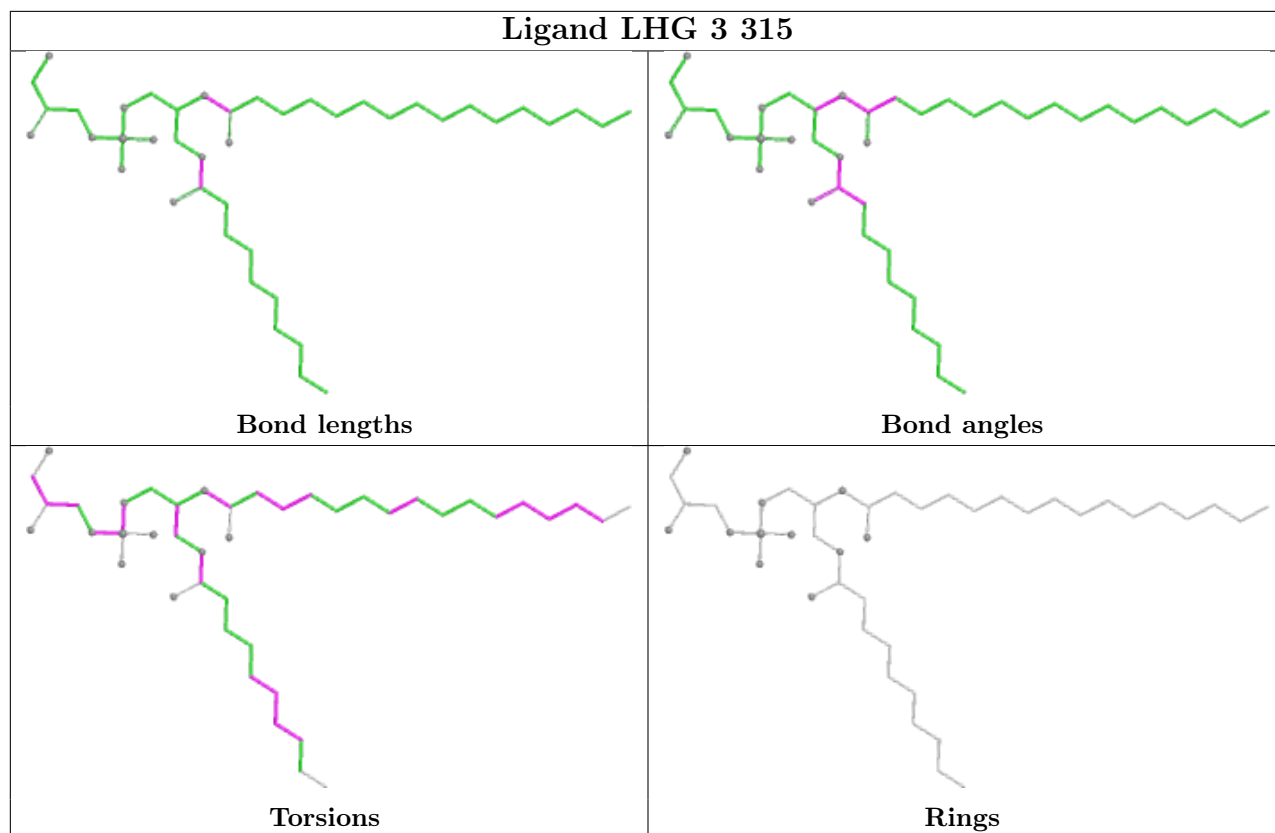


Rings

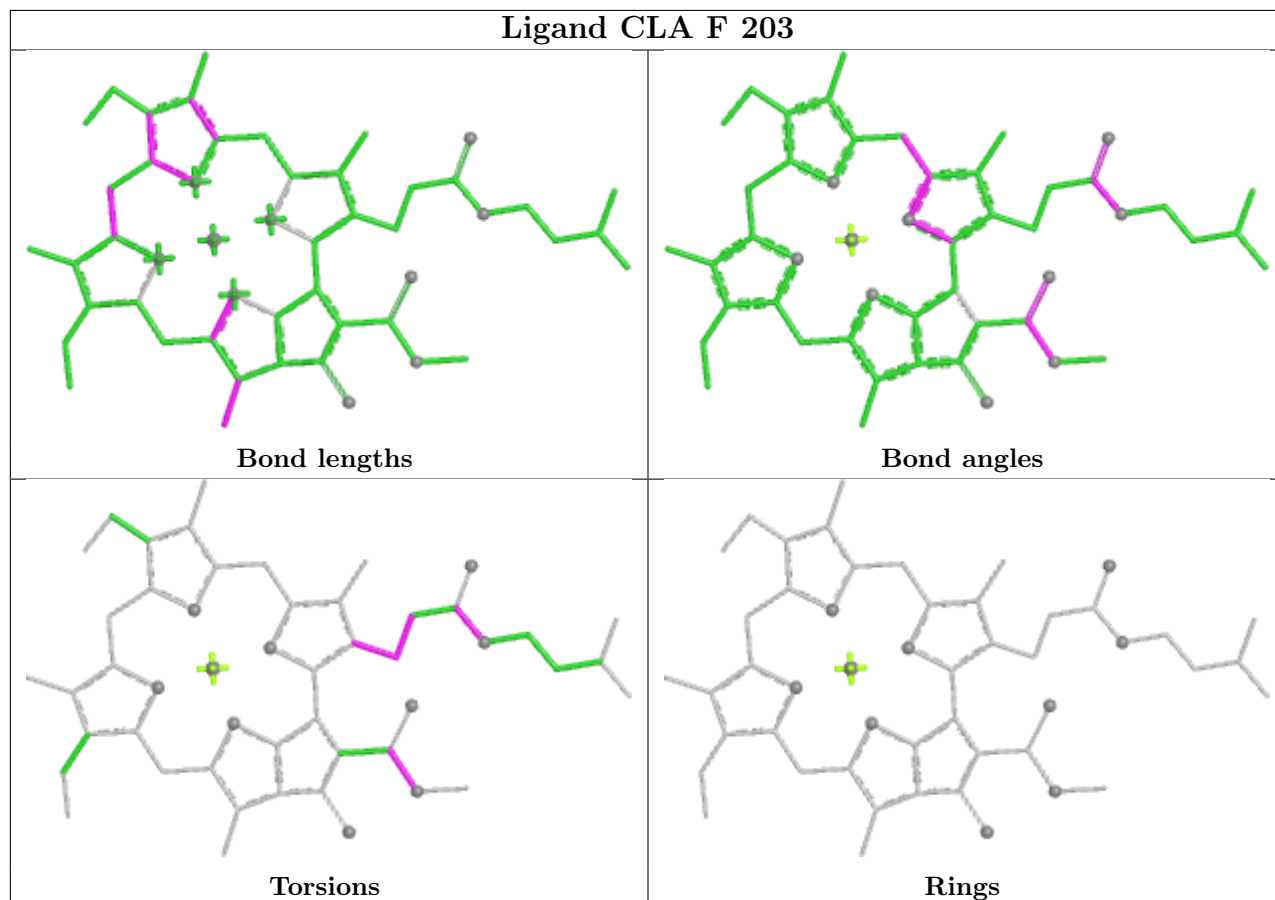
Ligand CLA 6 603



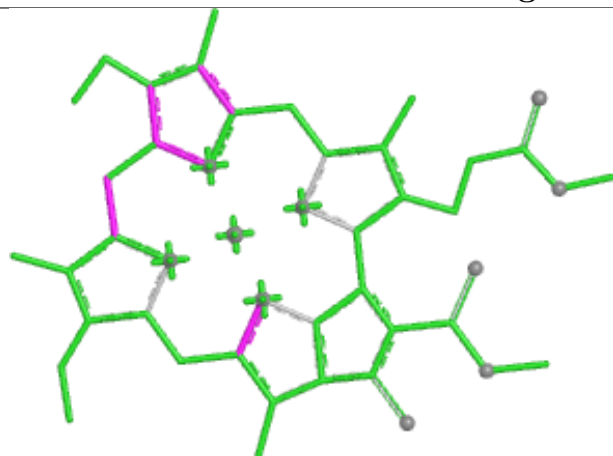
Ligand LHG 3 315



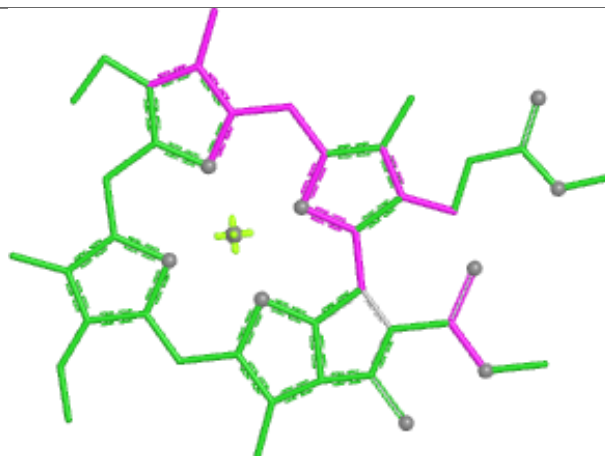
Ligand CLA F 203



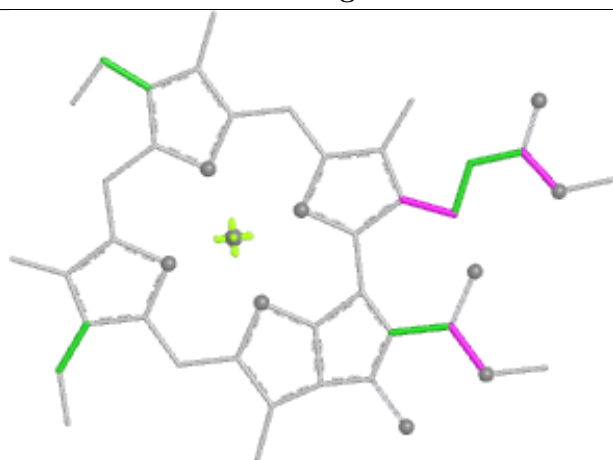
Ligand CLA 3 304



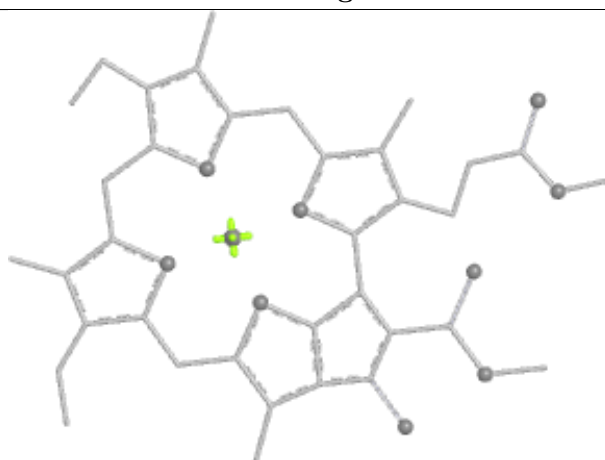
Bond lengths



Bond angles

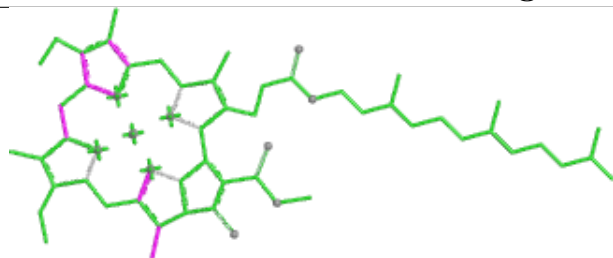


Torsions

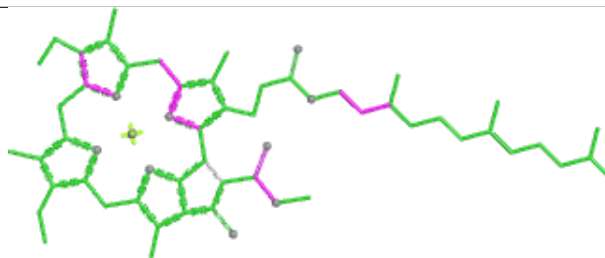


Rings

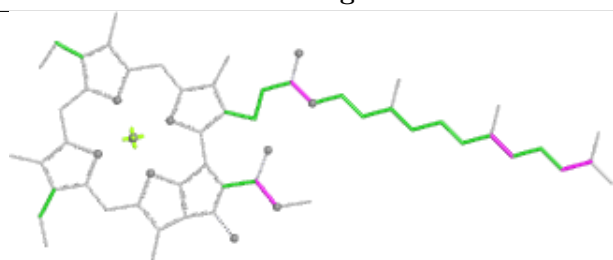
Ligand CLA 3 305



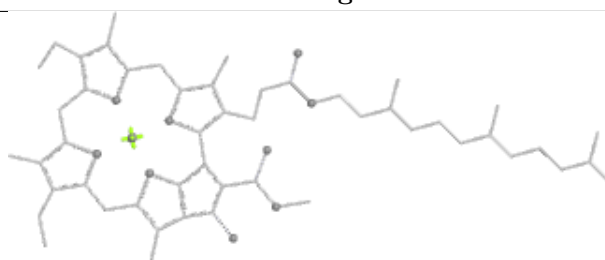
Bond lengths



Bond angles

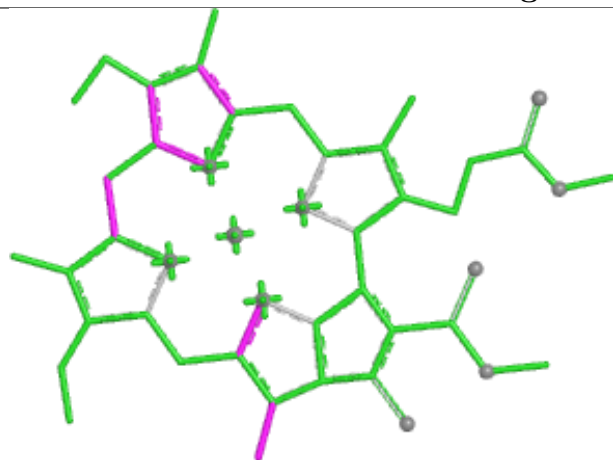


Torsions

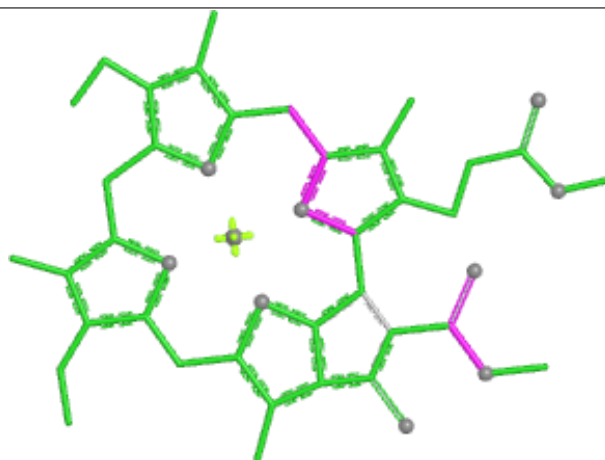


Rings

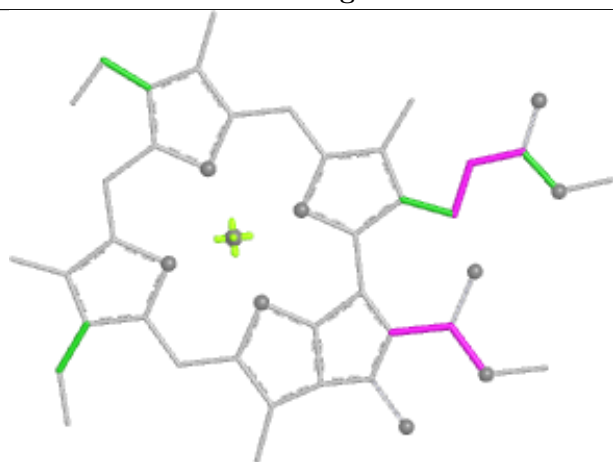
Ligand CLA t 304



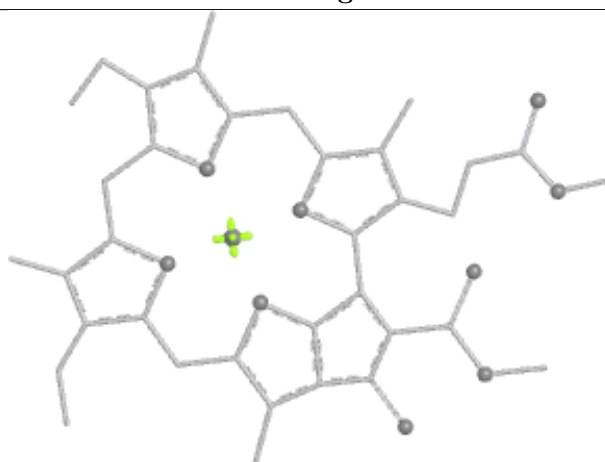
Bond lengths



Bond angles

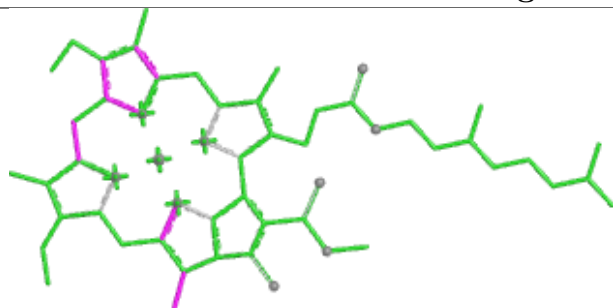


Torsions

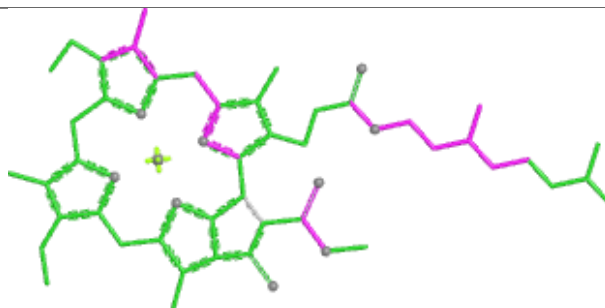


Rings

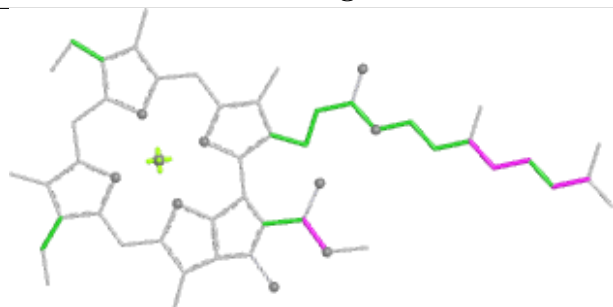
Ligand CLA h 602



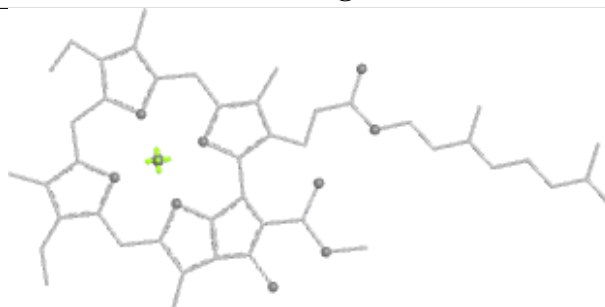
Bond lengths



Bond angles

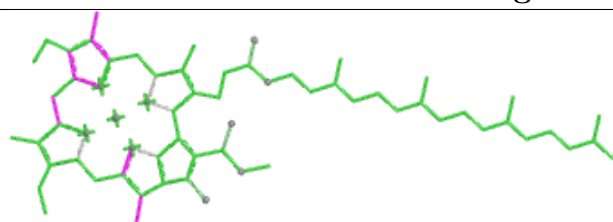


Torsions

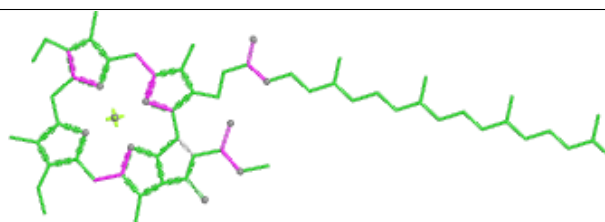


Rings

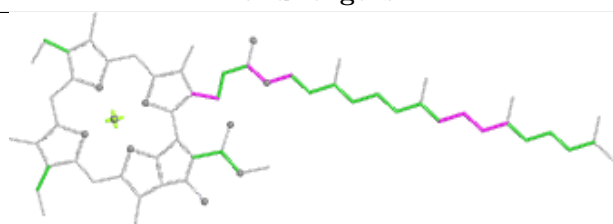
Ligand CLA R 103



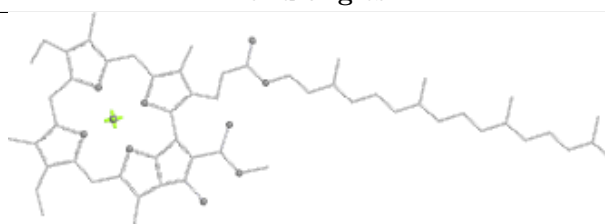
Bond lengths



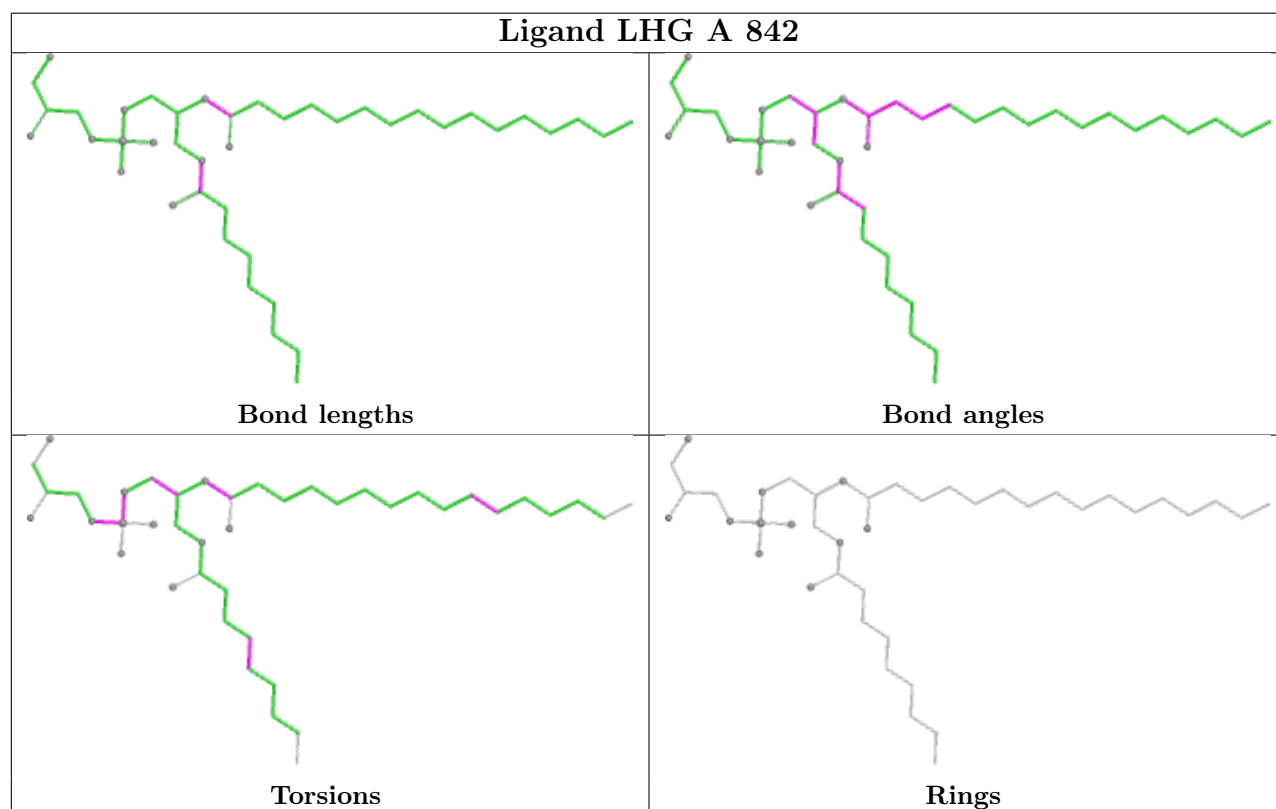
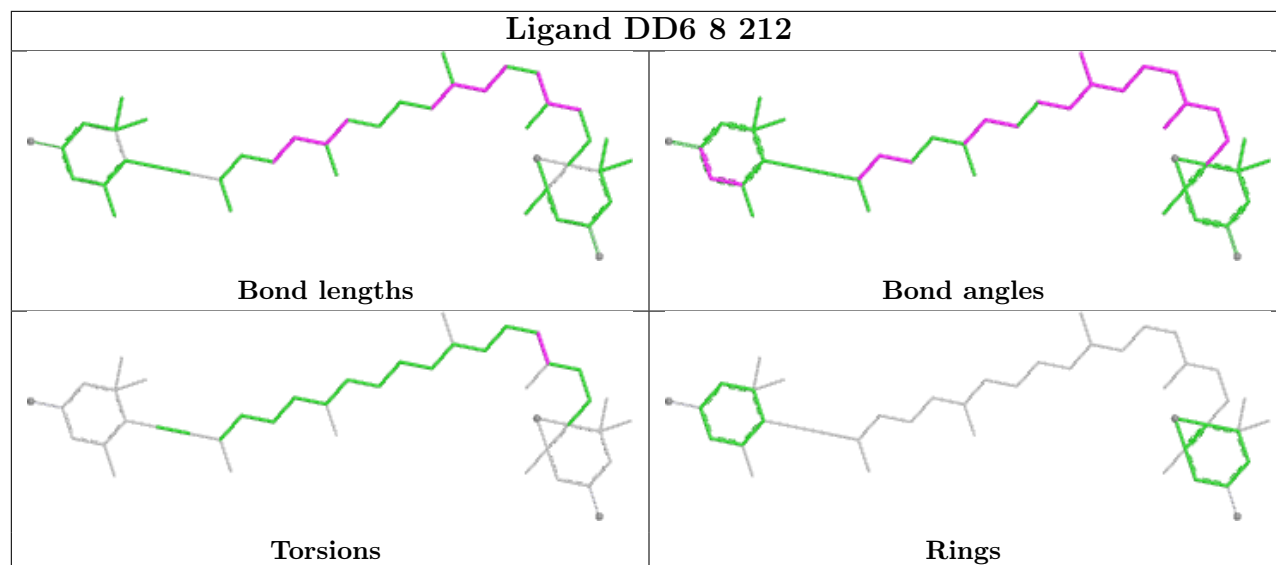
Bond angles



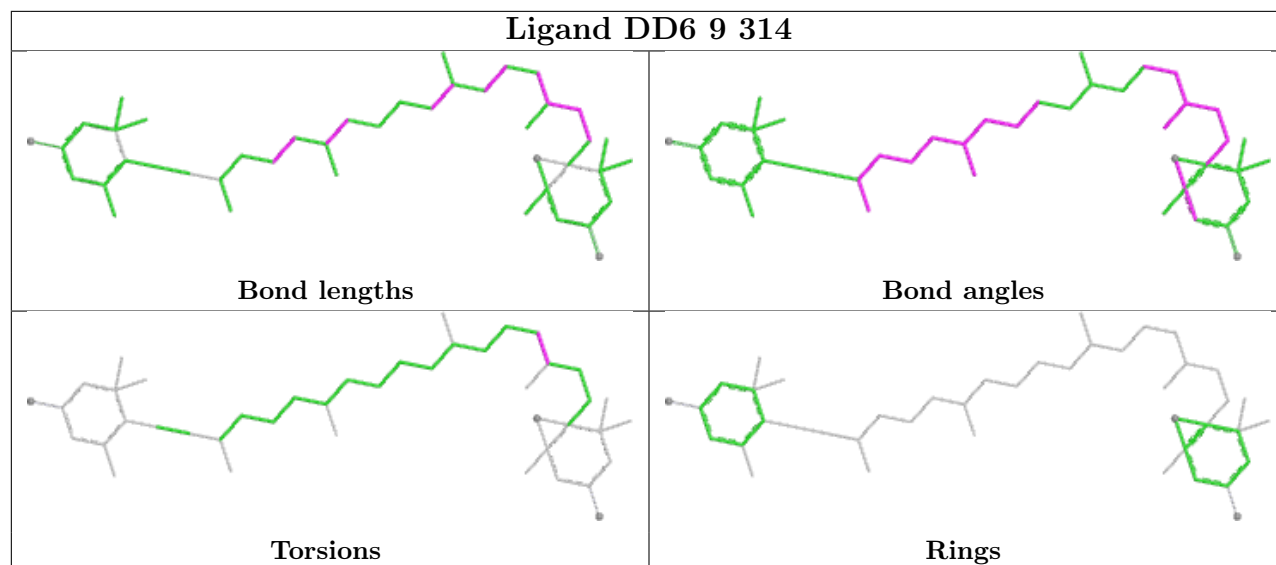
Torsions



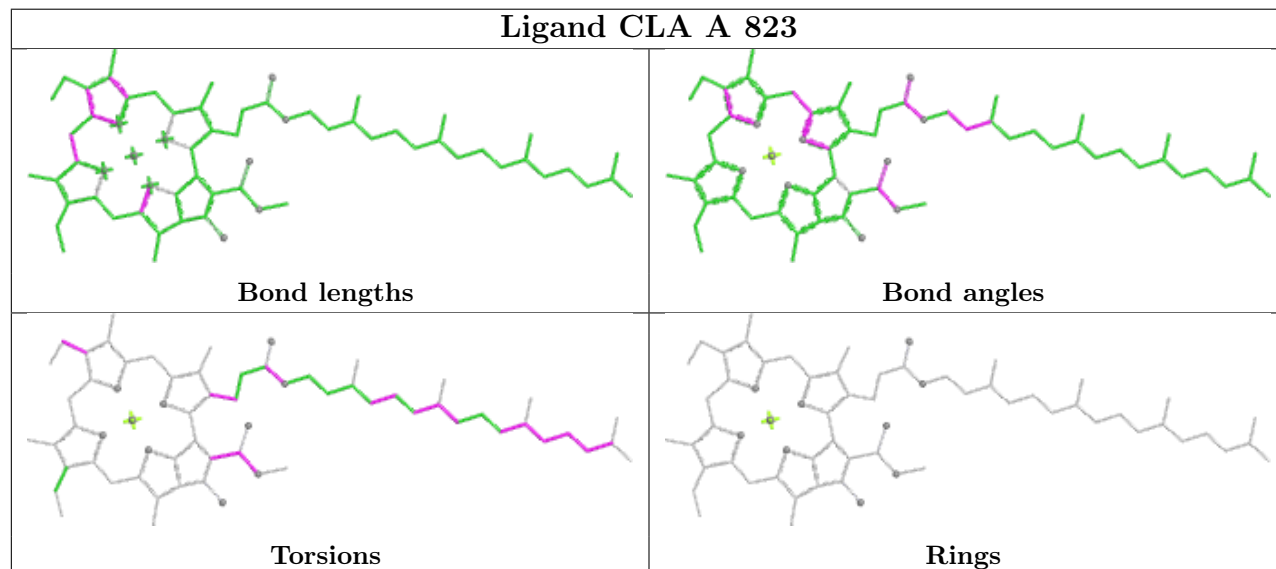
Rings



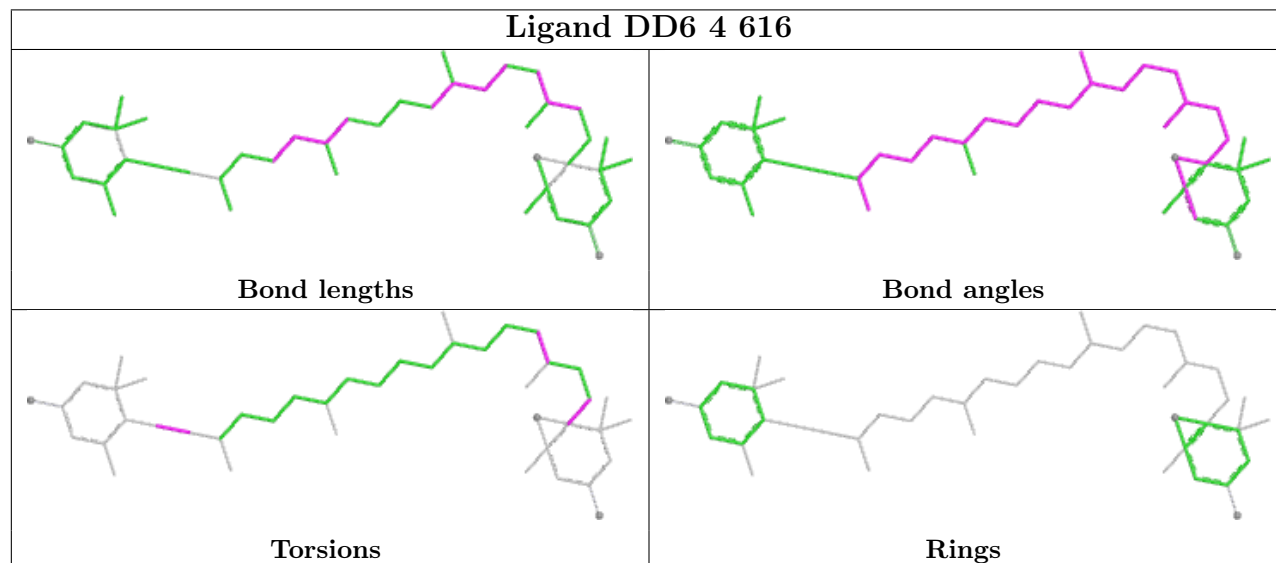
Ligand DD6 9 314



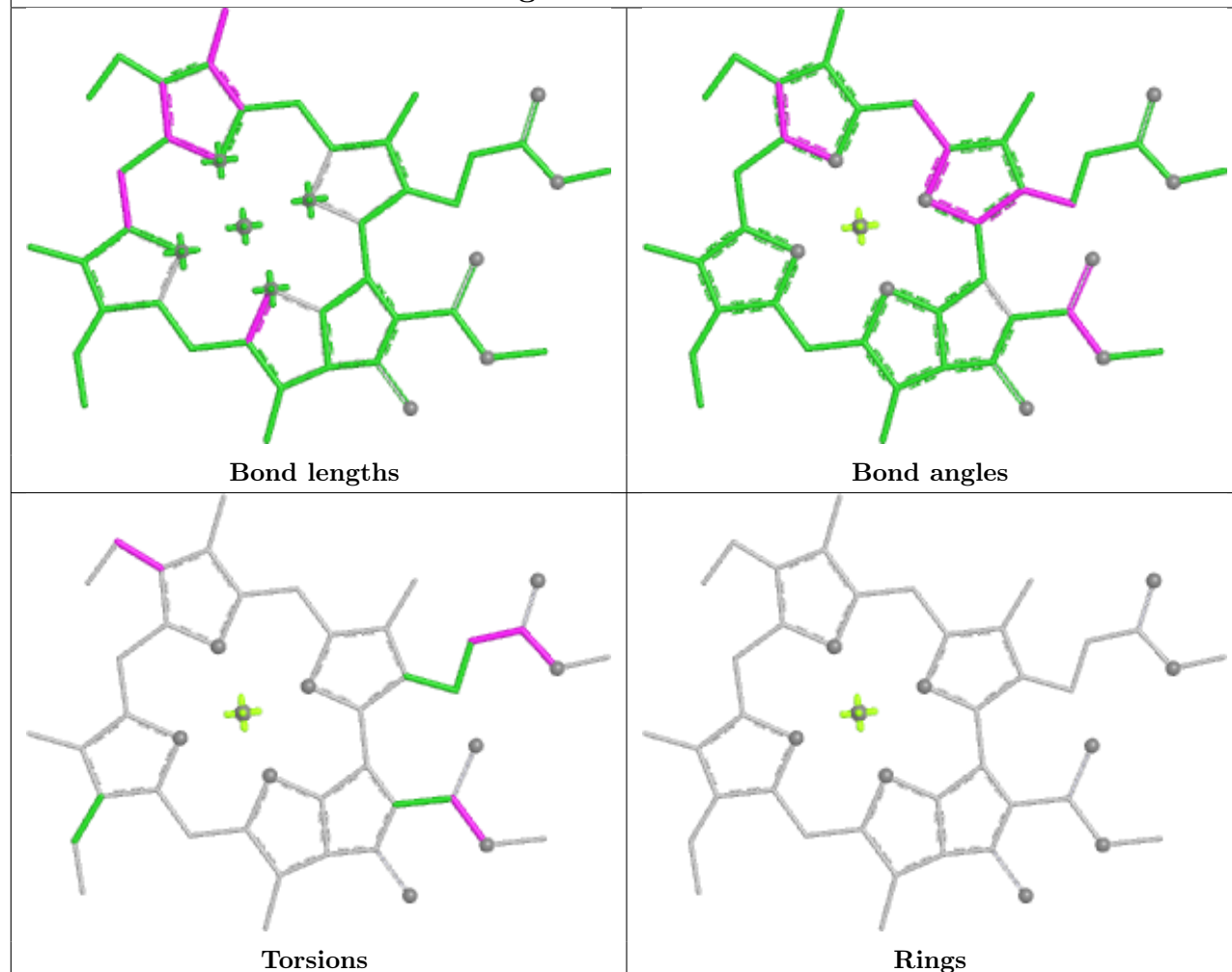
Ligand CLA A 823



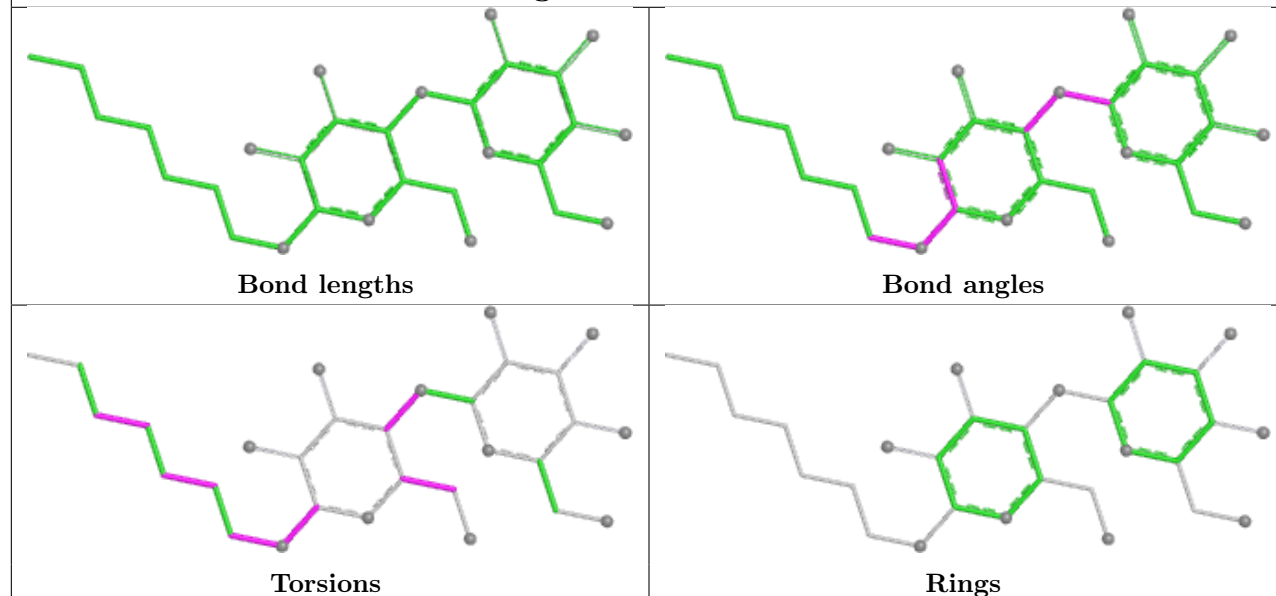
Ligand DD6 4 616



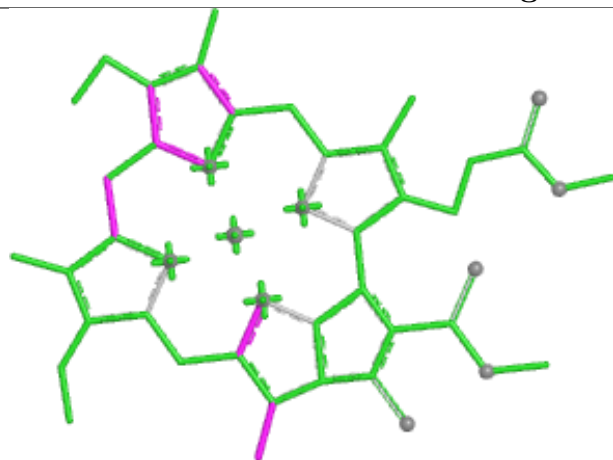
Ligand CLA c 603



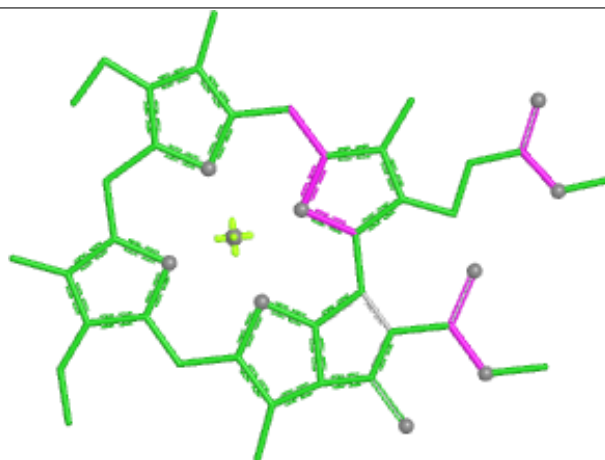
Ligand LMT 3 314



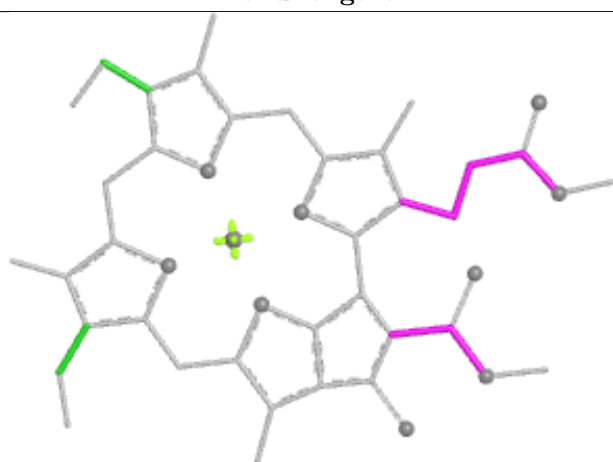
Ligand CLA t 302



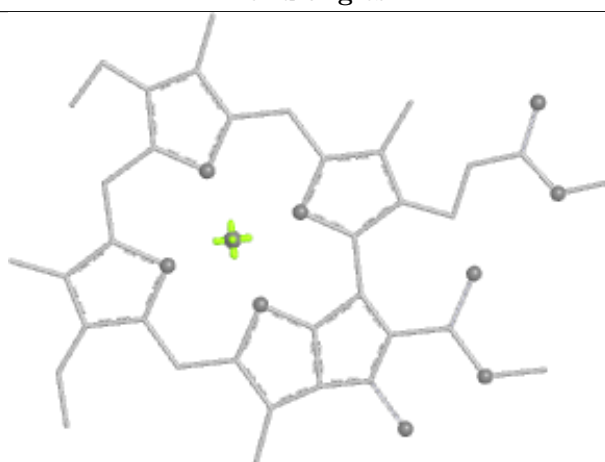
Bond lengths



Bond angles

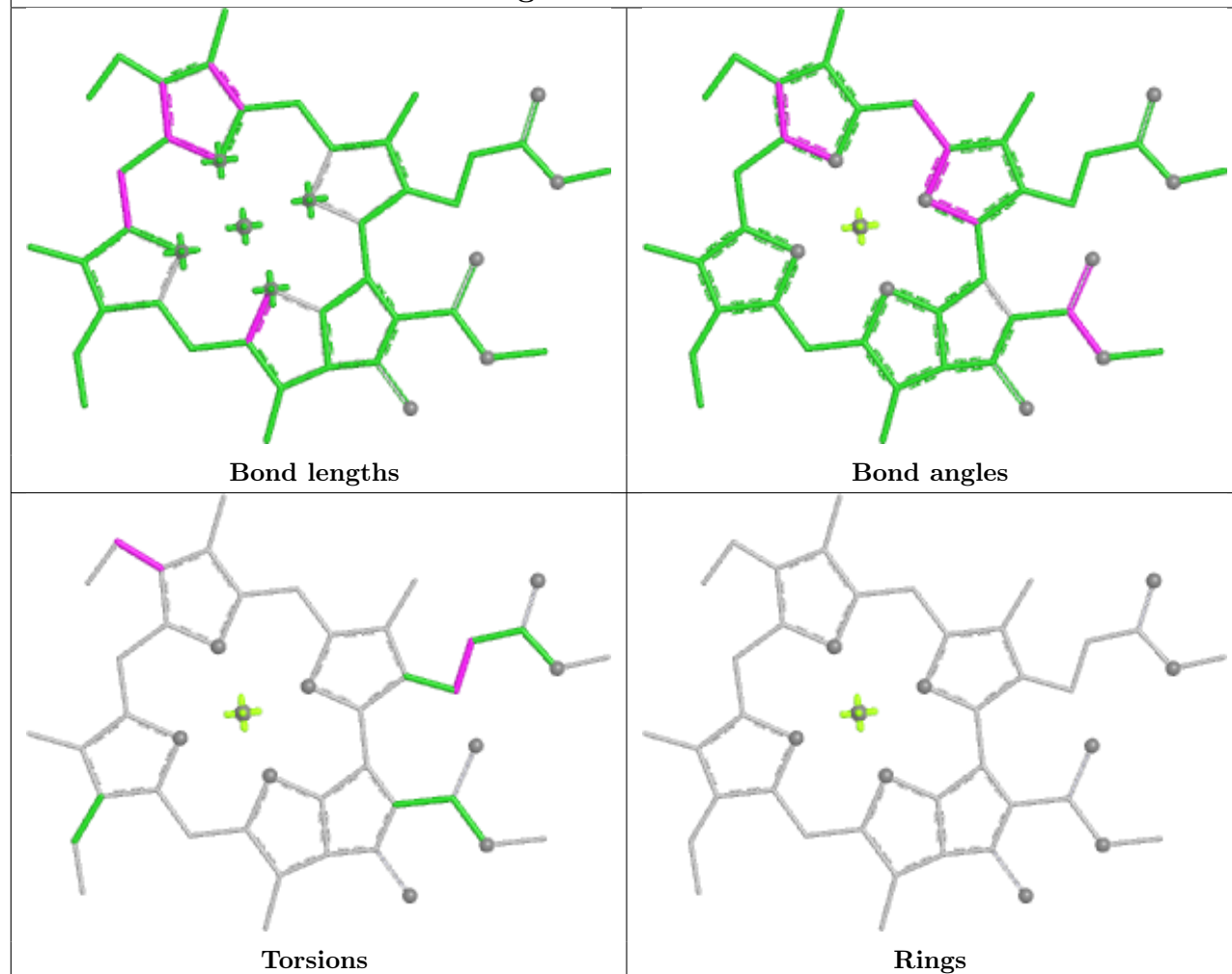


Torsions

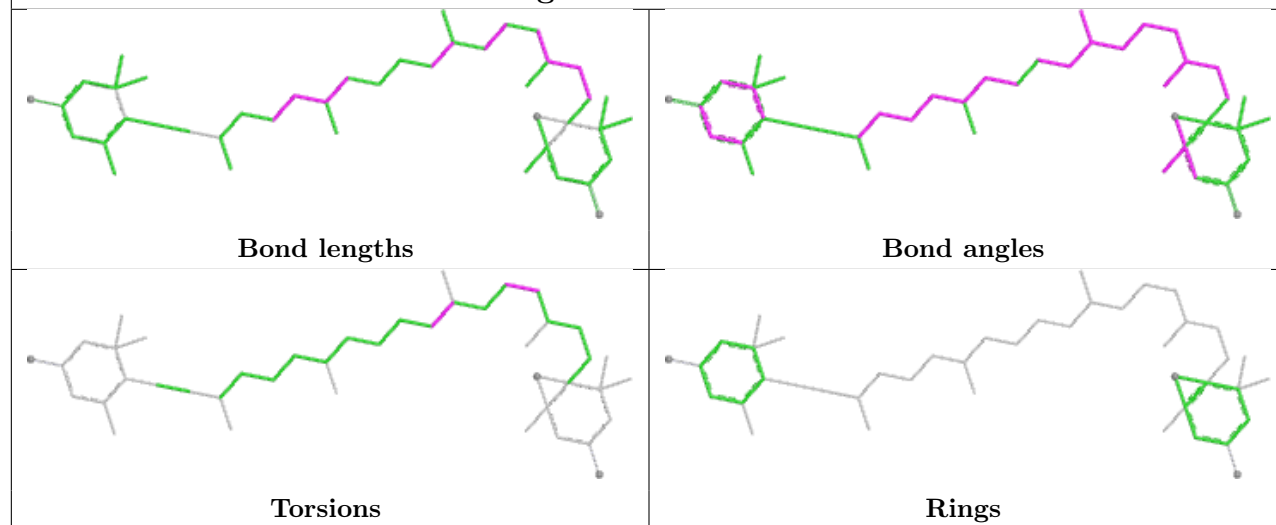


Rings

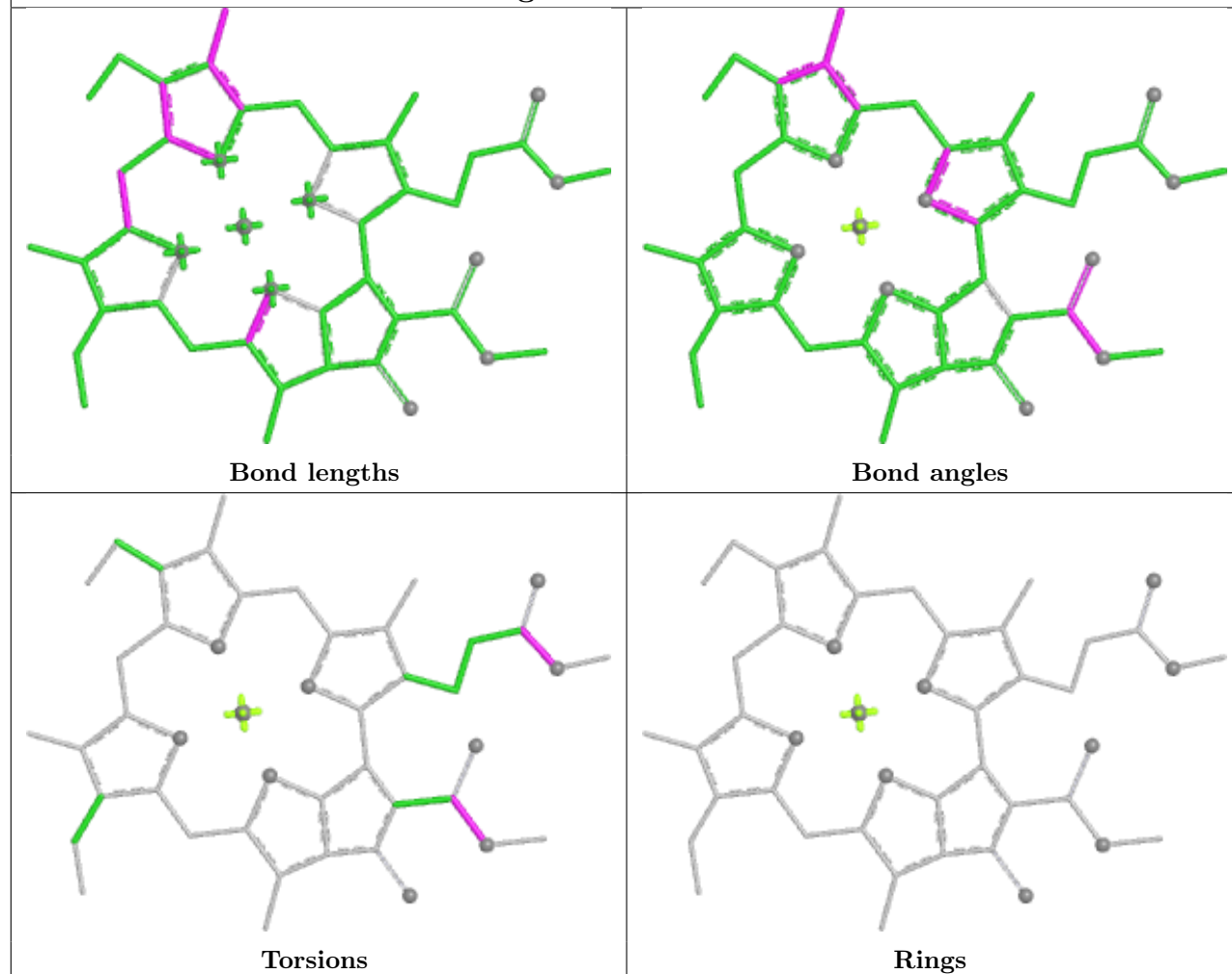
Ligand CLA 6 612



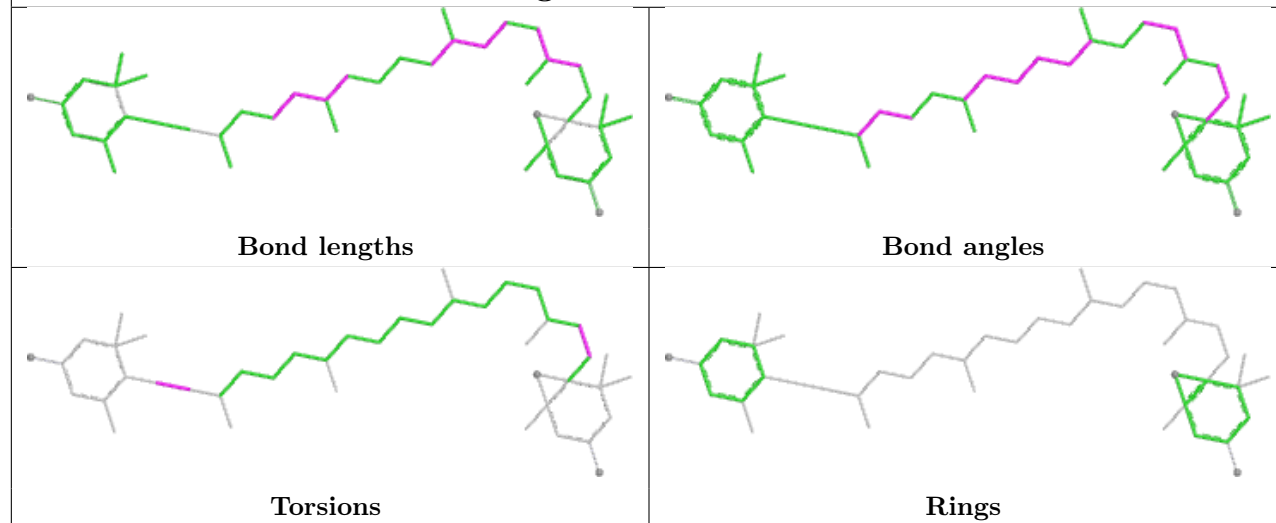
Ligand DD6 8 210



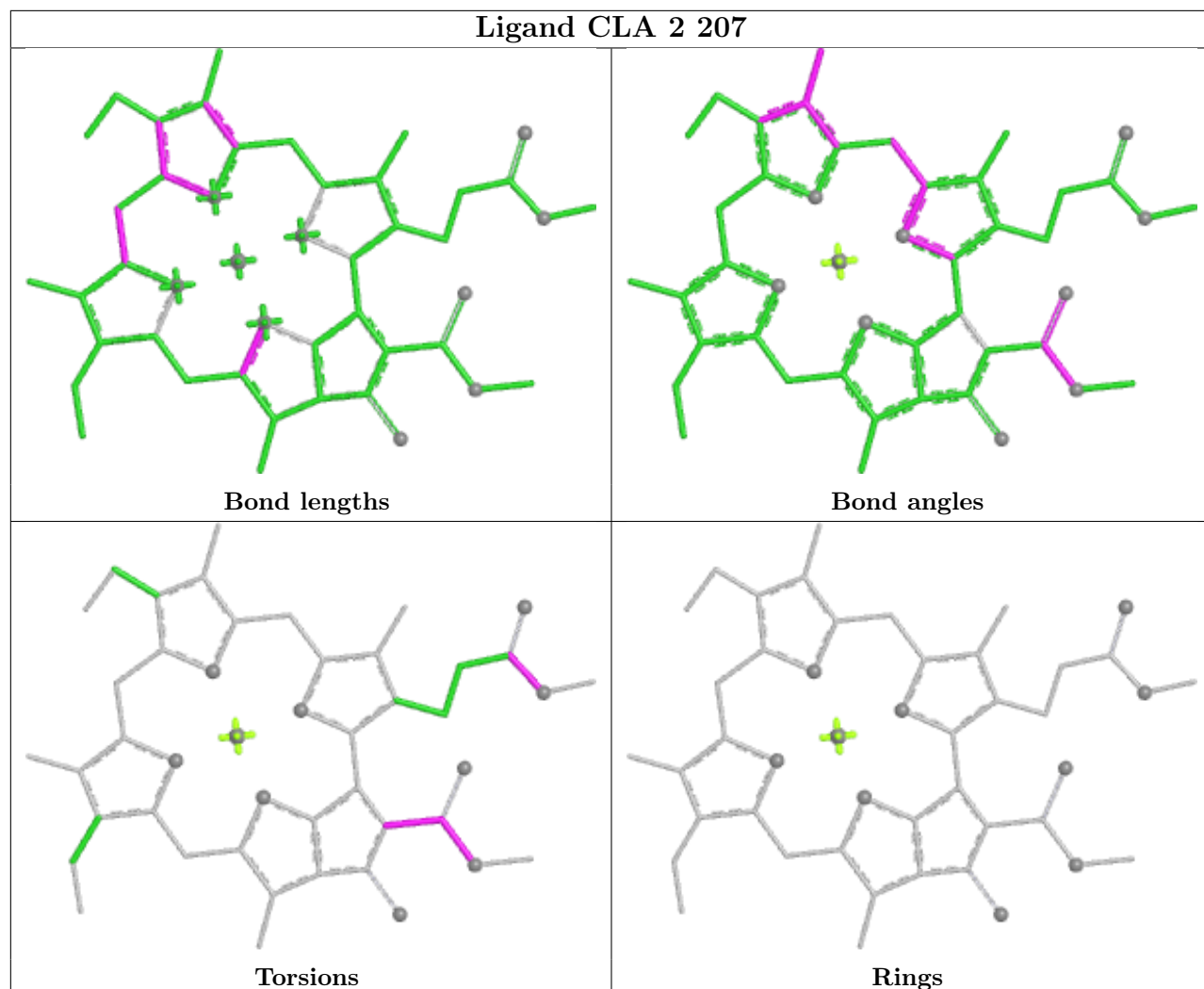
Ligand CLA 2 205



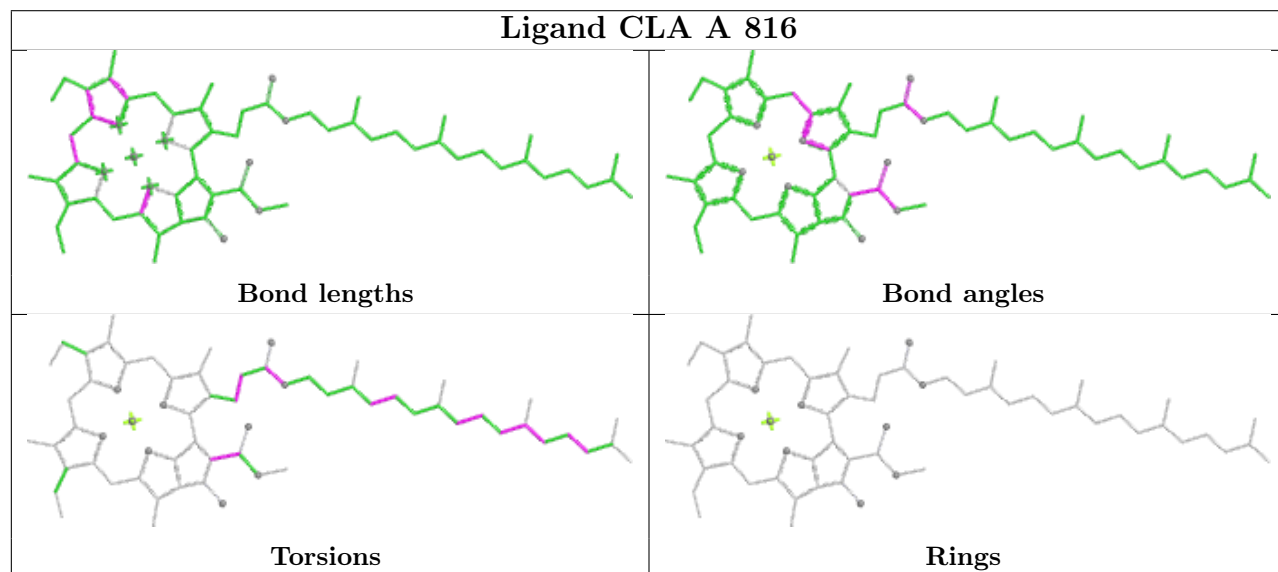
Ligand DD6 h 616



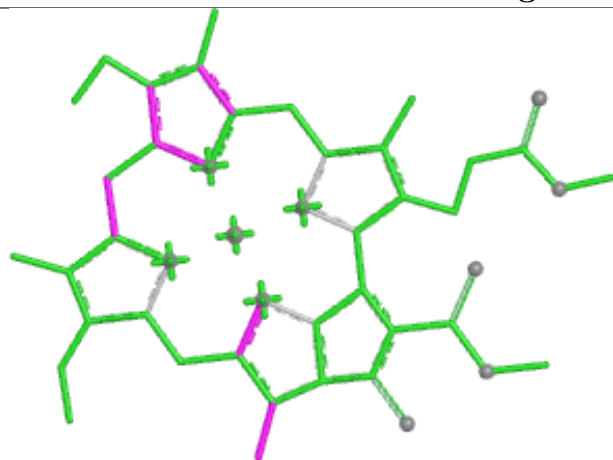
Ligand CLA 2 207



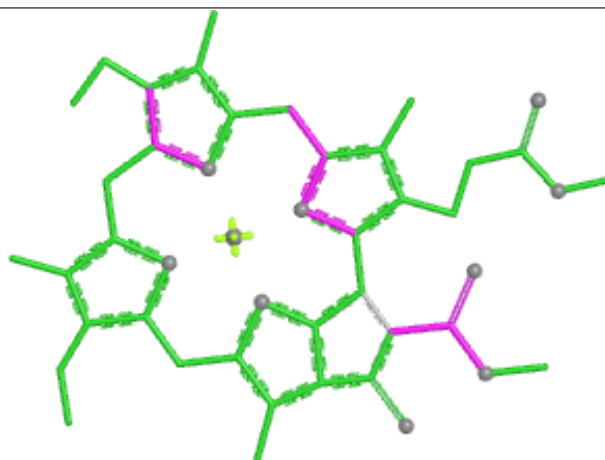
Ligand CLA A 816



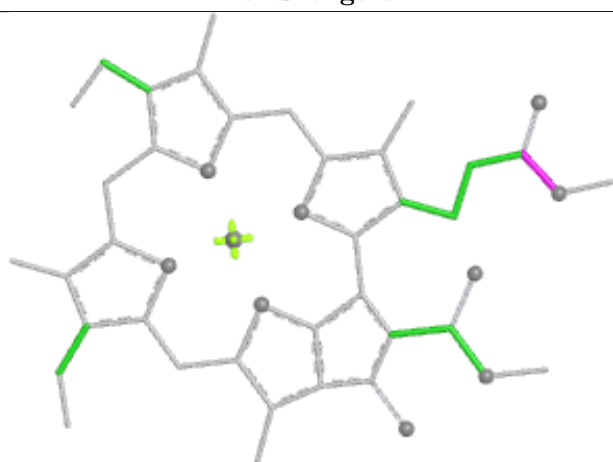
Ligand CLA 4 606



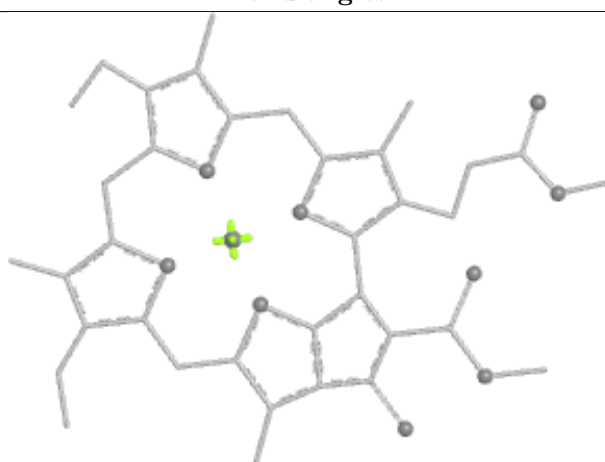
Bond lengths



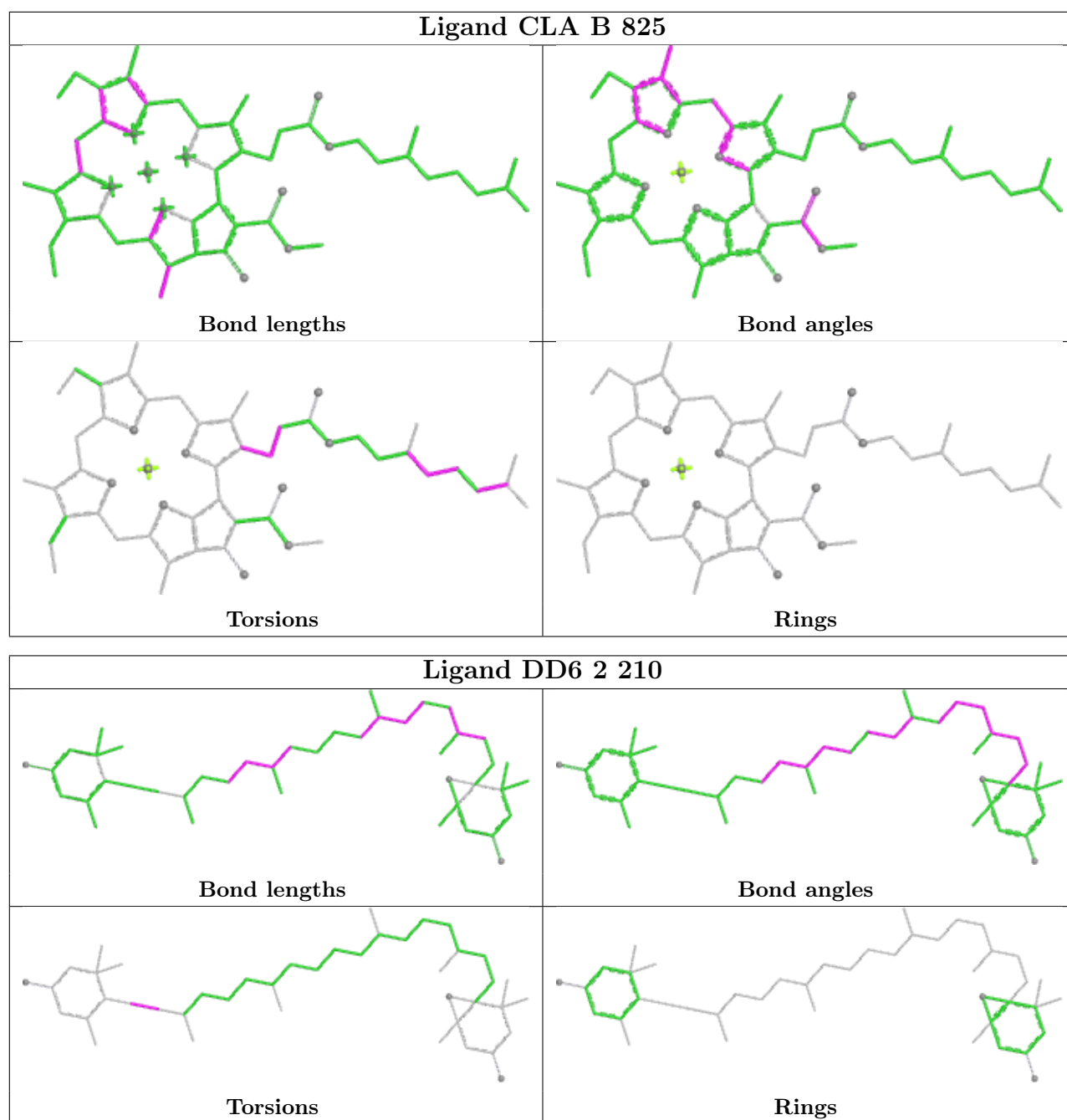
Bond angles

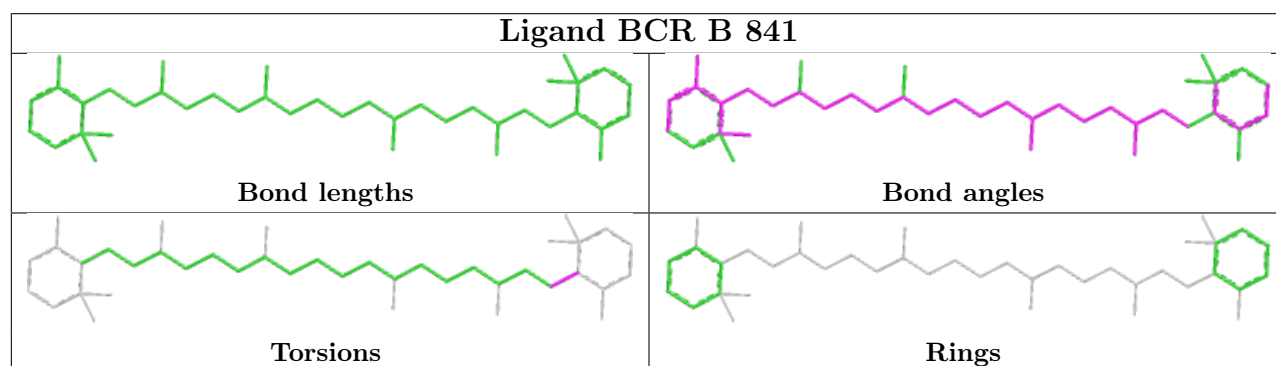
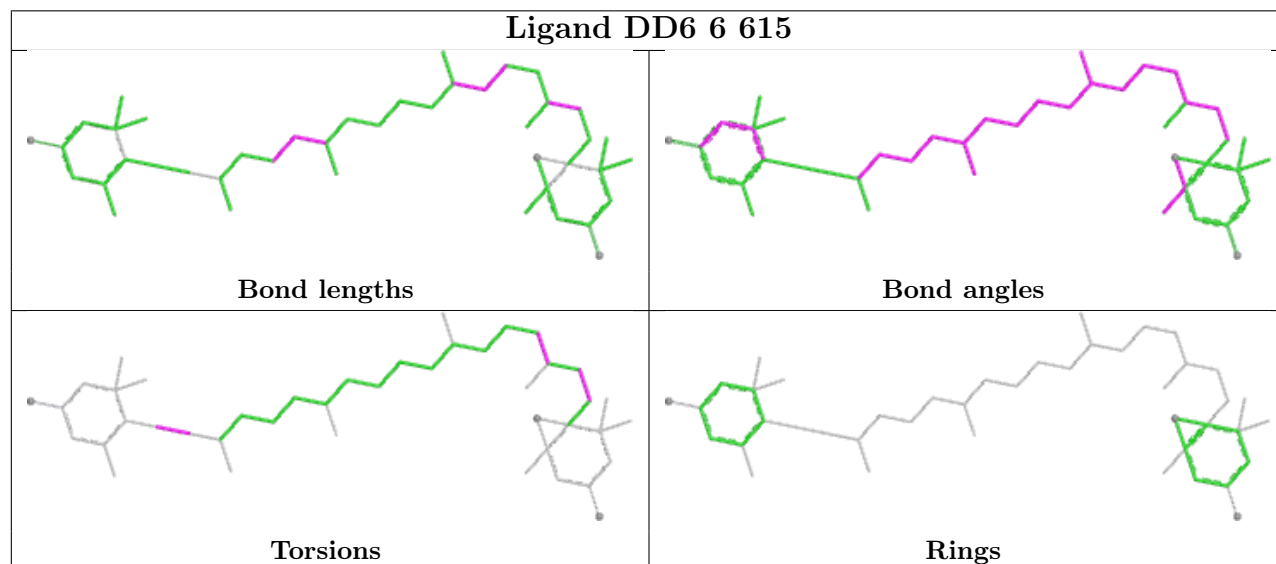
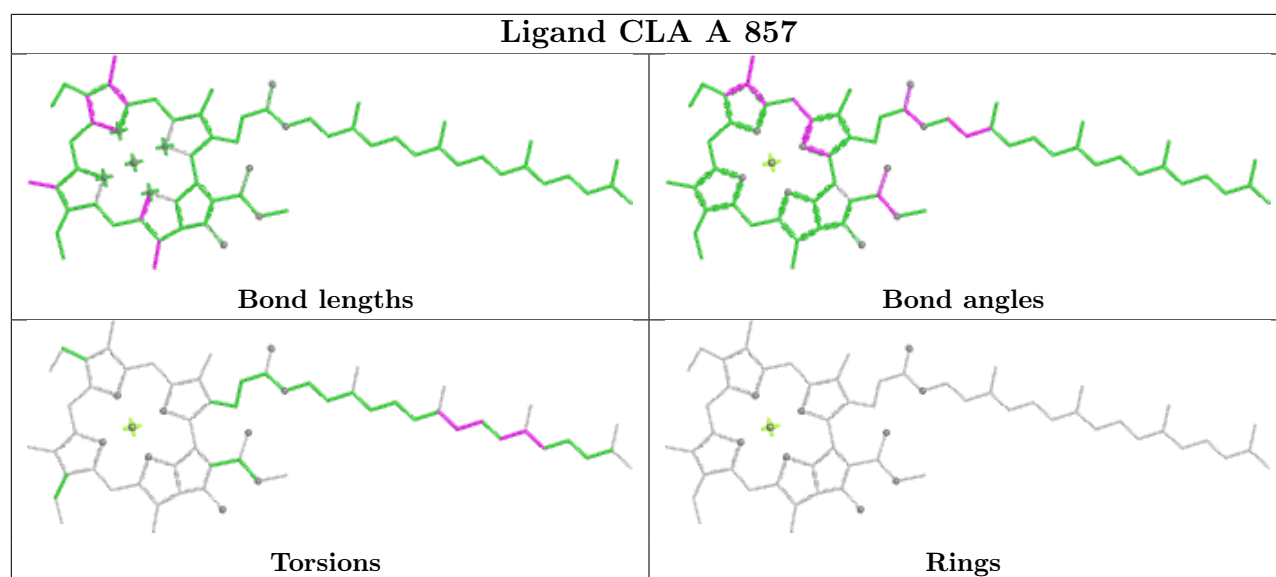


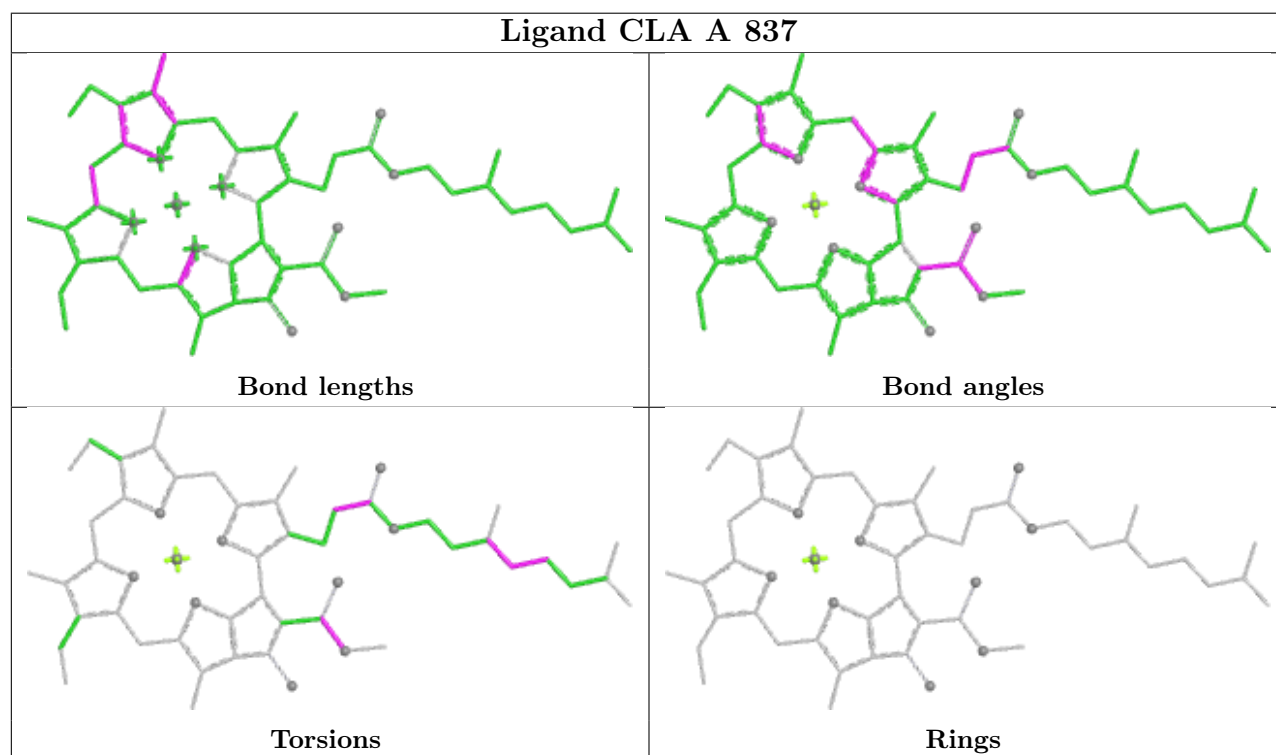
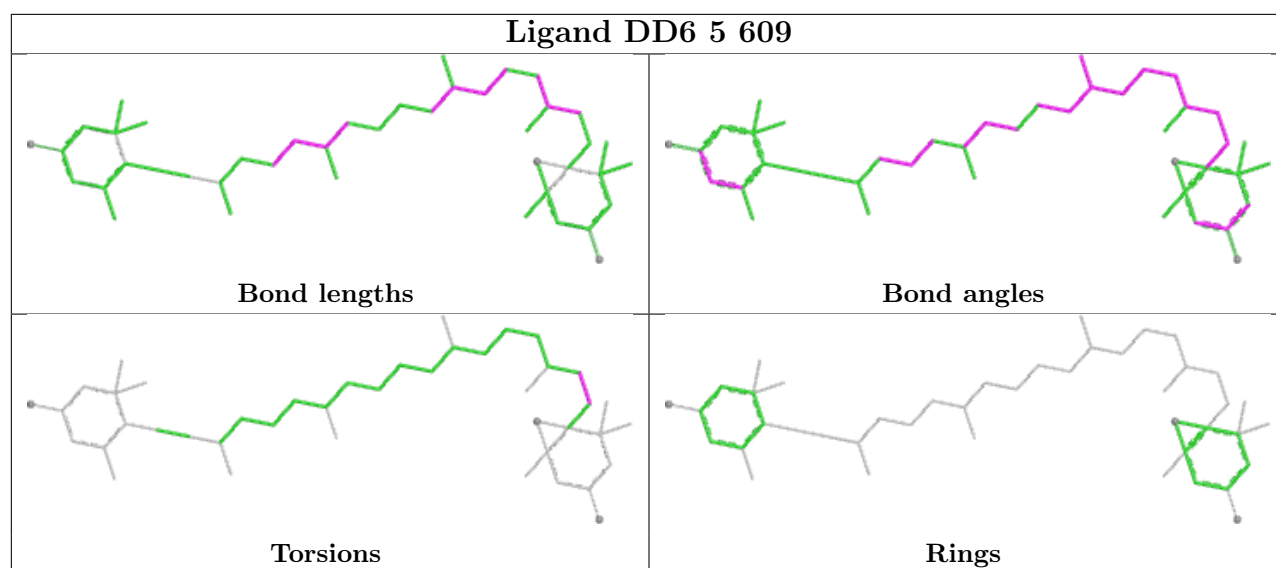
Torsions



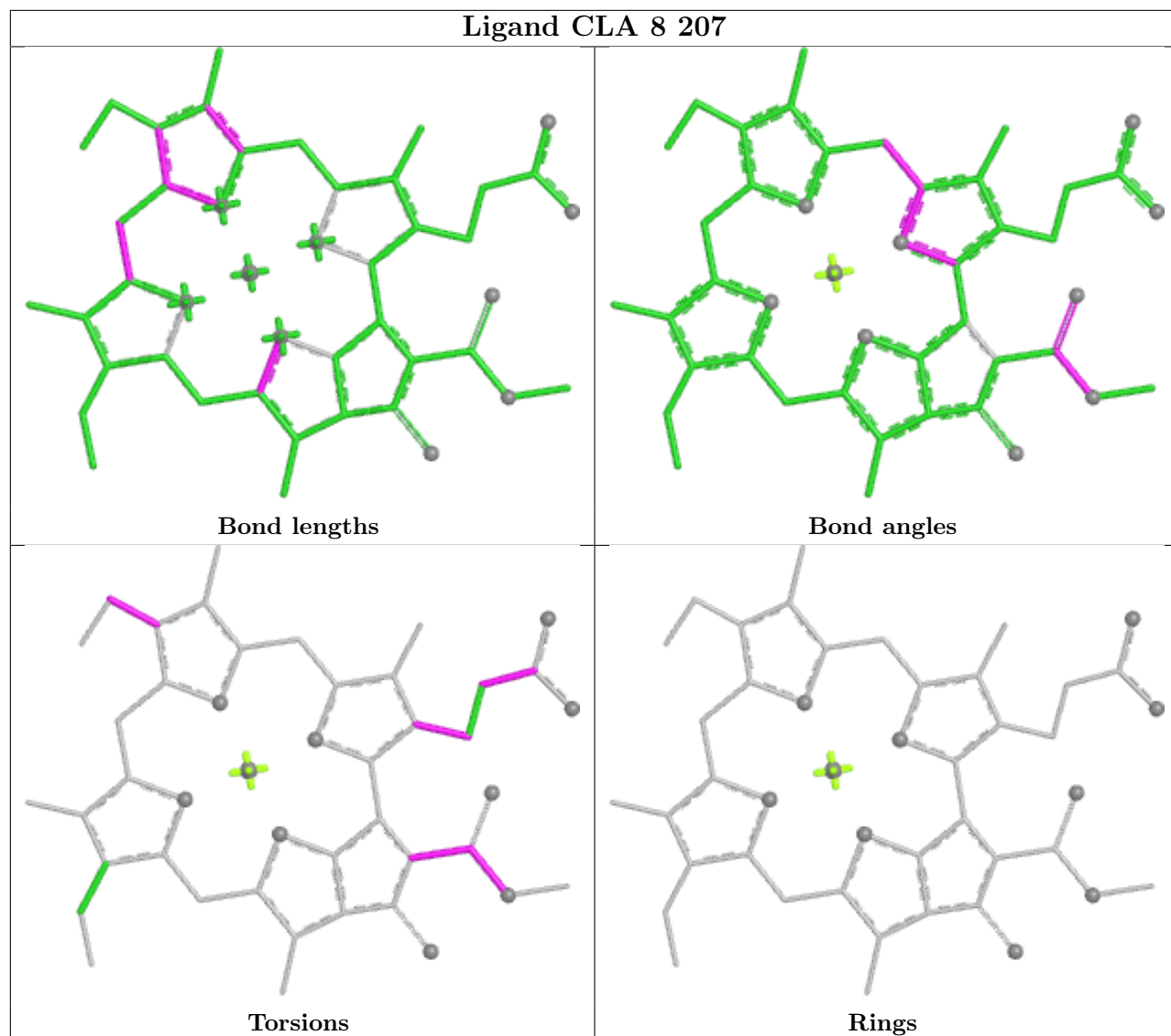
Rings



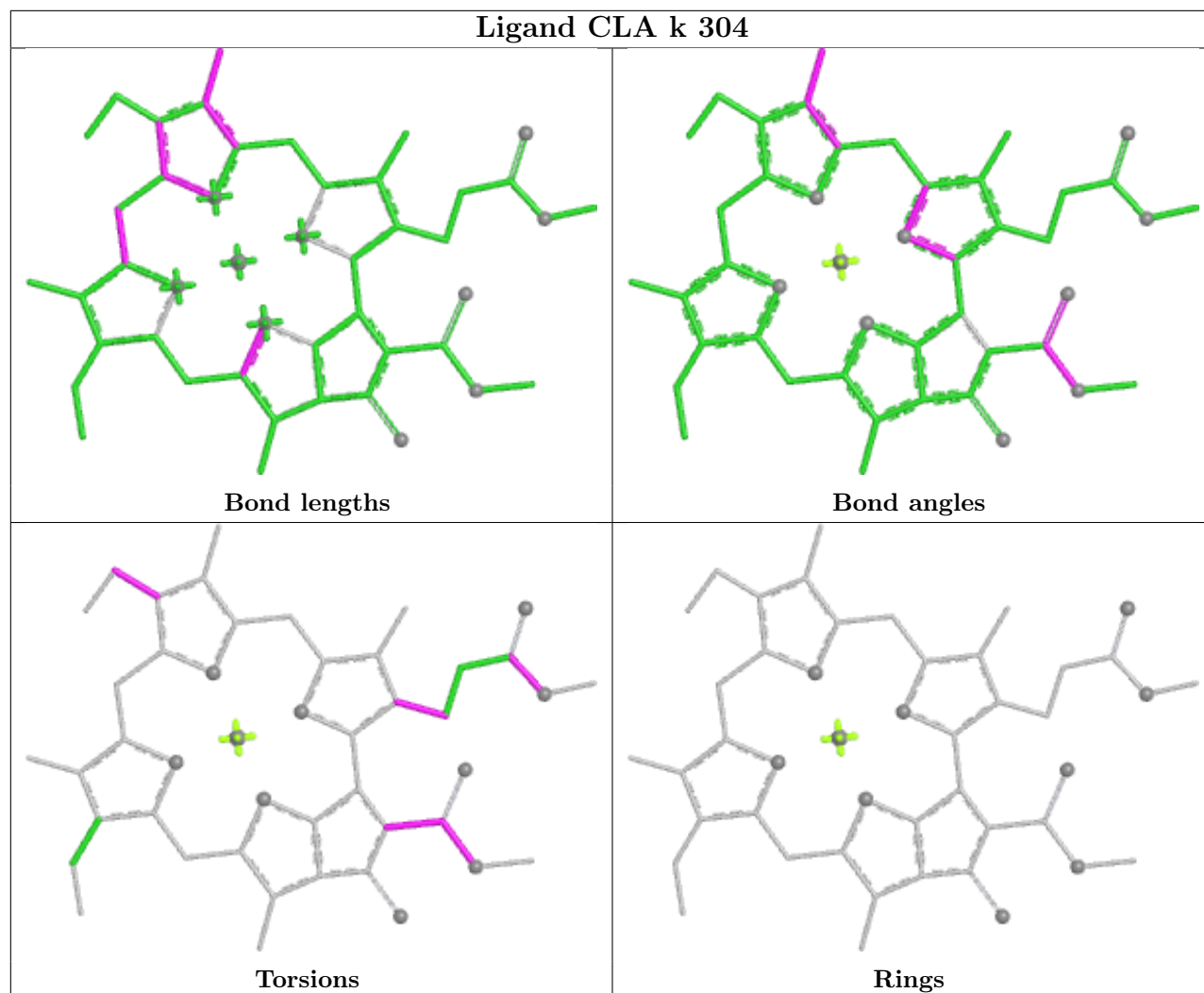




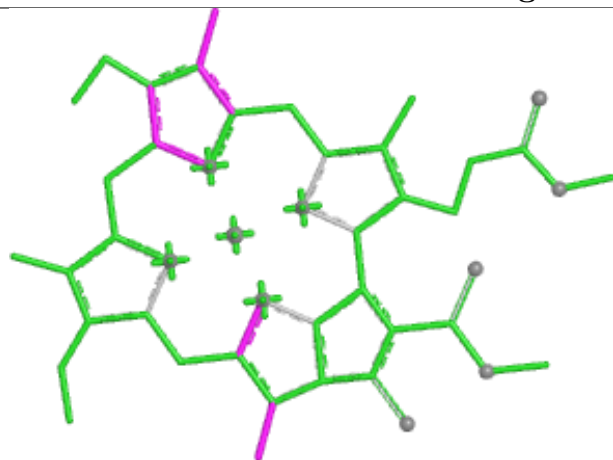
Ligand CLA 8 207



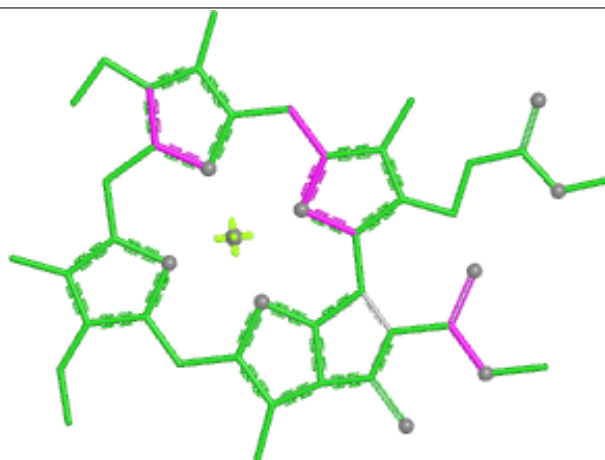
Ligand CLA k 304



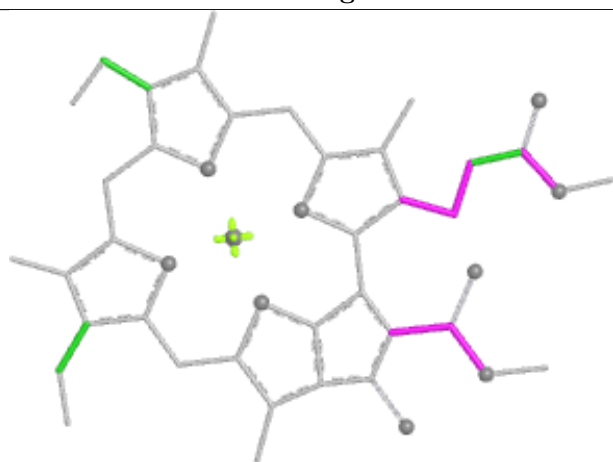
Ligand CLA 9 308



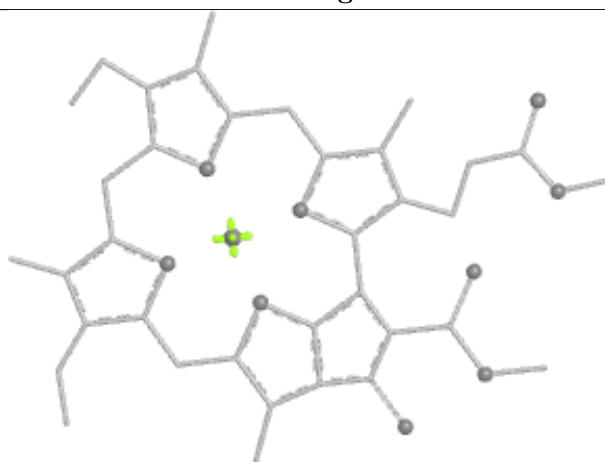
Bond lengths



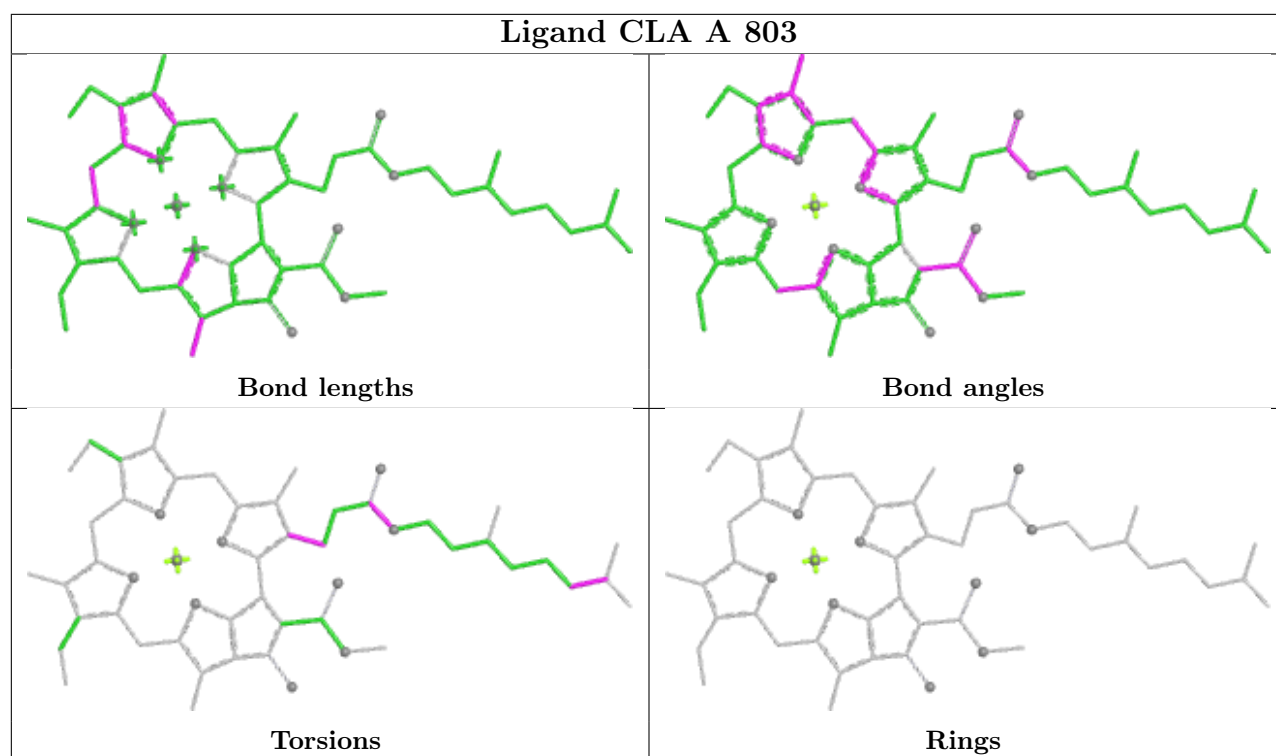
Bond angles



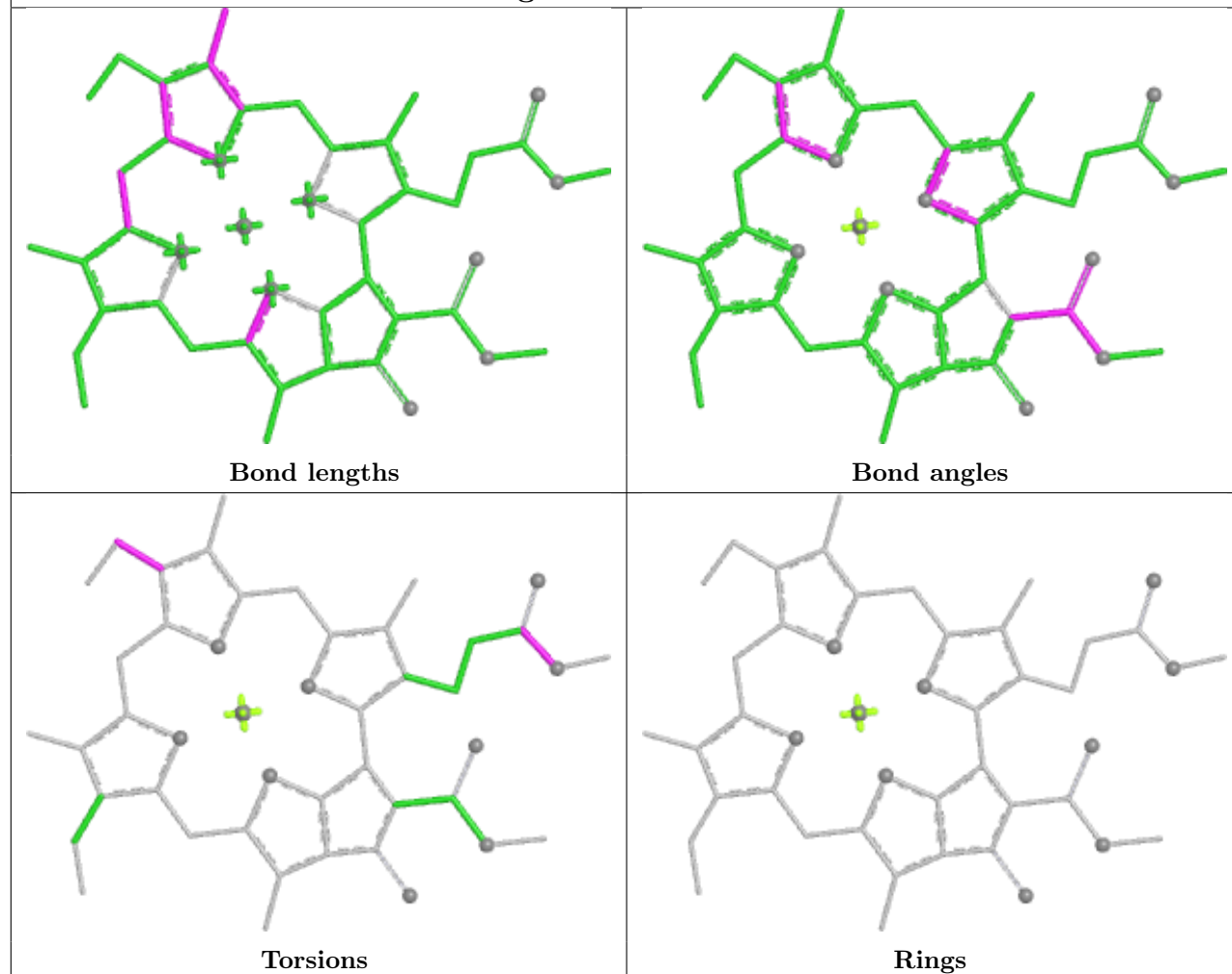
Torsions



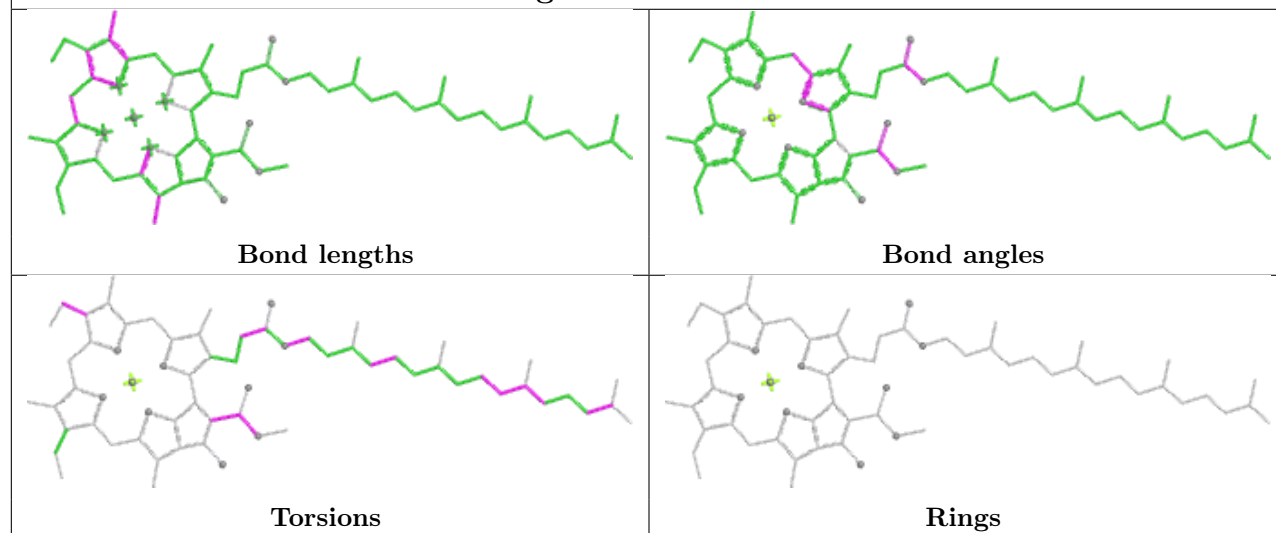
Rings

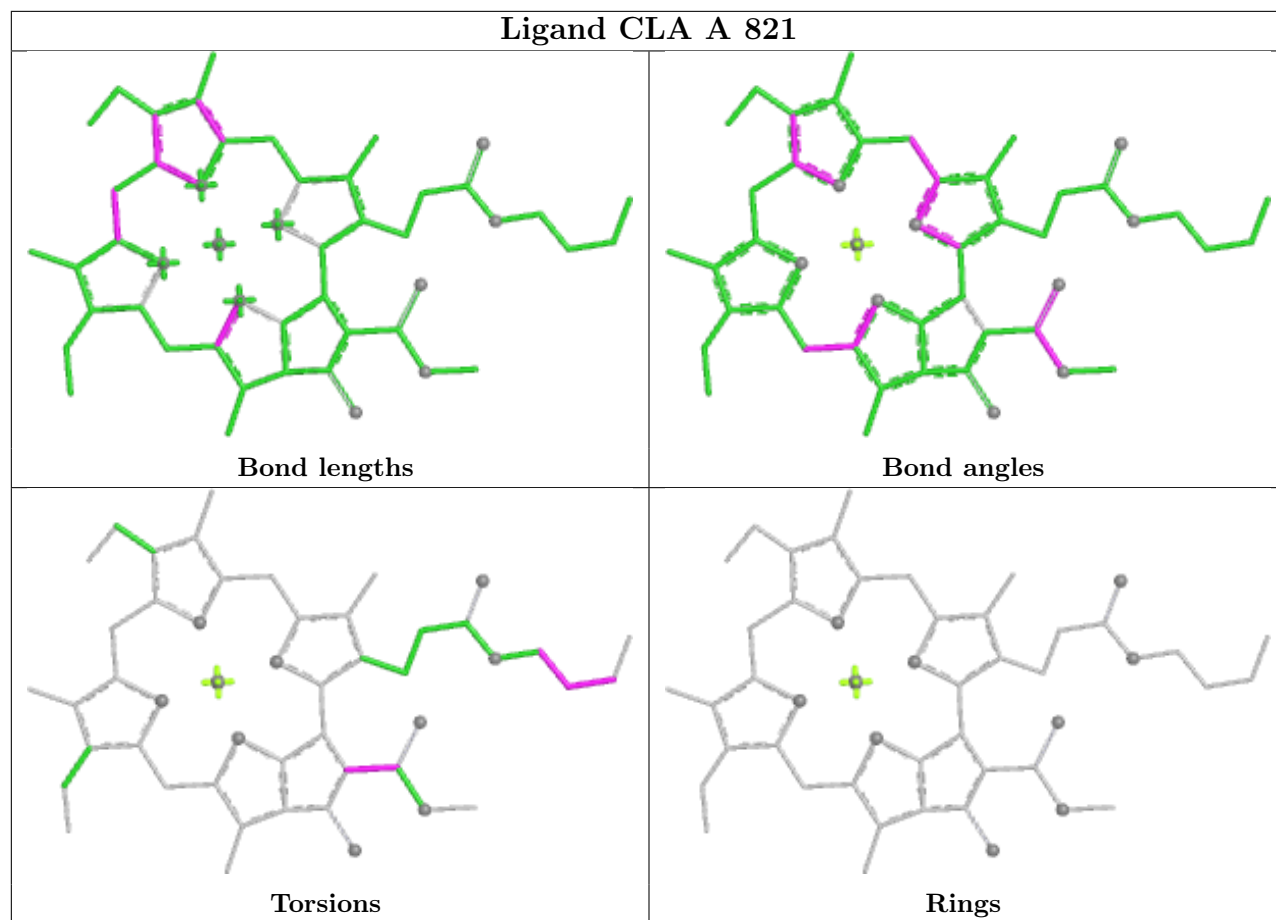


Ligand CLA 6 605

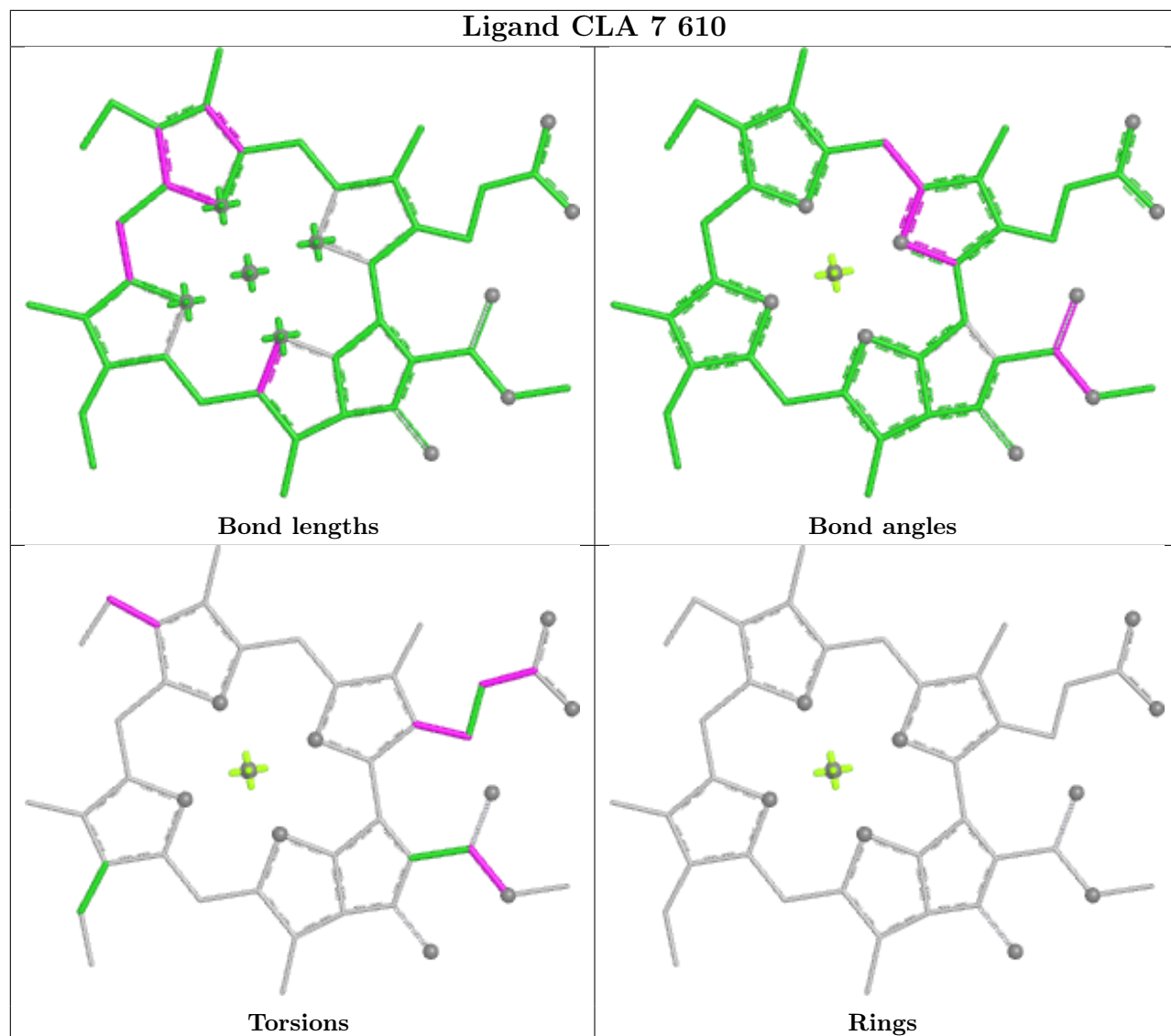


Ligand CLA 1 317

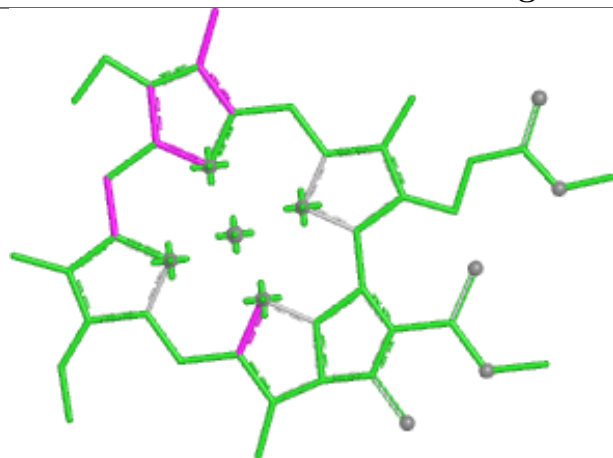




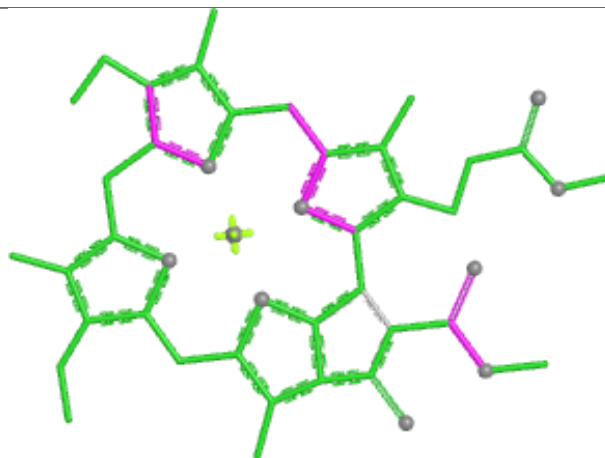
Ligand CLA 7 610



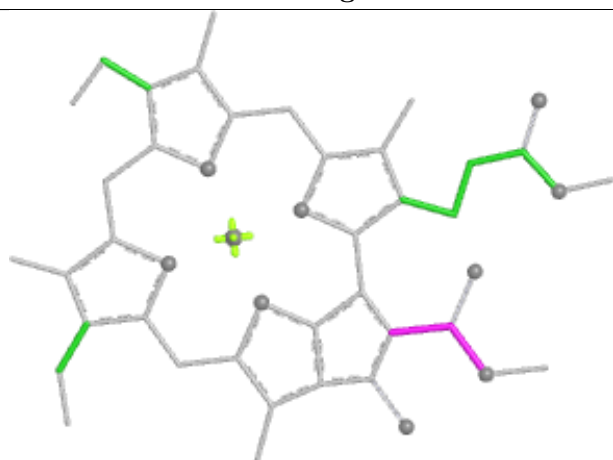
Ligand CLA 6 608



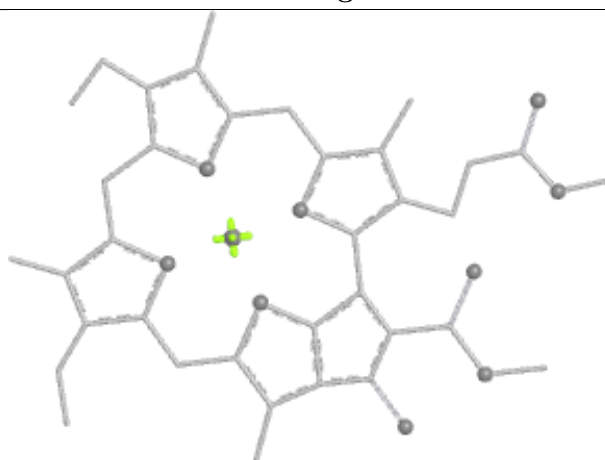
Bond lengths



Bond angles

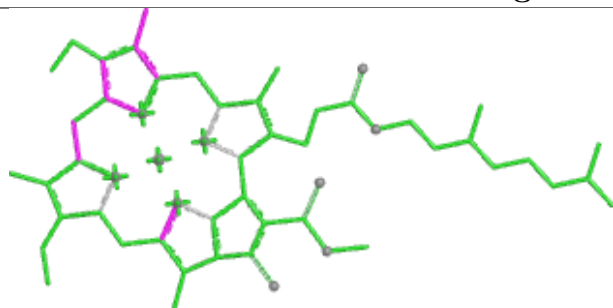


Torsions

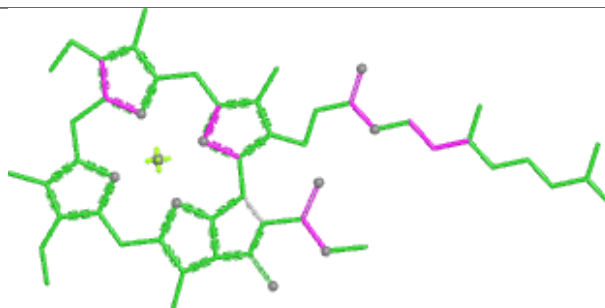


Rings

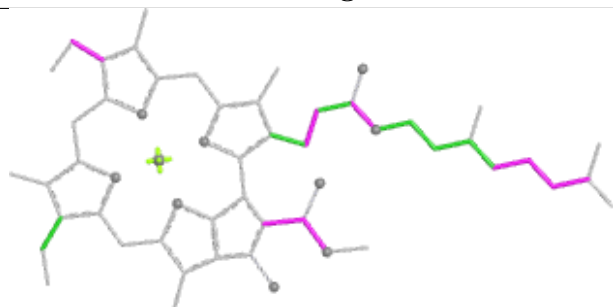
Ligand CLA A 822



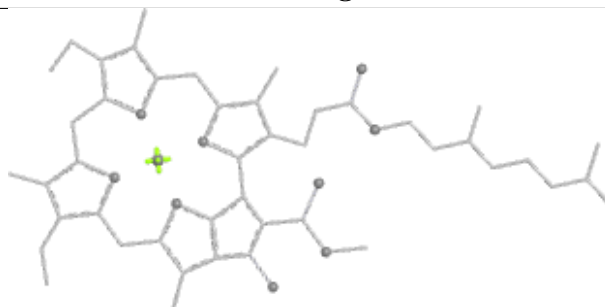
Bond lengths



Bond angles

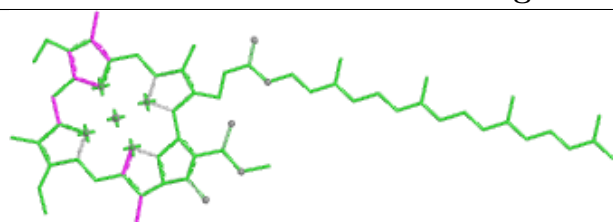


Torsions

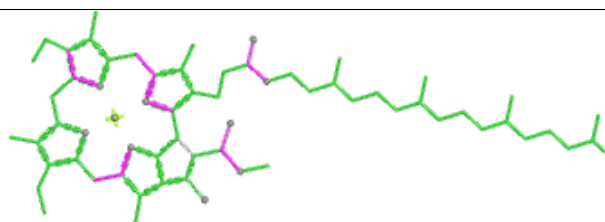


Rings

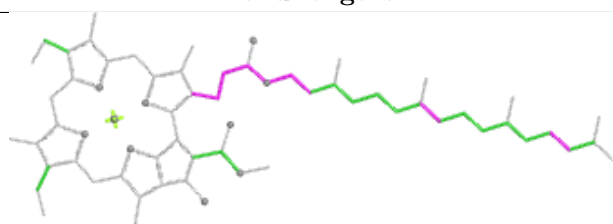
Ligand CLA A 804



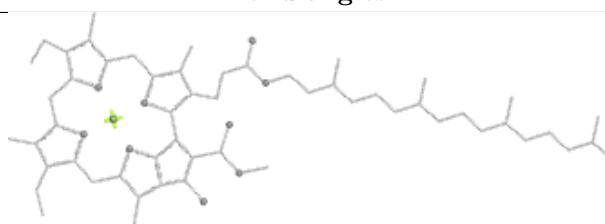
Bond lengths



Bond angles

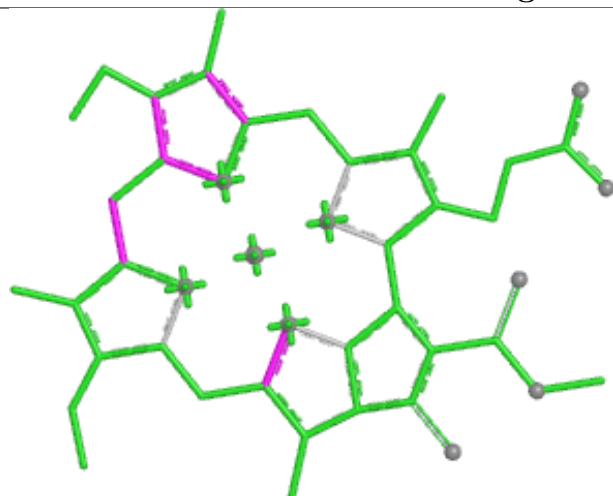


Torsions

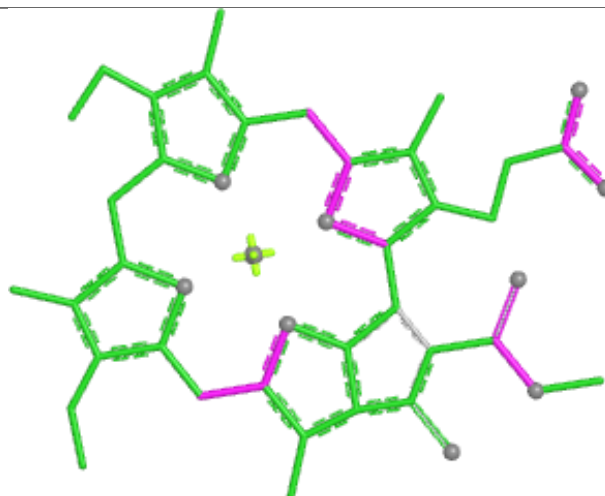


Rings

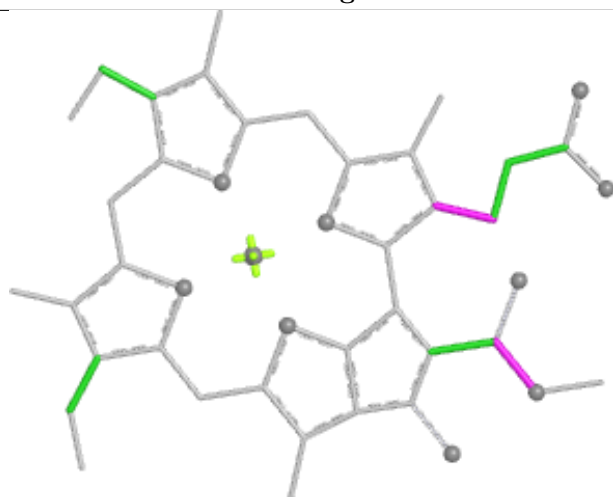
Ligand CLA k 309



Bond lengths



Bond angles

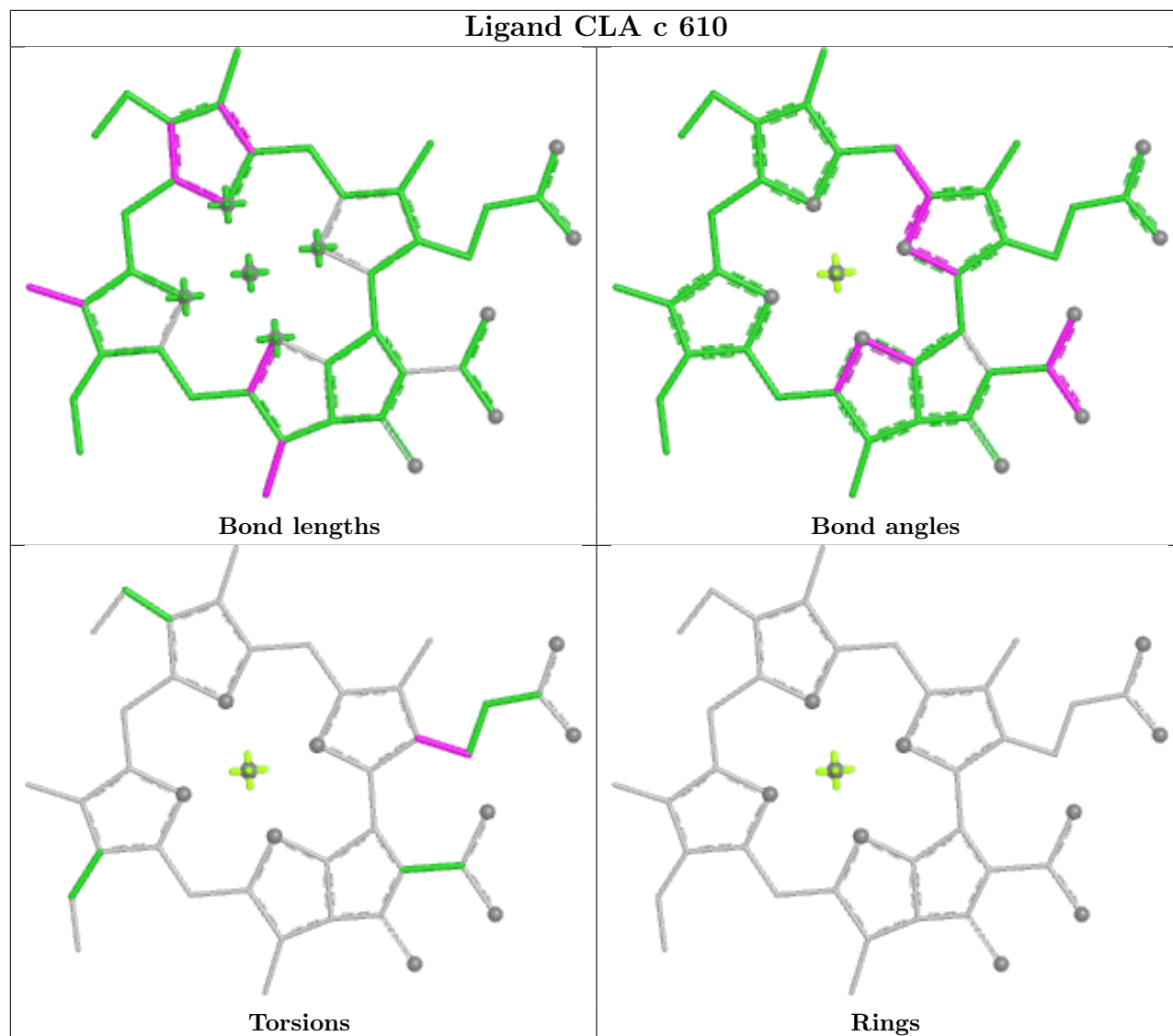


Torsions

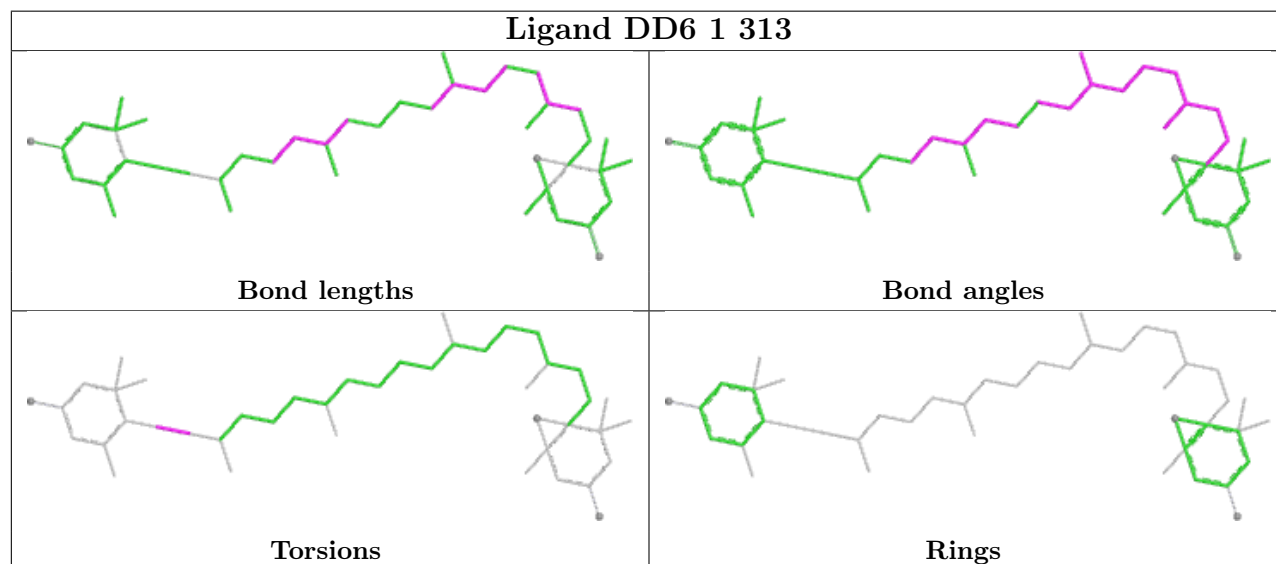


Rings

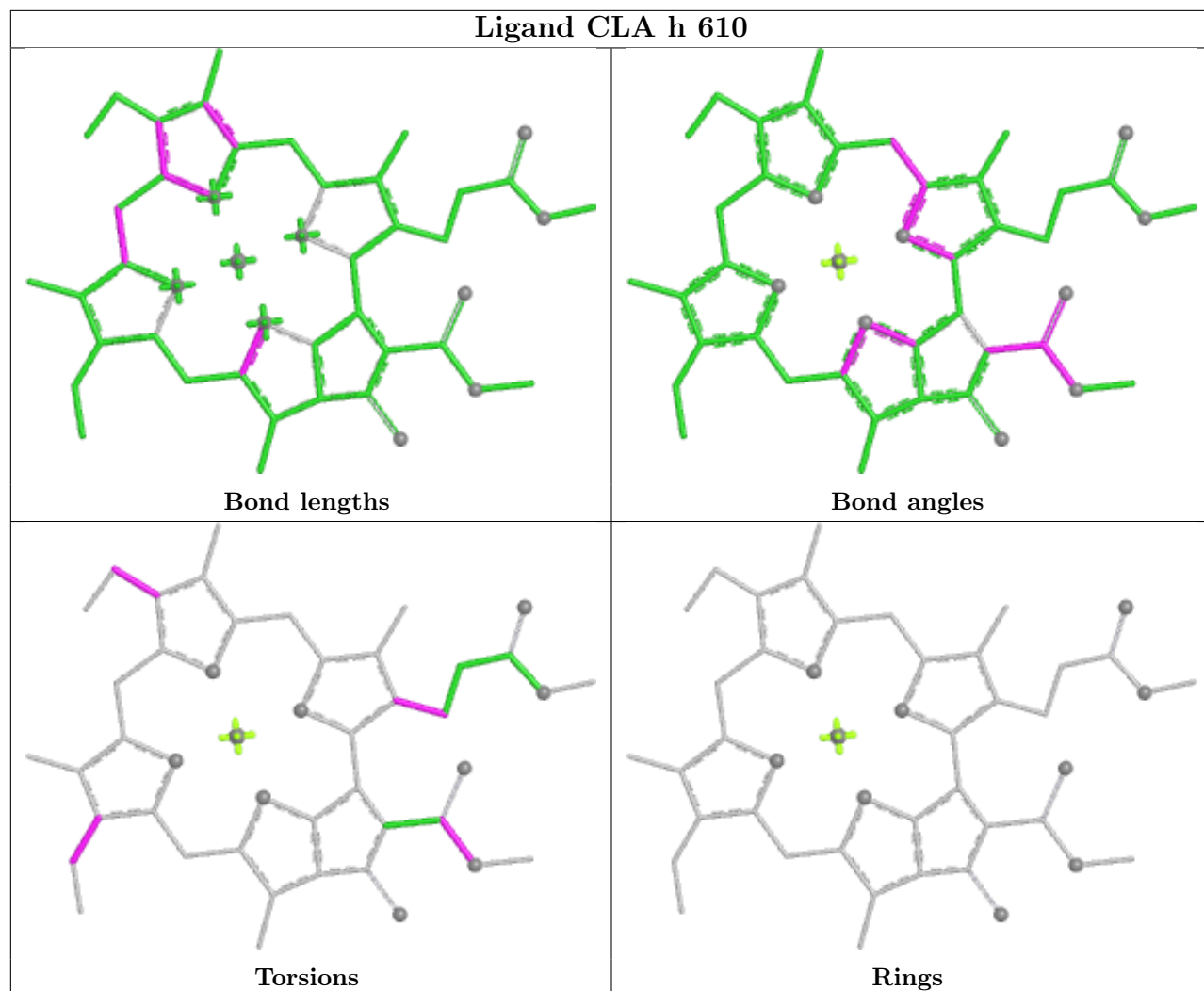
Ligand CLA c 610



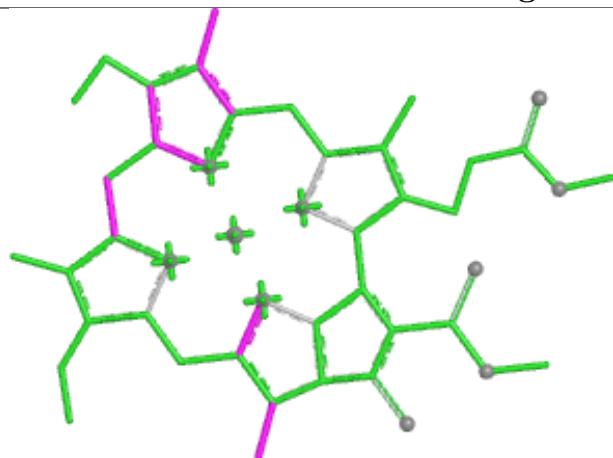
Ligand DD6 1 313



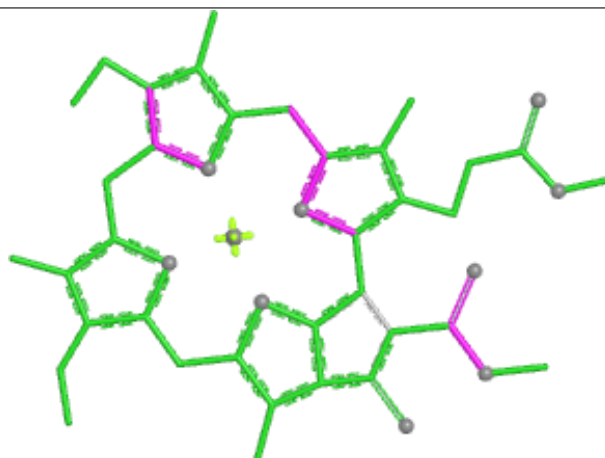
Ligand CLA h 610



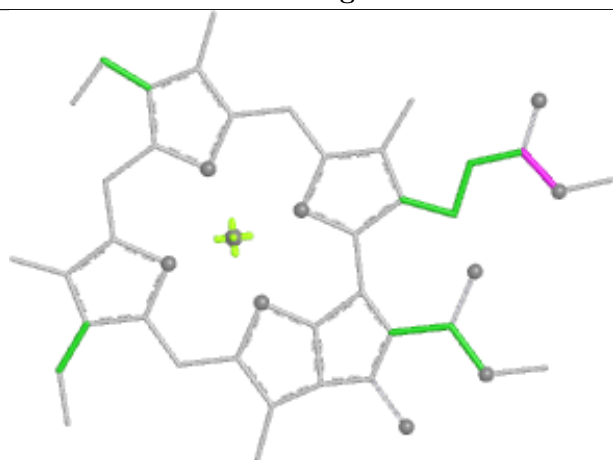
Ligand CLA 4 603



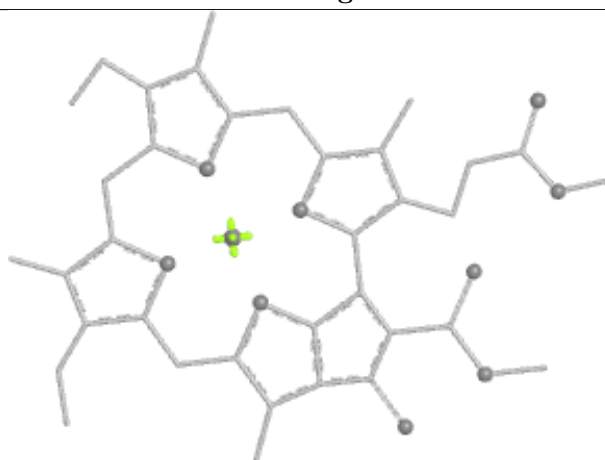
Bond lengths



Bond angles

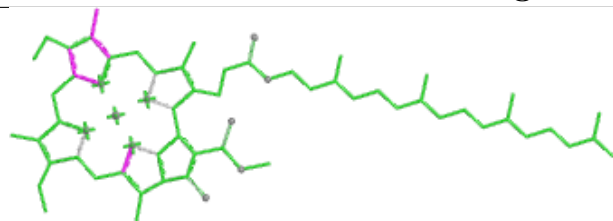


Torsions

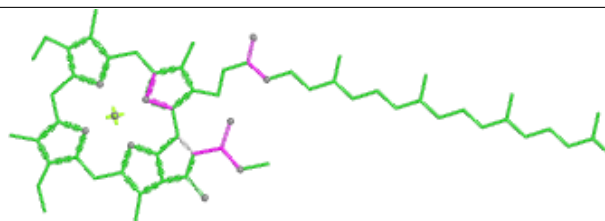


Rings

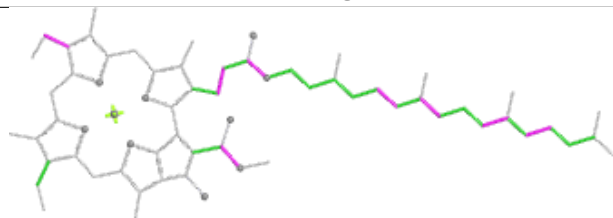
Ligand CLA A 836



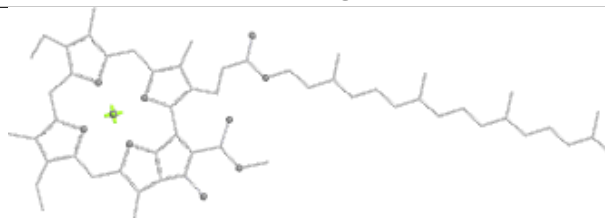
Bond lengths



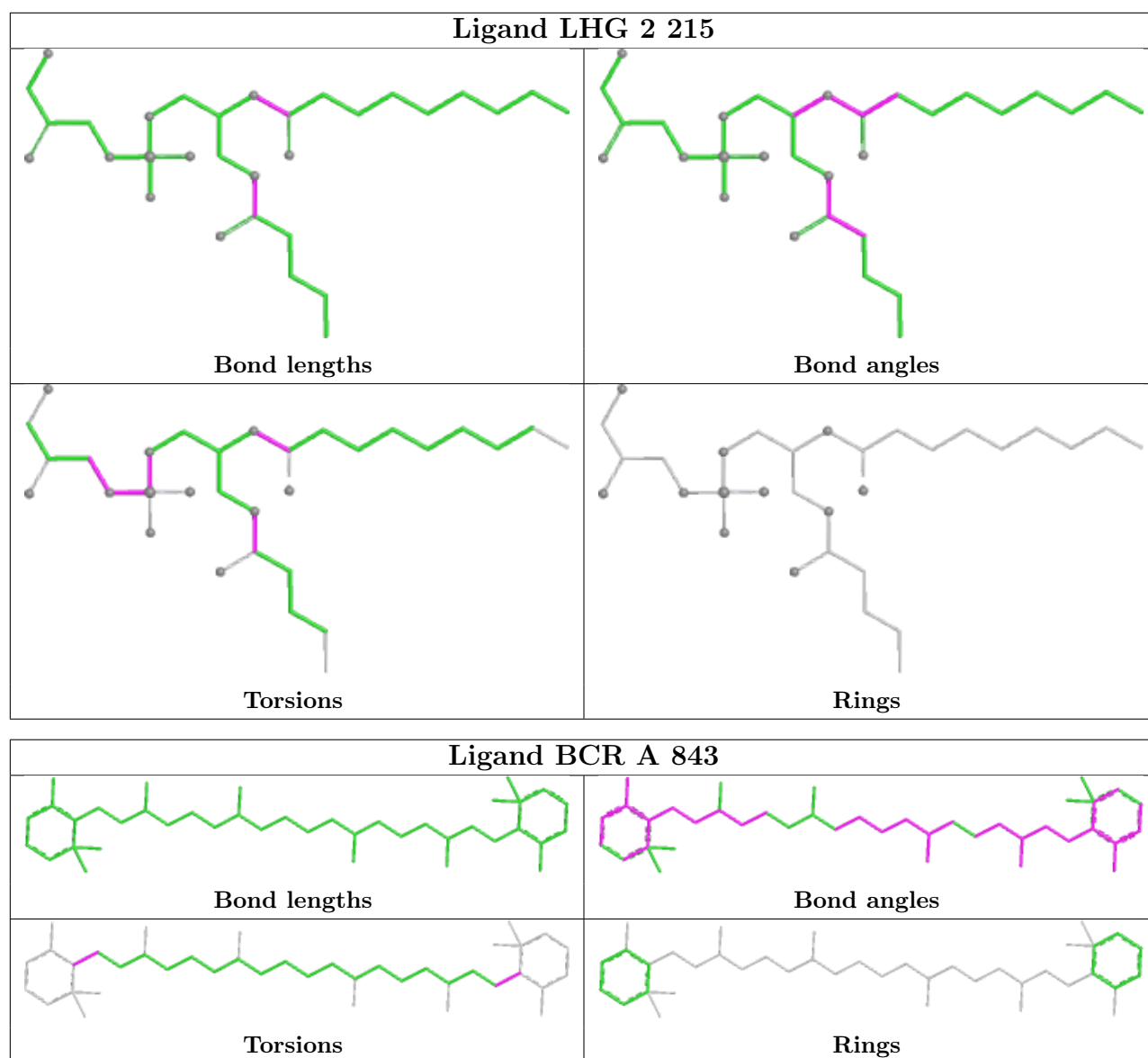
Bond angles

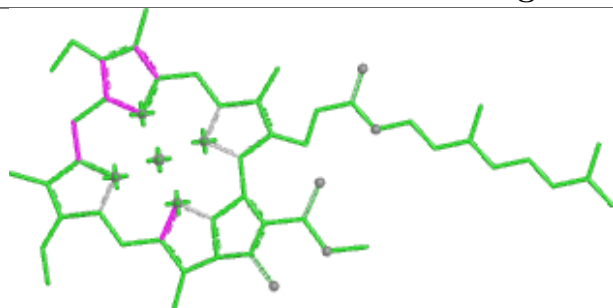


Torsions

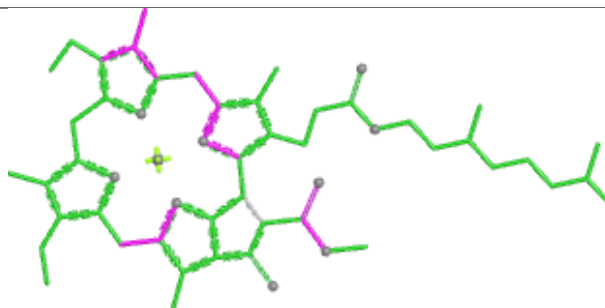


Rings

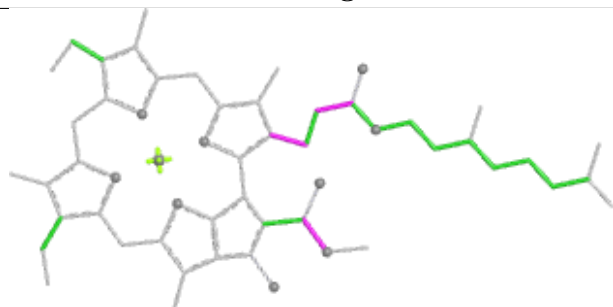


Ligand CLA k 311

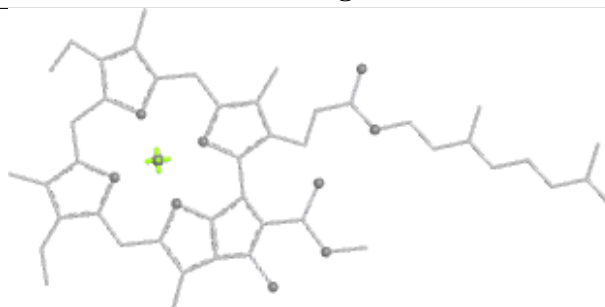
Bond lengths



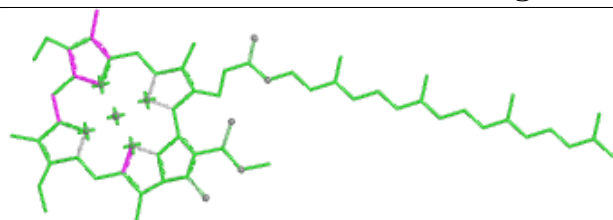
Bond angles



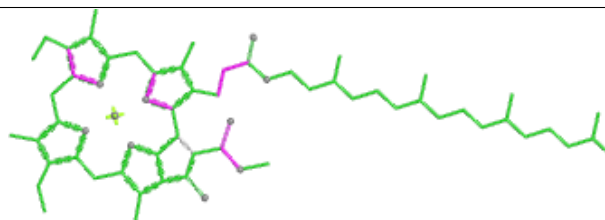
Torsions



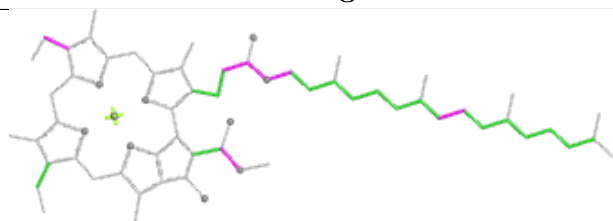
Rings

Ligand CLA A 808

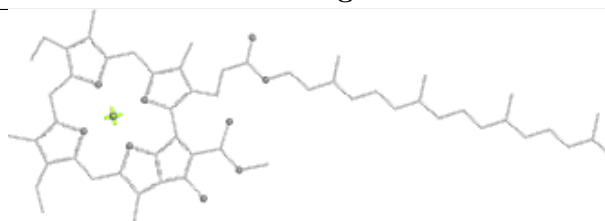
Bond lengths



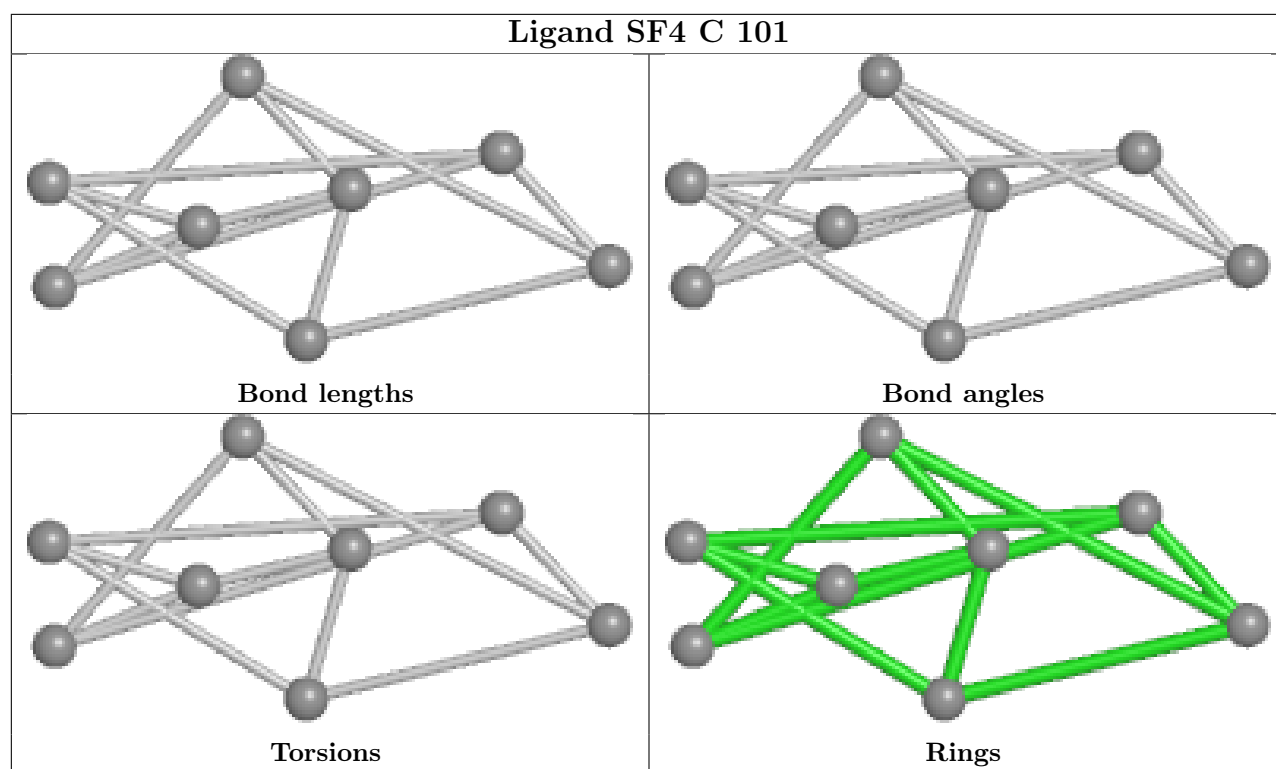
Bond angles



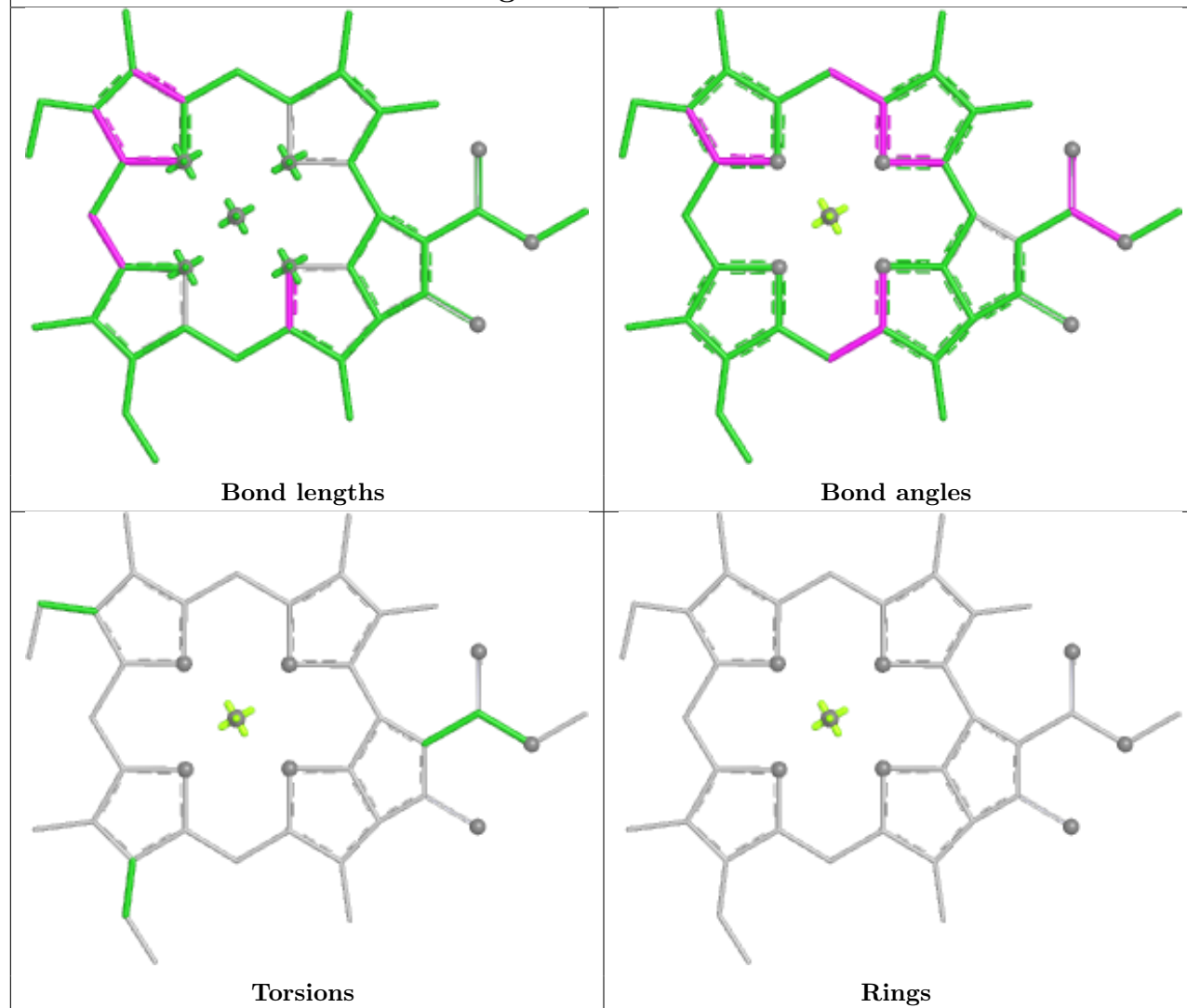
Torsions



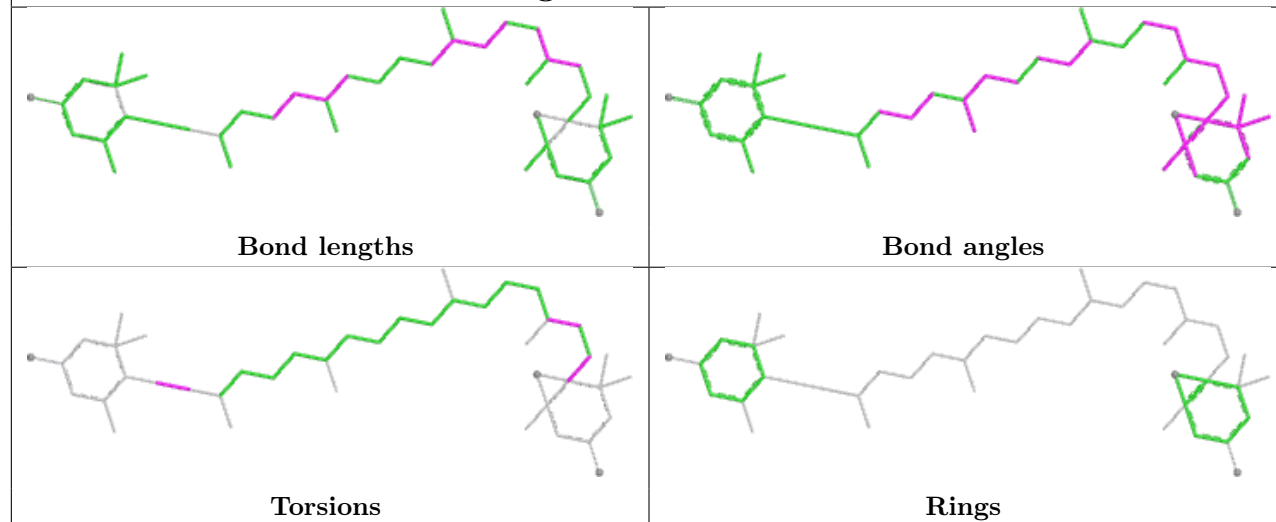
Rings

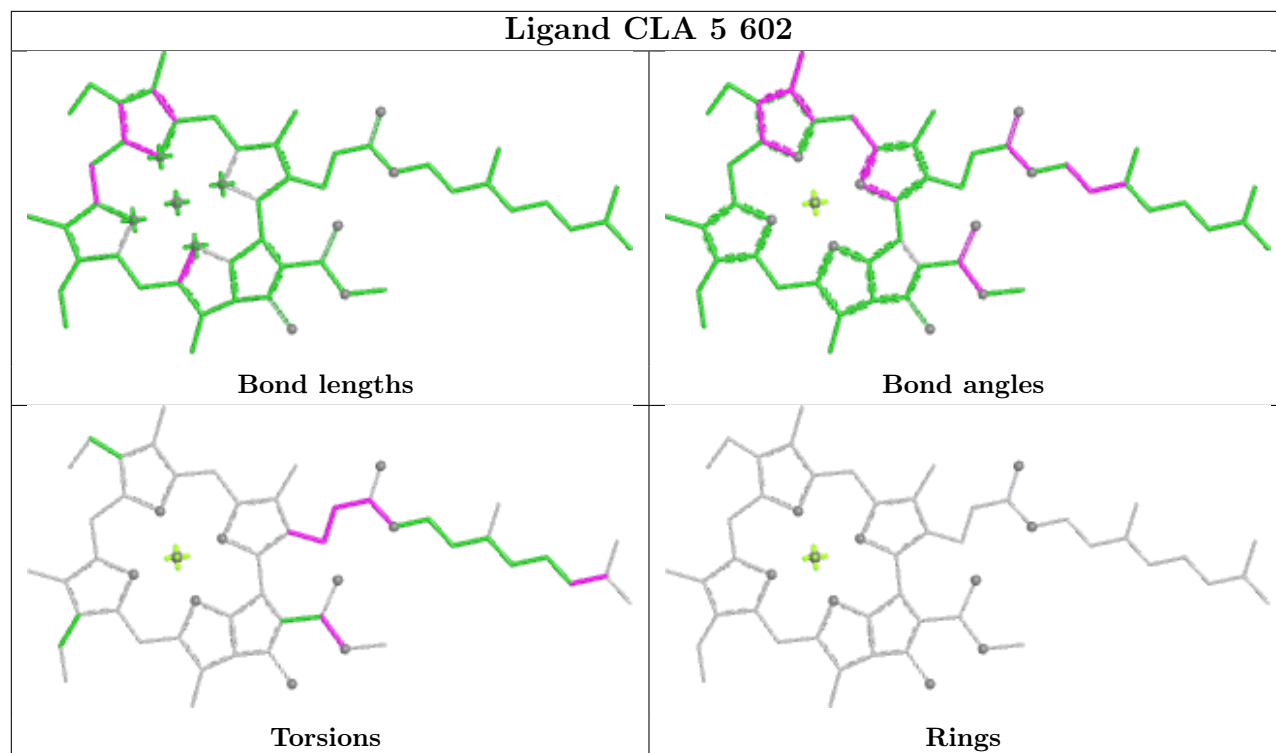
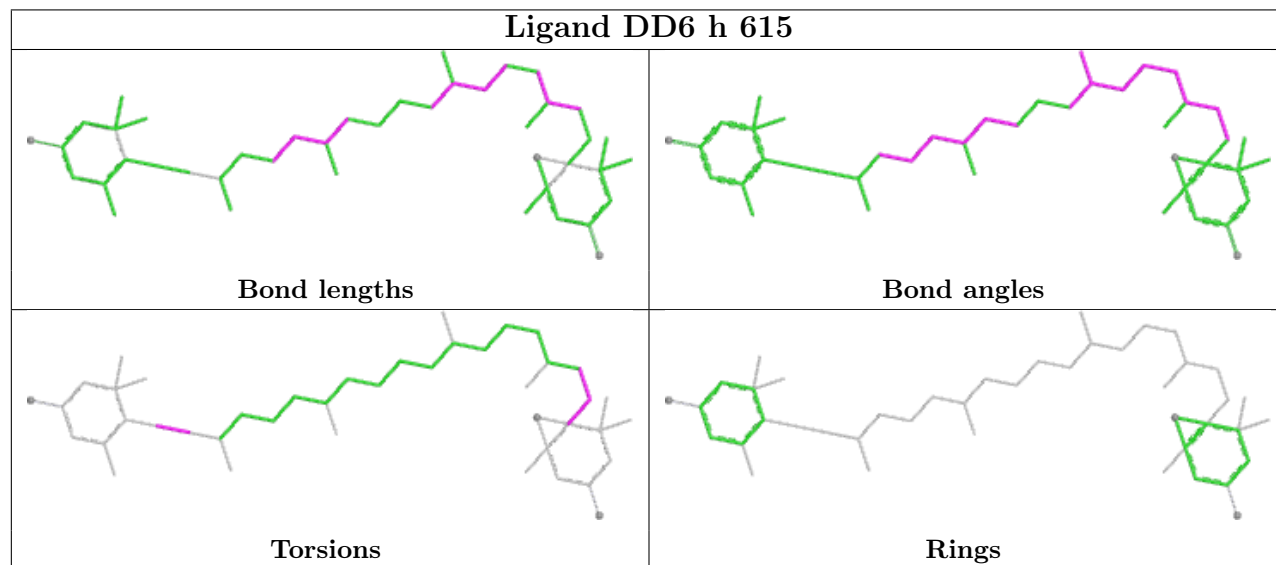


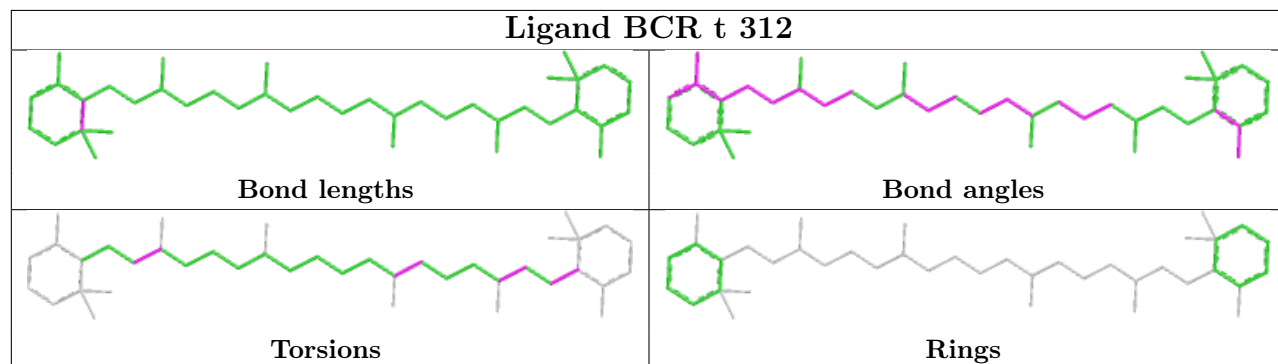
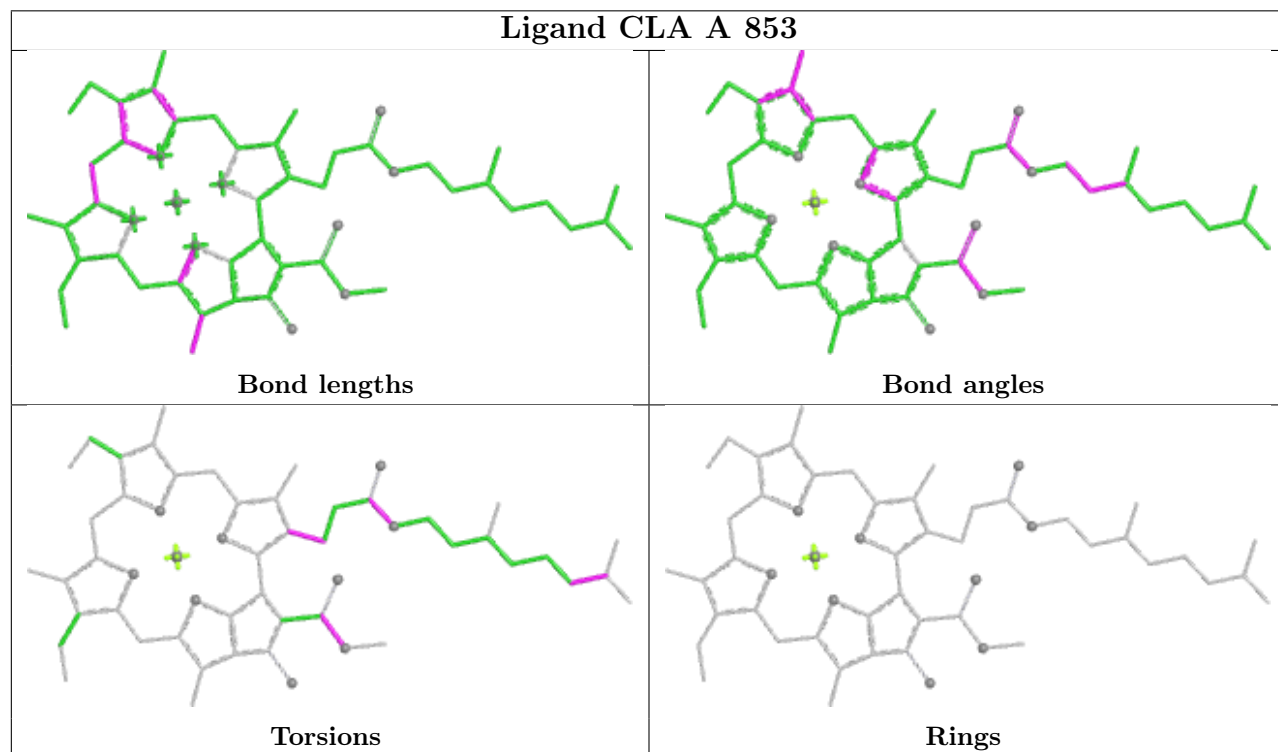
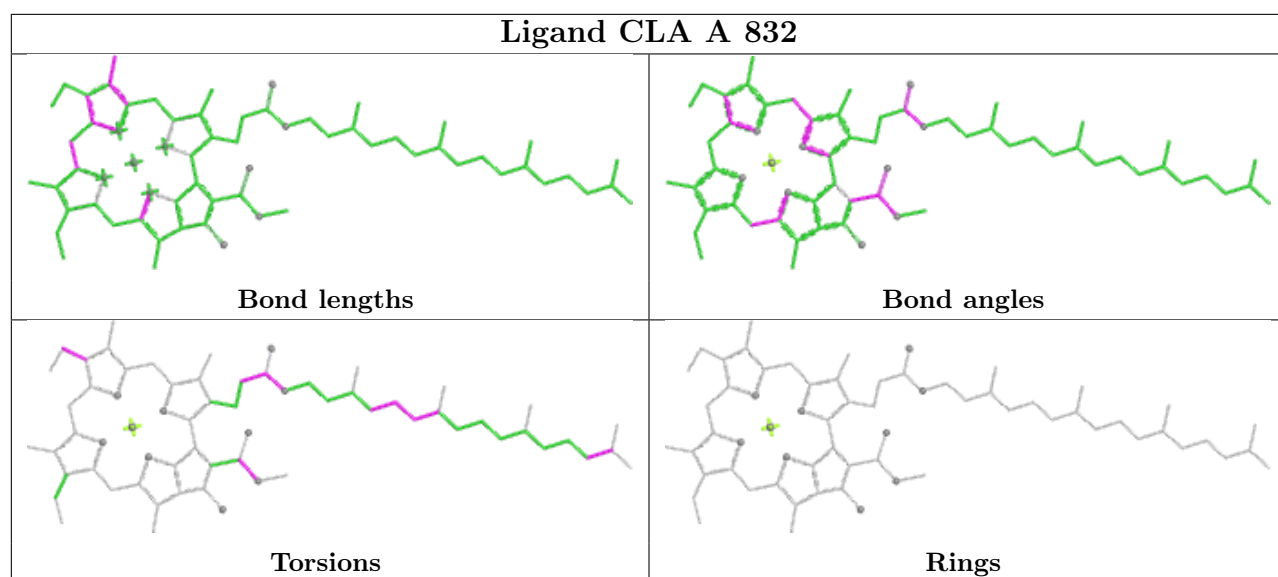
Ligand CLA 3 309



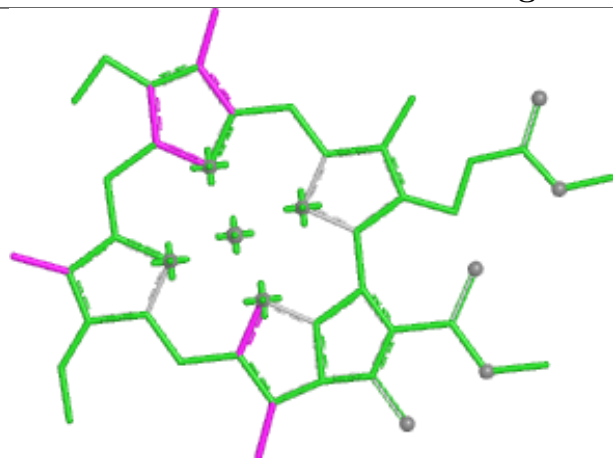
Ligand DD6 6 616



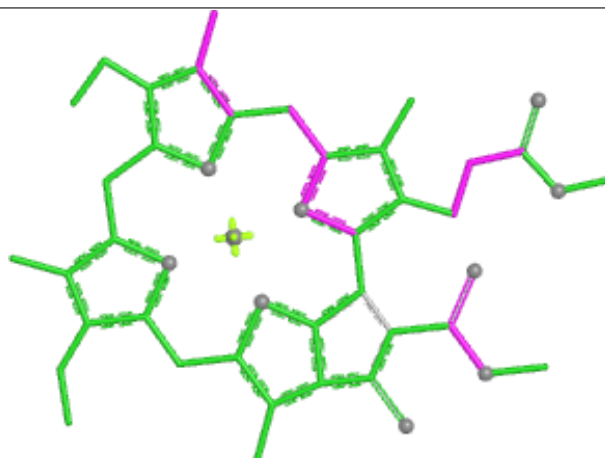
Ligand CLA 5 602**Ligand DD6 h 615**



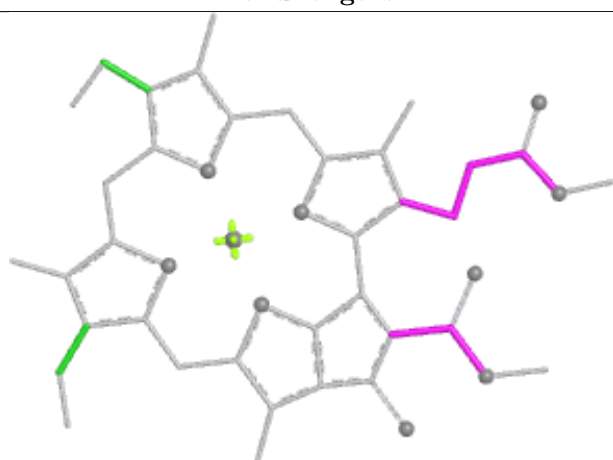
Ligand CLA 9 305



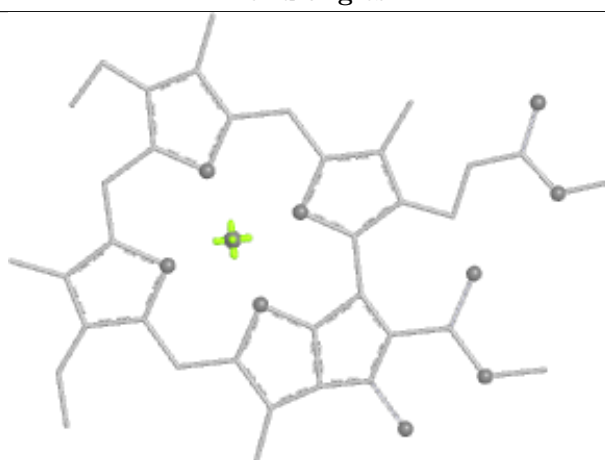
Bond lengths



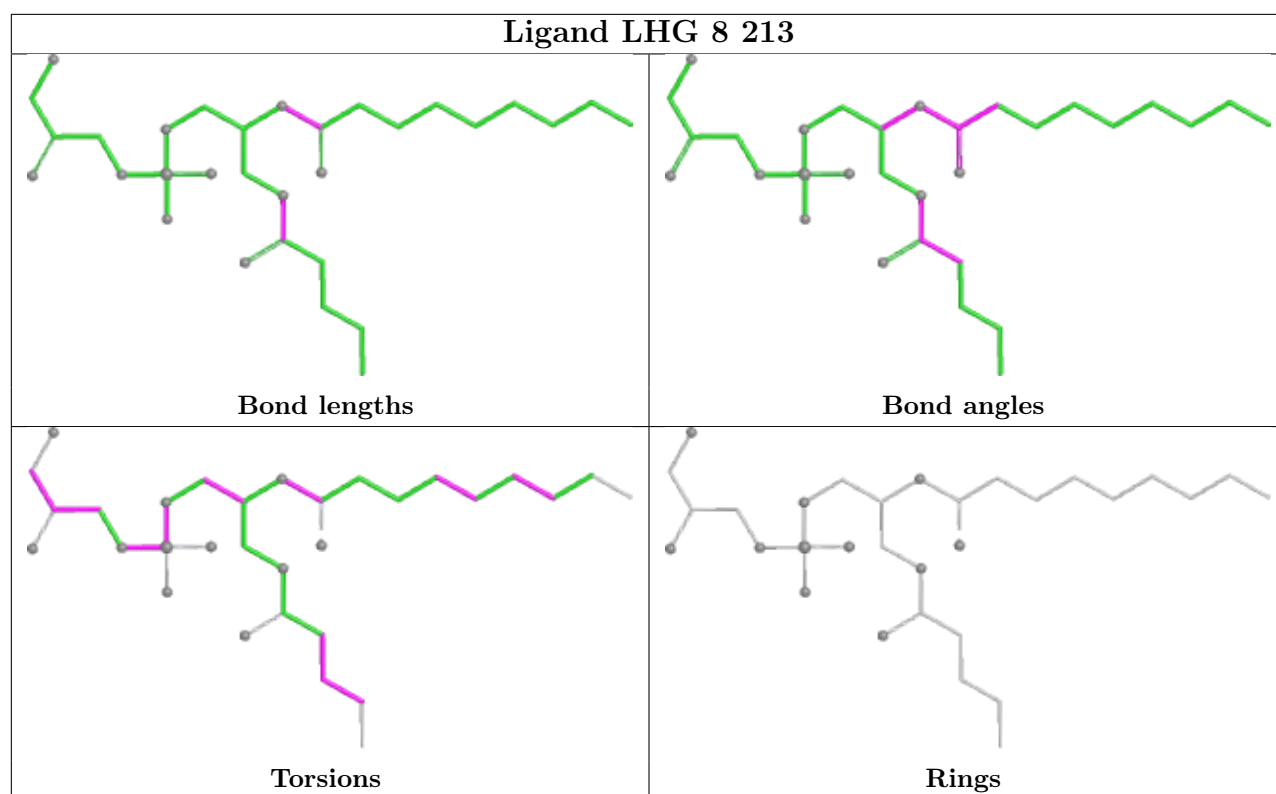
Bond angles



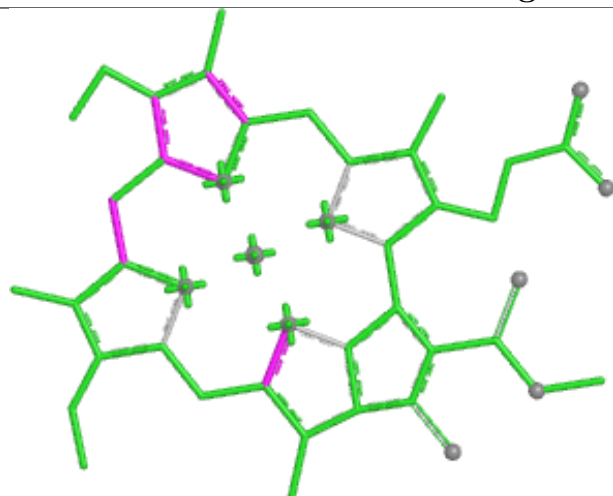
Torsions



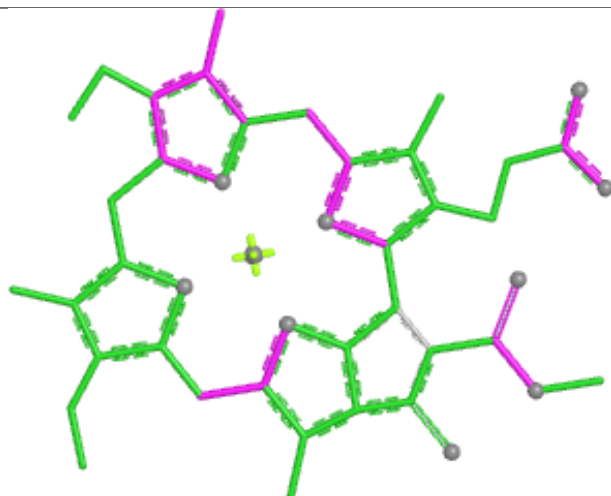
Rings



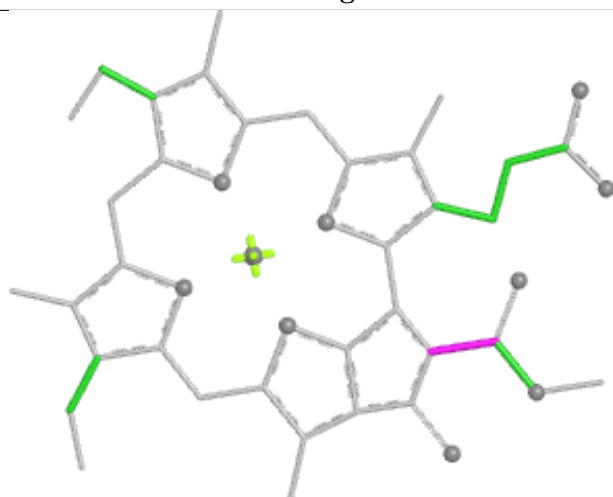
Ligand CLA 7 607



Bond lengths



Bond angles

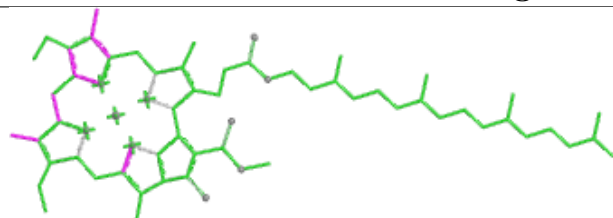


Torsions

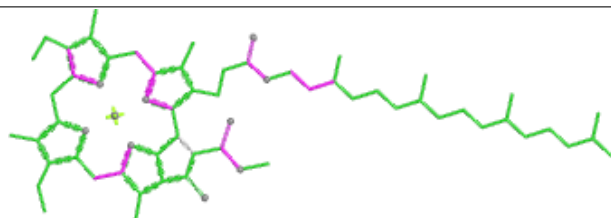


Rings

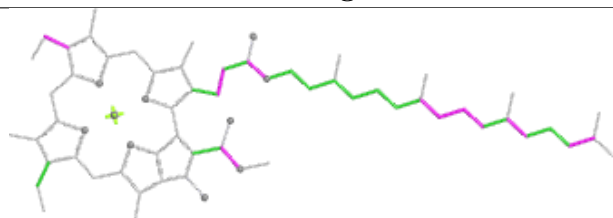
Ligand CLA A 812



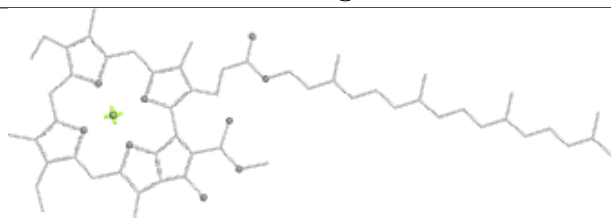
Bond lengths



Bond angles

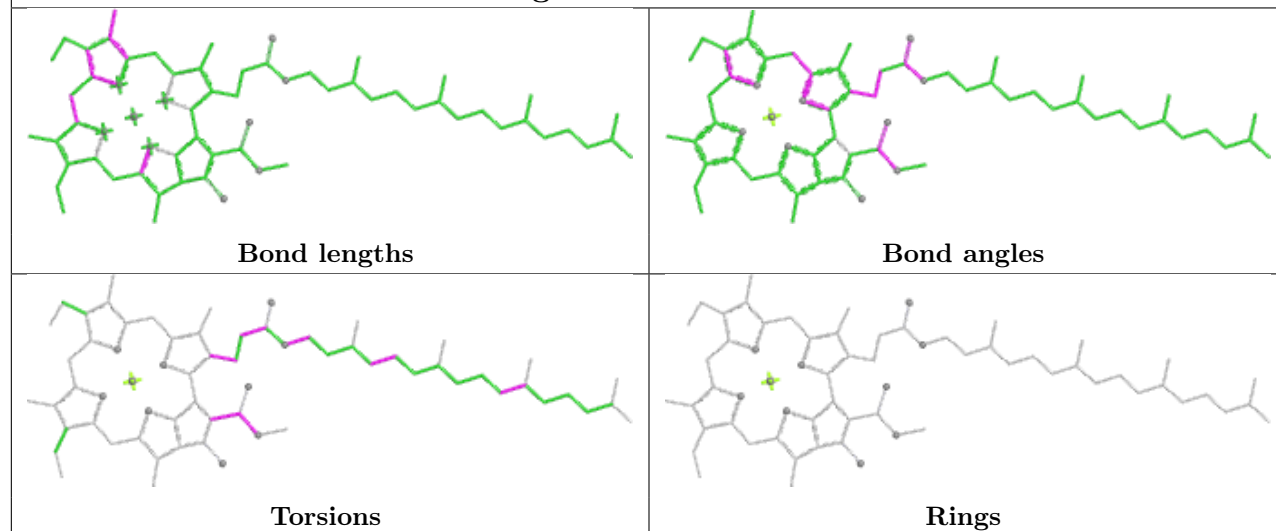


Torsions

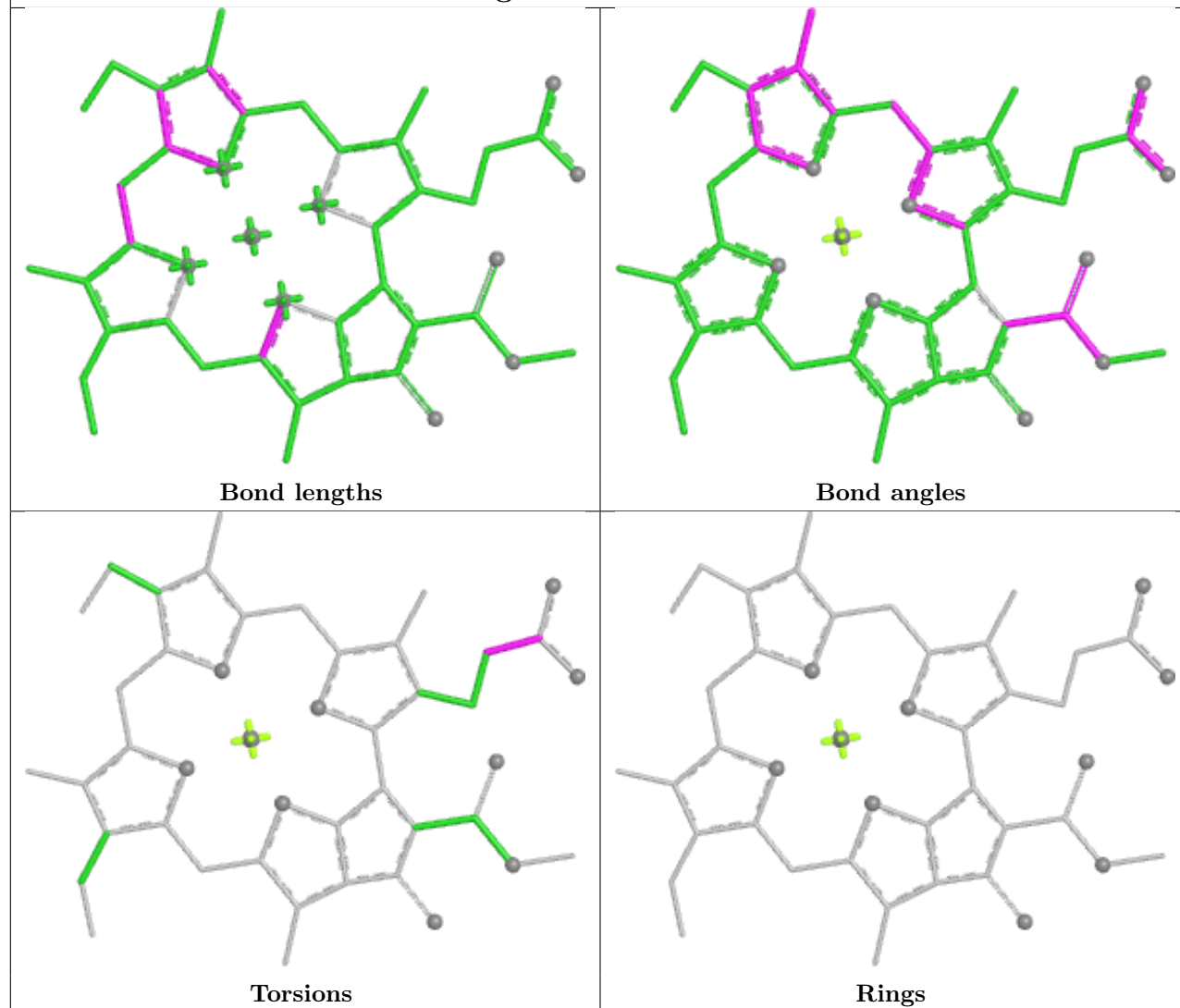


Rings

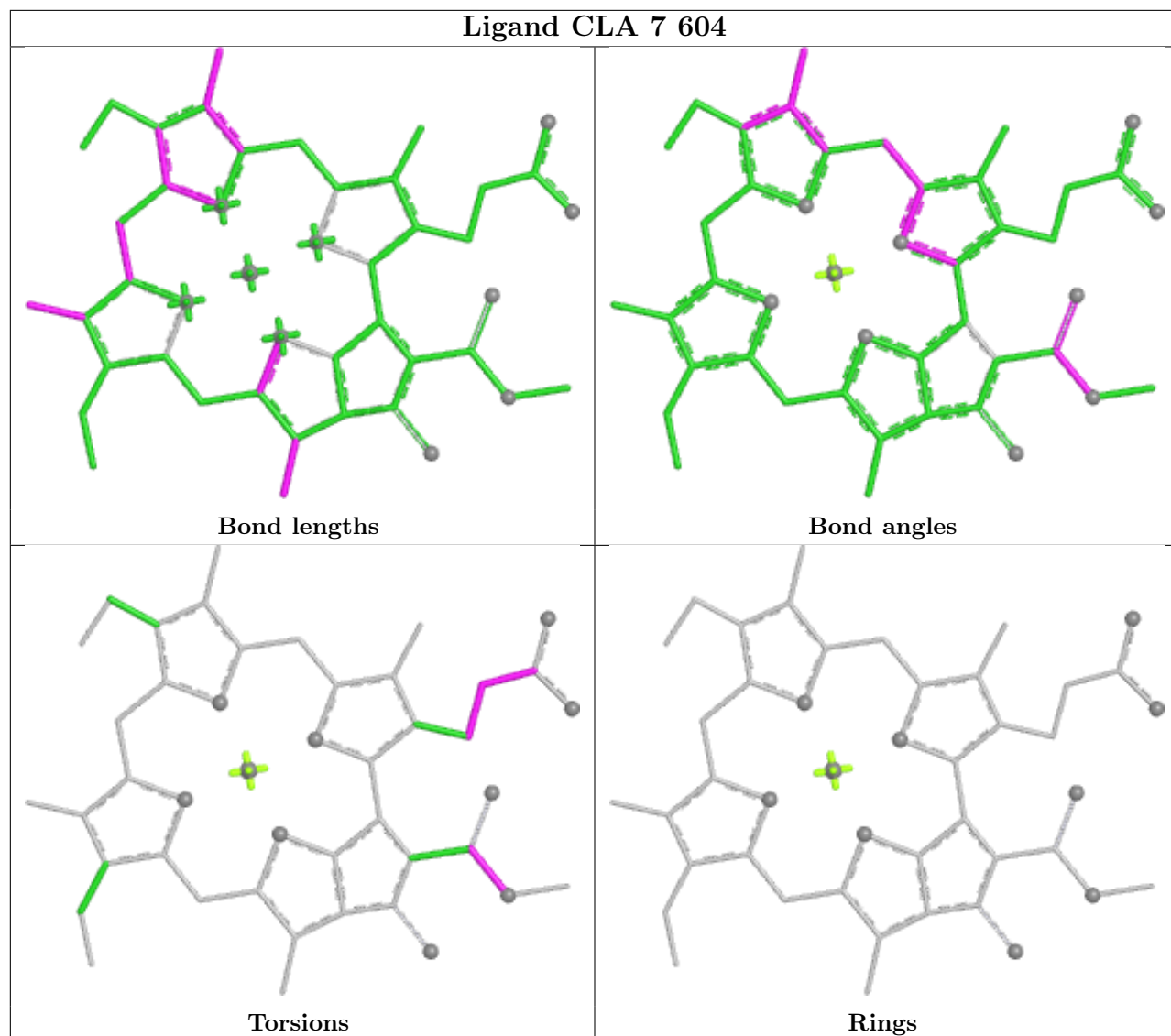
Ligand CLA B 809



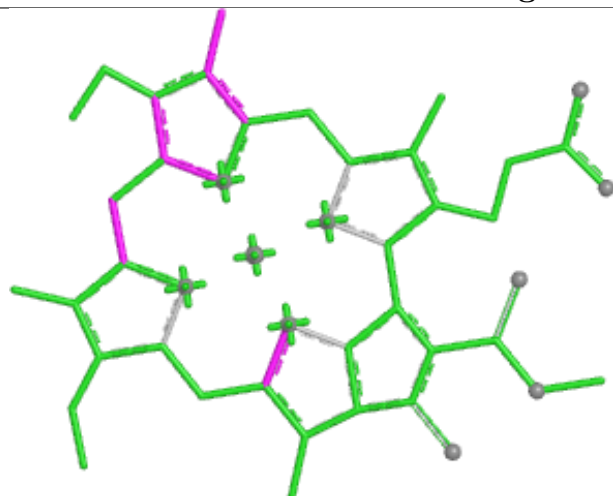
Ligand CLA 7 603



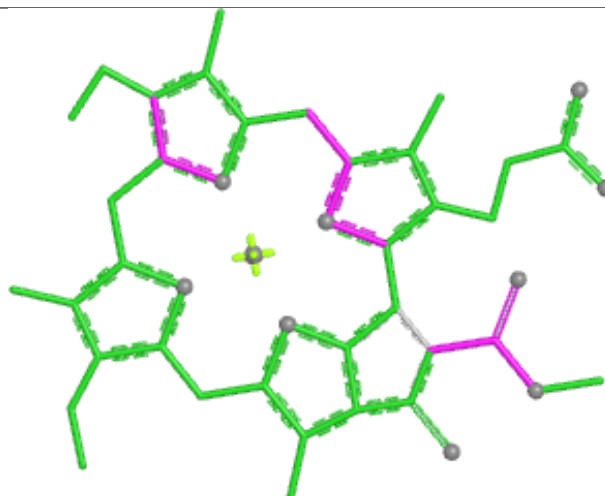
Ligand CLA 7 604



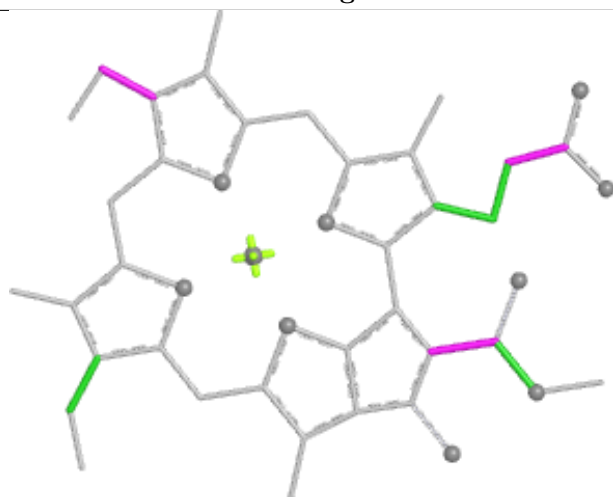
Ligand CLA 3 302



Bond lengths



Bond angles

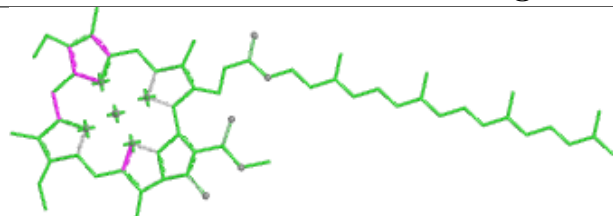


Torsions

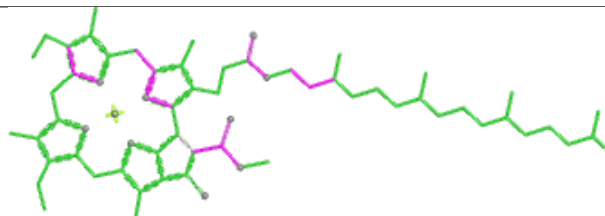


Rings

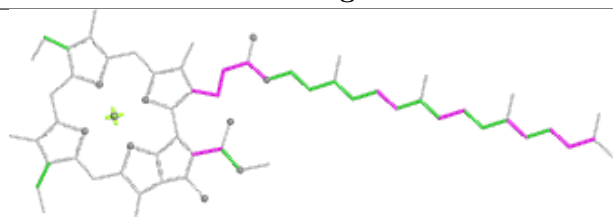
Ligand CLA A 807



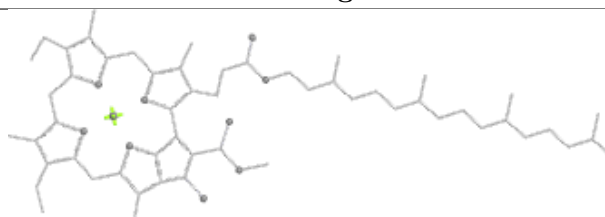
Bond lengths



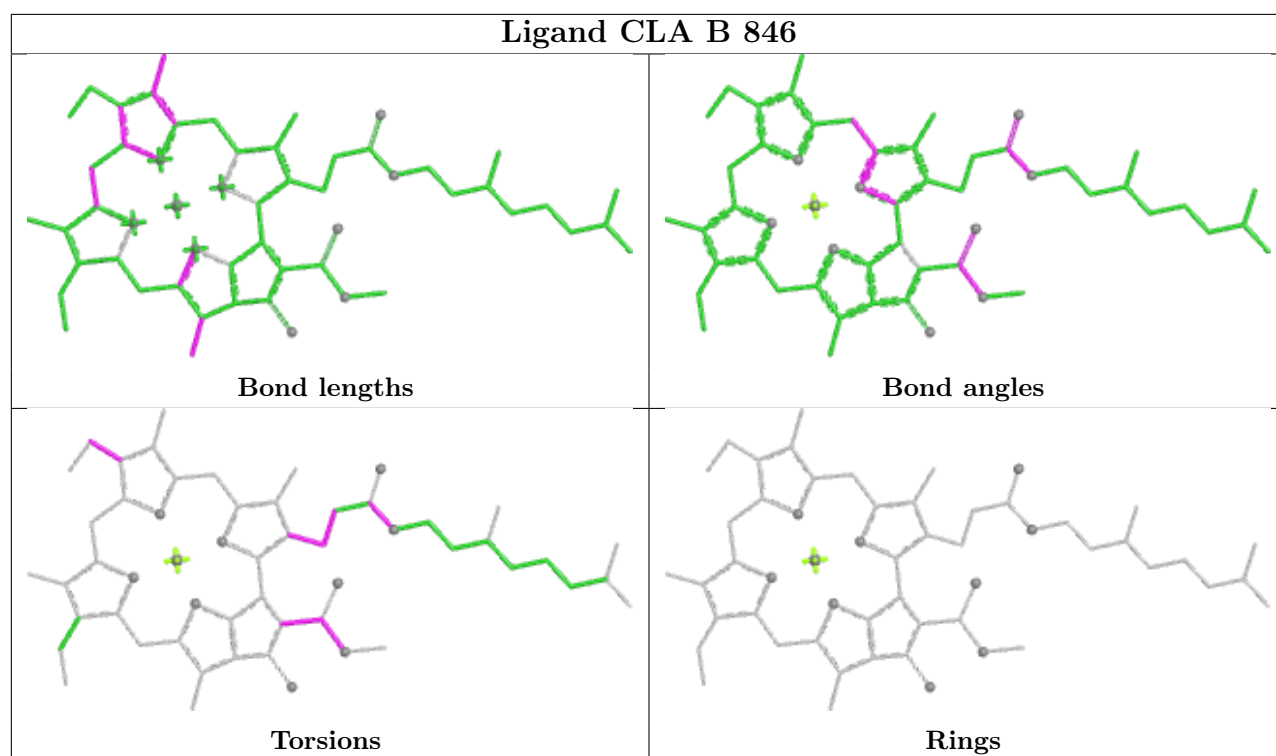
Bond angles



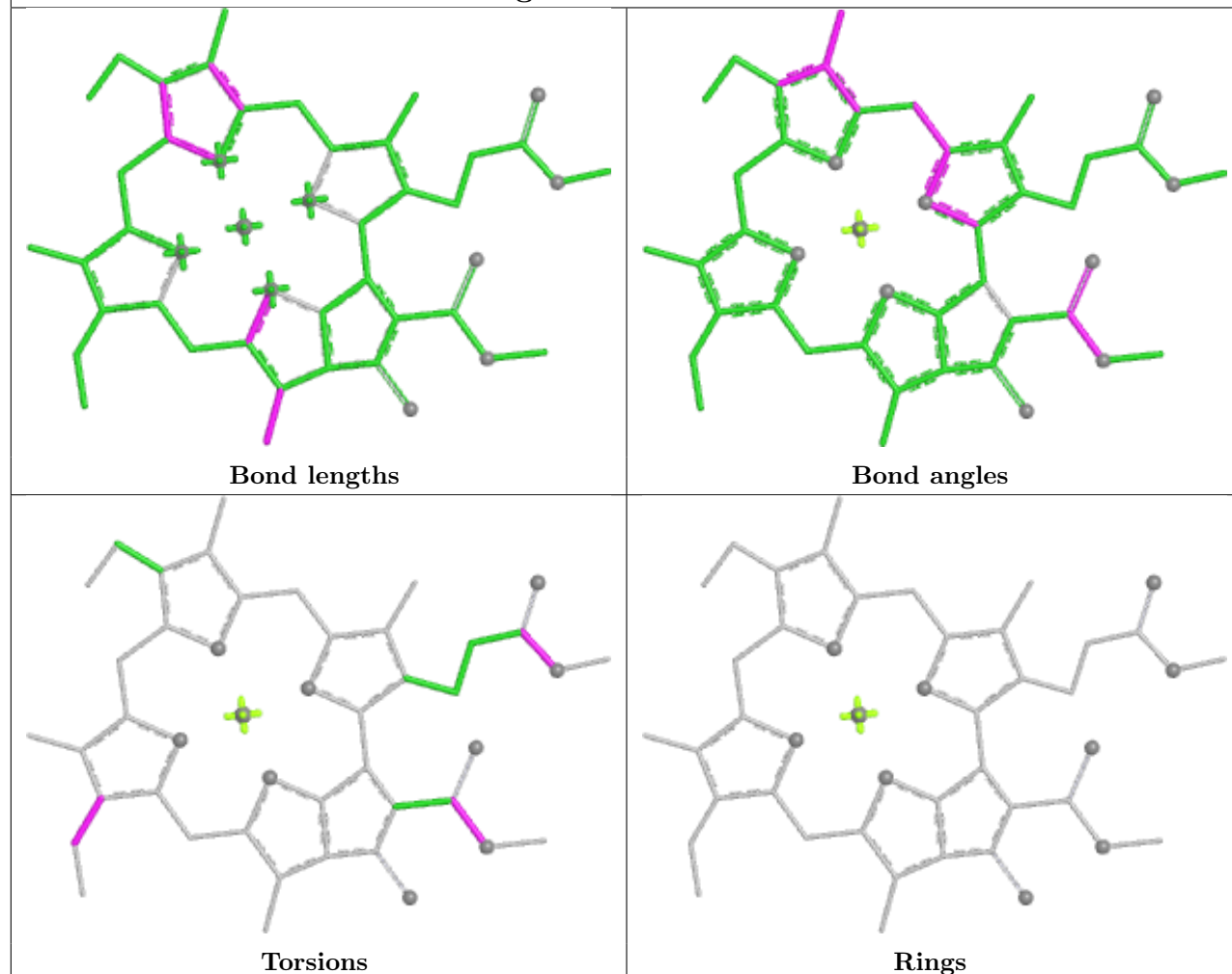
Torsions



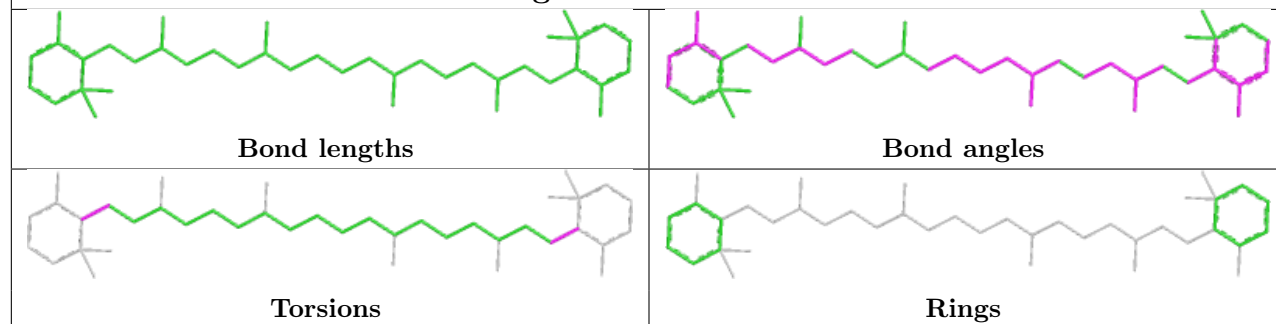
Rings



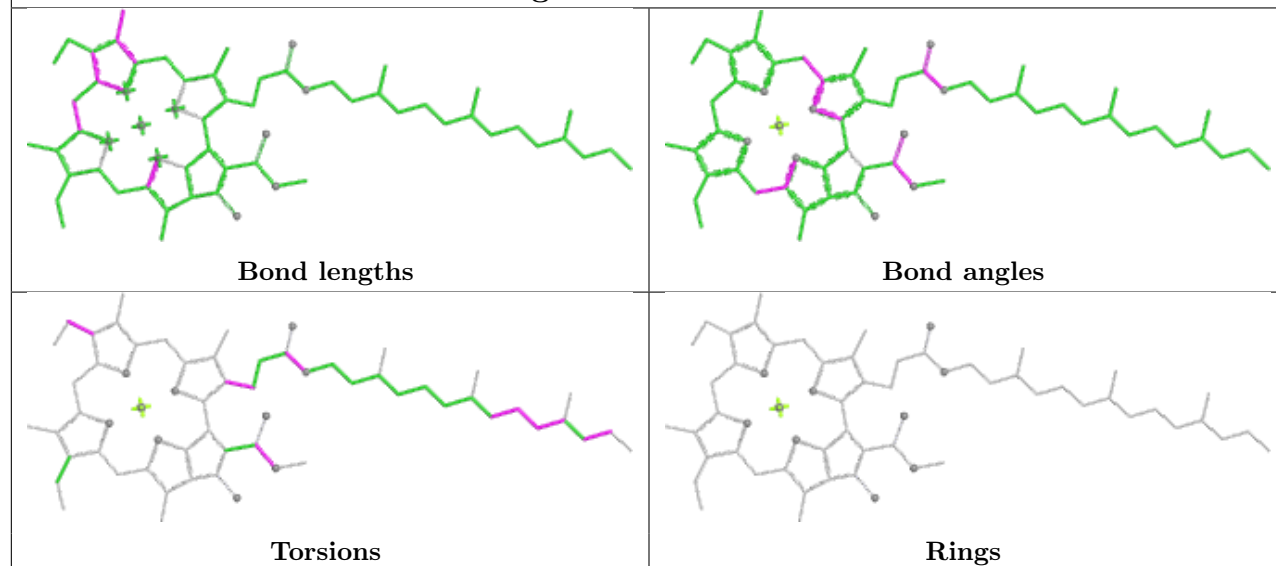
Ligand CLA L 205



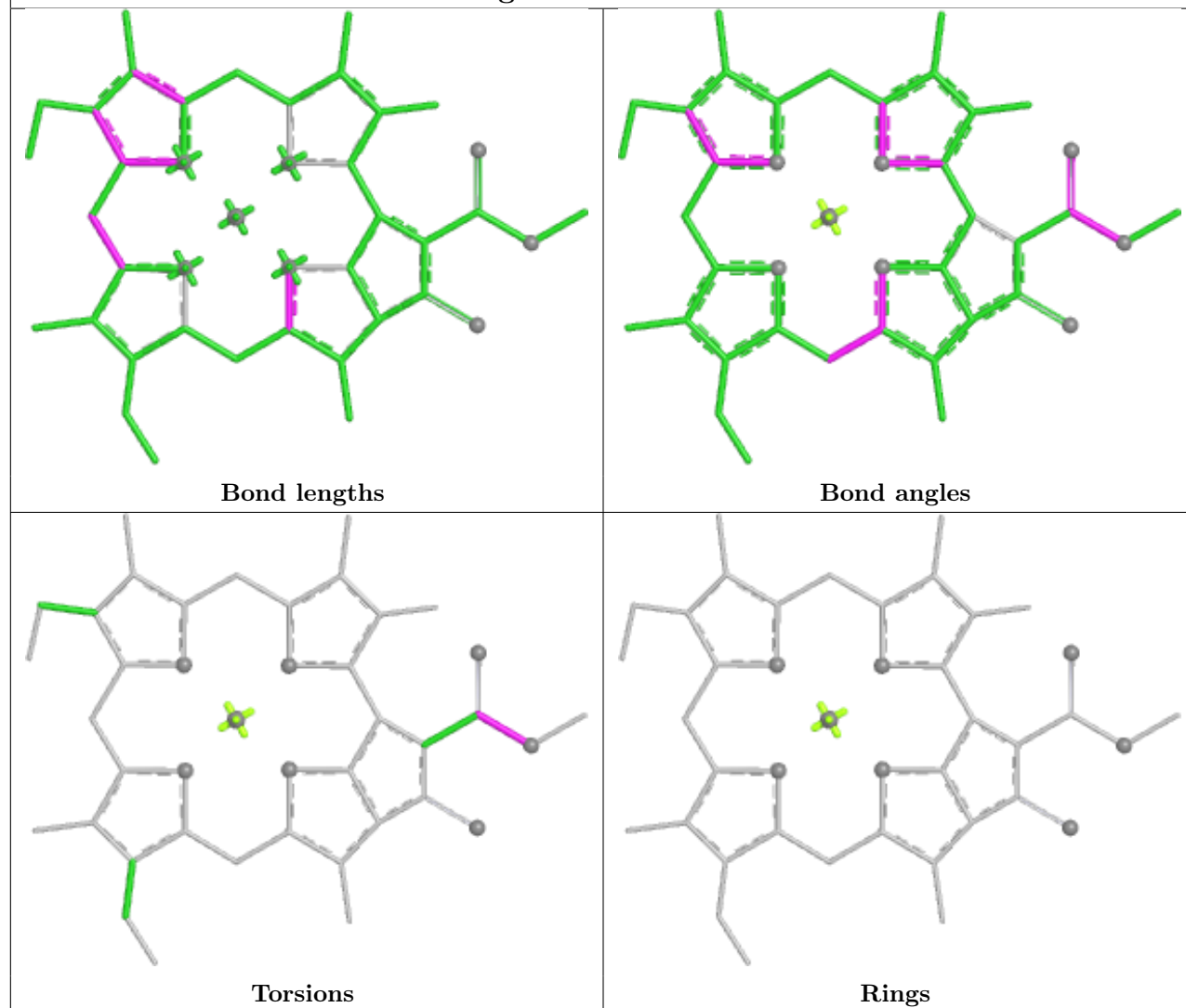
Ligand BCR L 206



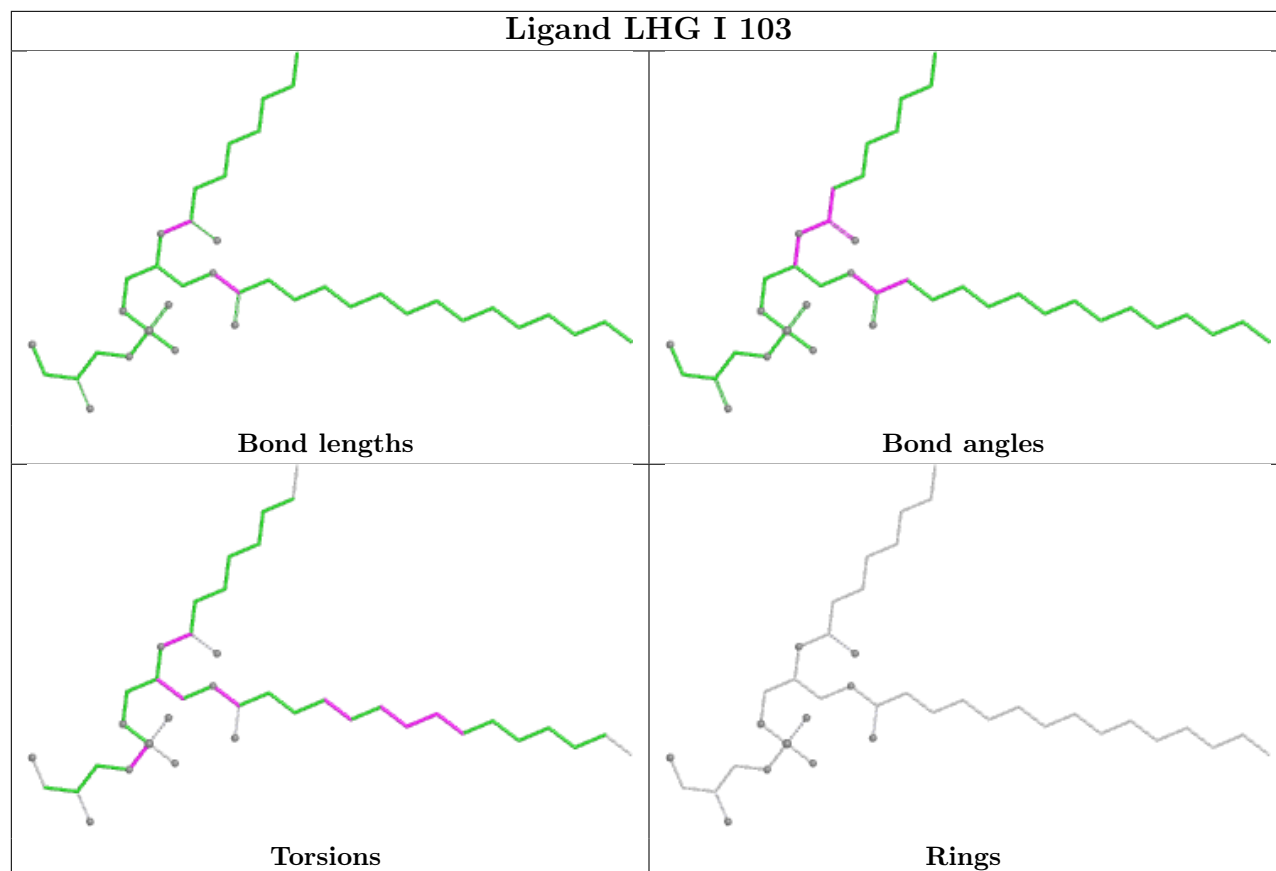
Ligand CLA A 810



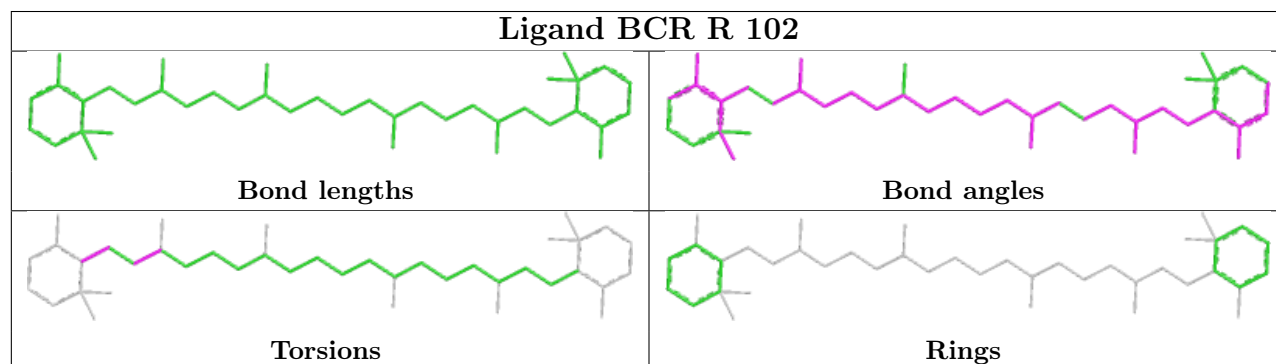
Ligand CLA 4 610

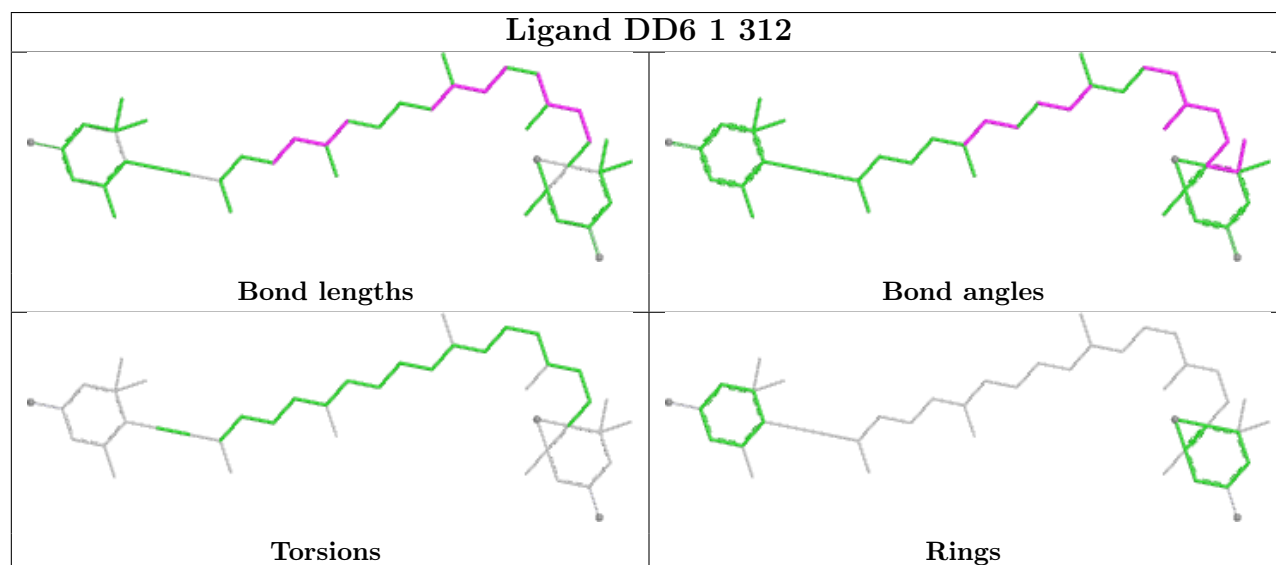
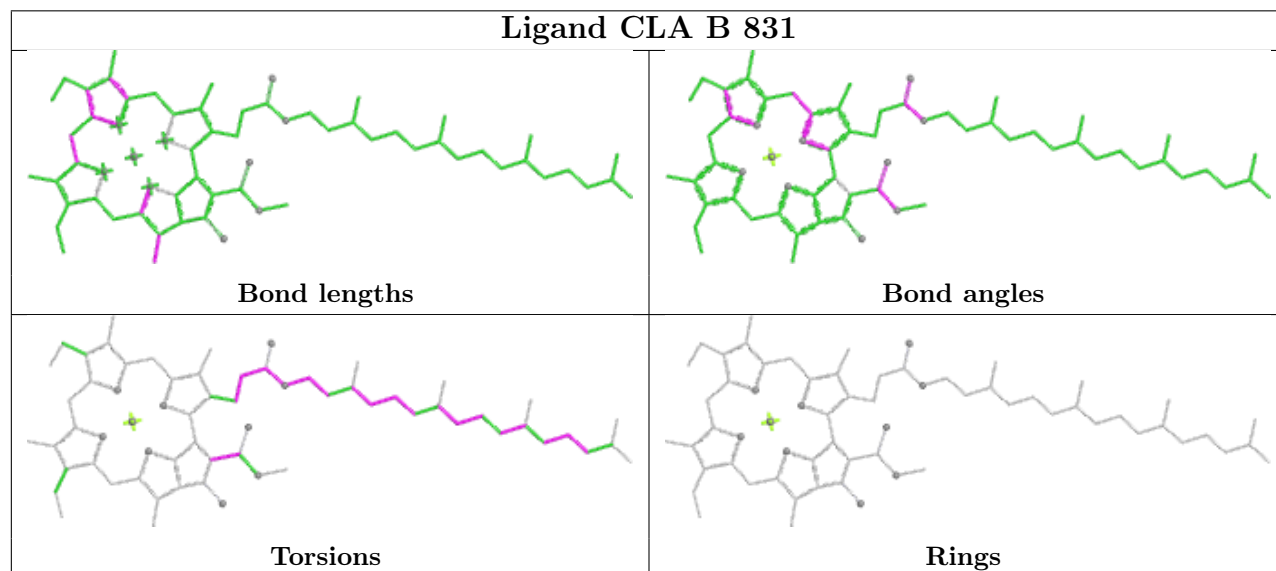
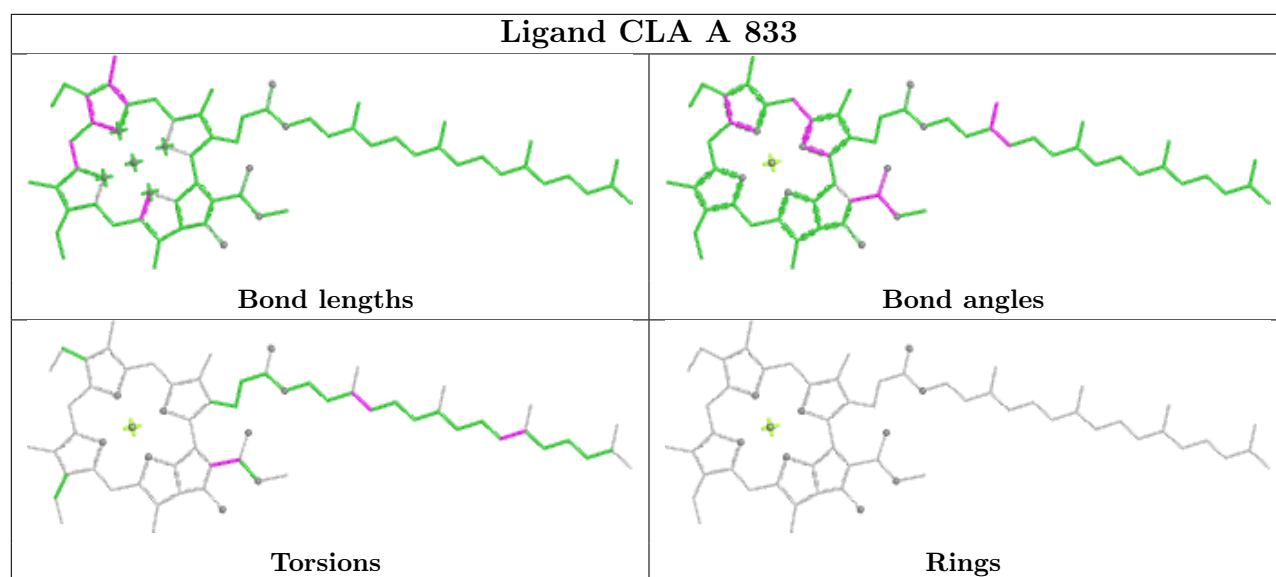


Ligand LHG I 103

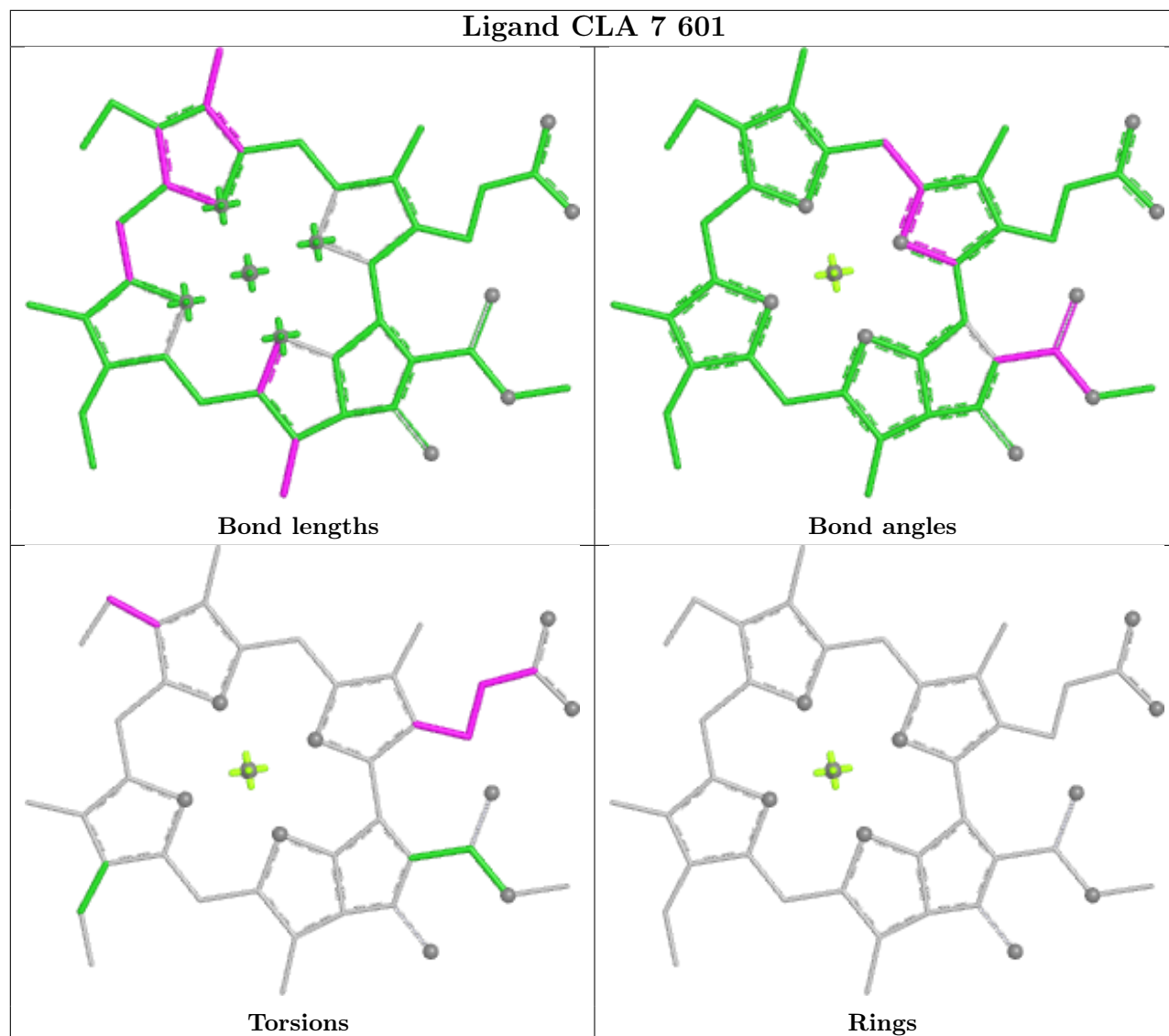


Ligand BCR R 102

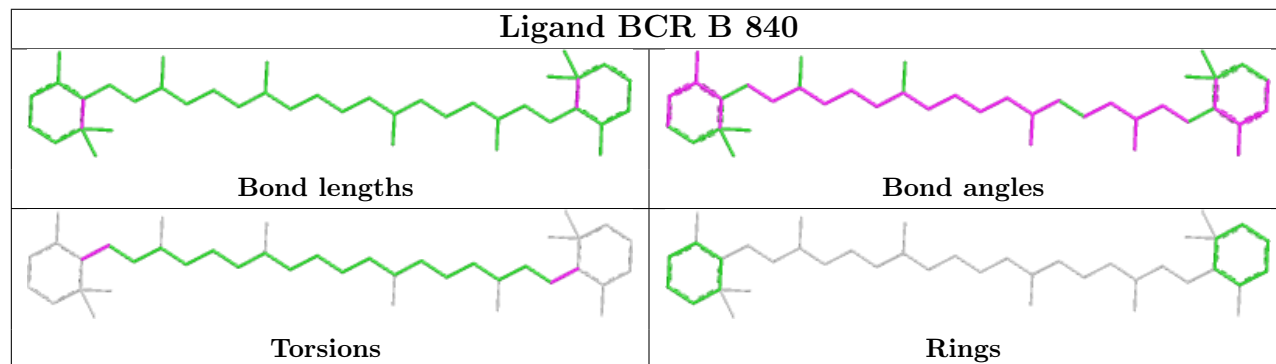


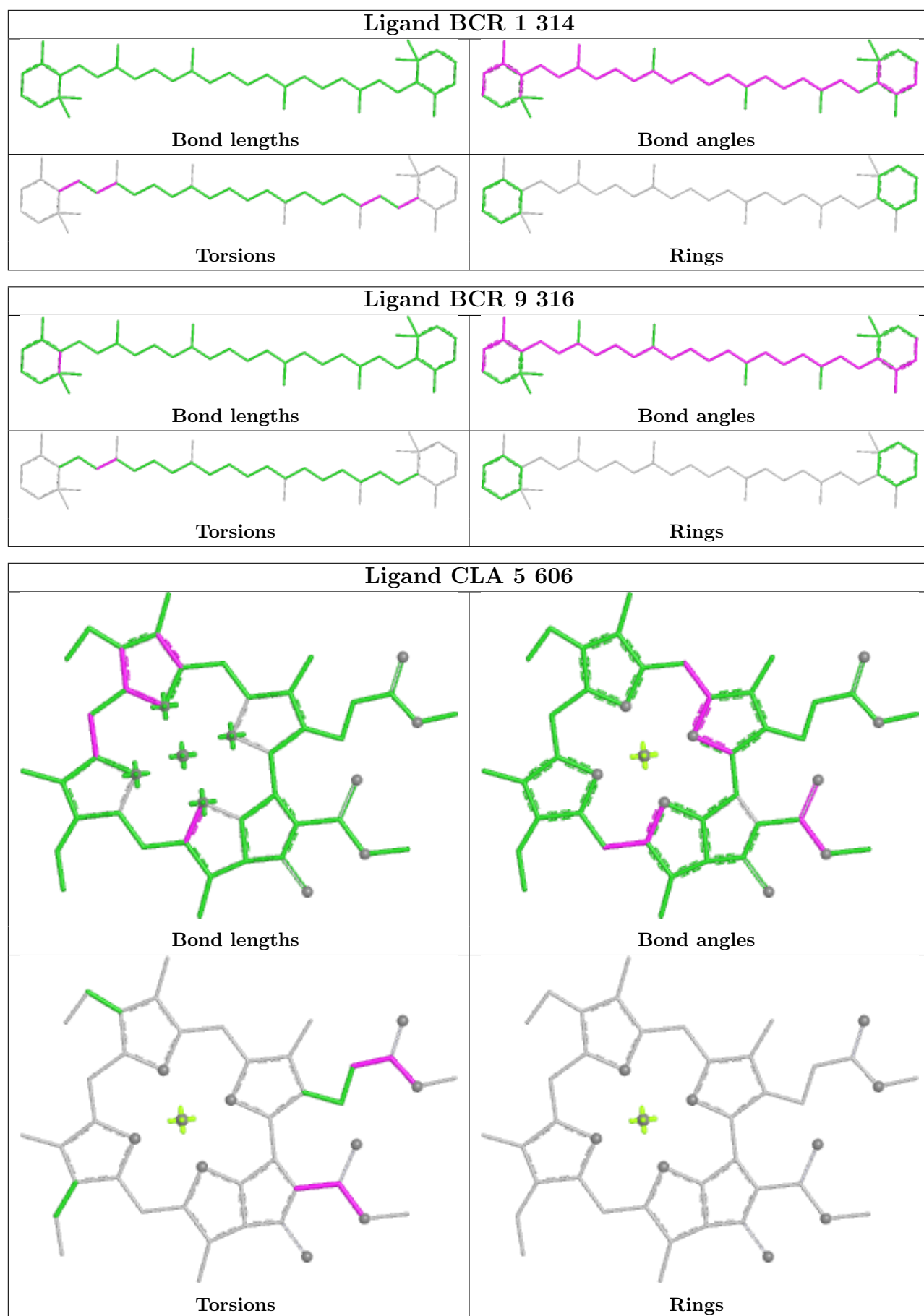


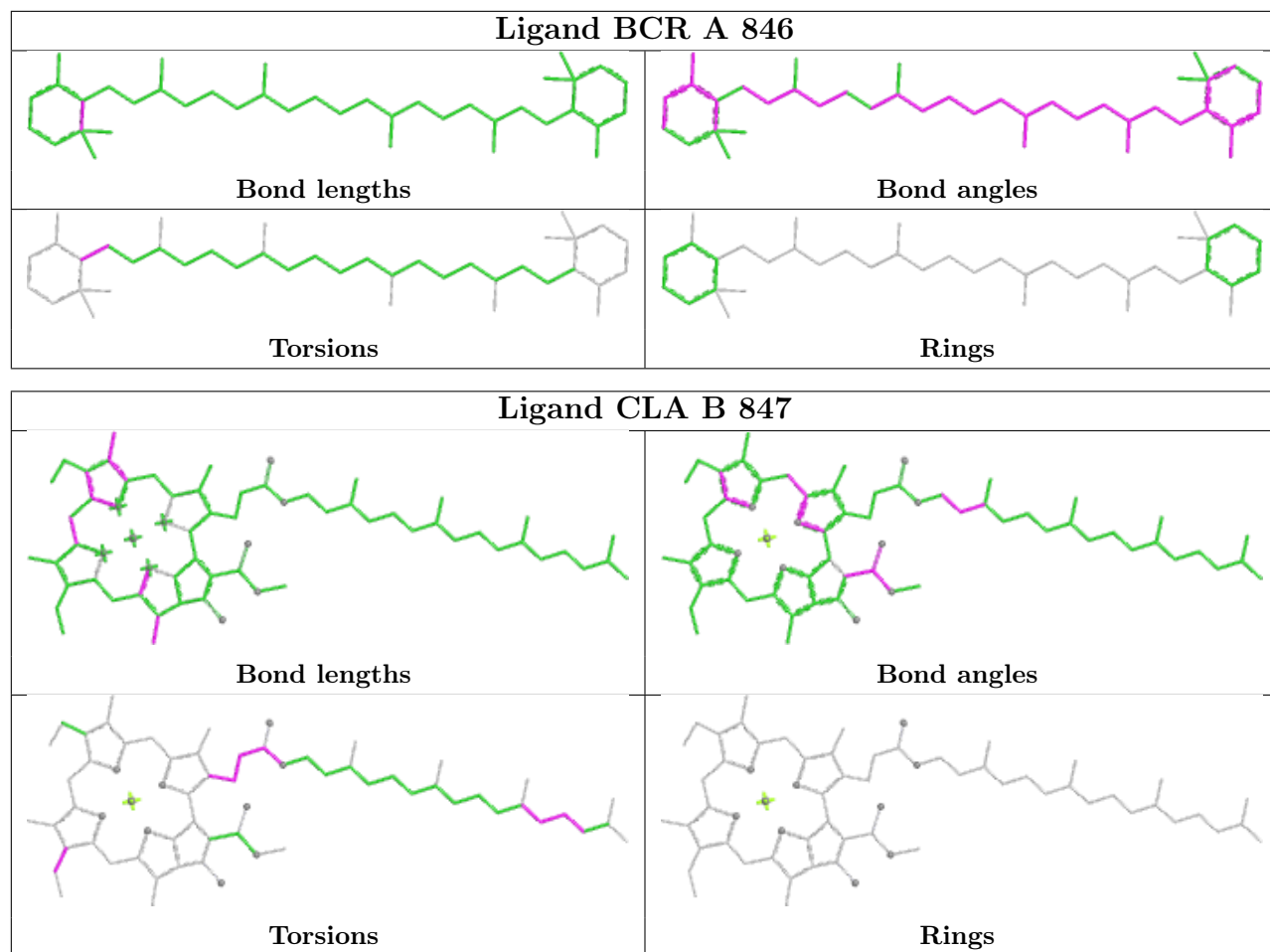
Ligand CLA 7 601



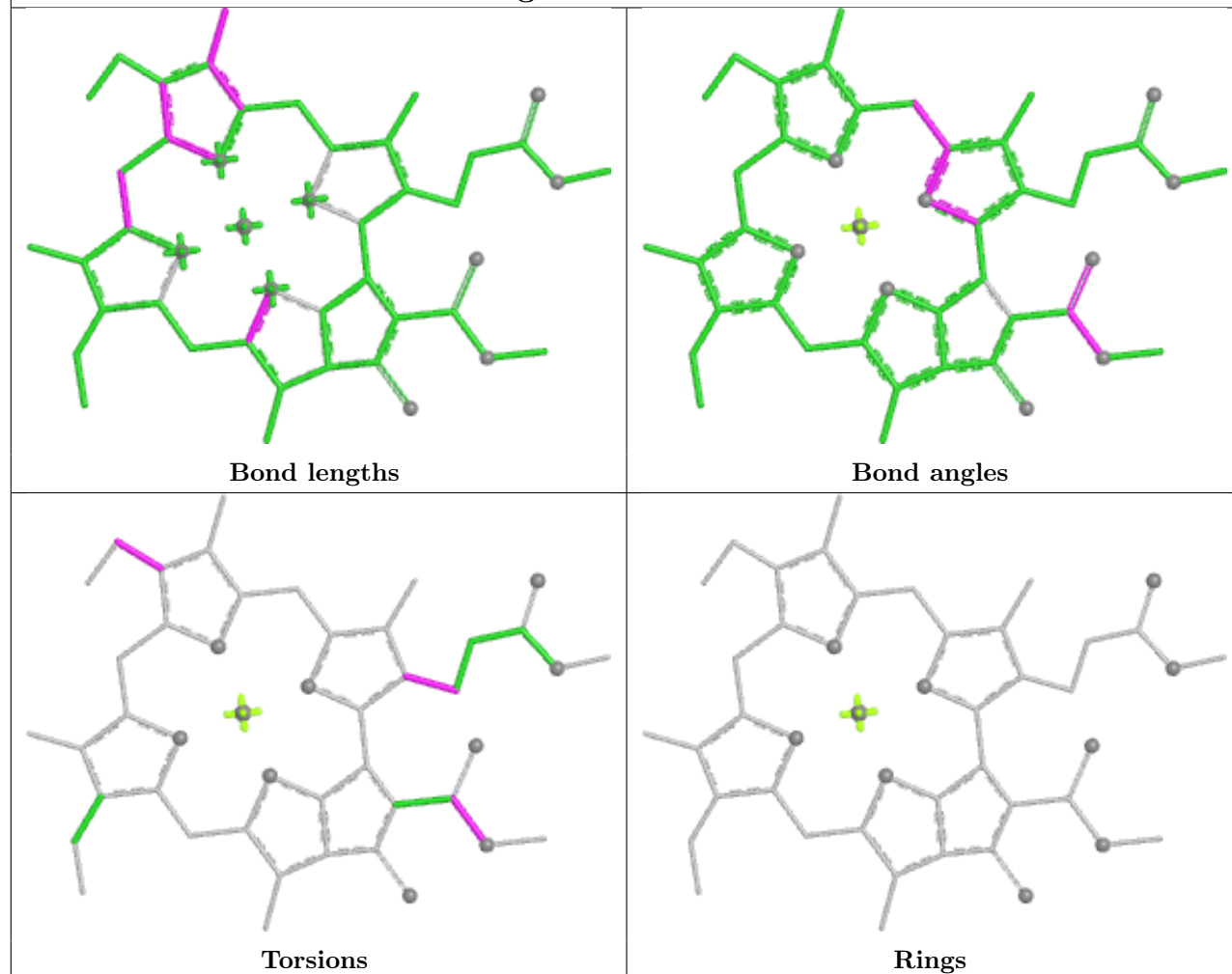
Ligand BCR B 840



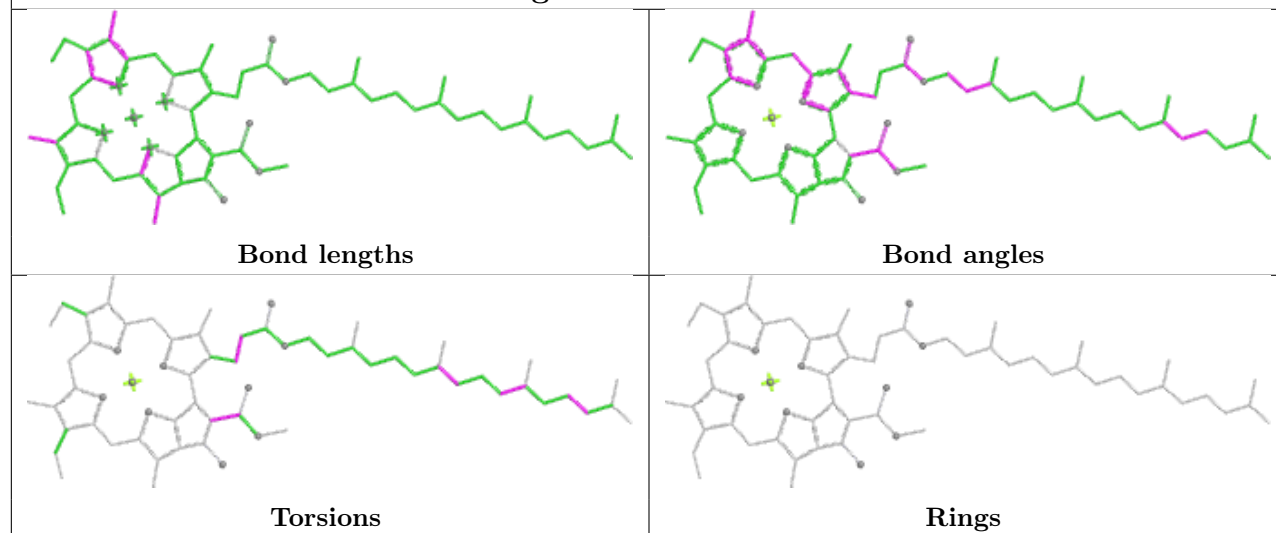


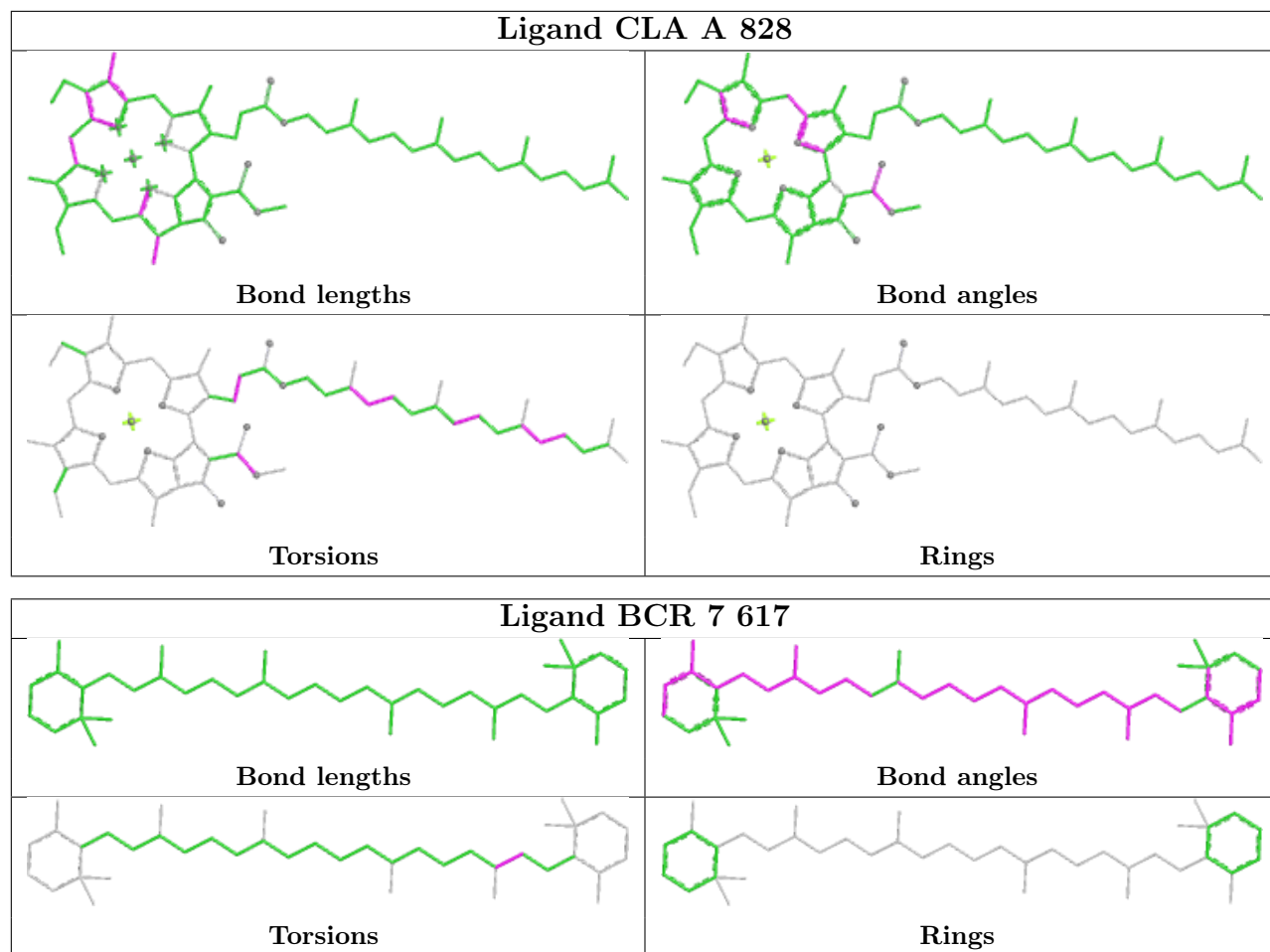


Ligand CLA 1 308

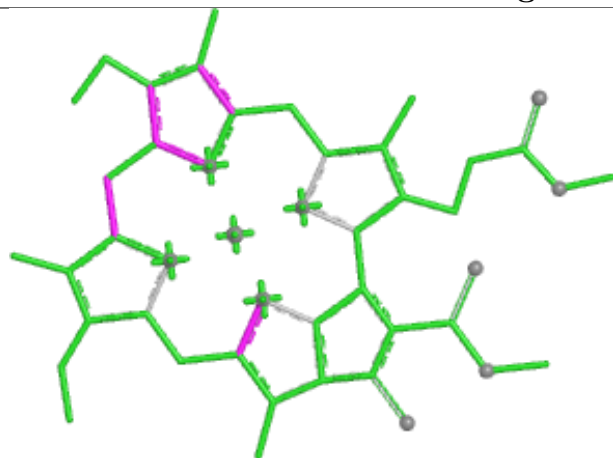


Ligand CLA A 860

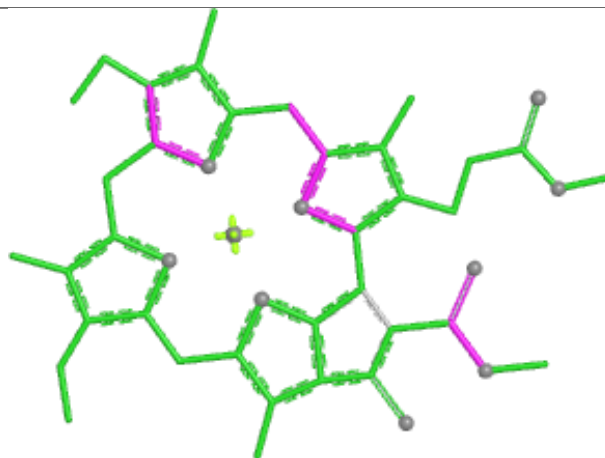




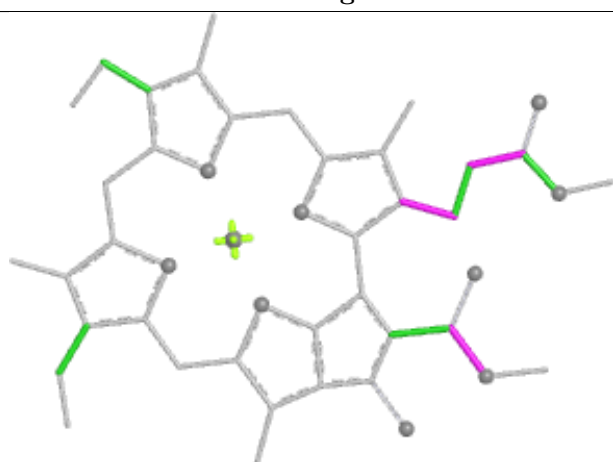
Ligand CLA k 305



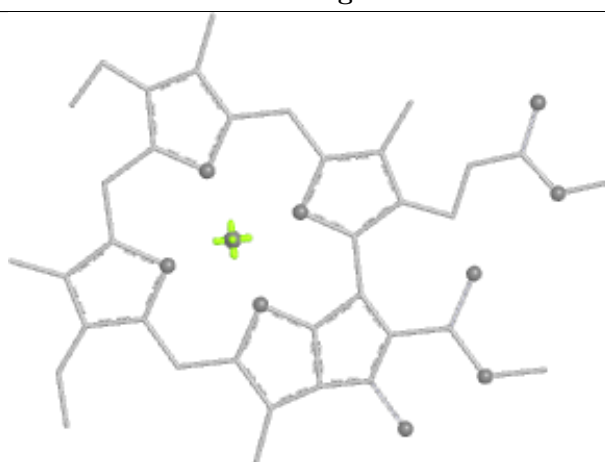
Bond lengths



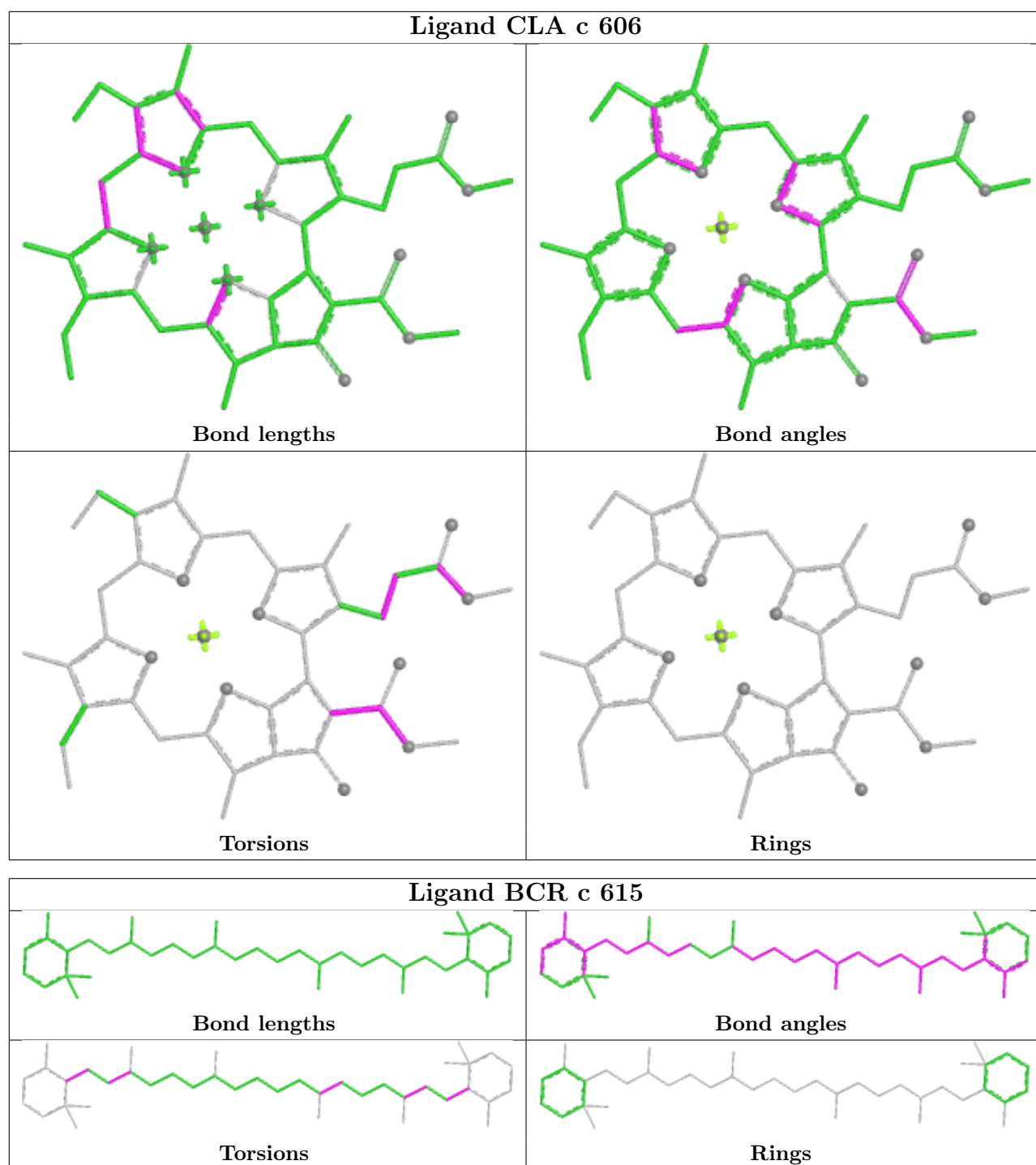
Bond angles



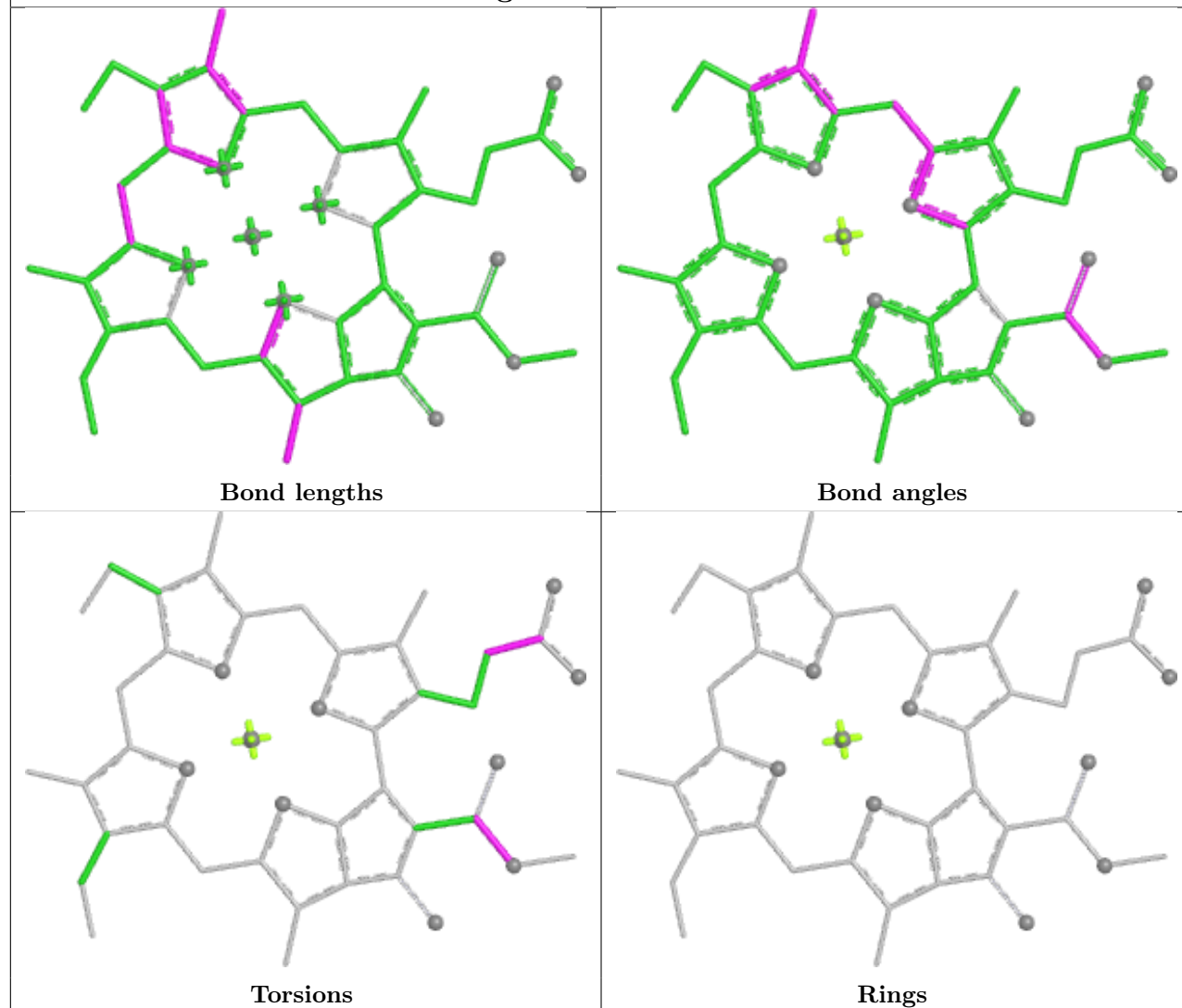
Torsions



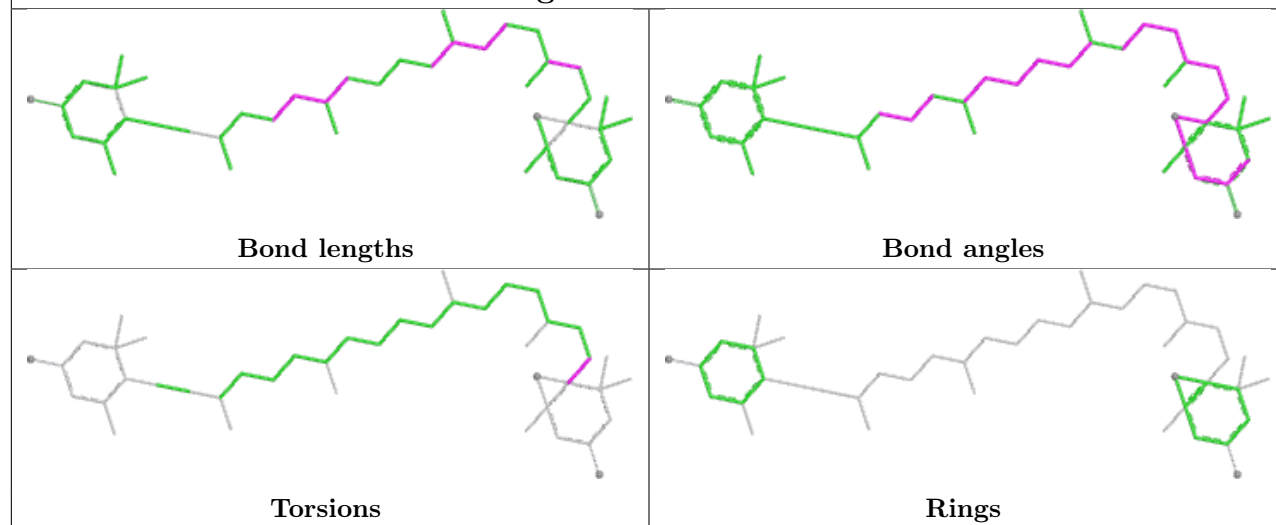
Rings



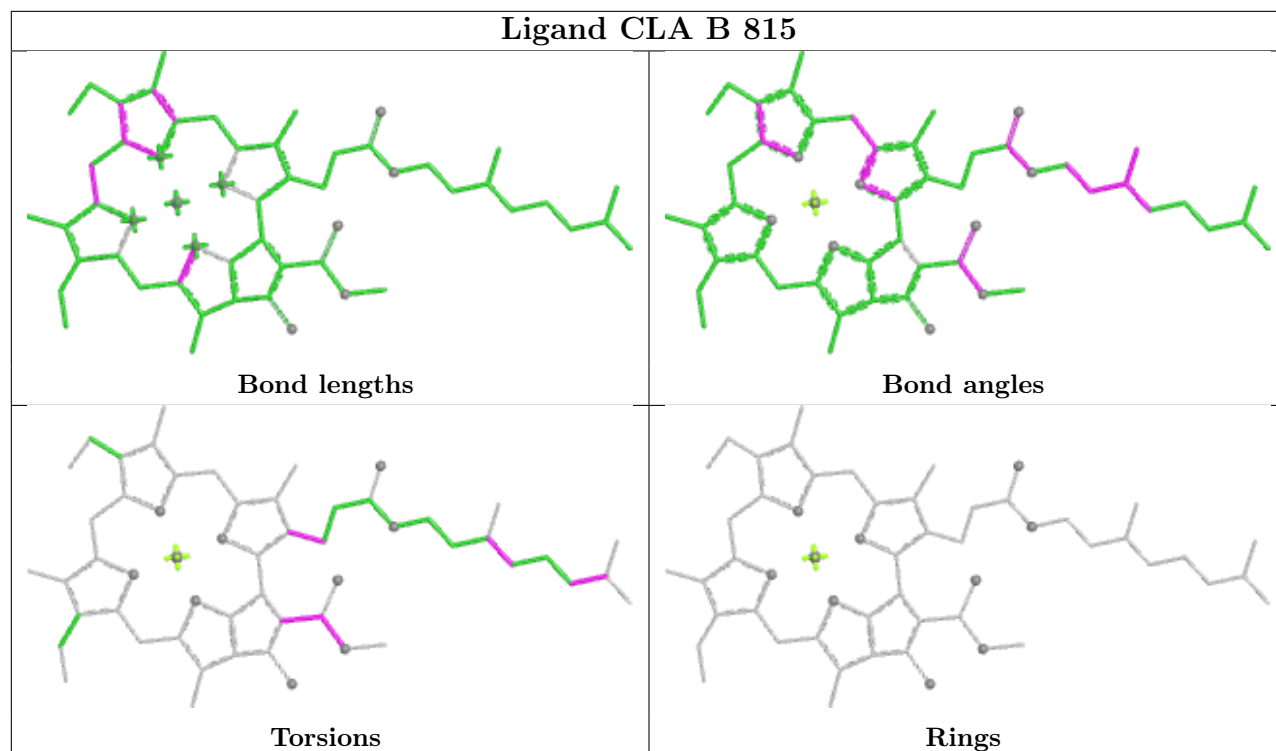
Ligand CLA 9 311



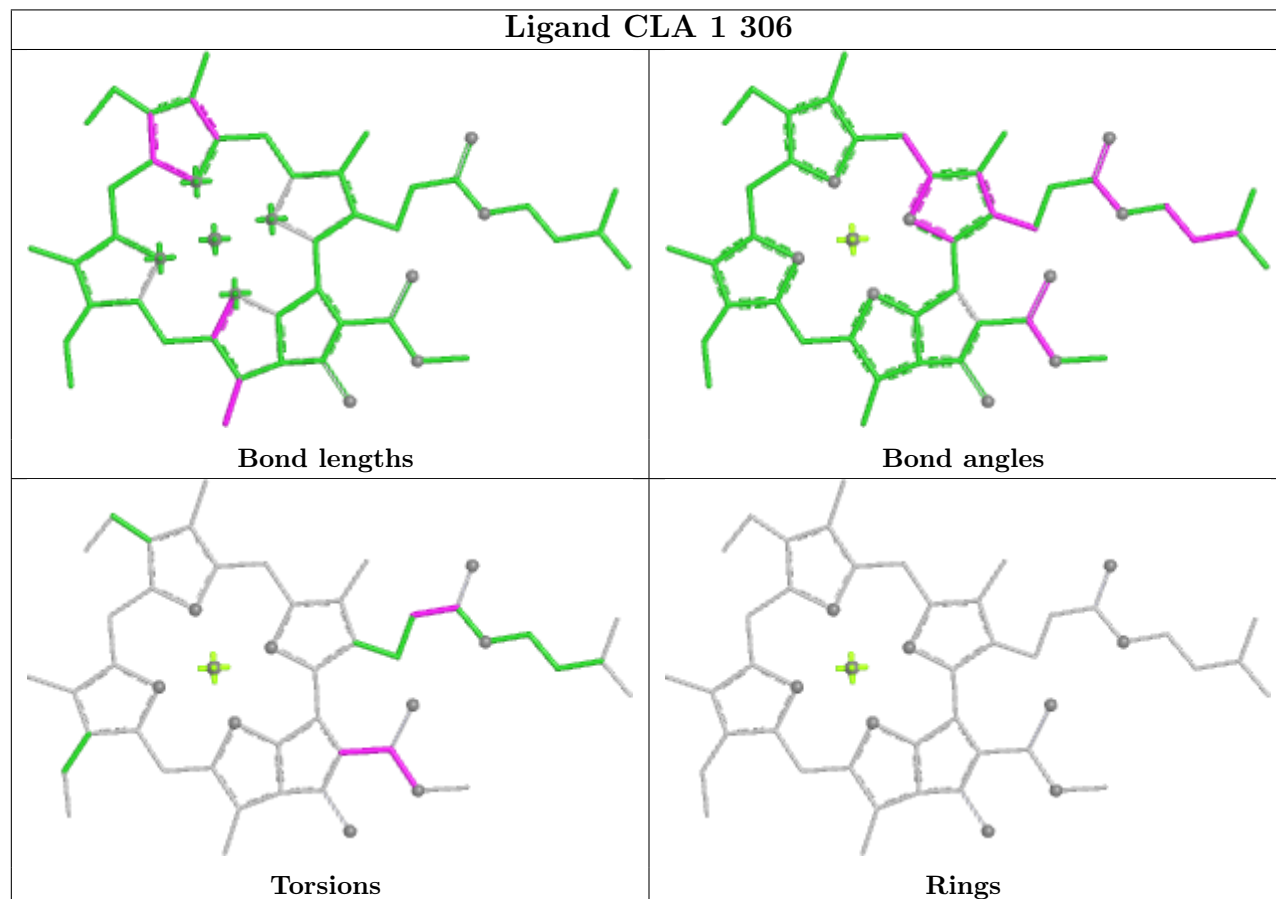
Ligand DD6 3 312

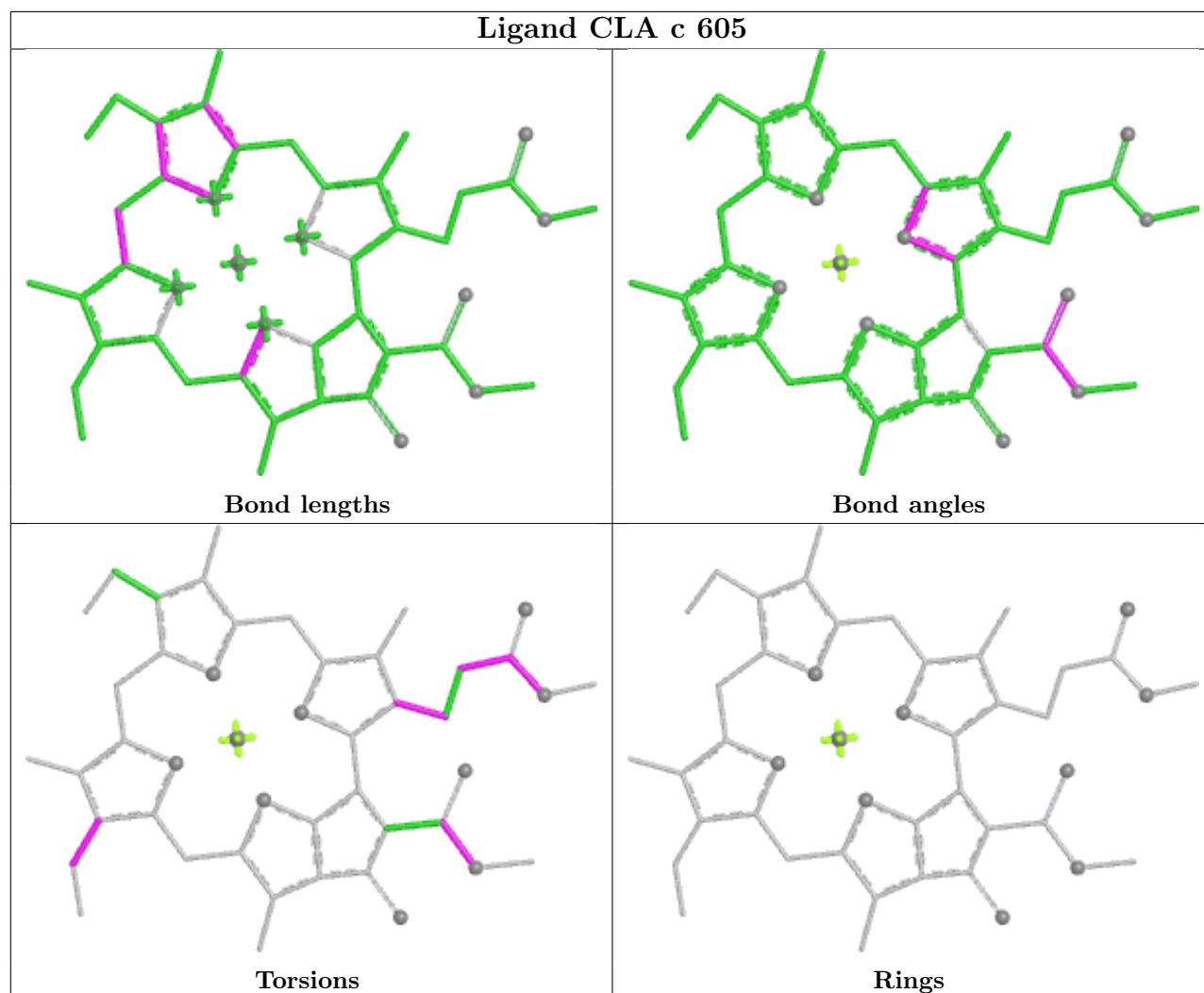
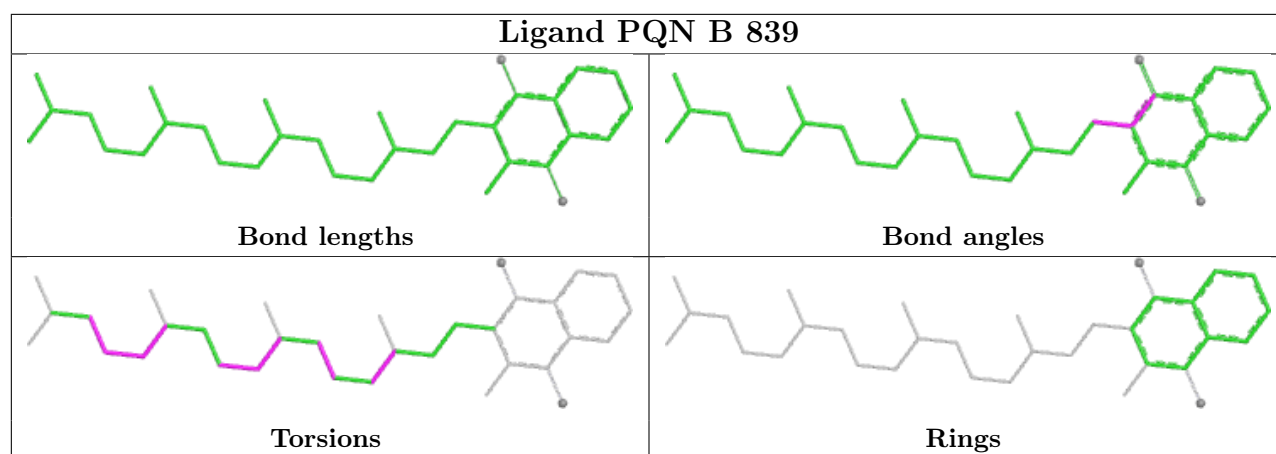


Ligand CLA B 815

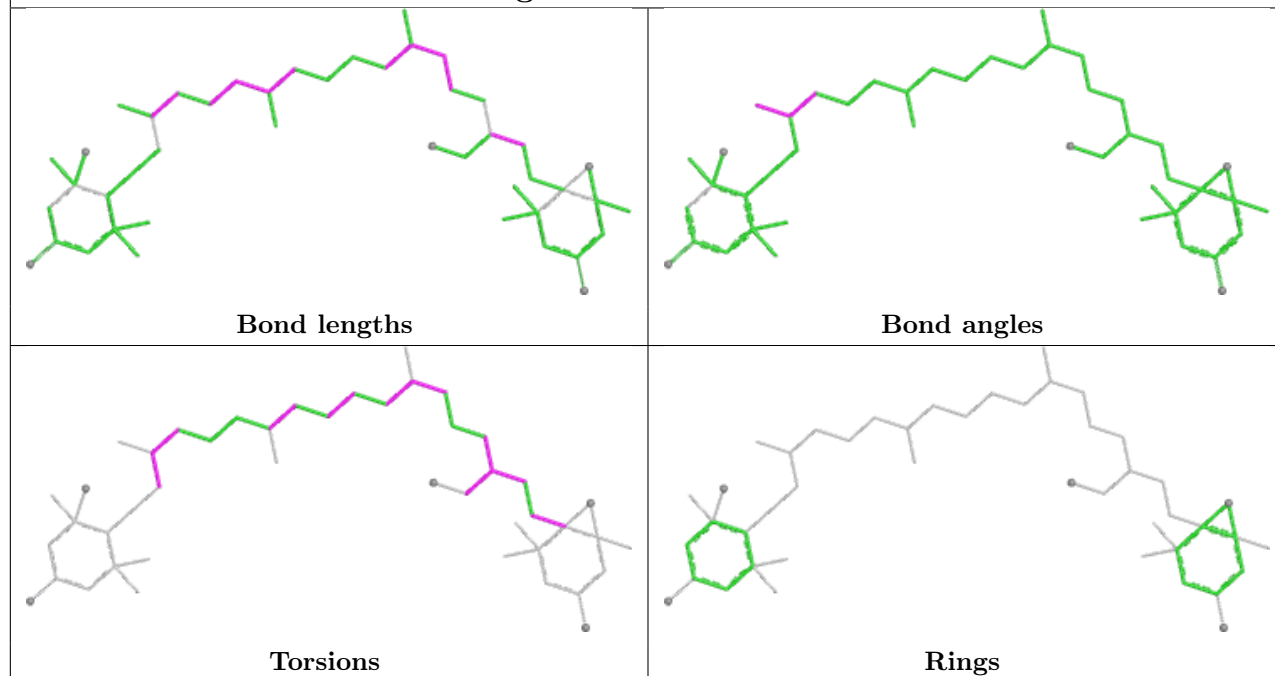


Ligand CLA 1 306

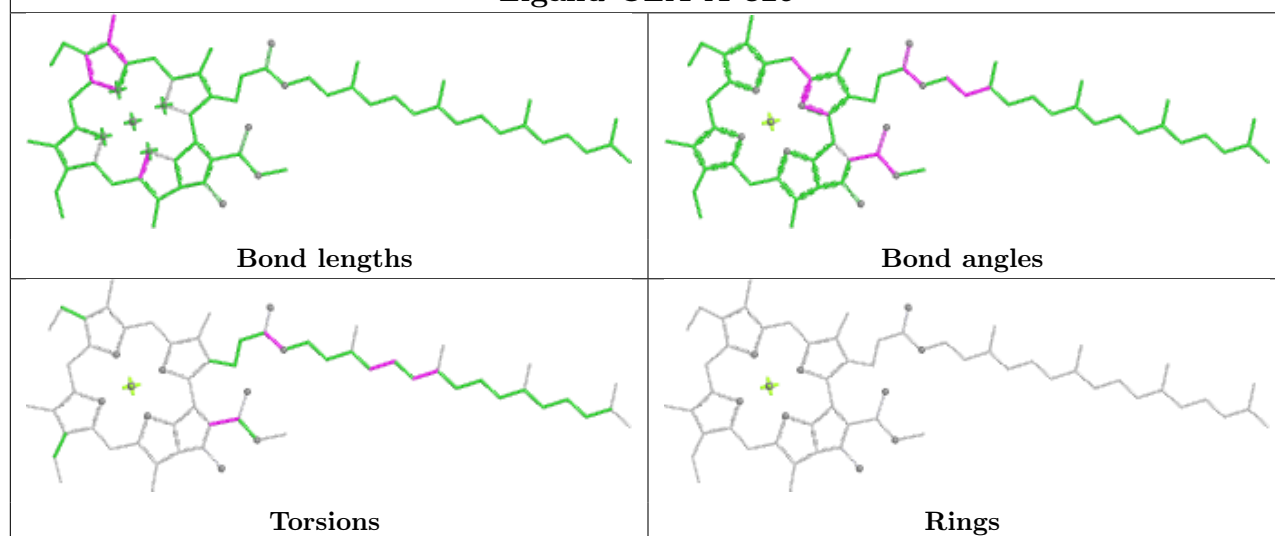




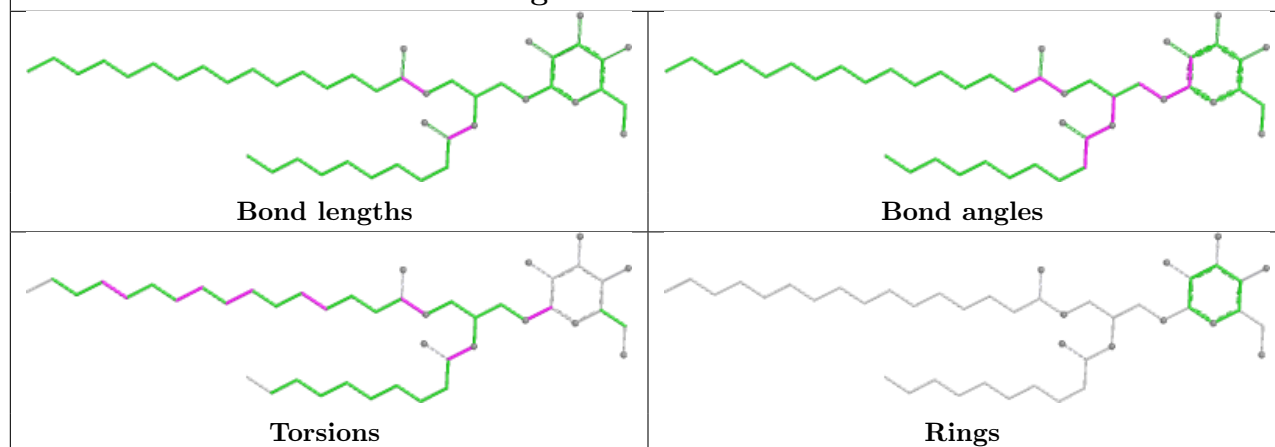
Ligand A1L1G 3 310



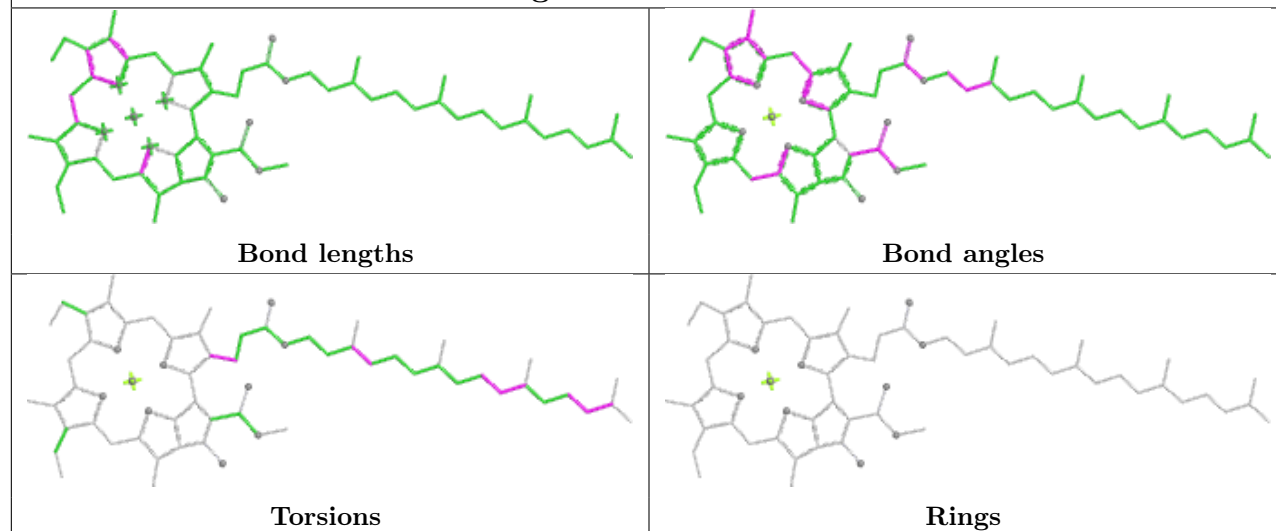
Ligand CLA A 829



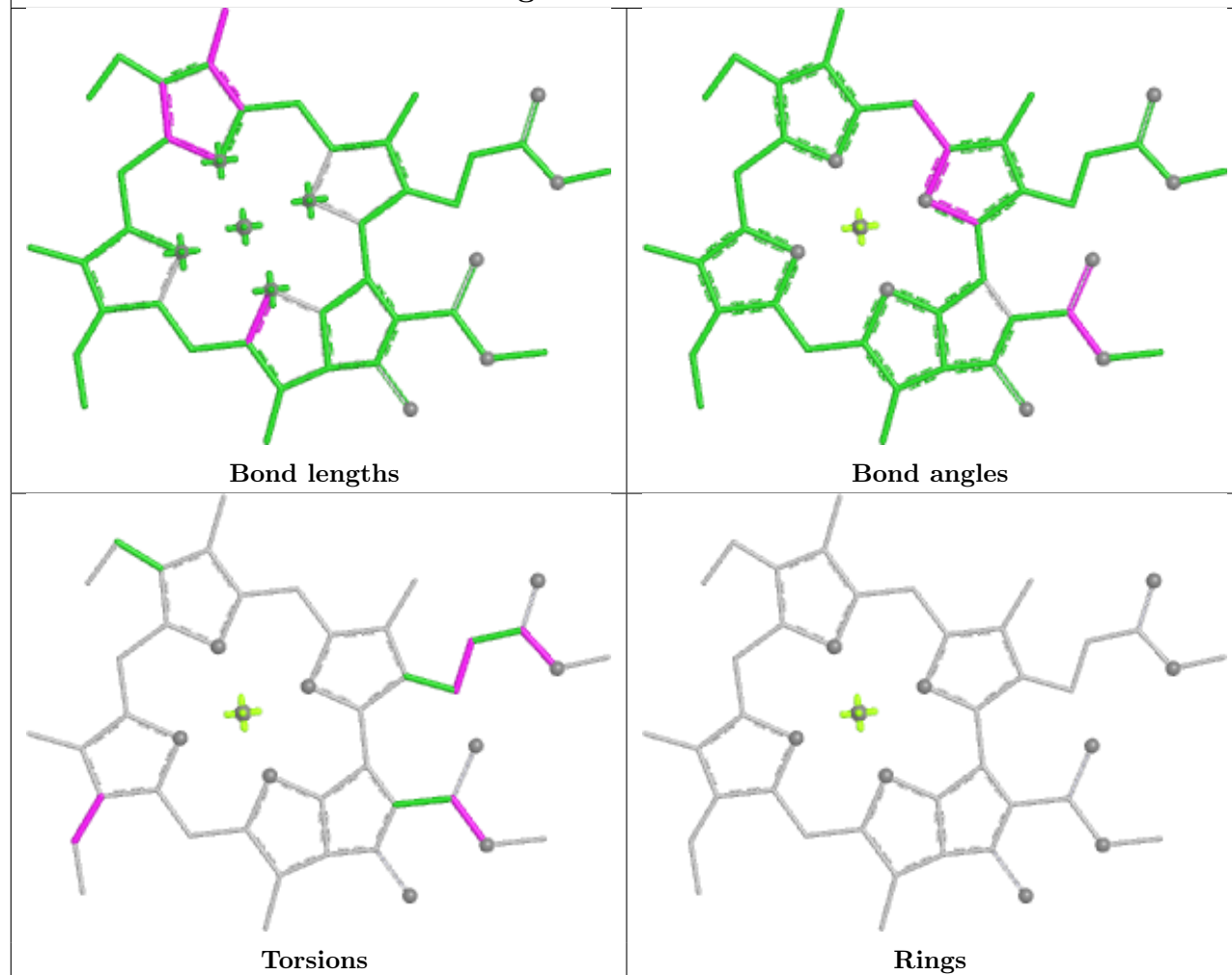
Ligand LMG 2 214



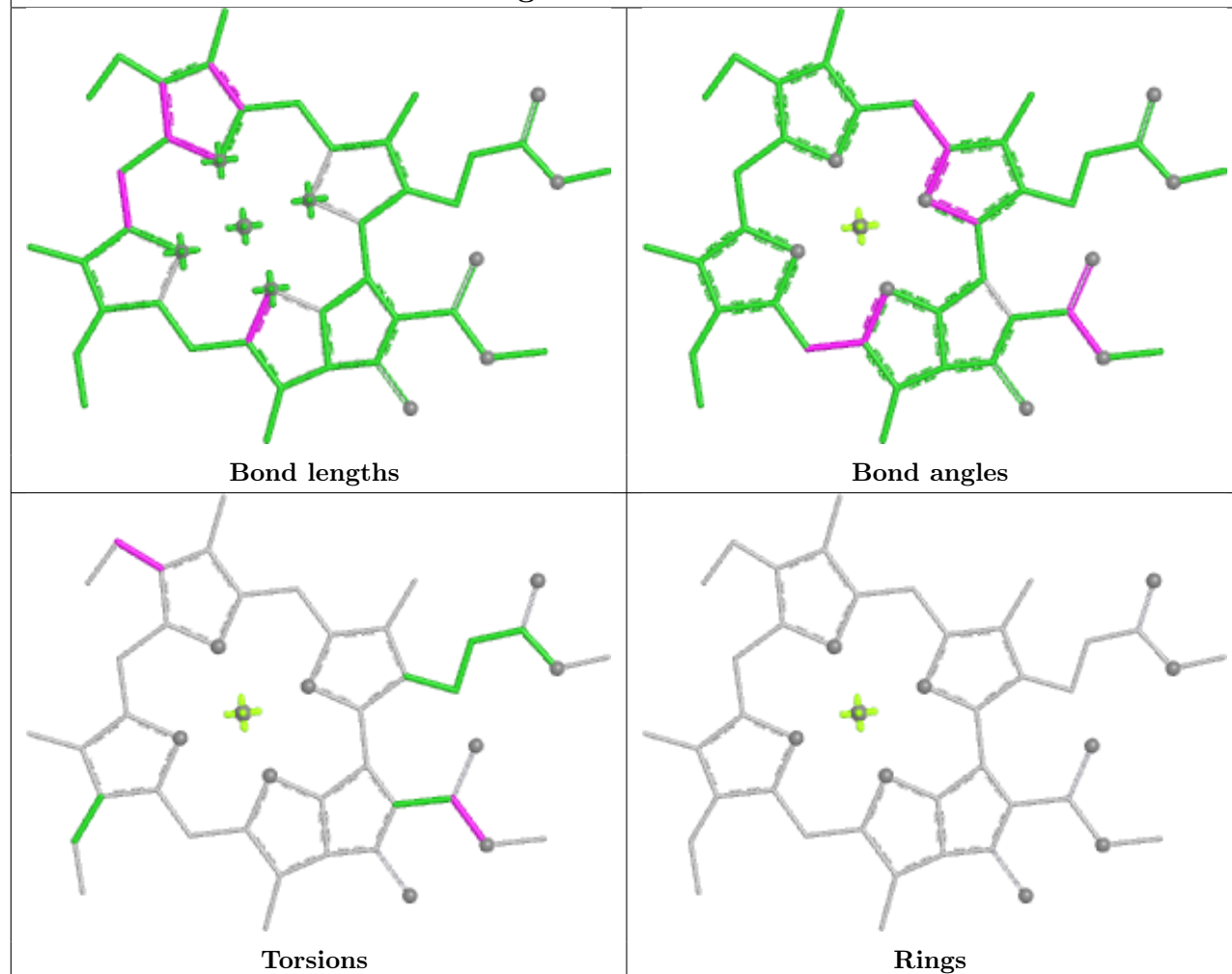
Ligand CLA A 826



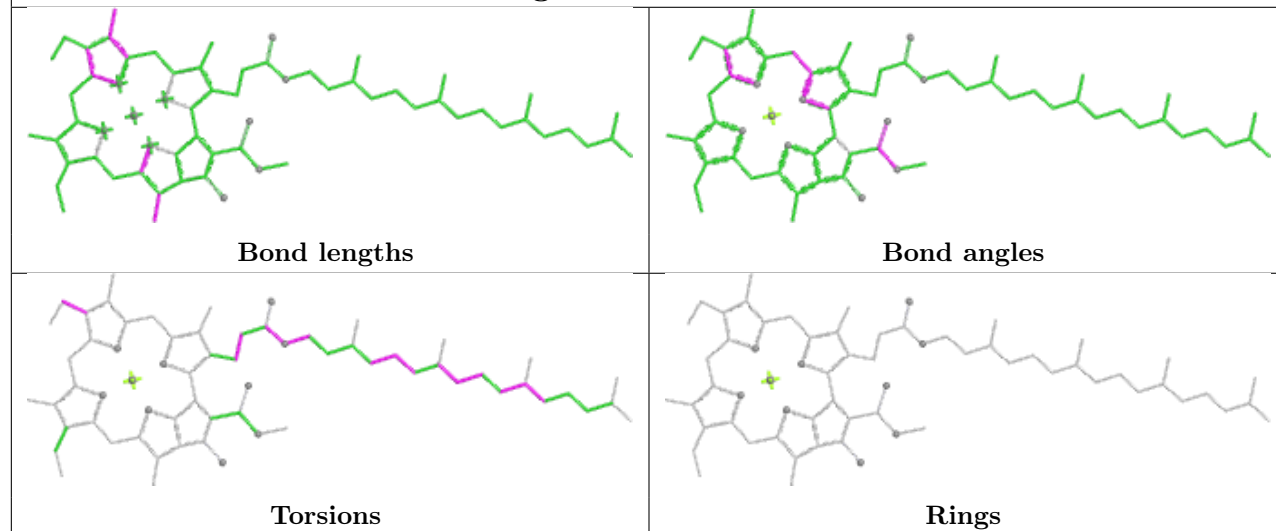
Ligand CLA 6 606



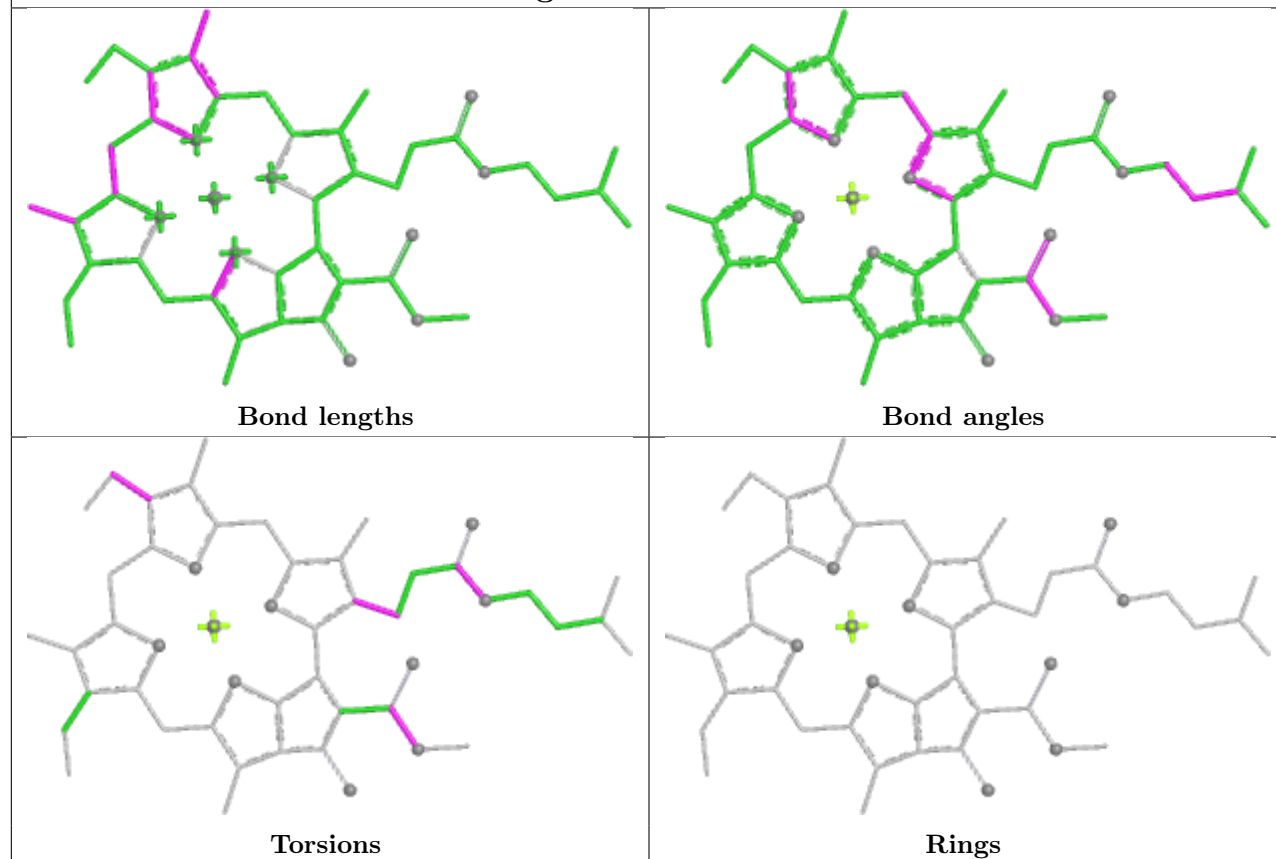
Ligand CLA 8 201



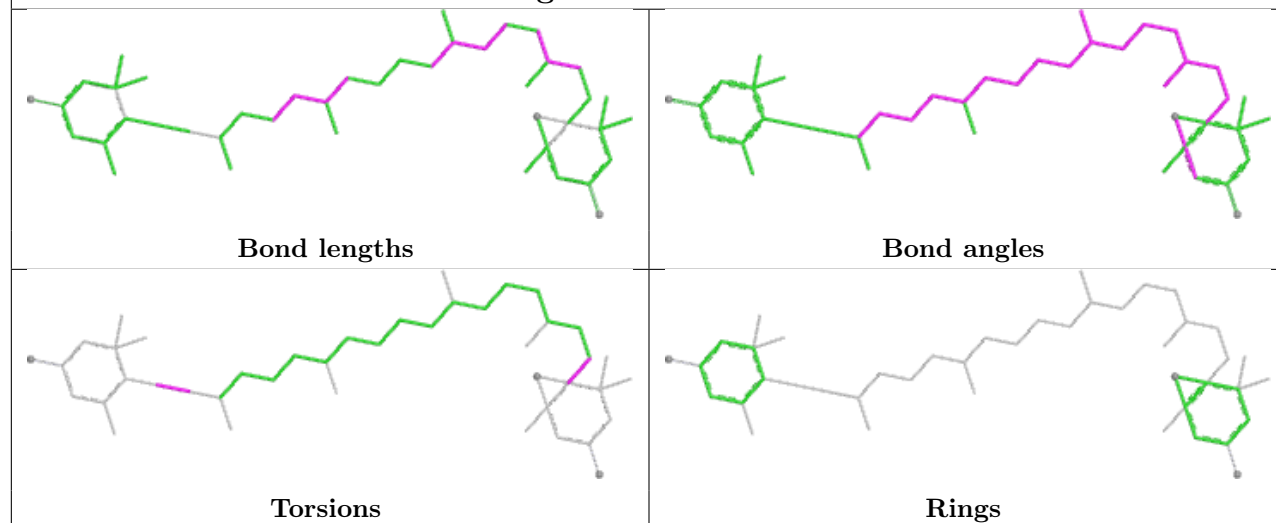
Ligand CLA B 801

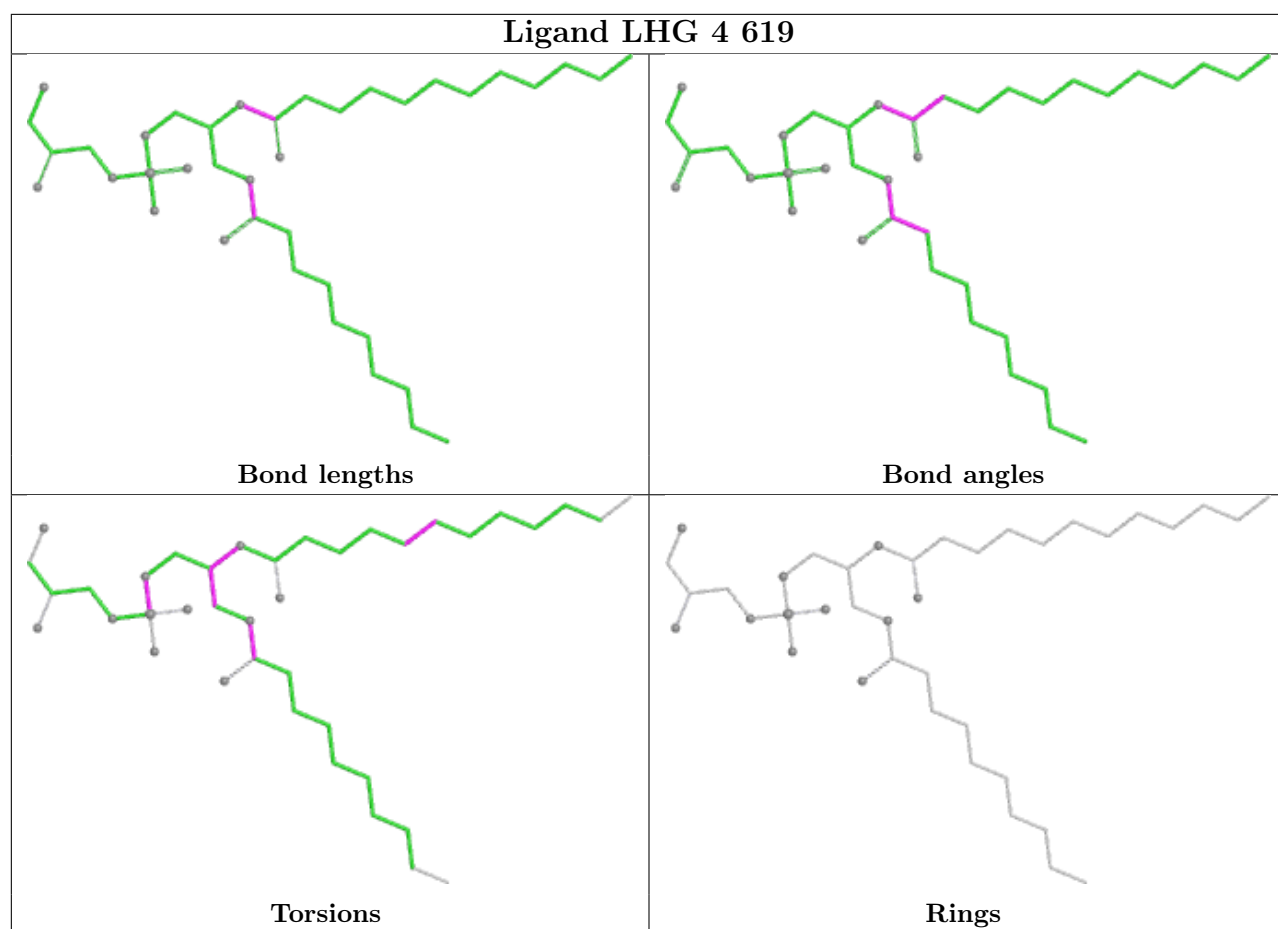


Ligand CLA 6 609

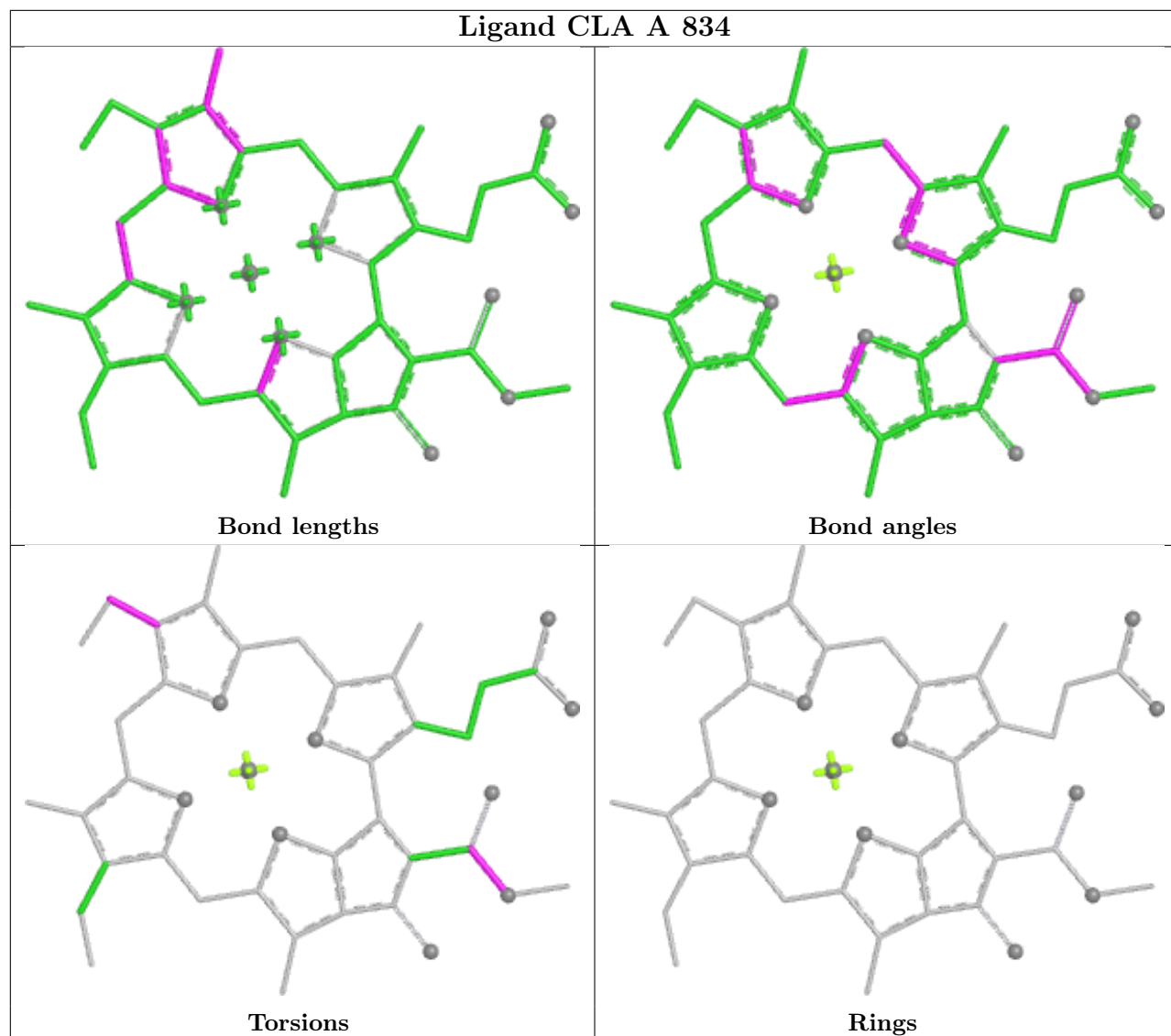


Ligand DD6 J 102

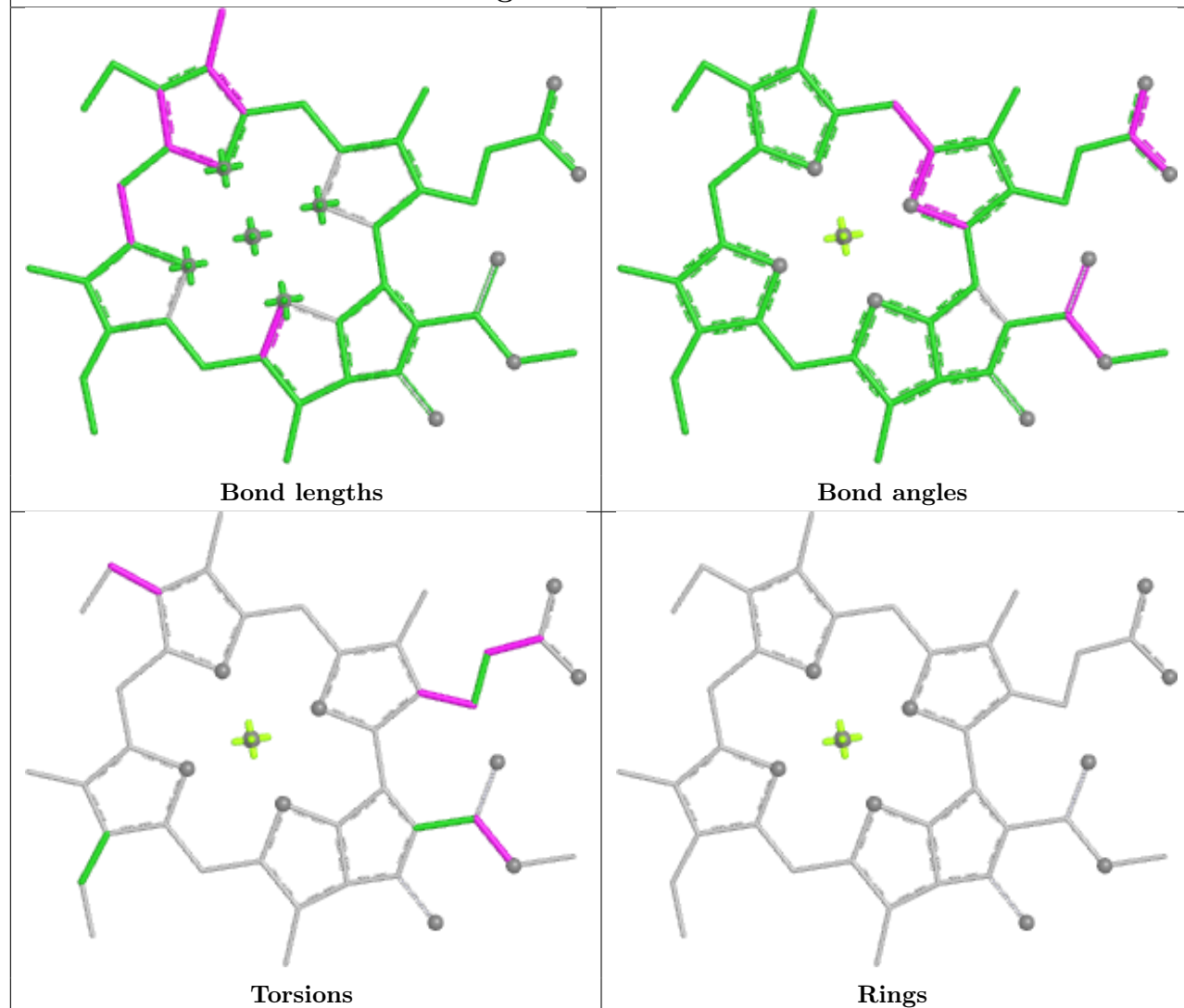




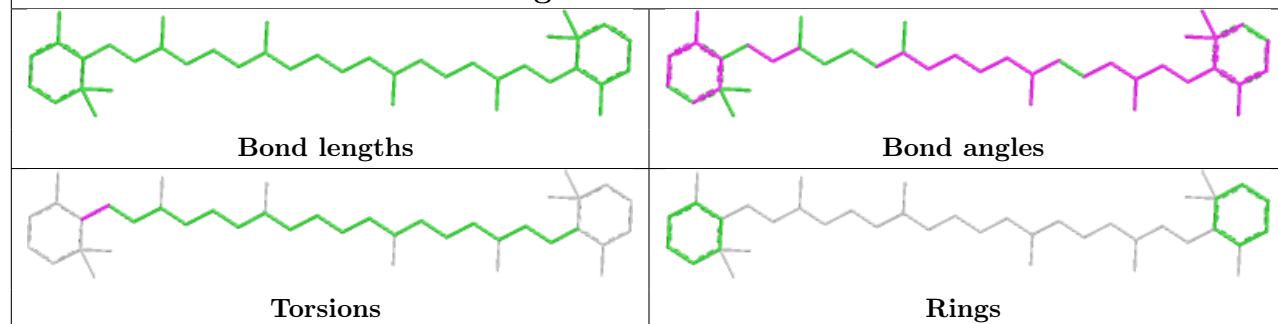
Ligand CLA A 834

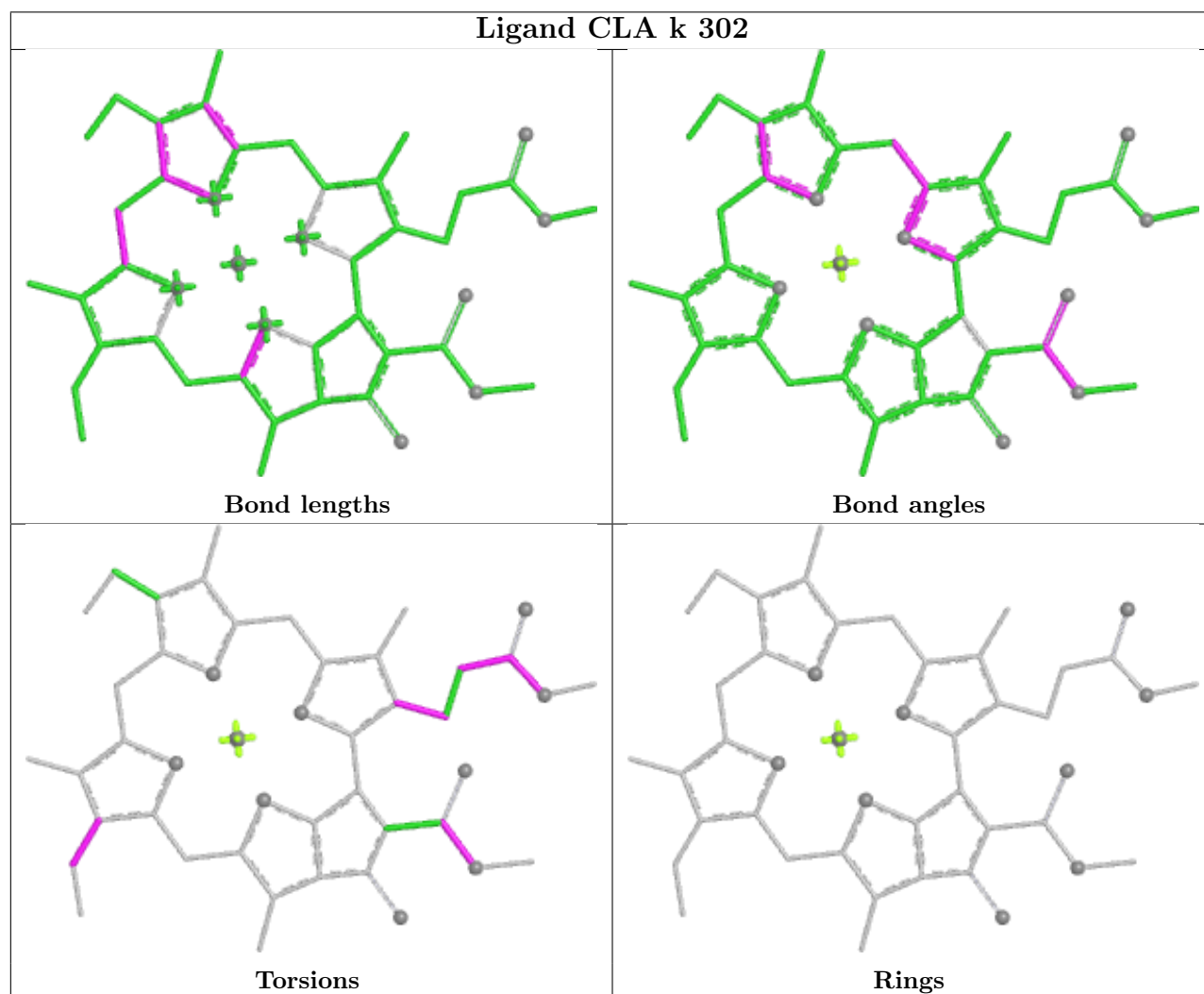
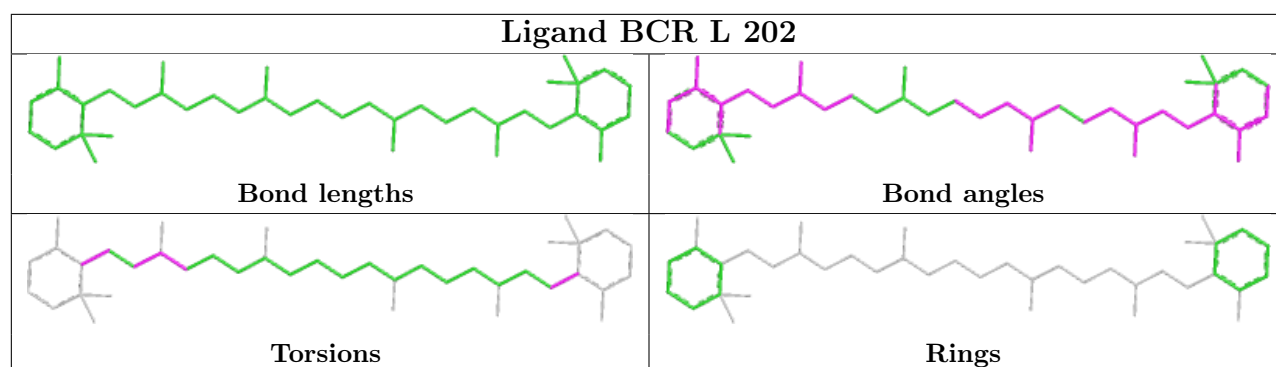


Ligand CLA 8 205

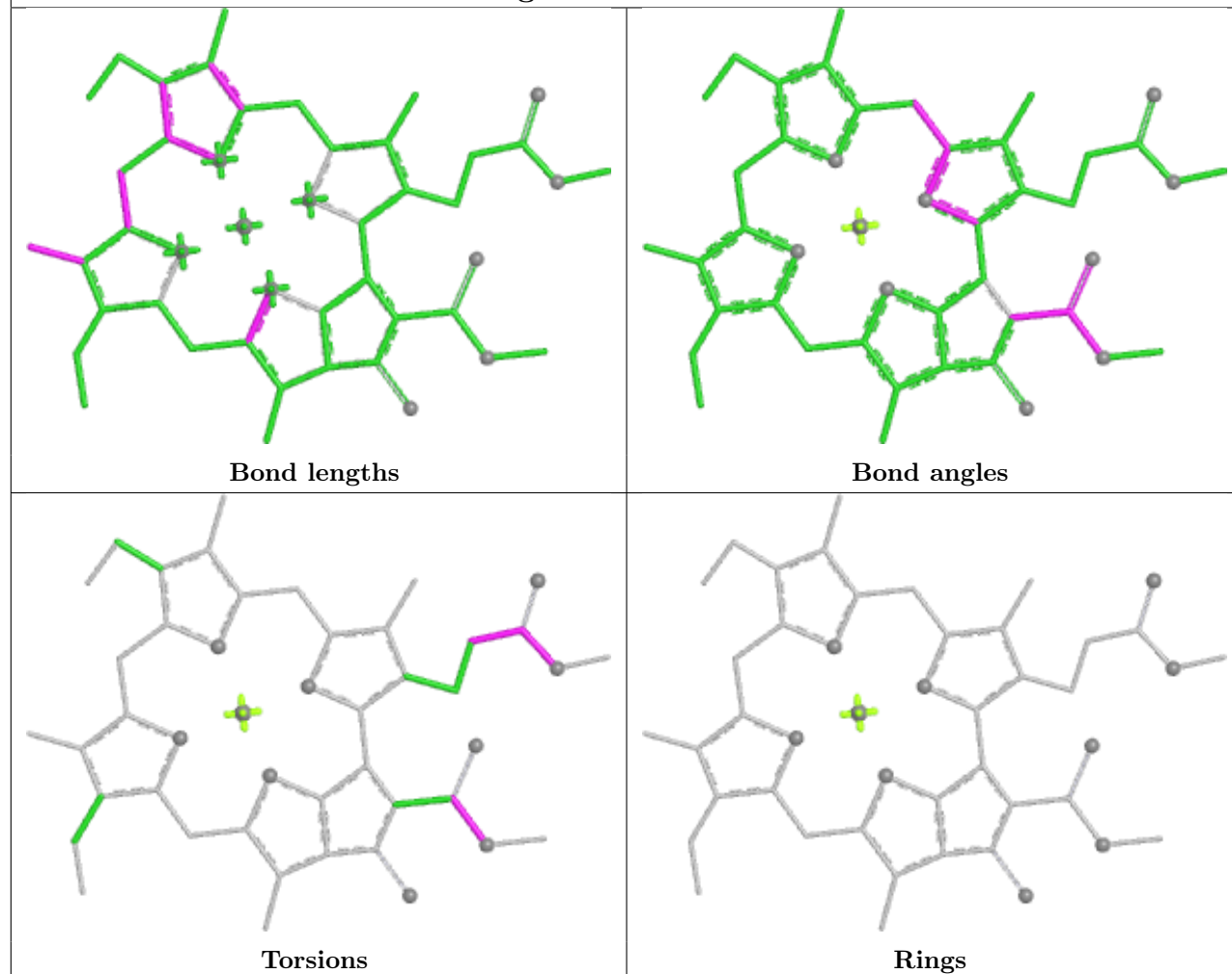


Ligand BCR J 104

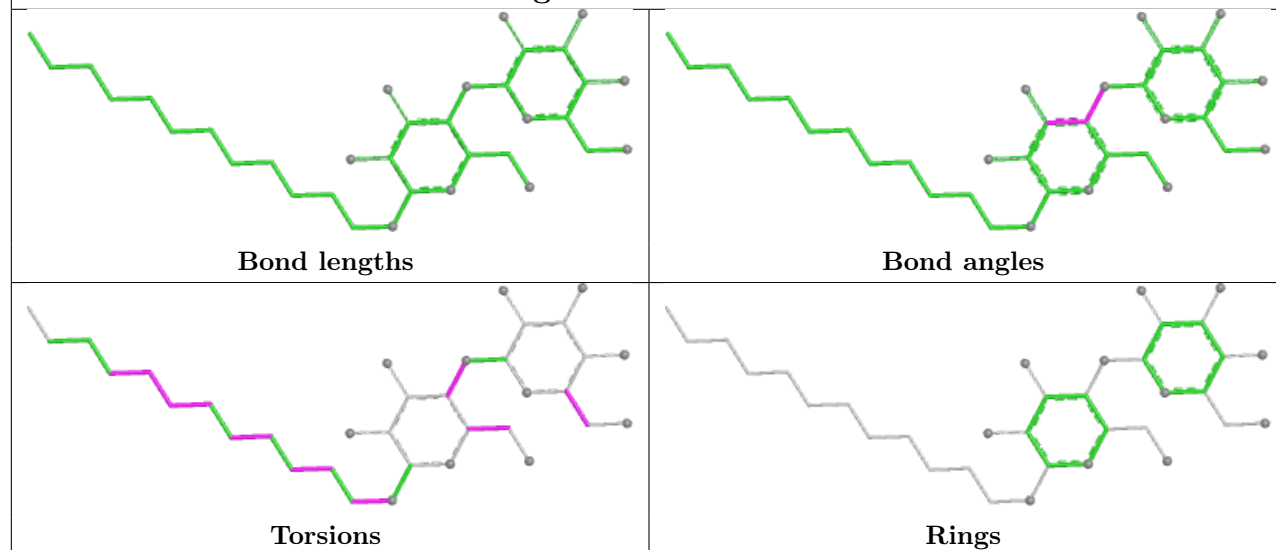




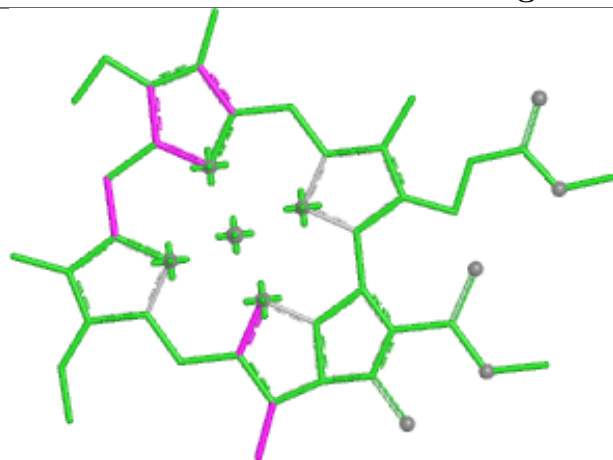
Ligand CLA 4 609



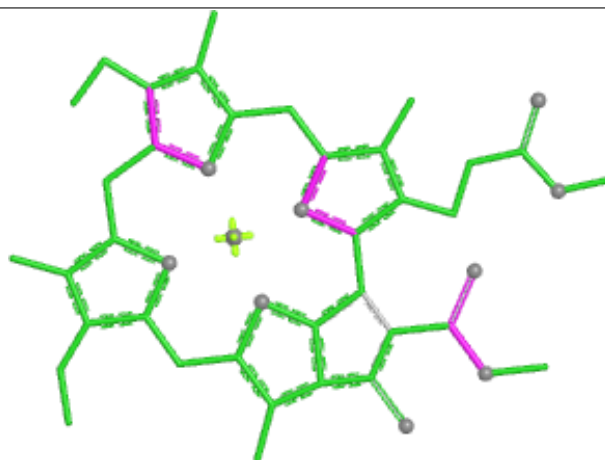
Ligand LMT 1 315



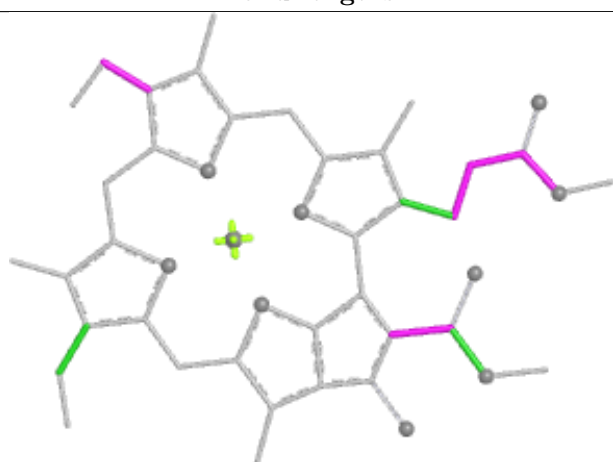
Ligand CLA k 307



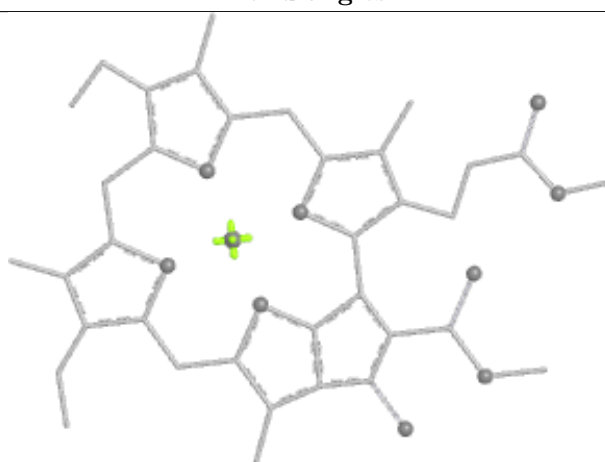
Bond lengths



Bond angles

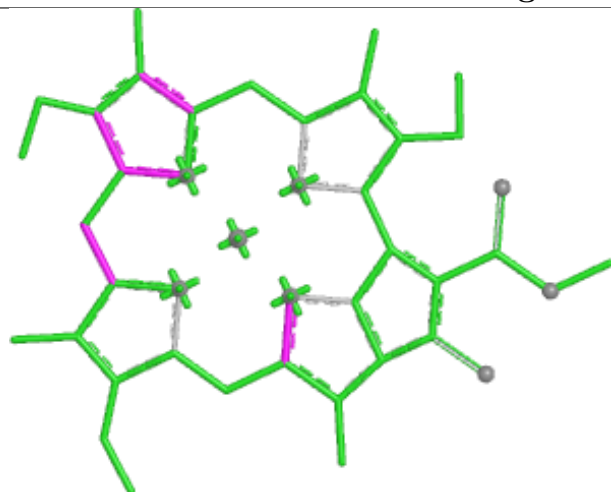


Torsions

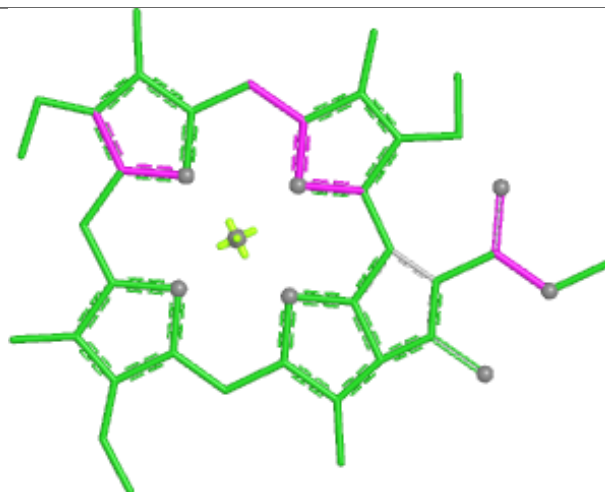


Rings

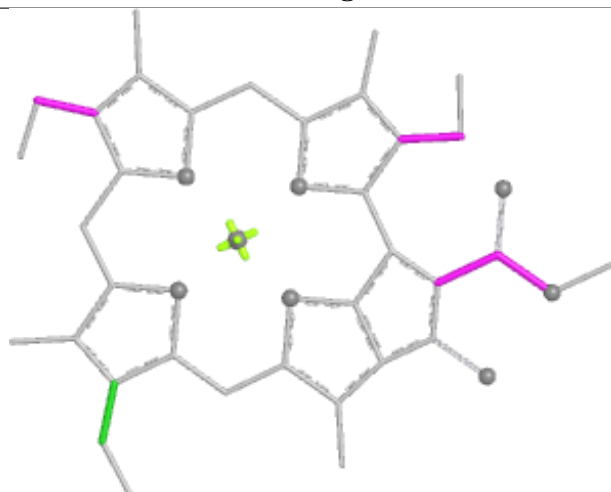
Ligand CLA J 103



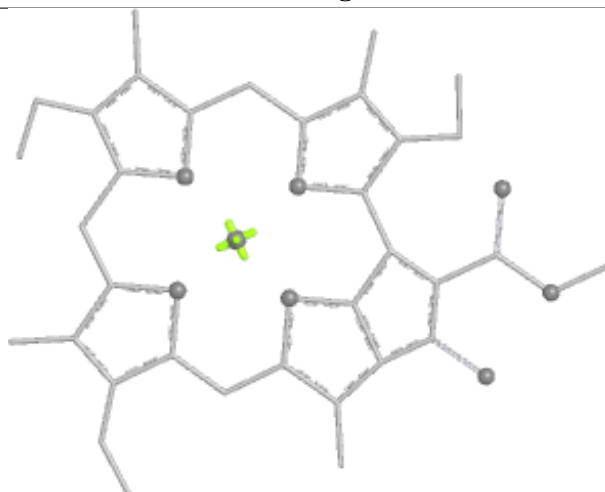
Bond lengths



Bond angles

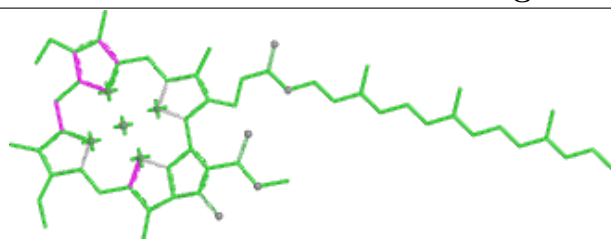


Torsions

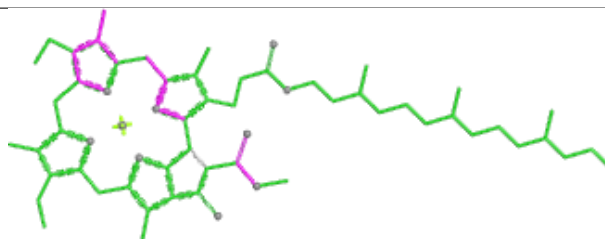


Rings

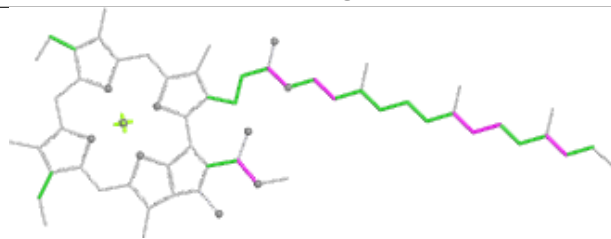
Ligand CLA A 827



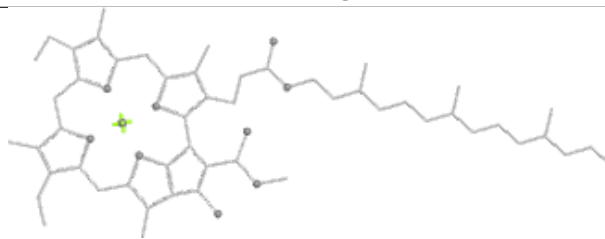
Bond lengths



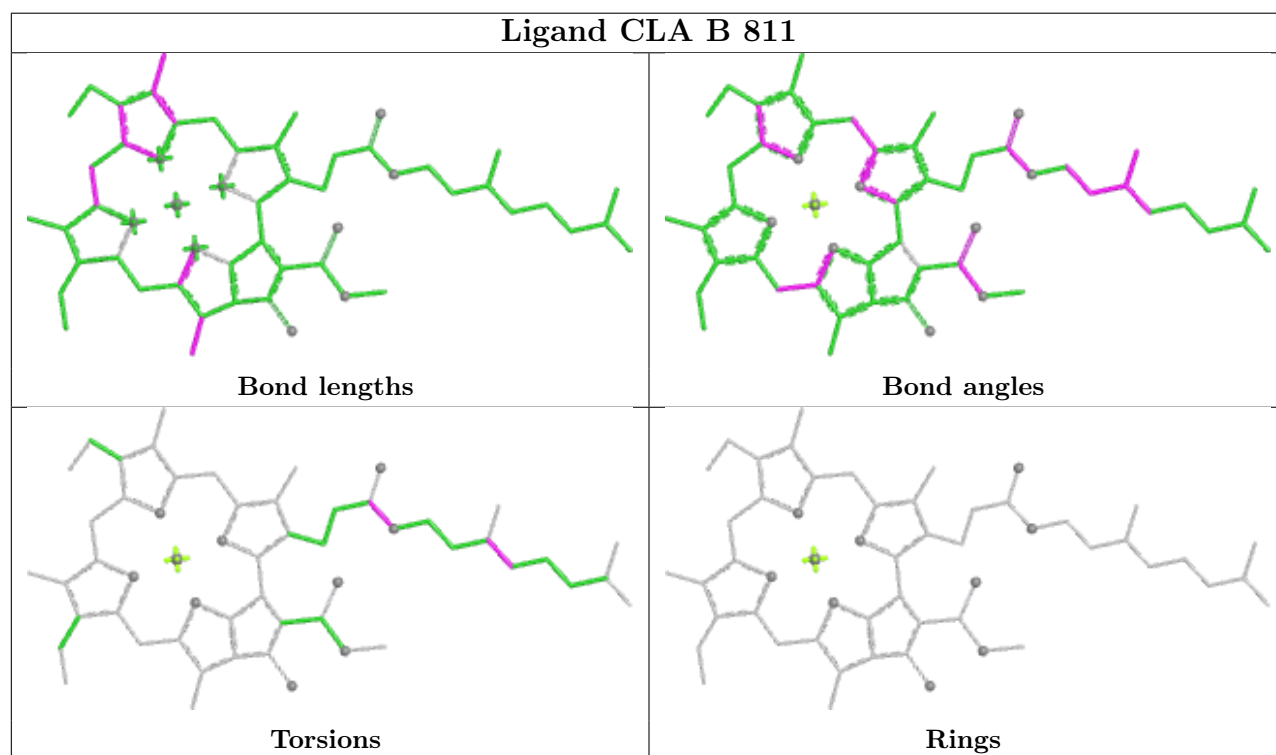
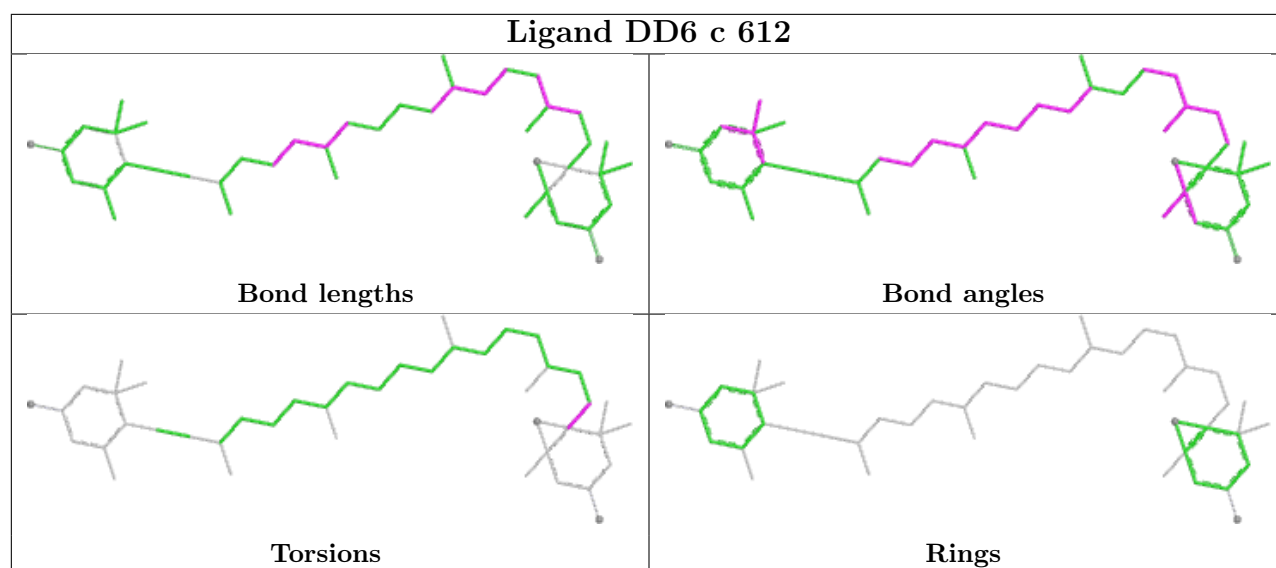
Bond angles

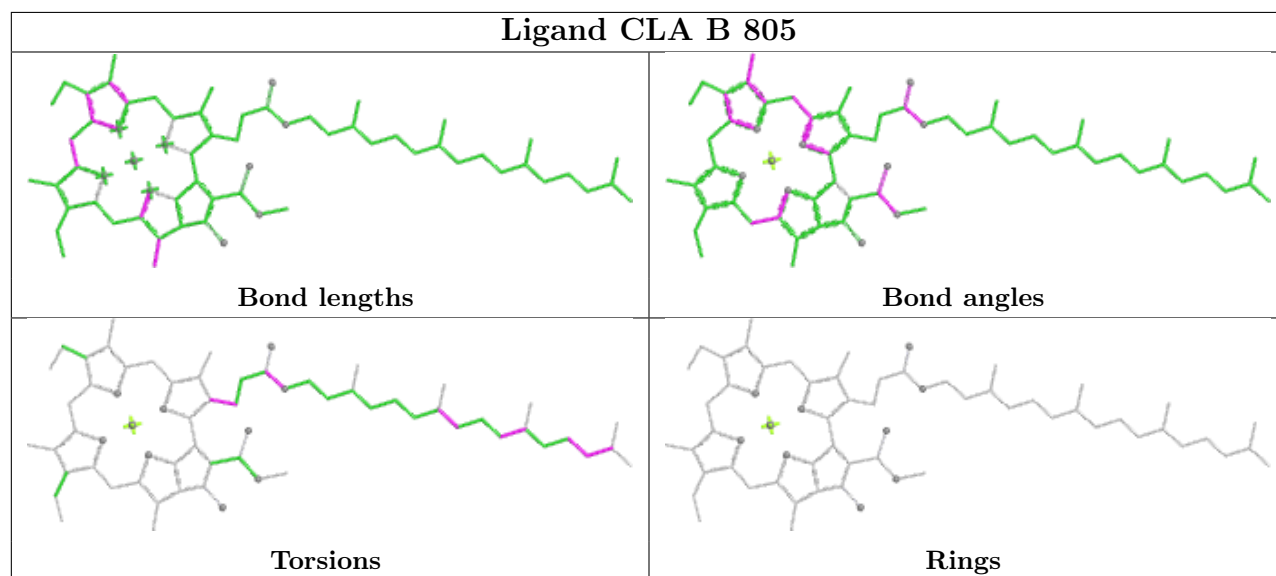
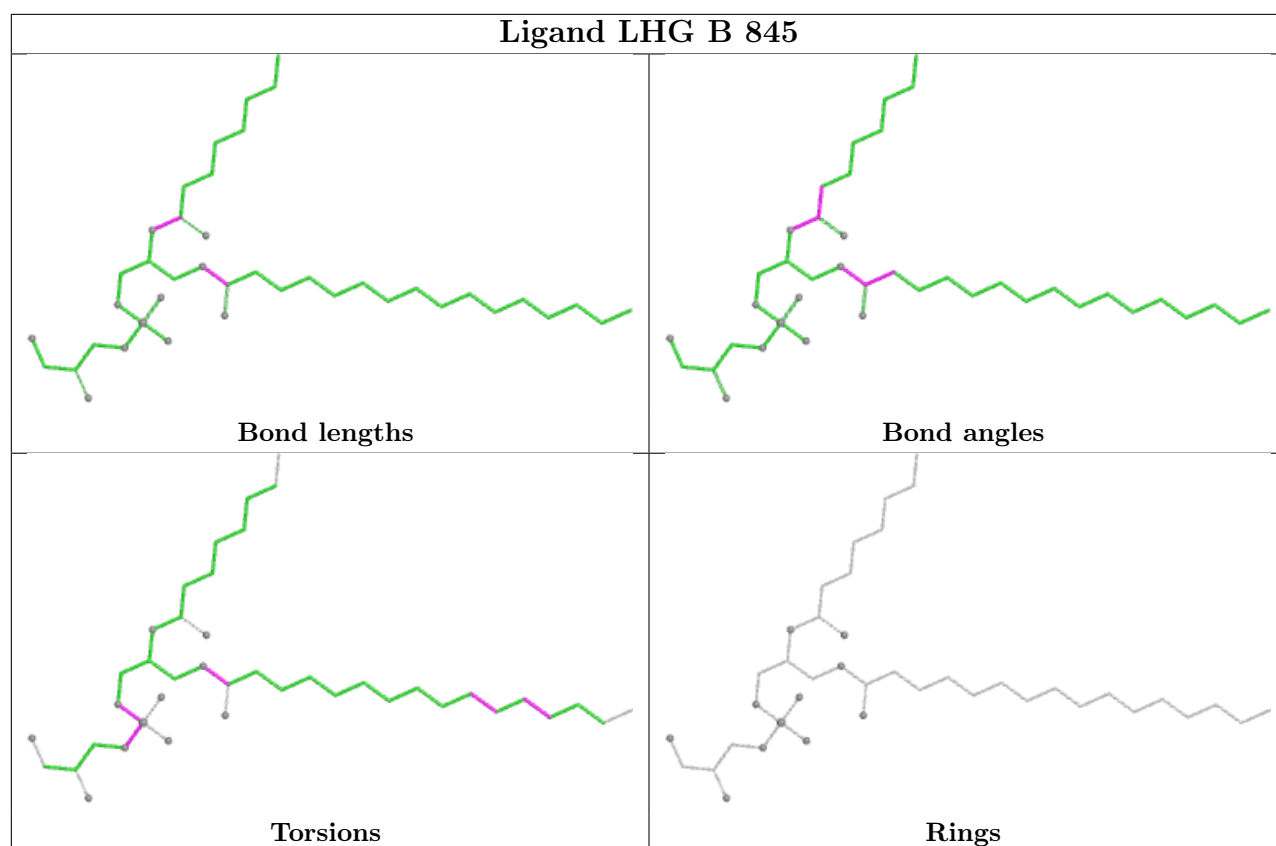


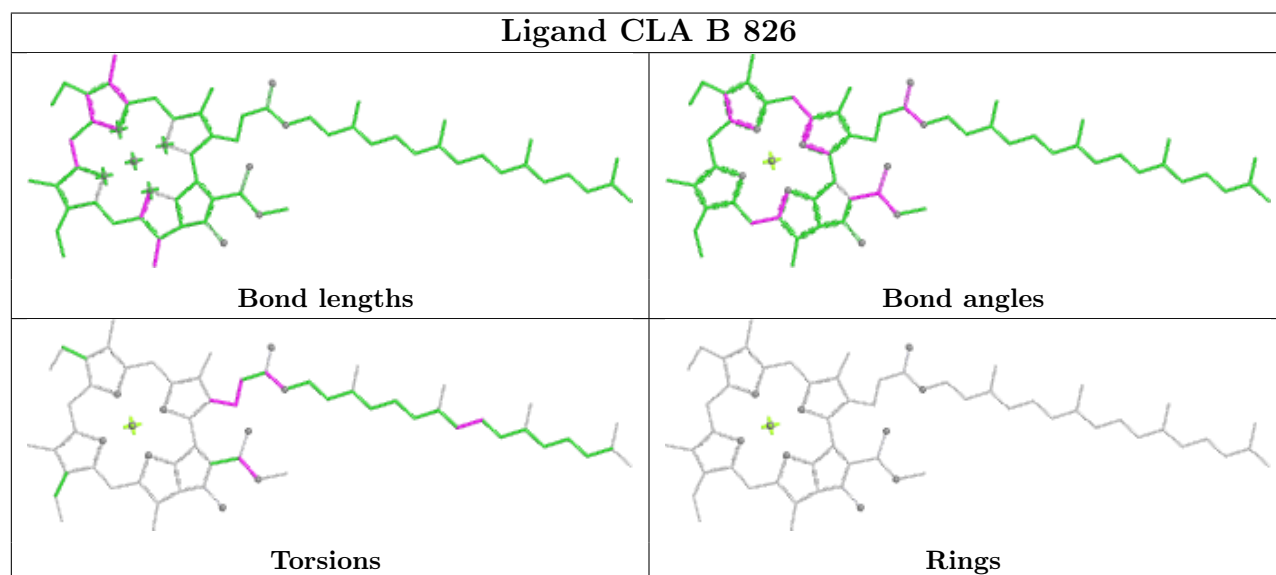
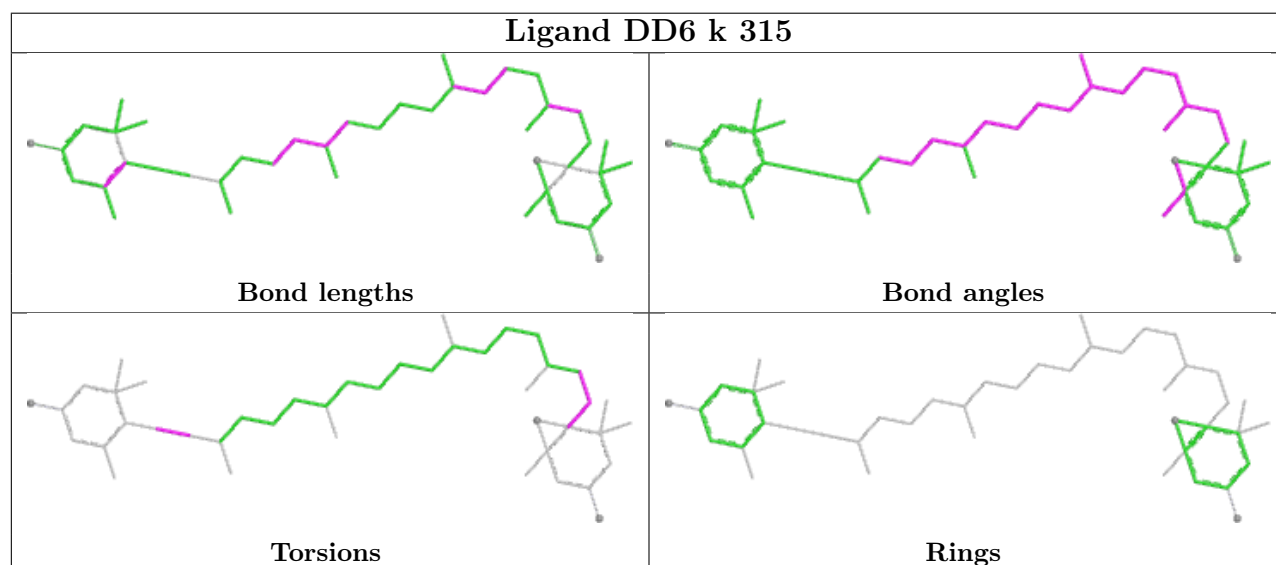
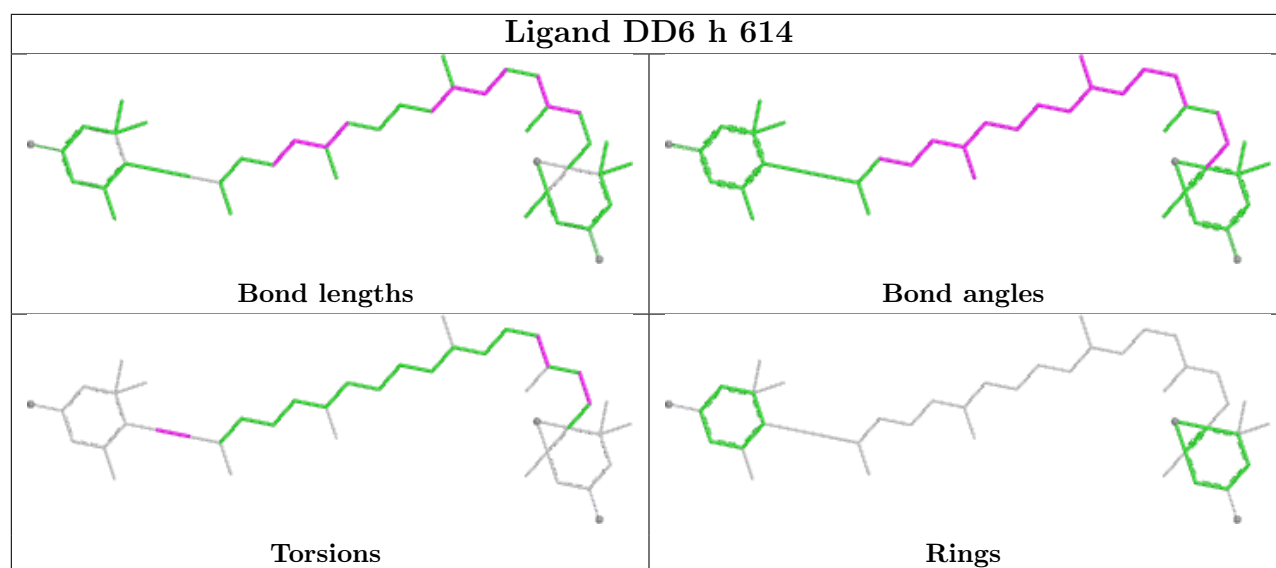
Torsions



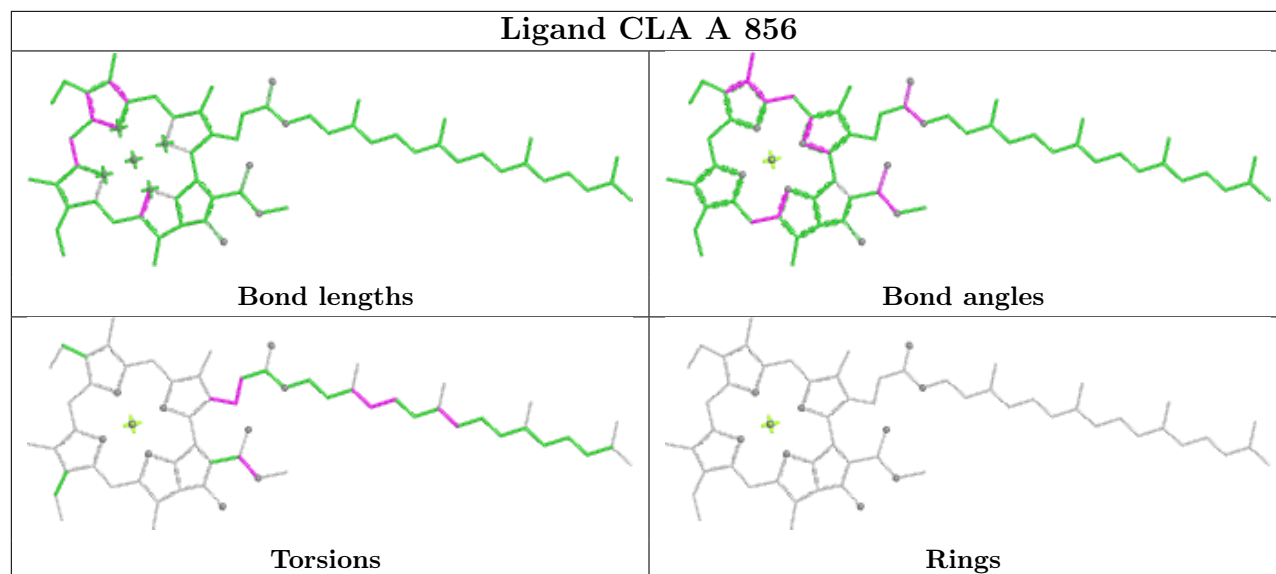
Rings



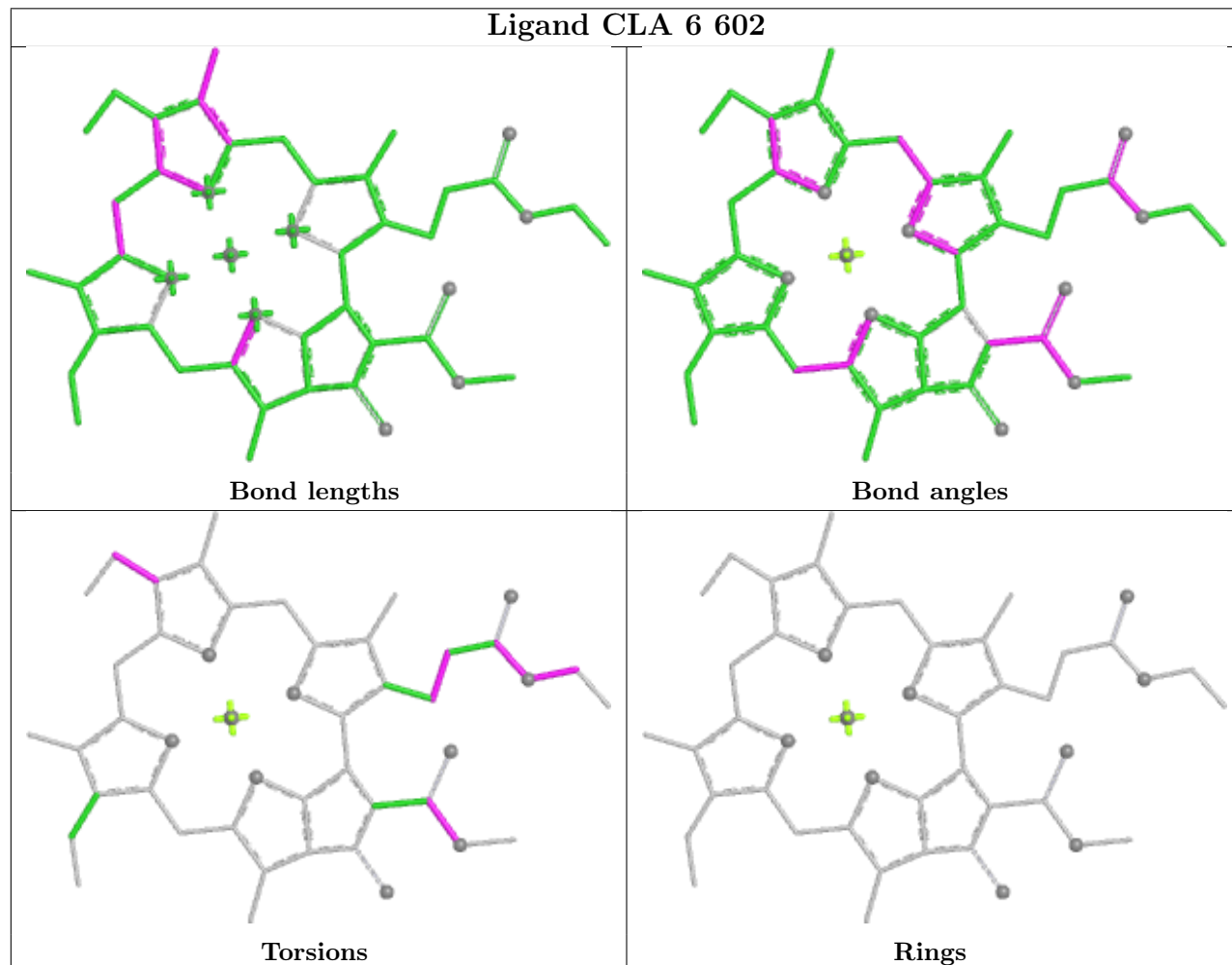


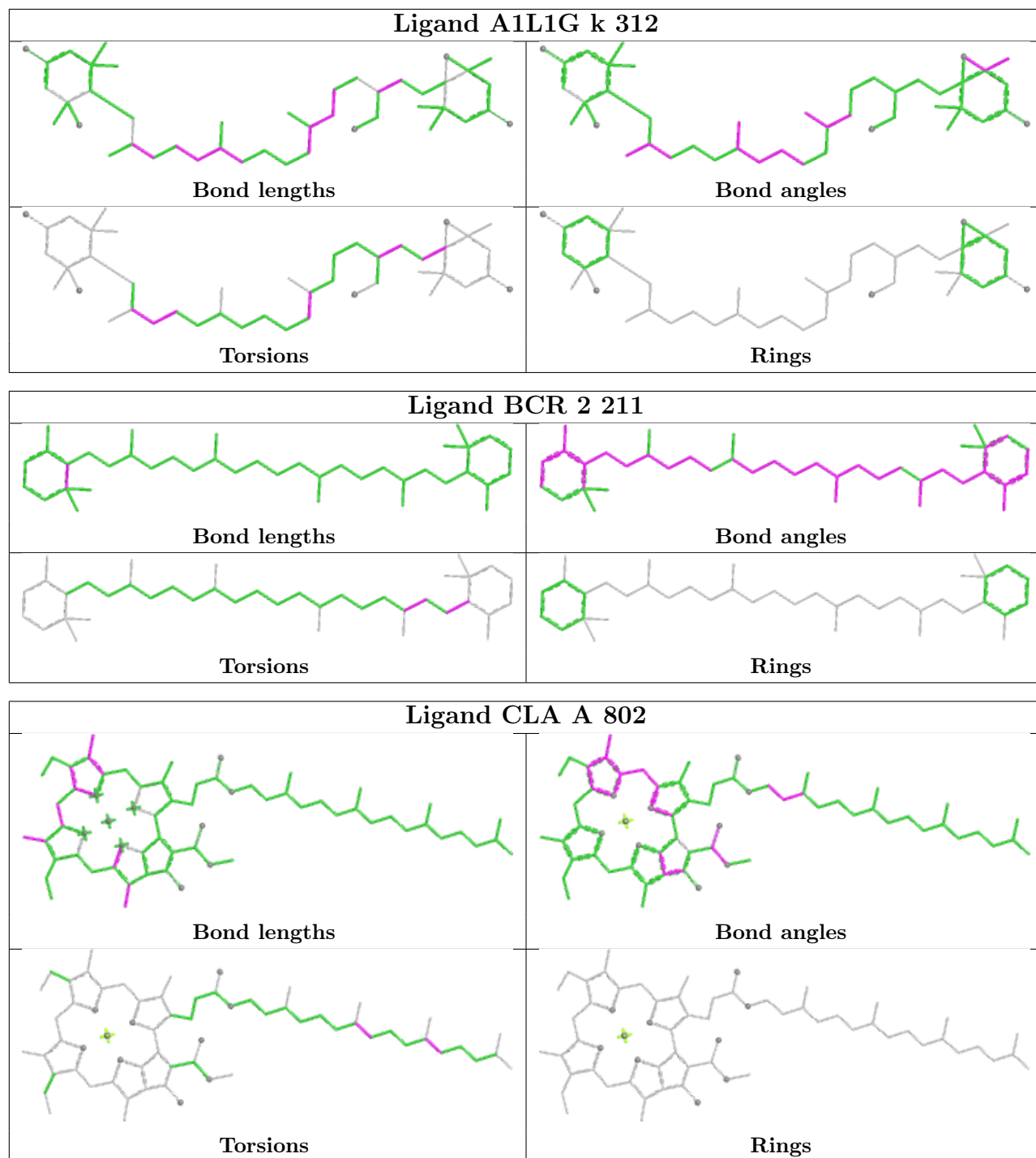


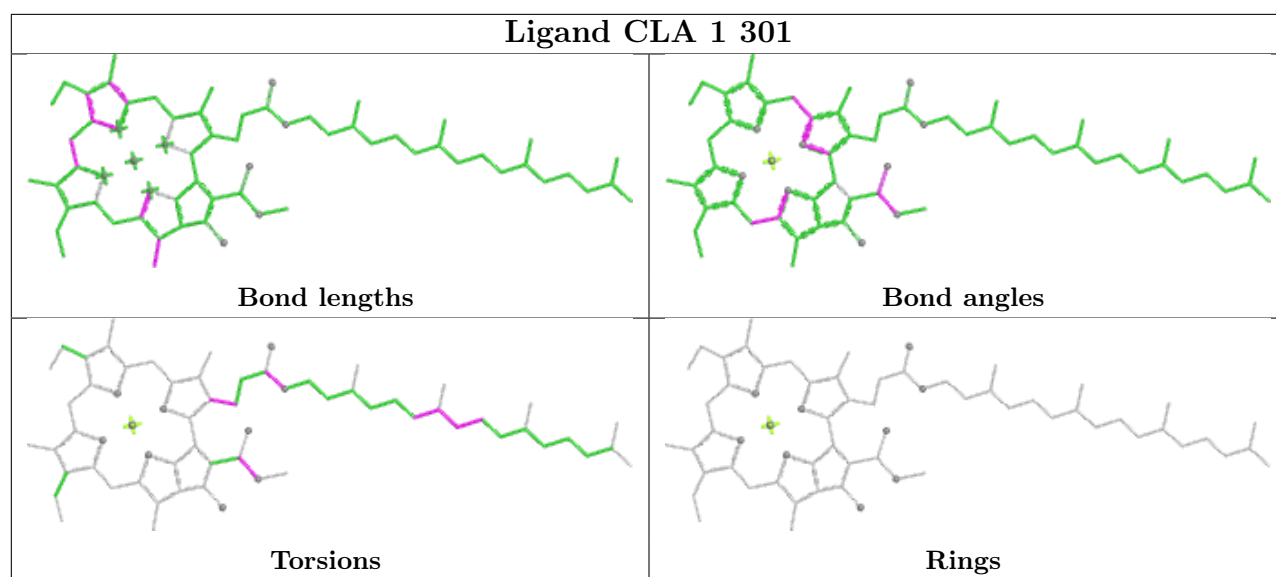
Ligand CLA A 856



Ligand CLA 6 602







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.

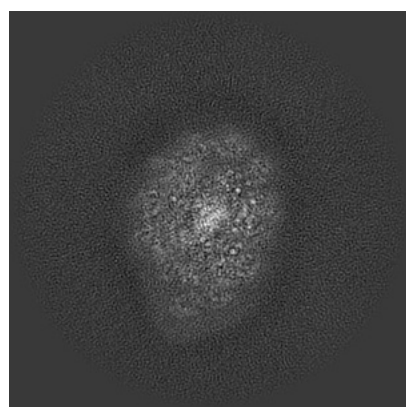
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63625. These allow visual inspection of the internal detail of the map and identification of artifacts.

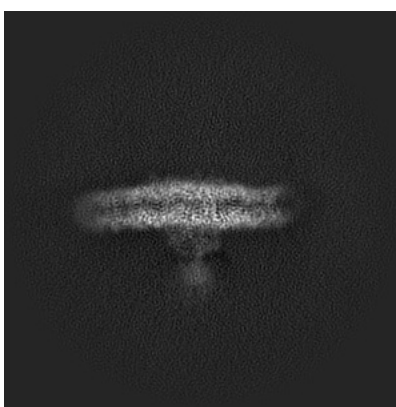
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

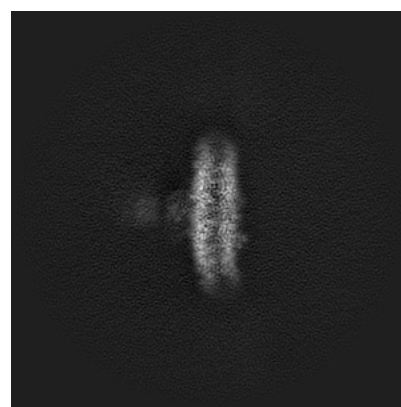
6.1.1 Primary map



X



Y

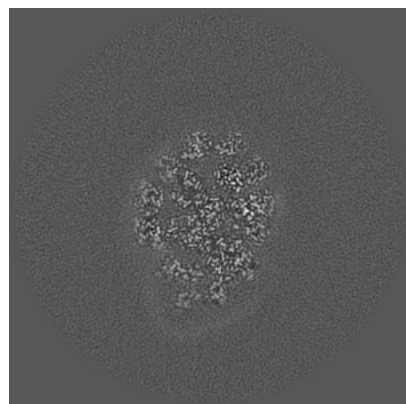


Z

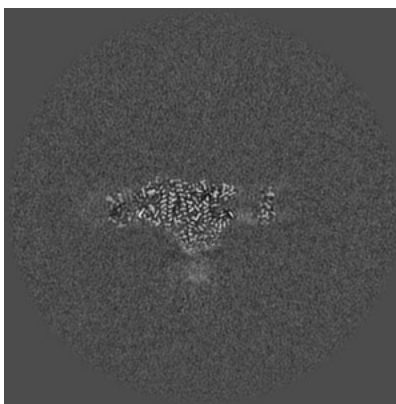
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

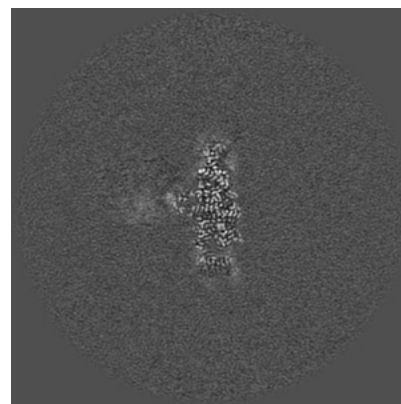
6.2.1 Primary map



X Index: 220



Y Index: 220

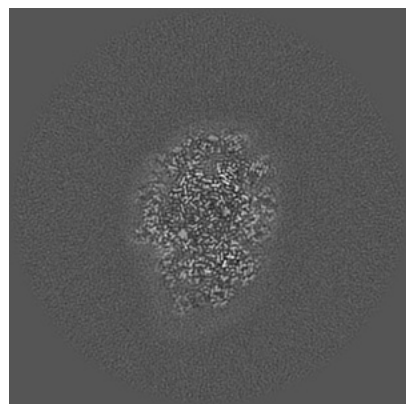


Z Index: 220

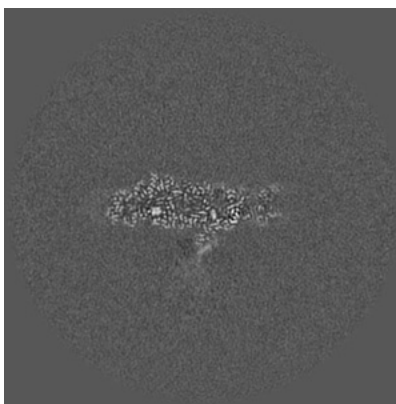
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

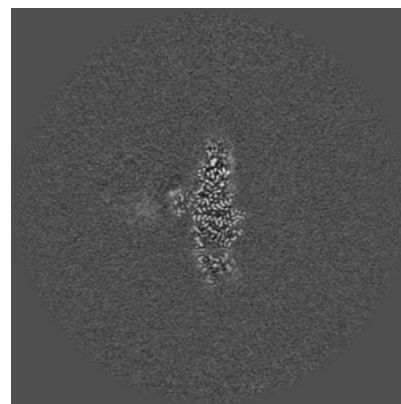
6.3.1 Primary map



X Index: 213



Y Index: 234

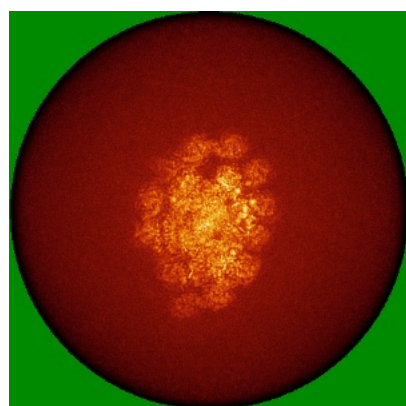


Z Index: 224

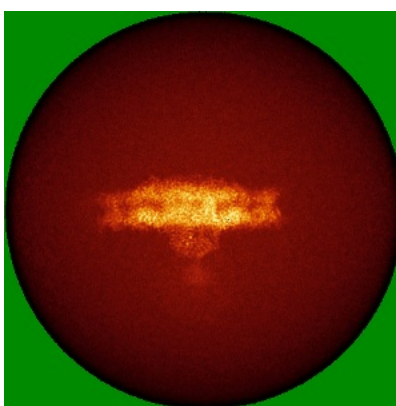
The images above show the largest variance slices of the map in three orthogonal directions.

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

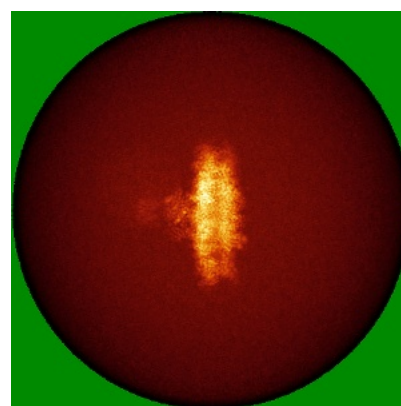
6.4.1 Primary map



X



Y

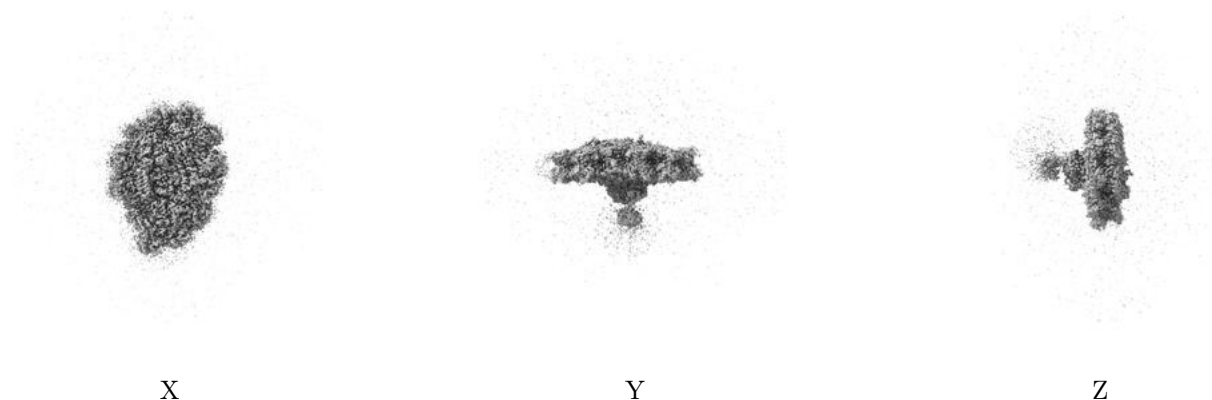


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

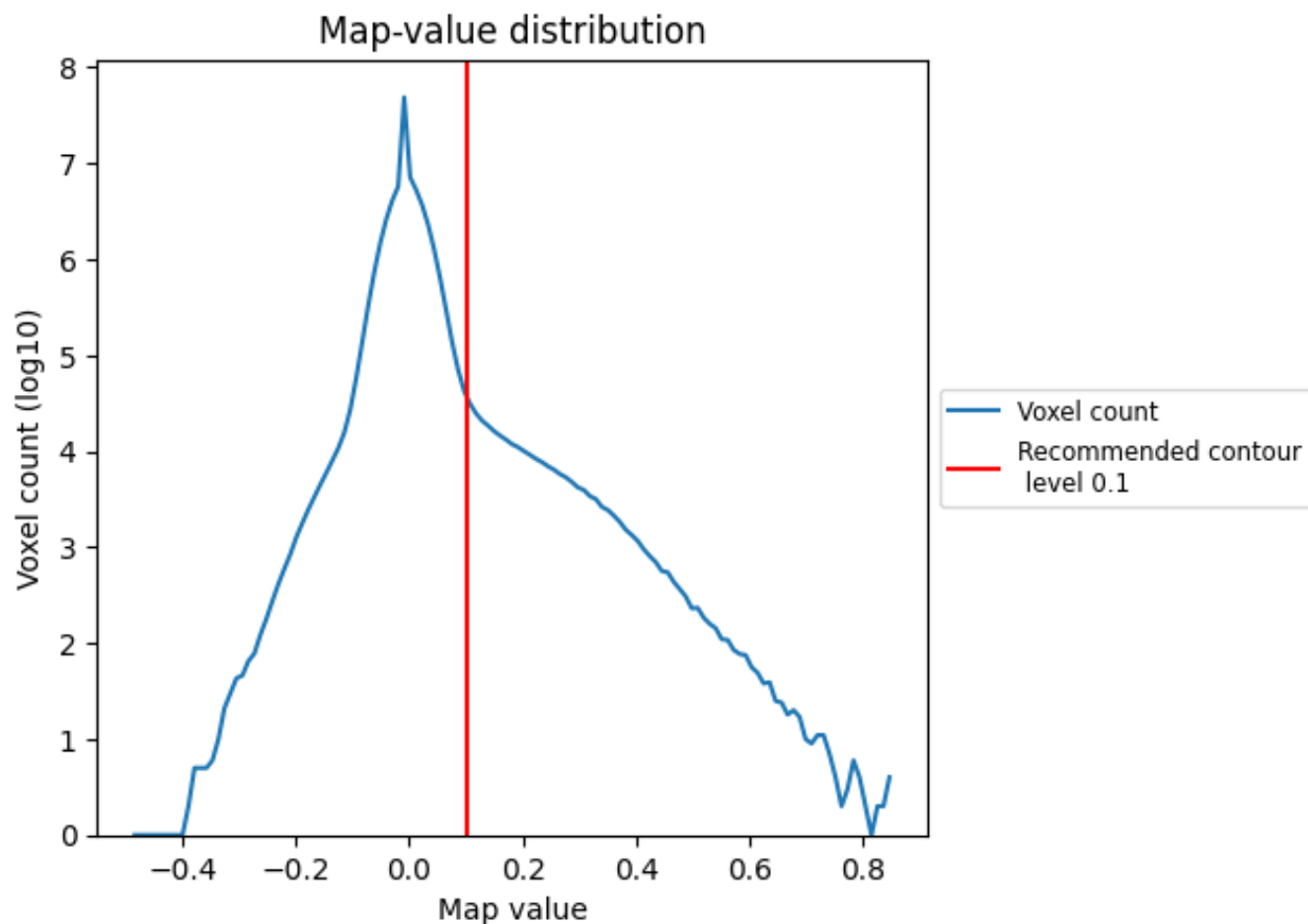
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

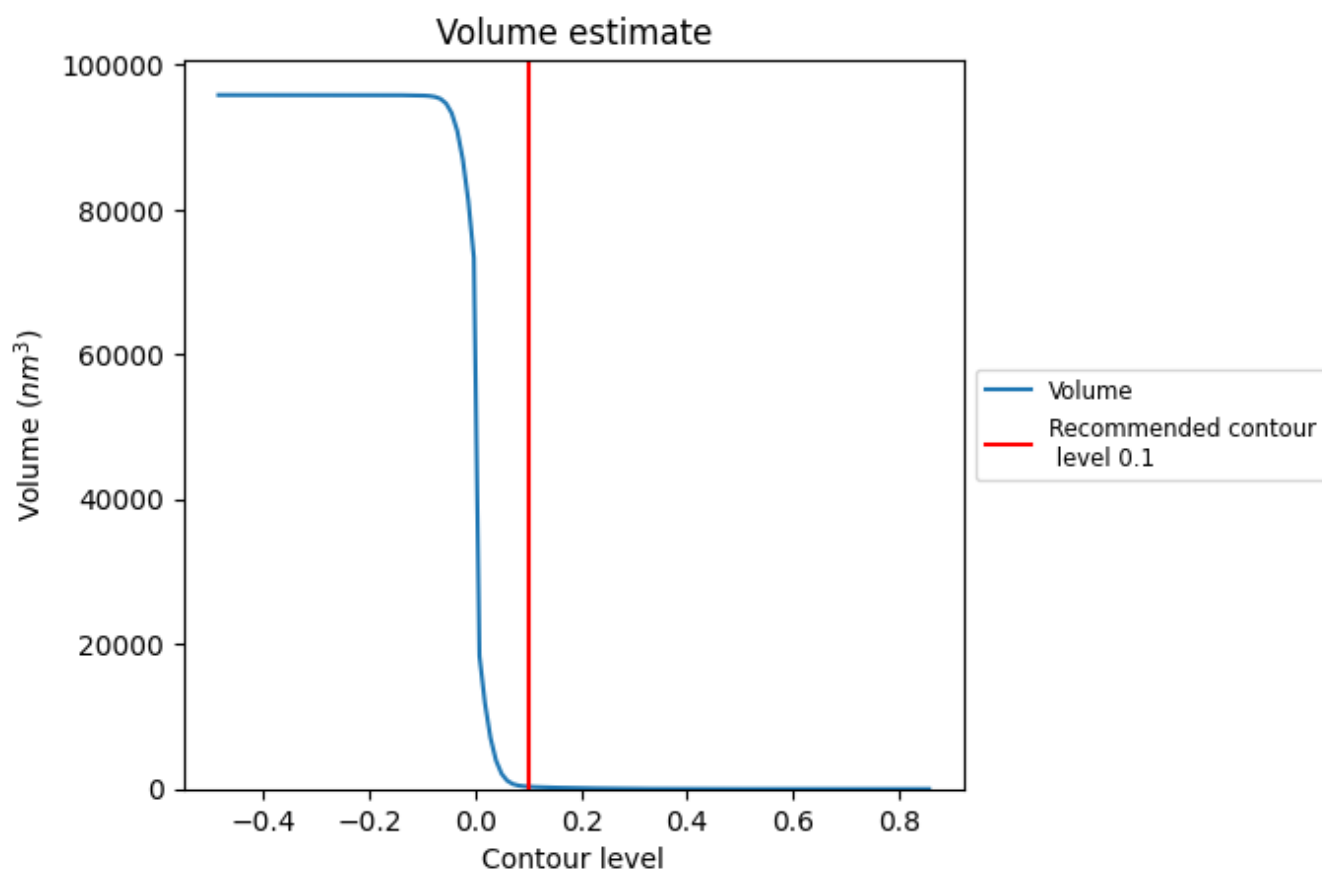
This section contains the results of statistical analysis of the map.

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.

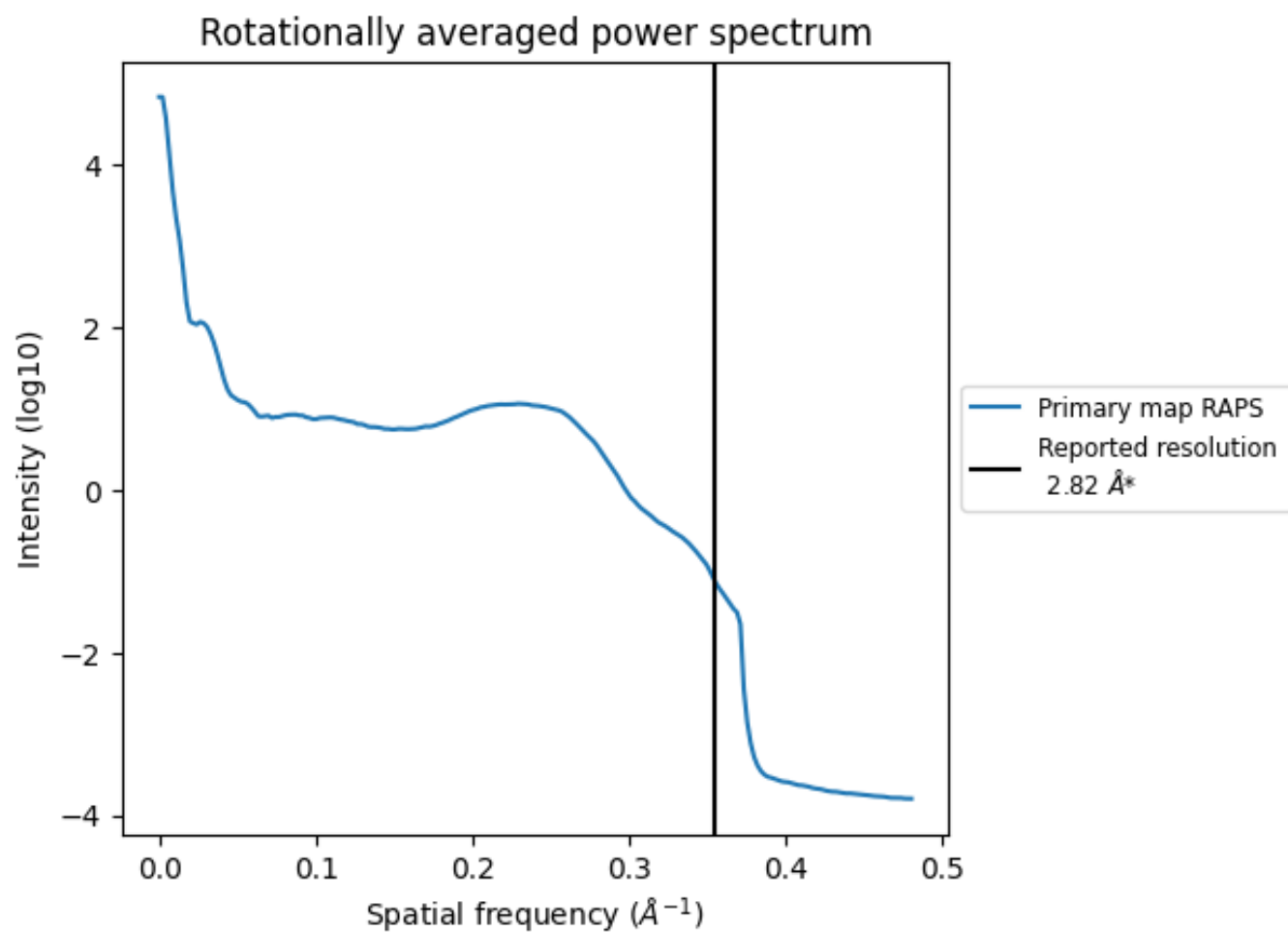
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; this corresponds to an approximate mass of 295 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 0.355 Å⁻¹

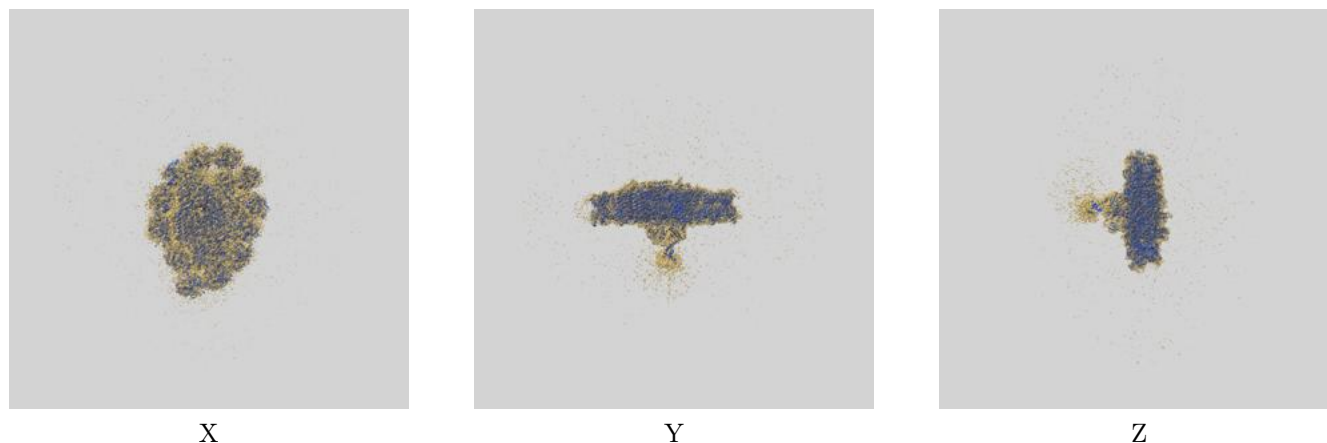
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

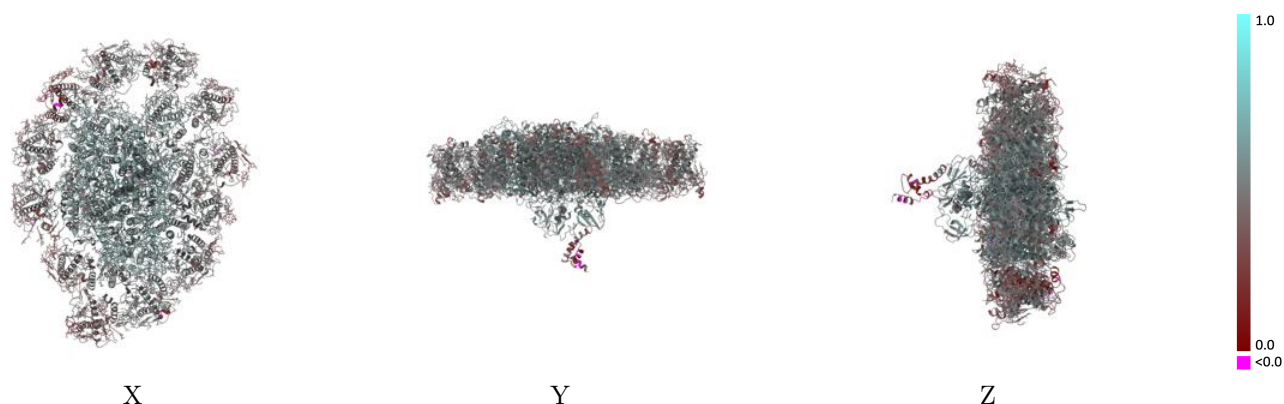
This section contains information regarding the fit between EMDB map EMD-63625 and PDB model 9M4F. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



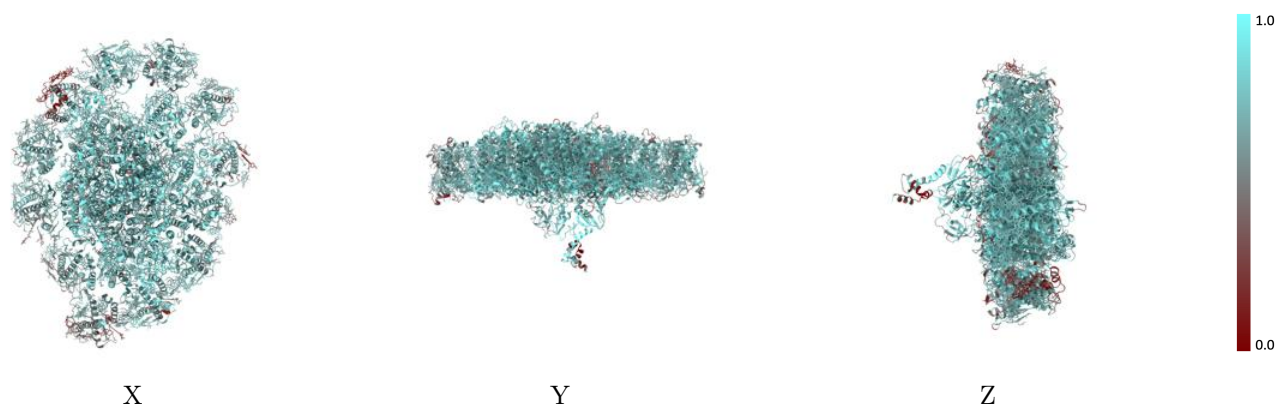
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



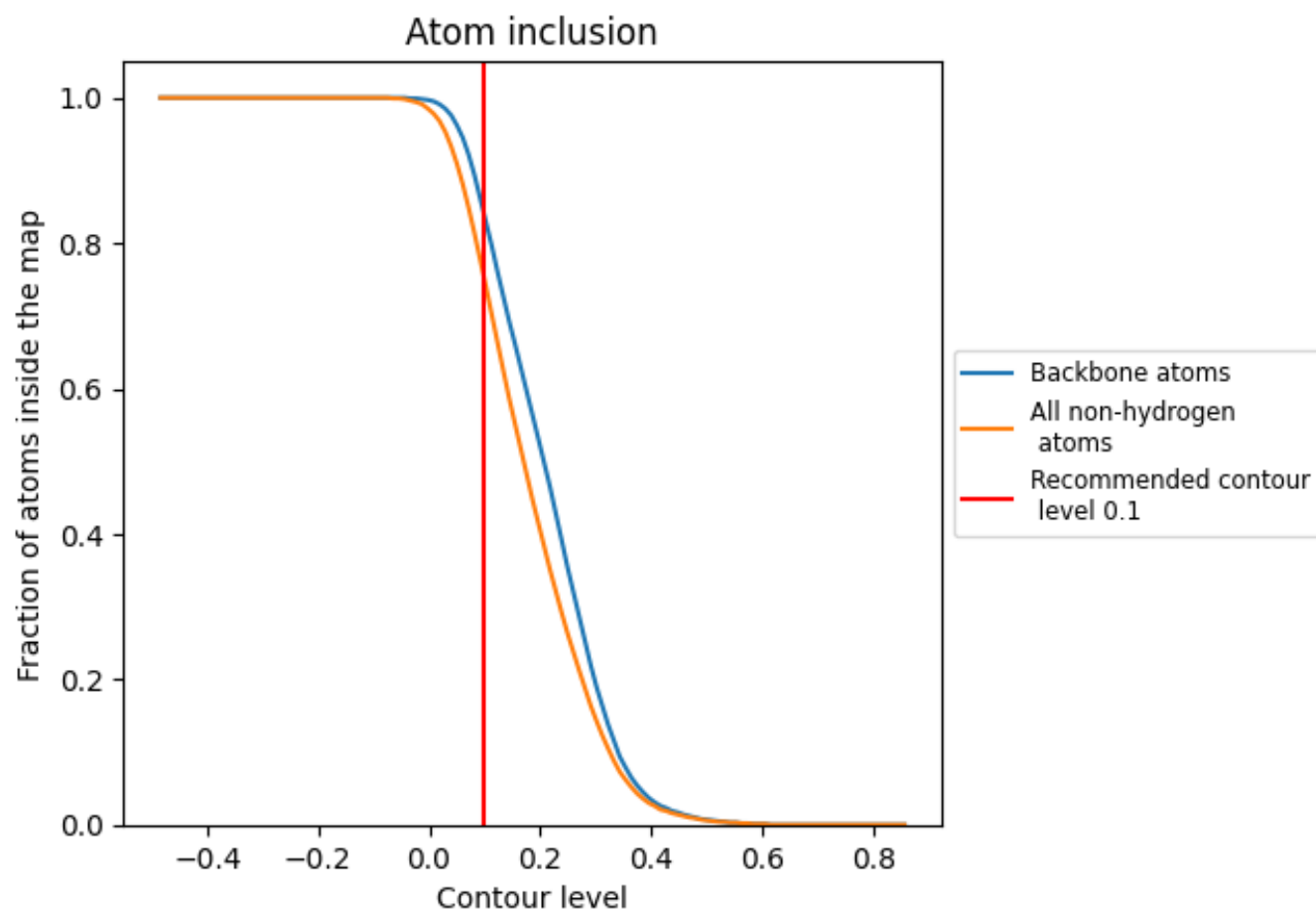
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.4950
1	 0.7410	 0.4690
2	 0.6780	 0.4260
3	 0.8430	 0.5220
4	 0.7210	 0.4510
5	 0.5160	 0.3670
6	 0.6820	 0.4370
7	 0.6840	 0.4260
8	 0.6740	 0.4200
9	 0.5030	 0.3820
A	 0.8250	 0.5720
B	 0.8350	 0.5690
C	 0.8540	 0.5490
D	 0.7810	 0.5150
E	 0.7450	 0.5250
F	 0.7860	 0.5220
I	 0.7860	 0.5260
J	 0.8270	 0.5420
L	 0.8760	 0.5340
M	 0.8330	 0.5030
R	 0.7510	 0.4920
S	 0.5070	 0.2720
c	 0.7410	 0.4640
h	 0.7040	 0.4590
k	 0.6510	 0.4290
t	 0.6750	 0.4380

