



Full wwPDB EM Validation Report ⓘ

Nov 9, 2025 – 12:43 AM JST

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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

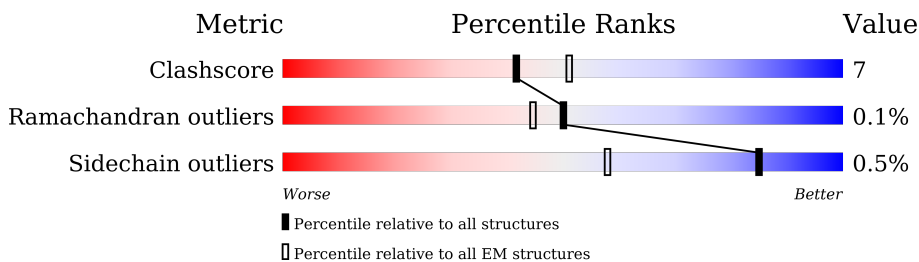
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	220	74% 6% 20%
2	2	194	62% 9% 29%
3	3	205	68% 9% 23%
4	4	231	66% 15% 19%
5	5	216	69% 8% 23%
6	6	212	64% 11% 23%
6	h	212	67% 10% 22%
7	7	207	68% 13% 20%
8	8	179	77% 13% 10%

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Mol	Chain	Length	Quality of chain
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	-	-	-
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	-	-	-

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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 [i](#)

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		

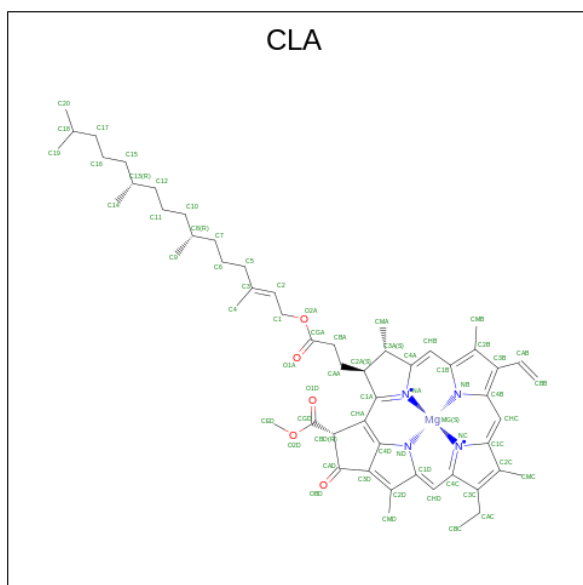
- Molecule 22 is a protein called PsaR.

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

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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 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
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 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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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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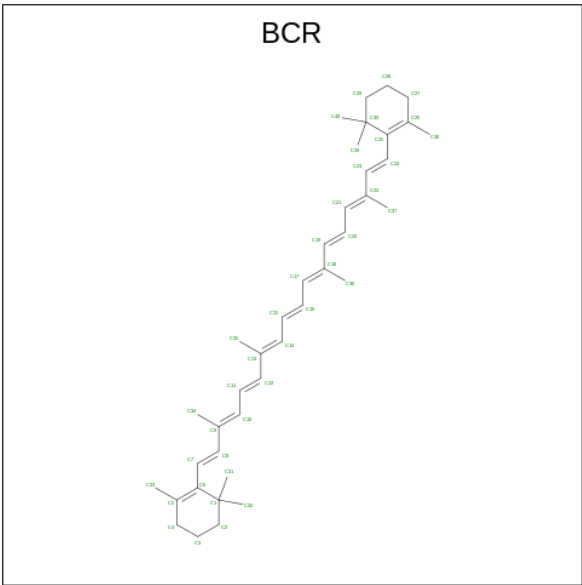
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			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
			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).



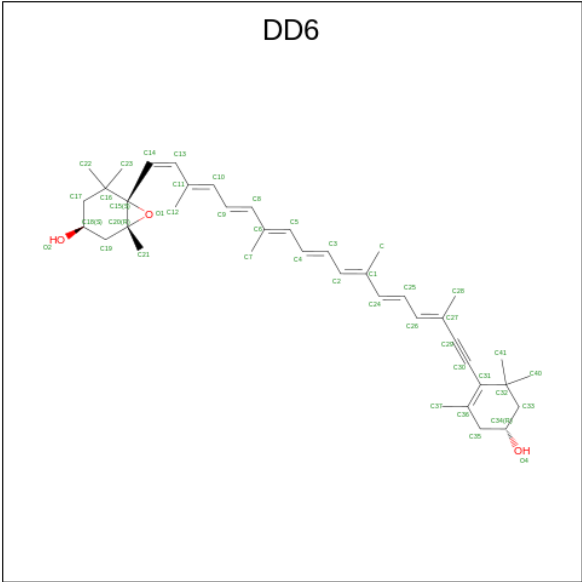
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	9	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	t	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C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

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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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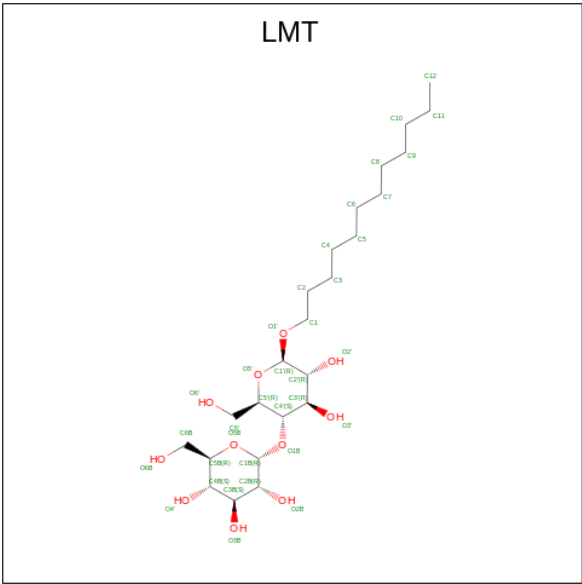
Mol	Chain	Residues	Atoms			AltConf
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	6	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			43	40	3	
26	7	1	Total	C	O	0
			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).



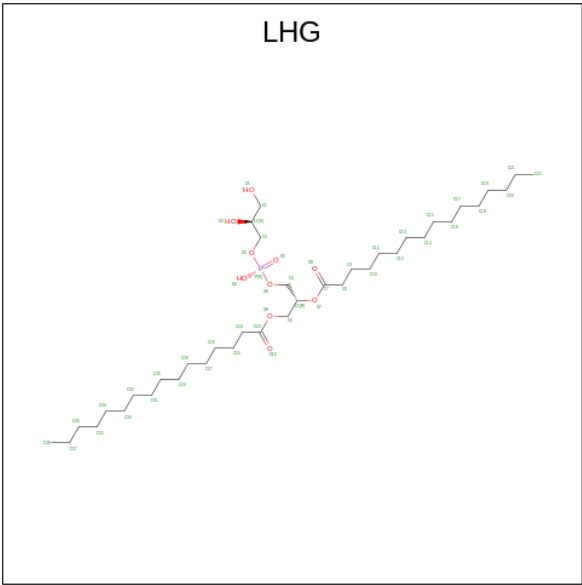
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			35	24	11	

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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).



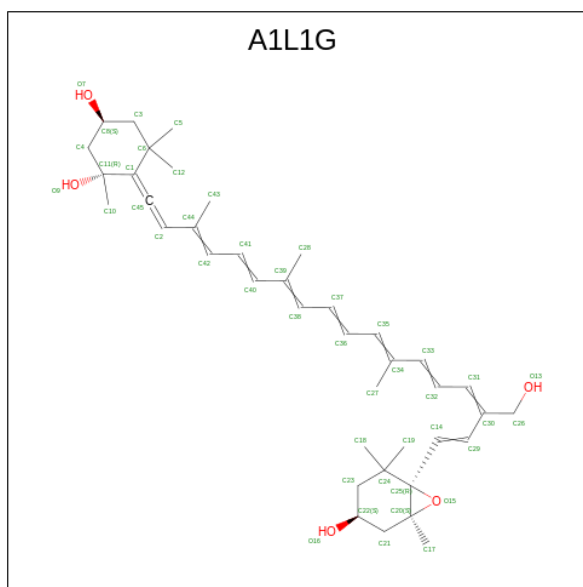
Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			31	20	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	4	1	Total	C	O	P	0
			39	28	10	1	
28	8	1	Total	C	O	P	0
			31	20	10	1	

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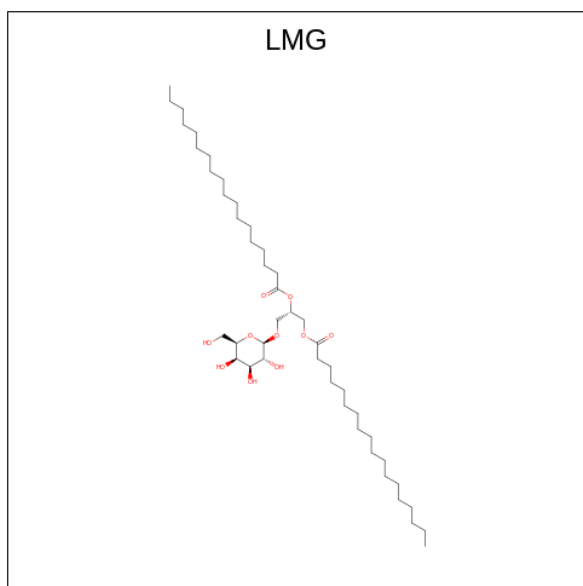
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	37	10	1	
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			41	30	10	1	
28	A	1	Total	C	O	P	0
			37	26	10	1	
28	B	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			41	30	10	1	
28	I	1	Total	C	O	P	0
			40	29	10	1	
28	J	1	Total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

- 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).



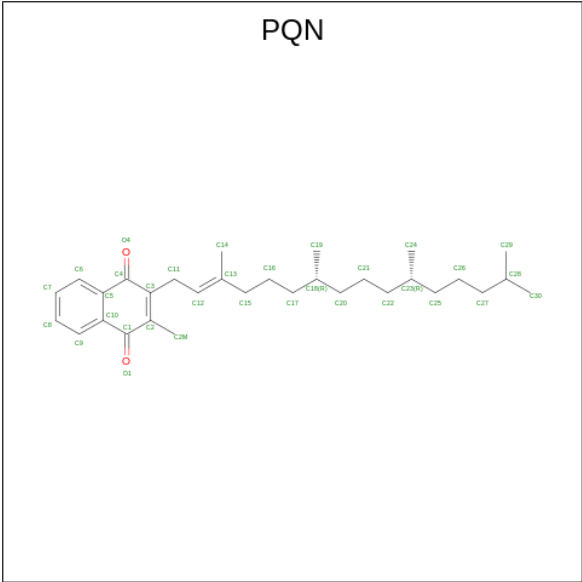
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			45	40	5	
29	3	1	Total	C	O	0
			45	40	5	
29	7	1	Total	C	O	0
			45	40	5	
29	9	1	Total	C	O	0
			45	40	5	
29	k	1	Total	C	O	0
			45	40	5	

- 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).



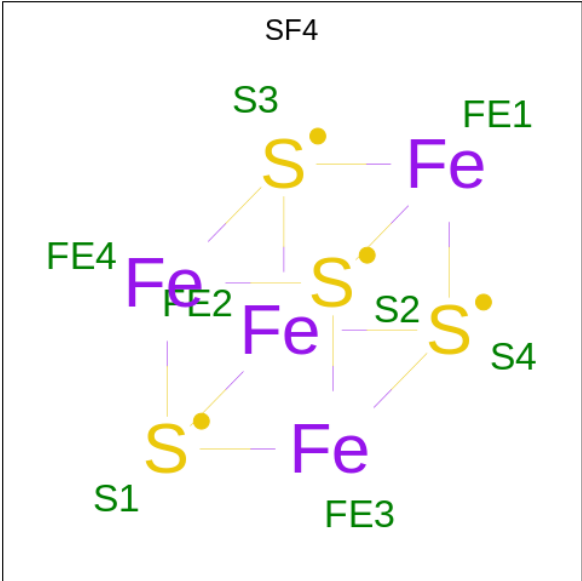
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			45	35	10	
30	t	1	Total	C	O	0
			34	24	10	
30	A	1	Total	C	O	0
			38	28	10	

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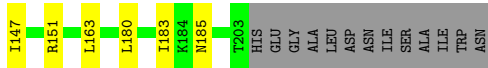
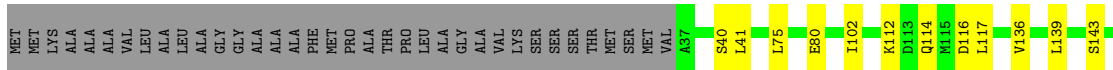
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Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	



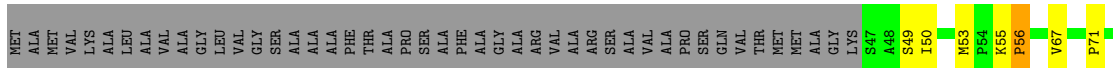
- Molecule 5: light-harvesting protein XLH5

Chain 5: 69% 8% 23%



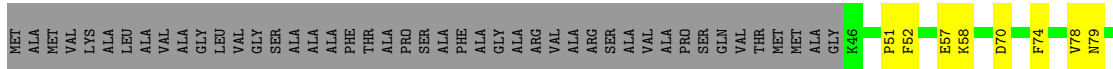
- Molecule 6: light-harvesting protein XLH6/10

Chain 6: 64% 11% 23%



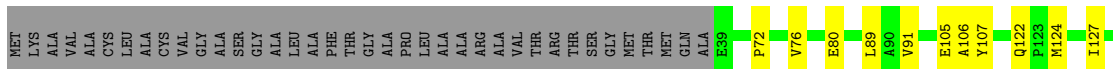
- Molecule 6: light-harvesting protein XLH6/10

Chain h: 67% 10% 22%



- Molecule 7: light-harvesting protein XLH7

Chain 7: 68% 13% 20%

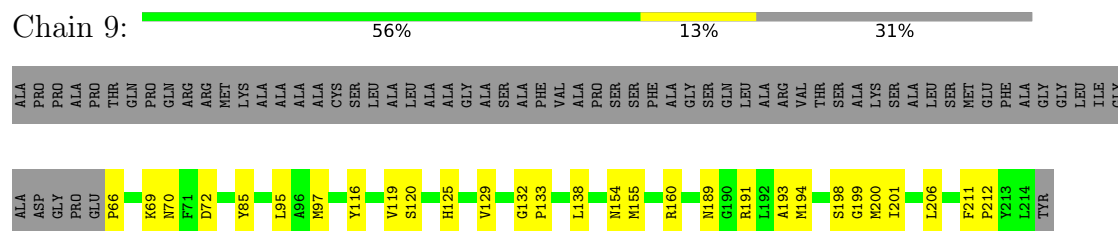


- Molecule 8: light-harvesting protein XLH8

Chain 8: 77% 13% 10%



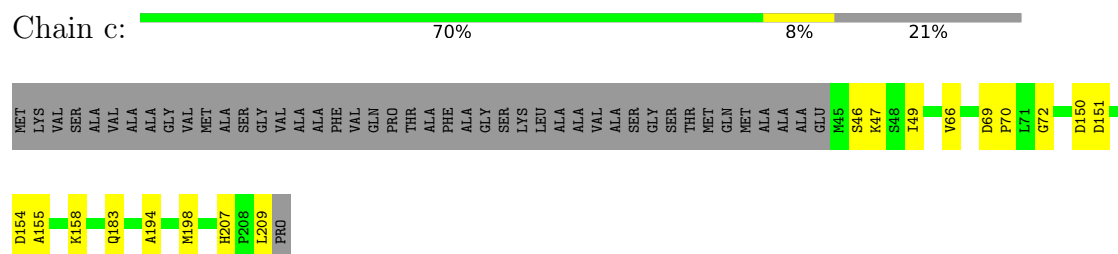
- Molecule 9: light-harvesting protein XLH9/13



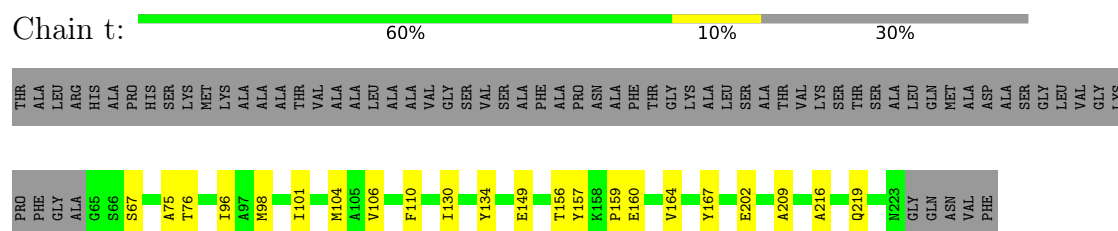
- Molecule 9: light-harvesting protein XLH9/13



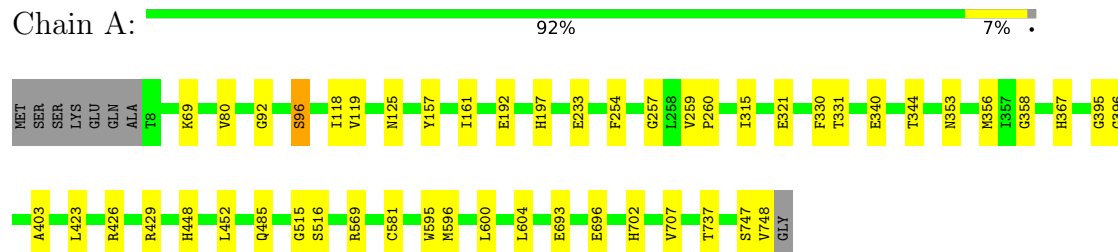
- Molecule 10: light-harvesting protein XLH11



- Molecule 11: light-harvesting protein XLH12

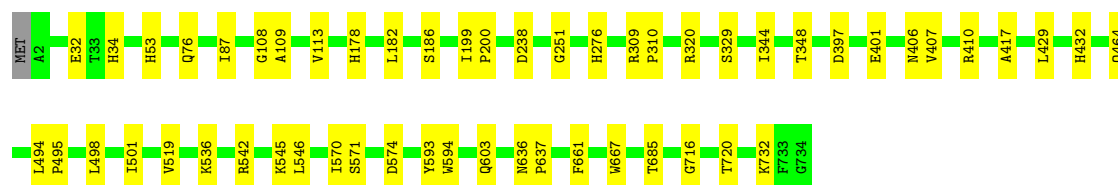


- Molecule 12: PsaA




- Molecule 13: PsaB

Chain B:  93% 7%




• Molecule 14: PsaC

Chain C:  89% 10%




• Molecule 15: PsaD

Chain D:  84% 11% 5%




• Molecule 16: PsaE

Chain E:  87% 11%




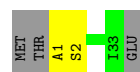
• Molecule 17: PsaF

Chain F:  77% 9% 13%



• Molecule 18: PsaI

Chain I:  86% 6% 8%

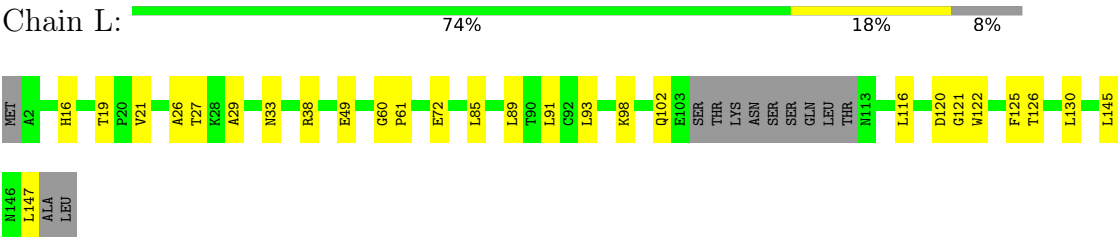


• Molecule 19: PsaJ

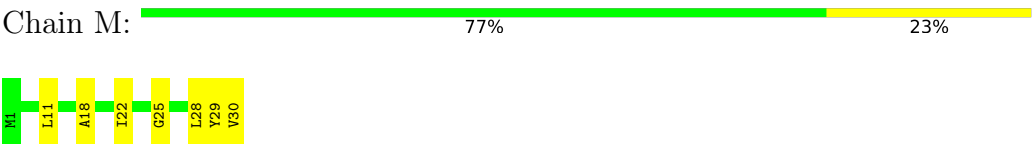
Chain J:  76% 19% 5%



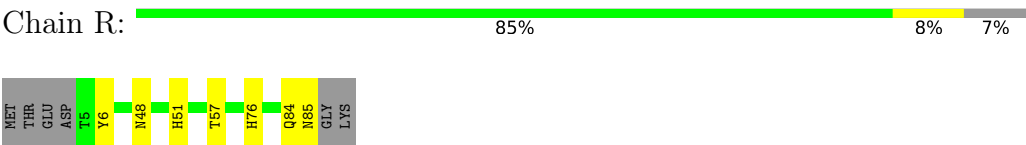
● Molecule 20: PsaL



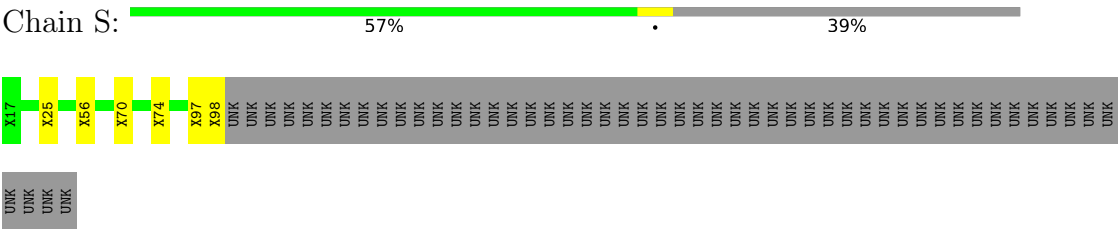
● Molecule 21: PsaM



● 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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.18	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	174/220 (79%)	169 (97%)	5 (3%)	0	100	100
2	2	135/194 (70%)	121 (90%)	13 (10%)	1 (1%)	19	46
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%)	22	49
6	h	163/212 (77%)	154 (94%)	8 (5%)	1 (1%)	22	49
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%)	19	46
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	24
17	F	159/185 (86%)	153 (96%)	5 (3%)	1 (1%)	22	49
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%)	50	76

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%)	54	82
3	3	121/152 (80%)	121 (100%)	0	100	100
4	4	143/173 (83%)	142 (99%)	1 (1%)	81	94
5	5	130/162 (80%)	130 (100%)	0	100	100
6	6	129/159 (81%)	125 (97%)	4 (3%)	35	68
6	h	131/159 (82%)	131 (100%)	0	100	100
7	7	137/163 (84%)	135 (98%)	2 (2%)	60	85
8	8	127/141 (90%)	126 (99%)	1 (1%)	79	93
9	9	125/168 (74%)	124 (99%)	1 (1%)	79	93
9	k	128/168 (76%)	127 (99%)	1 (1%)	79	93
10	c	129/156 (83%)	128 (99%)	1 (1%)	79	93
11	t	133/178 (75%)	132 (99%)	1 (1%)	79	93
12	A	603/609 (99%)	601 (100%)	2 (0%)	91	97
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%)	52	81
21	M	25/25 (100%)	25 (100%)	0	100	100
22	R	68/73 (93%)	67 (98%)	1 (2%)	60	85
All	All	3512/3985 (88%)	3493 (100%)	19 (0%)	85	95

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	$\# Z > 2$
25	BCR	L	206	-	41,41,41	0.73	0	56,56,56	2.09	18 (32%)
24	CLA	1	301	1	65,73,73	1.52	6 (9%)	76,113,113	1.25	7 (9%)
25	BCR	B	841	-	41,41,41	0.75	0	56,56,56	2.08	22 (39%)
25	BCR	I	102	-	41,41,41	0.72	0	56,56,56	2.32	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	804	13	65,73,73	1.54	6 (9%)	76,113,113	1.47	10 (13%)
24	CLA	A	827	12	62,70,73	1.52	5 (8%)	72,109,113	1.31	7 (9%)
29	A1L1G	7	614	-	38,47,47	1.53	8 (21%)	49,71,71	1.10	2 (4%)
26	DD6	c	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.70	8 (15%)
26	DD6	5	608	-	39,45,45	1.53	8 (20%)	52,67,67	1.77	11 (21%)
26	DD6	7	618	-	39,45,45	1.72	6 (15%)	52,67,67	1.72	13 (25%)
24	CLA	k	306	9	46,54,73	1.76	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	1	308	1	46,54,73	1.86	6 (13%)	53,90,113	1.33	7 (13%)
24	CLA	4	602	4	60,68,73	1.54	5 (8%)	70,107,113	1.32	8 (11%)
24	CLA	5	607	5	45,53,73	1.86	8 (17%)	52,89,113	1.56	8 (15%)
24	CLA	4	607	4	46,54,73	1.77	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	B	813	13	46,54,73	1.77	5 (10%)	53,90,113	1.50	8 (15%)
29	A1L1G	3	310	-	38,47,47	1.49	8 (21%)	49,71,71	0.99	3 (6%)
28	LHG	3	315	-	42,42,48	0.99	2 (4%)	45,48,54	1.03	4 (8%)
24	CLA	k	303	-	55,63,73	1.63	5 (9%)	64,101,113	1.55	13 (20%)
24	CLA	A	831	12	65,73,73	1.49	5 (7%)	76,113,113	1.22	7 (9%)
24	CLA	J	103	19	42,50,73	1.86	5 (11%)	48,85,113	1.43	7 (14%)
27	LMT	1	316	-	36,36,36	0.69	0	47,47,47	0.94	2 (4%)
24	CLA	3	305	3	60,68,73	1.57	5 (8%)	70,107,113	1.25	8 (11%)
26	DD6	R	105	-	39,45,45	1.55	10 (25%)	52,67,67	1.87	12 (23%)
24	CLA	B	838	28	65,73,73	1.50	7 (10%)	76,113,113	1.36	9 (11%)
24	CLA	A	807	12	65,73,73	1.48	5 (7%)	76,113,113	1.28	9 (11%)
24	CLA	B	824	13	65,73,73	1.55	5 (7%)	76,113,113	1.40	11 (14%)
24	CLA	L	205	-	46,54,73	1.75	6 (13%)	53,90,113	1.39	7 (13%)
26	DD6	4	616	-	39,45,45	1.51	8 (20%)	52,67,67	1.83	13 (25%)
26	DD6	h	614	-	39,45,45	1.53	8 (20%)	52,67,67	1.59	10 (19%)
24	CLA	9	302	9	46,54,73	1.74	6 (13%)	53,90,113	1.56	6 (11%)
24	CLA	8	202	8	46,54,73	1.78	5 (10%)	53,90,113	1.44	7 (13%)
27	LMT	A	850	-	36,36,36	0.68	0	47,47,47	0.64	0
24	CLA	3	301	3	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
24	CLA	A	819	12	45,53,73	1.81	6 (13%)	52,89,113	1.44	8 (15%)
24	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.44	8 (10%)
24	CLA	B	829	13	65,73,73	1.47	7 (10%)	76,113,113	1.50	9 (11%)
24	CLA	A	805	12	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
28	LHG	A	852	-	36,36,48	1.07	2 (5%)	39,42,54	1.02	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	816	13	65,73,73	1.52	7 (10%)	76,113,113	1.36	9 (11%)
24	CLA	7	605	7	46,54,73	1.81	5 (10%)	53,90,113	1.43	7 (13%)
24	CLA	t	310	-	46,54,73	1.80	5 (10%)	53,90,113	1.41	7 (13%)
24	CLA	2	207	-	46,54,73	1.77	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	k	310	9	41,49,73	1.92	5 (12%)	47,84,113	1.50	8 (17%)
24	CLA	A	828	12	65,73,73	1.50	6 (9%)	76,113,113	1.26	7 (9%)
24	CLA	k	309	9	45,53,73	1.83	5 (11%)	52,89,113	1.41	8 (15%)
28	LHG	I	103	-	39,39,48	1.03	2 (5%)	42,45,54	1.15	4 (9%)
24	CLA	B	810	13	54,62,73	1.66	7 (12%)	67,100,113	1.47	13 (19%)
26	DD6	A	848	-	39,45,45	1.46	8 (20%)	52,67,67	1.92	10 (19%)
24	CLA	A	817	12	65,73,73	1.49	8 (12%)	76,113,113	1.26	8 (10%)
24	CLA	6	606	6	46,54,73	1.78	5 (10%)	53,90,113	1.34	7 (13%)
24	CLA	3	308	3	46,54,73	1.76	6 (13%)	53,90,113	1.45	8 (15%)
26	DD6	4	617	-	39,45,45	1.50	8 (20%)	52,67,67	1.85	12 (23%)
24	CLA	A	837	12	55,63,73	1.65	5 (9%)	64,101,113	1.38	9 (14%)
24	CLA	c	603	10	46,54,73	1.75	6 (13%)	53,90,113	1.44	8 (15%)
24	CLA	t	304	-	46,54,73	1.77	6 (13%)	53,90,113	1.40	7 (13%)
24	CLA	c	604	-	46,54,73	1.81	6 (13%)	53,90,113	1.37	6 (11%)
24	CLA	A	811	12	46,54,73	1.79	6 (13%)	53,90,113	1.38	7 (13%)
26	DD6	c	614	-	39,45,45	1.50	8 (20%)	52,67,67	2.15	11 (21%)
30	LMG	t	314	-	34,34,55	1.12	2 (5%)	42,42,63	1.21	4 (9%)
24	CLA	2	201	2	45,53,73	1.83	6 (13%)	52,89,113	1.59	8 (15%)
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.37	20 (35%)
24	CLA	h	605	6	46,54,73	1.81	5 (10%)	53,90,113	1.38	8 (15%)
24	CLA	4	608	-	50,58,73	1.71	5 (10%)	58,95,113	1.51	10 (17%)
28	LHG	B	845	24	40,40,48	1.02	2 (5%)	43,46,54	0.97	1 (2%)
24	CLA	A	856	-	65,73,73	1.53	7 (10%)	76,113,113	1.31	6 (7%)
24	CLA	A	812	12	65,73,73	1.51	7 (10%)	76,113,113	1.31	8 (10%)
24	CLA	B	820	13	55,63,73	1.64	6 (10%)	64,101,113	1.37	9 (14%)
24	CLA	5	606	-	46,54,73	1.81	5 (10%)	53,90,113	1.42	7 (13%)
24	CLA	3	304	3	46,54,73	1.79	5 (10%)	53,90,113	1.66	8 (15%)
24	CLA	2	206	2	46,54,73	1.78	6 (13%)	53,90,113	1.44	8 (15%)
26	DD6	k	315	-	39,45,45	1.50	8 (20%)	52,67,67	2.04	12 (23%)
25	BCR	k	316	-	41,41,41	0.73	0	56,56,56	2.32	20 (35%)
24	CLA	A	826	12	65,73,73	1.48	5 (7%)	76,113,113	1.36	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	J	105	-	37,37,48	1.05	2 (5%)	40,43,54	1.11	3 (7%)
24	CLA	B	817	13	65,73,73	1.52	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	1	313	-	39,45,45	1.52	8 (20%)	52,67,67	1.56	8 (15%)
24	CLA	7	612	7	46,54,73	1.82	5 (10%)	53,90,113	1.41	7 (13%)
24	CLA	B	833	13	58,66,73	1.57	5 (8%)	67,104,113	1.45	9 (13%)
24	CLA	h	603	6	44,53,73	1.81	5 (11%)	50,89,113	1.44	7 (14%)
24	CLA	c	602	10	65,73,73	1.48	5 (7%)	76,113,113	1.28	9 (11%)
24	CLA	t	302	11	46,54,73	1.81	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	1	309	1	44,53,73	1.83	6 (13%)	50,89,113	1.40	7 (14%)
24	CLA	9	307	9	46,54,73	1.74	7 (15%)	53,90,113	1.54	8 (15%)
26	DD6	6	615	-	39,45,45	1.45	8 (20%)	52,67,67	1.88	15 (28%)
29	A1L1G	9	312	-	38,47,47	1.54	8 (21%)	49,71,71	1.24	6 (12%)
25	BCR	1	314	-	41,41,41	0.74	0	56,56,56	2.16	18 (32%)
24	CLA	B	830	13	58,66,73	1.63	6 (10%)	67,104,113	1.33	8 (11%)
24	CLA	A	804	12	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
26	DD6	6	617	-	39,45,45	1.55	9 (23%)	52,67,67	1.63	9 (17%)
24	CLA	A	801	12	65,73,73	1.51	6 (9%)	76,113,113	1.44	10 (13%)
25	BCR	7	617	-	41,41,41	0.77	0	56,56,56	1.98	21 (37%)
25	BCR	B	840	-	41,41,41	0.79	0	56,56,56	2.01	23 (41%)
28	LHG	2	215	-	30,30,48	1.16	2 (6%)	33,36,54	1.13	3 (9%)
25	BCR	1	310	-	41,41,41	0.76	0	56,56,56	2.17	21 (37%)
24	CLA	B	818	-	65,73,73	1.52	6 (9%)	76,113,113	1.24	9 (11%)
24	CLA	B	848	13	65,73,73	1.49	5 (7%)	76,113,113	1.26	7 (9%)
24	CLA	1	305	1	45,53,73	1.80	8 (17%)	52,89,113	1.83	8 (15%)
24	CLA	A	802	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	7 (9%)
24	CLA	9	305	-	46,54,73	1.74	5 (10%)	53,90,113	1.60	8 (15%)
26	DD6	5	609	-	39,45,45	1.50	8 (20%)	52,67,67	1.77	9 (17%)
25	BCR	R	101	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	22 (39%)
24	CLA	6	603	6	46,54,73	1.79	5 (10%)	53,90,113	1.35	7 (13%)
26	DD6	3	313	-	39,45,45	1.54	8 (20%)	52,67,67	1.61	10 (19%)
24	CLA	7	609	7	46,54,73	1.80	5 (10%)	53,90,113	1.43	7 (13%)
24	CLA	4	610	4	41,49,73	1.90	5 (12%)	47,84,113	1.46	6 (12%)
24	CLA	A	808	12	65,73,73	1.53	5 (7%)	76,113,113	1.26	7 (9%)
24	CLA	8	204	8	45,53,73	1.84	7 (15%)	52,89,113	1.48	8 (15%)
26	DD6	9	313	-	39,45,45	1.56	8 (20%)	52,67,67	1.61	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	F	204	-	41,41,41	0.75	0	56,56,56	2.01	16 (28%)
24	CLA	A	824	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	7 (9%)
24	CLA	1	302	1	45,53,73	1.78	8 (17%)	52,89,113	1.41	8 (15%)
26	DD6	h	615	-	39,45,45	1.50	8 (20%)	52,67,67	1.71	10 (19%)
24	CLA	3	309	3	41,49,73	1.87	5 (12%)	47,84,113	1.51	7 (14%)
24	CLA	2	204	2	60,68,73	1.56	6 (10%)	70,107,113	1.32	7 (10%)
24	CLA	B	828	13	50,58,73	1.75	7 (14%)	58,95,113	1.36	8 (13%)
24	CLA	6	608	6	46,54,73	1.77	5 (10%)	53,90,113	1.36	7 (13%)
32	SF4	C	102	14	0,12,12	-	-	-	-	-
24	CLA	F	201	-	65,73,73	1.52	5 (7%)	76,113,113	1.26	8 (10%)
24	CLA	5	602	5	55,63,73	1.66	5 (9%)	64,101,113	1.42	9 (14%)
25	BCR	R	102	-	41,41,41	0.75	0	56,56,56	2.15	21 (37%)
27	LMT	3	314	-	31,31,36	0.70	0	42,42,47	1.19	3 (7%)
24	CLA	9	301	9	46,54,73	1.80	6 (13%)	53,90,113	1.55	7 (13%)
25	BCR	B	849	-	41,41,41	0.64	0	56,56,56	2.24	20 (35%)
24	CLA	B	847	13	65,73,73	1.54	7 (10%)	76,113,113	1.22	8 (10%)
29	A1L1G	2	213	-	38,47,47	1.51	8 (21%)	49,71,71	1.03	5 (10%)
24	CLA	6	601	6	45,53,73	1.84	5 (11%)	52,89,113	1.44	8 (15%)
24	CLA	7	606	7	60,68,73	1.56	5 (8%)	70,107,113	1.45	7 (10%)
24	CLA	7	607	7	45,53,73	1.82	5 (11%)	52,89,113	1.51	8 (15%)
31	PQN	B	839	-	34,34,34	0.35	0	42,45,45	0.60	1 (2%)
24	CLA	9	308	-	46,54,73	1.79	6 (13%)	53,90,113	1.39	6 (11%)
24	CLA	A	840	28	65,73,73	1.50	5 (7%)	76,113,113	1.31	9 (11%)
24	CLA	t	303	11	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
24	CLA	B	846	13	55,63,73	1.63	6 (10%)	64,101,113	1.30	8 (12%)
28	LHG	L	201	-	28,28,48	1.22	2 (7%)	31,34,54	1.13	2 (6%)
24	CLA	A	816	12	65,73,73	1.49	5 (7%)	76,113,113	1.28	9 (11%)
24	CLA	1	304	26	55,63,73	1.63	7 (12%)	64,101,113	1.23	7 (10%)
24	CLA	8	203	-	50,58,73	1.74	7 (14%)	58,95,113	1.44	10 (17%)
24	CLA	c	605	10	46,54,73	1.82	5 (10%)	53,90,113	1.40	6 (11%)
25	BCR	2	211	-	41,41,41	0.76	0	56,56,56	2.12	22 (39%)
24	CLA	c	609	-	60,68,73	1.59	5 (8%)	70,107,113	1.44	10 (14%)
24	CLA	A	823	12	65,73,73	1.52	7 (10%)	76,113,113	1.20	8 (10%)
27	LMT	1	315	-	36,36,36	0.67	0	47,47,47	0.79	1 (2%)
25	BCR	A	846	-	41,41,41	0.74	1 (2%)	56,56,56	2.38	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	806	12	65,73,73	1.53	5 (7%)	76,113,113	1.24	8 (10%)
24	CLA	B	832	-	45,53,73	1.84	6 (13%)	52,89,113	1.33	6 (11%)
24	CLA	c	610	10	43,52,73	1.89	6 (13%)	49,88,113	1.40	8 (16%)
24	CLA	h	607	6	46,54,73	1.79	6 (13%)	53,90,113	1.30	7 (13%)
26	DD6	t	311	-	39,45,45	1.56	8 (20%)	52,67,67	1.54	7 (13%)
25	BCR	A	843	-	41,41,41	0.72	0	56,56,56	2.34	21 (37%)
28	LHG	A	849	-	40,40,48	1.03	2 (5%)	43,46,54	1.05	2 (4%)
24	CLA	h	611	6	41,49,73	1.80	6 (14%)	47,84,113	1.82	8 (17%)
24	CLA	9	304	9	46,54,73	1.74	6 (13%)	53,90,113	1.61	7 (13%)
24	CLA	B	835	13	47,55,73	1.75	5 (10%)	54,91,113	1.55	7 (12%)
24	CLA	t	306	11	45,53,73	1.82	5 (11%)	52,89,113	1.45	7 (13%)
24	CLA	B	825	13	55,63,73	1.61	5 (9%)	64,101,113	1.35	7 (10%)
24	CLA	5	601	5	45,53,73	1.82	5 (11%)	52,89,113	1.40	8 (15%)
24	CLA	3	302	3	45,53,73	1.79	6 (13%)	52,89,113	1.49	8 (15%)
24	CLA	8	207	-	45,53,73	1.86	5 (11%)	52,89,113	1.42	7 (13%)
24	CLA	6	604	-	46,54,73	1.79	6 (13%)	53,90,113	1.36	7 (13%)
24	CLA	4	601	4	41,50,73	1.89	6 (14%)	46,85,113	1.30	7 (15%)
24	CLA	c	607	10	46,54,73	1.70	7 (15%)	53,90,113	1.47	8 (15%)
24	CLA	4	604	-	46,54,73	1.85	6 (13%)	53,90,113	1.37	6 (11%)
26	DD6	7	616	-	39,45,45	1.63	8 (20%)	52,67,67	1.71	8 (15%)
30	LMG	2	214	-	45,45,55	0.95	2 (4%)	53,53,63	1.37	5 (9%)
26	DD6	4	615	-	39,45,45	1.56	9 (23%)	52,67,67	1.60	7 (13%)
24	CLA	6	610	6	46,54,73	1.83	6 (13%)	53,90,113	1.30	6 (11%)
24	CLA	7	608	-	45,53,73	1.82	5 (11%)	52,89,113	1.59	7 (13%)
24	CLA	h	609	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	h	610	6	46,54,73	1.84	5 (10%)	53,90,113	1.36	8 (15%)
24	CLA	1	317	-	65,73,73	1.53	6 (9%)	76,113,113	1.22	8 (10%)
24	CLA	k	302	9	46,54,73	1.78	5 (10%)	53,90,113	1.53	7 (13%)
24	CLA	A	833	12	65,73,73	1.53	6 (9%)	76,113,113	1.28	9 (11%)
29	A1L1G	k	312	-	38,47,47	1.48	8 (21%)	49,71,71	1.08	4 (8%)
24	CLA	1	307	1	45,53,73	1.84	5 (11%)	52,89,113	1.39	6 (11%)
24	CLA	A	836	12	65,73,73	1.54	6 (9%)	76,113,113	1.19	8 (10%)
26	DD6	9	317	-	39,45,45	1.48	8 (20%)	52,67,67	2.09	16 (30%)
24	CLA	B	814	13	50,58,73	1.73	7 (14%)	58,95,113	1.45	9 (15%)
25	BCR	L	202	-	41,41,41	0.68	0	56,56,56	2.28	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	806	13	65,73,73	1.50	5 (7%)	76,113,113	1.29	7 (9%)
24	CLA	4	611	-	46,54,73	1.79	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	J	104	-	41,41,41	0.69	0	56,56,56	2.28	23 (41%)
24	CLA	A	803	12	55,63,73	1.63	6 (10%)	64,101,113	1.42	9 (14%)
26	DD6	k	313	-	39,45,45	1.48	8 (20%)	52,67,67	1.70	11 (21%)
26	DD6	h	616	-	39,45,45	1.56	8 (20%)	52,67,67	1.72	9 (17%)
24	CLA	8	205	8	45,53,73	1.80	5 (11%)	52,89,113	1.37	8 (15%)
24	CLA	8	209	-	41,49,73	1.89	5 (12%)	47,84,113	1.49	7 (14%)
24	CLA	h	608	6	46,54,73	1.80	6 (13%)	53,90,113	1.34	6 (11%)
24	CLA	B	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
25	BCR	t	312	-	41,41,41	0.76	0	56,56,56	1.79	9 (16%)
24	CLA	6	612	-	46,54,73	1.79	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	J	101	-	41,41,41	0.88	0	56,56,56	2.37	19 (33%)
24	CLA	A	860	12	65,73,73	1.45	7 (10%)	76,113,113	1.51	11 (14%)
27	LMT	h	617	-	29,29,36	0.74	0	40,40,47	0.85	2 (5%)
24	CLA	B	815	13	55,63,73	1.63	5 (9%)	64,101,113	1.38	9 (14%)
24	CLA	B	809	13	65,73,73	1.50	6 (9%)	76,113,113	1.32	9 (11%)
24	CLA	B	834	13	65,73,73	1.52	5 (7%)	76,113,113	1.24	8 (10%)
24	CLA	6	602	6	47,55,73	1.77	6 (12%)	54,91,113	1.38	8 (14%)
24	CLA	A	820	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
24	CLA	h	612	-	45,53,73	1.83	7 (15%)	52,89,113	1.46	8 (15%)
24	CLA	A	832	12	65,73,73	1.51	6 (9%)	76,113,113	1.26	9 (11%)
26	DD6	2	210	-	39,45,45	1.50	8 (20%)	52,67,67	1.73	8 (15%)
24	CLA	5	604	5	46,54,73	1.80	5 (10%)	53,90,113	1.33	7 (13%)
24	CLA	L	204	20	65,73,73	1.53	6 (9%)	76,113,113	1.25	9 (11%)
24	CLA	B	827	13	65,73,73	1.51	6 (9%)	76,113,113	1.29	9 (11%)
24	CLA	t	305	11	46,54,73	1.78	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	k	305	9	46,54,73	1.80	5 (10%)	53,90,113	1.39	6 (11%)
24	CLA	h	606	6	46,54,73	1.77	6 (13%)	53,90,113	1.39	7 (13%)
24	CLA	7	611	7	46,54,73	1.80	6 (13%)	53,90,113	1.44	7 (13%)
24	CLA	2	203	-	50,58,73	1.71	5 (10%)	58,95,113	1.39	8 (13%)
24	CLA	A	838	12	65,73,73	1.52	6 (9%)	76,113,113	1.26	8 (10%)
24	CLA	L	203	20	55,63,73	1.60	5 (9%)	64,101,113	1.45	10 (15%)
26	DD6	1	311	24	39,45,45	1.59	8 (20%)	52,67,67	1.61	12 (23%)
24	CLA	1	303	1	46,54,73	1.77	5 (10%)	53,90,113	1.39	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	3	312	-	39,45,45	1.47	8 (20%)	52,67,67	1.84	9 (17%)
28	LHG	B	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	A	822	12	55,63,73	1.66	6 (10%)	64,101,113	1.31	8 (12%)
24	CLA	B	805	13	65,73,73	1.48	5 (7%)	76,113,113	1.32	7 (9%)
24	CLA	c	601	10	43,51,73	1.87	6 (13%)	49,86,113	1.40	8 (16%)
26	DD6	c	612	-	39,45,45	1.48	8 (20%)	52,67,67	2.07	11 (21%)
24	CLA	7	610	7	45,53,73	1.82	5 (11%)	52,89,113	1.39	7 (13%)
24	CLA	9	306	9	46,54,73	1.81	6 (13%)	53,90,113	1.50	8 (15%)
24	CLA	A	853	12	55,63,73	1.61	6 (10%)	64,101,113	1.43	8 (12%)
26	DD6	2	212	-	39,45,45	1.53	8 (20%)	52,67,67	1.67	8 (15%)
24	CLA	8	208	8	45,53,73	1.78	6 (13%)	52,89,113	1.58	6 (11%)
24	CLA	A	829	12	65,73,73	1.52	6 (9%)	76,113,113	1.30	9 (11%)
24	CLA	A	847	-	55,63,73	1.65	5 (9%)	64,101,113	1.43	8 (12%)
25	BCR	I	101	-	41,41,41	0.78	1 (2%)	56,56,56	2.28	25 (44%)
24	CLA	B	802	13	65,73,73	1.49	6 (9%)	76,113,113	1.17	7 (9%)
24	CLA	B	811	13	55,63,73	1.65	7 (12%)	64,101,113	1.38	10 (15%)
24	CLA	c	608	10	65,73,73	1.51	6 (9%)	76,113,113	1.23	8 (10%)
24	CLA	c	606	10	46,54,73	1.80	5 (10%)	53,90,113	1.41	6 (11%)
32	SF4	C	101	14	0,12,12	-	-	-	-	-
24	CLA	4	609	4	46,54,73	1.79	6 (13%)	53,90,113	1.39	8 (15%)
24	CLA	A	830	12	55,63,73	1.66	8 (14%)	64,101,113	1.89	13 (20%)
24	CLA	9	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	7 (13%)
25	BCR	c	615	-	41,41,41	0.71	0	56,56,56	2.64	21 (37%)
24	CLA	9	303	-	46,54,73	1.79	8 (17%)	53,90,113	1.51	7 (13%)
24	CLA	A	810	12	62,70,73	1.55	6 (9%)	72,109,113	1.24	8 (11%)
24	CLA	2	208	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	6 (11%)
25	BCR	A	859	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
24	CLA	h	602	6	55,63,73	1.62	6 (10%)	64,101,113	2.06	13 (20%)
24	CLA	h	604	-	46,54,73	1.78	5 (10%)	53,90,113	1.38	7 (13%)
24	CLA	B	819	13	46,54,73	1.80	5 (10%)	53,90,113	1.38	7 (13%)
28	LHG	4	619	-	38,38,48	1.05	2 (5%)	41,44,54	0.99	2 (4%)
24	CLA	2	202	2	55,63,73	1.67	5 (9%)	64,101,113	1.35	8 (12%)
24	CLA	2	205	2	46,54,73	1.76	5 (10%)	53,90,113	1.46	6 (11%)
24	CLA	2	209	-	46,54,73	1.80	5 (10%)	53,90,113	1.38	7 (13%)
26	DD6	h	613	-	39,45,45	1.50	8 (20%)	52,67,67	1.56	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	842	-	41,41,41	0.75	0	56,56,56	2.12	14 (25%)
24	CLA	R	104	22	45,53,73	1.76	7 (15%)	52,89,113	1.61	7 (13%)
24	CLA	t	301	11	45,53,73	1.80	5 (11%)	52,89,113	1.69	8 (15%)
24	CLA	A	818	12	65,73,73	1.50	5 (7%)	76,113,113	1.31	10 (13%)
24	CLA	k	301	9	46,54,73	1.77	5 (10%)	53,90,113	1.42	7 (13%)
26	DD6	9	314	-	39,45,45	1.65	7 (17%)	52,67,67	2.20	11 (21%)
24	CLA	5	603	5	45,53,73	1.83	5 (11%)	52,89,113	1.45	8 (15%)
24	CLA	6	609	-	50,58,73	1.74	8 (16%)	58,95,113	1.39	8 (13%)
24	CLA	6	611	6	43,52,73	1.83	7 (16%)	49,88,113	1.55	6 (12%)
24	CLA	c	611	10	41,49,73	1.88	5 (12%)	47,84,113	1.50	7 (14%)
24	CLA	5	605	5	46,54,73	1.78	5 (10%)	53,90,113	1.40	7 (13%)
24	CLA	9	310	9	46,54,73	1.79	6 (13%)	53,90,113	1.52	6 (11%)
24	CLA	B	808	13	65,73,73	1.52	9 (13%)	76,113,113	1.25	10 (13%)
24	CLA	k	304	9	46,54,73	1.82	6 (13%)	53,90,113	1.51	6 (11%)
26	DD6	k	314	-	39,45,45	1.53	9 (23%)	52,67,67	1.75	7 (13%)
24	CLA	R	103	22	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
27	LMT	A	851	-	26,26,36	0.82	0	37,37,47	1.05	5 (13%)
24	CLA	9	309	9	46,54,73	1.75	5 (10%)	53,90,113	1.48	7 (13%)
24	CLA	B	831	-	65,73,73	1.53	6 (9%)	76,113,113	1.24	8 (10%)
24	CLA	t	308	11	46,54,73	1.85	6 (13%)	53,90,113	1.31	7 (13%)
24	CLA	k	308	-	41,49,73	1.89	5 (12%)	47,84,113	1.78	7 (14%)
27	LMT	A	854	-	36,36,36	0.68	0	47,47,47	0.88	0
24	CLA	6	607	6	46,54,73	1.80	5 (10%)	53,90,113	1.35	7 (13%)
25	BCR	A	845	-	40,40,41	0.81	0	52,54,56	2.22	18 (34%)
24	CLA	A	815	-	45,53,73	1.83	5 (11%)	52,89,113	1.40	8 (15%)
24	CLA	3	303	-	55,63,73	1.64	5 (9%)	64,101,113	1.38	9 (14%)
25	BCR	A	844	-	41,41,41	0.84	0	56,56,56	2.12	18 (32%)
24	CLA	A	814	12	50,58,73	1.72	5 (10%)	58,95,113	1.43	8 (13%)
30	LMG	A	855	-	38,38,55	1.07	2 (5%)	46,46,63	1.08	2 (4%)
24	CLA	4	603	4	46,54,73	1.80	6 (13%)	53,90,113	1.40	7 (13%)
24	CLA	7	602	7	50,58,73	1.72	5 (10%)	58,95,113	1.67	12 (20%)
26	DD6	6	616	-	39,45,45	1.54	8 (20%)	52,67,67	2.05	12 (23%)
32	SF4	A	858	12,13	0,12,12	-	-	-	-	-
28	LHG	A	842	24	41,41,48	1.09	2 (4%)	44,47,54	1.28	5 (11%)
26	DD6	9	315	-	39,45,45	1.58	9 (23%)	52,67,67	1.74	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	J	102	-	39,45,45	1.53	8 (20%)	52,67,67	1.65	11 (21%)
26	DD6	3	311	-	39,45,45	1.51	8 (20%)	52,67,67	1.63	10 (19%)
28	LHG	1	318	-	42,42,48	0.97	3 (7%)	45,48,54	1.39	4 (8%)
24	CLA	h	601	6	45,53,73	1.83	5 (11%)	52,89,113	1.51	8 (15%)
24	CLA	A	809	12	46,54,73	1.76	5 (10%)	53,90,113	1.40	7 (13%)
25	BCR	9	316	-	41,41,41	0.76	0	56,56,56	2.36	18 (32%)
26	DD6	4	614	-	39,45,45	1.52	8 (20%)	52,67,67	1.80	11 (21%)
28	LHG	A	841	-	47,47,48	0.93	2 (4%)	50,53,54	0.98	3 (6%)
24	CLA	4	605	4	46,54,73	1.76	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	B	837	13	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
24	CLA	F	203	17	50,58,73	1.71	5 (10%)	58,95,113	1.44	7 (12%)
31	PQN	A	839	-	34,34,34	0.35	0	42,45,45	0.61	1 (2%)
24	CLA	A	857	12	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
24	CLA	A	835	12	51,59,73	1.70	6 (11%)	59,96,113	1.40	9 (15%)
24	CLA	4	612	4	46,54,73	1.75	6 (13%)	53,90,113	1.51	6 (11%)
26	DD6	1	312	-	39,45,45	1.57	9 (23%)	52,67,67	1.51	7 (13%)
28	LHG	8	213	-	30,30,48	1.19	2 (6%)	33,36,54	1.47	4 (12%)
24	CLA	1	306	1	50,58,73	1.71	5 (10%)	58,95,113	1.43	10 (17%)
26	DD6	t	313	-	39,45,45	1.46	8 (20%)	52,67,67	1.72	11 (21%)
26	DD6	6	614	-	39,45,45	1.61	8 (20%)	52,67,67	1.46	6 (11%)
24	CLA	6	605	6	46,54,73	1.80	5 (10%)	53,90,113	1.39	7 (13%)
24	CLA	7	603	7	45,53,73	1.82	5 (11%)	52,89,113	1.45	8 (15%)
24	CLA	B	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	11 (14%)
24	CLA	8	206	8	46,54,73	1.80	5 (10%)	53,90,113	1.45	7 (13%)
24	CLA	B	807	13	65,73,73	1.50	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	8	211	-	39,45,45	1.51	8 (20%)	52,67,67	1.78	9 (17%)
24	CLA	A	834	12	45,53,73	1.83	5 (11%)	52,89,113	1.47	8 (15%)
26	DD6	8	212	-	39,45,45	1.50	8 (20%)	52,67,67	1.64	10 (19%)
26	DD6	8	210	-	39,45,45	1.68	8 (20%)	52,67,67	2.09	12 (23%)
24	CLA	A	825	-	65,73,73	1.48	5 (7%)	76,113,113	1.28	8 (10%)
24	CLA	7	601	7	45,53,73	1.84	7 (15%)	52,89,113	1.42	8 (15%)
24	CLA	8	201	8	46,54,73	1.81	5 (10%)	53,90,113	1.36	7 (13%)
24	CLA	B	812	13	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
26	DD6	7	615	-	39,45,45	1.49	8 (20%)	52,67,67	1.82	12 (23%)
24	CLA	t	307	-	46,54,73	1.80	5 (10%)	53,90,113	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	k	307	9	46,54,73	1.81	6 (13%)	53,90,113	1.33	6 (11%)
24	CLA	3	307	-	45,53,73	1.81	6 (13%)	52,89,113	1.48	7 (13%)
24	CLA	B	821	13	53,61,73	1.65	6 (11%)	61,98,113	1.39	11 (18%)
24	CLA	t	309	-	46,54,73	1.81	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	B	826	13	65,73,73	1.55	7 (10%)	76,113,113	1.22	8 (10%)
24	CLA	3	306	3	65,73,73	1.51	6 (9%)	76,113,113	1.24	8 (10%)
24	CLA	4	613	4	46,54,73	1.82	6 (13%)	53,90,113	1.38	7 (13%)
25	BCR	M	101	-	41,41,41	0.74	0	56,56,56	2.14	16 (28%)
26	DD6	6	613	-	39,45,45	1.52	8 (20%)	52,67,67	1.66	8 (15%)
24	CLA	A	813	12	65,73,73	1.51	6 (9%)	76,113,113	1.23	9 (11%)
24	CLA	B	836	-	65,73,73	1.53	6 (9%)	76,113,113	1.21	7 (9%)
24	CLA	F	202	-	46,54,73	1.80	5 (10%)	53,90,113	1.37	7 (13%)
24	CLA	7	604	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
24	CLA	B	823	-	64,72,73	1.50	6 (9%)	74,111,113	1.30	9 (12%)
25	BCR	4	618	-	41,41,41	0.79	0	56,56,56	2.38	20 (35%)
24	CLA	A	821	12	49,57,73	1.72	5 (10%)	55,93,113	1.41	7 (12%)
24	CLA	k	311	-	55,63,73	1.64	5 (9%)	64,101,113	1.40	7 (10%)
24	CLA	4	606	4	46,54,73	1.77	5 (10%)	53,90,113	1.38	8 (15%)
26	DD6	7	613	-	39,45,45	1.48	8 (20%)	52,67,67	1.86	11 (21%)

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
25	BCR	L	206	-	-	4/29/63/63	0/2/2/2
24	CLA	1	301	1	1/1/15/20	11/37/115/115	-
25	BCR	B	841	-	-	2/29/63/63	0/2/2/2
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
24	CLA	B	804	13	1/1/15/20	13/37/115/115	-
24	CLA	A	827	12	1/1/14/20	11/34/112/115	-
29	A1L1G	7	614	-	-	12/29/85/85	0/3/3/3
26	DD6	c	613	-	-	0/26/80/80	0/3/3/3
26	DD6	5	608	-	-	4/26/80/80	0/3/3/3
26	DD6	7	618	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	k	306	9	1/1/11/20	5/15/93/115	-
24	CLA	1	308	1	1/1/11/20	5/15/93/115	-
24	CLA	4	602	4	1/1/14/20	11/31/109/115	-
24	CLA	5	607	5	1/1/11/20	5/13/91/115	-
24	CLA	4	607	4	1/1/11/20	8/15/93/115	-
24	CLA	B	813	13	1/1/11/20	8/15/93/115	-
29	A1L1G	3	310	-	-	16/29/85/85	0/3/3/3
28	LHG	3	315	-	-	26/47/47/53	-
24	CLA	A	831	12	1/1/15/20	12/37/115/115	-
24	CLA	J	103	19	1/1/10/20	6/10/88/115	-
24	CLA	k	303	-	-	10/25/103/115	-
27	LMT	1	316	-	-	8/21/61/61	0/2/2/2
24	CLA	3	305	3	1/1/14/20	8/31/109/115	-
26	DD6	R	105	-	-	6/26/80/80	0/3/3/3
24	CLA	B	838	28	1/1/15/20	7/37/115/115	-
24	CLA	A	807	12	1/1/15/20	16/37/115/115	-
24	CLA	B	824	13	1/1/15/20	9/37/115/115	-
24	CLA	L	205	-	1/1/11/20	6/15/93/115	-
26	DD6	4	616	-	-	4/26/80/80	0/3/3/3
26	DD6	h	614	-	-	4/26/80/80	0/3/3/3
24	CLA	9	302	9	1/1/11/20	7/15/93/115	-
24	CLA	8	202	8	1/1/11/20	9/15/93/115	-
27	LMT	A	850	-	-	10/21/61/61	0/2/2/2
24	CLA	3	301	3	-	15/37/115/115	-
24	CLA	A	819	12	1/1/11/20	2/13/91/115	-
24	CLA	B	803	-	1/1/15/20	8/37/115/115	-
24	CLA	B	829	13	1/1/15/20	9/37/115/115	-
24	CLA	A	805	12	1/1/15/20	11/37/115/115	-
28	LHG	A	852	-	-	9/41/41/53	-
24	CLA	B	816	13	1/1/15/20	12/37/115/115	-
24	CLA	7	605	7	1/1/11/20	4/15/93/115	-
24	CLA	t	310	-	1/1/11/20	6/15/93/115	-
24	CLA	2	207	-	1/1/11/20	6/15/93/115	-
24	CLA	k	310	9	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	828	12	1/1/15/20	12/37/115/115	-
24	CLA	k	309	9	1/1/11/20	5/13/91/115	-
28	LHG	I	103	-	-	13/44/44/53	-
24	CLA	B	810	13	1/1/13/20	8/25/101/115	-
26	DD6	A	848	-	-	1/26/80/80	0/3/3/3
24	CLA	A	817	12	1/1/15/20	11/37/115/115	-
24	CLA	6	606	6	1/1/11/20	9/15/93/115	-
24	CLA	3	308	3	1/1/11/20	8/15/93/115	-
26	DD6	4	617	-	-	1/26/80/80	0/3/3/3
24	CLA	A	837	12	1/1/13/20	8/25/103/115	-
24	CLA	c	603	10	1/1/11/20	9/15/93/115	-
24	CLA	t	304	-	1/1/11/20	5/15/93/115	-
24	CLA	c	604	-	1/1/11/20	8/15/93/115	-
24	CLA	A	811	12	1/1/11/20	6/15/93/115	-
26	DD6	c	614	-	-	1/26/80/80	0/3/3/3
30	LMG	t	314	-	-	6/29/49/70	0/1/1/1
24	CLA	2	201	2	1/1/11/20	9/13/91/115	-
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
24	CLA	h	605	6	1/1/11/20	4/15/93/115	-
24	CLA	4	608	-	1/1/12/20	7/19/97/115	-
28	LHG	B	845	24	-	9/45/45/53	-
24	CLA	A	856	-	-	11/37/115/115	-
24	CLA	A	812	12	1/1/15/20	13/37/115/115	-
24	CLA	B	820	13	1/1/13/20	10/25/103/115	-
24	CLA	5	606	-	1/1/11/20	6/15/93/115	-
24	CLA	3	304	3	1/1/11/20	6/15/93/115	-
24	CLA	2	206	2	1/1/11/20	5/15/93/115	-
26	DD6	k	315	-	-	3/26/80/80	0/3/3/3
25	BCR	k	316	-	-	3/29/63/63	0/2/2/2
24	CLA	A	826	12	1/1/15/20	11/37/115/115	-
28	LHG	J	105	-	-	12/42/42/53	-
24	CLA	B	817	13	1/1/15/20	18/37/115/115	-
26	DD6	1	313	-	-	1/26/80/80	0/3/3/3
24	CLA	7	612	7	1/1/11/20	8/15/93/115	-
24	CLA	B	833	13	1/1/13/20	6/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	603	6	1/1/11/20	4/13/91/115	-
24	CLA	c	602	10	1/1/15/20	12/37/115/115	-
24	CLA	t	302	11	1/1/11/20	12/15/93/115	-
24	CLA	1	309	1	1/1/11/20	2/13/91/115	-
24	CLA	9	307	9	1/1/11/20	7/15/93/115	-
26	DD6	6	615	-	-	4/26/80/80	0/3/3/3
29	A1L1G	9	312	-	-	13/29/85/85	0/3/3/3
25	BCR	1	314	-	-	8/29/63/63	0/2/2/2
24	CLA	B	830	13	1/1/13/20	8/29/107/115	-
24	CLA	A	804	12	1/1/15/20	15/37/115/115	-
26	DD6	6	617	-	-	1/26/80/80	0/3/3/3
24	CLA	A	801	12	1/1/15/20	16/37/115/115	-
25	BCR	7	617	-	-	2/29/63/63	0/2/2/2
25	BCR	B	840	-	-	4/29/63/63	0/2/2/2
28	LHG	2	215	-	-	9/35/35/53	-
25	BCR	1	310	-	-	3/29/63/63	0/2/2/2
24	CLA	B	818	-	1/1/15/20	12/37/115/115	-
24	CLA	B	848	13	1/1/15/20	10/37/115/115	-
24	CLA	1	305	1	1/1/11/20	7/13/91/115	-
24	CLA	A	802	-	1/1/15/20	6/37/115/115	-
24	CLA	9	305	-	-	10/15/93/115	-
26	DD6	5	609	-	-	1/26/80/80	0/3/3/3
25	BCR	R	101	-	-	4/29/63/63	0/2/2/2
24	CLA	6	603	6	1/1/11/20	8/15/93/115	-
26	DD6	3	313	-	-	3/26/80/80	0/3/3/3
24	CLA	7	609	7	1/1/11/20	7/15/93/115	-
24	CLA	4	610	4	1/1/10/20	2/8/86/115	-
24	CLA	A	808	12	1/1/15/20	9/37/115/115	-
24	CLA	8	204	8	1/1/11/20	4/13/91/115	-
26	DD6	9	313	-	-	3/26/80/80	0/3/3/3
25	BCR	F	204	-	-	2/29/63/63	0/2/2/2
24	CLA	A	824	-	1/1/15/20	15/37/115/115	-
24	CLA	1	302	1	1/1/11/20	6/13/91/115	-
26	DD6	h	615	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	3	309	3	1/1/10/20	2/8/86/115	-
24	CLA	2	204	2	1/1/14/20	10/31/109/115	-
24	CLA	B	828	13	1/1/12/20	9/19/97/115	-
24	CLA	6	608	6	1/1/11/20	4/15/93/115	-
32	SF4	C	102	14	-	-	0/6/5/5
24	CLA	F	201	-	1/1/15/20	12/37/115/115	-
24	CLA	5	602	5	1/1/13/20	10/25/103/115	-
25	BCR	R	102	-	-	4/29/63/63	0/2/2/2
27	LMT	3	314	-	-	9/16/56/61	0/2/2/2
24	CLA	9	301	9	1/1/11/20	8/15/93/115	-
25	BCR	B	849	-	-	4/29/63/63	0/2/2/2
24	CLA	B	847	13	1/1/15/20	14/37/115/115	-
29	A1L1G	2	213	-	-	19/29/85/85	0/3/3/3
24	CLA	6	601	6	1/1/11/20	6/13/91/115	-
24	CLA	7	606	7	1/1/14/20	12/31/109/115	-
24	CLA	7	607	7	1/1/11/20	3/13/91/115	-
31	PQN	B	839	-	-	10/23/43/43	0/2/2/2
24	CLA	9	308	-	1/1/11/20	8/15/93/115	-
24	CLA	A	840	28	1/1/15/20	11/37/115/115	-
24	CLA	t	303	11	1/1/15/20	15/37/115/115	-
24	CLA	B	846	13	1/1/13/20	8/25/103/115	-
28	LHG	L	201	-	-	15/33/33/53	-
24	CLA	A	816	12	1/1/15/20	13/37/115/115	-
24	CLA	1	304	26	1/1/13/20	11/25/103/115	-
24	CLA	8	203	-	1/1/12/20	8/19/97/115	-
24	CLA	c	605	10	1/1/11/20	10/15/93/115	-
25	BCR	2	211	-	-	4/29/63/63	0/2/2/2
24	CLA	c	609	-	1/1/14/20	11/31/109/115	-
24	CLA	A	823	12	1/1/15/20	19/37/115/115	-
27	LMT	1	315	-	-	12/21/61/61	0/2/2/2
25	BCR	A	846	-	-	2/29/63/63	0/2/2/2
24	CLA	A	806	12	1/1/15/20	10/37/115/115	-
24	CLA	B	832	-	1/1/11/20	9/13/91/115	-
24	CLA	c	610	10	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	607	6	1/1/11/20	4/15/93/115	-
26	DD6	t	311	-	-	2/26/80/80	0/3/3/3
25	BCR	A	843	-	-	4/29/63/63	0/2/2/2
28	LHG	A	849	-	-	13/45/45/53	-
24	CLA	h	611	6	-	4/8/86/115	-
24	CLA	9	304	9	1/1/11/20	6/15/93/115	-
24	CLA	B	835	13	1/1/11/20	7/16/94/115	-
24	CLA	t	306	11	1/1/11/20	8/13/91/115	-
24	CLA	B	825	13	1/1/13/20	8/25/103/115	-
24	CLA	5	601	5	1/1/11/20	3/13/91/115	-
24	CLA	3	302	3	1/1/11/20	3/13/91/115	-
24	CLA	8	207	-	1/1/11/20	7/13/91/115	-
24	CLA	6	604	-	1/1/11/20	4/15/93/115	-
24	CLA	4	601	4	1/1/10/20	3/9/87/115	-
24	CLA	c	607	10	1/1/11/20	3/15/93/115	-
24	CLA	4	604	-	1/1/11/20	8/15/93/115	-
26	DD6	7	616	-	-	2/26/80/80	0/3/3/3
30	LMG	2	214	-	-	8/40/60/70	0/1/1/1
26	DD6	4	615	-	-	1/26/80/80	0/3/3/3
24	CLA	6	610	6	1/1/11/20	4/15/93/115	-
24	CLA	7	608	-	1/1/11/20	6/13/91/115	-
24	CLA	h	609	-	1/1/11/20	5/15/93/115	-
24	CLA	h	610	6	1/1/11/20	7/15/93/115	-
24	CLA	1	317	-	1/1/15/20	14/37/115/115	-
24	CLA	k	302	9	1/1/11/20	9/15/93/115	-
24	CLA	A	833	12	1/1/15/20	5/37/115/115	-
29	A1L1G	k	312	-	-	8/29/85/85	0/3/3/3
24	CLA	1	307	1	1/1/11/20	4/13/91/115	-
24	CLA	A	836	12	1/1/15/20	13/37/115/115	-
26	DD6	9	317	-	-	2/26/80/80	0/3/3/3
24	CLA	B	814	13	1/1/12/20	3/19/97/115	-
25	BCR	L	202	-	-	6/29/63/63	0/2/2/2
24	CLA	B	806	13	1/1/15/20	9/37/115/115	-
24	CLA	4	611	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	J	104	-	-	2/29/63/63	0/2/2/2
24	CLA	A	803	12	-	6/25/103/115	-
26	DD6	k	313	-	-	1/26/80/80	0/3/3/3
26	DD6	h	616	-	-	2/26/80/80	0/3/3/3
24	CLA	8	205	8	1/1/11/20	7/13/91/115	-
24	CLA	8	209	-	1/1/10/20	3/8/86/115	-
24	CLA	h	608	6	1/1/11/20	5/15/93/115	-
24	CLA	B	801	-	1/1/15/20	13/37/115/115	-
25	BCR	t	312	-	-	8/29/63/63	0/2/2/2
24	CLA	6	612	-	1/1/11/20	1/15/93/115	-
25	BCR	J	101	-	-	2/29/63/63	0/2/2/2
24	CLA	A	860	12	1/1/15/20	6/37/115/115	-
27	LMT	h	617	-	-	7/14/54/61	0/2/2/2
24	CLA	B	815	13	1/1/13/20	11/25/103/115	-
24	CLA	B	809	13	1/1/15/20	10/37/115/115	-
24	CLA	B	834	13	1/1/15/20	10/37/115/115	-
24	CLA	6	602	6	1/1/11/20	6/16/94/115	-
24	CLA	A	820	-	1/1/15/20	10/37/115/115	-
24	CLA	h	612	-	1/1/11/20	7/13/91/115	-
24	CLA	A	832	12	-	12/37/115/115	-
26	DD6	2	210	-	-	1/26/80/80	0/3/3/3
24	CLA	5	604	5	1/1/11/20	1/15/93/115	-
24	CLA	L	204	20	-	9/37/115/115	-
24	CLA	B	827	13	1/1/15/20	12/37/115/115	-
24	CLA	t	305	11	1/1/11/20	6/15/93/115	-
24	CLA	k	305	9	1/1/11/20	6/15/93/115	-
24	CLA	h	606	6	1/1/11/20	5/15/93/115	-
24	CLA	7	611	7	1/1/11/20	7/15/93/115	-
24	CLA	2	203	-	1/1/12/20	5/19/97/115	-
24	CLA	A	838	12	1/1/15/20	10/37/115/115	-
24	CLA	L	203	20	1/1/13/20	10/25/103/115	-
26	DD6	1	311	24	-	0/26/80/80	0/3/3/3
24	CLA	1	303	1	1/1/11/20	6/15/93/115	-
26	DD6	3	312	-	-	1/26/80/80	0/3/3/3
28	LHG	B	844	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	822	12	1/1/13/20	14/25/103/115	-
24	CLA	B	805	13	1/1/15/20	11/37/115/115	-
24	CLA	c	601	10	1/1/10/20	5/11/89/115	-
26	DD6	c	612	-	-	1/26/80/80	0/3/3/3
24	CLA	7	610	7	1/1/11/20	6/13/91/115	-
24	CLA	9	306	9	1/1/11/20	5/15/93/115	-
24	CLA	A	853	12	1/1/13/20	7/25/103/115	-
26	DD6	2	212	-	-	1/26/80/80	0/3/3/3
24	CLA	8	208	8	1/1/11/20	5/13/91/115	-
24	CLA	A	829	12	1/1/15/20	8/37/115/115	-
24	CLA	A	847	-	1/1/13/20	10/25/103/115	-
25	BCR	I	101	-	-	4/29/63/63	0/2/2/2
24	CLA	B	802	13	1/1/15/20	17/37/115/115	-
24	CLA	B	811	13	1/1/13/20	5/25/103/115	-
24	CLA	c	608	10	1/1/15/20	13/37/115/115	-
24	CLA	c	606	10	1/1/11/20	6/15/93/115	-
32	SF4	C	101	14	-	-	0/6/5/5
24	CLA	4	609	4	1/1/11/20	6/15/93/115	-
24	CLA	A	830	12	-	8/25/103/115	-
24	CLA	9	311	-	1/1/11/20	6/13/91/115	-
25	BCR	c	615	-	-	10/29/63/63	0/2/2/2
24	CLA	9	303	-	1/1/11/20	8/15/93/115	-
24	CLA	A	810	12	1/1/14/20	13/34/112/115	-
24	CLA	2	208	-	1/1/11/20	6/15/93/115	-
25	BCR	A	859	-	-	4/29/63/63	0/2/2/2
24	CLA	h	602	6	1/1/13/20	7/25/103/115	-
24	CLA	h	604	-	1/1/11/20	5/15/93/115	-
24	CLA	B	819	13	1/1/11/20	2/15/93/115	-
28	LHG	4	619	-	-	8/43/43/53	-
24	CLA	2	202	2	1/1/13/20	6/25/103/115	-
24	CLA	2	205	2	-	4/15/93/115	-
24	CLA	2	209	-	1/1/11/20	7/15/93/115	-
26	DD6	h	613	-	-	1/26/80/80	0/3/3/3
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
24	CLA	R	104	22	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	t	301	11	1/1/11/20	4/13/91/115	-
24	CLA	A	818	12	1/1/15/20	15/37/115/115	-
24	CLA	k	301	9	1/1/11/20	4/15/93/115	-
26	DD6	9	314	-	-	2/26/80/80	0/3/3/3
24	CLA	5	603	5	1/1/11/20	4/13/91/115	-
24	CLA	6	609	-	1/1/12/20	7/19/97/115	-
24	CLA	6	611	6	1/1/11/20	4/11/89/115	-
24	CLA	c	611	10	1/1/10/20	4/8/86/115	-
24	CLA	5	605	5	1/1/11/20	9/15/93/115	-
24	CLA	9	310	9	1/1/11/20	6/15/93/115	-
24	CLA	B	808	13	1/1/15/20	8/37/115/115	-
24	CLA	k	304	9	1/1/11/20	7/15/93/115	-
26	DD6	k	314	-	-	2/26/80/80	0/3/3/3
24	CLA	R	103	22	1/1/15/20	9/37/115/115	-
27	LMT	A	851	-	-	4/11/51/61	0/2/2/2
24	CLA	9	309	9	1/1/11/20	9/15/93/115	-
24	CLA	B	831	-	1/1/15/20	19/37/115/115	-
24	CLA	t	308	11	1/1/11/20	6/15/93/115	-
24	CLA	k	308	-	1/1/10/20	6/8/86/115	-
27	LMT	A	854	-	-	9/21/61/61	0/2/2/2
24	CLA	6	607	6	1/1/11/20	4/15/93/115	-
25	BCR	A	845	-	-	5/29/60/63	0/2/2/2
24	CLA	A	815	-	1/1/11/20	6/13/91/115	-
24	CLA	3	303	-	1/1/13/20	7/25/103/115	-
25	BCR	A	844	-	-	6/29/63/63	0/2/2/2
24	CLA	A	814	12	1/1/12/20	7/19/97/115	-
30	LMG	A	855	-	-	5/33/53/70	0/1/1/1
24	CLA	4	603	4	1/1/11/20	3/15/93/115	-
24	CLA	7	602	7	1/1/12/20	9/19/97/115	-
26	DD6	6	616	-	-	4/26/80/80	0/3/3/3
32	SF4	A	858	12,13	-	-	0/6/5/5
28	LHG	A	842	24	-	10/46/46/53	-
26	DD6	9	315	-	-	4/26/80/80	0/3/3/3
26	DD6	J	102	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	3	311	-	-	1/26/80/80	0/3/3/3
28	LHG	1	318	-	-	15/47/47/53	-
24	CLA	h	601	6	1/1/11/20	5/13/91/115	-
24	CLA	A	809	12	1/1/11/20	6/15/93/115	-
25	BCR	9	316	-	-	2/29/63/63	0/2/2/2
26	DD6	4	614	-	-	1/26/80/80	0/3/3/3
28	LHG	A	841	-	-	19/52/52/53	-
24	CLA	4	605	4	1/1/11/20	4/15/93/115	-
24	CLA	B	837	13	1/1/15/20	15/37/115/115	-
24	CLA	F	203	17	1/1/12/20	7/19/97/115	-
31	PQN	A	839	-	-	5/23/43/43	0/2/2/2
24	CLA	A	857	12	1/1/15/20	9/37/115/115	-
24	CLA	A	835	12	1/1/12/20	5/21/99/115	-
24	CLA	4	612	4	1/1/11/20	5/15/93/115	-
26	DD6	1	312	-	-	0/26/80/80	0/3/3/3
28	LHG	8	213	-	-	17/35/35/53	-
24	CLA	1	306	1	1/1/12/20	4/19/97/115	-
26	DD6	t	313	-	-	0/26/80/80	0/3/3/3
26	DD6	6	614	-	-	1/26/80/80	0/3/3/3
24	CLA	6	605	6	-	2/15/93/115	-
24	CLA	7	603	7	1/1/11/20	2/13/91/115	-
24	CLA	B	822	-	1/1/15/20	12/37/115/115	-
24	CLA	8	206	8	1/1/11/20	8/15/93/115	-
24	CLA	B	807	13	-	7/37/115/115	-
26	DD6	8	211	-	-	3/26/80/80	0/3/3/3
24	CLA	A	834	12	1/1/11/20	4/13/91/115	-
26	DD6	8	212	-	-	2/26/80/80	0/3/3/3
26	DD6	8	210	-	-	3/26/80/80	0/3/3/3
24	CLA	A	825	-	1/1/15/20	6/37/115/115	-
24	CLA	7	601	7	1/1/11/20	6/13/91/115	-
24	CLA	8	201	8	1/1/11/20	4/15/93/115	-
24	CLA	B	812	13	1/1/15/20	16/37/115/115	-
26	DD6	7	615	-	-	3/26/80/80	0/3/3/3
24	CLA	t	307	-	1/1/11/20	7/15/93/115	-
24	CLA	k	307	9	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	3	307	-	1/1/11/20	4/13/91/115	-
24	CLA	B	821	13	1/1/12/20	11/23/101/115	-
24	CLA	t	309	-	1/1/11/20	4/15/93/115	-
24	CLA	B	826	13	1/1/15/20	8/37/115/115	-
24	CLA	3	306	3	1/1/15/20	10/37/115/115	-
24	CLA	4	613	4	1/1/11/20	11/15/93/115	-
25	BCR	M	101	-	-	9/29/63/63	0/2/2/2
26	DD6	6	613	-	-	2/26/80/80	0/3/3/3
24	CLA	A	813	12	1/1/15/20	12/37/115/115	-
24	CLA	B	836	-	1/1/15/20	12/37/115/115	-
24	CLA	F	202	-	1/1/11/20	3/15/93/115	-
24	CLA	7	604	-	1/1/11/20	6/13/91/115	-
24	CLA	B	823	-	1/1/14/20	7/36/114/115	-
25	BCR	4	618	-	-	1/29/63/63	0/2/2/2
24	CLA	A	821	12	1/1/11/20	2/18/96/115	-
24	CLA	k	311	-	1/1/13/20	7/25/103/115	-
24	CLA	4	606	4	1/1/11/20	2/15/93/115	-
26	DD6	7	613	-	-	0/26/80/80	0/3/3/3

All (1747) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	308	CLA	C4B-NB	8.30	1.42	1.35
24	B	824	CLA	C4B-NB	8.24	1.42	1.35
24	4	604	CLA	C4B-NB	8.21	1.42	1.35
24	t	308	CLA	C4B-NB	8.18	1.42	1.35
24	1	308	CLA	C4B-NB	8.11	1.42	1.35
24	h	610	CLA	C4B-NB	8.02	1.42	1.35
24	k	310	CLA	C4B-NB	8.01	1.42	1.35
24	3	305	CLA	C4B-NB	7.97	1.42	1.35
24	5	602	CLA	C4B-NB	7.95	1.42	1.35
24	4	613	CLA	C4B-NB	7.95	1.42	1.35
24	B	828	CLA	C4B-NB	7.94	1.42	1.35
24	7	605	CLA	C4B-NB	7.94	1.42	1.35
24	A	806	CLA	C4B-NB	7.94	1.42	1.35
24	8	206	CLA	C4B-NB	7.94	1.42	1.35
24	8	207	CLA	C4B-NB	7.93	1.42	1.35
24	6	601	CLA	C4B-NB	7.93	1.42	1.35
24	1	307	CLA	C4B-NB	7.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	202	CLA	C4B-NB	7.92	1.42	1.35
24	c	601	CLA	C4B-NB	7.91	1.42	1.35
24	c	610	CLA	C4B-NB	7.91	1.42	1.35
24	k	304	CLA	C4B-NB	7.90	1.42	1.35
24	5	607	CLA	C4B-NB	7.90	1.42	1.35
24	6	610	CLA	C4B-NB	7.90	1.42	1.35
24	2	208	CLA	C4B-NB	7.90	1.42	1.35
24	B	826	CLA	C4B-NB	7.90	1.42	1.35
24	t	307	CLA	C4B-NB	7.89	1.42	1.35
24	B	836	CLA	C4B-NB	7.88	1.42	1.35
24	A	833	CLA	C4B-NB	7.86	1.42	1.35
24	B	831	CLA	C4B-NB	7.85	1.42	1.35
24	8	204	CLA	C4B-NB	7.85	1.42	1.35
24	3	304	CLA	C4B-NB	7.85	1.42	1.35
24	9	308	CLA	C4B-NB	7.84	1.42	1.35
24	7	608	CLA	C4B-NB	7.84	1.42	1.35
24	2	201	CLA	C4B-NB	7.83	1.42	1.35
24	t	302	CLA	C4B-NB	7.83	1.42	1.35
24	2	202	CLA	C4B-NB	7.82	1.42	1.35
24	k	307	CLA	C4B-NB	7.82	1.42	1.35
24	5	606	CLA	C4B-NB	7.82	1.42	1.35
24	7	611	CLA	C4B-NB	7.82	1.42	1.35
24	A	836	CLA	C4B-NB	7.82	1.42	1.35
24	t	309	CLA	C4B-NB	7.82	1.42	1.35
24	1	301	CLA	C4B-NB	7.82	1.42	1.35
24	4	610	CLA	C4B-NB	7.81	1.42	1.35
24	8	201	CLA	C4B-NB	7.81	1.42	1.35
24	c	605	CLA	C4B-NB	7.81	1.42	1.35
24	k	302	CLA	C4B-NB	7.81	1.42	1.35
24	7	609	CLA	C4B-NB	7.80	1.42	1.35
24	B	834	CLA	C4B-NB	7.80	1.42	1.35
24	A	834	CLA	C4B-NB	7.80	1.42	1.35
24	A	838	CLA	C4B-NB	7.79	1.42	1.35
24	B	819	CLA	C4B-NB	7.79	1.42	1.35
24	B	818	CLA	C4B-NB	7.79	1.42	1.35
24	B	830	CLA	C4B-NB	7.79	1.42	1.35
24	h	608	CLA	C4B-NB	7.78	1.42	1.35
24	8	209	CLA	C4B-NB	7.78	1.42	1.35
24	4	601	CLA	C4B-NB	7.78	1.42	1.35
24	6	607	CLA	C4B-NB	7.77	1.42	1.35
24	c	604	CLA	C4B-NB	7.77	1.42	1.35
24	F	201	CLA	C4B-NB	7.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	601	CLA	C4B-NB	7.76	1.42	1.35
24	h	601	CLA	C4B-NB	7.76	1.42	1.35
24	B	811	CLA	C4B-NB	7.76	1.42	1.35
24	2	209	CLA	C4B-NB	7.75	1.42	1.35
24	h	605	CLA	C4B-NB	7.75	1.42	1.35
24	5	603	CLA	C4B-NB	7.75	1.42	1.35
24	6	604	CLA	C4B-NB	7.74	1.42	1.35
24	9	306	CLA	C4B-NB	7.74	1.42	1.35
24	h	609	CLA	C4B-NB	7.74	1.42	1.35
24	A	808	CLA	C4B-NB	7.74	1.42	1.35
24	A	847	CLA	C4B-NB	7.74	1.42	1.35
24	A	837	CLA	C4B-NB	7.74	1.42	1.35
24	1	309	CLA	C4B-NB	7.73	1.42	1.35
24	B	817	CLA	C4B-NB	7.73	1.42	1.35
24	6	605	CLA	C4B-NB	7.72	1.42	1.35
24	A	815	CLA	C4B-NB	7.72	1.42	1.35
24	1	317	CLA	C4B-NB	7.71	1.42	1.35
24	c	606	CLA	C4B-NB	7.71	1.42	1.35
24	t	301	CLA	C4B-NB	7.70	1.42	1.35
24	6	612	CLA	C4B-NB	7.70	1.42	1.35
24	5	604	CLA	C4B-NB	7.70	1.42	1.35
24	8	202	CLA	C4B-NB	7.70	1.42	1.35
24	6	602	CLA	C4B-NB	7.70	1.42	1.35
24	B	808	CLA	C4B-NB	7.69	1.42	1.35
24	c	609	CLA	C4B-NB	7.69	1.42	1.35
24	k	309	CLA	C4B-NB	7.69	1.42	1.35
24	A	814	CLA	C4B-NB	7.68	1.42	1.35
24	7	607	CLA	C4B-NB	7.68	1.42	1.35
24	5	601	CLA	C4B-NB	7.68	1.42	1.35
24	A	810	CLA	C4B-NB	7.68	1.42	1.35
24	R	103	CLA	C4B-NB	7.68	1.42	1.35
24	A	829	CLA	C4B-NB	7.67	1.42	1.35
24	c	608	CLA	C4B-NB	7.67	1.42	1.35
24	B	813	CLA	C4B-NB	7.67	1.42	1.35
24	A	818	CLA	C4B-NB	7.67	1.42	1.35
24	9	301	CLA	C4B-NB	7.66	1.42	1.35
24	4	611	CLA	C4B-NB	7.66	1.42	1.35
24	A	811	CLA	C4B-NB	7.66	1.42	1.35
24	3	307	CLA	C4B-NB	7.66	1.42	1.35
24	h	607	CLA	C4B-NB	7.66	1.42	1.35
24	B	827	CLA	C4B-NB	7.66	1.42	1.35
24	2	206	CLA	C4B-NB	7.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	204	CLA	C4B-NB	7.66	1.42	1.35
24	J	103	CLA	C4B-NB	7.66	1.42	1.35
24	t	304	CLA	C4B-NB	7.65	1.42	1.35
24	A	822	CLA	C4B-NB	7.65	1.42	1.35
24	6	608	CLA	C4B-NB	7.65	1.42	1.35
24	t	305	CLA	C4B-NB	7.65	1.42	1.35
24	5	605	CLA	C4B-NB	7.64	1.42	1.35
24	4	607	CLA	C4B-NB	7.64	1.42	1.35
24	t	310	CLA	C4B-NB	7.63	1.42	1.35
24	7	603	CLA	C4B-NB	7.63	1.42	1.35
24	B	847	CLA	C4B-NB	7.63	1.42	1.35
24	A	804	CLA	C4B-NB	7.63	1.42	1.35
24	t	306	CLA	C4B-NB	7.62	1.42	1.35
24	4	606	CLA	C4B-NB	7.61	1.42	1.35
24	9	310	CLA	C4B-NB	7.61	1.42	1.35
24	3	309	CLA	C4B-NB	7.61	1.42	1.35
24	8	203	CLA	C4B-NB	7.61	1.42	1.35
24	A	820	CLA	C4B-NB	7.61	1.42	1.35
24	B	832	CLA	C4B-NB	7.61	1.42	1.35
24	A	830	CLA	C4B-NB	7.60	1.42	1.35
24	k	311	CLA	C4B-NB	7.60	1.42	1.35
24	9	303	CLA	C4B-NB	7.60	1.42	1.35
24	A	856	CLA	C4B-NB	7.60	1.42	1.35
24	c	611	CLA	C4B-NB	7.59	1.42	1.35
24	1	306	CLA	C4B-NB	7.59	1.42	1.35
24	B	846	CLA	C4B-NB	7.59	1.42	1.35
24	4	603	CLA	C4B-NB	7.59	1.42	1.35
24	3	301	CLA	C4B-NB	7.59	1.42	1.35
24	F	203	CLA	C4B-NB	7.59	1.42	1.35
24	6	606	CLA	C4B-NB	7.58	1.42	1.35
24	A	805	CLA	C4B-NB	7.58	1.42	1.35
24	B	835	CLA	C4B-NB	7.58	1.42	1.35
24	2	205	CLA	C4B-NB	7.57	1.42	1.35
24	k	305	CLA	C4B-NB	7.57	1.42	1.35
24	B	814	CLA	C4B-NB	7.57	1.42	1.35
24	6	603	CLA	C4B-NB	7.57	1.42	1.35
24	A	821	CLA	C4B-NB	7.56	1.42	1.35
24	h	603	CLA	C4B-NB	7.56	1.42	1.35
24	A	801	CLA	C4B-NB	7.55	1.41	1.35
24	8	205	CLA	C4B-NB	7.55	1.41	1.35
24	B	816	CLA	C4B-NB	7.55	1.41	1.35
24	h	604	CLA	C4B-NB	7.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	819	CLA	C4B-NB	7.54	1.41	1.35
24	t	303	CLA	C4B-NB	7.54	1.41	1.35
24	3	303	CLA	C4B-NB	7.54	1.41	1.35
24	6	611	CLA	C4B-NB	7.54	1.41	1.35
24	2	203	CLA	C4B-NB	7.54	1.41	1.35
24	A	816	CLA	C4B-NB	7.54	1.41	1.35
24	3	306	CLA	C4B-NB	7.53	1.41	1.35
24	7	610	CLA	C4B-NB	7.53	1.41	1.35
24	B	822	CLA	C4B-NB	7.52	1.41	1.35
24	4	612	CLA	C4B-NB	7.52	1.41	1.35
24	8	208	CLA	C4B-NB	7.52	1.41	1.35
24	B	820	CLA	C4B-NB	7.52	1.41	1.35
24	1	303	CLA	C4B-NB	7.52	1.41	1.35
24	B	815	CLA	C4B-NB	7.51	1.41	1.35
24	A	824	CLA	C4B-NB	7.51	1.41	1.35
24	4	608	CLA	C4B-NB	7.50	1.41	1.35
24	9	311	CLA	C4B-NB	7.50	1.41	1.35
24	k	301	CLA	C4B-NB	7.50	1.41	1.35
24	A	809	CLA	C4B-NB	7.50	1.41	1.35
24	A	813	CLA	C4B-NB	7.50	1.41	1.35
24	B	807	CLA	C4B-NB	7.49	1.41	1.35
24	A	853	CLA	C4B-NB	7.49	1.41	1.35
24	h	612	CLA	C4B-NB	7.49	1.41	1.35
24	2	207	CLA	C4B-NB	7.49	1.41	1.35
24	A	803	CLA	C4B-NB	7.49	1.41	1.35
24	A	826	CLA	C4B-NB	7.48	1.41	1.35
24	B	825	CLA	C4B-NB	7.48	1.41	1.35
24	A	835	CLA	C4B-NB	7.47	1.41	1.35
24	4	609	CLA	C4B-NB	7.47	1.41	1.35
24	h	602	CLA	C4B-NB	7.47	1.41	1.35
24	1	304	CLA	C4B-NB	7.47	1.41	1.35
24	7	606	CLA	C4B-NB	7.47	1.41	1.35
24	B	809	CLA	C4B-NB	7.46	1.41	1.35
24	A	823	CLA	C4B-NB	7.46	1.41	1.35
24	B	806	CLA	C4B-NB	7.46	1.41	1.35
24	B	848	CLA	C4B-NB	7.45	1.41	1.35
24	A	828	CLA	C4B-NB	7.44	1.41	1.35
24	k	306	CLA	C4B-NB	7.43	1.41	1.35
24	A	832	CLA	C4B-NB	7.43	1.41	1.35
24	A	827	CLA	C4B-NB	7.42	1.41	1.35
24	4	605	CLA	C4B-NB	7.42	1.41	1.35
24	7	604	CLA	C4B-NB	7.41	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	805	CLA	C4B-NB	7.40	1.41	1.35
24	6	609	CLA	C4B-NB	7.40	1.41	1.35
24	k	303	CLA	C4B-NB	7.39	1.41	1.35
24	A	812	CLA	C4B-NB	7.39	1.41	1.35
24	h	611	CLA	C4B-NB	7.39	1.41	1.35
24	1	305	CLA	C4B-NB	7.39	1.41	1.35
24	A	840	CLA	C4B-NB	7.39	1.41	1.35
24	9	304	CLA	C4B-NB	7.38	1.41	1.35
24	B	802	CLA	C4B-NB	7.38	1.41	1.35
24	3	302	CLA	C4B-NB	7.38	1.41	1.35
24	9	305	CLA	C4B-NB	7.38	1.41	1.35
24	c	602	CLA	C4B-NB	7.37	1.41	1.35
24	A	807	CLA	C4B-NB	7.37	1.41	1.35
24	A	831	CLA	C4B-NB	7.37	1.41	1.35
24	B	801	CLA	C4B-NB	7.36	1.41	1.35
24	7	612	CLA	C4B-NB	7.36	1.41	1.35
24	7	602	CLA	C4B-NB	7.35	1.41	1.35
24	B	823	CLA	C4B-NB	7.35	1.41	1.35
24	A	825	CLA	C4B-NB	7.34	1.41	1.35
24	3	308	CLA	C4B-NB	7.33	1.41	1.35
24	B	812	CLA	C4B-NB	7.33	1.41	1.35
24	4	602	CLA	C4B-NB	7.33	1.41	1.35
24	2	204	CLA	C4B-NB	7.32	1.41	1.35
24	B	837	CLA	C4B-NB	7.32	1.41	1.35
24	B	838	CLA	C4B-NB	7.30	1.41	1.35
24	L	205	CLA	C4B-NB	7.30	1.41	1.35
24	9	302	CLA	C4B-NB	7.30	1.41	1.35
24	h	606	CLA	C4B-NB	7.30	1.41	1.35
24	B	833	CLA	C4B-NB	7.29	1.41	1.35
24	c	603	CLA	C4B-NB	7.29	1.41	1.35
24	9	307	CLA	C4B-NB	7.29	1.41	1.35
24	B	821	CLA	C4B-NB	7.28	1.41	1.35
24	9	309	CLA	C4B-NB	7.25	1.41	1.35
24	L	203	CLA	C4B-NB	7.23	1.41	1.35
24	A	817	CLA	C4B-NB	7.22	1.41	1.35
24	R	104	CLA	C4B-NB	7.21	1.41	1.35
24	A	802	CLA	C4B-NB	7.20	1.41	1.35
24	A	857	CLA	C4B-NB	7.17	1.41	1.35
24	B	829	CLA	C4B-NB	7.17	1.41	1.35
24	A	860	CLA	C4B-NB	7.16	1.41	1.35
24	B	810	CLA	C4B-NB	7.14	1.41	1.35
24	1	302	CLA	C4B-NB	7.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	804	CLA	C4B-NB	7.02	1.41	1.35
24	c	607	CLA	C4B-NB	6.93	1.41	1.35
24	B	803	CLA	C4B-NB	6.59	1.41	1.35
26	7	618	DD6	C10-C11	4.87	1.42	1.35
26	7	618	DD6	C5-C6	4.86	1.42	1.35
28	A	842	LHG	O7-C7	4.82	1.47	1.34
26	7	618	DD6	C2-C1	4.75	1.42	1.35
26	9	314	DD6	C2-C1	4.65	1.41	1.35
26	8	210	DD6	C2-C1	4.57	1.41	1.35
26	8	210	DD6	C10-C11	4.56	1.41	1.35
26	7	616	DD6	C2-C1	4.55	1.41	1.35
26	9	314	DD6	C10-C11	4.49	1.41	1.35
26	7	616	DD6	C5-C6	4.43	1.41	1.35
26	8	210	DD6	C5-C6	4.43	1.41	1.35
26	6	614	DD6	C5-C6	4.42	1.41	1.35
29	7	614	A1L1G	C42-C44	4.41	1.41	1.35
29	9	312	A1L1G	C42-C44	4.40	1.41	1.35
28	8	213	LHG	O8-C23	4.38	1.46	1.33
24	A	801	CLA	C1D-ND	4.31	1.43	1.37
26	9	314	DD6	C5-C6	4.31	1.41	1.35
28	L	201	LHG	O8-C23	4.30	1.45	1.33
26	6	614	DD6	C10-C11	4.28	1.41	1.35
28	A	849	LHG	O8-C23	4.28	1.45	1.33
26	1	311	DD6	C10-C11	4.26	1.41	1.35
26	6	614	DD6	C2-C1	4.26	1.41	1.35
28	4	619	LHG	O7-C7	4.26	1.46	1.34
26	1	311	DD6	C2-C1	4.26	1.41	1.35
26	7	616	DD6	C10-C11	4.25	1.41	1.35
28	B	845	LHG	O7-C7	4.25	1.46	1.34
24	B	804	CLA	C1D-ND	4.24	1.43	1.37
30	A	855	LMG	O7-C10	4.23	1.46	1.34
28	3	315	LHG	O8-C23	4.23	1.45	1.33
28	A	852	LHG	O8-C23	4.23	1.45	1.33
29	2	213	A1L1G	C42-C44	4.22	1.41	1.35
26	t	311	DD6	C2-C1	4.20	1.41	1.35
24	2	208	CLA	C1D-ND	4.20	1.42	1.37
24	c	610	CLA	C1D-ND	4.20	1.42	1.37
30	t	314	LMG	O8-C28	4.19	1.45	1.33
28	2	215	LHG	O8-C23	4.19	1.45	1.33
26	1	311	DD6	C5-C6	4.19	1.41	1.35
29	k	312	A1L1G	C42-C44	4.19	1.41	1.35
26	9	315	DD6	C2-C1	4.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	103	LHG	O8-C23	4.18	1.45	1.33
29	3	310	A1L1G	C42-C44	4.18	1.41	1.35
28	B	844	LHG	O8-C23	4.18	1.45	1.33
26	t	311	DD6	C10-C11	4.17	1.41	1.35
26	1	312	DD6	C2-C1	4.17	1.41	1.35
28	A	852	LHG	O7-C7	4.17	1.46	1.34
28	J	105	LHG	O8-C23	4.16	1.45	1.33
28	A	849	LHG	O7-C7	4.16	1.46	1.34
26	h	616	DD6	C5-C6	4.16	1.41	1.35
28	4	619	LHG	O8-C23	4.16	1.45	1.33
30	A	855	LMG	O8-C28	4.15	1.45	1.33
28	L	201	LHG	O7-C7	4.15	1.46	1.34
26	9	313	DD6	C5-C6	4.15	1.41	1.35
24	8	207	CLA	C1D-ND	4.14	1.42	1.37
26	3	313	DD6	C2-C1	4.13	1.41	1.35
28	A	841	LHG	O8-C23	4.13	1.45	1.33
26	h	616	DD6	C10-C11	4.13	1.41	1.35
26	1	312	DD6	C5-C6	4.13	1.41	1.35
26	9	315	DD6	C10-C11	4.12	1.41	1.35
24	7	612	CLA	C1D-ND	4.12	1.42	1.37
28	1	318	LHG	O8-C23	4.12	1.45	1.33
24	k	308	CLA	C1D-ND	4.10	1.42	1.37
26	h	614	DD6	C10-C11	4.10	1.41	1.35
26	9	315	DD6	C5-C6	4.10	1.41	1.35
24	4	609	CLA	C1D-ND	4.10	1.42	1.37
30	2	214	LMG	O8-C28	4.09	1.45	1.33
26	4	615	DD6	C10-C11	4.08	1.41	1.35
24	B	816	CLA	C1D-ND	4.08	1.42	1.37
24	c	609	CLA	C1D-ND	4.08	1.42	1.37
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	A	842	LHG	O8-C23	4.07	1.45	1.33
28	B	845	LHG	O8-C23	4.07	1.45	1.33
26	6	616	DD6	C10-C11	4.06	1.41	1.35
24	k	305	CLA	C1D-ND	4.05	1.42	1.37
24	7	608	CLA	C1D-ND	4.04	1.42	1.37
28	J	105	LHG	O7-C7	4.04	1.45	1.34
24	7	601	CLA	C1D-ND	4.03	1.42	1.37
26	1	312	DD6	C10-C11	4.03	1.41	1.35
28	2	215	LHG	O7-C7	4.03	1.45	1.34
26	t	311	DD6	C5-C6	4.03	1.41	1.35
26	9	313	DD6	C2-C1	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	103	LHG	O7-C7	4.02	1.45	1.34
24	1	308	CLA	C1D-ND	4.01	1.42	1.37
24	7	611	CLA	C1D-ND	4.01	1.42	1.37
26	9	313	DD6	C10-C11	4.01	1.41	1.35
24	t	309	CLA	C1D-ND	4.01	1.42	1.37
28	8	213	LHG	O7-C7	4.01	1.45	1.34
26	2	212	DD6	C2-C1	4.00	1.41	1.35
24	2	207	CLA	C1D-ND	4.00	1.42	1.37
24	8	202	CLA	C1D-ND	4.00	1.42	1.37
26	R	105	DD6	C2-C1	4.00	1.41	1.35
26	4	615	DD6	C5-C6	3.99	1.41	1.35
24	h	604	CLA	C1D-ND	3.99	1.42	1.37
24	6	603	CLA	C1D-ND	3.99	1.42	1.37
24	9	309	CLA	C1D-ND	3.99	1.42	1.37
26	6	617	DD6	C5-C6	3.98	1.41	1.35
30	t	314	LMG	O7-C10	3.98	1.45	1.34
24	1	307	CLA	C1D-ND	3.98	1.42	1.37
26	6	617	DD6	C2-C1	3.98	1.41	1.35
24	8	203	CLA	C1D-ND	3.98	1.42	1.37
26	h	616	DD6	C2-C1	3.98	1.41	1.35
24	t	310	CLA	C1D-ND	3.96	1.42	1.37
24	7	605	CLA	C1D-ND	3.96	1.42	1.37
24	5	606	CLA	C1D-ND	3.96	1.42	1.37
26	4	615	DD6	C2-C1	3.95	1.41	1.35
24	t	308	CLA	C1D-ND	3.95	1.42	1.37
24	5	601	CLA	C1D-ND	3.95	1.42	1.37
24	k	311	CLA	C1D-ND	3.95	1.42	1.37
24	h	610	CLA	C1D-ND	3.95	1.42	1.37
29	9	312	A1L1G	C38-C39	3.95	1.41	1.35
24	8	201	CLA	C1D-ND	3.94	1.42	1.37
26	R	105	DD6	C5-C6	3.94	1.41	1.35
24	2	202	CLA	C1D-ND	3.94	1.42	1.37
24	t	301	CLA	C1D-ND	3.94	1.42	1.37
26	h	614	DD6	C5-C6	3.94	1.41	1.35
24	2	209	CLA	C1D-ND	3.93	1.42	1.37
26	3	311	DD6	C2-C1	3.93	1.41	1.35
24	6	601	CLA	C1D-ND	3.93	1.42	1.37
24	h	609	CLA	C1D-ND	3.93	1.42	1.37
26	4	614	DD6	C10-C11	3.93	1.41	1.35
26	k	315	DD6	C2-C1	3.93	1.41	1.35
30	2	214	LMG	O7-C10	3.93	1.45	1.34
24	3	307	CLA	C1D-ND	3.92	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	605	CLA	C1D-ND	3.92	1.42	1.37
26	3	313	DD6	C10-C11	3.92	1.41	1.35
24	6	610	CLA	C1D-ND	3.92	1.42	1.37
28	3	315	LHG	O7-C7	3.92	1.45	1.34
24	A	814	CLA	C1D-ND	3.92	1.42	1.37
26	2	210	DD6	C2-C1	3.92	1.41	1.35
24	F	203	CLA	C1D-ND	3.92	1.42	1.37
24	1	309	CLA	C1D-ND	3.92	1.42	1.37
26	8	212	DD6	C2-C1	3.91	1.41	1.35
24	A	829	CLA	C1D-ND	3.91	1.42	1.37
24	h	602	CLA	C1D-ND	3.91	1.42	1.37
24	c	604	CLA	C1D-ND	3.91	1.42	1.37
26	3	313	DD6	C5-C6	3.91	1.41	1.35
26	6	613	DD6	C2-C1	3.91	1.41	1.35
24	5	607	CLA	C1D-ND	3.91	1.42	1.37
24	k	301	CLA	C1D-ND	3.91	1.42	1.37
24	A	832	CLA	C1D-ND	3.90	1.42	1.37
24	c	605	CLA	C1D-ND	3.90	1.42	1.37
26	5	608	DD6	C5-C6	3.90	1.41	1.35
24	A	806	CLA	C1D-ND	3.90	1.42	1.37
24	8	204	CLA	C1D-ND	3.90	1.42	1.37
29	7	614	A1L1G	C38-C39	3.90	1.41	1.35
24	B	831	CLA	C1D-ND	3.90	1.42	1.37
24	2	206	CLA	C1D-ND	3.89	1.42	1.37
24	7	607	CLA	C1D-ND	3.89	1.42	1.37
24	A	856	CLA	C1D-ND	3.89	1.42	1.37
24	7	609	CLA	C1D-ND	3.89	1.42	1.37
24	A	805	CLA	C1D-ND	3.88	1.42	1.37
24	t	302	CLA	C1D-ND	3.88	1.42	1.37
26	2	212	DD6	C10-C11	3.88	1.40	1.35
24	k	310	CLA	C1D-ND	3.88	1.42	1.37
24	9	301	CLA	C1D-ND	3.88	1.42	1.37
24	A	812	CLA	C1D-ND	3.88	1.42	1.37
26	8	211	DD6	C2-C1	3.88	1.40	1.35
24	5	604	CLA	C1D-ND	3.87	1.42	1.37
24	c	611	CLA	C1D-ND	3.87	1.42	1.37
29	7	614	A1L1G	C35-C34	3.87	1.40	1.35
24	4	610	CLA	C1D-ND	3.87	1.42	1.37
24	7	603	CLA	C1D-ND	3.87	1.42	1.37
24	2	203	CLA	C1D-ND	3.87	1.42	1.37
26	J	102	DD6	C10-C11	3.87	1.40	1.35
26	h	614	DD6	C2-C1	3.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	612	CLA	C1D-ND	3.87	1.42	1.37
24	B	827	CLA	C1D-ND	3.87	1.42	1.37
24	h	601	CLA	C1D-ND	3.86	1.42	1.37
24	h	603	CLA	C1D-ND	3.86	1.42	1.37
24	c	606	CLA	C1D-ND	3.86	1.42	1.37
26	4	614	DD6	C5-C6	3.86	1.40	1.35
24	h	605	CLA	C1D-ND	3.86	1.42	1.37
24	A	816	CLA	C1D-ND	3.86	1.42	1.37
26	1	313	DD6	C5-C6	3.86	1.40	1.35
26	J	102	DD6	C5-C6	3.86	1.40	1.35
24	B	806	CLA	C1D-ND	3.86	1.42	1.37
24	B	815	CLA	C1D-ND	3.86	1.42	1.37
26	6	617	DD6	C10-C11	3.86	1.40	1.35
29	9	312	A1L1G	C35-C34	3.86	1.40	1.35
24	4	611	CLA	C1D-ND	3.86	1.42	1.37
24	2	204	CLA	C1D-ND	3.86	1.42	1.37
24	A	837	CLA	C1D-ND	3.86	1.42	1.37
24	3	309	CLA	C1D-ND	3.85	1.42	1.37
26	2	212	DD6	C5-C6	3.85	1.40	1.35
24	A	834	CLA	C1D-ND	3.85	1.42	1.37
24	A	824	CLA	C1D-ND	3.85	1.42	1.37
24	B	819	CLA	C1D-ND	3.85	1.42	1.37
26	c	614	DD6	C10-C11	3.85	1.40	1.35
24	A	819	CLA	C1D-ND	3.85	1.42	1.37
24	1	303	CLA	C1D-ND	3.85	1.42	1.37
24	A	823	CLA	C1D-ND	3.84	1.42	1.37
24	h	611	CLA	C1D-ND	3.84	1.42	1.37
24	B	833	CLA	C1D-ND	3.84	1.42	1.37
26	4	617	DD6	C5-C6	3.84	1.40	1.35
24	B	847	CLA	C1D-ND	3.84	1.42	1.37
24	6	609	CLA	C1D-ND	3.84	1.42	1.37
24	9	310	CLA	C1D-ND	3.84	1.42	1.37
24	A	815	CLA	C1D-ND	3.84	1.42	1.37
24	A	818	CLA	C1D-ND	3.83	1.42	1.37
24	A	833	CLA	C1D-ND	3.83	1.42	1.37
24	B	807	CLA	C1D-ND	3.83	1.42	1.37
26	8	212	DD6	C5-C6	3.83	1.40	1.35
24	3	301	CLA	C1D-ND	3.83	1.42	1.37
24	t	304	CLA	C1D-ND	3.83	1.42	1.37
26	h	615	DD6	C2-C1	3.82	1.40	1.35
24	B	834	CLA	C1D-ND	3.82	1.42	1.37
24	3	302	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	616	DD6	C2-C1	3.82	1.40	1.35
26	8	211	DD6	C10-C11	3.82	1.40	1.35
24	7	610	CLA	C1D-ND	3.82	1.42	1.37
24	1	317	CLA	C1D-ND	3.82	1.42	1.37
24	6	612	CLA	C1D-ND	3.82	1.42	1.37
24	A	822	CLA	C1D-ND	3.82	1.42	1.37
24	B	813	CLA	C1D-ND	3.82	1.42	1.37
24	k	309	CLA	C1D-ND	3.82	1.42	1.37
24	4	613	CLA	C1D-ND	3.81	1.42	1.37
24	A	807	CLA	C1D-ND	3.81	1.42	1.37
29	2	213	A1L1G	C38-C39	3.81	1.40	1.35
24	4	612	CLA	C1D-ND	3.81	1.42	1.37
24	3	303	CLA	C1D-ND	3.80	1.42	1.37
24	A	810	CLA	C1D-ND	3.80	1.42	1.37
26	4	614	DD6	C2-C1	3.80	1.40	1.35
24	A	840	CLA	C1D-ND	3.80	1.42	1.37
24	B	837	CLA	C1D-ND	3.80	1.42	1.37
24	B	826	CLA	C1D-ND	3.80	1.42	1.37
26	1	313	DD6	C2-C1	3.80	1.40	1.35
26	4	616	DD6	C5-C6	3.80	1.40	1.35
24	6	604	CLA	C1D-ND	3.79	1.42	1.37
24	B	822	CLA	C1D-ND	3.79	1.42	1.37
24	t	306	CLA	C1D-ND	3.79	1.42	1.37
24	6	607	CLA	C1D-ND	3.79	1.42	1.37
24	k	304	CLA	C1D-ND	3.79	1.42	1.37
24	B	820	CLA	C1D-ND	3.79	1.42	1.37
26	1	313	DD6	C10-C11	3.79	1.40	1.35
26	6	613	DD6	C5-C6	3.79	1.40	1.35
24	J	103	CLA	C1D-ND	3.79	1.42	1.37
24	F	202	CLA	C1D-ND	3.78	1.42	1.37
24	t	307	CLA	C1D-ND	3.78	1.42	1.37
24	A	803	CLA	C1D-ND	3.78	1.42	1.37
24	A	817	CLA	C1D-ND	3.78	1.42	1.37
24	4	602	CLA	C1D-ND	3.78	1.42	1.37
24	5	603	CLA	C1D-ND	3.78	1.42	1.37
24	A	828	CLA	C1D-ND	3.78	1.42	1.37
26	3	311	DD6	C5-C6	3.78	1.40	1.35
24	A	808	CLA	C1D-ND	3.78	1.42	1.37
24	B	808	CLA	C1D-ND	3.77	1.42	1.37
24	A	827	CLA	C1D-ND	3.77	1.42	1.37
24	7	606	CLA	C1D-ND	3.77	1.42	1.37
24	A	835	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	836	CLA	C1D-ND	3.77	1.42	1.37
24	B	805	CLA	C1D-ND	3.77	1.42	1.37
24	B	817	CLA	C1D-ND	3.77	1.42	1.37
26	J	102	DD6	C2-C1	3.77	1.40	1.35
26	h	613	DD6	C2-C1	3.77	1.40	1.35
24	1	306	CLA	C1D-ND	3.77	1.42	1.37
24	8	209	CLA	C1D-ND	3.77	1.42	1.37
24	B	812	CLA	C1D-ND	3.77	1.42	1.37
24	A	820	CLA	C1D-ND	3.77	1.42	1.37
24	B	824	CLA	C1D-ND	3.77	1.42	1.37
26	k	314	DD6	C10-C11	3.77	1.40	1.35
24	5	605	CLA	C1D-ND	3.76	1.42	1.37
26	h	613	DD6	C10-C11	3.76	1.40	1.35
24	A	831	CLA	C1D-ND	3.76	1.42	1.37
24	B	801	CLA	C1D-ND	3.76	1.42	1.37
24	A	809	CLA	C1D-ND	3.76	1.42	1.37
26	3	311	DD6	C10-C11	3.76	1.40	1.35
24	A	826	CLA	C1D-ND	3.76	1.42	1.37
24	4	603	CLA	C1D-ND	3.76	1.42	1.37
24	t	303	CLA	C1D-ND	3.76	1.42	1.37
24	4	605	CLA	C1D-ND	3.75	1.42	1.37
24	A	811	CLA	C1D-ND	3.75	1.42	1.37
28	1	318	LHG	O7-C7	3.75	1.44	1.34
24	h	607	CLA	C1D-ND	3.75	1.42	1.37
24	8	205	CLA	C1D-ND	3.75	1.42	1.37
26	c	613	DD6	C2-C1	3.75	1.40	1.35
24	2	205	CLA	C1D-ND	3.75	1.42	1.37
26	3	312	DD6	C2-C1	3.75	1.40	1.35
26	5	608	DD6	C2-C1	3.75	1.40	1.35
24	A	804	CLA	C1D-ND	3.74	1.42	1.37
26	5	608	DD6	C10-C11	3.74	1.40	1.35
24	A	825	CLA	C1D-ND	3.74	1.42	1.37
24	1	301	CLA	C1D-ND	3.73	1.42	1.37
24	B	838	CLA	C1D-ND	3.73	1.42	1.37
24	4	604	CLA	C1D-ND	3.73	1.42	1.37
24	9	302	CLA	C1D-ND	3.73	1.42	1.37
24	k	307	CLA	C1D-ND	3.73	1.42	1.37
26	c	612	DD6	C10-C11	3.72	1.40	1.35
26	6	616	DD6	C2-C1	3.72	1.40	1.35
26	k	313	DD6	C5-C6	3.72	1.40	1.35
24	B	823	CLA	C1D-ND	3.72	1.42	1.37
26	2	210	DD6	C5-C6	3.72	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	k	312	A1L1G	C38-C39	3.72	1.40	1.35
24	c	603	CLA	C1D-ND	3.72	1.42	1.37
24	A	838	CLA	C1D-ND	3.72	1.42	1.37
24	F	201	CLA	C1D-ND	3.71	1.42	1.37
26	5	609	DD6	C5-C6	3.71	1.40	1.35
26	9	317	DD6	C5-C6	3.71	1.40	1.35
26	k	314	DD6	C5-C6	3.71	1.40	1.35
26	7	615	DD6	C5-C6	3.71	1.40	1.35
24	L	203	CLA	C1D-ND	3.71	1.42	1.37
24	5	602	CLA	C1D-ND	3.71	1.42	1.37
24	A	821	CLA	C1D-ND	3.71	1.42	1.37
24	A	847	CLA	C1D-ND	3.71	1.42	1.37
26	h	613	DD6	C5-C6	3.71	1.40	1.35
24	c	608	CLA	C1D-ND	3.71	1.42	1.37
24	6	608	CLA	C1D-ND	3.71	1.42	1.37
24	k	303	CLA	C1D-ND	3.70	1.42	1.37
26	6	616	DD6	C5-C6	3.70	1.40	1.35
24	9	304	CLA	C1D-ND	3.70	1.42	1.37
24	B	830	CLA	C1D-ND	3.70	1.42	1.37
24	B	802	CLA	C1D-ND	3.70	1.42	1.37
24	9	303	CLA	C1D-ND	3.70	1.42	1.37
24	3	306	CLA	C1D-ND	3.70	1.42	1.37
24	k	302	CLA	C1D-ND	3.70	1.42	1.37
29	2	213	A1L1G	C35-C34	3.70	1.40	1.35
26	5	609	DD6	C2-C1	3.69	1.40	1.35
26	c	613	DD6	C5-C6	3.69	1.40	1.35
24	2	201	CLA	C1D-ND	3.69	1.42	1.37
24	6	602	CLA	C1D-ND	3.69	1.42	1.37
24	t	305	CLA	C1D-ND	3.69	1.42	1.37
24	B	809	CLA	C1D-ND	3.69	1.42	1.37
26	4	617	DD6	C10-C11	3.69	1.40	1.35
24	4	607	CLA	C1D-ND	3.69	1.42	1.37
24	B	811	CLA	C1D-ND	3.69	1.42	1.37
24	h	606	CLA	C1D-ND	3.69	1.42	1.37
26	5	609	DD6	C10-C11	3.69	1.40	1.35
26	8	211	DD6	C5-C6	3.69	1.40	1.35
24	8	206	CLA	C1D-ND	3.68	1.42	1.37
24	A	860	CLA	C1D-ND	3.68	1.42	1.37
24	B	832	CLA	C1D-ND	3.68	1.42	1.37
24	B	804	CLA	C4D-ND	-3.68	1.32	1.37
24	9	308	CLA	C1D-ND	3.68	1.42	1.37
26	k	313	DD6	C2-C1	3.68	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	305	CLA	C1D-ND	3.68	1.42	1.37
24	3	304	CLA	C1D-ND	3.67	1.42	1.37
24	c	607	CLA	C1D-ND	3.67	1.42	1.37
26	2	210	DD6	C10-C11	3.67	1.40	1.35
26	k	313	DD6	C10-C11	3.67	1.40	1.35
24	L	205	CLA	C1D-ND	3.67	1.42	1.37
24	6	606	CLA	C1D-ND	3.67	1.42	1.37
24	B	836	CLA	C1D-ND	3.66	1.42	1.37
26	k	314	DD6	C2-C1	3.66	1.40	1.35
24	1	304	CLA	C1D-ND	3.66	1.42	1.37
24	L	204	CLA	C1D-ND	3.66	1.42	1.37
26	c	614	DD6	C2-C1	3.66	1.40	1.35
24	B	846	CLA	C1D-ND	3.65	1.42	1.37
24	8	208	CLA	C1D-ND	3.65	1.42	1.37
24	c	602	CLA	C1D-ND	3.65	1.42	1.37
26	c	613	DD6	C10-C11	3.65	1.40	1.35
24	B	835	CLA	C1D-ND	3.65	1.42	1.37
24	7	602	CLA	C1D-ND	3.65	1.42	1.37
26	h	615	DD6	C5-C6	3.64	1.40	1.35
26	6	613	DD6	C10-C11	3.64	1.40	1.35
24	h	608	CLA	C1D-ND	3.64	1.42	1.37
24	c	601	CLA	C1D-ND	3.64	1.42	1.37
26	h	615	DD6	C10-C11	3.64	1.40	1.35
24	7	602	CLA	C4D-ND	-3.64	1.32	1.37
26	8	212	DD6	C10-C11	3.63	1.40	1.35
26	7	615	DD6	C10-C11	3.63	1.40	1.35
29	k	312	A1L1G	C35-C34	3.63	1.40	1.35
29	3	310	A1L1G	C38-C39	3.63	1.40	1.35
24	4	606	CLA	C1D-ND	3.63	1.42	1.37
24	B	825	CLA	C1D-ND	3.62	1.42	1.37
24	B	821	CLA	C1D-ND	3.61	1.42	1.37
26	7	613	DD6	C10-C11	3.61	1.40	1.35
24	B	818	CLA	C1D-ND	3.61	1.42	1.37
24	B	848	CLA	C1D-ND	3.61	1.42	1.37
26	4	616	DD6	C10-C11	3.60	1.40	1.35
26	c	614	DD6	C5-C6	3.60	1.40	1.35
24	R	103	CLA	C1D-ND	3.60	1.42	1.37
24	B	810	CLA	CAB-C3B	-3.59	1.44	1.51
26	7	615	DD6	C2-C1	3.59	1.40	1.35
24	6	611	CLA	C1D-ND	3.59	1.42	1.37
24	A	813	CLA	C1D-ND	3.59	1.42	1.37
24	1	302	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	612	DD6	C5-C6	3.58	1.40	1.35
26	3	312	DD6	C5-C6	3.58	1.40	1.35
24	A	853	CLA	C1D-ND	3.58	1.42	1.37
26	7	613	DD6	C2-C1	3.58	1.40	1.35
26	7	613	DD6	C5-C6	3.58	1.40	1.35
24	4	601	CLA	C1D-ND	3.57	1.42	1.37
24	B	828	CLA	C1D-ND	3.57	1.42	1.37
24	k	306	CLA	C1D-ND	3.56	1.42	1.37
26	R	105	DD6	C10-C11	3.56	1.40	1.35
24	4	608	CLA	C1D-ND	3.56	1.42	1.37
26	c	612	DD6	C2-C1	3.56	1.40	1.35
24	7	604	CLA	C1D-ND	3.56	1.42	1.37
29	3	310	A1L1G	C35-C34	3.55	1.40	1.35
24	R	104	CLA	C1D-ND	3.55	1.42	1.37
26	4	617	DD6	C2-C1	3.53	1.40	1.35
24	B	814	CLA	C1D-ND	3.50	1.42	1.37
24	3	305	CLA	C1D-ND	3.50	1.42	1.37
24	9	311	CLA	C1D-ND	3.50	1.42	1.37
24	3	308	CLA	C1D-ND	3.50	1.42	1.37
26	9	317	DD6	C2-C1	3.49	1.40	1.35
26	A	848	DD6	C5-C6	3.49	1.40	1.35
24	A	830	CLA	C4D-ND	-3.48	1.32	1.37
26	9	317	DD6	C10-C11	3.48	1.40	1.35
26	3	312	DD6	C10-C11	3.48	1.40	1.35
26	A	848	DD6	C2-C1	3.48	1.40	1.35
26	k	315	DD6	C5-C6	3.47	1.40	1.35
24	A	802	CLA	C4D-ND	-3.47	1.32	1.37
26	6	615	DD6	C5-C6	3.47	1.40	1.35
24	A	857	CLA	C1D-ND	3.47	1.42	1.37
26	6	615	DD6	C10-C11	3.46	1.40	1.35
26	t	313	DD6	C10-C11	3.46	1.40	1.35
26	t	313	DD6	C5-C6	3.45	1.40	1.35
24	9	306	CLA	C1D-ND	3.44	1.42	1.37
26	A	848	DD6	C10-C11	3.44	1.40	1.35
24	B	810	CLA	C1D-ND	3.43	1.42	1.37
24	B	803	CLA	C1D-ND	3.41	1.42	1.37
26	t	313	DD6	C2-C1	3.41	1.40	1.35
24	B	810	CLA	C4D-ND	-3.40	1.33	1.37
24	9	306	CLA	C4D-ND	-3.39	1.33	1.37
24	9	307	CLA	C1D-ND	3.37	1.41	1.37
24	B	829	CLA	C1D-ND	3.35	1.41	1.37
24	A	830	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	803	CLA	C4D-ND	-3.32	1.33	1.37
24	7	612	CLA	C4D-ND	-3.32	1.33	1.37
24	9	307	CLA	C4D-ND	-3.31	1.33	1.37
26	k	315	DD6	C10-C11	3.31	1.40	1.35
24	1	305	CLA	C4D-ND	-3.30	1.33	1.37
26	6	615	DD6	C2-C1	3.30	1.40	1.35
24	7	603	CLA	CHC-C1C	3.27	1.43	1.35
24	B	835	CLA	C4D-ND	-3.24	1.33	1.37
24	B	804	CLA	CHC-C1C	3.24	1.43	1.35
24	B	829	CLA	C4D-ND	-3.24	1.33	1.37
24	L	204	CLA	C4D-ND	-3.24	1.33	1.37
24	L	205	CLA	C4D-ND	-3.23	1.33	1.37
24	B	812	CLA	CHC-C1C	3.23	1.43	1.35
24	7	612	CLA	CHC-C1C	3.22	1.43	1.35
24	3	308	CLA	C4D-ND	-3.22	1.33	1.37
24	5	602	CLA	CHC-C1C	3.22	1.43	1.35
24	B	806	CLA	CHC-C1C	3.20	1.43	1.35
24	6	609	CLA	CHC-C1C	3.19	1.43	1.35
24	t	301	CLA	CHC-C1C	3.18	1.43	1.35
24	c	608	CLA	C4D-ND	-3.18	1.33	1.37
24	6	611	CLA	C4D-ND	-3.18	1.33	1.37
24	4	611	CLA	CHC-C1C	3.18	1.43	1.35
24	k	311	CLA	CHC-C1C	3.18	1.43	1.35
24	h	606	CLA	C4D-ND	-3.17	1.33	1.37
24	c	603	CLA	CHC-C1C	3.17	1.43	1.35
24	B	848	CLA	C4D-ND	-3.17	1.33	1.37
24	7	602	CLA	CHC-C1C	3.16	1.43	1.35
24	A	840	CLA	C4D-ND	-3.16	1.33	1.37
24	k	302	CLA	CHC-C1C	3.16	1.43	1.35
24	7	607	CLA	CHC-C1C	3.16	1.43	1.35
24	A	820	CLA	CHC-C1C	3.16	1.43	1.35
24	9	311	CLA	C4D-ND	-3.15	1.33	1.37
24	B	817	CLA	CHC-C1C	3.15	1.43	1.35
24	3	306	CLA	C4D-ND	-3.15	1.33	1.37
24	9	301	CLA	CHC-C1C	3.15	1.43	1.35
24	B	830	CLA	C4D-ND	-3.15	1.33	1.37
24	B	832	CLA	CHC-C1C	3.14	1.43	1.35
24	t	302	CLA	C4D-ND	-3.14	1.33	1.37
24	B	832	CLA	C4D-ND	-3.14	1.33	1.37
24	A	805	CLA	CHC-C1C	3.14	1.43	1.35
24	t	306	CLA	C4D-ND	-3.13	1.33	1.37
24	R	104	CLA	C4D-ND	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	307	CLA	CHC-C1C	3.13	1.43	1.35
24	c	607	CLA	C4D-ND	-3.13	1.33	1.37
24	B	831	CLA	CHC-C1C	3.13	1.43	1.35
24	A	826	CLA	CHC-C1C	3.13	1.43	1.35
24	c	601	CLA	CHC-C1C	3.13	1.43	1.35
24	4	608	CLA	C4D-ND	-3.13	1.33	1.37
24	B	825	CLA	CHC-C1C	3.13	1.43	1.35
24	5	603	CLA	CHC-C1C	3.12	1.43	1.35
24	h	609	CLA	C4D-ND	-3.12	1.33	1.37
24	1	302	CLA	C4D-ND	-3.12	1.33	1.37
24	B	823	CLA	C4D-ND	-3.12	1.33	1.37
24	A	811	CLA	C4D-ND	-3.12	1.33	1.37
24	8	206	CLA	C4D-ND	-3.12	1.33	1.37
24	B	806	CLA	C4D-ND	-3.11	1.33	1.37
24	A	822	CLA	CHC-C1C	3.11	1.42	1.35
24	6	612	CLA	CHC-C1C	3.11	1.42	1.35
24	B	819	CLA	CHC-C1C	3.11	1.42	1.35
24	5	604	CLA	CHC-C1C	3.11	1.42	1.35
24	A	804	CLA	CHC-C1C	3.11	1.42	1.35
24	9	305	CLA	C4D-ND	-3.11	1.33	1.37
24	c	604	CLA	CHC-C1C	3.11	1.42	1.35
24	c	601	CLA	C4D-ND	-3.10	1.33	1.37
24	h	609	CLA	CHC-C1C	3.10	1.42	1.35
24	A	808	CLA	CHC-C1C	3.10	1.42	1.35
24	k	303	CLA	C4D-ND	-3.10	1.33	1.37
24	B	819	CLA	C4D-ND	-3.10	1.33	1.37
24	A	802	CLA	CHC-C1C	3.10	1.42	1.35
24	B	805	CLA	CHC-C1C	3.10	1.42	1.35
24	A	827	CLA	CHC-C1C	3.10	1.42	1.35
24	L	203	CLA	CHC-C1C	3.10	1.42	1.35
24	B	835	CLA	CHC-C1C	3.10	1.42	1.35
24	t	306	CLA	CHC-C1C	3.10	1.42	1.35
24	h	608	CLA	C4D-ND	-3.10	1.33	1.37
24	1	308	CLA	CHC-C1C	3.10	1.42	1.35
24	2	207	CLA	CHC-C1C	3.10	1.42	1.35
24	4	609	CLA	C4D-ND	-3.10	1.33	1.37
24	A	803	CLA	CHC-C1C	3.10	1.42	1.35
24	B	824	CLA	CHC-C1C	3.10	1.42	1.35
24	A	813	CLA	C4D-ND	-3.10	1.33	1.37
24	1	306	CLA	C4D-ND	-3.09	1.33	1.37
24	4	603	CLA	CHC-C1C	3.09	1.42	1.35
24	B	808	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	815	CLA	CHC-C1C	3.09	1.42	1.35
24	5	607	CLA	C4D-ND	-3.09	1.33	1.37
24	2	209	CLA	CHC-C1C	3.09	1.42	1.35
24	k	310	CLA	CHC-C1C	3.09	1.42	1.35
24	5	604	CLA	C4D-ND	-3.09	1.33	1.37
24	B	836	CLA	CHC-C1C	3.09	1.42	1.35
24	A	834	CLA	CHC-C1C	3.08	1.42	1.35
24	c	602	CLA	C4D-ND	-3.08	1.33	1.37
24	8	209	CLA	C4D-ND	-3.08	1.33	1.37
24	B	838	CLA	CHC-C1C	3.08	1.42	1.35
24	A	822	CLA	C4D-ND	-3.08	1.33	1.37
24	J	103	CLA	C4D-ND	-3.08	1.33	1.37
24	4	610	CLA	C4D-ND	-3.08	1.33	1.37
24	2	202	CLA	C4D-ND	-3.08	1.33	1.37
24	A	860	CLA	C4D-ND	-3.08	1.33	1.37
24	A	821	CLA	CHC-C1C	3.08	1.42	1.35
24	8	208	CLA	C4D-ND	-3.08	1.33	1.37
24	t	305	CLA	CHC-C1C	3.08	1.42	1.35
24	F	202	CLA	CHC-C1C	3.08	1.42	1.35
24	2	203	CLA	C4D-ND	-3.08	1.33	1.37
24	B	848	CLA	CHC-C1C	3.08	1.42	1.35
24	4	604	CLA	CHC-C1C	3.08	1.42	1.35
24	3	304	CLA	C4D-ND	-3.07	1.33	1.37
24	4	606	CLA	CHC-C1C	3.07	1.42	1.35
26	7	618	DD6	C9-C8	3.07	1.42	1.34
24	A	812	CLA	CHC-C1C	3.07	1.42	1.35
24	A	840	CLA	CHC-C1C	3.07	1.42	1.35
24	k	307	CLA	C4D-ND	-3.07	1.33	1.37
24	A	837	CLA	CHC-C1C	3.07	1.42	1.35
24	1	317	CLA	CHC-C1C	3.07	1.42	1.35
24	3	309	CLA	CHC-C1C	3.07	1.42	1.35
24	A	838	CLA	CHC-C1C	3.07	1.42	1.35
24	6	602	CLA	CHC-C1C	3.07	1.42	1.35
24	t	309	CLA	CHC-C1C	3.07	1.42	1.35
24	A	847	CLA	CHC-C1C	3.07	1.42	1.35
24	6	606	CLA	C4D-ND	-3.07	1.33	1.37
24	B	847	CLA	C4D-ND	-3.07	1.33	1.37
24	4	608	CLA	CHC-C1C	3.06	1.42	1.35
24	c	604	CLA	C4D-ND	-3.06	1.33	1.37
24	7	610	CLA	C4D-ND	-3.06	1.33	1.37
24	1	304	CLA	C4D-ND	-3.06	1.33	1.37
24	c	602	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	834	CLA	CHC-C1C	3.06	1.42	1.35
24	h	605	CLA	CHC-C1C	3.06	1.42	1.35
24	A	853	CLA	CHC-C1C	3.06	1.42	1.35
24	A	803	CLA	C4D-ND	-3.06	1.33	1.37
24	B	813	CLA	CHC-C1C	3.06	1.42	1.35
24	h	603	CLA	CHC-C1C	3.06	1.42	1.35
24	B	814	CLA	C4D-ND	-3.06	1.33	1.37
24	B	817	CLA	C4D-ND	-3.06	1.33	1.37
24	A	815	CLA	CHC-C1C	3.06	1.42	1.35
24	B	818	CLA	CHC-C1C	3.06	1.42	1.35
24	7	610	CLA	CHC-C1C	3.06	1.42	1.35
24	A	810	CLA	C4D-ND	-3.06	1.33	1.37
24	t	303	CLA	CHC-C1C	3.06	1.42	1.35
24	2	205	CLA	C4D-ND	-3.06	1.33	1.37
24	4	603	CLA	C4D-ND	-3.06	1.33	1.37
24	B	826	CLA	C4D-ND	-3.05	1.33	1.37
24	A	814	CLA	CHC-C1C	3.05	1.42	1.35
24	A	817	CLA	C4D-ND	-3.05	1.33	1.37
24	A	856	CLA	CHC-C1C	3.05	1.42	1.35
24	k	306	CLA	CHC-C1C	3.05	1.42	1.35
24	6	602	CLA	C4D-ND	-3.05	1.33	1.37
24	B	828	CLA	CHC-C1C	3.05	1.42	1.35
24	2	206	CLA	CHC-C1C	3.05	1.42	1.35
24	9	303	CLA	C4D-ND	-3.05	1.33	1.37
24	B	818	CLA	C4D-ND	-3.05	1.33	1.37
24	t	304	CLA	CHC-C1C	3.05	1.42	1.35
24	B	821	CLA	CHC-C1C	3.05	1.42	1.35
24	3	309	CLA	C4D-ND	-3.05	1.33	1.37
24	B	823	CLA	CHC-C1C	3.05	1.42	1.35
24	A	825	CLA	C4D-ND	-3.05	1.33	1.37
24	6	607	CLA	CHC-C1C	3.05	1.42	1.35
24	k	309	CLA	CHC-C1C	3.05	1.42	1.35
24	B	838	CLA	C4D-ND	-3.05	1.33	1.37
24	c	606	CLA	CHC-C1C	3.05	1.42	1.35
24	A	813	CLA	CHC-C1C	3.05	1.42	1.35
24	7	607	CLA	C4D-ND	-3.05	1.33	1.37
24	A	806	CLA	CHC-C1C	3.05	1.42	1.35
24	A	823	CLA	C4D-ND	-3.05	1.33	1.37
24	9	302	CLA	CHC-C1C	3.05	1.42	1.35
24	3	306	CLA	CHC-C1C	3.05	1.42	1.35
24	F	201	CLA	C4D-ND	-3.05	1.33	1.37
24	5	606	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	304	CLA	CHC-C1C	3.04	1.42	1.35
24	c	605	CLA	CHC-C1C	3.04	1.42	1.35
24	A	824	CLA	CHC-C1C	3.04	1.42	1.35
24	h	604	CLA	CHC-C1C	3.04	1.42	1.35
24	2	209	CLA	C4D-ND	-3.04	1.33	1.37
24	c	606	CLA	C4D-ND	-3.04	1.33	1.37
24	B	829	CLA	CHC-C1C	3.04	1.42	1.35
24	c	608	CLA	CHC-C1C	3.04	1.42	1.35
24	6	605	CLA	CHC-C1C	3.04	1.42	1.35
24	L	204	CLA	CHC-C1C	3.04	1.42	1.35
24	A	821	CLA	C4D-ND	-3.04	1.33	1.37
24	5	605	CLA	CHC-C1C	3.04	1.42	1.35
24	A	817	CLA	CHC-C1C	3.04	1.42	1.35
24	B	811	CLA	CHC-C1C	3.04	1.42	1.35
24	8	207	CLA	CHC-C1C	3.04	1.42	1.35
24	c	611	CLA	CHC-C1C	3.04	1.42	1.35
24	F	201	CLA	CHC-C1C	3.04	1.42	1.35
24	J	103	CLA	CHC-C1C	3.04	1.42	1.35
24	4	610	CLA	CHC-C1C	3.04	1.42	1.35
24	B	836	CLA	C4D-ND	-3.04	1.33	1.37
24	4	607	CLA	CHC-C1C	3.04	1.42	1.35
24	3	302	CLA	CHC-C1C	3.04	1.42	1.35
24	B	827	CLA	CHC-C1C	3.04	1.42	1.35
24	A	836	CLA	C4D-ND	-3.04	1.33	1.37
24	A	818	CLA	CHC-C1C	3.03	1.42	1.35
24	B	847	CLA	CHC-C1C	3.03	1.42	1.35
24	4	604	CLA	C4D-ND	-3.03	1.33	1.37
24	A	815	CLA	C4D-ND	-3.03	1.33	1.37
24	1	301	CLA	CHC-C1C	3.03	1.42	1.35
24	A	809	CLA	CHC-C1C	3.03	1.42	1.35
24	5	603	CLA	C4D-ND	-3.03	1.33	1.37
24	7	608	CLA	CHC-C1C	3.03	1.42	1.35
24	4	611	CLA	C4D-ND	-3.03	1.33	1.37
24	B	815	CLA	C4D-ND	-3.03	1.33	1.37
24	B	846	CLA	C4D-ND	-3.03	1.33	1.37
24	R	103	CLA	C4D-ND	-3.03	1.33	1.37
24	R	103	CLA	CHC-C1C	3.03	1.42	1.35
24	B	813	CLA	C4D-ND	-3.03	1.33	1.37
24	9	311	CLA	CHC-C1C	3.03	1.42	1.35
24	B	826	CLA	CHC-C1C	3.03	1.42	1.35
24	6	604	CLA	CHC-C1C	3.03	1.42	1.35
24	h	607	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	303	CLA	CHC-C1C	3.03	1.42	1.35
24	A	828	CLA	CHC-C1C	3.03	1.42	1.35
24	8	205	CLA	C4D-ND	-3.03	1.33	1.37
24	t	310	CLA	CHC-C1C	3.03	1.42	1.35
24	k	305	CLA	CHC-C1C	3.03	1.42	1.35
24	c	605	CLA	C4D-ND	-3.03	1.33	1.37
24	A	819	CLA	C4D-ND	-3.03	1.33	1.37
24	2	203	CLA	CHC-C1C	3.02	1.42	1.35
24	4	601	CLA	CHC-C1C	3.02	1.42	1.35
24	7	604	CLA	C4D-ND	-3.02	1.33	1.37
24	B	834	CLA	C4D-ND	-3.02	1.33	1.37
24	B	811	CLA	C4D-ND	-3.02	1.33	1.37
24	1	304	CLA	CHC-C1C	3.02	1.42	1.35
24	k	301	CLA	C4D-ND	-3.02	1.33	1.37
24	A	823	CLA	CHC-C1C	3.02	1.42	1.35
24	3	301	CLA	CHC-C1C	3.02	1.42	1.35
24	k	302	CLA	C4D-ND	-3.02	1.33	1.37
24	h	602	CLA	CHC-C1C	3.02	1.42	1.35
24	3	308	CLA	CHC-C1C	3.02	1.42	1.35
24	1	305	CLA	C1D-ND	3.02	1.41	1.37
24	4	602	CLA	CHC-C1C	3.02	1.42	1.35
24	h	601	CLA	C4D-ND	-3.02	1.33	1.37
24	B	820	CLA	CHC-C1C	3.02	1.42	1.35
24	k	309	CLA	C4D-ND	-3.02	1.33	1.37
24	h	608	CLA	CHC-C1C	3.02	1.42	1.35
24	t	307	CLA	C4D-ND	-3.02	1.33	1.37
24	A	820	CLA	C4D-ND	-3.02	1.33	1.37
24	4	607	CLA	C4D-ND	-3.01	1.33	1.37
24	A	833	CLA	CHC-C1C	3.01	1.42	1.35
24	A	812	CLA	C4D-ND	-3.01	1.33	1.37
24	4	606	CLA	C4D-ND	-3.01	1.33	1.37
24	7	606	CLA	C4D-ND	-3.01	1.33	1.37
24	9	309	CLA	C4D-ND	-3.01	1.33	1.37
24	B	812	CLA	C4D-ND	-3.01	1.33	1.37
24	4	602	CLA	C4D-ND	-3.01	1.33	1.37
24	c	611	CLA	C4D-ND	-3.01	1.33	1.37
24	3	303	CLA	C4D-ND	-3.01	1.33	1.37
24	B	820	CLA	C4D-ND	-3.01	1.33	1.37
24	A	831	CLA	C4D-ND	-3.01	1.33	1.37
24	6	603	CLA	CHC-C1C	3.01	1.42	1.35
24	4	605	CLA	C4D-ND	-3.01	1.33	1.37
24	8	201	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	831	CLA	CHC-C1C	3.00	1.42	1.35
24	A	808	CLA	C4D-ND	-3.00	1.33	1.37
24	1	309	CLA	CHC-C1C	3.00	1.42	1.35
24	3	305	CLA	CHC-C1C	3.00	1.42	1.35
24	5	601	CLA	C4D-ND	-3.00	1.33	1.37
24	k	310	CLA	C4D-ND	-3.00	1.33	1.37
24	A	835	CLA	CHC-C1C	3.00	1.42	1.35
24	9	310	CLA	C4D-ND	-3.00	1.33	1.37
24	B	828	CLA	C4D-ND	-3.00	1.33	1.37
24	8	201	CLA	CHC-C1C	3.00	1.42	1.35
24	t	308	CLA	CHC-C1C	3.00	1.42	1.35
24	B	803	CLA	CHC-C1C	3.00	1.42	1.35
24	B	814	CLA	CMB-C2B	-3.00	1.45	1.51
24	h	610	CLA	C4D-ND	-3.00	1.33	1.37
24	A	804	CLA	C4D-ND	-3.00	1.33	1.37
24	A	857	CLA	C4D-ND	-3.00	1.33	1.37
24	1	307	CLA	CHC-C1C	3.00	1.42	1.35
24	8	206	CLA	CHC-C1C	3.00	1.42	1.35
24	4	613	CLA	C4D-ND	-3.00	1.33	1.37
24	F	203	CLA	CHC-C1C	3.00	1.42	1.35
24	5	601	CLA	CHC-C1C	3.00	1.42	1.35
24	2	202	CLA	CHC-C1C	3.00	1.42	1.35
24	t	307	CLA	CHC-C1C	3.00	1.42	1.35
24	A	807	CLA	CHC-C1C	3.00	1.42	1.35
24	h	604	CLA	C4D-ND	-3.00	1.33	1.37
24	c	610	CLA	C4D-ND	-3.00	1.33	1.37
24	B	807	CLA	C4D-ND	-3.00	1.33	1.37
24	B	833	CLA	C4D-ND	-3.00	1.33	1.37
24	7	608	CLA	C4D-ND	-3.00	1.33	1.37
24	3	303	CLA	CHC-C1C	2.99	1.42	1.35
24	A	810	CLA	CHC-C1C	2.99	1.42	1.35
24	h	603	CLA	C4D-ND	-2.99	1.33	1.37
24	h	612	CLA	C4D-ND	-2.99	1.33	1.37
24	A	809	CLA	C4D-ND	-2.99	1.33	1.37
24	8	203	CLA	CHC-C1C	2.99	1.42	1.35
24	A	811	CLA	CHC-C1C	2.99	1.42	1.35
24	B	807	CLA	CHC-C1C	2.99	1.42	1.35
24	6	609	CLA	C4D-ND	-2.99	1.33	1.37
24	t	305	CLA	C4D-ND	-2.99	1.33	1.37
24	h	610	CLA	CHC-C1C	2.99	1.42	1.35
24	4	605	CLA	CHC-C1C	2.99	1.42	1.35
24	6	603	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	834	CLA	C4D-ND	-2.98	1.33	1.37
24	B	833	CLA	CHC-C1C	2.98	1.42	1.35
24	1	307	CLA	C4D-ND	-2.98	1.33	1.37
24	1	317	CLA	C4D-ND	-2.98	1.33	1.37
24	3	301	CLA	C4D-ND	-2.98	1.33	1.37
24	A	838	CLA	C4D-ND	-2.98	1.33	1.37
24	A	816	CLA	CHC-C1C	2.98	1.42	1.35
24	8	203	CLA	C4D-ND	-2.98	1.33	1.37
24	1	303	CLA	CHC-C1C	2.98	1.42	1.35
24	8	209	CLA	CHC-C1C	2.98	1.42	1.35
24	A	853	CLA	C4D-ND	-2.98	1.33	1.37
24	7	604	CLA	CHC-C1C	2.98	1.42	1.35
24	B	837	CLA	CHC-C1C	2.98	1.42	1.35
24	3	307	CLA	C4D-ND	-2.97	1.33	1.37
24	B	822	CLA	CHC-C1C	2.97	1.42	1.35
24	4	609	CLA	CHC-C1C	2.97	1.42	1.35
24	9	308	CLA	C4D-ND	-2.97	1.33	1.37
24	7	606	CLA	CHC-C1C	2.97	1.42	1.35
24	6	601	CLA	C4D-ND	-2.97	1.33	1.37
24	A	847	CLA	C4D-ND	-2.97	1.33	1.37
24	3	304	CLA	CHC-C1C	2.97	1.42	1.35
24	3	305	CLA	C4D-ND	-2.97	1.33	1.37
24	4	613	CLA	CHC-C1C	2.97	1.42	1.35
24	t	302	CLA	CHC-C1C	2.97	1.42	1.35
24	k	306	CLA	C4D-ND	-2.97	1.33	1.37
24	A	832	CLA	CHC-C1C	2.96	1.42	1.35
24	8	202	CLA	CHC-C1C	2.96	1.42	1.35
24	B	821	CLA	C4D-ND	-2.96	1.33	1.37
24	6	610	CLA	CHC-C1C	2.96	1.42	1.35
24	8	205	CLA	CHC-C1C	2.96	1.42	1.35
24	A	807	CLA	C4D-ND	-2.96	1.33	1.37
24	B	825	CLA	C4D-ND	-2.96	1.33	1.37
24	6	601	CLA	CHC-C1C	2.96	1.42	1.35
24	9	302	CLA	C4D-ND	-2.96	1.33	1.37
24	6	607	CLA	C4D-ND	-2.96	1.33	1.37
24	4	612	CLA	C4D-ND	-2.96	1.33	1.37
24	h	606	CLA	CHC-C1C	2.96	1.42	1.35
24	h	612	CLA	CHC-C1C	2.96	1.42	1.35
24	h	605	CLA	C4D-ND	-2.95	1.33	1.37
24	h	607	CLA	C4D-ND	-2.95	1.33	1.37
26	8	210	DD6	C9-C8	2.95	1.42	1.34
24	7	601	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	802	CLA	C4D-ND	-2.95	1.33	1.37
24	2	205	CLA	CHC-C1C	2.95	1.42	1.35
24	c	609	CLA	CHC-C1C	2.95	1.42	1.35
24	B	816	CLA	CHC-C1C	2.95	1.42	1.35
24	7	609	CLA	CHC-C1C	2.95	1.42	1.35
24	4	601	CLA	C4D-ND	-2.95	1.33	1.37
24	6	610	CLA	C4D-ND	-2.95	1.33	1.37
24	A	805	CLA	C4D-ND	-2.95	1.33	1.37
24	6	611	CLA	CHC-C1C	2.95	1.42	1.35
24	B	846	CLA	CHC-C1C	2.95	1.42	1.35
24	7	611	CLA	C4D-ND	-2.95	1.33	1.37
24	A	837	CLA	C4D-ND	-2.95	1.33	1.37
24	B	802	CLA	CHC-C1C	2.95	1.42	1.35
24	7	605	CLA	CHC-C1C	2.95	1.42	1.35
24	A	819	CLA	CHC-C1C	2.94	1.42	1.35
24	B	830	CLA	CHC-C1C	2.94	1.42	1.35
24	7	601	CLA	CHC-C1C	2.94	1.42	1.35
24	B	809	CLA	CHC-C1C	2.94	1.42	1.35
24	6	608	CLA	CHC-C1C	2.94	1.42	1.35
24	A	801	CLA	CHC-C1C	2.94	1.42	1.35
24	3	307	CLA	CHC-C1C	2.94	1.42	1.35
24	B	805	CLA	C4D-ND	-2.94	1.33	1.37
24	F	202	CLA	C4D-ND	-2.94	1.33	1.37
24	2	208	CLA	CHC-C1C	2.94	1.42	1.35
24	k	304	CLA	CHC-C1C	2.94	1.42	1.35
24	1	301	CLA	C4D-ND	-2.94	1.33	1.37
24	6	605	CLA	C4D-ND	-2.94	1.33	1.37
26	7	618	DD6	C25-C24	2.94	1.42	1.34
24	B	808	CLA	C4D-ND	-2.94	1.33	1.37
24	A	828	CLA	C4D-ND	-2.94	1.33	1.37
24	A	833	CLA	C4D-ND	-2.94	1.33	1.37
24	9	309	CLA	CHC-C1C	2.94	1.42	1.35
24	6	604	CLA	C4D-ND	-2.94	1.33	1.37
24	2	206	CLA	C4D-ND	-2.93	1.33	1.37
24	A	825	CLA	CHC-C1C	2.93	1.42	1.35
24	7	603	CLA	C4D-ND	-2.93	1.33	1.37
24	A	806	CLA	C4D-ND	-2.93	1.33	1.37
24	B	801	CLA	CHC-C1C	2.93	1.42	1.35
24	9	301	CLA	C4D-ND	-2.92	1.33	1.37
24	A	836	CLA	CHC-C1C	2.92	1.42	1.35
24	L	205	CLA	CHC-C1C	2.92	1.42	1.35
24	9	307	CLA	CHC-C1C	2.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	860	CLA	CHC-C1C	2.92	1.42	1.35
24	A	818	CLA	C4D-ND	-2.92	1.33	1.37
24	2	207	CLA	C4D-ND	-2.92	1.33	1.37
24	B	814	CLA	CHC-C1C	2.92	1.42	1.35
24	A	829	CLA	CHC-C1C	2.92	1.42	1.35
24	1	306	CLA	CHC-C1C	2.92	1.42	1.35
24	t	303	CLA	C4D-ND	-2.91	1.33	1.37
24	t	308	CLA	C4D-ND	-2.91	1.33	1.37
24	k	308	CLA	CHC-C1C	2.91	1.42	1.35
24	A	835	CLA	C4D-ND	-2.91	1.33	1.37
24	B	809	CLA	C4D-ND	-2.91	1.33	1.37
24	6	606	CLA	CHC-C1C	2.91	1.42	1.35
24	A	832	CLA	C4D-ND	-2.91	1.33	1.37
24	h	601	CLA	CHC-C1C	2.91	1.42	1.35
24	2	204	CLA	C4D-ND	-2.91	1.33	1.37
24	k	301	CLA	CHC-C1C	2.91	1.42	1.35
24	A	827	CLA	C4D-ND	-2.91	1.33	1.37
24	c	603	CLA	C4D-ND	-2.91	1.33	1.37
24	8	204	CLA	CHC-C1C	2.90	1.42	1.35
24	B	837	CLA	C4D-ND	-2.90	1.33	1.37
24	7	611	CLA	CHC-C1C	2.90	1.42	1.35
24	c	610	CLA	CHC-C1C	2.90	1.42	1.35
24	5	605	CLA	C4D-ND	-2.90	1.33	1.37
24	6	608	CLA	C4D-ND	-2.90	1.33	1.37
24	A	856	CLA	C4D-ND	-2.90	1.33	1.37
24	B	827	CLA	C4D-ND	-2.89	1.33	1.37
24	B	810	CLA	CHC-C1C	2.89	1.42	1.35
24	A	826	CLA	C4D-ND	-2.89	1.33	1.37
24	8	207	CLA	C4D-ND	-2.89	1.33	1.37
24	B	831	CLA	C4D-ND	-2.89	1.33	1.37
24	1	303	CLA	C4D-ND	-2.89	1.33	1.37
24	9	305	CLA	CHC-C1C	2.89	1.42	1.35
24	6	612	CLA	C4D-ND	-2.88	1.33	1.37
24	A	814	CLA	C4D-ND	-2.88	1.33	1.37
24	7	609	CLA	C4D-ND	-2.88	1.33	1.37
24	1	308	CLA	C4D-ND	-2.87	1.33	1.37
24	k	308	CLA	C4D-ND	-2.87	1.33	1.37
24	B	801	CLA	C4D-ND	-2.87	1.33	1.37
24	8	208	CLA	CHC-C1C	2.87	1.42	1.35
24	1	309	CLA	C4D-ND	-2.87	1.33	1.37
24	k	311	CLA	C4D-ND	-2.87	1.33	1.37
24	B	824	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	203	CLA	C4D-ND	-2.87	1.33	1.37
24	9	304	CLA	C4D-ND	-2.87	1.33	1.37
24	5	606	CLA	C4D-ND	-2.87	1.33	1.37
24	B	822	CLA	C4D-ND	-2.87	1.33	1.37
24	5	602	CLA	C4D-ND	-2.86	1.33	1.37
24	t	309	CLA	C4D-ND	-2.86	1.33	1.37
24	4	612	CLA	CHC-C1C	2.86	1.42	1.35
24	2	201	CLA	C4D-ND	-2.86	1.33	1.37
24	7	605	CLA	C4D-ND	-2.86	1.33	1.37
24	t	310	CLA	C4D-ND	-2.86	1.33	1.37
24	R	104	CLA	CHC-C1C	2.86	1.42	1.35
24	A	829	CLA	C4D-ND	-2.86	1.33	1.37
24	2	201	CLA	CHC-C1C	2.85	1.42	1.35
24	3	302	CLA	C4D-ND	-2.85	1.33	1.37
24	h	602	CLA	C4D-ND	-2.85	1.33	1.37
24	k	305	CLA	C4D-ND	-2.85	1.33	1.37
24	A	824	CLA	C4D-ND	-2.85	1.33	1.37
24	c	609	CLA	C4D-ND	-2.85	1.33	1.37
24	2	204	CLA	CHC-C1C	2.84	1.42	1.35
24	1	305	CLA	CMB-C2B	-2.83	1.45	1.51
24	A	802	CLA	C1D-ND	2.83	1.41	1.37
24	8	204	CLA	C4D-ND	-2.82	1.33	1.37
26	8	210	DD6	C25-C24	2.82	1.41	1.34
26	7	616	DD6	C25-C24	2.82	1.41	1.34
26	9	314	DD6	C25-C24	2.82	1.41	1.34
24	9	303	CLA	CHC-C1C	2.82	1.42	1.35
24	A	857	CLA	CHC-C1C	2.82	1.42	1.35
24	c	607	CLA	CHC-C1C	2.81	1.42	1.35
24	9	306	CLA	CHC-C1C	2.81	1.42	1.35
24	A	816	CLA	C4D-ND	-2.81	1.33	1.37
24	L	203	CLA	C4D-ND	-2.80	1.33	1.37
24	k	304	CLA	C4D-ND	-2.80	1.33	1.37
24	9	310	CLA	CHC-C1C	2.80	1.42	1.35
26	6	614	DD6	C9-C8	2.79	1.41	1.34
24	A	830	CLA	CMB-C2B	-2.79	1.45	1.51
24	8	202	CLA	C4D-ND	-2.79	1.33	1.37
26	9	314	DD6	C9-C8	2.78	1.41	1.34
24	1	302	CLA	CHC-C1C	2.78	1.42	1.35
24	t	301	CLA	C4D-ND	-2.78	1.33	1.37
24	9	308	CLA	CHC-C1C	2.78	1.42	1.35
26	9	317	DD6	C24-C1	-2.77	1.40	1.45
24	5	607	CLA	CHC-C1C	2.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	311	DD6	C9-C8	2.76	1.41	1.34
24	t	304	CLA	C4D-ND	-2.75	1.33	1.37
24	A	830	CLA	CHC-C1C	2.74	1.42	1.35
24	A	801	CLA	C4D-ND	-2.74	1.33	1.37
26	t	313	DD6	C24-C1	-2.74	1.40	1.45
24	9	303	CLA	CMB-C2B	-2.74	1.45	1.51
26	6	615	DD6	C24-C1	-2.73	1.40	1.45
24	B	816	CLA	C4D-ND	-2.73	1.33	1.37
24	7	606	CLA	CMB-C2B	-2.72	1.46	1.51
24	4	604	CLA	CMB-C2B	-2.71	1.46	1.51
24	h	611	CLA	CHC-C1C	2.71	1.41	1.35
26	1	311	DD6	C25-C24	2.70	1.41	1.34
26	t	311	DD6	C25-C24	2.69	1.41	1.34
24	B	809	CLA	CMB-C2B	-2.69	1.46	1.51
26	9	313	DD6	C9-C8	2.68	1.41	1.34
24	2	208	CLA	C4D-ND	-2.68	1.34	1.37
26	9	315	DD6	C25-C24	2.68	1.41	1.34
29	7	614	A1L1G	C41-C40	2.68	1.41	1.34
26	A	848	DD6	C8-C6	-2.68	1.40	1.45
24	B	826	CLA	CMB-C2B	-2.67	1.46	1.51
26	6	614	DD6	C25-C24	2.66	1.41	1.34
26	A	848	DD6	C13-C11	-2.66	1.40	1.45
24	2	205	CLA	CMB-C2B	-2.66	1.46	1.51
26	7	616	DD6	C9-C8	2.65	1.41	1.34
26	k	315	DD6	C24-C1	-2.65	1.40	1.45
24	A	802	CLA	CMB-C2B	-2.65	1.46	1.51
24	9	310	CLA	CMB-C2B	-2.65	1.46	1.51
26	1	312	DD6	C25-C24	2.65	1.41	1.34
26	4	615	DD6	C25-C24	2.64	1.41	1.34
24	A	829	CLA	CMB-C2B	-2.63	1.46	1.51
29	9	312	A1L1G	C41-C40	2.63	1.41	1.34
24	1	302	CLA	CMB-C2B	-2.62	1.46	1.51
26	9	317	DD6	C13-C11	-2.62	1.40	1.45
24	B	830	CLA	CMB-C2B	-2.61	1.46	1.51
24	4	603	CLA	CMB-C2B	-2.61	1.46	1.51
26	2	212	DD6	C25-C24	2.61	1.41	1.34
24	h	608	CLA	CMB-C2B	-2.61	1.46	1.51
26	9	315	DD6	C9-C8	2.61	1.41	1.34
26	6	616	DD6	C25-C24	2.61	1.41	1.34
24	7	611	CLA	CMB-C2B	-2.61	1.46	1.51
24	h	612	CLA	CMB-C2B	-2.61	1.46	1.51
26	h	614	DD6	C9-C8	2.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	311	DD6	C9-C8	2.60	1.41	1.34
29	2	213	A1L1G	C33-C34	-2.60	1.40	1.45
26	c	614	DD6	C13-C11	-2.60	1.40	1.45
26	c	612	DD6	C25-C24	2.60	1.41	1.34
26	t	313	DD6	C8-C6	-2.60	1.40	1.45
24	B	818	CLA	CMB-C2B	-2.60	1.46	1.51
24	h	605	CLA	CMB-C2B	-2.59	1.46	1.51
24	B	832	CLA	CMB-C2B	-2.59	1.46	1.51
26	h	616	DD6	C9-C8	2.58	1.41	1.34
26	k	315	DD6	C8-C6	-2.58	1.40	1.45
24	L	204	CLA	CMB-C2B	-2.58	1.46	1.51
26	4	616	DD6	C13-C11	-2.58	1.40	1.45
24	k	304	CLA	CMB-C2B	-2.58	1.46	1.51
26	A	848	DD6	C24-C1	-2.58	1.40	1.45
26	9	317	DD6	C8-C6	-2.58	1.40	1.45
24	h	611	CLA	C4D-ND	-2.58	1.34	1.37
24	1	305	CLA	C3B-C2B	-2.58	1.36	1.40
26	1	312	DD6	C9-C8	2.58	1.41	1.34
26	8	211	DD6	C25-C24	2.57	1.41	1.34
26	6	615	DD6	C8-C6	-2.57	1.40	1.45
26	4	615	DD6	C9-C8	2.57	1.41	1.34
24	A	818	CLA	CMB-C2B	-2.57	1.46	1.51
26	6	613	DD6	C8-C6	-2.57	1.40	1.45
24	B	847	CLA	CMB-C2B	-2.57	1.46	1.51
24	B	833	CLA	CMB-C2B	-2.56	1.46	1.51
26	3	313	DD6	C25-C24	2.56	1.41	1.34
26	2	210	DD6	C25-C24	2.56	1.41	1.34
24	9	305	CLA	CMB-C2B	-2.56	1.46	1.51
26	3	313	DD6	C9-C8	2.56	1.41	1.34
26	4	617	DD6	C24-C1	-2.56	1.40	1.45
24	9	308	CLA	CMB-C2B	-2.55	1.46	1.51
26	7	613	DD6	C24-C1	-2.55	1.40	1.45
26	R	105	DD6	C25-C24	2.55	1.41	1.34
26	h	615	DD6	C24-C1	-2.55	1.40	1.45
24	B	829	CLA	CMB-C2B	-2.55	1.46	1.51
24	B	810	CLA	CMB-C2B	-2.55	1.46	1.51
24	7	604	CLA	CMB-C2B	-2.55	1.46	1.51
26	9	313	DD6	C25-C24	2.54	1.41	1.34
24	1	308	CLA	CMB-C2B	-2.54	1.46	1.51
29	2	213	A1L1G	C41-C40	2.54	1.41	1.34
24	A	820	CLA	CMB-C2B	-2.54	1.46	1.51
24	A	836	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	824	CLA	CMB-C2B	-2.54	1.46	1.51
24	2	204	CLA	CMB-C2B	-2.54	1.46	1.51
29	9	312	A1L1G	C32-C33	2.54	1.41	1.34
26	7	615	DD6	C24-C1	-2.54	1.40	1.45
29	k	312	A1L1G	C41-C40	2.53	1.41	1.34
26	6	613	DD6	C13-C11	-2.53	1.40	1.45
26	J	102	DD6	C9-C8	2.53	1.41	1.34
24	c	611	CLA	CMB-C2B	-2.53	1.46	1.51
24	3	308	CLA	CMB-C2B	-2.53	1.46	1.51
24	B	801	CLA	CMB-C2B	-2.53	1.46	1.51
26	6	616	DD6	C13-C11	-2.53	1.40	1.45
26	6	613	DD6	C25-C24	2.53	1.41	1.34
25	B	843	BCR	C1-C6	-2.53	1.50	1.53
26	t	313	DD6	C13-C11	-2.53	1.40	1.45
26	7	615	DD6	C8-C6	-2.52	1.40	1.45
26	c	613	DD6	C13-C11	-2.52	1.40	1.45
26	k	313	DD6	C24-C1	-2.52	1.40	1.45
26	4	614	DD6	C9-C8	2.52	1.41	1.34
26	3	312	DD6	C8-C6	-2.52	1.40	1.45
26	2	210	DD6	C13-C11	-2.51	1.40	1.45
24	t	305	CLA	CMB-C2B	-2.51	1.46	1.51
24	B	822	CLA	CMB-C2B	-2.51	1.46	1.51
24	1	305	CLA	CMD-C2D	-2.51	1.45	1.50
24	A	832	CLA	CMB-C2B	-2.51	1.46	1.51
24	B	803	CLA	CMB-C2B	-2.51	1.46	1.51
24	A	822	CLA	CMB-C2B	-2.50	1.46	1.51
26	h	613	DD6	C25-C24	2.50	1.41	1.34
26	5	608	DD6	C9-C8	2.50	1.41	1.34
26	4	616	DD6	C8-C6	-2.50	1.40	1.45
26	k	315	DD6	C25-C24	2.50	1.41	1.34
26	7	613	DD6	C13-C11	-2.50	1.40	1.45
24	A	860	CLA	CMB-C2B	-2.50	1.46	1.51
26	1	313	DD6	C25-C24	2.50	1.41	1.34
26	c	614	DD6	C8-C6	-2.50	1.40	1.45
24	B	846	CLA	CMB-C2B	-2.50	1.46	1.51
26	6	616	DD6	C9-C8	2.49	1.41	1.34
26	6	617	DD6	C9-C8	2.49	1.41	1.34
26	8	211	DD6	C8-C6	-2.49	1.40	1.45
24	B	804	CLA	CMB-C2B	-2.49	1.46	1.51
24	8	203	CLA	CMB-C2B	-2.49	1.46	1.51
26	3	312	DD6	C13-C11	-2.49	1.40	1.45
24	1	317	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	617	DD6	C13-C11	-2.49	1.40	1.45
26	h	616	DD6	C25-C24	2.48	1.41	1.34
24	B	836	CLA	CMB-C2B	-2.48	1.46	1.51
26	c	612	DD6	C24-C1	-2.48	1.40	1.45
24	B	820	CLA	CMB-C2B	-2.48	1.46	1.51
24	h	607	CLA	CMB-C2B	-2.48	1.46	1.51
26	6	613	DD6	C24-C1	-2.48	1.40	1.45
26	5	609	DD6	C8-C6	-2.48	1.40	1.45
24	h	606	CLA	CMB-C2B	-2.48	1.46	1.51
24	k	306	CLA	CMB-C2B	-2.48	1.46	1.51
26	h	613	DD6	C24-C1	-2.48	1.40	1.45
26	c	613	DD6	C24-C1	-2.48	1.40	1.45
26	5	609	DD6	C24-C1	-2.48	1.40	1.45
26	7	613	DD6	C8-C6	-2.48	1.40	1.45
24	A	813	CLA	CMB-C2B	-2.47	1.46	1.51
26	6	617	DD6	C25-C24	2.47	1.40	1.34
26	h	613	DD6	C8-C6	-2.47	1.40	1.45
24	A	834	CLA	CMB-C2B	-2.47	1.46	1.51
24	7	601	CLA	CMB-C2B	-2.47	1.46	1.51
24	A	857	CLA	CMB-C2B	-2.47	1.46	1.51
29	k	312	A1L1G	C32-C33	2.47	1.40	1.34
29	3	310	A1L1G	C33-C34	-2.46	1.40	1.45
26	5	609	DD6	C25-C24	2.46	1.40	1.34
24	6	609	CLA	C3B-CAB	-2.46	1.42	1.47
26	8	211	DD6	C9-C8	2.46	1.40	1.34
26	4	616	DD6	C25-C24	2.46	1.40	1.34
26	8	211	DD6	C13-C11	-2.46	1.40	1.45
24	L	203	CLA	CMB-C2B	-2.46	1.46	1.51
29	3	310	A1L1G	C41-C40	2.46	1.40	1.34
26	5	608	DD6	C13-C11	-2.46	1.40	1.45
24	R	104	CLA	CMB-C2B	-2.46	1.46	1.51
24	9	306	CLA	CMB-C2B	-2.46	1.46	1.51
24	A	833	CLA	CMB-C2B	-2.46	1.46	1.51
26	3	311	DD6	C25-C24	2.46	1.40	1.34
24	3	301	CLA	CMB-C2B	-2.45	1.46	1.51
26	3	312	DD6	C24-C1	-2.45	1.40	1.45
26	4	617	DD6	C8-C6	-2.45	1.40	1.45
26	6	615	DD6	C13-C11	-2.45	1.40	1.45
26	J	102	DD6	C25-C24	2.45	1.40	1.34
26	h	613	DD6	C9-C8	2.45	1.40	1.34
24	B	828	CLA	CMB-C2B	-2.45	1.46	1.51
26	1	313	DD6	C9-C8	2.45	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	212	DD6	C9-C8	2.45	1.40	1.34
24	F	202	CLA	CMB-C2B	-2.45	1.46	1.51
26	c	613	DD6	C8-C6	-2.45	1.40	1.45
26	7	615	DD6	C13-C11	-2.45	1.40	1.45
26	5	608	DD6	C24-C1	-2.45	1.40	1.45
26	k	313	DD6	C13-C11	-2.45	1.40	1.45
24	9	311	CLA	CMB-C2B	-2.45	1.46	1.51
24	6	608	CLA	CMB-C2B	-2.45	1.46	1.51
24	3	303	CLA	CMB-C2B	-2.44	1.46	1.51
24	B	807	CLA	CMB-C2B	-2.44	1.46	1.51
26	9	317	DD6	C9-C8	2.44	1.40	1.34
26	k	313	DD6	C9-C8	2.44	1.40	1.34
29	7	614	A1L1G	C33-C34	-2.44	1.40	1.45
26	2	212	DD6	C13-C11	-2.44	1.40	1.45
26	5	608	DD6	C8-C6	-2.44	1.40	1.45
29	3	310	A1L1G	C40-C39	-2.44	1.40	1.45
24	A	804	CLA	CMB-C2B	-2.44	1.46	1.51
24	B	808	CLA	CMB-C2B	-2.44	1.46	1.51
24	B	803	CLA	CMC-C2C	-2.44	1.45	1.50
24	3	306	CLA	CMB-C2B	-2.44	1.46	1.51
24	h	611	CLA	CMB-C2B	-2.44	1.46	1.51
26	3	312	DD6	C25-C24	2.44	1.40	1.34
24	B	837	CLA	CMB-C2B	-2.44	1.46	1.51
26	4	614	DD6	C13-C11	-2.44	1.40	1.45
24	1	305	CLA	CHC-C1C	2.44	1.41	1.35
26	4	616	DD6	C9-C8	2.44	1.40	1.34
24	A	840	CLA	CMB-C2B	-2.44	1.46	1.51
26	k	314	DD6	C25-C24	2.44	1.40	1.34
24	A	838	CLA	CMB-C2B	-2.44	1.46	1.51
26	4	617	DD6	C9-C8	2.44	1.40	1.34
24	B	838	CLA	CMB-C2B	-2.43	1.46	1.51
26	c	614	DD6	C9-C8	2.43	1.40	1.34
24	B	816	CLA	CMB-C2B	-2.43	1.46	1.51
24	B	808	CLA	C3B-C2B	-2.43	1.37	1.40
24	c	603	CLA	CMB-C2B	-2.43	1.46	1.51
24	A	810	CLA	CMB-C2B	-2.43	1.46	1.51
24	A	835	CLA	CMB-C2B	-2.43	1.46	1.51
26	8	212	DD6	C25-C24	2.43	1.40	1.34
24	F	201	CLA	CMB-C2B	-2.43	1.46	1.51
26	c	613	DD6	C25-C24	2.43	1.40	1.34
26	6	617	DD6	C24-C1	-2.43	1.40	1.45
24	2	202	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	825	CLA	CMB-C2B	-2.43	1.46	1.51
24	B	848	CLA	CMB-C2B	-2.43	1.46	1.51
26	h	615	DD6	C8-C6	-2.42	1.40	1.45
24	t	310	CLA	CMB-C2B	-2.42	1.46	1.51
26	k	313	DD6	C8-C6	-2.42	1.40	1.45
26	5	609	DD6	C13-C11	-2.42	1.40	1.45
26	R	105	DD6	C8-C6	-2.42	1.40	1.45
24	4	607	CLA	CMB-C2B	-2.42	1.46	1.51
26	c	612	DD6	C9-C8	2.42	1.40	1.34
24	6	609	CLA	CMB-C2B	-2.42	1.46	1.51
29	7	614	A1L1G	C32-C33	2.42	1.40	1.34
24	B	816	CLA	C3B-C2B	-2.42	1.37	1.40
26	c	614	DD6	C24-C1	-2.42	1.40	1.45
26	3	311	DD6	C8-C6	-2.42	1.40	1.45
24	B	811	CLA	CMB-C2B	-2.42	1.46	1.51
26	J	102	DD6	C24-C1	-2.41	1.40	1.45
26	8	212	DD6	C9-C8	2.41	1.40	1.34
26	3	311	DD6	C13-C11	-2.41	1.40	1.45
24	B	835	CLA	CMB-C2B	-2.41	1.46	1.51
26	k	313	DD6	C25-C24	2.41	1.40	1.34
24	8	204	CLA	CMB-C2B	-2.41	1.46	1.51
26	2	210	DD6	C8-C6	-2.41	1.40	1.45
26	3	311	DD6	C9-C8	2.41	1.40	1.34
24	4	601	CLA	CMB-C2B	-2.41	1.46	1.51
26	R	105	DD6	C24-C1	-2.41	1.40	1.45
24	c	601	CLA	CMB-C2B	-2.41	1.46	1.51
26	5	608	DD6	C25-C24	2.41	1.40	1.34
26	h	614	DD6	C24-C1	-2.41	1.40	1.45
26	k	314	DD6	C9-C8	2.41	1.40	1.34
24	A	812	CLA	CMB-C2B	-2.41	1.46	1.51
29	3	310	A1L1G	C32-C33	2.41	1.40	1.34
24	3	302	CLA	CMB-C2B	-2.41	1.46	1.51
24	9	302	CLA	CMB-C2B	-2.41	1.46	1.51
26	1	313	DD6	C8-C6	-2.41	1.40	1.45
26	8	212	DD6	C8-C6	-2.41	1.40	1.45
26	c	614	DD6	C25-C24	2.40	1.40	1.34
24	A	809	CLA	CMB-C2B	-2.40	1.46	1.51
24	A	815	CLA	CMB-C2B	-2.40	1.46	1.51
24	A	828	CLA	CMB-C2B	-2.40	1.46	1.51
24	6	605	CLA	CMB-C2B	-2.40	1.46	1.51
26	6	613	DD6	C9-C8	2.40	1.40	1.34
24	8	205	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	617	DD6	C25-C24	2.40	1.40	1.34
26	R	105	DD6	C9-C8	2.40	1.40	1.34
24	6	602	CLA	CMB-C2B	-2.40	1.46	1.51
24	R	103	CLA	CMB-C2B	-2.40	1.46	1.51
26	h	613	DD6	C13-C11	-2.40	1.40	1.45
26	k	314	DD6	C8-C6	-2.40	1.40	1.45
26	1	313	DD6	C24-C1	-2.40	1.40	1.45
26	5	609	DD6	C9-C8	2.40	1.40	1.34
24	A	819	CLA	CMB-C2B	-2.40	1.46	1.51
24	c	608	CLA	CMB-C2B	-2.40	1.46	1.51
26	6	616	DD6	C24-C1	-2.40	1.40	1.45
24	4	613	CLA	CMB-C2B	-2.40	1.46	1.51
24	A	808	CLA	CMB-C2B	-2.40	1.46	1.51
24	A	811	CLA	CMB-C2B	-2.40	1.46	1.51
24	B	827	CLA	CMB-C2B	-2.39	1.46	1.51
24	B	819	CLA	CMB-C2B	-2.39	1.46	1.51
26	2	210	DD6	C9-C8	2.39	1.40	1.34
24	B	802	CLA	CMB-C2B	-2.39	1.46	1.51
24	A	837	CLA	CMB-C2B	-2.39	1.46	1.51
26	k	314	DD6	C13-C11	-2.39	1.40	1.45
24	h	612	CLA	C3B-C2B	-2.39	1.37	1.40
26	h	615	DD6	C9-C8	2.39	1.40	1.34
24	9	309	CLA	CMB-C2B	-2.39	1.46	1.51
24	6	606	CLA	CMB-C2B	-2.39	1.46	1.51
26	6	616	DD6	C8-C6	-2.39	1.40	1.45
24	3	305	CLA	CMB-C2B	-2.39	1.46	1.51
29	2	213	A1L1G	C32-C33	2.39	1.40	1.34
24	7	605	CLA	CMB-C2B	-2.39	1.46	1.51
26	J	102	DD6	C13-C11	-2.38	1.40	1.45
24	t	309	CLA	CMB-C2B	-2.38	1.46	1.51
24	A	801	CLA	CMB-C2B	-2.38	1.46	1.51
26	c	613	DD6	C9-C8	2.38	1.40	1.34
24	B	812	CLA	CMB-C2B	-2.38	1.46	1.51
24	B	821	CLA	CMB-C2B	-2.38	1.46	1.51
24	2	203	CLA	CMB-C2B	-2.38	1.46	1.51
24	4	610	CLA	CMB-C2B	-2.38	1.46	1.51
26	c	612	DD6	C8-C6	-2.38	1.40	1.45
26	8	212	DD6	C24-C1	-2.38	1.40	1.45
24	A	823	CLA	CMB-C2B	-2.38	1.46	1.51
29	2	213	A1L1G	C40-C39	-2.38	1.40	1.45
24	5	604	CLA	CMB-C2B	-2.38	1.46	1.51
26	h	614	DD6	C25-C24	2.38	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	614	DD6	C25-C24	2.38	1.40	1.34
24	L	205	CLA	CMB-C2B	-2.38	1.46	1.51
24	3	307	CLA	CMB-C2B	-2.38	1.46	1.51
24	8	207	CLA	CMB-C2B	-2.38	1.46	1.51
24	B	834	CLA	CMB-C2B	-2.38	1.46	1.51
26	c	612	DD6	C13-C11	-2.37	1.40	1.45
26	4	614	DD6	C24-C1	-2.37	1.40	1.45
26	k	315	DD6	C13-C11	-2.37	1.40	1.45
26	J	102	DD6	C8-C6	-2.37	1.40	1.45
24	5	602	CLA	CMB-C2B	-2.37	1.46	1.51
24	A	824	CLA	CMB-C2B	-2.37	1.46	1.51
24	A	830	CLA	C3B-C2B	-2.37	1.37	1.40
24	A	853	CLA	CMB-C2B	-2.37	1.46	1.51
24	6	603	CLA	CMB-C2B	-2.37	1.46	1.51
26	8	210	DD6	C13-C11	-2.37	1.40	1.45
26	7	613	DD6	C9-C8	2.37	1.40	1.34
24	c	609	CLA	CMB-C2B	-2.37	1.46	1.51
24	A	806	CLA	CMB-C2B	-2.37	1.46	1.51
26	6	617	DD6	C8-C6	-2.37	1.40	1.45
24	A	817	CLA	CMB-C2B	-2.37	1.46	1.51
26	2	210	DD6	C24-C1	-2.37	1.40	1.45
24	1	304	CLA	CMB-C2B	-2.37	1.46	1.51
24	5	603	CLA	CMB-C2B	-2.37	1.46	1.51
24	4	606	CLA	CMB-C2B	-2.37	1.46	1.51
24	3	309	CLA	CMB-C2B	-2.36	1.46	1.51
26	2	212	DD6	C8-C6	-2.36	1.40	1.45
24	J	103	CLA	CMB-C2B	-2.36	1.46	1.51
24	6	607	CLA	CMB-C2B	-2.36	1.46	1.51
26	3	312	DD6	C9-C8	2.36	1.40	1.34
24	k	307	CLA	CMB-C2B	-2.36	1.46	1.51
24	9	307	CLA	CMB-C2B	-2.36	1.46	1.51
24	A	826	CLA	CMB-C2B	-2.36	1.46	1.51
26	7	615	DD6	C9-C8	2.36	1.40	1.34
24	F	203	CLA	CMB-C2B	-2.36	1.46	1.51
24	B	823	CLA	CMB-C2B	-2.36	1.46	1.51
24	h	601	CLA	CMB-C2B	-2.36	1.46	1.51
26	7	618	DD6	C13-C14	2.36	1.37	1.32
24	2	208	CLA	CMB-C2B	-2.36	1.46	1.51
24	7	612	CLA	CMB-C2B	-2.36	1.46	1.51
24	h	610	CLA	CMB-C2B	-2.36	1.46	1.51
29	k	312	A1L1G	C33-C34	-2.36	1.40	1.45
24	2	206	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	301	CLA	CMB-C2B	-2.36	1.46	1.51
24	B	817	CLA	CMB-C2B	-2.35	1.46	1.51
24	7	602	CLA	CMB-C2B	-2.35	1.46	1.51
24	A	814	CLA	CMB-C2B	-2.35	1.46	1.51
24	6	610	CLA	CMB-C2B	-2.35	1.46	1.51
26	7	613	DD6	C25-C24	2.35	1.40	1.34
24	5	601	CLA	CMB-C2B	-2.35	1.46	1.51
24	A	831	CLA	CMB-C2B	-2.35	1.46	1.51
26	h	615	DD6	C13-C11	-2.35	1.40	1.45
24	k	310	CLA	CMB-C2B	-2.35	1.46	1.51
24	8	201	CLA	CMB-C2B	-2.35	1.46	1.51
24	A	821	CLA	CMB-C2B	-2.35	1.46	1.51
24	4	608	CLA	CMB-C2B	-2.35	1.46	1.51
24	6	612	CLA	CMB-C2B	-2.35	1.46	1.51
24	t	306	CLA	CMB-C2B	-2.35	1.46	1.51
26	8	211	DD6	C24-C1	-2.35	1.40	1.45
24	8	202	CLA	CMB-C2B	-2.35	1.46	1.51
24	9	304	CLA	CMB-C2B	-2.35	1.46	1.51
24	B	815	CLA	CMB-C2B	-2.35	1.46	1.51
24	B	831	CLA	CMB-C2B	-2.35	1.46	1.51
24	B	847	CLA	C3B-C2B	-2.34	1.37	1.40
24	B	805	CLA	CMB-C2B	-2.34	1.46	1.51
24	A	853	CLA	CMD-C2D	-2.34	1.45	1.50
24	1	303	CLA	CMB-C2B	-2.34	1.46	1.51
24	4	605	CLA	CMB-C2B	-2.34	1.46	1.51
24	A	847	CLA	CMB-C2B	-2.34	1.46	1.51
24	1	306	CLA	CMB-C2B	-2.34	1.46	1.51
24	3	304	CLA	CMB-C2B	-2.34	1.46	1.51
24	A	857	CLA	CMD-C2D	-2.34	1.45	1.50
24	4	612	CLA	CMB-C2B	-2.34	1.46	1.51
24	c	605	CLA	CMB-C2B	-2.34	1.46	1.51
24	A	803	CLA	CMB-C2B	-2.34	1.46	1.51
24	A	856	CLA	CMB-C2B	-2.34	1.46	1.51
24	h	609	CLA	CMB-C2B	-2.34	1.46	1.51
24	2	209	CLA	CMB-C2B	-2.33	1.46	1.51
24	5	605	CLA	CMB-C2B	-2.33	1.46	1.51
29	k	312	A1L1G	C40-C39	-2.33	1.40	1.45
24	8	208	CLA	CMB-C2B	-2.33	1.46	1.51
24	A	860	CLA	CMC-C2C	-2.33	1.45	1.50
24	7	610	CLA	CMB-C2B	-2.33	1.46	1.51
24	A	807	CLA	CMB-C2B	-2.33	1.46	1.51
24	5	606	CLA	CMB-C2B	-2.33	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	615	DD6	C25-C24	2.33	1.40	1.34
24	6	604	CLA	CMB-C2B	-2.33	1.46	1.51
24	k	302	CLA	CMB-C2B	-2.33	1.46	1.51
24	4	609	CLA	CMB-C2B	-2.33	1.46	1.51
24	B	806	CLA	CMB-C2B	-2.33	1.46	1.51
24	t	302	CLA	CMB-C2B	-2.33	1.46	1.51
24	7	609	CLA	CMB-C2B	-2.33	1.46	1.51
24	c	602	CLA	CMB-C2B	-2.32	1.46	1.51
24	c	604	CLA	CMB-C2B	-2.32	1.46	1.51
24	c	606	CLA	CMB-C2B	-2.32	1.46	1.51
24	A	805	CLA	CMB-C2B	-2.32	1.46	1.51
24	h	604	CLA	CMB-C2B	-2.32	1.46	1.51
24	k	305	CLA	CMB-C2B	-2.32	1.46	1.51
24	4	611	CLA	CMB-C2B	-2.32	1.46	1.51
24	h	603	CLA	CMB-C2B	-2.32	1.46	1.51
24	k	309	CLA	CMB-C2B	-2.32	1.46	1.51
26	k	314	DD6	C24-C1	-2.32	1.41	1.45
26	6	617	DD6	C13-C11	-2.32	1.41	1.45
26	h	614	DD6	C13-C11	-2.32	1.41	1.45
26	h	615	DD6	C25-C24	2.32	1.40	1.34
24	B	825	CLA	CMB-C2B	-2.32	1.46	1.51
24	6	611	CLA	CMB-C2B	-2.32	1.46	1.51
24	1	301	CLA	CMB-C2B	-2.32	1.46	1.51
24	8	206	CLA	CMB-C2B	-2.32	1.46	1.51
24	2	201	CLA	CMB-C2B	-2.31	1.46	1.51
26	1	313	DD6	C13-C11	-2.31	1.41	1.45
26	4	614	DD6	C8-C6	-2.31	1.41	1.45
24	c	610	CLA	CMB-C2B	-2.31	1.46	1.51
26	4	616	DD6	C24-C1	-2.31	1.41	1.45
24	B	830	CLA	C3B-C2B	-2.31	1.37	1.40
24	2	201	CLA	CMD-C2D	-2.31	1.45	1.50
24	A	816	CLA	CMB-C2B	-2.31	1.46	1.51
24	t	303	CLA	CMB-C2B	-2.31	1.46	1.51
24	k	303	CLA	CMB-C2B	-2.31	1.46	1.51
26	3	311	DD6	C24-C1	-2.30	1.41	1.45
25	R	101	BCR	C30-C25	-2.30	1.50	1.53
24	8	209	CLA	CMB-C2B	-2.30	1.46	1.51
26	A	848	DD6	C9-C8	2.30	1.40	1.34
24	t	304	CLA	CMB-C2B	-2.30	1.46	1.51
24	h	612	CLA	C3B-CAB	-2.30	1.43	1.47
24	7	603	CLA	CMB-C2B	-2.30	1.46	1.51
24	1	309	CLA	CMB-C2B	-2.30	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	315	DD6	C24-C1	-2.30	1.41	1.45
24	1	307	CLA	CMB-C2B	-2.30	1.46	1.51
24	t	307	CLA	CMB-C2B	-2.29	1.46	1.51
24	t	308	CLA	CMB-C2B	-2.29	1.46	1.51
29	3	310	A1L1G	C29-C30	-2.29	1.40	1.45
24	A	827	CLA	CMB-C2B	-2.29	1.46	1.51
26	1	312	DD6	C8-C6	-2.29	1.41	1.45
24	k	311	CLA	CMB-C2B	-2.28	1.46	1.51
24	B	813	CLA	CMB-C2B	-2.28	1.46	1.51
26	t	313	DD6	C25-C24	2.28	1.40	1.34
24	7	607	CLA	CMB-C2B	-2.28	1.46	1.51
26	6	615	DD6	C9-C8	2.28	1.40	1.34
26	R	105	DD6	C13-C14	2.27	1.37	1.32
26	k	315	DD6	C9-C8	2.27	1.40	1.34
24	9	301	CLA	CMB-C2B	-2.27	1.46	1.51
26	8	212	DD6	C13-C11	-2.27	1.41	1.45
24	B	828	CLA	CMD-C2D	-2.27	1.46	1.50
26	9	313	DD6	C24-C1	-2.27	1.41	1.45
24	6	611	CLA	CMD-C2D	-2.27	1.46	1.50
26	t	313	DD6	C9-C8	2.26	1.40	1.34
24	5	607	CLA	CMB-C2B	-2.26	1.46	1.51
24	7	608	CLA	CMB-C2B	-2.26	1.46	1.51
26	A	848	DD6	C25-C24	2.26	1.40	1.34
24	6	601	CLA	CMB-C2B	-2.26	1.46	1.51
24	2	207	CLA	CMB-C2B	-2.26	1.46	1.51
26	k	314	DD6	C26-C27	2.26	1.41	1.37
24	c	603	CLA	C3B-C2B	-2.26	1.37	1.40
24	A	802	CLA	CMC-C2C	-2.26	1.46	1.50
26	h	616	DD6	C13-C11	-2.25	1.41	1.45
26	9	313	DD6	C8-C6	-2.25	1.41	1.45
26	9	315	DD6	C13-C11	-2.25	1.41	1.45
26	3	313	DD6	C8-C6	-2.25	1.41	1.45
24	c	607	CLA	CMB-C2B	-2.25	1.47	1.51
26	h	616	DD6	C8-C6	-2.25	1.41	1.45
26	h	614	DD6	C8-C6	-2.24	1.41	1.45
24	B	816	CLA	C3B-CAB	-2.24	1.43	1.47
26	3	313	DD6	C13-C11	-2.24	1.41	1.45
26	t	311	DD6	C13-C11	-2.24	1.41	1.45
24	6	609	CLA	C3B-C2B	-2.24	1.37	1.40
26	h	616	DD6	C24-C1	-2.24	1.41	1.45
24	4	609	CLA	CMC-C2C	-2.24	1.46	1.50
29	9	312	A1L1G	C33-C34	-2.23	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	614	A1L1G	C29-C30	-2.23	1.40	1.45
24	h	602	CLA	CMB-C2B	-2.23	1.47	1.51
24	9	301	CLA	CMD-C2D	-2.23	1.46	1.50
26	1	312	DD6	C24-C1	-2.23	1.41	1.45
26	8	210	DD6	C13-C14	2.23	1.37	1.32
26	9	314	DD6	C13-C14	2.23	1.37	1.32
26	3	313	DD6	C24-C1	-2.23	1.41	1.45
26	6	615	DD6	C25-C24	2.23	1.40	1.34
24	L	204	CLA	C3B-C2B	-2.22	1.37	1.40
24	4	604	CLA	C3B-C2B	-2.22	1.37	1.40
24	1	302	CLA	C3B-CAB	-2.22	1.43	1.47
24	B	832	CLA	C3B-C2B	-2.22	1.37	1.40
26	4	615	DD6	C8-C6	-2.22	1.41	1.45
26	t	311	DD6	C8-C6	-2.22	1.41	1.45
24	4	602	CLA	CMB-C2B	-2.21	1.47	1.51
26	9	317	DD6	C25-C24	2.21	1.40	1.34
24	4	603	CLA	C3B-C2B	-2.21	1.37	1.40
26	4	615	DD6	C24-C1	-2.21	1.41	1.45
24	B	826	CLA	C3B-C2B	-2.21	1.37	1.40
24	t	301	CLA	CMB-C2B	-2.20	1.47	1.51
24	A	802	CLA	CMD-C2D	-2.20	1.46	1.50
26	2	212	DD6	C24-C1	-2.20	1.41	1.45
24	B	838	CLA	C3B-CAB	-2.20	1.43	1.47
24	k	308	CLA	CMB-C2B	-2.20	1.47	1.51
24	h	611	CLA	CMD-C2D	-2.19	1.46	1.50
24	A	836	CLA	C3B-C2B	-2.19	1.37	1.40
24	B	829	CLA	CMD-C2D	-2.19	1.46	1.50
24	B	801	CLA	CMD-C2D	-2.19	1.46	1.50
24	9	302	CLA	CMD-C2D	-2.18	1.46	1.50
24	1	302	CLA	C3B-C2B	-2.17	1.37	1.40
24	A	835	CLA	C3B-C2B	-2.17	1.37	1.40
26	9	313	DD6	C13-C11	-2.17	1.41	1.45
26	4	615	DD6	C13-C11	-2.17	1.41	1.45
26	7	616	DD6	C13-C11	-2.17	1.41	1.45
24	A	830	CLA	CMD-C2D	-2.16	1.46	1.50
24	A	823	CLA	C3B-C2B	-2.16	1.37	1.40
24	6	611	CLA	CMC-C2C	-2.16	1.46	1.50
24	B	838	CLA	C3B-C2B	-2.16	1.37	1.40
24	1	302	CLA	CMD-C2D	-2.16	1.46	1.50
24	B	828	CLA	C3B-C2B	-2.16	1.37	1.40
29	7	614	A1L1G	C40-C39	-2.16	1.41	1.45
24	B	814	CLA	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	312	DD6	C13-C11	-2.15	1.41	1.45
24	B	803	CLA	C3B-CAB	-2.15	1.43	1.47
24	A	823	CLA	C3B-CAB	-2.15	1.43	1.47
26	6	614	DD6	C13-C11	-2.14	1.41	1.45
26	9	315	DD6	C8-C6	-2.14	1.41	1.45
24	A	822	CLA	C3B-C2B	-2.14	1.37	1.40
24	A	804	CLA	C3B-C2B	-2.14	1.37	1.40
26	8	210	DD6	C24-C1	-2.14	1.41	1.45
24	A	860	CLA	CMD-C2D	-2.14	1.46	1.50
24	h	607	CLA	C3B-C2B	-2.14	1.37	1.40
24	h	608	CLA	C3B-C2B	-2.14	1.37	1.40
24	2	204	CLA	C3B-C2B	-2.13	1.37	1.40
24	7	601	CLA	CMD-C2D	-2.13	1.46	1.50
29	2	213	A1L1G	C29-C30	-2.13	1.40	1.45
26	6	617	DD6	C13-C14	2.13	1.37	1.32
29	9	312	A1L1G	C40-C39	-2.13	1.41	1.45
26	R	105	DD6	C13-C11	-2.13	1.41	1.45
24	A	812	CLA	CMC-C2C	-2.13	1.46	1.50
24	1	308	CLA	C3B-C2B	-2.12	1.37	1.40
24	A	812	CLA	C3B-C2B	-2.12	1.37	1.40
24	A	817	CLA	C3B-CAB	-2.12	1.43	1.47
24	B	820	CLA	C3B-C2B	-2.12	1.37	1.40
26	t	311	DD6	C24-C1	-2.12	1.41	1.45
25	I	101	BCR	C30-C25	-2.11	1.50	1.53
24	A	832	CLA	C3B-C2B	-2.11	1.37	1.40
24	5	607	CLA	C3B-C2B	-2.11	1.37	1.40
24	6	610	CLA	C3B-C2B	-2.11	1.37	1.40
24	R	104	CLA	CMC-C2C	-2.11	1.46	1.50
26	7	616	DD6	C8-C6	-2.11	1.41	1.45
24	A	833	CLA	C3B-C2B	-2.10	1.37	1.40
24	8	208	CLA	CMD-C2D	-2.10	1.46	1.50
24	4	613	CLA	C3B-C2B	-2.10	1.37	1.40
24	k	304	CLA	C3B-C2B	-2.10	1.37	1.40
24	B	821	CLA	CMD-C2D	-2.10	1.46	1.50
24	1	304	CLA	C3B-C2B	-2.10	1.37	1.40
24	R	104	CLA	CMD-C2D	-2.10	1.46	1.50
24	A	817	CLA	C3B-C2B	-2.09	1.37	1.40
24	B	809	CLA	C3B-C2B	-2.09	1.37	1.40
24	5	607	CLA	MG-NC	2.09	2.11	2.06
24	4	612	CLA	CMD-C2D	-2.09	1.46	1.50
24	B	823	CLA	CMD-C2D	-2.09	1.46	1.50
24	4	601	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	810	CLA	CMD-C2D	-2.09	1.46	1.50
29	k	312	A1L1G	C29-C30	-2.09	1.40	1.45
24	B	808	CLA	C3B-CAB	-2.09	1.43	1.47
24	B	811	CLA	C3B-C2B	-2.09	1.37	1.40
24	B	811	CLA	CMD-C2D	-2.09	1.46	1.50
26	6	614	DD6	C24-C1	-2.08	1.41	1.45
24	9	311	CLA	CMD-C2D	-2.08	1.46	1.50
24	t	304	CLA	CMD-C2D	-2.08	1.46	1.50
24	A	813	CLA	CMD-C2D	-2.08	1.46	1.50
24	1	305	CLA	C4B-CHC	-2.08	1.35	1.41
24	7	601	CLA	C3B-C2B	-2.08	1.37	1.40
24	5	607	CLA	C4B-CHC	-2.08	1.35	1.41
24	8	203	CLA	C3B-C2B	-2.08	1.37	1.40
24	9	303	CLA	C3B-C2B	-2.08	1.37	1.40
29	9	312	A1L1G	C29-C30	-2.08	1.40	1.45
24	c	601	CLA	C3B-C2B	-2.08	1.37	1.40
26	9	315	DD6	C13-C14	2.08	1.37	1.32
26	1	311	DD6	C8-C6	-2.07	1.41	1.45
26	1	312	DD6	C13-C14	2.07	1.37	1.32
24	9	303	CLA	CMD-C2D	-2.07	1.46	1.50
26	1	311	DD6	C13-C11	-2.07	1.41	1.45
24	9	307	CLA	CMC-C2C	-2.07	1.46	1.50
25	A	846	BCR	C1-C6	-2.06	1.50	1.53
24	B	803	CLA	CMD-C2D	-2.06	1.46	1.50
26	R	105	DD6	C36-C31	-2.06	1.32	1.34
24	B	836	CLA	C3B-C2B	-2.06	1.37	1.40
24	9	308	CLA	CMD-C2D	-2.06	1.46	1.50
24	B	847	CLA	C3B-CAB	-2.06	1.43	1.47
24	B	808	CLA	CMC-C2C	-2.06	1.46	1.50
24	c	608	CLA	C3B-C2B	-2.05	1.37	1.40
24	9	307	CLA	CMD-C2D	-2.05	1.46	1.50
24	1	304	CLA	CMD-C2D	-2.05	1.46	1.50
24	9	306	CLA	CMD-C2D	-2.05	1.46	1.50
24	7	604	CLA	CMD-C2D	-2.05	1.46	1.50
24	9	304	CLA	CMD-C2D	-2.05	1.46	1.50
24	A	801	CLA	CMD-C2D	-2.05	1.46	1.50
24	B	814	CLA	CMD-C2D	-2.05	1.46	1.50
24	8	204	CLA	C3B-C2B	-2.05	1.37	1.40
24	B	818	CLA	C3B-C2B	-2.05	1.37	1.40
24	2	206	CLA	C3B-C2B	-2.05	1.37	1.40
26	6	614	DD6	C8-C6	-2.05	1.41	1.45
24	A	829	CLA	C3B-C2B	-2.05	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	829	CLA	CMC-C2C	-2.05	1.46	1.50
24	L	205	CLA	CMD-C2D	-2.05	1.46	1.50
24	A	824	CLA	CMD-C2D	-2.04	1.46	1.50
24	A	856	CLA	C3B-C2B	-2.04	1.37	1.40
24	A	810	CLA	C3B-C2B	-2.04	1.37	1.40
24	6	604	CLA	CMD-C2D	-2.04	1.46	1.50
24	k	307	CLA	CMD-C2D	-2.04	1.46	1.50
24	A	811	CLA	C3B-C2B	-2.04	1.37	1.40
24	6	609	CLA	CMC-C2C	-2.04	1.46	1.50
24	A	857	CLA	CMC-C2C	-2.04	1.46	1.50
26	7	616	DD6	C13-C14	2.04	1.37	1.32
24	9	310	CLA	CMD-C2D	-2.03	1.46	1.50
24	R	103	CLA	CMD-C2D	-2.03	1.46	1.50
24	B	804	CLA	C3B-CAB	-2.03	1.43	1.47
24	A	819	CLA	C3B-C2B	-2.03	1.37	1.40
24	c	604	CLA	C3B-C2B	-2.03	1.37	1.40
24	3	306	CLA	C3B-C2B	-2.03	1.37	1.40
24	t	308	CLA	C3B-C2B	-2.03	1.37	1.40
24	3	307	CLA	CMD-C2D	-2.02	1.46	1.50
26	1	311	DD6	C24-C1	-2.02	1.41	1.45
24	3	308	CLA	CMD-C2D	-2.02	1.46	1.50
26	9	314	DD6	C13-C11	-2.02	1.41	1.45
24	8	204	CLA	CMD-C2D	-2.02	1.46	1.50
24	3	302	CLA	C3B-C2B	-2.02	1.37	1.40
24	1	309	CLA	CMD-C2D	-2.02	1.46	1.50
24	1	317	CLA	C3B-C2B	-2.02	1.37	1.40
24	B	802	CLA	CMD-C2D	-2.02	1.46	1.50
24	A	828	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	808	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	827	CLA	CMD-C2D	-2.01	1.46	1.50
24	B	831	CLA	CMD-C2D	-2.01	1.46	1.50
24	c	607	CLA	CMD-C2D	-2.01	1.46	1.50
24	c	607	CLA	C3B-CAB	-2.01	1.43	1.47
24	B	846	CLA	CMD-C2D	-2.01	1.46	1.50
24	6	602	CLA	C3B-C2B	-2.01	1.37	1.40
24	1	301	CLA	CMD-C2D	-2.01	1.46	1.50
28	1	318	LHG	O7-C5	-2.01	1.41	1.46
24	B	826	CLA	CMD-C2D	-2.01	1.46	1.50
24	A	856	CLA	C3B-CAB	-2.01	1.43	1.47
24	h	602	CLA	CMD-C2D	-2.01	1.46	1.50
24	8	203	CLA	CMC-C2C	-2.01	1.46	1.50
24	9	303	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
24	h	606	CLA	CMD-C2D	-2.00	1.46	1.50
24	A	817	CLA	CMD-C2D	-2.00	1.46	1.50
26	4	615	DD6	C13-C14	2.00	1.37	1.32
24	c	610	CLA	CMC-C2C	-2.00	1.46	1.50
24	7	611	CLA	C3B-C2B	-2.00	1.37	1.40
24	A	830	CLA	MG-NA	2.00	2.11	2.06
24	A	803	CLA	CMD-C2D	-2.00	1.46	1.50

All (2909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	830	CLA	C4A-NA-C1A	9.33	110.90	106.71
26	9	314	DD6	C3-C2-C1	-8.92	114.58	127.31
26	8	210	DD6	C14-C13-C11	-8.74	111.97	125.53
25	c	615	BCR	C20-C21-C22	-8.66	114.95	127.31
26	k	315	DD6	C3-C2-C1	-8.60	115.04	127.31
24	1	305	CLA	C4A-NA-C1A	7.90	110.26	106.71
25	B	843	BCR	C11-C10-C9	-7.16	117.09	127.31
24	h	602	CLA	C5-C3-C2	7.14	135.57	121.12
26	6	616	DD6	C3-C2-C1	-7.14	117.13	127.31
26	R	105	DD6	C9-C10-C11	-6.97	117.36	127.31
26	9	315	DD6	C3-C2-C1	-6.96	117.37	127.31
24	9	305	CLA	C4A-NA-C1A	6.89	109.80	106.71
25	k	316	BCR	C15-C14-C13	-6.87	117.51	127.31
26	4	617	DD6	C4-C5-C6	-6.76	117.66	127.31
25	A	843	BCR	C28-C27-C26	-6.74	102.03	114.08
26	7	613	DD6	C3-C2-C1	-6.72	117.72	127.31
25	M	101	BCR	C20-C21-C22	-6.72	117.72	127.31
26	c	612	DD6	C9-C10-C11	-6.70	117.74	127.31
25	c	615	BCR	C16-C17-C18	-6.65	117.83	127.31
25	A	846	BCR	C28-C27-C26	-6.60	102.29	114.08
26	k	314	DD6	C3-C2-C1	-6.59	117.91	127.31
26	9	317	DD6	C4-C5-C6	-6.55	117.97	127.31
25	B	842	BCR	C24-C23-C22	-6.55	116.34	126.23
26	2	210	DD6	C3-C2-C1	-6.45	118.11	127.31
25	L	202	BCR	C28-C27-C26	-6.31	102.80	114.08
26	h	615	DD6	C3-C2-C1	-6.25	118.39	127.31
25	9	316	BCR	C7-C8-C9	-6.25	116.79	126.23
25	4	618	BCR	C16-C17-C18	-6.23	118.42	127.31
25	1	314	BCR	C16-C17-C18	-6.22	118.43	127.31
26	A	848	DD6	C4-C5-C6	-6.22	118.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	104	CLA	C4A-NA-C1A	6.20	109.50	106.71
26	6	617	DD6	C3-C2-C1	-6.17	118.51	127.31
26	c	614	DD6	C3-C2-C1	-6.13	118.57	127.31
24	h	611	CLA	C4A-NA-C1A	6.13	109.46	106.71
26	t	313	DD6	C3-C2-C1	-6.12	118.57	127.31
25	J	104	BCR	C28-C27-C26	-6.11	103.16	114.08
24	A	860	CLA	C4A-NA-C1A	6.10	109.45	106.71
25	B	849	BCR	C28-C27-C26	-6.10	103.18	114.08
24	9	310	CLA	C4A-NA-C1A	6.09	109.45	106.71
26	5	609	DD6	C3-C2-C1	-6.07	118.64	127.31
24	B	803	CLA	C4A-NA-C1A	6.05	109.43	106.71
24	L	203	CLA	C4A-NA-C1A	5.96	109.38	106.71
26	6	613	DD6	C3-C2-C1	-5.95	118.81	127.31
25	4	618	BCR	C20-C21-C22	-5.93	118.85	127.31
26	c	612	DD6	C3-C2-C1	-5.93	118.85	127.31
26	5	608	DD6	C3-C2-C1	-5.91	118.87	127.31
26	9	317	DD6	C3-C2-C1	-5.83	119.00	127.31
24	B	837	CLA	C4A-NA-C1A	5.82	109.32	106.71
26	3	313	DD6	C3-C2-C1	-5.81	119.01	127.31
24	k	302	CLA	C4A-NA-C1A	5.79	109.31	106.71
26	c	613	DD6	C3-C2-C1	-5.75	119.10	127.31
24	9	304	CLA	C4A-NA-C1A	5.74	109.29	106.71
24	3	301	CLA	C4A-NA-C1A	5.74	109.29	106.71
26	6	615	DD6	C9-C10-C11	-5.74	119.12	127.31
24	3	304	CLA	CMB-C2B-C1B	-5.73	119.66	128.46
24	A	857	CLA	C4A-NA-C1A	5.73	109.28	106.71
24	h	601	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	9	316	BCR	C11-C10-C9	-5.70	119.17	127.31
25	B	843	BCR	C15-C14-C13	-5.70	119.18	127.31
24	k	308	CLA	CMB-C2B-C1B	-5.69	119.71	128.46
24	h	602	CLA	C1-C2-C3	5.69	135.89	126.04
25	M	101	BCR	C16-C17-C18	-5.67	119.21	127.31
24	B	829	CLA	C4A-NA-C1A	5.67	109.26	106.71
26	A	848	DD6	C3-C2-C1	-5.54	119.40	127.31
25	L	202	BCR	C3-C4-C5	-5.53	104.20	114.08
26	5	608	DD6	C4-C5-C6	-5.53	119.42	127.31
25	B	841	BCR	C33-C5-C6	-5.52	118.33	124.53
24	B	835	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	1	314	BCR	C11-C10-C9	-5.50	119.46	127.31
24	B	809	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	7	617	BCR	C15-C14-C13	-5.48	119.48	127.31
25	A	845	BCR	C11-C10-C9	-5.47	119.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	615	DD6	C3-C2-C1	-5.46	119.51	127.31
25	A	843	BCR	C3-C4-C5	-5.46	104.33	114.08
24	A	837	CLA	C4A-NA-C1A	5.45	109.16	106.71
24	3	302	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	1	310	BCR	C16-C17-C18	-5.43	119.56	127.31
24	A	802	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
24	9	307	CLA	C4A-NA-C1A	5.41	109.14	106.71
26	J	102	DD6	C3-C2-C1	-5.41	119.59	127.31
24	B	822	CLA	C4A-NA-C1A	5.41	109.14	106.71
24	t	301	CLA	C4A-NA-C1A	5.40	109.14	106.71
24	9	302	CLA	C4A-NA-C1A	5.40	109.13	106.71
25	A	844	BCR	C16-C17-C18	-5.37	119.64	127.31
25	t	312	BCR	C38-C26-C25	-5.37	118.50	124.53
25	J	101	BCR	C1-C6-C5	-5.37	115.05	122.61
25	B	843	BCR	C24-C23-C22	-5.36	118.13	126.23
25	M	101	BCR	C15-C14-C13	-5.36	119.65	127.31
24	F	203	CLA	C4A-NA-C1A	5.36	109.12	106.71
24	6	611	CLA	C4A-NA-C1A	5.36	109.12	106.71
24	9	303	CLA	C4A-NA-C1A	5.36	109.11	106.71
24	B	806	CLA	C4A-NA-C1A	5.36	109.11	106.71
24	2	204	CLA	C4A-NA-C1A	5.35	109.11	106.71
26	7	616	DD6	C9-C10-C11	-5.35	119.68	127.31
26	c	612	DD6	C14-C13-C11	-5.34	117.25	125.53
26	h	613	DD6	C3-C2-C1	-5.34	119.70	127.31
24	k	304	CLA	C4A-NA-C1A	5.33	109.10	106.71
24	4	612	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
24	t	301	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
25	I	102	BCR	C28-C27-C26	-5.29	104.62	114.08
26	k	315	DD6	C14-C13-C11	-5.29	117.33	125.53
25	9	316	BCR	C16-C17-C18	-5.28	119.78	127.31
26	t	311	DD6	C3-C2-C1	-5.27	119.79	127.31
26	3	311	DD6	C3-C2-C1	-5.27	119.79	127.31
24	8	204	CLA	C4A-NA-C1A	5.25	109.07	106.71
24	B	838	CLA	C4A-NA-C1A	5.25	109.07	106.71
26	6	615	DD6	C3-C2-C1	-5.25	119.81	127.31
25	J	104	BCR	C3-C4-C5	-5.25	104.70	114.08
24	h	602	CLA	C4-C3-C2	-5.25	110.22	123.68
26	2	212	DD6	C3-C2-C1	-5.23	119.84	127.31
25	9	316	BCR	C15-C14-C13	-5.23	119.85	127.31
25	L	206	BCR	C28-C27-C26	-5.22	104.75	114.08
24	B	833	CLA	C4A-NA-C1A	5.21	109.05	106.71
26	4	616	DD6	C3-C2-C1	-5.21	119.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	615	BCR	C7-C8-C9	-5.20	118.37	126.23
25	F	204	BCR	C15-C14-C13	-5.20	119.89	127.31
25	B	849	BCR	C3-C4-C5	-5.20	104.80	114.08
26	6	616	DD6	C9-C10-C11	-5.20	119.89	127.31
24	B	801	CLA	C4A-NA-C1A	5.19	109.04	106.71
26	9	314	DD6	C9-C10-C11	-5.19	119.91	127.31
24	5	603	CLA	C4A-NA-C1A	5.18	109.04	106.71
24	7	604	CLA	C4A-NA-C1A	5.18	109.04	106.71
25	J	101	BCR	C36-C18-C17	-5.17	115.68	122.92
26	1	313	DD6	C3-C2-C1	-5.16	119.95	127.31
24	t	303	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
26	4	614	DD6	C3-C2-C1	-5.13	119.98	127.31
24	A	814	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	B	805	CLA	C4A-NA-C1A	5.13	109.01	106.71
26	7	616	DD6	C3-C2-C1	-5.13	119.99	127.31
24	7	605	CLA	C4A-NA-C1A	5.12	109.01	106.71
24	A	815	CLA	C4A-NA-C1A	5.11	109.00	106.71
24	8	203	CLA	C4A-NA-C1A	5.10	109.00	106.71
24	c	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	4	618	BCR	C24-C23-C22	-5.10	118.53	126.23
26	3	312	DD6	C4-C5-C6	-5.09	120.04	127.31
26	c	614	DD6	O1-C20-C19	-5.09	109.56	113.38
26	c	612	DD6	C4-C5-C6	-5.07	120.07	127.31
24	7	606	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
25	c	615	BCR	C38-C26-C25	-5.05	118.85	124.53
26	8	211	DD6	C3-C2-C1	-5.05	120.10	127.31
24	5	606	CLA	C4A-NA-C1A	5.05	108.98	106.71
24	B	807	CLA	C4A-NA-C1A	5.05	108.97	106.71
24	6	601	CLA	C4A-NA-C1A	5.04	108.97	106.71
24	A	808	CLA	C4A-NA-C1A	5.04	108.97	106.71
24	h	602	CLA	CMB-C2B-C1B	-5.04	120.71	128.46
26	A	848	DD6	C15-C14-C13	-5.04	115.35	125.99
24	R	103	CLA	C4A-NA-C1A	5.03	108.97	106.71
26	3	312	DD6	C3-C2-C1	-5.03	120.13	127.31
25	k	316	BCR	C20-C21-C22	-5.01	120.17	127.31
24	k	310	CLA	C4A-NA-C1A	5.00	108.96	106.71
26	9	313	DD6	C4-C5-C6	-5.00	120.17	127.31
26	4	614	DD6	C4-C5-C6	-4.98	120.21	127.31
25	J	101	BCR	C4-C5-C6	-4.97	115.52	122.73
24	B	812	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	4	615	DD6	C3-C2-C1	-4.96	120.23	127.31
24	4	608	CLA	C4A-NA-C1A	4.96	108.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	616	DD6	C4-C5-C6	-4.96	120.24	127.31
24	6	612	CLA	C4A-NA-C1A	4.96	108.93	106.71
24	A	826	CLA	C4A-NA-C1A	4.95	108.93	106.71
26	8	212	DD6	C3-C2-C1	-4.95	120.25	127.31
26	c	614	DD6	C4-C5-C6	-4.94	120.25	127.31
24	B	814	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
24	A	805	CLA	C4A-NA-C1A	4.94	108.93	106.71
25	J	101	BCR	C7-C8-C9	-4.93	118.78	126.23
24	A	804	CLA	C4A-NA-C1A	4.93	108.92	106.71
25	J	101	BCR	C11-C10-C9	-4.93	120.27	127.31
24	9	301	CLA	C4A-NA-C1A	4.93	108.92	106.71
24	7	608	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
26	8	211	DD6	C15-C14-C13	-4.92	115.60	125.99
25	2	211	BCR	C15-C14-C13	-4.92	120.30	127.31
24	3	304	CLA	CMB-C2B-C3B	4.91	133.87	124.68
25	L	206	BCR	C30-C25-C26	-4.90	115.71	122.61
24	A	832	CLA	C4A-NA-C1A	4.90	108.91	106.71
25	9	316	BCR	C20-C21-C22	-4.90	120.32	127.31
25	B	842	BCR	C11-C10-C9	-4.89	120.34	127.31
25	B	842	BCR	C7-C8-C9	-4.88	118.86	126.23
24	9	311	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
24	t	304	CLA	C4A-NA-C1A	4.87	108.89	106.71
24	A	817	CLA	C4A-NA-C1A	4.86	108.89	106.71
24	B	848	CLA	C4A-NA-C1A	4.85	108.89	106.71
24	B	804	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
25	A	846	BCR	C7-C8-C9	-4.84	118.92	126.23
26	1	312	DD6	C3-C2-C1	-4.84	120.41	127.31
24	k	308	CLA	CMB-C2B-C3B	4.84	133.73	124.68
26	8	210	DD6	C3-C2-C1	-4.83	120.41	127.31
26	6	616	DD6	C14-C13-C11	-4.83	118.04	125.53
24	A	812	CLA	C4A-NA-C1A	4.82	108.88	106.71
26	h	616	DD6	C9-C10-C11	-4.82	120.43	127.31
26	4	616	DD6	C4-C5-C6	-4.82	120.43	127.31
24	7	609	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	B	825	CLA	C4A-NA-C1A	4.81	108.87	106.71
26	2	212	DD6	C9-C10-C11	-4.81	120.45	127.31
24	3	309	CLA	C4A-NA-C1A	4.80	108.86	106.71
24	6	609	CLA	C4A-NA-C1A	4.80	108.86	106.71
26	9	317	DD6	C15-C14-C13	-4.80	115.85	125.99
25	A	845	BCR	C7-C8-C9	-4.79	118.99	126.23
26	k	313	DD6	C3-C2-C1	-4.79	120.47	127.31
24	t	310	CLA	C4A-NA-C1A	4.79	108.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	307	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	B	842	BCR	C16-C17-C18	-4.78	120.49	127.31
24	B	829	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
24	A	835	CLA	C4A-NA-C1A	4.76	108.84	106.71
26	3	311	DD6	C15-C14-C13	-4.75	115.95	125.99
25	k	316	BCR	C11-C10-C9	-4.74	120.55	127.31
26	k	314	DD6	C9-C10-C11	-4.74	120.55	127.31
24	2	205	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
25	c	615	BCR	C24-C23-C22	-4.73	119.09	126.23
24	B	820	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	4	608	CLA	C1-C2-C3	-4.72	119.11	126.75
24	8	208	CLA	C4A-NA-C1A	4.72	108.83	106.71
26	6	615	DD6	C4-C5-C6	-4.71	120.59	127.31
24	2	206	CLA	C4A-NA-C1A	4.71	108.82	106.71
24	A	834	CLA	C4A-NA-C1A	4.71	108.82	106.71
26	1	311	DD6	C3-C2-C1	-4.70	120.60	127.31
24	2	207	CLA	C4A-NA-C1A	4.70	108.82	106.71
24	9	309	CLA	C4A-NA-C1A	4.69	108.81	106.71
24	7	604	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
24	A	816	CLA	C4A-NA-C1A	4.68	108.81	106.71
24	6	608	CLA	C4A-NA-C1A	4.67	108.81	106.71
24	7	608	CLA	C4A-NA-C1A	4.67	108.80	106.71
24	B	847	CLA	C4A-NA-C1A	4.66	108.80	106.71
24	B	827	CLA	C4A-NA-C1A	4.66	108.80	106.71
25	c	615	BCR	C33-C5-C6	-4.66	119.30	124.53
24	c	607	CLA	C4A-NA-C1A	4.66	108.80	106.71
24	B	824	CLA	C4A-NA-C1A	4.65	108.80	106.71
26	7	615	DD6	C4-C5-C6	-4.64	120.69	127.31
24	9	302	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
25	A	845	BCR	C15-C14-C13	-4.63	120.70	127.31
25	B	849	BCR	C27-C26-C25	-4.63	116.01	122.73
24	B	802	CLA	C4A-NA-C1A	4.63	108.79	106.71
26	9	314	DD6	C25-C24-C1	-4.61	113.46	126.42
24	1	309	CLA	C4A-NA-C1A	4.60	108.78	106.71
26	2	210	DD6	C9-C10-C11	-4.60	120.74	127.31
25	A	844	BCR	C24-C23-C22	-4.60	119.28	126.23
26	6	613	DD6	C15-C14-C13	-4.60	116.27	125.99
24	2	208	CLA	C4A-NA-C1A	4.59	108.77	106.71
24	k	305	CLA	C4A-NA-C1A	4.59	108.77	106.71
24	F	201	CLA	C4A-NA-C1A	4.59	108.77	106.71
26	c	614	DD6	C9-C10-C11	-4.59	120.76	127.31
24	A	806	CLA	C4A-NA-C1A	4.59	108.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	301	CLA	CMB-C2B-C3B	4.59	133.26	124.68
25	4	618	BCR	C28-C27-C26	-4.58	105.89	114.08
24	k	311	CLA	C4A-NA-C1A	4.58	108.76	106.71
26	9	313	DD6	C3-C2-C1	-4.57	120.79	127.31
24	9	301	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	7	607	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	5	602	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
24	2	201	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
25	c	615	BCR	C11-C10-C9	-4.54	120.83	127.31
26	h	614	DD6	C3-C2-C1	-4.54	120.83	127.31
25	A	845	BCR	C24-C23-C22	-4.54	119.37	126.23
24	A	831	CLA	C4A-NA-C1A	4.54	108.75	106.71
24	4	610	CLA	C4A-NA-C1A	4.54	108.75	106.71
24	9	308	CLA	C4A-NA-C1A	4.53	108.74	106.71
24	7	602	CLA	CAC-C3C-C4C	4.53	130.69	124.81
25	B	841	BCR	C37-C22-C23	4.53	125.22	118.08
25	R	102	BCR	C38-C26-C25	-4.53	119.44	124.53
25	J	101	BCR	C36-C18-C19	4.53	125.21	118.08
30	2	214	LMG	O1-C1-C2	4.53	115.37	108.30
24	c	609	CLA	C1-C2-C3	-4.53	118.21	126.04
24	h	603	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
26	7	615	DD6	C9-C10-C11	-4.53	120.85	127.31
24	8	207	CLA	C4A-NA-C1A	4.52	108.74	106.71
24	A	801	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	A	820	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
24	A	807	CLA	C4A-NA-C1A	4.52	108.74	106.71
24	t	306	CLA	C4A-NA-C1A	4.50	108.73	106.71
24	4	612	CLA	CMB-C2B-C3B	4.50	133.10	124.68
24	A	860	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
26	c	614	DD6	C15-C14-C13	-4.50	116.48	125.99
24	A	803	CLA	C4A-NA-C1A	4.50	108.73	106.71
26	7	618	DD6	C4-C5-C6	-4.49	120.90	127.31
24	A	802	CLA	CMB-C2B-C3B	4.49	133.08	124.68
24	4	607	CLA	C4A-NA-C1A	4.49	108.72	106.71
26	c	613	DD6	C15-C14-C13	-4.49	116.50	125.99
24	A	821	CLA	C4A-NA-C1A	4.49	108.72	106.71
24	A	820	CLA	C4A-NA-C1A	4.48	108.72	106.71
24	A	829	CLA	C4A-NA-C1A	4.48	108.72	106.71
24	8	208	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
24	A	853	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
25	I	102	BCR	C37-C22-C23	4.46	125.10	118.08
24	k	301	CLA	C4A-NA-C1A	4.46	108.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	315	DD6	C9-C10-C11	-4.46	120.95	127.31
25	F	204	BCR	C11-C10-C9	-4.46	120.95	127.31
24	6	611	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
24	t	305	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
25	A	846	BCR	C37-C22-C23	4.46	125.10	118.08
24	A	809	CLA	C4A-NA-C1A	4.45	108.71	106.71
24	5	601	CLA	C4A-NA-C1A	4.45	108.70	106.71
24	t	307	CLA	C4A-NA-C1A	4.45	108.70	106.71
24	A	825	CLA	C4A-NA-C1A	4.44	108.70	106.71
24	A	847	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
26	3	312	DD6	C14-C13-C11	-4.44	118.65	125.53
24	4	603	CLA	C4A-NA-C1A	4.44	108.70	106.71
25	I	101	BCR	C4-C5-C6	-4.43	116.29	122.73
24	A	828	CLA	C4A-NA-C1A	4.43	108.70	106.71
24	A	819	CLA	C4A-NA-C1A	4.43	108.70	106.71
25	F	204	BCR	C7-C8-C9	-4.42	119.55	126.23
26	4	616	DD6	O1-C20-C19	-4.42	110.06	113.38
24	A	801	CLA	C1D-ND-C4D	-4.42	103.20	106.33
24	A	818	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
24	6	604	CLA	C4A-NA-C1A	4.41	108.69	106.71
24	7	611	CLA	C4A-NA-C1A	4.41	108.69	106.71
26	3	312	DD6	C9-C10-C11	-4.41	121.01	127.31
26	1	312	DD6	C9-C10-C11	-4.40	121.03	127.31
24	c	611	CLA	C4A-NA-C1A	4.40	108.68	106.71
25	1	310	BCR	C28-C27-C26	-4.40	106.23	114.08
26	A	848	DD6	C9-C10-C11	-4.40	121.04	127.31
24	A	824	CLA	C4A-NA-C1A	4.39	108.68	106.71
24	L	204	CLA	C4A-NA-C1A	4.39	108.68	106.71
25	4	618	BCR	C15-C14-C13	-4.39	121.05	127.31
26	7	613	DD6	C15-C14-C13	-4.38	116.73	125.99
24	6	602	CLA	C4A-NA-C1A	4.38	108.67	106.71
25	A	843	BCR	C16-C17-C18	-4.38	121.06	127.31
25	A	845	BCR	C8-C7-C6	-4.37	119.61	127.09
25	A	844	BCR	C15-C14-C13	-4.37	121.07	127.31
26	7	618	DD6	C3-C2-C1	-4.37	121.07	127.31
25	1	314	BCR	C33-C5-C6	-4.37	119.62	124.53
24	4	605	CLA	C4A-NA-C1A	4.36	108.66	106.71
24	c	603	CLA	C4A-NA-C1A	4.36	108.66	106.71
24	4	604	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
28	A	842	LHG	O7-C7-C8	4.34	120.86	111.50
26	k	314	DD6	C4-C5-C6	-4.34	121.11	127.31
28	I	103	LHG	O7-C7-C8	4.34	120.85	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	602	CLA	CMB-C2B-C3B	4.34	132.79	124.68
24	5	605	CLA	C4A-NA-C1A	4.34	108.66	106.71
25	A	844	BCR	C11-C10-C9	-4.33	121.13	127.31
24	A	840	CLA	C4A-NA-C1A	4.33	108.65	106.71
24	B	819	CLA	C4A-NA-C1A	4.33	108.65	106.71
24	k	311	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	B	849	BCR	C37-C22-C23	4.32	124.88	118.08
24	7	603	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
24	h	604	CLA	C4A-NA-C1A	4.30	108.64	106.71
24	7	608	CLA	CMB-C2B-C3B	4.30	132.73	124.68
25	R	102	BCR	C37-C22-C23	4.30	124.84	118.08
24	A	827	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
24	A	824	CLA	CMB-C2B-C1B	-4.29	121.86	128.46
26	4	617	DD6	C3-C2-C1	-4.29	121.19	127.31
24	t	303	CLA	CMB-C2B-C3B	4.28	132.69	124.68
25	A	859	BCR	C20-C21-C22	-4.28	121.20	127.31
24	h	611	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
24	2	205	CLA	C4A-NA-C1A	4.27	108.63	106.71
24	A	827	CLA	C4A-NA-C1A	4.27	108.63	106.71
25	M	101	BCR	C24-C23-C22	-4.27	119.79	126.23
25	k	316	BCR	C3-C4-C5	-4.26	106.47	114.08
24	1	303	CLA	C4A-NA-C1A	4.26	108.62	106.71
24	B	804	CLA	CMB-C2B-C3B	4.25	132.63	124.68
24	B	818	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
26	8	211	DD6	C4-C5-C6	-4.24	121.25	127.31
25	B	843	BCR	C33-C5-C4	4.24	121.77	113.62
24	3	303	CLA	C4A-NA-C1A	4.24	108.61	106.71
26	8	212	DD6	C15-C14-C13	-4.24	117.03	125.99
24	L	205	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
25	A	844	BCR	C20-C21-C22	-4.24	121.26	127.31
24	A	857	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
24	1	301	CLA	C4A-NA-C1A	4.23	108.61	106.71
28	1	318	LHG	C5-O7-C7	-4.23	107.38	117.79
24	B	831	CLA	C4A-NA-C1A	4.23	108.61	106.71
24	7	601	CLA	C4A-NA-C1A	4.23	108.61	106.71
27	3	314	LMT	C1-O1'-C1'	4.22	120.84	113.84
24	8	209	CLA	C4A-NA-C1A	4.21	108.60	106.71
24	A	856	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
24	B	846	CLA	C4A-NA-C1A	4.21	108.60	106.71
24	F	202	CLA	C4A-NA-C1A	4.20	108.59	106.71
24	B	817	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
26	c	613	DD6	C4-C5-C6	-4.19	121.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	105	LHG	O7-C7-C8	4.18	120.52	111.50
25	A	845	BCR	C16-C17-C18	-4.18	121.34	127.31
24	h	609	CLA	C4A-NA-C1A	4.18	108.58	106.71
25	B	840	BCR	C16-C17-C18	-4.17	121.36	127.31
24	B	835	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
25	2	211	BCR	C28-C27-C26	-4.16	106.64	114.08
24	2	201	CLA	CMB-C2B-C3B	4.16	132.47	124.68
26	R	105	DD6	C3-C2-C1	-4.16	121.37	127.31
24	B	833	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
24	c	606	CLA	C4A-NA-C1A	4.16	108.58	106.71
24	4	606	CLA	C4A-NA-C1A	4.15	108.57	106.71
25	I	101	BCR	C3-C4-C5	-4.15	106.66	114.08
25	A	846	BCR	C1-C6-C5	-4.15	116.77	122.61
26	h	613	DD6	C15-C14-C13	-4.15	117.22	125.99
24	8	201	CLA	C4A-NA-C1A	4.15	108.57	106.71
24	c	601	CLA	C4A-NA-C1A	4.15	108.57	106.71
25	J	104	BCR	C37-C22-C23	4.14	124.61	118.08
25	I	102	BCR	C4-C5-C6	-4.14	116.72	122.73
25	B	849	BCR	C16-C17-C18	-4.14	121.40	127.31
25	B	840	BCR	C20-C21-C22	-4.14	121.40	127.31
24	1	307	CLA	C4A-NA-C1A	4.14	108.57	106.71
26	h	614	DD6	C4-C5-C6	-4.14	121.41	127.31
25	1	314	BCR	C7-C8-C9	-4.14	119.99	126.23
24	7	602	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
24	9	304	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
24	c	604	CLA	C4A-NA-C1A	4.13	108.56	106.71
24	8	206	CLA	C4A-NA-C1A	4.12	108.56	106.71
24	B	813	CLA	C4A-NA-C1A	4.12	108.56	106.71
24	8	202	CLA	C4A-NA-C1A	4.11	108.56	106.71
26	2	212	DD6	C4-C5-C6	-4.11	121.45	127.31
24	9	311	CLA	CMB-C2B-C3B	4.11	132.36	124.68
24	B	805	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
26	7	613	DD6	C4-C5-C6	-4.10	121.45	127.31
25	B	843	BCR	C38-C26-C25	-4.10	119.92	124.53
24	h	605	CLA	C4A-NA-C1A	4.10	108.55	106.71
25	A	844	BCR	C33-C5-C6	-4.10	119.92	124.53
24	A	853	CLA	C4A-NA-C1A	4.10	108.55	106.71
24	A	826	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	8	213	LHG	O7-C7-C8	4.10	120.33	111.50
24	4	611	CLA	C4A-NA-C1A	4.09	108.55	106.71
24	c	609	CLA	C4A-NA-C1A	4.09	108.54	106.71
25	R	102	BCR	C23-C24-C25	-4.08	115.73	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	609	CLA	C4A-NA-C1A	4.08	108.54	106.71
24	A	847	CLA	C4A-NA-C1A	4.08	108.54	106.71
25	1	310	BCR	C33-C5-C6	-4.08	119.94	124.53
28	B	844	LHG	O7-C7-C8	4.08	120.30	111.50
26	k	315	DD6	C9-C10-C11	-4.08	121.49	127.31
24	3	307	CLA	C4A-NA-C1A	4.08	108.54	106.71
24	4	602	CLA	C4A-NA-C1A	4.08	108.54	106.71
24	A	805	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
24	J	103	CLA	C4A-NA-C1A	4.07	108.54	106.71
24	2	207	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
28	B	845	LHG	O7-C7-C8	4.07	120.27	111.50
24	A	801	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
25	J	101	BCR	C15-C14-C13	-4.07	121.51	127.31
24	1	308	CLA	C4A-NA-C1A	4.06	108.53	106.71
24	B	808	CLA	C4A-NA-C1A	4.05	108.53	106.71
25	I	102	BCR	C36-C18-C19	4.05	124.46	118.08
28	1	318	LHG	O7-C7-C8	4.05	120.23	111.50
24	B	816	CLA	O2D-CGD-O1D	-4.05	115.93	123.84
26	R	105	DD6	C4-C5-C6	-4.05	121.54	127.31
26	9	314	DD6	C24-C1-C2	4.04	125.15	118.94
26	9	314	DD6	C25-C26-C27	-4.04	114.84	126.58
24	B	823	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
26	7	615	DD6	C15-C14-C13	-4.04	117.46	125.99
24	A	838	CLA	C4A-NA-C1A	4.04	108.52	106.71
24	B	816	CLA	C4A-NA-C1A	4.04	108.52	106.71
24	h	602	CLA	C4A-NA-C1A	4.03	108.52	106.71
24	7	610	CLA	C4A-NA-C1A	4.03	108.52	106.71
24	A	810	CLA	C4A-NA-C1A	4.03	108.52	106.71
24	h	607	CLA	C4A-NA-C1A	4.03	108.52	106.71
25	k	316	BCR	C38-C26-C25	-4.02	120.01	124.53
24	5	607	CLA	C4A-NA-C1A	4.02	108.52	106.71
26	1	312	DD6	C4-C5-C6	-4.02	121.57	127.31
24	8	205	CLA	C4A-NA-C1A	4.02	108.51	106.71
24	9	305	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
24	2	203	CLA	C4A-NA-C1A	4.01	108.51	106.71
24	9	311	CLA	C4A-NA-C1A	4.01	108.51	106.71
24	7	607	CLA	CMB-C2B-C3B	4.01	132.18	124.68
24	5	602	CLA	CMB-C2B-C3B	4.01	132.18	124.68
25	B	842	BCR	C15-C14-C13	-4.01	121.59	127.31
24	B	825	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
24	3	308	CLA	C4A-NA-C1A	4.00	108.51	106.71
24	A	823	CLA	C4A-NA-C1A	4.00	108.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	856	CLA	C4A-NA-C1A	4.00	108.51	106.71
30	t	314	LMG	O7-C10-C11	4.00	120.13	111.50
24	3	306	CLA	C4A-NA-C1A	4.00	108.50	106.71
24	9	301	CLA	CMB-C2B-C3B	4.00	132.16	124.68
24	k	308	CLA	C4A-NA-C1A	4.00	108.50	106.71
24	c	605	CLA	C4A-NA-C1A	3.99	108.50	106.71
24	B	824	CLA	C4-C3-C5	3.99	121.99	115.27
25	A	846	BCR	C36-C18-C19	3.99	124.36	118.08
24	h	608	CLA	C4A-NA-C1A	3.99	108.50	106.71
24	k	304	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
24	R	104	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
25	L	202	BCR	C37-C22-C23	3.98	124.35	118.08
24	h	612	CLA	C4A-NA-C1A	3.98	108.50	106.71
24	A	803	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
26	7	616	DD6	C14-C13-C11	-3.98	119.36	125.53
24	B	816	CLA	O2D-CGD-CBD	3.98	118.33	111.27
24	7	603	CLA	C4A-NA-C1A	3.97	108.49	106.71
24	A	853	CLA	CMB-C2B-C3B	3.97	132.11	124.68
25	L	206	BCR	C38-C26-C27	3.96	121.23	113.62
24	B	829	CLA	CMB-C2B-C3B	3.96	132.09	124.68
26	h	614	DD6	C15-C14-C13	-3.96	117.62	125.99
24	h	603	CLA	CMB-C2B-C3B	3.96	132.09	124.68
24	9	302	CLA	CMB-C2B-C3B	3.95	132.07	124.68
25	I	101	BCR	C30-C25-C26	-3.95	117.05	122.61
25	k	316	BCR	C24-C23-C22	-3.95	120.27	126.23
24	4	613	CLA	C4A-NA-C1A	3.95	108.48	106.71
25	7	617	BCR	C33-C5-C6	-3.95	120.10	124.53
25	R	102	BCR	C28-C27-C26	-3.94	107.04	114.08
24	A	836	CLA	C4A-NA-C1A	3.94	108.48	106.71
24	6	605	CLA	C4A-NA-C1A	3.94	108.48	106.71
26	h	616	DD6	C3-C2-C1	-3.94	121.69	127.31
26	5	609	DD6	C9-C10-C11	-3.94	121.69	127.31
30	A	855	LMG	O7-C10-C11	3.94	119.98	111.50
24	h	606	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
28	A	849	LHG	O7-C7-C8	3.93	119.97	111.50
24	3	308	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
24	8	208	CLA	CMB-C2B-C3B	3.93	132.03	124.68
24	A	818	CLA	C4A-NA-C1A	3.93	108.47	106.71
24	B	811	CLA	C4A-NA-C1A	3.93	108.47	106.71
25	R	102	BCR	C34-C9-C8	-3.93	111.89	118.08
24	A	856	CLA	CMB-C2B-C3B	3.92	132.02	124.68
25	L	206	BCR	C16-C17-C18	-3.92	121.72	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	618	BCR	C11-C10-C9	-3.92	121.72	127.31
26	8	210	DD6	C9-C10-C11	-3.92	121.72	127.31
26	J	102	DD6	C4-C5-C6	-3.91	121.72	127.31
26	5	609	DD6	C15-C14-C13	-3.91	117.72	125.99
25	t	312	BCR	C11-C10-C9	-3.91	121.72	127.31
24	k	303	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	9	316	BCR	C28-C27-C26	-3.91	107.09	114.08
25	I	101	BCR	C20-C21-C22	-3.91	121.73	127.31
25	L	206	BCR	C27-C26-C25	-3.91	117.05	122.73
25	L	206	BCR	C20-C21-C22	-3.91	121.73	127.31
24	k	306	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
24	B	828	CLA	C4A-NA-C1A	3.90	108.46	106.71
25	J	104	BCR	C16-C17-C18	-3.90	121.74	127.31
24	8	206	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	8	211	DD6	O1-C20-C19	-3.90	110.45	113.38
26	6	616	DD6	C4-C5-C6	-3.90	121.74	127.31
24	7	606	CLA	CMB-C2B-C3B	3.90	131.97	124.68
25	B	840	BCR	C37-C22-C23	3.89	124.21	118.08
25	A	843	BCR	C7-C8-C9	-3.89	120.35	126.23
24	9	309	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
25	L	206	BCR	C7-C8-C9	-3.89	120.36	126.23
25	B	841	BCR	C7-C8-C9	-3.89	120.36	126.23
30	2	214	LMG	O7-C10-C11	3.89	119.88	111.50
24	1	317	CLA	C4A-NA-C1A	3.89	108.45	106.71
24	9	303	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
24	B	806	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
24	7	611	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
24	A	847	CLA	CMB-C2B-C3B	3.88	131.94	124.68
25	c	615	BCR	C3-C4-C5	-3.88	107.14	114.08
26	4	617	DD6	C9-C10-C11	-3.88	121.77	127.31
24	c	607	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
25	9	316	BCR	C24-C23-C22	-3.88	120.37	126.23
24	h	612	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
26	7	618	DD6	O1-C20-C19	-3.88	110.47	113.38
26	6	614	DD6	C3-C2-C1	-3.88	121.78	127.31
25	A	843	BCR	C20-C21-C22	-3.88	121.78	127.31
24	A	834	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
25	t	312	BCR	C7-C8-C9	-3.87	120.38	126.23
24	7	604	CLA	CMB-C2B-C3B	3.87	131.92	124.68
24	3	303	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
24	t	305	CLA	C4A-NA-C1A	3.86	108.44	106.71
26	t	313	DD6	C4-C5-C6	-3.86	121.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	829	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
24	A	822	CLA	C4A-NA-C1A	3.86	108.44	106.71
24	t	302	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
24	6	611	CLA	CMB-C2B-C3B	3.85	131.89	124.68
24	9	307	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
24	2	202	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
24	B	813	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
24	B	824	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
24	7	602	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
25	I	101	BCR	C37-C22-C23	3.85	124.14	118.08
26	6	617	DD6	C9-C10-C11	-3.85	121.82	127.31
25	B	843	BCR	C20-C21-C22	-3.84	121.82	127.31
24	A	827	CLA	CMB-C2B-C3B	3.84	131.87	124.68
24	k	302	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	I	101	BCR	C16-C17-C18	-3.84	121.83	127.31
25	J	104	BCR	C27-C26-C25	-3.84	117.16	122.73
24	k	309	CLA	C4A-NA-C1A	3.83	108.43	106.71
24	c	610	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
26	4	614	DD6	C15-C14-C13	-3.83	117.89	125.99
24	9	310	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	R	102	BCR	C36-C18-C19	3.83	124.11	118.08
24	B	812	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
24	k	311	CLA	CMB-C2B-C3B	3.82	131.83	124.68
24	B	836	CLA	C4A-NA-C1A	3.82	108.42	106.71
26	h	616	DD6	C15-C14-C13	-3.82	117.91	125.99
25	k	316	BCR	C7-C8-C9	-3.81	120.48	126.23
24	c	611	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
24	B	832	CLA	C4A-NA-C1A	3.81	108.42	106.71
25	R	101	BCR	C37-C22-C23	3.81	124.07	118.08
25	A	859	BCR	C16-C17-C18	-3.80	121.88	127.31
24	B	815	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
25	B	840	BCR	C7-C8-C9	-3.80	120.49	126.23
24	3	309	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
25	A	859	BCR	C37-C22-C23	3.80	124.06	118.08
25	A	843	BCR	C33-C5-C6	-3.79	120.27	124.53
25	I	102	BCR	C20-C21-C22	-3.79	121.89	127.31
26	4	616	DD6	C15-C14-C13	-3.79	117.98	125.99
25	I	101	BCR	C33-C5-C4	3.79	120.89	113.62
24	A	802	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
24	B	804	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
26	4	614	DD6	C34-C35-C36	-3.79	104.31	111.85
25	J	101	BCR	C16-C17-C18	-3.78	121.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	312	BCR	C33-C5-C6	-3.78	120.28	124.53
28	2	215	LHG	O7-C7-C8	3.78	119.65	111.50
24	t	305	CLA	CMB-C2B-C3B	3.78	131.74	124.68
24	t	303	CLA	C4A-NA-C1A	3.77	108.40	106.71
24	A	860	CLA	CMB-C2B-C3B	3.77	131.74	124.68
26	4	615	DD6	C14-C13-C11	-3.76	119.69	125.53
24	7	612	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
24	4	603	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
25	J	101	BCR	C37-C22-C23	3.76	124.00	118.08
24	7	606	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
24	A	802	CLA	C4A-NA-C1A	3.75	108.39	106.71
24	3	305	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
26	1	313	DD6	C15-C14-C13	-3.75	118.06	125.99
24	B	814	CLA	CMB-C2B-C3B	3.75	131.69	124.68
25	A	843	BCR	C27-C26-C25	-3.75	117.29	122.73
25	J	104	BCR	C4-C5-C6	-3.75	117.29	122.73
26	7	618	DD6	C9-C10-C11	-3.75	121.96	127.31
25	1	310	BCR	C15-C14-C13	-3.74	121.97	127.31
26	6	613	DD6	C4-C5-C6	-3.74	121.97	127.31
24	4	611	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
24	B	817	CLA	CMB-C2B-C3B	3.74	131.67	124.68
24	B	836	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	2	211	BCR	C38-C26-C25	-3.73	120.33	124.53
24	A	857	CLA	CMB-C2B-C3B	3.73	131.66	124.68
24	2	203	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
28	4	619	LHG	O7-C7-C8	3.73	119.54	111.50
24	B	822	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
24	6	606	CLA	C4A-NA-C1A	3.73	108.38	106.71
24	h	603	CLA	C4A-NA-C1A	3.73	108.38	106.71
25	2	211	BCR	C11-C10-C9	-3.73	121.99	127.31
26	c	614	DD6	C25-C26-C27	-3.72	115.77	126.58
24	A	814	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
24	3	301	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	F	204	BCR	C16-C17-C18	-3.72	122.00	127.31
28	8	213	LHG	C5-O7-C7	-3.72	108.64	117.79
25	R	101	BCR	C38-C26-C25	-3.72	120.36	124.53
24	6	605	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	A	846	BCR	C20-C21-C22	-3.71	122.01	127.31
26	h	615	DD6	C14-C13-C11	-3.71	119.77	125.53
24	A	824	CLA	CMB-C2B-C3B	3.71	131.62	124.68
24	t	309	CLA	C4A-NA-C1A	3.71	108.37	106.71
26	2	212	DD6	C15-C14-C13	-3.71	118.15	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	820	CLA	CMB-C2B-C3B	3.71	131.62	124.68
24	A	828	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	1	302	CLA	C4A-NA-C1A	3.71	108.37	106.71
24	A	811	CLA	C4A-NA-C1A	3.71	108.37	106.71
28	A	852	LHG	O7-C7-C8	3.71	119.49	111.50
24	B	804	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
24	2	205	CLA	CMB-C2B-C3B	3.71	131.61	124.68
30	2	214	LMG	C7-O1-C1	-3.71	106.50	113.74
25	1	314	BCR	C24-C23-C22	-3.70	120.64	126.23
26	3	312	DD6	O1-C20-C19	-3.70	110.60	113.38
24	A	830	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
26	6	615	DD6	C14-C13-C11	-3.70	119.79	125.53
24	7	603	CLA	CMB-C2B-C3B	3.70	131.59	124.68
26	6	613	DD6	C9-C10-C11	-3.69	122.04	127.31
24	B	827	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
25	B	841	BCR	C11-C10-C9	-3.69	122.04	127.31
25	t	312	BCR	C15-C14-C13	-3.69	122.04	127.31
24	3	305	CLA	C4A-NA-C1A	3.69	108.36	106.71
26	9	313	DD6	O1-C20-C19	-3.69	110.61	113.38
25	9	316	BCR	C33-C5-C6	-3.69	120.39	124.53
25	I	101	BCR	C36-C18-C19	3.69	123.89	118.08
25	A	843	BCR	C37-C22-C23	3.68	123.88	118.08
24	7	602	CLA	CMB-C2B-C3B	3.68	131.57	124.68
25	L	206	BCR	C37-C22-C23	3.68	123.87	118.08
24	A	826	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
24	4	607	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	I	102	BCR	C16-C17-C18	-3.67	122.07	127.31
24	3	307	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	A	840	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	B	834	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
25	F	204	BCR	C38-C26-C25	-3.67	120.41	124.53
24	A	821	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
24	6	603	CLA	C4A-NA-C1A	3.67	108.35	106.71
24	k	308	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
26	7	616	DD6	C4-C5-C6	-3.66	122.08	127.31
26	k	313	DD6	C14-C13-C11	-3.66	119.85	125.53
26	6	614	DD6	C4-C5-C6	-3.66	122.08	127.31
26	k	313	DD6	C4-C5-C6	-3.66	122.09	127.31
26	t	313	DD6	C15-C14-C13	-3.66	118.26	125.99
24	B	814	CLA	C4A-NA-C1A	3.65	108.35	106.71
24	c	607	CLA	CMB-C2B-C3B	3.65	131.51	124.68
26	t	313	DD6	C9-C10-C11	-3.65	122.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	306	CLA	C4A-NA-C1A	3.65	108.35	106.71
24	9	304	CLA	CMB-C2B-C3B	3.65	131.51	124.68
24	4	612	CLA	C4A-NA-C1A	3.65	108.35	106.71
24	t	302	CLA	C4A-NA-C1A	3.65	108.35	106.71
24	2	207	CLA	CMB-C2B-C3B	3.65	131.50	124.68
24	A	818	CLA	CMB-C2B-C3B	3.64	131.49	124.68
24	3	306	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
24	h	611	CLA	CMB-C2B-C3B	3.64	131.48	124.68
25	R	101	BCR	C16-C17-C18	-3.64	122.12	127.31
24	8	202	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
24	c	608	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	3	311	DD6	C9-C10-C11	-3.63	122.13	127.31
25	B	840	BCR	C36-C18-C19	3.63	123.80	118.08
24	5	607	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	A	859	BCR	C7-C8-C9	-3.63	120.75	126.23
24	h	602	CLA	C6-C5-C3	3.63	122.97	113.45
24	t	304	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
24	c	606	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	R	101	BCR	C20-C21-C22	-3.63	122.14	127.31
24	B	829	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
26	2	210	DD6	C15-C14-C13	-3.62	118.33	125.99
25	A	846	BCR	C16-C17-C18	-3.62	122.14	127.31
26	8	212	DD6	C9-C10-C11	-3.62	122.14	127.31
25	J	101	BCR	C33-C5-C4	3.62	120.57	113.62
24	t	309	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
24	2	209	CLA	C4A-NA-C1A	3.62	108.33	106.71
24	L	205	CLA	CMB-C2B-C3B	3.62	131.45	124.68
26	7	615	DD6	C14-C13-C11	-3.62	119.92	125.53
24	B	826	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
24	6	603	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
24	B	810	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
24	4	606	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
24	2	201	CLA	C4A-NA-C1A	3.61	108.33	106.71
26	R	105	DD6	C12-C11-C10	-3.61	117.87	122.92
25	1	314	BCR	C15-C14-C13	-3.60	122.17	127.31
28	L	201	LHG	O7-C7-C8	3.60	119.26	111.50
26	c	614	DD6	C34-C35-C36	-3.60	104.68	111.85
25	A	846	BCR	C27-C26-C25	-3.60	117.50	122.73
24	F	203	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
24	3	307	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
26	8	210	DD6	C13-C11-C10	3.58	124.44	118.94
24	A	813	CLA	C4A-NA-C1A	3.58	108.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	BCR	C38-C26-C27	3.58	120.49	113.62
24	B	809	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
24	h	604	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
24	c	603	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
24	A	860	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
24	4	601	CLA	C4A-NA-C1A	3.57	108.31	106.71
24	B	823	CLA	CMB-C2B-C3B	3.57	131.36	124.68
25	F	204	BCR	C20-C21-C22	-3.57	122.21	127.31
24	B	803	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	I	101	BCR	C1-C6-C5	-3.57	117.59	122.61
24	A	809	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
24	5	604	CLA	C4A-NA-C1A	3.57	108.31	106.71
24	c	602	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
24	B	823	CLA	C4A-NA-C1A	3.56	108.31	106.71
24	A	826	CLA	CMB-C2B-C3B	3.56	131.34	124.68
25	J	104	BCR	C7-C8-C9	-3.56	120.85	126.23
26	9	315	DD6	C14-C13-C11	-3.56	120.00	125.53
24	2	209	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
25	B	840	BCR	C30-C25-C26	-3.56	117.60	122.61
24	t	306	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
24	A	856	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
24	F	202	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
24	B	821	CLA	C4A-NA-C1A	3.56	108.31	106.71
25	B	841	BCR	C36-C18-C19	3.56	123.68	118.08
24	B	824	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	B	818	CLA	C4A-NA-C1A	3.55	108.30	106.71
24	R	103	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	9	316	BCR	C38-C26-C25	-3.55	120.54	124.53
24	A	829	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
24	k	301	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
24	9	306	CLA	C4A-NA-C1A	3.55	108.30	106.71
24	k	303	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
26	c	614	DD6	O1-C20-C21	3.55	119.31	115.06
25	A	845	BCR	C38-C26-C25	-3.55	120.55	124.53
24	B	835	CLA	CMB-C2B-C3B	3.55	131.31	124.68
24	A	813	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
24	A	816	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
26	9	314	DD6	C-C1-C2	-3.55	117.96	122.92
24	R	104	CLA	CMB-C2B-C3B	3.55	131.31	124.68
24	9	308	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
24	h	609	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	c	614	DD6	C21-C20-C15	-3.54	116.33	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	104	BCR	C36-C18-C19	3.54	123.66	118.08
25	M	101	BCR	C7-C8-C9	-3.54	120.89	126.23
29	7	614	A1L1G	O15-C20-C21	-3.54	110.72	113.38
25	A	859	BCR	C24-C23-C22	-3.54	120.89	126.23
25	I	101	BCR	C38-C26-C27	3.53	120.41	113.62
26	1	311	DD6	C15-C14-C13	-3.53	118.52	125.99
25	A	843	BCR	C33-C5-C4	3.53	120.40	113.62
24	B	833	CLA	CMB-C2B-C3B	3.53	131.28	124.68
24	B	825	CLA	CMB-C2B-C3B	3.53	131.28	124.68
24	1	306	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
24	A	831	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
24	A	816	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
26	h	615	DD6	C9-C10-C11	-3.53	122.28	127.31
24	B	811	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
24	h	610	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
25	B	843	BCR	C33-C5-C6	-3.52	120.57	124.53
26	2	210	DD6	C4-C5-C6	-3.52	122.28	127.31
24	1	303	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
25	M	101	BCR	C28-C27-C26	-3.52	107.79	114.08
25	A	846	BCR	C4-C5-C6	-3.52	117.62	122.73
24	A	803	CLA	CMB-C2B-C3B	3.52	131.26	124.68
24	A	833	CLA	C4A-NA-C1A	3.52	108.29	106.71
25	J	104	BCR	C20-C21-C22	-3.52	122.29	127.31
25	k	316	BCR	C16-C17-C18	-3.51	122.29	127.31
26	k	313	DD6	C9-C10-C11	-3.51	122.29	127.31
24	5	604	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
26	c	613	DD6	C9-C10-C11	-3.51	122.30	127.31
28	A	841	LHG	O7-C7-C8	3.51	119.07	111.50
26	c	614	DD6	C25-C24-C1	-3.51	116.55	126.42
24	t	308	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
24	9	306	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
25	A	859	BCR	C36-C18-C19	3.51	123.60	118.08
26	9	314	DD6	O1-C20-C19	-3.51	110.75	113.38
24	1	301	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
24	B	805	CLA	CMB-C2B-C3B	3.51	131.24	124.68
24	B	810	CLA	CAB-C3B-C4B	-3.51	123.08	128.46
24	A	805	CLA	CMB-C2B-C3B	3.51	131.24	124.68
24	A	830	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	2	211	BCR	C21-C20-C19	-3.50	112.29	123.22
24	1	317	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
28	A	842	LHG	C10-C9-C8	-3.50	100.60	113.19
24	B	817	CLA	C4A-NA-C1A	3.50	108.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	834	CLA	C4A-NA-C1A	3.50	108.28	106.71
24	L	204	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
25	I	101	BCR	C7-C8-C9	-3.50	120.94	126.23
24	B	827	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
24	h	605	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	B	841	BCR	C3-C4-C5	-3.50	107.83	114.08
25	B	849	BCR	C20-C21-C22	-3.50	122.32	127.31
24	9	309	CLA	CMB-C2B-C3B	3.50	131.22	124.68
25	L	202	BCR	C34-C9-C10	-3.50	118.03	122.92
25	B	843	BCR	C4-C5-C6	-3.49	117.66	122.73
26	9	317	DD6	C25-C24-C1	-3.49	116.60	126.42
26	5	608	DD6	C9-C10-C11	-3.49	122.33	127.31
25	B	849	BCR	C36-C18-C19	3.49	123.57	118.08
28	8	213	LHG	O8-C23-C24	3.48	122.84	111.91
24	h	608	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	J	101	BCR	C20-C21-C22	-3.48	122.34	127.31
24	B	807	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	R	101	BCR	C36-C18-C19	3.48	123.56	118.08
24	8	209	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
24	B	801	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
24	B	826	CLA	C4A-NA-C1A	3.48	108.27	106.71
24	3	308	CLA	CMB-C2B-C3B	3.48	131.18	124.68
26	4	614	DD6	C9-C10-C11	-3.47	122.35	127.31
25	F	204	BCR	C33-C5-C6	-3.47	120.63	124.53
25	c	615	BCR	C20-C19-C18	-3.47	116.67	126.42
24	c	605	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
26	k	314	DD6	O1-C20-C19	-3.46	110.78	113.38
24	8	206	CLA	CMB-C2B-C3B	3.46	131.15	124.68
24	A	807	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
24	6	604	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
24	A	825	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
24	9	307	CLA	CMB-C2B-C3B	3.45	131.14	124.68
25	L	206	BCR	C36-C18-C19	3.45	123.52	118.08
24	k	303	CLA	C4-C3-C5	3.45	121.08	115.27
25	k	316	BCR	C28-C27-C26	-3.45	107.92	114.08
25	1	310	BCR	C20-C21-C22	-3.45	122.39	127.31
26	6	616	DD6	O1-C20-C19	-3.45	110.79	113.38
25	R	102	BCR	C20-C21-C22	-3.45	122.39	127.31
24	B	831	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
26	4	617	DD6	C4-C3-C2	-3.45	116.42	123.47
26	8	210	DD6	C4-C5-C6	-3.44	122.39	127.31
24	B	815	CLA	C4A-NA-C1A	3.44	108.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	102	BCR	C31-C1-C6	-3.44	104.72	110.30
24	7	606	CLA	O2D-CGD-CBD	3.44	117.38	111.27
24	A	838	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
24	k	309	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
24	5	607	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	B	842	BCR	C33-C5-C6	-3.44	120.67	124.53
25	4	618	BCR	C3-C4-C5	-3.44	107.94	114.08
25	k	316	BCR	C15-C16-C17	-3.43	116.44	123.47
25	2	211	BCR	C33-C5-C6	-3.43	120.67	124.53
24	B	812	CLA	CMB-C2B-C3B	3.43	131.10	124.68
24	A	811	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
24	h	606	CLA	C4A-NA-C1A	3.43	108.25	106.71
25	1	310	BCR	C38-C26-C27	3.43	120.20	113.62
24	6	607	CLA	C4A-NA-C1A	3.43	108.25	106.71
24	c	604	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
24	B	813	CLA	CMB-C2B-C3B	3.42	131.08	124.68
24	B	818	CLA	CMB-C2B-C3B	3.42	131.08	124.68
24	5	606	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	t	311	DD6	C4-C5-C6	-3.42	122.44	127.31
24	4	610	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	3	311	DD6	C4-C5-C6	-3.41	122.44	127.31
24	k	303	CLA	CMB-C2B-C3B	3.41	131.06	124.68
24	h	612	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	L	202	BCR	C36-C18-C19	3.41	123.45	118.08
25	1	310	BCR	C11-C10-C9	-3.41	122.44	127.31
29	k	312	A1L1G	C43-C44-C42	-3.41	118.15	122.92
26	7	618	DD6	C14-C13-C11	-3.41	120.25	125.53
26	4	615	DD6	C9-C10-C11	-3.41	122.45	127.31
29	9	312	A1L1G	C43-C44-C42	-3.41	118.15	122.92
24	4	609	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
24	J	103	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
24	B	815	CLA	CMB-C2B-C3B	3.40	131.04	124.68
24	c	601	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	A	846	BCR	C33-C5-C4	3.40	120.14	113.62
24	c	610	CLA	CMB-C2B-C3B	3.40	131.03	124.68
26	t	311	DD6	C15-C14-C13	-3.39	118.82	125.99
26	8	211	DD6	C9-C10-C11	-3.39	122.47	127.31
24	t	310	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
24	A	847	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
25	J	101	BCR	C15-C16-C17	-3.39	116.53	123.47
24	1	302	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
24	B	808	CLA	O2D-CGD-O1D	-3.39	117.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	202	BCR	C7-C8-C9	-3.39	121.12	126.23
24	1	304	CLA	C4A-NA-C1A	3.39	108.23	106.71
24	6	612	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
24	1	309	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	B	820	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	k	306	CLA	CMB-C2B-C3B	3.38	131.00	124.68
25	R	101	BCR	C38-C26-C27	3.38	120.11	113.62
24	5	605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	7	601	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	7	609	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
24	5	601	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
25	R	102	BCR	C11-C10-C9	-3.37	122.50	127.31
25	2	211	BCR	C7-C8-C9	-3.37	121.14	126.23
24	4	604	CLA	C4A-NA-C1A	3.37	108.22	106.71
24	B	819	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
26	6	616	DD6	C21-C20-C15	-3.37	116.62	122.26
26	7	613	DD6	C25-C26-C27	-3.37	116.81	126.58
25	B	849	BCR	C16-C15-C14	-3.37	116.58	123.47
24	9	306	CLA	CHB-C4A-NA	3.37	129.17	124.51
24	6	608	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
24	A	837	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
24	6	601	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	B	843	BCR	C11-C12-C13	-3.36	116.97	126.42
24	4	604	CLA	CMB-C2B-C3B	3.36	130.97	124.68
24	c	609	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
24	A	833	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	A	845	BCR	C28-C27-C26	-3.35	108.09	114.08
25	A	843	BCR	C36-C18-C19	3.35	123.36	118.08
25	c	615	BCR	C23-C22-C21	3.35	124.08	118.94
25	B	841	BCR	C20-C21-C22	-3.35	122.53	127.31
25	F	204	BCR	C24-C23-C22	-3.35	121.17	126.23
24	2	206	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
24	4	613	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
24	t	302	CLA	CMB-C2B-C3B	3.35	130.94	124.68
24	A	822	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
24	B	806	CLA	CMB-C2B-C3B	3.34	130.93	124.68
25	2	211	BCR	C38-C26-C27	3.34	120.04	113.62
26	h	613	DD6	C4-C5-C6	-3.34	122.54	127.31
24	A	803	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
24	h	606	CLA	CMB-C2B-C3B	3.34	130.93	124.68
24	A	812	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	7	605	CLA	CMB-C2B-C1B	-3.34	123.33	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	602	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	7	612	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	6	606	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
26	2	210	DD6	C14-C13-C11	-3.33	120.36	125.53
24	9	306	CLA	C1B-CHB-C4A	-3.33	123.51	130.12
25	1	310	BCR	C16-C15-C14	-3.33	116.65	123.47
24	8	207	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
24	F	201	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
24	A	836	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
24	5	603	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
24	3	303	CLA	CMB-C2B-C3B	3.32	130.90	124.68
24	k	304	CLA	CMB-C2B-C3B	3.32	130.89	124.68
24	1	304	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
26	6	614	DD6	C15-C14-C13	-3.32	118.98	125.99
24	A	806	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
24	7	606	CLA	C4A-NA-C1A	3.31	108.20	106.71
25	A	844	BCR	C38-C26-C25	-3.31	120.81	124.53
24	A	807	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	7	610	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
24	L	203	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
24	k	302	CLA	CMB-C2B-C3B	3.31	130.87	124.68
24	A	810	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	4	618	BCR	C38-C26-C27	3.31	119.97	113.62
24	6	610	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
24	B	810	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
24	1	307	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
26	9	314	DD6	C14-C13-C11	-3.30	120.41	125.53
24	B	848	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
24	4	605	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
24	A	819	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
24	7	606	CLA	C1B-CHB-C4A	-3.30	123.59	130.12
24	3	304	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
24	8	203	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
24	A	805	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
24	9	305	CLA	CMB-C2B-C3B	3.29	130.84	124.68
24	k	305	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
24	B	846	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
24	1	306	CLA	C4A-NA-C1A	3.29	108.18	106.71
24	3	309	CLA	CMB-C2B-C3B	3.29	130.83	124.68
24	L	203	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	I	102	BCR	C1-C6-C7	3.29	125.07	115.78
24	3	306	CLA	CMB-C2B-C3B	3.28	130.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	614	DD6	C33-C34-C35	-3.28	105.81	110.30
30	t	314	LMG	C8-O7-C10	-3.28	109.71	117.79
24	B	827	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	B	821	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	c	608	CLA	C4A-NA-C1A	3.28	108.18	106.71
24	B	803	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	2	211	BCR	C33-C5-C4	3.28	119.92	113.62
25	R	101	BCR	C30-C25-C26	-3.27	118.00	122.61
25	L	202	BCR	C33-C5-C6	-3.27	120.85	124.53
24	A	840	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
24	3	302	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	A	845	BCR	C38-C26-C27	3.26	119.88	113.62
28	A	842	LHG	C6-C5-C4	-3.26	104.08	111.79
24	A	838	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
27	3	314	LMT	O1'-C1'-C2'	3.26	113.39	108.30
24	2	203	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	B	849	BCR	C7-C8-C9	-3.26	121.31	126.23
26	7	613	DD6	C25-C24-C1	-3.26	117.27	126.42
26	R	105	DD6	C12-C11-C13	3.25	123.20	118.08
24	B	837	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
24	8	205	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
24	4	611	CLA	CMB-C2B-C3B	3.25	130.76	124.68
26	1	313	DD6	C4-C5-C6	-3.25	122.67	127.31
24	A	817	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
24	4	602	CLA	C4-C3-C5	3.25	120.73	115.27
24	A	827	CLA	C1B-CHB-C4A	-3.25	123.69	130.12
24	F	203	CLA	CMB-C2B-C3B	3.24	130.74	124.68
25	B	841	BCR	C16-C17-C18	-3.24	122.68	127.31
24	B	828	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
24	7	611	CLA	CMB-C2B-C3B	3.24	130.74	124.68
24	4	602	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
24	A	819	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	h	601	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
24	3	307	CLA	CMB-C2B-C3B	3.23	130.73	124.68
25	I	102	BCR	C33-C5-C4	3.23	119.83	113.62
24	A	833	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
24	7	612	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
26	7	616	DD6	C25-C26-C27	-3.23	117.20	126.58
24	7	607	CLA	C4A-NA-C1A	3.23	108.16	106.71
24	B	816	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
25	I	101	BCR	C27-C26-C25	-3.23	118.04	122.73
24	8	201	CLA	CMB-C2B-C1B	-3.23	123.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	317	DD6	C12-C11-C13	3.23	123.17	118.08
25	2	211	BCR	C15-C16-C17	-3.22	116.87	123.47
25	J	101	BCR	C11-C12-C13	-3.22	117.36	126.42
24	A	821	CLA	CMB-C2B-C3B	3.22	130.71	124.68
24	B	834	CLA	CMB-C2B-C3B	3.22	130.71	124.68
24	L	205	CLA	C4A-NA-C1A	3.22	108.16	106.71
24	A	828	CLA	CMB-C2B-C3B	3.22	130.71	124.68
24	A	840	CLA	CMB-C2B-C3B	3.22	130.70	124.68
24	k	303	CLA	O2D-CGD-CBD	3.22	116.99	111.27
25	B	843	BCR	C8-C7-C6	-3.22	118.16	127.20
24	B	810	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
25	M	101	BCR	C20-C19-C18	-3.22	117.38	126.42
25	k	316	BCR	C33-C5-C6	-3.22	120.92	124.53
24	8	204	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
24	A	835	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	c	615	BCR	C37-C22-C21	-3.22	118.42	122.92
24	A	801	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
24	B	834	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	I	102	BCR	C8-C9-C10	-3.22	114.01	118.94
24	9	310	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	A	814	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	c	602	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	4	615	DD6	C4-C5-C6	-3.21	122.73	127.31
24	B	838	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
24	A	808	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	B	843	BCR	C1-C6-C5	-3.21	118.09	122.61
26	8	212	DD6	C4-C5-C6	-3.21	122.73	127.31
24	9	307	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
24	h	611	CLA	CAA-C2A-C3A	-3.21	108.62	116.10
25	R	102	BCR	C8-C9-C10	3.20	123.86	118.94
24	2	206	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
26	7	613	DD6	C34-C35-C36	-3.20	105.48	111.85
24	c	606	CLA	CMB-C2B-C3B	3.20	130.67	124.68
26	6	617	DD6	C14-C13-C11	-3.20	120.56	125.53
24	B	835	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	h	610	CLA	CMB-C2B-C3B	3.20	130.66	124.68
24	7	610	CLA	CMB-C2B-C3B	3.19	130.65	124.68
24	A	829	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	1	310	BCR	C23-C24-C25	-3.19	118.24	127.20
25	c	615	BCR	C16-C15-C14	-3.19	116.94	123.47
25	F	204	BCR	C3-C4-C5	-3.19	108.38	114.08
26	k	315	DD6	C10-C9-C8	-3.19	113.26	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	603	CLA	CMB-C2B-C3B	3.19	130.65	124.68
24	B	815	CLA	C4-C3-C5	3.19	120.64	115.27
24	A	835	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
24	h	602	CLA	C1-O2A-CGA	3.19	124.81	116.44
24	A	804	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
28	3	315	LHG	O7-C7-C8	3.19	118.37	111.50
24	3	301	CLA	CMB-C2B-C3B	3.19	130.64	124.68
24	h	604	CLA	CMB-C2B-C3B	3.18	130.64	124.68
25	4	618	BCR	C33-C5-C6	-3.18	120.95	124.53
24	1	306	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	B	843	BCR	C15-C16-C17	-3.18	116.96	123.47
25	1	310	BCR	C33-C5-C4	3.18	119.72	113.62
24	t	304	CLA	CMB-C2B-C3B	3.18	130.62	124.68
24	c	603	CLA	CMB-C2B-C3B	3.17	130.62	124.68
24	A	834	CLA	CMB-C2B-C3B	3.17	130.62	124.68
25	L	202	BCR	C38-C26-C27	3.17	119.71	113.62
24	B	823	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
26	A	848	DD6	C25-C26-C27	-3.17	117.39	126.58
24	4	612	CLA	C1B-CHB-C4A	-3.17	123.85	130.12
25	L	202	BCR	C30-C25-C26	-3.17	118.16	122.61
25	A	845	BCR	C20-C21-C22	-3.17	122.79	127.31
24	4	601	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
25	9	316	BCR	C33-C5-C4	3.16	119.69	113.62
25	2	211	BCR	C16-C17-C18	-3.16	122.80	127.31
24	B	805	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
24	B	838	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
24	h	610	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
26	3	313	DD6	C25-C26-C27	-3.16	117.41	126.58
24	1	302	CLA	C1B-CHB-C4A	-3.16	123.87	130.12
25	1	314	BCR	C20-C21-C22	-3.15	122.81	127.31
24	c	608	CLA	CMB-C2B-C3B	3.15	130.58	124.68
24	A	837	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
24	9	307	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
24	c	605	CLA	CMB-C2B-C3B	3.15	130.57	124.68
24	1	306	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
24	t	309	CLA	CMB-C2B-C3B	3.14	130.56	124.68
25	4	618	BCR	C20-C19-C18	-3.14	117.58	126.42
24	4	606	CLA	CMB-C2B-C3B	3.14	130.56	124.68
24	A	816	CLA	CMB-C2B-C3B	3.14	130.56	124.68
24	B	822	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	c	615	BCR	C15-C14-C13	-3.14	122.83	127.31
24	B	826	CLA	C1B-CHB-C4A	-3.14	123.90	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	309	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	9	317	DD6	C4-C3-C2	-3.14	117.05	123.47
24	6	605	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
25	7	617	BCR	C15-C16-C17	-3.14	117.05	123.47
25	I	101	BCR	C24-C23-C22	-3.13	121.50	126.23
24	3	302	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
25	1	310	BCR	C8-C7-C6	-3.13	118.41	127.20
24	A	807	CLA	CMB-C2B-C3B	3.13	130.54	124.68
24	t	306	CLA	CMB-C2B-C3B	3.13	130.53	124.68
24	B	822	CLA	CMB-C2B-C3B	3.13	130.53	124.68
26	t	311	DD6	C9-C10-C11	-3.13	122.85	127.31
24	2	208	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
24	k	310	CLA	O2D-CGD-CBD	3.12	116.82	111.27
24	B	847	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
24	h	610	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
24	1	308	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
24	B	836	CLA	CMB-C2B-C3B	3.12	130.52	124.68
25	B	842	BCR	C33-C5-C4	3.12	119.61	113.62
24	2	202	CLA	CMB-C2B-C3B	3.12	130.52	124.68
24	4	608	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
24	9	303	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	1	301	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	B	846	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	9	317	DD6	C10-C9-C8	-3.12	113.49	123.22
24	t	307	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
25	B	849	BCR	C29-C30-C25	3.12	115.28	110.48
24	B	803	CLA	CMB-C2B-C3B	3.12	130.51	124.68
24	L	204	CLA	CHD-C1D-ND	-3.12	121.59	124.45
24	h	611	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
24	c	604	CLA	CMB-C2B-C3B	3.11	130.50	124.68
26	5	609	DD6	C4-C5-C6	-3.11	122.87	127.31
24	6	605	CLA	CMB-C2B-C3B	3.11	130.50	124.68
24	4	609	CLA	CMB-C2B-C3B	3.11	130.50	124.68
24	7	604	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	2	209	CLA	CMB-C2B-C3B	3.11	130.49	124.68
24	A	831	CLA	CMB-C2B-C3B	3.11	130.49	124.68
24	A	857	CLA	C1-C2-C3	-3.11	120.67	126.04
25	2	211	BCR	C23-C24-C25	-3.11	118.47	127.20
24	A	809	CLA	CMB-C2B-C3B	3.11	130.49	124.68
24	8	206	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
24	A	813	CLA	CMB-C2B-C3B	3.11	130.49	124.68
26	h	613	DD6	C9-C10-C11	-3.11	122.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	822	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
24	8	202	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
24	A	824	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	B	817	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	1	314	BCR	C3-C4-C5	-3.10	108.54	114.08
24	6	605	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	4	602	CLA	CMB-C2B-C3B	3.10	130.48	124.68
24	4	607	CLA	CMB-C2B-C3B	3.10	130.47	124.68
24	A	832	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	9	311	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
24	8	202	CLA	CMB-C2B-C3B	3.10	130.47	124.68
24	k	303	CLA	C1B-CHB-C4A	-3.10	123.99	130.12
24	c	611	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	J	102	DD6	C15-C14-C13	-3.10	119.45	125.99
24	B	818	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	k	301	CLA	CMB-C2B-C3B	3.09	130.47	124.68
25	4	618	BCR	C7-C8-C9	-3.09	121.56	126.23
24	k	310	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
24	7	602	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
24	B	836	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	8	203	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	A	818	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	B	815	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
25	I	102	BCR	C15-C16-C17	-3.08	117.16	123.47
24	4	613	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
24	c	610	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
25	A	846	BCR	C30-C25-C24	3.08	124.48	115.78
24	R	103	CLA	CMB-C2B-C3B	3.08	130.44	124.68
25	R	101	BCR	C33-C5-C6	-3.08	121.07	124.53
24	5	602	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
24	9	308	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
24	3	301	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	B	803	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	A	833	CLA	C4-C3-C5	3.07	120.44	115.27
24	h	602	CLA	O2A-C1-C2	-3.07	100.56	108.64
24	3	304	CLA	C4A-NA-C1A	3.07	108.09	106.71
24	4	603	CLA	CMB-C2B-C3B	3.07	130.42	124.68
24	A	811	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	B	807	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	A	834	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
25	B	842	BCR	C38-C26-C25	-3.07	121.08	124.53
24	A	838	CLA	C1B-CHB-C4A	-3.07	124.05	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	613	DD6	C9-C10-C11	-3.06	122.94	127.31
25	1	314	BCR	C30-C25-C26	-3.06	118.30	122.61
24	J	103	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	B	830	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
25	4	618	BCR	C33-C5-C4	3.06	119.49	113.62
24	t	303	CLA	C4-C3-C5	3.06	120.42	115.27
24	1	303	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	k	305	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	B	830	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	4	609	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
24	A	801	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
24	7	607	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
24	1	309	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	B	821	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	6	607	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
24	A	812	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	A	857	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
24	5	604	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	I	102	BCR	C27-C26-C25	-3.05	118.31	122.73
25	R	101	BCR	C28-C27-C26	-3.04	108.64	114.08
24	8	202	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
24	B	816	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
24	R	103	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
24	2	201	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
24	3	305	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	h	609	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	1	305	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
24	A	825	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	B	841	BCR	C33-C5-C4	3.04	119.45	113.62
24	5	606	CLA	CMB-C2B-C3B	3.04	130.36	124.68
24	7	605	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	6	604	CLA	CMB-C2B-C3B	3.04	130.36	124.68
24	1	317	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	5	602	CLA	C4A-NA-C1A	3.04	108.07	106.71
24	7	605	CLA	CMB-C2B-C3B	3.04	130.36	124.68
24	2	209	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	6	610	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
25	B	840	BCR	C1-C6-C5	-3.03	118.34	122.61
24	B	833	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	4	604	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
24	A	803	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
24	B	821	CLA	O2D-CGD-O1D	-3.03	117.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	312	BCR	C16-C17-C18	-3.03	122.99	127.31
24	A	813	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
24	A	825	CLA	CMB-C2B-C3B	3.03	130.34	124.68
24	9	304	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
24	A	817	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
26	4	614	DD6	C25-C26-C27	-3.03	117.79	126.58
25	7	617	BCR	C3-C4-C5	-3.03	108.67	114.08
24	6	610	CLA	CMB-C2B-C3B	3.03	130.34	124.68
24	h	605	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	k	304	CLA	C1B-CHB-C4A	-3.03	124.13	130.12
24	c	606	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
25	J	104	BCR	C39-C30-C25	-3.02	105.39	110.30
24	1	302	CLA	CMB-C2B-C3B	3.02	130.34	124.68
24	A	830	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
24	A	815	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	B	849	BCR	C12-C13-C14	-3.02	114.30	118.94
24	A	823	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	t	305	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
24	7	601	CLA	CMB-C2B-C3B	3.02	130.33	124.68
24	k	304	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	h	615	DD6	C7-C6-C8	3.02	122.84	118.08
24	k	306	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
24	h	611	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	9	303	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	1	304	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	t	308	CLA	CMB-C2B-C3B	3.02	130.32	124.68
24	B	823	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
26	k	313	DD6	O1-C20-C19	-3.02	111.12	113.38
24	4	613	CLA	CMB-C2B-C3B	3.01	130.32	124.68
24	t	310	CLA	CMB-C2B-C3B	3.01	130.32	124.68
24	A	811	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
29	9	312	A1L1G	C17-C20-C25	-3.01	117.21	122.26
26	c	612	DD6	C12-C11-C10	-3.01	118.70	122.92
25	R	102	BCR	C16-C17-C18	-3.01	123.01	127.31
24	8	209	CLA	CHD-C1D-ND	-3.01	121.68	124.45
24	7	601	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
24	9	303	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
24	1	308	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
24	k	306	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	7	607	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	3	303	CLA	C1-C2-C3	-3.00	120.85	126.04
24	1	305	CLA	C2A-C1A-CHA	3.00	129.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	305	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	3	313	DD6	C21-C20-C19	-3.00	110.90	114.28
24	6	612	CLA	CMB-C2B-C3B	3.00	130.29	124.68
24	4	606	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	c	607	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	1	304	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	7	617	BCR	C33-C5-C4	3.00	119.38	113.62
25	B	841	BCR	C15-C16-C17	-3.00	117.33	123.47
24	k	308	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
26	1	311	DD6	C41-C32-C31	3.00	115.23	110.47
25	A	844	BCR	C7-C8-C9	-3.00	121.71	126.23
24	B	801	CLA	CMB-C2B-C3B	2.99	130.28	124.68
26	k	313	DD6	C19-C18-C17	2.99	116.55	110.77
26	A	848	DD6	C4-C3-C2	-2.99	117.34	123.47
24	A	856	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
24	B	837	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	c	615	BCR	C30-C25-C24	2.99	124.24	115.78
24	k	307	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
24	B	813	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
24	1	304	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	B	813	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	J	103	CLA	CMB-C2B-C3B	2.99	130.27	124.68
24	A	830	CLA	CHB-C4A-NA	2.99	128.64	124.51
24	B	802	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	1	305	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	B	826	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	t	308	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	9	304	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	6	607	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
24	B	820	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	A	817	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	7	617	BCR	C7-C8-C9	-2.98	121.73	126.23
24	4	602	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	9	309	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	6	602	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	B	830	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
26	h	615	DD6	C10-C9-C8	-2.98	113.92	123.22
26	3	312	DD6	C19-C18-C17	2.98	116.53	110.77
24	6	602	CLA	CHD-C1D-ND	-2.98	121.72	124.45
24	c	602	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	B	808	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	6	609	CLA	C1B-CHB-C4A	-2.98	124.22	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	606	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	B	834	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	7	612	CLA	CMB-C2B-C3B	2.98	130.25	124.68
24	h	612	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
24	8	207	CLA	CMB-C2B-C3B	2.97	130.24	124.68
24	c	607	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
24	t	309	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	7	611	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
24	8	209	CLA	CMB-C2B-C3B	2.97	130.23	124.68
24	B	838	CLA	CMB-C2B-C3B	2.97	130.23	124.68
25	L	202	BCR	C20-C21-C22	-2.97	123.08	127.31
24	B	812	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	t	306	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
24	B	813	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	5	605	CLA	CMB-C2B-C3B	2.97	130.23	124.68
24	t	303	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
24	6	609	CLA	CMB-C2B-C3B	2.96	130.22	124.68
24	2	202	CLA	C4-C3-C5	2.96	120.26	115.27
24	A	803	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	B	819	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	I	102	BCR	C1-C6-C5	-2.96	118.44	122.61
24	L	204	CLA	O2D-CGD-CBD	2.96	116.53	111.27
25	7	617	BCR	C28-C27-C26	-2.96	108.80	114.08
24	B	811	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	1	310	BCR	C3-C4-C5	-2.96	108.80	114.08
24	8	204	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	A	833	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
24	2	209	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
24	A	810	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
24	A	847	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	1	317	CLA	CMB-C2B-C3B	2.96	130.21	124.68
24	h	606	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
24	A	820	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	2	201	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
25	1	314	BCR	C16-C15-C14	-2.95	117.42	123.47
24	9	310	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
24	B	818	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
24	4	602	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	t	310	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	A	825	CLA	CHD-C1D-ND	-2.95	121.74	124.45
24	c	609	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
25	B	840	BCR	C36-C18-C17	-2.95	118.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	101	BCR	C33-C5-C4	2.95	119.28	113.62
24	2	204	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	B	825	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	1	307	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
24	A	811	CLA	CMB-C2B-C3B	2.95	130.19	124.68
25	A	846	BCR	C38-C26-C27	2.95	119.28	113.62
24	t	307	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
24	4	604	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	h	601	CLA	CMB-C2B-C3B	2.95	130.19	124.68
26	1	311	DD6	C4-C5-C6	-2.94	123.11	127.31
24	6	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	t	313	DD6	C10-C9-C8	-2.94	114.03	123.22
24	3	309	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	c	604	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	B	817	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	c	608	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	1	301	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	6	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
24	5	604	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	6	616	DD6	C-C1-C2	-2.94	118.81	122.92
24	h	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	B	807	CLA	CMB-C2B-C3B	2.94	130.18	124.68
24	B	836	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
24	6	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	A	810	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
24	h	607	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
24	h	605	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
24	R	104	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	1	310	BCR	C27-C26-C25	-2.93	118.47	122.73
24	4	605	CLA	CMB-C2B-C3B	2.93	130.17	124.68
24	3	304	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
29	3	310	A1L1G	C43-C44-C42	-2.93	118.81	122.92
25	L	202	BCR	C27-C26-C25	-2.93	118.47	122.73
25	M	101	BCR	C10-C11-C12	-2.93	114.07	123.22
24	A	857	CLA	CHB-C4A-NA	2.93	128.57	124.51
24	R	104	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
24	B	828	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	A	848	DD6	C25-C24-C1	-2.93	118.19	126.42
24	5	601	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	A	810	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	t	309	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
24	A	825	CLA	C1B-CHB-C4A	-2.93	124.32	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	202	BCR	C11-C10-C9	-2.93	123.13	127.31
24	k	301	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
24	B	816	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	h	604	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
25	A	846	BCR	C15-C16-C17	-2.93	117.48	123.47
24	3	305	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
24	B	816	CLA	CMB-C2B-C3B	2.92	130.15	124.68
24	5	607	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	2	203	CLA	CHD-C1D-ND	-2.92	121.77	124.45
24	1	303	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
24	5	605	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
24	c	601	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
24	B	801	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
24	c	601	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	B	815	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	A	846	BCR	C11-C10-C9	-2.92	123.14	127.31
25	4	618	BCR	C27-C26-C25	-2.92	118.50	122.73
24	B	821	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	4	601	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	B	831	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	t	307	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
24	k	307	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
24	c	608	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	h	608	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	A	807	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	7	601	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
24	1	317	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
24	2	204	CLA	CMB-C2B-C1B	-2.91	123.98	128.46
24	L	204	CLA	CMB-C2B-C1B	-2.91	123.98	128.46
24	6	601	CLA	CMB-C2B-C3B	2.91	130.13	124.68
24	5	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	J	103	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	c	609	CLA	CMB-C2B-C3B	2.91	130.13	124.68
24	4	611	CLA	CHD-C1D-ND	-2.91	121.78	124.45
24	B	831	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	A	817	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	5	603	CLA	CMB-C2B-C3B	2.91	130.12	124.68
26	5	609	DD6	C19-C18-C17	2.91	116.39	110.77
24	8	203	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	A	828	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	1	305	CLA	CAA-CBA-CGA	-2.91	104.79	112.51
28	3	315	LHG	O8-C23-C24	2.91	121.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	609	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	c	604	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	6	608	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	6	611	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	B	847	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
24	5	607	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	4	611	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	R	101	BCR	C1-C6-C5	-2.91	118.52	122.61
24	3	302	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	2	211	BCR	C8-C7-C6	-2.90	119.04	127.20
24	B	846	CLA	CMB-C2B-C3B	2.90	130.11	124.68
24	A	812	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
24	1	306	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	R	101	BCR	C7-C8-C9	-2.90	121.85	126.23
24	8	206	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	t	302	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
26	k	315	DD6	C7-C6-C8	2.90	122.65	118.08
24	A	821	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	c	605	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	B	820	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	B	835	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	B	811	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
24	B	804	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	A	806	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	F	202	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	B	810	CLA	CHD-C1D-ND	-2.90	121.79	124.45
25	R	102	BCR	C1-C6-C5	-2.90	118.53	122.61
24	7	608	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
24	A	828	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	B	832	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	7	609	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	9	306	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	7	610	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
24	k	310	CLA	CHD-C1D-ND	-2.90	121.79	124.45
26	k	315	DD6	C8-C6-C5	-2.90	114.50	118.94
24	B	848	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	8	205	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	7	612	CLA	CHD-C1D-ND	-2.89	121.80	124.45
24	A	856	CLA	CHD-C1D-ND	-2.89	121.80	124.45
24	B	819	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	A	809	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
24	B	811	CLA	CMB-C2B-C3B	2.89	130.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	613	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	F	202	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	c	605	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
24	L	205	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
24	B	803	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	2	208	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	A	827	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
24	6	606	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
24	c	611	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	c	603	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
24	B	832	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
24	2	206	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	8	204	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	A	808	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	A	816	CLA	O2D-CGD-CBD	2.88	116.39	111.27
25	J	104	BCR	C16-C15-C14	-2.88	117.57	123.47
24	9	304	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	B	829	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
24	B	820	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	L	203	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	4	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	1	310	BCR	C38-C26-C25	-2.88	121.30	124.53
24	6	603	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	A	804	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
24	B	809	CLA	CMB-C2B-C3B	2.88	130.06	124.68
24	A	819	CLA	CMB-C2B-C3B	2.88	130.06	124.68
24	8	201	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	5	606	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
24	A	814	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
24	k	309	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	A	823	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	1	309	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	A	812	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	4	606	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
24	A	819	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
24	9	305	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	A	838	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	2	206	CLA	O2D-CGD-CBD	2.87	116.37	111.27
25	4	618	BCR	C8-C7-C6	-2.87	119.14	127.20
25	A	843	BCR	C16-C15-C14	-2.87	117.59	123.47
24	5	602	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
24	4	605	CLA	O2D-CGD-O1D	-2.87	118.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	314	LMT	C1B-O1B-C4'	-2.87	110.87	117.96
24	F	203	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	2	203	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	8	208	CLA	CHB-C4A-NA	2.87	128.47	124.51
24	B	838	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
25	A	844	BCR	C8-C7-C6	-2.86	119.16	127.20
25	L	202	BCR	C16-C17-C18	-2.86	123.22	127.31
25	J	104	BCR	C30-C25-C26	-2.86	118.58	122.61
24	A	821	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
24	A	831	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
24	B	848	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	2	211	BCR	C3-C4-C5	-2.86	108.97	114.08
24	B	824	CLA	O2D-CGD-CBD	2.86	116.35	111.27
24	h	608	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	h	604	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
24	h	605	CLA	CMB-C2B-C3B	2.86	130.02	124.68
24	k	303	CLA	CHD-C1D-ND	-2.86	121.83	124.45
24	F	201	CLA	CMB-C2B-C3B	2.86	130.02	124.68
24	1	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	5	605	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	8	207	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
25	J	104	BCR	C29-C30-C25	2.85	114.87	110.48
24	A	808	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	B	804	CLA	C1-O2A-CGA	2.85	123.93	116.44
25	7	617	BCR	C38-C26-C27	2.85	119.09	113.62
24	6	608	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	A	831	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	7	618	DD6	C25-C26-C27	-2.85	118.30	126.58
24	B	824	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	9	310	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	3	305	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	J	101	BCR	C37-C22-C21	-2.85	118.93	122.92
24	1	301	CLA	CHD-C1D-ND	-2.85	121.84	124.45
24	B	809	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	B	825	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
24	9	308	CLA	CMB-C2B-C3B	2.85	130.00	124.68
24	A	829	CLA	O2D-CGD-CBD	2.85	116.33	111.27
24	7	605	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
28	A	849	LHG	O8-C23-C24	2.85	120.84	111.91
24	k	311	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
24	8	203	CLA	CMB-C2B-C3B	2.84	130.00	124.68
24	5	603	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	9	306	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	A	835	CLA	CMB-C2B-C3B	2.84	129.99	124.68
24	A	836	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
26	5	609	DD6	C14-C13-C11	-2.84	121.12	125.53
28	L	201	LHG	O8-C23-C24	2.84	120.82	111.91
24	A	818	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
26	8	210	DD6	C7-C6-C5	-2.84	118.95	122.92
24	A	829	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
24	A	840	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
24	4	610	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	A	853	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	3	306	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	A	833	CLA	CMB-C2B-C3B	2.83	129.98	124.68
24	c	609	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
24	k	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	B	814	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
25	J	101	BCR	C24-C23-C22	-2.83	121.95	126.23
24	7	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	h	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	A	802	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	B	842	BCR	C3-C4-C5	-2.83	109.02	114.08
25	I	102	BCR	C7-C8-C9	-2.83	121.96	126.23
24	8	201	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	t	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	c	606	CLA	CHD-C1D-ND	-2.83	121.85	124.45
24	A	820	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
24	2	206	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	A	832	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
24	B	827	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	7	617	BCR	C16-C17-C18	-2.83	123.28	127.31
24	2	203	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
24	h	601	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	7	608	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	I	101	BCR	C38-C26-C25	-2.83	121.36	124.53
24	B	836	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	7	604	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	h	603	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	B	814	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
24	t	307	CLA	CMB-C2B-C3B	2.82	129.96	124.68
26	3	313	DD6	C10-C9-C8	-2.82	114.41	123.22
24	B	831	CLA	O2D-CGD-O1D	-2.82	118.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	843	BCR	C30-C25-C26	-2.82	118.64	122.61
26	8	212	DD6	C12-C11-C13	2.82	122.52	118.08
24	A	820	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	L	204	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	A	822	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	h	601	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	2	207	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	A	809	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	9	315	DD6	C25-C24-C1	-2.82	118.50	126.42
24	t	310	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
24	B	808	CLA	O2A-CGA-O1A	-2.82	116.49	123.59
24	3	303	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
24	3	303	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	A	837	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	6	615	DD6	C4-C3-C2	-2.81	117.71	123.47
25	L	202	BCR	C1-C6-C7	2.81	123.73	115.78
24	7	609	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
24	h	609	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
31	B	839	PQN	C11-C3-C4	-2.81	115.49	118.50
24	A	838	CLA	CHD-C1D-ND	-2.81	121.87	124.45
25	A	845	BCR	C11-C12-C13	-2.81	118.52	126.42
24	1	301	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	3	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	A	813	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	B	833	CLA	C4-C3-C5	2.81	119.99	115.27
25	7	617	BCR	C24-C23-C22	-2.81	122.00	126.23
24	B	846	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
24	2	208	CLA	CMB-C2B-C3B	2.81	129.93	124.68
24	1	308	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	B	840	BCR	C4-C5-C6	-2.81	118.66	122.73
24	4	605	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	7	617	BCR	C10-C11-C12	-2.80	114.47	123.22
24	6	606	CLA	CMB-C2B-C3B	2.80	129.93	124.68
24	c	606	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
24	B	805	CLA	CHD-C1D-ND	-2.80	121.88	124.45
24	8	208	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	6	604	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
24	4	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	2	202	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	8	205	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	k	311	CLA	CHD-C1D-ND	-2.80	121.88	124.45
24	2	207	CLA	C1B-CHB-C4A	-2.80	124.57	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	610	CLA	CMB-C2B-C3B	2.80	129.91	124.68
24	6	609	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
24	2	202	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
24	F	201	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
24	A	830	CLA	CMB-C2B-C3B	2.80	129.91	124.68
25	9	316	BCR	C3-C4-C5	-2.80	109.08	114.08
24	9	305	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
24	B	830	CLA	C4A-NA-C1A	2.80	107.96	106.71
25	B	841	BCR	C28-C27-C26	-2.80	109.08	114.08
24	9	301	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
24	B	810	CLA	CMB-C2B-C3B	2.80	130.16	124.69
24	A	857	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	k	310	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
24	A	822	CLA	CMB-C2B-C3B	2.79	129.91	124.68
24	7	609	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
24	8	206	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	R	105	DD6	C26-C25-C24	-2.79	114.51	123.22
24	2	202	CLA	C4A-NA-C1A	2.79	107.96	106.71
24	8	209	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
24	6	606	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	B	840	BCR	C37-C22-C21	-2.79	119.02	122.92
25	7	617	BCR	C30-C25-C26	-2.79	118.69	122.61
24	3	308	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
24	A	806	CLA	CMB-C2B-C3B	2.79	129.89	124.68
24	c	608	CLA	CHD-C1D-ND	-2.79	121.89	124.45
24	k	303	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
24	c	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	5	601	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	B	819	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
24	8	201	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	1	307	CLA	CMB-C2B-C3B	2.78	129.89	124.68
24	7	602	CLA	CAC-C3C-C2C	-2.78	122.77	127.53
24	B	810	CLA	C4A-NA-C1A	2.78	107.96	106.71
24	A	832	CLA	CHD-C1D-ND	-2.78	121.90	124.45
24	k	302	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	8	210	DD6	O1-C20-C19	2.78	115.47	113.38
24	A	832	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
24	R	103	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	A	843	BCR	C36-C18-C17	-2.78	119.03	122.92
24	t	305	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	8	205	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
24	A	860	CLA	CHB-C4A-NA	2.78	128.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	309	CLA	CHD-C1D-ND	-2.78	121.90	124.45
24	k	308	CLA	O2D-CGD-CBD	2.78	116.20	111.27
25	B	840	BCR	C33-C5-C4	2.77	118.94	113.62
26	1	313	DD6	C10-C9-C8	-2.77	114.56	123.22
24	8	208	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
24	h	607	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
24	A	804	CLA	CHD-C1D-ND	-2.77	121.91	124.45
24	h	607	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
29	9	312	A1L1G	C28-C39-C38	-2.77	119.04	122.92
24	7	607	CLA	CHD-C1D-ND	-2.77	121.91	124.45
24	B	830	CLA	C4-C3-C5	2.77	119.93	115.27
25	7	617	BCR	C38-C26-C25	-2.77	121.42	124.53
24	4	608	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	9	314	DD6	C12-C11-C10	-2.77	119.04	122.92
24	A	823	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
24	4	601	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	h	605	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	M	101	BCR	C16-C15-C14	-2.77	117.81	123.47
24	B	828	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
25	k	316	BCR	C38-C26-C27	2.77	118.93	113.62
24	1	307	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	A	815	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
24	2	204	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	B	809	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	B	811	CLA	C4-C3-C5	2.76	119.92	115.27
24	8	209	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	6	617	DD6	C4-C5-C6	-2.76	123.37	127.31
24	k	309	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	I	102	BCR	C30-C25-C24	2.76	123.58	115.78
24	h	602	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
24	B	832	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
24	2	206	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
24	c	604	CLA	CHD-C1D-ND	-2.76	121.92	124.45
24	t	306	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	6	607	CLA	CHD-C1D-ND	-2.76	121.92	124.45
24	2	205	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	R	103	CLA	CHD-C1D-ND	-2.75	121.92	124.45
24	B	826	CLA	CMB-C2B-C3B	2.75	129.83	124.68
26	7	618	DD6	C7-C6-C5	-2.75	119.07	122.92
24	A	821	CLA	CHD-C1D-ND	-2.75	121.92	124.45
26	2	212	DD6	C14-C13-C11	-2.75	121.26	125.53
24	F	201	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	828	CLA	CMB-C2B-C3B	2.75	129.83	124.68
24	A	816	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
24	B	806	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	B	837	CLA	CMB-C2B-C3B	2.75	129.82	124.68
24	4	608	CLA	CHD-C1D-ND	-2.75	121.93	124.45
24	B	807	CLA	CHD-C1D-ND	-2.75	121.93	124.45
26	A	848	DD6	O1-C20-C19	-2.75	111.32	113.38
24	5	607	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	8	201	CLA	CHD-C1D-ND	-2.75	121.93	124.45
24	t	302	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
24	5	601	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
24	4	610	CLA	CHD-C1D-ND	-2.74	121.93	124.45
24	A	801	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	5	606	CLA	CHD-C1D-ND	-2.74	121.93	124.45
24	3	307	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
24	4	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
28	1	318	LHG	O8-C23-C24	2.74	120.50	111.91
24	3	306	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
24	B	837	CLA	C4-C3-C5	2.74	119.88	115.27
24	4	607	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	B	840	BCR	C11-C10-C9	-2.74	123.40	127.31
24	A	857	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
24	c	609	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	5	606	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
24	k	301	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	A	810	CLA	CHD-C1D-ND	-2.73	121.94	124.45
24	A	812	CLA	CHD-C1D-ND	-2.73	121.94	124.45
25	4	618	BCR	C38-C26-C25	-2.73	121.46	124.53
24	B	813	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	B	801	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
24	4	602	CLA	CHD-C1D-ND	-2.73	121.95	124.45
24	A	813	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
26	4	617	DD6	C3-C4-C5	2.73	129.06	123.47
24	A	808	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
26	t	313	DD6	C14-C13-C11	-2.73	121.30	125.53
24	L	205	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
24	A	834	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	7	617	BCR	C8-C7-C6	-2.72	119.56	127.20
25	R	102	BCR	C33-C5-C6	2.72	127.58	124.53
24	c	610	CLA	C4A-NA-C1A	2.72	107.93	106.71
25	B	841	BCR	C8-C7-C6	-2.72	119.57	127.20
24	3	309	CLA	CHD-C1D-ND	-2.72	121.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	616	DD6	C10-C9-C8	-2.72	114.74	123.22
26	9	317	DD6	C21-C20-C15	-2.72	117.71	122.26
24	B	847	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
24	6	610	CLA	C4A-NA-C1A	2.72	107.93	106.71
24	6	603	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
24	B	823	CLA	CHD-C1D-ND	-2.71	121.96	124.45
24	8	207	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
24	B	827	CLA	O2D-CGD-CBD	2.71	116.09	111.27
24	B	848	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
24	4	613	CLA	CHD-C1D-ND	-2.71	121.96	124.45
24	1	305	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
24	t	304	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	7	602	CLA	C1-C2-C3	-2.71	122.36	126.75
24	c	611	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	A	806	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	1	306	CLA	C1-C2-C3	-2.71	122.36	126.75
24	9	301	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	k	302	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	4	610	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	h	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	B	826	CLA	CHD-C1D-ND	-2.71	121.97	124.45
24	9	309	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	4	607	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	8	203	CLA	C1-C2-C3	-2.71	122.37	126.75
25	4	618	BCR	C16-C15-C14	-2.70	117.93	123.47
26	5	608	DD6	C14-C13-C11	-2.70	121.34	125.53
24	k	310	CLA	CMB-C2B-C3B	2.70	129.74	124.68
24	A	860	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
26	3	313	DD6	C-C1-C2	-2.70	119.14	122.92
24	6	601	CLA	CHD-C1D-ND	-2.70	121.97	124.45
25	1	314	BCR	C33-C5-C4	2.70	118.81	113.62
24	6	601	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
25	A	844	BCR	C33-C5-C4	2.70	118.80	113.62
24	2	205	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
24	B	824	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
24	B	822	CLA	C5-C3-C2	2.70	126.58	121.12
24	9	302	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	9	307	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	I	101	BCR	C16-C15-C14	-2.70	117.95	123.47
29	2	213	A1L1G	C37-C36-C35	2.70	129.00	123.47
24	t	305	CLA	CHD-C1D-ND	-2.70	121.98	124.45
25	A	843	BCR	C4-C5-C6	-2.70	118.82	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	612	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
24	A	823	CLA	CMB-C2B-C3B	2.69	129.72	124.68
24	A	809	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	F	201	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	A	826	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	B	811	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	4	605	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	A	834	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	A	860	CLA	C1-C2-C3	-2.69	121.39	126.04
24	1	308	CLA	CMB-C2B-C3B	2.69	129.71	124.68
24	B	835	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
24	A	804	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
28	I	103	LHG	C5-O7-C7	-2.69	111.18	117.79
24	h	609	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	B	833	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
25	F	204	BCR	C28-C27-C26	-2.68	109.28	114.08
26	4	617	DD6	C15-C14-C13	-2.68	120.32	125.99
24	6	610	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	9	311	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	A	837	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
26	c	612	DD6	O1-C20-C19	2.68	115.40	113.38
24	3	306	CLA	CHD-C1D-ND	-2.68	121.99	124.45
24	B	801	CLA	CHD-C1D-ND	-2.68	121.99	124.45
24	t	301	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	2	207	CLA	CHD-C1D-ND	-2.68	121.99	124.45
24	5	605	CLA	CHD-C1D-ND	-2.68	121.99	124.45
26	7	615	DD6	C25-C26-C27	-2.68	118.81	126.58
25	c	615	BCR	C38-C26-C27	2.68	118.76	113.62
24	4	608	CLA	CMB-C2B-C3B	2.68	129.69	124.68
24	k	305	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
26	R	105	DD6	C33-C34-C35	2.67	113.96	110.30
29	7	614	A1L1G	C28-C39-C38	-2.67	119.18	122.92
24	4	603	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
24	5	603	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
24	F	202	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
26	5	609	DD6	C34-C35-C36	-2.67	106.53	111.85
24	k	301	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	3	307	CLA	O2D-CGD-CBD	2.67	116.02	111.27
26	k	314	DD6	C14-C13-C11	-2.67	121.39	125.53
24	5	602	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	k	311	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	1	302	CLA	O2D-CGD-O1D	-2.67	118.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	602	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	B	818	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	3	309	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
26	h	616	DD6	C3-C4-C5	2.67	128.94	123.47
24	t	303	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	A	830	CLA	C1D-ND-C4D	2.67	108.23	106.33
24	B	830	CLA	CMB-C2B-C3B	2.67	129.67	124.68
24	4	608	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
24	k	305	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	B	820	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	L	205	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	t	304	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
25	R	102	BCR	C15-C16-C17	-2.66	118.02	123.47
24	c	611	CLA	CHD-C1D-ND	-2.66	122.01	124.45
24	6	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	6	616	DD6	C22-C16-C17	-2.66	104.36	108.98
24	9	308	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	A	859	BCR	C16-C15-C14	-2.66	118.03	123.47
24	6	605	CLA	CHD-C1D-ND	-2.66	122.01	124.45
26	J	102	DD6	C10-C9-C8	-2.66	114.93	123.22
24	B	831	CLA	CHD-C1D-ND	-2.66	122.01	124.45
24	B	808	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
25	1	310	BCR	C7-C8-C9	-2.65	122.23	126.23
25	1	314	BCR	C34-C9-C10	-2.65	119.21	122.92
26	7	616	DD6	C25-C24-C1	-2.65	118.97	126.42
24	6	608	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	F	204	BCR	C38-C26-C27	2.65	118.71	113.62
24	k	310	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	6	602	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	7	611	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	A	808	CLA	CHD-C1D-ND	-2.65	122.02	124.45
24	A	836	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
27	A	851	LMT	C2'-C3'-C4'	2.65	115.73	109.68
26	6	617	DD6	O1-C20-C21	-2.65	111.89	115.06
26	7	618	DD6	C3-C4-C5	2.65	128.89	123.47
27	1	316	LMT	C1B-O1B-C4'	-2.65	111.42	117.96
24	7	603	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
25	A	844	BCR	C28-C27-C26	-2.64	109.36	114.08
26	7	613	DD6	C10-C9-C8	-2.64	114.97	123.22
24	9	302	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
24	L	203	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
24	3	301	CLA	CHD-C1D-ND	-2.64	122.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	302	CLA	CHD-C1D-ND	-2.64	122.03	124.45
24	6	607	CLA	CMB-C2B-C3B	2.64	129.62	124.68
24	B	834	CLA	CHD-C1D-ND	-2.64	122.03	124.45
26	c	613	DD6	C25-C24-C1	-2.64	119.00	126.42
24	B	838	CLA	CHD-C1D-ND	-2.64	122.03	124.45
24	R	104	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	3	304	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	B	849	BCR	C30-C25-C26	-2.64	118.90	122.61
24	9	307	CLA	CHD-C1D-ND	-2.63	122.03	124.45
25	I	102	BCR	C37-C22-C21	-2.63	119.23	122.92
26	c	614	DD6	C14-C13-C11	-2.63	121.45	125.53
25	B	842	BCR	C37-C22-C21	-2.63	119.24	122.92
24	3	302	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
24	c	602	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
26	k	315	DD6	C12-C11-C10	-2.63	119.24	122.92
25	L	206	BCR	C38-C26-C25	-2.63	121.58	124.53
24	k	302	CLA	CHD-C1D-ND	-2.63	122.04	124.45
25	J	104	BCR	C2-C1-C6	2.63	114.52	110.48
29	k	312	A1L1G	O15-C20-C17	-2.63	111.91	115.06
24	A	824	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
26	k	313	DD6	C26-C25-C24	-2.62	115.03	123.22
25	B	840	BCR	C38-C26-C27	2.62	118.66	113.62
24	t	303	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
24	A	814	CLA	CHD-C1D-ND	-2.62	122.04	124.45
28	I	103	LHG	O8-C23-C24	2.62	120.14	111.91
24	4	608	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
26	4	616	DD6	C25-C26-C27	-2.62	118.97	126.58
25	J	104	BCR	C12-C13-C14	-2.62	114.92	118.94
24	h	602	CLA	CHD-C1D-ND	-2.62	122.05	124.45
24	B	822	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
24	A	835	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
26	6	617	DD6	C37-C36-C31	-2.62	120.80	124.35
25	R	102	BCR	C38-C26-C27	2.62	118.64	113.62
24	B	810	CLA	CAA-C2A-C1A	-2.61	103.41	111.97
24	B	832	CLA	CHD-C1D-ND	-2.61	122.05	124.45
24	F	203	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
24	A	813	CLA	CHD-C1D-ND	-2.61	122.05	124.45
24	A	814	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
24	7	603	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	2	205	CLA	CHD-C1D-ND	-2.61	122.05	124.45
26	9	317	DD6	C13-C11-C10	-2.61	114.93	118.94
24	A	826	CLA	O2D-CGD-CBD	2.61	115.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	609	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	c	612	DD6	C40-C32-C31	-2.61	106.32	110.47
24	c	610	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
26	h	615	DD6	C8-C6-C5	-2.61	114.94	118.94
24	h	601	CLA	CHD-C1D-ND	-2.61	122.06	124.45
26	t	313	DD6	C25-C24-C1	-2.60	119.10	126.42
26	9	315	DD6	C21-C20-C19	-2.60	111.35	114.28
24	3	308	CLA	CHD-C1D-ND	-2.60	122.06	124.45
24	A	827	CLA	CHD-C1D-ND	-2.60	122.06	124.45
25	B	841	BCR	C37-C22-C21	-2.60	119.28	122.92
24	2	202	CLA	CHD-C1D-ND	-2.60	122.06	124.45
25	t	312	BCR	C33-C5-C4	2.60	118.61	113.62
24	B	810	CLA	CAB-C3B-C2B	2.60	129.78	124.69
25	L	202	BCR	C38-C26-C25	-2.60	121.61	124.53
24	9	302	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	R	102	BCR	C37-C22-C21	-2.60	119.28	122.92
24	A	837	CLA	CHD-C1D-ND	-2.60	122.07	124.45
24	J	103	CLA	CHD-C1D-ND	-2.60	122.07	124.45
24	2	208	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
24	k	303	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	A	826	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
25	9	316	BCR	C38-C26-C27	2.60	118.60	113.62
26	c	612	DD6	O1-C20-C21	-2.60	111.95	115.06
24	9	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	c	601	CLA	CHD-C1D-ND	-2.60	122.07	124.45
24	B	829	CLA	C1-C2-C3	-2.59	121.56	126.04
24	A	847	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	J	104	BCR	C38-C26-C25	2.59	127.44	124.53
26	1	311	DD6	C37-C36-C31	-2.59	120.82	124.35
24	B	824	CLA	CHD-C1D-ND	-2.59	122.07	124.45
24	B	802	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
25	7	617	BCR	C21-C20-C19	-2.59	115.13	123.22
24	B	806	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
26	6	615	DD6	C26-C25-C24	-2.59	115.14	123.22
28	J	105	LHG	C5-O7-C7	-2.59	111.43	117.79
25	M	101	BCR	C38-C26-C25	-2.59	121.62	124.53
24	B	805	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
30	A	855	LMG	O8-C28-C29	2.59	120.02	111.91
24	A	801	CLA	C4A-NA-C1A	2.58	107.87	106.71
24	h	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	5	602	CLA	CHD-C1D-ND	-2.58	122.08	124.45
24	8	204	CLA	C1B-CHB-C4A	-2.58	125.00	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	811	CLA	CHD-C1D-ND	-2.58	122.08	124.45
24	2	204	CLA	CMB-C2B-C3B	2.58	129.50	124.68
26	3	312	DD6	C4-C3-C2	-2.58	118.19	123.47
24	B	815	CLA	CHD-C1D-ND	-2.58	122.09	124.45
25	L	206	BCR	C36-C18-C17	-2.58	119.31	122.92
25	I	102	BCR	C15-C14-C13	-2.58	123.64	127.31
26	7	616	DD6	C-C1-C2	-2.57	119.32	122.92
25	A	859	BCR	C30-C25-C26	-2.57	118.99	122.61
26	3	313	DD6	C7-C6-C8	2.57	122.13	118.08
24	t	301	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
24	B	807	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
25	B	849	BCR	C37-C22-C21	-2.57	119.32	122.92
24	5	601	CLA	CHD-C1D-ND	-2.57	122.09	124.45
25	R	101	BCR	C24-C23-C22	-2.57	122.35	126.23
24	B	837	CLA	CHD-C1D-ND	-2.57	122.09	124.45
24	A	815	CLA	CHD-C1D-ND	-2.57	122.09	124.45
25	M	101	BCR	C11-C10-C9	-2.57	123.65	127.31
24	6	612	CLA	CHD-C1D-ND	-2.57	122.10	124.45
24	h	603	CLA	O2D-CGD-O1D	-2.57	118.26	124.09
28	3	315	LHG	C5-O7-C7	-2.57	111.48	117.79
25	1	314	BCR	C28-C27-C26	-2.56	109.50	114.08
25	I	101	BCR	C28-C27-C26	-2.56	109.50	114.08
24	6	601	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
24	B	837	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
24	B	819	CLA	CHD-C1D-ND	-2.56	122.10	124.45
26	4	617	DD6	O1-C20-C21	-2.56	111.99	115.06
24	t	306	CLA	CHD-C1D-ND	-2.56	122.11	124.45
26	t	313	DD6	C7-C6-C8	2.56	122.10	118.08
26	k	315	DD6	C25-C24-C1	-2.55	119.24	126.42
24	A	817	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	A	846	BCR	C3-C4-C5	-2.55	109.52	114.08
24	A	822	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	c	615	BCR	C33-C5-C4	2.55	118.52	113.62
24	6	611	CLA	O2D-CGD-O1D	-2.55	118.29	124.09
24	B	811	CLA	C1-C2-C3	-2.55	121.63	126.04
25	F	204	BCR	C11-C12-C13	-2.55	119.25	126.42
24	4	601	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
26	h	613	DD6	C10-C9-C8	-2.55	115.26	123.22
24	h	609	CLA	CHD-C1D-ND	-2.55	122.11	124.45
24	3	301	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
24	A	830	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	B	843	BCR	C7-C8-C9	-2.55	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	853	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
24	t	307	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	2	213	A1L1G	O15-C20-C17	-2.54	112.01	115.06
25	B	841	BCR	C11-C12-C13	-2.54	119.27	126.42
24	c	610	CLA	C1D-ND-C4D	-2.54	104.53	106.33
24	c	607	CLA	CHD-C1D-ND	-2.54	122.12	124.45
24	A	806	CLA	CHD-C1D-ND	-2.54	122.12	124.45
24	B	806	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	J	102	DD6	O1-C20-C19	-2.54	111.47	113.38
24	k	303	CLA	C4A-NA-C1A	2.54	107.85	106.71
26	9	313	DD6	C19-C18-C17	2.54	115.68	110.77
24	7	602	CLA	CBC-CAC-C3C	2.54	119.44	112.43
24	F	202	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	A	844	BCR	C3-C4-C5	-2.54	109.54	114.08
26	8	212	DD6	C34-C35-C36	-2.54	106.80	111.85
24	A	805	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
24	2	209	CLA	CHD-C1D-ND	-2.54	122.12	124.45
24	h	607	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	4	617	DD6	C14-C13-C11	-2.54	121.59	125.53
24	A	816	CLA	CHD-C1D-ND	-2.53	122.13	124.45
24	A	802	CLA	C1-C2-C3	-2.53	121.66	126.04
25	9	316	BCR	C16-C15-C14	-2.53	118.29	123.47
25	k	316	BCR	C11-C12-C13	-2.53	119.31	126.42
24	k	307	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
26	k	313	DD6	C10-C9-C8	-2.53	115.33	123.22
24	2	204	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	A	818	CLA	CHD-C1D-ND	-2.53	122.13	124.45
24	F	203	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	h	604	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	I	102	BCR	C29-C30-C25	2.52	114.37	110.48
26	7	616	DD6	C12-C11-C10	-2.52	119.39	122.92
25	B	840	BCR	C27-C26-C25	-2.52	119.07	122.73
24	A	805	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	L	206	BCR	C33-C5-C6	-2.52	121.70	124.53
24	1	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	B	812	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
25	k	316	BCR	C23-C24-C25	-2.52	120.13	127.20
24	B	821	CLA	C1-C2-C3	-2.52	121.69	126.04
24	7	611	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	B	841	BCR	C24-C23-C22	-2.52	122.43	126.23
24	A	802	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	R	101	BCR	C23-C24-C25	-2.51	120.14	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	302	CLA	CHD-C1D-ND	-2.51	122.14	124.45
24	1	309	CLA	O2D-CGD-O1D	-2.51	118.38	124.09
24	4	602	CLA	CHB-C4A-NA	2.51	127.99	124.51
24	B	804	CLA	C4D-CHA-C1A	2.51	124.30	121.25
25	A	843	BCR	C11-C10-C9	-2.51	123.73	127.31
25	M	101	BCR	C37-C22-C21	-2.51	119.41	122.92
24	B	812	CLA	CHD-C1D-ND	-2.50	122.15	124.45
24	B	808	CLA	O2D-CGD-CBD	2.50	115.72	111.27
25	B	842	BCR	C1-C6-C5	-2.50	119.09	122.61
26	R	105	DD6	C15-C14-C13	2.50	131.28	125.99
24	L	203	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	B	822	CLA	C4-C3-C2	-2.50	117.26	123.68
24	B	808	CLA	C1-C2-C3	-2.50	121.72	126.04
24	A	803	CLA	O2D-CGD-CBD	2.50	115.71	111.27
24	1	317	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	I	101	BCR	C37-C22-C21	-2.49	119.43	122.92
24	9	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	c	615	BCR	C7-C6-C5	-2.49	115.42	121.46
24	A	836	CLA	CHD-C1D-ND	-2.49	122.16	124.45
26	8	212	DD6	C10-C9-C8	-2.49	115.44	123.22
24	B	831	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	B	802	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	5	603	CLA	CHD-C1D-ND	-2.49	122.17	124.45
25	B	843	BCR	C34-C9-C10	-2.49	119.43	122.92
24	7	602	CLA	O2D-CGD-CBD	2.49	115.69	111.27
24	8	203	CLA	O2D-CGD-CBD	2.49	115.69	111.27
25	A	844	BCR	C16-C15-C14	-2.49	118.37	123.47
24	A	815	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
24	1	306	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	B	810	CLA	C1-C2-C3	-2.49	121.74	126.04
29	k	312	A1L1G	C28-C39-C38	-2.49	119.44	122.92
24	B	830	CLA	CHD-C1D-ND	-2.49	122.17	124.45
27	h	617	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
24	A	823	CLA	CHD-C1D-ND	-2.49	122.17	124.45
24	1	306	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
29	k	312	A1L1G	C36-C37-C38	2.48	128.56	123.47
24	1	306	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
25	I	101	BCR	C15-C16-C17	-2.48	118.39	123.47
26	h	616	DD6	C25-C26-C27	-2.48	119.38	126.58
24	c	601	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
24	5	602	CLA	C1-C2-C3	-2.48	121.75	126.04
25	2	211	BCR	C10-C11-C12	-2.48	115.48	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	206	BCR	C37-C22-C21	-2.48	119.45	122.92
25	I	102	BCR	C19-C18-C17	-2.48	115.14	118.94
26	8	210	DD6	C25-C24-C1	-2.47	119.47	126.42
24	t	308	CLA	CHD-C1D-ND	-2.47	122.18	124.45
25	B	843	BCR	C16-C17-C18	-2.47	123.78	127.31
24	A	813	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	k	307	CLA	CMB-C2B-C3B	2.47	129.30	124.68
24	B	813	CLA	CHD-C1D-ND	-2.47	122.19	124.45
24	L	203	CLA	C1-C2-C3	-2.47	121.78	126.04
24	h	606	CLA	CHD-C1D-ND	-2.47	122.19	124.45
24	B	817	CLA	CHD-C1D-ND	-2.46	122.19	124.45
24	A	830	CLA	C2A-C1A-CHA	2.46	128.16	123.86
25	B	841	BCR	C30-C25-C26	-2.46	119.15	122.61
26	h	615	DD6	C9-C8-C6	2.46	133.33	126.42
26	6	617	DD6	C25-C26-C27	-2.46	119.44	126.58
24	B	809	CLA	CHD-C1D-ND	-2.46	122.19	124.45
24	B	847	CLA	CMB-C2B-C3B	2.46	129.28	124.68
25	A	844	BCR	C34-C9-C8	2.46	121.95	118.08
26	9	315	DD6	C12-C11-C10	-2.46	119.48	122.92
24	6	610	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	I	101	BCR	C8-C9-C10	-2.45	115.17	118.94
25	k	316	BCR	C20-C19-C18	-2.45	119.52	126.42
26	9	317	DD6	C19-C18-C17	2.45	115.51	110.77
24	t	301	CLA	CHD-C1D-ND	-2.45	122.20	124.45
24	A	840	CLA	CHD-C1D-ND	-2.45	122.20	124.45
24	A	853	CLA	CHD-C1D-ND	-2.45	122.20	124.45
24	B	829	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	B	848	CLA	CHD-C1D-ND	-2.45	122.20	124.45
24	A	804	CLA	CMB-C2B-C3B	2.45	129.25	124.68
26	4	616	DD6	C9-C10-C11	-2.44	123.82	127.31
24	A	833	CLA	CHD-C1D-ND	-2.44	122.21	124.45
26	5	608	DD6	C15-C14-C13	-2.44	120.83	125.99
24	7	610	CLA	CHD-C1D-ND	-2.44	122.21	124.45
24	A	807	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	9	315	DD6	C25-C26-C27	-2.44	119.50	126.58
24	2	204	CLA	CHD-C1D-ND	-2.44	122.21	124.45
28	A	841	LHG	O8-C23-C24	2.44	119.56	111.91
25	B	841	BCR	C19-C18-C17	-2.44	115.20	118.94
24	c	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	2	211	BCR	C36-C18-C19	2.44	121.92	118.08
24	6	606	CLA	CHD-C1D-ND	-2.44	122.22	124.45
24	t	310	CLA	CHD-C1D-ND	-2.44	122.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	614	DD6	C9-C10-C11	-2.44	123.83	127.31
24	B	817	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	B	840	BCR	C24-C23-C22	-2.43	122.56	126.23
24	7	609	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	A	812	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	B	808	CLA	CMB-C2B-C3B	2.43	129.23	124.68
25	c	615	BCR	C24-C25-C26	-2.43	115.57	121.46
24	k	308	CLA	C1D-ND-C4D	-2.43	104.61	106.33
26	8	211	DD6	C33-C34-C35	-2.43	106.98	110.30
26	8	210	DD6	C34-C35-C36	-2.43	107.01	111.85
24	1	306	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	7	608	CLA	CHD-C1D-ND	-2.43	122.22	124.45
30	2	214	LMG	C8-O7-C10	-2.43	111.81	117.79
24	t	301	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	8	205	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	4	607	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	c	603	CLA	CHD-C1D-ND	-2.43	122.22	124.45
24	B	822	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
24	9	311	CLA	CHD-C1D-ND	-2.42	122.23	124.45
25	k	316	BCR	C33-C5-C4	2.42	118.27	113.62
24	B	847	CLA	CHD-C1D-ND	-2.42	122.23	124.45
24	8	204	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	9	314	DD6	C15-C14-C13	-2.42	120.87	125.99
25	L	202	BCR	C1-C6-C5	-2.42	119.20	122.61
26	3	313	DD6	C25-C24-C1	-2.42	119.62	126.42
28	2	215	LHG	O8-C23-C24	2.42	119.50	111.91
25	k	316	BCR	C2-C1-C6	2.42	114.20	110.48
26	7	613	DD6	C7-C6-C8	2.41	121.88	118.08
29	9	312	A1L1G	C3-C6-C1	2.41	111.56	109.21
25	L	206	BCR	C16-C15-C14	-2.41	118.53	123.47
25	B	840	BCR	C28-C27-C26	-2.41	109.77	114.08
24	A	832	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	B	810	CLA	O2D-CGD-CBD	2.41	115.56	111.27
26	6	615	DD6	O1-C20-C21	-2.41	112.17	115.06
26	9	315	DD6	C-C1-C2	-2.41	119.55	122.92
25	R	101	BCR	C3-C4-C5	-2.41	109.77	114.08
24	B	802	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	5	605	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	A	859	BCR	C37-C22-C21	-2.41	119.55	122.92
25	A	845	BCR	C23-C24-C25	-2.40	120.45	127.20
25	A	843	BCR	C29-C30-C25	2.40	114.18	110.48
25	B	843	BCR	C2-C1-C6	-2.40	106.78	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
24	A	835	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	4	616	DD6	C25-C24-C1	-2.40	119.67	126.42
26	2	212	DD6	C-C1-C2	-2.40	119.56	122.92
25	B	843	BCR	C3-C4-C5	-2.40	109.79	114.08
26	7	618	DD6	C25-C24-C1	-2.40	119.68	126.42
25	c	615	BCR	C36-C18-C17	-2.40	119.56	122.92
25	L	202	BCR	C15-C16-C17	-2.40	118.56	123.47
24	7	603	CLA	CHD-C1D-ND	-2.40	122.25	124.45
24	A	840	CLA	O2D-CGD-CBD	2.40	115.53	111.27
25	B	840	BCR	C3-C4-C5	-2.40	109.80	114.08
26	9	315	DD6	C41-C32-C31	-2.39	106.66	110.47
24	A	860	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
26	k	315	DD6	C3-C4-C5	-2.39	118.57	123.47
27	A	851	LMT	O3'-C3'-C2'	-2.39	104.82	110.35
25	A	846	BCR	C23-C22-C21	-2.39	115.27	118.94
25	I	102	BCR	C38-C26-C27	2.39	118.21	113.62
26	4	616	DD6	C4-C3-C2	-2.39	118.58	123.47
24	3	302	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	4	618	BCR	C30-C25-C26	-2.39	119.25	122.61
25	2	211	BCR	C29-C30-C25	2.39	114.16	110.48
25	M	101	BCR	C36-C18-C17	-2.39	119.58	122.92
25	1	310	BCR	C24-C23-C22	-2.39	122.63	126.23
25	B	843	BCR	C38-C26-C27	2.38	118.19	113.62
25	J	101	BCR	C28-C27-C26	-2.38	109.82	114.08
26	7	618	DD6	C-C1-C2	-2.38	119.59	122.92
24	1	305	CLA	O1A-CGA-CBA	2.38	130.73	123.08
24	B	833	CLA	CHB-C4A-NA	2.38	127.81	124.51
31	A	839	PQN	C11-C3-C4	-2.38	115.95	118.50
24	B	846	CLA	CHD-C1D-ND	-2.38	122.27	124.45
26	4	614	DD6	C25-C24-C1	-2.38	119.73	126.42
24	L	204	CLA	CMB-C2B-C3B	2.38	129.13	124.68
25	1	310	BCR	C35-C13-C12	2.38	121.83	118.08
25	A	846	BCR	C37-C22-C21	-2.38	119.59	122.92
26	6	616	DD6	O1-C20-C21	2.38	117.91	115.06
24	k	302	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	c	613	DD6	C25-C26-C27	-2.38	119.68	126.58
24	c	601	CLA	CBA-CAA-C2A	-2.38	109.00	114.02
24	9	301	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	t	309	CLA	CHD-C1D-ND	-2.38	122.27	124.45
24	9	306	CLA	C2A-C1A-CHA	2.37	128.01	123.86
25	B	843	BCR	C35-C13-C14	-2.37	119.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	212	DD6	C25-C26-C27	-2.37	119.69	126.58
24	4	603	CLA	CHD-C1D-ND	-2.37	122.27	124.45
24	L	203	CLA	CHD-C1D-ND	-2.37	122.27	124.45
25	I	102	BCR	C31-C1-C6	2.37	114.14	110.30
26	9	313	DD6	C10-C9-C8	-2.37	115.82	123.22
24	B	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	k	306	CLA	CHD-C1D-ND	-2.37	122.28	124.45
25	M	101	BCR	C3-C4-C5	-2.37	109.85	114.08
24	3	306	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	A	816	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
26	h	616	DD6	C4-C3-C2	-2.37	118.62	123.47
25	L	202	BCR	C23-C24-C25	-2.37	120.55	127.20
24	A	831	CLA	CHD-C1D-ND	-2.37	122.28	124.45
24	h	603	CLA	CHD-C1D-ND	-2.37	122.28	124.45
26	6	615	DD6	C7-C6-C8	2.36	121.80	118.08
24	k	303	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	B	842	BCR	C23-C22-C21	2.36	122.57	118.94
26	6	615	DD6	C33-C32-C31	2.36	114.41	109.62
24	B	827	CLA	CHD-C1D-ND	-2.36	122.28	124.45
24	A	853	CLA	C1-C2-C3	-2.36	121.96	126.04
26	c	613	DD6	C10-C9-C8	-2.36	115.84	123.22
26	8	212	DD6	C12-C11-C10	-2.36	119.61	122.92
24	B	801	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	3	308	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	A	819	CLA	CHD-C1D-ND	-2.36	122.29	124.45
26	2	210	DD6	C-C1-C2	-2.36	119.62	122.92
25	F	204	BCR	C15-C16-C17	-2.36	118.64	123.47
24	k	305	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	A	817	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	A	848	DD6	C12-C11-C13	2.36	121.79	118.08
24	A	816	CLA	CHB-C4A-NA	2.35	127.77	124.51
26	8	211	DD6	C34-C35-C36	-2.35	107.17	111.85
24	k	309	CLA	CHB-C4A-NA	2.35	127.77	124.51
26	J	102	DD6	C25-C24-C1	-2.35	119.80	126.42
24	B	832	CLA	CMB-C2B-C3B	2.35	129.08	124.68
26	5	609	DD6	C10-C9-C8	-2.35	115.88	123.22
25	9	316	BCR	C23-C24-C25	-2.35	120.60	127.20
25	B	840	BCR	C15-C16-C17	-2.35	118.66	123.47
24	4	606	CLA	CHD-C1D-ND	-2.35	122.30	124.45
26	9	317	DD6	C25-C26-C27	-2.35	119.76	126.58
24	5	604	CLA	CHD-C1D-ND	-2.35	122.30	124.45
24	8	204	CLA	CHD-C1D-ND	-2.35	122.30	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	838	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
28	B	844	LHG	C5-O7-C7	-2.35	112.02	117.79
24	8	203	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	2	206	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	A	808	CLA	CAA-CBA-CGA	-2.34	106.40	113.25
24	2	201	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	7	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	h	608	CLA	CHD-C1D-ND	-2.34	122.30	124.45
26	9	317	DD6	C34-C35-C36	-2.34	107.19	111.85
24	A	860	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	J	104	BCR	C23-C22-C21	-2.34	115.35	118.94
24	A	824	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	t	305	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	1	313	DD6	C7-C6-C8	2.34	121.76	118.08
24	7	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	4	609	CLA	CHD-C1D-ND	-2.34	122.31	124.45
24	A	803	CLA	CHB-C4A-NA	2.34	127.74	124.51
24	h	607	CLA	CMB-C2B-C3B	2.34	129.05	124.68
24	A	830	CLA	O2D-CGD-CBD	2.34	115.42	111.27
25	B	849	BCR	C38-C26-C27	2.34	118.10	113.62
24	6	609	CLA	CHB-C4A-NA	2.34	127.74	124.51
26	6	613	DD6	C10-C9-C8	-2.33	115.93	123.22
26	7	615	DD6	C4-C3-C2	-2.33	118.69	123.47
25	A	859	BCR	C36-C18-C17	-2.33	119.66	122.92
24	7	604	CLA	CHD-C1D-ND	-2.33	122.31	124.45
26	k	313	DD6	C4-C3-C2	-2.33	118.70	123.47
26	5	608	DD6	C25-C24-C1	-2.33	119.87	126.42
26	3	313	DD6	C4-C5-C6	-2.33	123.99	127.31
26	t	313	DD6	C26-C25-C24	-2.33	115.95	123.22
26	4	614	DD6	C14-C13-C11	-2.33	121.92	125.53
25	A	844	BCR	C15-C16-C17	-2.33	118.71	123.47
25	A	843	BCR	C38-C26-C25	-2.33	121.92	124.53
24	B	810	CLA	CHB-C4A-NA	2.32	127.73	124.51
25	F	204	BCR	C33-C5-C4	2.32	118.08	113.62
25	R	102	BCR	C19-C18-C17	-2.32	115.38	118.94
24	A	807	CLA	O2D-CGD-CBD	2.32	115.39	111.27
24	6	609	CLA	CHD-C1D-ND	-2.32	122.32	124.45
25	A	846	BCR	C15-C14-C13	-2.32	124.00	127.31
25	A	843	BCR	C23-C24-C25	-2.32	120.68	127.20
24	A	840	CLA	C1-C2-C3	-2.32	122.03	126.04
24	B	814	CLA	CHD-C1D-ND	-2.32	122.32	124.45
24	A	838	CLA	O2A-CGA-O1A	-2.32	117.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	210	DD6	C25-C26-C27	-2.32	119.85	126.58
25	7	617	BCR	C11-C10-C9	-2.32	124.00	127.31
26	h	614	DD6	C33-C34-C35	2.32	113.48	110.30
24	B	818	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
25	A	845	BCR	C30-C25-C26	-2.32	119.35	122.61
25	7	617	BCR	C37-C22-C23	2.32	121.73	118.08
28	J	105	LHG	O8-C23-C24	2.32	119.18	111.91
25	A	846	BCR	C19-C18-C17	-2.32	115.39	118.94
24	B	808	CLA	CHB-C4A-NA	2.32	127.71	124.51
26	R	105	DD6	C19-C18-C17	2.31	115.24	110.77
26	9	313	DD6	C4-C3-C2	-2.31	118.74	123.47
24	4	604	CLA	CHD-C1D-ND	-2.31	122.33	124.45
24	B	829	CLA	O2D-CGD-CBD	2.31	115.38	111.27
24	2	208	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	1	313	DD6	C9-C10-C11	-2.31	124.01	127.31
28	A	852	LHG	O8-C23-C24	2.31	119.16	111.91
24	B	804	CLA	CHA-C1A-NA	-2.31	121.11	126.40
25	A	846	BCR	C29-C30-C25	2.31	114.04	110.48
24	7	612	CLA	O1D-CGD-CBD	2.31	129.21	124.48
25	J	104	BCR	C36-C18-C17	-2.31	119.69	122.92
25	B	841	BCR	C32-C1-C6	-2.31	106.56	110.30
24	9	304	CLA	CBA-CAA-C2A	-2.31	107.05	113.86
24	B	812	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	c	609	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	h	606	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	c	610	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	A	844	BCR	C21-C20-C19	-2.30	116.02	123.22
24	B	802	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	3	311	DD6	C25-C26-C27	-2.30	119.89	126.58
24	B	821	CLA	CHD-C1D-ND	-2.30	122.34	124.45
24	9	311	CLA	CHB-C4A-NA	2.30	127.70	124.51
24	B	803	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	A	825	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	A	846	BCR	C24-C23-C22	-2.30	122.76	126.23
25	A	846	BCR	C24-C25-C26	-2.30	115.89	121.46
24	k	306	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	2	211	BCR	C16-C15-C14	-2.30	118.76	123.47
25	4	618	BCR	C1-C6-C5	-2.30	119.37	122.61
24	A	811	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	2	211	BCR	C4-C5-C6	-2.30	119.39	122.73
26	7	618	DD6	C34-C35-C36	-2.30	107.28	111.85
24	A	847	CLA	O2A-CGA-O1A	-2.30	117.79	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	206	BCR	C30-C25-C24	2.30	122.28	115.78
24	B	814	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
25	A	846	BCR	C12-C13-C14	-2.30	115.42	118.94
25	B	849	BCR	C8-C9-C10	-2.30	115.42	118.94
24	9	303	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
25	R	101	BCR	C16-C15-C14	-2.29	118.77	123.47
25	J	104	BCR	C33-C5-C4	2.29	118.02	113.62
26	8	210	DD6	C20-C19-C18	2.29	117.29	112.75
24	B	816	CLA	C1-C2-C3	-2.29	122.08	126.04
24	A	829	CLA	CHD-C1D-ND	-2.29	122.35	124.45
26	1	313	DD6	C12-C11-C13	2.29	121.69	118.08
24	A	837	CLA	O2D-CGD-CBD	2.29	115.34	111.27
26	3	311	DD6	C10-C9-C8	-2.29	116.07	123.22
24	A	819	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	B	840	BCR	C15-C14-C13	-2.29	124.05	127.31
26	t	311	DD6	C25-C24-C1	-2.29	120.00	126.42
24	6	607	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	c	607	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	1	317	CLA	CHB-C4A-NA	2.28	127.67	124.51
30	2	214	LMG	O8-C28-C29	2.28	119.07	111.91
24	8	202	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	A	821	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	h	602	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	B	849	BCR	C24-C23-C22	-2.28	122.79	126.23
26	5	608	DD6	C20-C19-C18	2.28	117.26	112.75
24	3	302	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	9	316	BCR	C37-C22-C21	-2.28	119.73	122.92
26	R	105	DD6	C4-C3-C2	-2.28	118.81	123.47
25	J	104	BCR	C23-C24-C25	-2.28	120.81	127.20
25	9	316	BCR	C11-C12-C13	-2.28	120.02	126.42
26	4	616	DD6	C33-C34-C35	-2.28	107.19	110.30
24	1	303	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	B	840	BCR	C16-C15-C14	-2.27	118.82	123.47
24	B	815	CLA	CHB-C4A-NA	2.27	127.66	124.51
24	A	834	CLA	O2D-CGD-CBD	2.27	115.31	111.27
26	h	614	DD6	C10-C9-C8	-2.27	116.13	123.22
24	2	207	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	1	317	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
26	h	613	DD6	C25-C26-C27	-2.27	119.98	126.58
24	6	612	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	J	101	BCR	C30-C25-C24	2.27	122.20	115.78
24	h	610	CLA	C4A-NA-C1A	2.27	107.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	827	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	c	612	DD6	C25-C24-C1	-2.27	120.04	126.42
26	4	616	DD6	C12-C11-C13	2.27	121.65	118.08
24	A	817	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
27	A	851	LMT	C1B-O1B-C4'	-2.27	112.35	117.96
24	L	203	CLA	O2D-CGD-CBD	2.27	115.30	111.27
26	6	615	DD6	O1-C20-C19	2.27	115.08	113.38
28	A	841	LHG	C5-O7-C7	-2.27	112.21	117.79
24	7	605	CLA	CHD-C1D-ND	-2.27	122.37	124.45
24	A	804	CLA	CHB-C4A-NA	2.27	127.64	124.51
24	A	815	CLA	CMB-C2B-C3B	2.27	128.92	124.68
24	A	830	CLA	C4D-CHA-C1A	2.26	124.00	121.25
24	B	825	CLA	CHD-C1D-ND	-2.26	122.37	124.45
24	1	304	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
26	1	311	DD6	C25-C26-C27	-2.26	120.01	126.58
24	A	860	CLA	C16-C15-C13	-2.26	108.61	115.92
25	2	211	BCR	C37-C22-C23	2.26	121.64	118.08
25	c	615	BCR	C34-C9-C10	-2.26	119.76	122.92
24	k	301	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	A	843	BCR	C2-C1-C6	2.26	113.96	110.48
24	3	303	CLA	CHD-C1D-ND	-2.26	122.38	124.45
24	B	834	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	6	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	A	832	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	7	617	BCR	C27-C26-C25	-2.26	119.45	122.73
24	B	830	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
25	B	841	BCR	C23-C22-C21	-2.25	115.48	118.94
26	J	102	DD6	C25-C26-C27	-2.25	120.04	126.58
26	6	616	DD6	C12-C11-C10	-2.25	119.77	122.92
26	7	613	DD6	C12-C11-C13	2.25	121.62	118.08
24	A	836	CLA	O2D-CGD-CBD	2.25	115.27	111.27
25	1	314	BCR	C36-C18-C17	-2.25	119.77	122.92
25	R	102	BCR	C7-C6-C5	2.25	126.91	121.46
25	F	204	BCR	C23-C24-C25	-2.25	120.89	127.20
26	h	615	DD6	C25-C24-C1	-2.25	120.10	126.42
24	1	308	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	t	313	DD6	C4-C3-C2	-2.24	118.88	123.47
24	A	813	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
26	R	105	DD6	C37-C36-C31	-2.24	121.30	124.35
24	B	817	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	h	605	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	B	829	CLA	C2A-C1A-CHA	2.24	127.78	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	101	BCR	C27-C26-C25	-2.24	119.48	122.73
25	B	849	BCR	C4-C5-C6	-2.24	119.48	122.73
24	J	103	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	B	814	CLA	C1-C2-C3	-2.24	123.13	126.75
24	c	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	t	304	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	A	846	BCR	C16-C15-C14	-2.24	118.89	123.47
25	B	849	BCR	C10-C11-C12	-2.24	116.24	123.22
24	h	601	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	7	615	DD6	C10-C9-C8	-2.23	116.25	123.22
24	R	103	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	J	102	DD6	C9-C10-C11	-2.23	124.12	127.31
27	1	315	LMT	O1B-C4'-C3'	2.23	113.22	107.28
26	4	614	DD6	C4-C3-C2	-2.23	118.90	123.47
26	1	312	DD6	C12-C11-C10	-2.23	119.80	122.92
24	B	805	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	I	102	BCR	C24-C25-C26	-2.23	116.06	121.46
25	I	101	BCR	C31-C1-C6	-2.23	106.68	110.30
24	A	807	CLA	CHD-C1D-ND	-2.23	122.41	124.45
24	A	803	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	7	615	DD6	C25-C24-C1	-2.23	120.15	126.42
24	h	604	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	B	837	CLA	CHB-C4A-NA	2.23	127.59	124.51
26	2	210	DD6	O1-C20-C19	-2.23	111.71	113.38
24	8	205	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	k	310	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	t	308	CLA	C4A-NA-C1A	2.23	107.71	106.71
24	A	801	CLA	C2A-C1A-CHA	2.23	127.75	123.86
26	k	313	DD6	C7-C6-C8	2.23	121.58	118.08
25	B	849	BCR	C2-C1-C6	2.23	113.91	110.48
24	A	835	CLA	CHD-C1D-ND	-2.23	122.41	124.45
26	1	311	DD6	C10-C9-C8	-2.22	116.27	123.22
25	7	617	BCR	C20-C21-C22	-2.22	124.14	127.31
24	8	203	CLA	CHB-C4A-NA	2.22	127.59	124.51
26	k	314	DD6	C-C1-C2	-2.22	119.81	122.92
24	B	836	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	B	838	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	1	311	DD6	C7-C6-C8	2.22	121.58	118.08
24	A	805	CLA	O2D-CGD-CBD	2.22	115.22	111.27
25	A	859	BCR	C8-C7-C6	-2.22	120.96	127.20
24	B	828	CLA	C1-C2-C3	-2.22	123.16	126.75
25	R	101	BCR	C15-C16-C17	-2.22	118.93	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	303	CLA	C4-C3-C2	-2.22	117.98	123.68
25	A	845	BCR	C4-C5-C6	-2.22	122.33	124.51
24	B	806	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	B	846	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	9	312	A1L1G	C36-C37-C38	2.22	128.02	123.47
25	L	206	BCR	C11-C10-C9	-2.22	124.14	127.31
24	A	832	CLA	O2D-CGD-CBD	2.22	115.21	111.27
27	A	851	LMT	C1'-O5'-C5'	-2.22	109.34	113.69
24	B	828	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	A	830	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
24	B	820	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	c	615	BCR	C1-C6-C7	2.22	122.05	115.78
24	1	302	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	3	305	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	L	202	BCR	C23-C22-C21	-2.21	115.55	118.94
25	4	618	BCR	C4-C5-C6	-2.21	119.52	122.73
24	6	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	B	820	CLA	C1-C2-C3	-2.21	122.22	126.04
24	5	607	CLA	CHD-C1D-ND	-2.21	122.42	124.45
24	A	826	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	A	829	CLA	CHB-C4A-NA	2.21	127.57	124.51
26	9	317	DD6	C3-C4-C5	2.21	128.00	123.47
24	4	603	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	h	610	CLA	CHB-C4A-NA	2.21	127.57	124.51
29	3	310	A1L1G	C28-C39-C38	-2.21	119.83	122.92
25	I	102	BCR	C12-C13-C14	-2.21	115.55	118.94
24	A	828	CLA	CHD-C1D-ND	-2.21	122.42	124.45
24	4	611	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	8	206	CLA	CHB-C4A-NA	2.21	127.56	124.51
24	4	609	CLA	CHB-C4A-NA	2.21	127.56	124.51
24	B	811	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	c	613	DD6	C34-C35-C36	-2.21	107.46	111.85
24	B	827	CLA	CHB-C4A-NA	2.21	127.56	124.51
26	8	211	DD6	C10-C9-C8	-2.21	116.33	123.22
24	A	805	CLA	CHB-C4A-NA	2.20	127.56	124.51
25	R	102	BCR	C4-C5-C6	-2.20	119.53	122.73
25	B	841	BCR	C21-C20-C19	-2.20	116.34	123.22
24	A	814	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	3	313	DD6	C9-C8-C6	2.20	132.60	126.42
24	9	305	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	B	831	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	8	212	DD6	C7-C6-C8	2.20	121.55	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	316	BCR	C8-C7-C6	-2.20	121.02	127.20
24	9	307	CLA	O2D-CGD-CBD	2.20	115.18	111.27
25	A	844	BCR	C10-C11-C12	-2.20	116.35	123.22
24	c	609	CLA	C4-C3-C5	2.20	118.97	115.27
26	6	615	DD6	C32-C33-C34	2.20	118.61	113.64
24	9	310	CLA	CHB-C4A-NA	2.20	127.55	124.51
26	k	315	DD6	O1-C20-C21	-2.20	112.42	115.06
25	R	101	BCR	C4-C5-C6	-2.20	119.54	122.73
28	2	215	LHG	C5-O7-C7	-2.20	112.38	117.79
26	7	618	DD6	C12-C11-C10	-2.20	119.85	122.92
24	A	820	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	3	305	CLA	C1-C2-C3	-2.19	122.25	126.04
25	I	101	BCR	C19-C18-C17	-2.19	115.57	118.94
24	6	601	CLA	CHB-C4A-NA	2.19	127.55	124.51
24	B	821	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	4	618	BCR	C37-C22-C21	-2.19	119.85	122.92
24	4	612	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	R	105	DD6	C20-C19-C18	2.19	117.09	112.75
26	c	612	DD6	C-C1-C2	-2.19	119.85	122.92
24	8	202	CLA	C2A-C1A-CHA	2.19	127.69	123.86
26	7	613	DD6	C-C1-C2	-2.19	119.85	122.92
24	6	609	CLA	C1-C2-C3	-2.19	123.20	126.75
24	h	610	CLA	C1D-ND-C4D	-2.19	104.78	106.33
26	1	311	DD6	C-C1-C2	-2.19	119.85	122.92
25	I	102	BCR	C24-C23-C22	-2.19	122.92	126.23
24	8	201	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	3	311	DD6	C25-C24-C1	-2.19	120.26	126.42
24	4	601	CLA	CHD-C1D-ND	-2.19	122.44	124.45
24	B	833	CLA	CHD-C1D-ND	-2.19	122.44	124.45
24	2	201	CLA	C2D-C1D-ND	-2.19	108.49	110.10
26	h	615	DD6	C37-C36-C31	-2.19	121.38	124.35
24	4	607	CLA	CHB-C4A-NA	2.19	127.54	124.51
24	7	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
24	7	611	CLA	CHB-C4A-NA	2.19	127.54	124.51
24	A	801	CLA	C4D-C3D-CAD	-2.19	105.52	108.10
24	3	304	CLA	CHB-C4A-NA	2.19	127.53	124.51
25	A	844	BCR	C38-C26-C27	2.19	117.81	113.62
25	2	211	BCR	C1-C6-C5	-2.18	119.54	122.61
26	3	311	DD6	C7-C6-C8	2.18	121.52	118.08
24	t	309	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	B	821	CLA	CAC-C3C-C4C	2.18	127.64	124.81
24	k	311	CLA	CHB-C4A-NA	2.18	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	102	BCR	C10-C11-C12	-2.18	116.42	123.22
25	I	101	BCR	C12-C13-C14	-2.18	115.60	118.94
24	2	202	CLA	C1-C2-C3	-2.18	122.28	126.04
25	M	101	BCR	C38-C26-C27	2.18	117.80	113.62
26	6	617	DD6	C25-C24-C1	-2.18	120.30	126.42
24	A	826	CLA	C1-C2-C3	-2.18	122.28	126.04
24	B	822	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	A	845	BCR	C27-C26-C25	-2.18	119.57	122.73
24	3	303	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	A	810	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
25	F	204	BCR	C35-C13-C14	-2.18	119.88	122.92
24	7	604	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	A	830	CLA	C2D-C1D-ND	-2.17	108.50	110.10
24	A	838	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	4	606	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	B	824	CLA	C1-C2-C3	-2.17	122.28	126.04
25	B	841	BCR	C15-C14-C13	-2.17	124.21	127.31
25	L	202	BCR	C8-C7-C6	-2.17	121.10	127.20
24	A	809	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	6	617	DD6	C10-C9-C8	-2.17	116.44	123.22
29	9	312	A1L1G	C27-C34-C35	-2.17	119.89	122.92
24	B	809	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	k	315	DD6	C26-C25-C24	-2.17	116.45	123.22
28	1	318	LHG	C9-C8-C7	-2.17	105.74	113.62
24	4	605	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	A	810	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	t	312	BCR	C8-C7-C6	-2.17	121.12	127.20
24	3	301	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	t	306	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	A	831	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	B	825	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	J	104	BCR	C1-C6-C5	-2.16	119.57	122.61
25	I	102	BCR	C23-C22-C21	-2.16	115.62	118.94
25	R	101	BCR	C37-C22-C21	-2.16	119.89	122.92
24	6	608	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	8	211	DD6	C12-C11-C13	2.16	121.48	118.08
24	B	815	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	t	314	LMG	O8-C28-C29	2.16	118.68	111.91
24	A	833	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	7	617	BCR	C34-C9-C8	2.16	121.48	118.08
25	1	314	BCR	C38-C26-C27	2.16	117.76	113.62
24	8	207	CLA	CHD-C1D-ND	-2.16	122.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	615	DD6	C-C1-C24	2.16	121.48	118.08
24	4	613	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	1	311	DD6	C32-C31-C36	-2.16	119.59	122.63
24	A	837	CLA	CHB-C4A-NA	2.16	127.49	124.51
24	B	816	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
24	A	820	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
25	1	314	BCR	C11-C12-C13	-2.15	120.37	126.42
24	9	309	CLA	C2A-C1A-CHA	2.15	127.62	123.86
26	k	314	DD6	C26-C25-C24	-2.15	116.50	123.22
28	4	619	LHG	O8-C23-C24	2.15	118.66	111.91
26	J	102	DD6	C7-C6-C8	2.15	121.47	118.08
26	3	312	DD6	C26-C25-C24	-2.15	116.50	123.22
25	t	312	BCR	C38-C26-C27	2.15	117.75	113.62
24	4	608	CLA	CHB-C4A-NA	2.15	127.48	124.51
24	6	602	CLA	O2D-CGD-CBD	2.15	115.09	111.27
24	7	606	CLA	CED-O2D-CGD	2.15	120.80	115.94
25	A	859	BCR	C33-C5-C6	-2.15	122.11	124.53
24	2	203	CLA	C1-C2-C3	-2.15	123.28	126.75
25	A	843	BCR	C37-C22-C21	-2.15	119.91	122.92
24	A	853	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	J	102	DD6	C12-C11-C13	2.15	121.46	118.08
24	B	818	CLA	O2D-CGD-CBD	2.15	115.08	111.27
26	5	608	DD6	C41-C32-C31	-2.15	107.06	110.47
24	c	602	CLA	CHB-C4A-NA	2.15	127.48	124.51
24	A	818	CLA	CHB-C4A-NA	2.15	127.48	124.51
24	A	825	CLA	O2D-CGD-CBD	2.15	115.08	111.27
24	3	308	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
26	6	613	DD6	C12-C11-C13	2.14	121.46	118.08
24	k	309	CLA	O2A-CGA-O1A	-2.14	117.95	123.30
26	7	618	DD6	C33-C32-C31	2.14	113.96	109.62
25	M	101	BCR	C33-C5-C6	-2.14	122.12	124.53
26	6	615	DD6	C25-C26-C27	-2.14	120.36	126.58
25	2	211	BCR	C27-C26-C25	-2.14	119.62	122.73
26	9	315	DD6	C4-C5-C6	-2.14	124.25	127.31
24	c	603	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
24	B	847	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	1	310	BCR	C30-C25-C26	-2.14	119.60	122.61
26	4	616	DD6	C-C1-C2	-2.14	119.93	122.92
26	h	614	DD6	C4-C3-C2	-2.14	119.09	123.47
26	8	212	DD6	C25-C26-C27	-2.14	120.38	126.58
24	B	811	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	A	836	CLA	CMB-C2B-C3B	2.14	128.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	613	DD6	C26-C25-C24	-2.14	116.55	123.22
24	B	834	CLA	O2D-CGD-CBD	2.13	115.06	111.27
26	h	613	DD6	C7-C6-C8	2.13	121.44	118.08
24	A	804	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	2	201	CLA	C3A-C2A-C1A	2.13	104.53	101.34
26	h	616	DD6	C12-C11-C10	-2.13	119.94	122.92
26	h	613	DD6	C12-C11-C13	2.13	121.44	118.08
26	9	317	DD6	C20-C19-C18	2.13	116.97	112.75
25	A	846	BCR	C30-C25-C26	-2.13	119.61	122.61
24	8	204	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
25	I	101	BCR	C10-C11-C12	-2.13	116.58	123.22
24	8	203	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
28	I	103	LHG	O7-C7-O9	-2.13	118.56	123.70
24	3	302	CLA	O2D-CGD-CBD	2.13	115.05	111.27
24	A	836	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
24	h	605	CLA	O2D-CGD-CBD	2.13	115.05	111.27
24	1	307	CLA	CHB-C4A-NA	2.13	127.45	124.51
24	B	803	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	6	605	CLA	O2D-CGD-CBD	2.12	115.04	111.27
26	5	609	DD6	C7-C6-C8	2.12	121.42	118.08
24	A	834	CLA	CHB-C4A-NA	2.12	127.45	124.51
26	J	102	DD6	C4-C3-C2	-2.12	119.12	123.47
24	A	835	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	5	608	DD6	C10-C9-C8	-2.12	116.59	123.22
26	4	617	DD6	C26-C25-C24	-2.12	116.59	123.22
24	A	833	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	B	822	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	9	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
24	B	807	CLA	O2D-CGD-CBD	2.12	115.04	111.27
24	B	821	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	c	608	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	9	301	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	1	304	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	2	212	DD6	C25-C24-C1	-2.12	120.46	126.42
24	6	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	9	316	BCR	C34-C9-C10	-2.12	119.96	122.92
24	A	801	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	h	615	DD6	C26-C25-C24	-2.12	116.61	123.22
24	B	847	CLA	O2D-CGD-CBD	2.12	115.03	111.27
24	B	814	CLA	CHB-C4A-NA	2.12	127.44	124.51
27	1	316	LMT	C2'-C3'-C4'	-2.12	104.85	109.68
24	4	601	CLA	CHB-C4A-NA	2.12	127.44	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	607	CLA	O2D-CGD-CBD	2.11	115.03	111.27
24	6	606	CLA	CHB-C4A-NA	2.11	127.44	124.51
24	F	203	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	B	848	CLA	CHB-C4A-NA	2.11	127.44	124.51
24	B	820	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	3	304	CLA	CHA-C1A-NA	-2.11	121.56	126.40
25	B	840	BCR	C38-C26-C25	-2.11	122.16	124.53
24	8	205	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
29	2	213	A1L1G	C27-C34-C35	-2.11	119.97	122.92
25	L	202	BCR	C33-C5-C4	2.11	117.67	113.62
25	1	310	BCR	C10-C11-C12	-2.11	116.63	123.22
24	A	815	CLA	O2D-CGD-CBD	2.11	115.02	111.27
26	4	614	DD6	C10-C9-C8	-2.11	116.63	123.22
24	5	606	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	h	612	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	1	312	DD6	C23-C16-C15	2.11	115.74	110.05
24	6	601	CLA	O2A-CGA-O1A	-2.11	118.04	123.30
24	B	838	CLA	O2D-CGD-CBD	2.11	115.01	111.27
24	A	829	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	A	818	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	h	610	CLA	O2D-CGD-CBD	2.11	115.01	111.27
24	B	821	CLA	O2D-CGD-CBD	2.11	115.01	111.27
26	4	615	DD6	C7-C6-C8	2.11	121.40	118.08
26	t	313	DD6	C12-C11-C13	2.11	121.40	118.08
27	h	617	LMT	O5B-C5B-C4B	2.11	113.52	109.69
24	c	605	CLA	CHD-C1D-ND	-2.11	122.52	124.45
24	A	812	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
24	c	602	CLA	O2D-CGD-CBD	2.10	115.01	111.27
24	A	822	CLA	C1-C2-C3	-2.10	122.41	126.04
24	B	826	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	A	859	BCR	C8-C9-C10	-2.10	115.72	118.94
25	A	859	BCR	C3-C4-C5	-2.10	110.33	114.08
26	c	612	DD6	C33-C32-C31	2.10	113.88	109.62
26	k	313	DD6	C-C1-C24	2.10	121.39	118.08
26	4	617	DD6	C25-C24-C1	-2.10	120.52	126.42
24	F	201	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	9	313	DD6	C14-C13-C11	-2.10	122.27	125.53
27	A	851	LMT	C1'-C2'-C3'	2.10	114.36	110.00
24	F	202	CLA	CHB-C4A-NA	2.10	127.41	124.51
24	1	301	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	B	802	CLA	CHB-C4A-NA	2.09	127.41	124.51
26	A	848	DD6	C10-C9-C8	-2.09	116.68	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	311	DD6	C12-C11-C13	2.09	121.38	118.08
24	3	305	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	A	847	CLA	C4-C3-C5	2.09	118.79	115.27
24	A	815	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	A	807	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	B	835	CLA	O2D-CGD-CBD	2.09	114.99	111.27
24	t	302	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	t	301	CLA	CAA-C2A-C1A	2.09	118.83	111.97
24	A	837	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
25	A	845	BCR	C3-C4-C5	-2.09	107.79	112.24
26	1	312	DD6	C12-C11-C13	2.09	121.37	118.08
25	1	314	BCR	C27-C26-C25	-2.09	119.70	122.73
24	8	207	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	L	204	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	R	104	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
24	B	804	CLA	O1D-CGD-CBD	2.09	128.76	124.48
24	c	609	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	A	818	CLA	O2D-CGD-CBD	2.09	114.98	111.27
24	B	810	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	7	615	DD6	C12-C11-C10	-2.09	120.00	122.92
26	t	311	DD6	C-C1-C2	-2.09	120.00	122.92
24	t	310	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	7	607	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
24	h	607	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	B	827	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	A	845	BCR	C16-C15-C14	-2.08	119.20	123.47
24	B	809	CLA	CBA-CAA-C2A	-2.08	107.71	113.86
24	9	303	CLA	C2A-C1A-CHA	2.08	127.50	123.86
25	B	842	BCR	C4-C5-C6	-2.08	119.71	122.73
24	A	806	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	1	310	BCR	C21-C20-C19	-2.08	116.72	123.22
25	J	101	BCR	C3-C4-C5	-2.08	110.36	114.08
24	7	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	A	832	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	L	206	BCR	C15-C16-C17	-2.08	119.22	123.47
25	A	846	BCR	C33-C5-C6	-2.08	122.19	124.53
24	c	608	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	A	824	CLA	C1-C2-C3	-2.08	122.45	126.04
24	A	819	CLA	O2D-CGD-CBD	2.08	114.96	111.27
24	3	306	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	7	607	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	B	823	CLA	O2D-CGD-CBD	2.08	114.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	823	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
24	c	611	CLA	CMA-C3A-C2A	-2.08	111.25	116.10
24	B	818	CLA	CHB-C4A-NA	2.08	127.38	124.51
26	6	616	DD6	C15-C14-C13	-2.08	121.61	125.99
30	t	314	LMG	O7-C10-O9	-2.08	118.69	123.70
24	B	808	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	I	102	BCR	C7-C6-C5	-2.07	116.44	121.46
25	B	841	BCR	C12-C13-C14	-2.07	115.76	118.94
26	8	210	DD6	C33-C32-C31	2.07	113.82	109.62
26	7	615	DD6	C7-C6-C8	2.07	121.34	118.08
24	A	840	CLA	CHB-C4A-NA	2.07	127.38	124.51
24	6	608	CLA	CHD-C1D-ND	-2.07	122.55	124.45
26	7	615	DD6	C34-C35-C36	-2.07	107.73	111.85
24	7	603	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
24	7	602	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	A	842	LHG	O8-C23-C24	2.07	118.40	111.91
24	A	823	CLA	CHB-C4A-NA	2.07	127.37	124.51
26	h	614	DD6	C26-C25-C24	-2.07	116.76	123.22
24	5	603	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	1	308	CLA	CHB-C4A-NA	2.07	127.37	124.51
26	9	314	DD6	C4-C3-C2	2.07	127.71	123.47
24	k	303	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	4	609	CLA	O2D-CGD-CBD	2.07	114.94	111.27
26	2	210	DD6	C25-C24-C1	-2.06	120.62	126.42
28	A	842	LHG	O7-C7-O9	-2.06	118.72	123.70
24	t	308	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	A	835	CLA	O2D-CGD-CBD	2.06	114.93	111.27
24	A	806	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	L	205	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	c	602	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	3	309	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	A	860	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
25	L	206	BCR	C3-C4-C5	-2.06	110.40	114.08
24	h	603	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	1	314	BCR	C20-C19-C18	-2.06	120.63	126.42
25	1	310	BCR	C37-C22-C23	2.06	121.32	118.08
24	h	612	CLA	CHD-C1D-ND	-2.06	122.56	124.45
24	B	833	CLA	C4-C3-C2	-2.06	118.40	123.68
26	6	615	DD6	C12-C11-C10	-2.06	120.04	122.92
26	4	615	DD6	C10-C9-C8	-2.05	116.81	123.22
26	3	312	DD6	C10-C9-C8	-2.05	116.81	123.22
25	J	104	BCR	C37-C22-C21	-2.05	120.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	602	CLA	CGD-CBD-CAD	2.05	117.38	110.73
24	5	604	CLA	CHB-C4A-NA	2.05	127.35	124.51
26	6	614	DD6	O1-C20-C19	-2.05	111.84	113.38
24	B	809	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	B	849	BCR	C23-C22-C21	-2.05	115.79	118.94
24	A	814	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	2	209	CLA	CHB-C4A-NA	2.05	127.35	124.51
28	8	213	LHG	O7-C7-O9	-2.05	118.75	123.70
24	A	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	B	823	CLA	CHB-C4A-NA	2.05	127.35	124.51
26	1	311	DD6	C12-C11-C13	2.05	121.31	118.08
26	3	311	DD6	C-C1-C2	-2.05	120.05	122.92
26	6	615	DD6	C10-C9-C8	-2.05	116.82	123.22
24	B	804	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	5	608	DD6	C4-C3-C2	-2.05	119.28	123.47
24	B	826	CLA	O2D-CGD-CBD	2.05	114.91	111.27
24	F	201	CLA	C1-C2-C3	-2.05	122.50	126.04
24	A	828	CLA	CHB-C4A-NA	2.05	127.34	124.51
24	k	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	8	209	CLA	CMA-C3A-C2A	-2.04	111.33	116.10
25	k	316	BCR	C34-C9-C8	2.04	121.30	118.08
26	h	614	DD6	C-C1-C24	2.04	121.30	118.08
25	k	316	BCR	C10-C11-C12	-2.04	116.85	123.22
24	3	303	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	L	203	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	h	611	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	4	606	CLA	O2D-CGD-CBD	2.04	114.89	111.27
26	6	614	DD6	C10-C9-C8	-2.04	116.86	123.22
25	B	842	BCR	C34-C9-C10	-2.04	120.07	122.92
24	6	603	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	c	610	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
29	3	310	A1L1G	C27-C34-C35	-2.04	120.07	122.92
26	1	312	DD6	C15-C14-C13	-2.04	121.69	125.99
24	9	306	CLA	CHD-C1D-ND	-2.03	122.58	124.45
24	6	604	CLA	CHB-C4A-NA	2.03	127.33	124.51
25	I	101	BCR	C21-C20-C19	-2.03	116.87	123.22
26	9	317	DD6	C7-C6-C5	-2.03	120.07	122.92
24	4	608	CLA	CBC-CAC-C3C	2.03	118.03	112.43
24	A	823	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	B	824	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	k	316	BCR	C37-C22-C21	-2.03	120.08	122.92
25	R	101	BCR	C36-C18-C17	-2.03	120.08	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
25	B	840	BCR	C11-C12-C13	-2.03	120.71	126.42
24	B	819	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	h	601	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
26	5	608	DD6	C19-C18-C17	2.03	114.69	110.77
24	B	812	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	7	605	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	L	202	BCR	C36-C18-C17	-2.03	120.08	122.92
26	9	313	DD6	C25-C26-C27	-2.03	120.69	126.58
24	5	601	CLA	CHB-C4A-NA	2.03	127.31	124.51
24	7	601	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	A	822	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	R	102	BCR	C15-C14-C13	-2.03	124.42	127.31
28	3	315	LHG	O8-C23-O10	-2.03	118.48	123.59
26	3	313	DD6	C12-C11-C13	2.03	121.27	118.08
24	B	828	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	7	608	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
25	B	843	BCR	C21-C20-C19	-2.02	116.90	123.22
26	9	317	DD6	C9-C10-C11	-2.02	124.42	127.31
26	1	311	DD6	C9-C8-C6	2.02	132.10	126.42
26	h	616	DD6	O1-C20-C19	-2.02	111.86	113.38
26	h	614	DD6	C7-C6-C8	2.02	121.27	118.08
26	1	313	DD6	C25-C24-C1	-2.02	120.73	126.42
24	B	846	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	6	603	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	k	307	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	4	615	DD6	C33-C32-C31	2.02	113.72	109.62
25	A	845	BCR	C21-C20-C19	-2.02	116.91	123.22
24	2	203	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	h	612	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
24	L	204	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	h	613	DD6	C25-C24-C1	-2.02	120.74	126.42
25	L	202	BCR	C37-C22-C21	-2.02	120.09	122.92
24	B	807	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	4	617	DD6	C7-C6-C5	-2.02	120.10	122.92
25	B	840	BCR	C33-C5-C6	-2.02	122.26	124.53
25	I	101	BCR	C23-C24-C25	-2.02	121.54	127.20
25	J	104	BCR	C40-C30-C25	2.02	113.57	110.30
26	t	311	DD6	C25-C26-C27	-2.02	120.73	126.58
24	5	601	CLA	O2A-CGA-O1A	-2.02	118.28	123.30
24	h	609	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	1	302	CLA	O2A-CGA-O1A	-2.01	118.28	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	824	CLA	CHB-C4A-NA	2.01	127.30	124.51
25	A	846	BCR	C21-C20-C19	-2.01	116.94	123.22
25	R	101	BCR	C15-C14-C13	-2.01	124.44	127.31
24	5	603	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
26	k	315	DD6	C9-C8-C6	2.01	132.07	126.42
26	h	614	DD6	C9-C10-C11	-2.01	124.44	127.31
26	4	617	DD6	C10-C9-C8	-2.01	116.94	123.22
25	7	617	BCR	C36-C18-C19	2.01	121.24	118.08
24	1	309	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	J	101	BCR	C29-C28-C27	-2.01	106.89	111.38
26	6	616	DD6	C23-C16-C15	2.01	115.47	110.05
24	3	307	CLA	CHB-C4A-NA	2.01	127.29	124.51
29	2	213	A1L1G	C28-C39-C40	2.01	121.24	118.08
29	2	213	A1L1G	C3-C6-C1	2.01	111.16	109.21
24	t	304	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	6	613	DD6	C14-C13-C11	-2.01	122.42	125.53
24	5	607	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
25	L	202	BCR	C7-C6-C5	-2.00	116.61	121.46
24	9	305	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
26	4	616	DD6	C7-C6-C8	2.00	121.23	118.08
25	R	102	BCR	C23-C22-C21	-2.00	115.87	118.94
24	7	601	CLA	O2D-CGD-CBD	2.00	114.82	111.27
24	A	818	CLA	C7-C6-C5	-2.00	107.93	113.36

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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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 (2325) 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

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Mol	Chain	Res	Type	Atoms
24	1	303	CLA	CHA-CBD-CGD-O1D
24	1	303	CLA	CHA-CBD-CGD-O2D
24	1	303	CLA	CBD-CGD-O2D-CED
24	1	304	CLA	CHA-CBD-CGD-O1D
24	1	304	CLA	CHA-CBD-CGD-O2D
24	1	304	CLA	CAD-CBD-CGD-O1D
24	1	305	CLA	CAD-CBD-CGD-O1D
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	CHA-CBD-CGD-O1D
24	2	201	CLA	CHA-CBD-CGD-O2D
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
24	2	203	CLA	CHA-CBD-CGD-O1D
24	2	203	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	208	CLA	CBA-CGA-O2A-C1
24	2	209	CLA	CBD-CGD-O2D-CED
24	2	209	CLA	O1D-CGD-O2D-CED
24	3	303	CLA	CHA-CBD-CGD-O1D
24	3	303	CLA	CHA-CBD-CGD-O2D
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	602	CLA	C2-C3-C5-C6
24	4	602	CLA	C4-C3-C5-C6
24	4	604	CLA	C3A-C2A-CAA-CBA
24	4	604	CLA	CBD-CGD-O2D-CED
24	4	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	4	608	CLA	O1A-CGA-O2A-C1
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	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
24	5	605	CLA	C3A-C2A-CAA-CBA
24	5	605	CLA	CBA-CGA-O2A-C1
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	606	CLA	CBD-CGD-O2D-CED
24	6	608	CLA	CBD-CGD-O2D-CED
24	6	611	CLA	C1A-C2A-CAA-CBA
24	6	611	CLA	C3A-C2A-CAA-CBA
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	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	CHA-CBD-CGD-O1D
24	8	201	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
24	8	206	CLA	CHA-CBD-CGD-O1D
24	8	206	CLA	CHA-CBD-CGD-O2D
24	8	207	CLA	C1A-C2A-CAA-CBA
24	8	207	CLA	C3A-C2A-CAA-CBA
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	CBA-CGA-O2A-C1
24	9	304	CLA	CBD-CGD-O2D-CED
24	9	305	CLA	CBD-CGD-O2D-CED
24	9	306	CLA	CHA-CBD-CGD-O1D
24	9	306	CLA	CHA-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	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-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	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
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	c	611	CLA	CHA-CBD-CGD-O1D
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

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Mol	Chain	Res	Type	Atoms
24	t	302	CLA	CBD-CGD-O2D-CED
24	t	303	CLA	C2-C3-C5-C6
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	CHA-CBD-CGD-O1D
24	t	305	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O2D
24	A	803	CLA	C3A-C2A-CAA-CBA
24	A	804	CLA	O2A-C1-C2-C3
24	A	807	CLA	C3A-C2A-CAA-CBA
24	A	807	CLA	CHA-CBD-CGD-O1D
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	CHA-CBD-CGD-O1D
24	A	809	CLA	CHA-CBD-CGD-O2D
24	A	809	CLA	CBD-CGD-O2D-CED
24	A	811	CLA	C3A-C2A-CAA-CBA
24	A	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	812	CLA	C11-C10-C8-C9
24	A	813	CLA	C1A-C2A-CAA-CBA
24	A	813	CLA	CHA-CBD-CGD-O1D
24	A	813	CLA	CHA-CBD-CGD-O2D
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	818	CLA	CHA-CBD-CGD-O1D
24	A	818	CLA	CHA-CBD-CGD-O2D
24	A	820	CLA	CBD-CGD-O2D-CED
24	A	822	CLA	CHA-CBD-CGD-O1D
24	A	822	CLA	CHA-CBD-CGD-O2D
24	A	822	CLA	CAD-CBD-CGD-O1D
24	A	823	CLA	C1A-C2A-CAA-CBA
24	A	823	CLA	C3A-C2A-CAA-CBA
24	A	824	CLA	C11-C12-C13-C14
24	A	827	CLA	O2A-C1-C2-C3
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	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	837	CLA	CHA-CBD-CGD-O1D
24	A	837	CLA	CHA-CBD-CGD-O2D
24	A	838	CLA	C2A-CAA-CBA-CGA
24	A	838	CLA	CAD-CBD-CGD-O1D
24	A	840	CLA	CHA-CBD-CGD-O1D
24	A	840	CLA	CHA-CBD-CGD-O2D
24	A	840	CLA	CAD-CBD-CGD-O1D
24	A	857	CLA	CHA-CBD-CGD-O1D
24	A	857	CLA	CHA-CBD-CGD-O2D
24	A	860	CLA	C11-C10-C8-C9
24	A	860	CLA	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
24	B	804	CLA	CHA-CBD-CGD-O1D
24	B	804	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
24	B	815	CLA	CHA-CBD-CGD-O2D
24	B	815	CLA	CAD-CBD-CGD-O1D
24	B	817	CLA	CHA-CBD-CGD-O1D
24	B	817	CLA	CHA-CBD-CGD-O2D
24	B	817	CLA	O2A-C1-C2-C3
24	B	820	CLA	C2A-CAA-CBA-CGA
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	821	CLA	CHA-CBD-CGD-O1D
24	B	821	CLA	CHA-CBD-CGD-O2D
24	B	826	CLA	C1A-C2A-CAA-CBA
24	B	826	CLA	C3A-C2A-CAA-CBA
24	B	826	CLA	C2A-CAA-CBA-CGA
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	C2-C3-C5-C6
24	B	830	CLA	C4-C3-C5-C6
24	B	833	CLA	C2-C3-C5-C6
24	B	833	CLA	C4-C3-C5-C6
24	B	834	CLA	CHA-CBD-CGD-O1D
24	B	834	CLA	CHA-CBD-CGD-O2D
24	B	835	CLA	C1A-C2A-CAA-CBA
24	B	835	CLA	CAD-CBD-CGD-O1D
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
24	B	846	CLA	C3A-C2A-CAA-CBA
24	F	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
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	C37-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	c	615	BCR	C36-C18-C19-C20
25	t	312	BCR	C23-C24-C25-C26
25	t	312	BCR	C23-C24-C25-C30
25	k	316	BCR	C1-C6-C7-C8
25	A	844	BCR	C17-C18-C19-C20
25	A	844	BCR	C36-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	843	BCR	C37-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
25	J	104	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
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	M	101	BCR	C23-C24-C25-C30
25	R	101	BCR	C5-C6-C7-C8
25	R	102	BCR	C5-C6-C7-C8
25	R	102	BCR	C7-C8-C9-C10
25	R	102	BCR	C7-C8-C9-C34
26	2	212	DD6	C11-C13-C14-C15
26	3	313	DD6	C13-C14-C15-C16
26	3	313	DD6	C13-C14-C15-C20
26	3	313	DD6	C27-C29-C30-C31
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	C10-C11-C13-C14
26	6	616	DD6	C12-C11-C13-C14
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-C16
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	k	315	DD6	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
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'
27	h	617	LMT	C2-C1-O1'-C1'
28	1	318	LHG	C1-C2-C3-O3
28	1	318	LHG	C3-O3-P-O4
28	1	318	LHG	C3-O3-P-O5
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	C4-O6-P-O3
28	3	315	LHG	C4-O6-P-O4
28	3	315	LHG	C4-O6-P-O5
28	8	213	LHG	C4-O6-P-O4
28	A	842	LHG	C3-O3-P-O4
28	A	842	LHG	C4-O6-P-O4
28	A	842	LHG	O6-C4-C5-O7
28	A	852	LHG	C4-O6-P-O4
28	B	844	LHG	C3-O3-P-O5
28	B	844	LHG	C4-O6-P-O5
28	B	845	LHG	C3-O3-P-O4
28	B	845	LHG	C4-O6-P-O5
28	I	103	LHG	C3-O3-P-O6
28	J	105	LHG	C3-O3-P-O4
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	C4-O6-P-O5
28	L	201	LHG	C8-C7-O7-C5
29	2	213	A1L1G	O13-C26-C30-C29
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	C32-C33-C34-C27
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

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Mol	Chain	Res	Type	Atoms
29	2	213	A1L1G	C37-C38-C39-C40
29	2	213	A1L1G	C28-C39-C40-C41
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
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

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Mol	Chain	Res	Type	Atoms
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	608	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
24	c	609	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	817	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	1	305	CLA	O1D-CGD-O2D-CED
24	4	602	CLA	O1D-CGD-O2D-CED
24	6	608	CLA	O1D-CGD-O2D-CED
24	9	304	CLA	O1D-CGD-O2D-CED
24	c	601	CLA	O1D-CGD-O2D-CED
24	t	305	CLA	O1D-CGD-O2D-CED
24	F	201	CLA	O1D-CGD-O2D-CED
24	J	103	CLA	O1D-CGD-O2D-CED
24	4	609	CLA	CBA-CGA-O2A-C1
24	9	307	CLA	CBA-CGA-O2A-C1
24	h	605	CLA	CBA-CGA-O2A-C1
24	B	832	CLA	C2C-C3C-CAC-CBC
27	A	854	LMT	O5B-C1B-O1B-C4'
24	3	305	CLA	O1D-CGD-O2D-CED
24	4	604	CLA	O1D-CGD-O2D-CED
24	5	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	9	308	CLA	O1D-CGD-O2D-CED
24	c	603	CLA	O1D-CGD-O2D-CED
24	t	302	CLA	O1D-CGD-O2D-CED
24	t	308	CLA	O1D-CGD-O2D-CED
24	k	305	CLA	O1D-CGD-O2D-CED
24	A	809	CLA	O1D-CGD-O2D-CED
24	A	820	CLA	O1D-CGD-O2D-CED
28	B	845	LHG	C24-C23-O8-C6
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	801	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
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

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Mol	Chain	Res	Type	Atoms
24	c	605	CLA	O1A-CGA-O2A-C1
24	k	302	CLA	O1A-CGA-O2A-C1
24	7	610	CLA	O1D-CGD-O2D-CED
27	h	617	LMT	O5B-C1B-O1B-C4'
24	7	604	CLA	O1D-CGD-O2D-CED
24	9	305	CLA	O1D-CGD-O2D-CED
24	h	602	CLA	O1D-CGD-O2D-CED
24	h	604	CLA	O1D-CGD-O2D-CED
24	B	809	CLA	O1D-CGD-O2D-CED
24	F	203	CLA	O1D-CGD-O2D-CED
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	4	608	CLA	O1D-CGD-O2D-CED
24	k	304	CLA	O1D-CGD-O2D-CED
24	A	814	CLA	O1D-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	7	605	CLA	CBA-CGA-O2A-C1
24	7	612	CLA	CBA-CGA-O2A-C1
24	8	206	CLA	CBA-CGA-O2A-C1
24	k	304	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
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	4	608	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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
28	A	841	LHG	C8-C7-O7-C5
24	h	601	CLA	O1D-CGD-O2D-CED
24	B	820	CLA	O1D-CGD-O2D-CED
24	2	203	CLA	CBD-CGD-O2D-CED
24	A	834	CLA	CBD-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	4	605	CLA	CBA-CGA-O2A-C1
24	4	612	CLA	CBA-CGA-O2A-C1
24	6	605	CLA	CBA-CGA-O2A-C1
24	6	606	CLA	CBA-CGA-O2A-C1
24	9	308	CLA	CBA-CGA-O2A-C1
24	h	608	CLA	CBA-CGA-O2A-C1
24	h	609	CLA	CBA-CGA-O2A-C1
24	c	607	CLA	CBA-CGA-O2A-C1
24	L	205	CLA	CBA-CGA-O2A-C1
24	2	202	CLA	C4-C3-C5-C6
24	2	202	CLA	C2-C3-C5-C6
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	A	801	CLA	C2A-CAA-CBA-CGA
24	B	829	CLA	C2A-CAA-CBA-CGA
24	B	836	CLA	C2A-CAA-CBA-CGA
24	A	823	CLA	O1A-CGA-O2A-C1
24	4	609	CLA	O1A-CGA-O2A-C1
24	7	612	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

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Mol	Chain	Res	Type	Atoms
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
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	1	304	CLA	O1D-CGD-O2D-CED
24	k	301	CLA	O1D-CGD-O2D-CED
24	A	810	CLA	O1D-CGD-O2D-CED
24	h	605	CLA	CBD-CGD-O2D-CED
24	h	610	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
24	A	847	CLA	O1D-CGD-O2D-CED
24	B	848	CLA	O1D-CGD-O2D-CED
28	I	103	LHG	O9-C7-O7-C5
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
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
27	A	854	LMT	O5B-C5B-C6B-O6B
28	3	315	LHG	C12-C13-C14-C15
24	4	609	CLA	CBD-CGD-O2D-CED
24	5	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	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	829	CLA	C3-C5-C6-C7
27	1	315	LMT	C3'-C4'-O1B-C1B
27	1	316	LMT	O5B-C5B-C6B-O6B
27	A	850	LMT	O5'-C5'-C6'-O6'
24	7	602	CLA	O1D-CGD-O2D-CED
24	B	813	CLA	O1D-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
24	8	205	CLA	CBD-CGD-O2D-CED
24	A	819	CLA	CBD-CGD-O2D-CED
24	A	832	CLA	CBD-CGD-O2D-CED
24	B	812	CLA	CBD-CGD-O2D-CED
27	3	314	LMT	O5'-C5'-C6'-O6'
27	A	850	LMT	O5B-C5B-C6B-O6B
27	A	854	LMT	C4B-C5B-C6B-O6B
27	h	617	LMT	C2B-C1B-O1B-C4'
24	8	209	CLA	O1D-CGD-O2D-CED
24	B	817	CLA	O1D-CGD-O2D-CED
24	A	816	CLA	C3-C5-C6-C7
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	B	816	CLA	O1A-CGA-O2A-C1
24	A	830	CLA	C4-C3-C5-C6
24	B	824	CLA	C4-C3-C5-C6
27	A	850	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
24	A	830	CLA	C2-C3-C5-C6
24	B	824	CLA	C2-C3-C5-C6
24	k	307	CLA	C2A-CAA-CBA-CGA
27	A	851	LMT	C4B-C5B-C6B-O6B
30	2	214	LMG	O6-C1-O1-C7
24	7	608	CLA	O1D-CGD-O2D-CED
24	c	609	CLA	O1D-CGD-O2D-CED
24	6	605	CLA	O1A-CGA-O2A-C1
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	7	611	CLA	CBA-CGA-O2A-C1
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	3	304	CLA	O1D-CGD-O2D-CED
24	A	808	CLA	O1D-CGD-O2D-CED
24	B	837	CLA	O1D-CGD-O2D-CED
24	4	613	CLA	CBD-CGD-O2D-CED
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	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
24	B	808	CLA	C3-C5-C6-C7
24	B	809	CLA	C3-C5-C6-C7
24	t	302	CLA	CBA-CGA-O2A-C1
24	c	611	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
24	B	811	CLA	CBA-CGA-O2A-C1
24	B	812	CLA	CBA-CGA-O2A-C1
24	B	823	CLA	CBA-CGA-O2A-C1
24	B	838	CLA	CBA-CGA-O2A-C1
28	A	852	LHG	C24-C23-O8-C6
28	3	315	LHG	C11-C10-C9-C8
24	2	207	CLA	O1A-CGA-O2A-C1
24	6	610	CLA	O1D-CGD-O2D-CED
24	t	303	CLA	C8-C10-C11-C12
24	B	834	CLA	C5-C6-C7-C8
24	L	204	CLA	C8-C10-C11-C12
24	R	103	CLA	C8-C10-C11-C12
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	F	201	CLA	C3-C5-C6-C7
24	A	828	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	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	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

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Mol	Chain	Res	Type	Atoms
24	B	828	CLA	O1D-CGD-O2D-CED
24	R	104	CLA	O1D-CGD-O2D-CED
24	B	804	CLA	C5-C6-C7-C8
25	2	211	BCR	C37-C22-C23-C24
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	845	BCR	C7-C8-C9-C34
25	A	845	BCR	C11-C12-C13-C35
25	B	843	BCR	C7-C8-C9-C34
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
29	9	312	A1L1G	C38-C39-C40-C41
27	1	315	LMT	O5'-C5'-C6'-O6'
28	3	315	LHG	C8-C7-O7-C5
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
24	B	812	CLA	C5-C6-C7-C8
24	R	103	CLA	C10-C11-C12-C13
24	k	306	CLA	O1D-CGD-O2D-CED
28	1	318	LHG	C13-C14-C15-C16
24	4	604	CLA	CBA-CGA-O2A-C1
24	A	827	CLA	CBD-CGD-O2D-CED
24	B	832	CLA	CBD-CGD-O2D-CED
27	1	316	LMT	C4B-C5B-C6B-O6B
24	1	308	CLA	O1D-CGD-O2D-CED
24	1	304	CLA	C5-C6-C7-C8
31	B	839	PQN	C23-C25-C26-C27
31	B	839	PQN	C25-C26-C27-C28
28	A	849	LHG	C7-C8-C9-C10
24	9	302	CLA	O1D-CGD-O2D-CED
24	c	605	CLA	O1D-CGD-O2D-CED
24	5	607	CLA	CBD-CGD-O2D-CED
24	t	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	815	CLA	CBD-CGD-O2D-CED
24	6	606	CLA	C2C-C3C-CAC-CBC
24	A	812	CLA	C8-C10-C11-C12
24	B	833	CLA	C5-C6-C7-C8
24	c	602	CLA	O1D-CGD-O2D-CED
24	B	815	CLA	O1D-CGD-O2D-CED
28	A	852	LHG	O10-C23-O8-C6
28	3	315	LHG	C7-C8-C9-C10
24	9	309	CLA	CBD-CGD-O2D-CED
24	8	204	CLA	O1D-CGD-O2D-CED
24	A	806	CLA	C5-C6-C7-C8
24	A	810	CLA	C8-C10-C11-C12
24	B	805	CLA	C15-C16-C17-C18
24	B	812	CLA	C15-C16-C17-C18
24	B	810	CLA	CBA-CGA-O2A-C1
24	9	309	CLA	O1A-CGA-O2A-C1
24	h	610	CLA	C2C-C3C-CAC-CBC
24	A	807	CLA	C8-C10-C11-C12
24	B	801	CLA	C5-C6-C7-C8
24	B	812	CLA	C8-C10-C11-C12
28	8	213	LHG	C23-C24-C25-C26
24	c	604	CLA	CBD-CGD-O2D-CED
24	t	301	CLA	CBD-CGD-O2D-CED
24	A	853	CLA	CBD-CGD-O2D-CED
24	3	305	CLA	C11-C10-C8-C7
24	4	602	CLA	C6-C7-C8-C10
24	t	303	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	3	301	CLA	C3-C5-C6-C7
24	A	840	CLA	O1A-CGA-O2A-C1
29	2	213	A1L1G	C40-C41-C42-C44
29	9	312	A1L1G	C40-C41-C42-C44
24	h	611	CLA	CBD-CGD-O2D-CED
24	2	201	CLA	C2A-CAA-CBA-CGA
24	A	804	CLA	C2A-CAA-CBA-CGA
24	A	812	CLA	C2A-CAA-CBA-CGA
24	B	801	CLA	C2A-CAA-CBA-CGA
24	6	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	A	840	CLA	C5-C6-C7-C8
24	B	802	CLA	C13-C15-C16-C17
24	6	607	CLA	O1A-CGA-O2A-C1
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	A	836	CLA	CBD-CGD-O2D-CED
24	A	828	CLA	C13-C15-C16-C17
24	B	827	CLA	C15-C16-C17-C18
24	B	806	CLA	O1D-CGD-O2D-CED
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	B	801	CLA	C3-C5-C6-C7
24	B	824	CLA	C5-C6-C7-C8
24	B	836	CLA	C13-C15-C16-C17
24	B	837	CLA	C10-C11-C12-C13
24	L	203	CLA	C2C-C3C-CAC-CBC
24	2	207	CLA	CBD-CGD-O2D-CED
24	F	203	CLA	O1A-CGA-O2A-C1
27	A	854	LMT	C2B-C1B-O1B-C4'
24	9	303	CLA	CBA-CGA-O2A-C1
24	B	819	CLA	CBA-CGA-O2A-C1
24	1	317	CLA	C10-C11-C12-C13
24	A	806	CLA	C15-C16-C17-C18
24	A	807	CLA	C15-C16-C17-C18
24	A	813	CLA	C15-C16-C17-C18
24	B	808	CLA	C13-C15-C16-C17
24	B	822	CLA	C10-C11-C12-C13
24	B	822	CLA	C13-C15-C16-C17
24	B	834	CLA	C13-C15-C16-C17
24	3	308	CLA	O1A-CGA-O2A-C1
28	2	215	LHG	C8-C7-O7-C5
24	3	306	CLA	C15-C16-C17-C18
24	A	807	CLA	C5-C6-C7-C8
24	A	813	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	810	CLA	C5-C6-C7-C8
24	B	831	CLA	C15-C16-C17-C18
28	1	318	LHG	C3-O3-P-O6
28	4	619	LHG	C4-O6-P-O3
28	8	213	LHG	C3-O3-P-O6
28	A	841	LHG	C3-O3-P-O6
28	A	842	LHG	C3-O3-P-O6
28	A	842	LHG	C4-O6-P-O3
28	A	849	LHG	C3-O3-P-O6
28	A	852	LHG	C4-O6-P-O3
28	B	844	LHG	C3-O3-P-O6
28	B	845	LHG	C3-O3-P-O6
28	B	845	LHG	C4-O6-P-O3
28	J	105	LHG	C3-O3-P-O6
28	L	201	LHG	C3-O3-P-O6
27	1	315	LMT	O5B-C5B-C6B-O6B
24	1	317	CLA	C3-C5-C6-C7
24	B	837	CLA	CBA-CGA-O2A-C1
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
28	2	215	LHG	O9-C7-O7-C5
28	3	315	LHG	O9-C7-O7-C5
24	B	811	CLA	C4-C3-C5-C6
24	B	815	CLA	C4-C3-C5-C6
24	A	836	CLA	C13-C15-C16-C17
24	B	823	CLA	C13-C15-C16-C17
24	B	810	CLA	O1A-CGA-O2A-C1
24	7	606	CLA	C2C-C3C-CAC-CBC
24	5	602	CLA	C2A-CAA-CBA-CGA
24	B	831	CLA	C3-C5-C6-C7
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	A	812	CLA	C10-C11-C12-C13
24	L	203	CLA	C4C-C3C-CAC-CBC
24	t	310	CLA	CBD-CGD-O2D-CED
24	k	301	CLA	CBA-CGA-O2A-C1
24	B	827	CLA	C13-C15-C16-C17
26	4	616	DD6	C9-C10-C11-C12
26	6	615	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
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	2	203	CLA	O1D-CGD-O2D-CED
24	A	803	CLA	C6-C7-C8-C9
24	A	830	CLA	C6-C7-C8-C10
28	A	841	LHG	C24-C25-C26-C27
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	5	606	CLA	O1D-CGD-O2D-CED
24	k	306	CLA	CBA-CGA-O2A-C1
29	3	310	A1L1G	C29-C30-C31-C32
28	3	315	LHG	C16-C17-C18-C19
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
26	R	105	DD6	C9-C10-C11-C13
27	A	851	LMT	C2'-C1'-O1'-C1
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
30	A	855	LMG	C2-C1-O1-C7
24	h	606	CLA	C2C-C3C-CAC-CBC
24	7	611	CLA	O1A-CGA-O2A-C1
24	A	823	CLA	C13-C15-C16-C17
24	A	827	CLA	C8-C10-C11-C12
24	B	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	823	CLA	C16-C17-C18-C19
24	4	609	CLA	O1D-CGD-O2D-CED
24	B	818	CLA	O1D-CGD-O2D-CED
24	B	834	CLA	O1D-CGD-O2D-CED
29	2	213	A1L1G	C14-C29-C30-C31
24	c	602	CLA	C14-C13-C15-C16
24	A	802	CLA	C14-C13-C15-C16
24	A	823	CLA	C6-C7-C8-C9
24	A	826	CLA	C11-C12-C13-C14
31	B	839	PQN	C24-C23-C25-C26
24	B	822	CLA	O1D-CGD-O2D-CED
28	1	318	LHG	C15-C16-C17-C18
24	h	608	CLA	C2A-CAA-CBA-CGA
24	A	828	CLA	C2A-CAA-CBA-CGA
24	B	813	CLA	C2A-CAA-CBA-CGA
25	1	314	BCR	C7-C8-C9-C34
27	A	850	LMT	C4-C5-C6-C7
28	8	213	LHG	C11-C12-C13-C14
28	3	315	LHG	O1-C1-C2-C3
28	8	213	LHG	O1-C1-C2-C3
25	1	314	BCR	C7-C8-C9-C10
25	t	312	BCR	C21-C22-C23-C24
24	B	821	CLA	O1D-CGD-O2D-CED
24	h	602	CLA	C6-C7-C8-C10
24	B	804	CLA	C16-C17-C18-C19
24	B	820	CLA	C6-C7-C8-C10
24	B	822	CLA	C16-C17-C18-C20
27	A	851	LMT	O5'-C1'-O1'-C1
31	B	839	PQN	C15-C16-C17-C18
24	2	209	CLA	CBA-CGA-O2A-C1
24	4	603	CLA	CBA-CGA-O2A-C1
24	9	302	CLA	CBA-CGA-O2A-C1
24	t	310	CLA	CBA-CGA-O2A-C1
24	B	826	CLA	O1D-CGD-O2D-CED
28	I	103	LHG	C25-C26-C27-C28
24	B	837	CLA	O1A-CGA-O2A-C1
24	A	813	CLA	C3-C5-C6-C7
24	B	820	CLA	CBA-CGA-O2A-C1
28	4	619	LHG	C24-C23-O8-C6
28	3	315	LHG	C17-C18-C19-C20
24	1	303	CLA	C3A-C2A-CAA-CBA
24	1	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
24	k	303	CLA	C3A-C2A-CAA-CBA
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
27	1	315	LMT	C2-C1-O1'-C1'
28	I	103	LHG	C28-C29-C30-C31
24	4	606	CLA	CBA-CGA-O2A-C1
24	A	812	CLA	O1D-CGD-O2D-CED
24	A	838	CLA	O1D-CGD-O2D-CED
27	h	617	LMT	C4B-C5B-C6B-O6B
24	t	302	CLA	O1A-CGA-O2A-C1
24	3	305	CLA	C11-C12-C13-C15
24	7	606	CLA	C11-C12-C13-C15
24	h	602	CLA	C6-C7-C8-C9
24	A	823	CLA	C16-C17-C18-C20
24	B	804	CLA	C16-C17-C18-C20
24	B	822	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	1	316	LMT	C6-C7-C8-C9
24	8	202	CLA	O1D-CGD-O2D-CED
24	2	208	CLA	CBD-CGD-O2D-CED
27	1	315	LMT	C7-C8-C9-C10
24	B	814	CLA	O2A-C1-C2-C3
28	J	105	LHG	C23-C24-C25-C26
24	B	822	CLA	O1A-CGA-O2A-C1
24	3	301	CLA	C4-C3-C5-C6
24	k	303	CLA	C4-C3-C5-C6
24	L	203	CLA	C4-C3-C5-C6
24	L	203	CLA	C2-C3-C5-C6
28	8	213	LHG	C8-C7-O7-C5
24	1	305	CLA	C2A-CAA-CBA-CGA
24	6	612	CLA	C2A-CAA-CBA-CGA
24	9	308	CLA	C2A-CAA-CBA-CGA
27	A	850	LMT	C6-C7-C8-C9
28	3	315	LHG	C28-C29-C30-C31
24	4	607	CLA	O1A-CGA-O2A-C1
24	7	606	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
27	A	850	LMT	C1-C2-C3-C4
27	3	314	LMT	C4'-C5'-C6'-O6'
24	B	807	CLA	C15-C16-C17-C18
24	9	301	CLA	O1A-CGA-O2A-C1
24	4	608	CLA	C2C-C3C-CAC-CBC
28	3	315	LHG	C26-C27-C28-C29
28	8	213	LHG	O9-C7-O7-C5
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	A	813	CLA	C10-C11-C12-C13
27	h	617	LMT	C1-C2-C3-C4
28	B	845	LHG	C33-C34-C35-C36
25	1	314	BCR	C1-C6-C7-C8
25	2	211	BCR	C23-C24-C25-C26
25	2	211	BCR	C23-C24-C25-C30
25	c	615	BCR	C23-C24-C25-C26
25	c	615	BCR	C23-C24-C25-C30
25	k	316	BCR	C5-C6-C7-C8
25	A	843	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	843	BCR	C23-C24-C25-C26
25	A	846	BCR	C1-C6-C7-C8
25	A	859	BCR	C5-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	M	101	BCR	C23-C24-C25-C26
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	9	305	CLA	CBA-CGA-O2A-C1
27	h	617	LMT	O5'-C5'-C6'-O6'
27	1	315	LMT	C3-C4-C5-C6
24	B	814	CLA	CBA-CGA-O2A-C1
24	A	826	CLA	C10-C11-C12-C13
24	B	817	CLA	C10-C11-C12-C13
24	B	826	CLA	O1A-CGA-O2A-C1
27	1	315	LMT	C1-C2-C3-C4
24	c	602	CLA	C15-C16-C17-C18
24	A	826	CLA	C4-C3-C5-C6
24	A	828	CLA	C4-C3-C5-C6
24	3	301	CLA	C2-C3-C5-C6
24	c	602	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	818	CLA	C2-C3-C5-C6
24	A	826	CLA	C2-C3-C5-C6
24	A	828	CLA	C2-C3-C5-C6
24	A	829	CLA	C6-C7-C8-C10
24	A	836	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	A	838	CLA	C12-C13-C15-C16
24	A	860	CLA	C11-C12-C13-C15
24	B	801	CLA	C11-C12-C13-C15
24	B	802	CLA	C2-C3-C5-C6
24	B	806	CLA	C11-C12-C13-C15
24	B	827	CLA	C6-C7-C8-C10
24	F	201	CLA	C6-C7-C8-C10
31	B	839	PQN	C22-C23-C25-C26
24	B	820	CLA	O1A-CGA-O2A-C1
28	3	315	LHG	C27-C28-C29-C30
24	A	832	CLA	O1D-CGD-O2D-CED
24	4	604	CLA	O1A-CGA-O2A-C1
24	c	602	CLA	CBA-CGA-O2A-C1
24	4	605	CLA	C2A-CAA-CBA-CGA
24	9	307	CLA	C2A-CAA-CBA-CGA
24	B	807	CLA	C2A-CAA-CBA-CGA
24	A	819	CLA	O1D-CGD-O2D-CED
24	B	807	CLA	C5-C6-C7-C8
28	A	842	LHG	C15-C16-C17-C18
24	A	856	CLA	CBD-CGD-O2D-CED
24	8	205	CLA	O1D-CGD-O2D-CED
24	A	813	CLA	C13-C15-C16-C17
24	1	304	CLA	C6-C7-C8-C9
24	A	806	CLA	C16-C17-C18-C19
27	3	314	LMT	C1-C2-C3-C4
28	B	844	LHG	C8-C7-O7-C5
27	h	617	LMT	O5B-C5B-C6B-O6B
24	B	806	CLA	C5-C6-C7-C8
28	B	844	LHG	O9-C7-O7-C5
27	3	314	LMT	C2'-C1'-O1'-C1
28	B	844	LHG	O7-C5-C6-O8
24	A	818	CLA	C4-C3-C5-C6
24	c	604	CLA	CBA-CGA-O2A-C1
24	k	303	CLA	C2-C3-C5-C6
24	A	820	CLA	C2-C3-C5-C6
24	B	811	CLA	C2-C3-C5-C6
24	B	815	CLA	C2-C3-C5-C6
26	4	614	DD6	C27-C29-C30-C31
26	7	618	DD6	C27-C29-C30-C31
26	8	211	DD6	C27-C29-C30-C31
26	h	615	DD6	C27-C29-C30-C31
26	k	315	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	A	848	DD6	C27-C29-C30-C31
26	J	102	DD6	C27-C29-C30-C31
24	t	303	CLA	C6-C7-C8-C9
24	A	807	CLA	C14-C13-C15-C16
24	A	810	CLA	C11-C12-C13-C14
24	A	816	CLA	C14-C13-C15-C16
24	A	817	CLA	C14-C13-C15-C16
24	A	827	CLA	C11-C10-C8-C9
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	805	CLA	C11-C10-C8-C9
24	B	806	CLA	C11-C12-C13-C14
24	B	817	CLA	C6-C7-C8-C9
24	B	827	CLA	C11-C10-C8-C9
31	A	839	PQN	C24-C23-C25-C26
24	A	807	CLA	C2A-CAA-CBA-CGA
25	A	844	BCR	C7-C8-C9-C34
25	M	101	BCR	C11-C12-C13-C35
24	B	812	CLA	O1D-CGD-O2D-CED
24	A	825	CLA	C15-C16-C17-C18
24	B	814	CLA	O1A-CGA-O2A-C1
28	4	619	LHG	O10-C23-O8-C6
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

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Mol	Chain	Res	Type	Atoms
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
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	1	304	CLA	C6-C7-C8-C10
24	3	301	CLA	C16-C17-C18-C20
24	7	606	CLA	C11-C12-C13-C14
24	A	803	CLA	C6-C7-C8-C10
24	A	806	CLA	C16-C17-C18-C20
24	A	830	CLA	C6-C7-C8-C9
28	A	849	LHG	C27-C28-C29-C30
24	A	831	CLA	C15-C16-C17-C18
24	B	847	CLA	C15-C16-C17-C18
28	1	318	LHG	C4-O6-P-O3
28	2	215	LHG	C3-O3-P-O6
28	3	315	LHG	C3-O3-P-O6
28	A	849	LHG	C4-O6-P-O3
24	B	816	CLA	C3-C5-C6-C7
24	A	826	CLA	C15-C16-C17-C18
28	A	842	LHG	O6-C4-C5-C6
24	3	305	CLA	C11-C12-C13-C14
25	A	845	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	820	CLA	C4-C3-C5-C6
24	B	802	CLA	C4-C3-C5-C6
24	B	838	CLA	C15-C16-C17-C18
28	A	842	LHG	C8-C7-O7-C5
24	B	837	CLA	C2A-CAA-CBA-CGA
24	A	807	CLA	C16-C17-C18-C20
24	4	613	CLA	O1D-CGD-O2D-CED
24	A	837	CLA	C3-C5-C6-C7
30	2	214	LMG	C33-C34-C35-C36
24	9	303	CLA	O1A-CGA-O2A-C1
24	c	602	CLA	O1A-CGA-O2A-C1
24	A	827	CLA	O1D-CGD-O2D-CED
24	B	832	CLA	O1D-CGD-O2D-CED
24	B	803	CLA	C2C-C3C-CAC-CBC
24	B	830	CLA	C10-C11-C12-C13
24	h	610	CLA	C4C-C3C-CAC-CBC
24	c	601	CLA	C2C-C3C-CAC-CBC
24	5	607	CLA	O1D-CGD-O2D-CED
24	A	815	CLA	O1D-CGD-O2D-CED
26	h	614	DD6	C9-C10-C11-C12
24	B	819	CLA	O1A-CGA-O2A-C1
24	A	805	CLA	C4-C3-C5-C6
31	B	839	PQN	C14-C13-C15-C16
24	A	810	CLA	C13-C15-C16-C17
24	4	608	CLA	C4C-C3C-CAC-CBC
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
28	A	849	LHG	C33-C34-C35-C36
24	1	301	CLA	C8-C10-C11-C12
24	2	204	CLA	C2-C1-O2A-CGA
24	B	831	CLA	C2-C1-O2A-CGA
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	A	829	CLA	CBA-CGA-O2A-C1
28	A	841	LHG	O6-C4-C5-O7
24	9	305	CLA	CAA-CBA-CGA-O2A
24	A	807	CLA	C16-C17-C18-C19
24	L	204	CLA	C10-C11-C12-C13
24	B	821	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	h	611	CLA	O1D-CGD-O2D-CED
26	8	212	DD6	C9-C10-C11-C13
26	h	614	DD6	C9-C10-C11-C13
24	B	810	CLA	CAA-CBA-CGA-O2A
30	t	314	LMG	O1-C7-C8-O7
27	1	316	LMT	C5-C6-C7-C8
24	B	818	CLA	C13-C15-C16-C17
24	h	604	CLA	CBA-CGA-O2A-C1
24	3	301	CLA	C16-C17-C18-C19
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	C2-C3-C5-C6
24	A	805	CLA	C11-C12-C13-C15
24	A	823	CLA	C6-C7-C8-C10
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	802	CLA	C6-C7-C8-C10
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
24	B	831	CLA	C11-C12-C13-C15
31	A	839	PQN	C17-C18-C20-C21
31	B	839	PQN	C12-C13-C15-C16
24	A	832	CLA	O1A-CGA-O2A-C1
24	2	204	CLA	C6-C7-C8-C9
24	c	602	CLA	C11-C10-C8-C9
24	A	805	CLA	C11-C12-C13-C14
24	A	818	CLA	C11-C12-C13-C14
24	A	818	CLA	C14-C13-C15-C16
24	A	824	CLA	C11-C10-C8-C9
24	A	825	CLA	C11-C10-C8-C9
24	A	827	CLA	C14-C13-C15-C16
24	A	828	CLA	C14-C13-C15-C16
24	A	856	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	857	CLA	C11-C10-C8-C9
24	B	801	CLA	C14-C13-C15-C16
24	B	802	CLA	C6-C7-C8-C9
24	B	803	CLA	C11-C12-C13-C14
24	B	847	CLA	C14-C13-C15-C16
24	L	204	CLA	C11-C12-C13-C14
24	R	103	CLA	C11-C12-C13-C14
29	9	312	A1L1G	C35-C36-C37-C38
24	t	303	CLA	C10-C11-C12-C13
24	t	302	CLA	C2A-CAA-CBA-CGA
24	2	207	CLA	O1D-CGD-O2D-CED
24	B	817	CLA	C16-C17-C18-C20
24	t	301	CLA	O1D-CGD-O2D-CED
24	A	853	CLA	O1D-CGD-O2D-CED
29	2	213	A1L1G	C32-C33-C34-C35
24	k	301	CLA	O1A-CGA-O2A-C1
24	7	609	CLA	CBA-CGA-O2A-C1
27	1	315	LMT	C5'-C4'-O1B-C1B
24	t	310	CLA	O1D-CGD-O2D-CED
28	L	201	LHG	C26-C27-C28-C29
24	k	306	CLA	O1A-CGA-O2A-C1
24	B	812	CLA	C13-C15-C16-C17
28	B	844	LHG	C10-C11-C12-C13
26	k	315	DD6	C11-C13-C14-C15
24	A	836	CLA	O1D-CGD-O2D-CED
28	L	201	LHG	C24-C23-O8-C6
24	B	837	CLA	C4-C3-C5-C6
30	t	314	LMG	C29-C30-C31-C32
24	A	840	CLA	C13-C15-C16-C17
28	A	842	LHG	O9-C7-O7-C5
24	B	824	CLA	O1A-CGA-O2A-C1
28	3	315	LHG	C24-C23-O8-C6
28	L	201	LHG	C5-C4-O6-P
24	8	206	CLA	C3A-C2A-CAA-CBA
24	h	610	CLA	C3A-C2A-CAA-CBA
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	4	603	CLA	O1A-CGA-O2A-C1
24	9	302	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	8	213	LHG	C24-C25-C26-C27
25	4	618	BCR	C15-C16-C17-C18
27	A	850	LMT	C2-C1-O1'-C1'
27	A	854	LMT	C2-C1-O1'-C1'
24	3	301	CLA	C10-C11-C12-C13
28	1	318	LHG	C28-C29-C30-C31
24	k	303	CLA	C6-C7-C8-C9
24	k	303	CLA	C6-C7-C8-C10
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
30	t	314	LMG	C7-C8-C9-O8
24	A	829	CLA	O1A-CGA-O2A-C1
24	B	831	CLA	O2A-C1-C2-C3
24	B	837	CLA	O2A-C1-C2-C3
24	5	602	CLA	O1A-CGA-O2A-C1
24	A	847	CLA	C4-C3-C5-C6
27	1	315	LMT	C5-C6-C7-C8
28	B	844	LHG	C4-O6-P-O3
30	2	214	LMG	O10-C28-O8-C9
30	2	214	LMG	C30-C31-C32-C33
24	4	606	CLA	O1A-CGA-O2A-C1
24	6	606	CLA	C2A-CAA-CBA-CGA
24	A	838	CLA	C13-C15-C16-C17
24	4	602	CLA	CBA-CGA-O2A-C1
28	A	842	LHG	C25-C26-C27-C28
24	5	602	CLA	C6-C7-C8-C10
24	4	609	CLA	CAA-CBA-CGA-O2A
24	2	208	CLA	O1D-CGD-O2D-CED
24	c	605	CLA	C2C-C3C-CAC-CBC
24	A	817	CLA	C2C-C3C-CAC-CBC
28	I	103	LHG	O7-C5-C6-O8
30	A	855	LMG	O1-C7-C8-O7
24	5	606	CLA	CBA-CGA-O2A-C1
27	A	850	LMT	C3-C4-C5-C6
29	9	312	A1L1G	O13-C26-C30-C31
24	R	103	CLA	C2-C1-O2A-CGA
24	A	856	CLA	O1D-CGD-O2D-CED
24	4	607	CLA	CAA-CBA-CGA-O2A
24	1	317	CLA	C14-C13-C15-C16
24	7	606	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	608	CLA	C11-C10-C8-C9
24	A	810	CLA	C11-C10-C8-C9
24	A	823	CLA	C11-C10-C8-C9
24	A	826	CLA	C6-C7-C8-C9
24	A	832	CLA	C6-C7-C8-C9
24	A	857	CLA	C11-C12-C13-C14
24	B	829	CLA	C14-C13-C15-C16
31	A	839	PQN	C19-C18-C20-C21
24	B	802	CLA	CBA-CGA-O2A-C1
24	B	847	CLA	C13-C15-C16-C17
27	A	854	LMT	C1-C2-C3-C4
24	A	832	CLA	C16-C17-C18-C19
24	B	817	CLA	C16-C17-C18-C19
25	A	843	BCR	C23-C24-C25-C30
25	L	202	BCR	C5-C6-C7-C8
28	A	849	LHG	C26-C27-C28-C29
24	9	301	CLA	CAA-CBA-CGA-O2A
25	t	312	BCR	C36-C18-C19-C20
25	A	845	BCR	C11-C12-C13-C14
24	B	838	CLA	C13-C15-C16-C17
24	2	209	CLA	O1A-CGA-O2A-C1
24	A	853	CLA	C6-C7-C8-C9
24	B	820	CLA	C6-C7-C8-C9
24	B	826	CLA	C8-C10-C11-C12
24	B	831	CLA	C5-C6-C7-C8
24	k	303	CLA	C2C-C3C-CAC-CBC
28	A	852	LHG	C30-C31-C32-C33
28	3	315	LHG	C18-C19-C20-C21
24	c	601	CLA	C2A-CAA-CBA-CGA
28	8	213	LHG	O6-C4-C5-C6
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	c	609	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	812	CLA	C12-C13-C15-C16
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

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Mol	Chain	Res	Type	Atoms
24	A	826	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	C11-C10-C8-C7
24	B	801	CLA	C12-C13-C15-C16
24	B	809	CLA	C11-C12-C13-C15
24	B	812	CLA	C12-C13-C15-C16
24	B	818	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	A	828	CLA	C3-C5-C6-C7
29	k	312	A1L1G	C40-C41-C42-C44
24	B	847	CLA	C2A-CAA-CBA-CGA
24	A	817	CLA	CBD-CGD-O2D-CED
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
27	A	854	LMT	C11-C10-C9-C8
24	3	308	CLA	CBD-CGD-O2D-CED
24	t	308	CLA	CAA-CBA-CGA-O2A
24	t	310	CLA	O1A-CGA-O2A-C1
30	A	855	LMG	C14-C15-C16-C17
24	1	302	CLA	CAD-CBD-CGD-O2D
24	1	304	CLA	CAD-CBD-CGD-O2D
24	1	305	CLA	CAD-CBD-CGD-O2D
24	2	209	CLA	CAD-CBD-CGD-O2D
24	3	306	CLA	CAD-CBD-CGD-O2D
24	3	307	CLA	CAD-CBD-CGD-O2D
24	8	205	CLA	CAD-CBD-CGD-O2D
24	8	207	CLA	CAD-CBD-CGD-O2D
24	9	302	CLA	CAD-CBD-CGD-O2D
24	9	304	CLA	CAD-CBD-CGD-O2D
24	h	609	CLA	CAD-CBD-CGD-O2D
24	c	603	CLA	CAD-CBD-CGD-O2D
24	c	607	CLA	CAD-CBD-CGD-O2D
24	c	608	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	t	304	CLA	CAD-CBD-CGD-O2D
24	t	306	CLA	CAD-CBD-CGD-O2D
24	k	309	CLA	CAD-CBD-CGD-O2D
24	A	838	CLA	CAD-CBD-CGD-O2D
24	B	809	CLA	CAD-CBD-CGD-O2D
24	B	823	CLA	CAD-CBD-CGD-O2D
24	B	829	CLA	CAD-CBD-CGD-O2D
24	B	831	CLA	CAD-CBD-CGD-O2D
24	B	835	CLA	CAD-CBD-CGD-O2D
24	B	848	CLA	CAD-CBD-CGD-O2D
29	9	312	A1L1G	C45-C2-C44-C43
30	2	214	LMG	C35-C36-C37-C38
24	k	303	CLA	CBA-CGA-O2A-C1
24	B	827	CLA	CBA-CGA-O2A-C1
28	4	619	LHG	C10-C11-C12-C13
31	B	839	PQN	C18-C20-C21-C22
24	B	808	CLA	C2-C3-C5-C6
28	B	844	LHG	C5-C4-O6-P
30	A	855	LMG	O1-C7-C8-C9
28	8	213	LHG	O6-C4-C5-O7
24	t	309	CLA	C2A-CAA-CBA-CGA
24	A	826	CLA	C16-C17-C18-C20
24	A	832	CLA	C16-C17-C18-C20
24	1	307	CLA	CHA-CBD-CGD-O1D
24	1	307	CLA	CHA-CBD-CGD-O2D
24	2	204	CLA	CHA-CBD-CGD-O1D
24	2	204	CLA	CHA-CBD-CGD-O2D
24	2	206	CLA	CHA-CBD-CGD-O1D
24	2	206	CLA	CHA-CBD-CGD-O2D
24	2	208	CLA	CHA-CBD-CGD-O1D
24	2	208	CLA	CHA-CBD-CGD-O2D
24	6	603	CLA	CHA-CBD-CGD-O1D
24	6	603	CLA	CHA-CBD-CGD-O2D
24	7	605	CLA	CHA-CBD-CGD-O1D
24	7	605	CLA	CHA-CBD-CGD-O2D
24	7	607	CLA	CHA-CBD-CGD-O1D
24	8	201	CLA	CHA-CBD-CGD-O2D
24	8	203	CLA	CHA-CBD-CGD-O1D
24	h	606	CLA	CHA-CBD-CGD-O1D
24	h	611	CLA	CHA-CBD-CGD-O1D
24	h	611	CLA	CHA-CBD-CGD-O2D
24	c	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	611	CLA	CHA-CBD-CGD-O2D
24	A	801	CLA	CHA-CBD-CGD-O1D
24	A	815	CLA	CHA-CBD-CGD-O1D
24	A	815	CLA	CHA-CBD-CGD-O2D
24	A	829	CLA	CHA-CBD-CGD-O1D
24	A	834	CLA	CHA-CBD-CGD-O1D
24	A	836	CLA	CHA-CBD-CGD-O1D
24	B	802	CLA	CHA-CBD-CGD-O1D
24	B	802	CLA	CHA-CBD-CGD-O2D
24	B	813	CLA	CHA-CBD-CGD-O1D
24	B	813	CLA	CHA-CBD-CGD-O2D
24	B	816	CLA	CHA-CBD-CGD-O1D
24	B	822	CLA	CHA-CBD-CGD-O1D
24	B	822	CLA	CHA-CBD-CGD-O2D
24	B	827	CLA	CHA-CBD-CGD-O1D
24	B	827	CLA	CHA-CBD-CGD-O2D
24	L	203	CLA	CHA-CBD-CGD-O1D
24	L	203	CLA	CHA-CBD-CGD-O2D
24	4	602	CLA	O1A-CGA-O2A-C1
24	h	606	CLA	C4C-C3C-CAC-CBC
26	8	210	DD6	C4-C5-C6-C8
28	3	315	LHG	O7-C5-C6-O8
28	A	841	LHG	O7-C5-C6-O8
28	L	201	LHG	O10-C23-O8-C6
28	A	849	LHG	O1-C1-C2-O2
28	B	845	LHG	C31-C32-C33-C34
24	A	856	CLA	C4-C3-C5-C6
24	B	808	CLA	C4-C3-C5-C6
28	3	315	LHG	O10-C23-O8-C6
26	2	210	DD6	C27-C29-C30-C31
26	6	613	DD6	C27-C29-C30-C31
26	6	616	DD6	C27-C29-C30-C31
26	9	313	DD6	C27-C29-C30-C31
26	h	614	DD6	C27-C29-C30-C31
26	h	616	DD6	C27-C29-C30-C31
28	A	849	LHG	C28-C29-C30-C31
24	1	301	CLA	C6-C7-C8-C9
24	3	306	CLA	C14-C13-C15-C16
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

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Mol	Chain	Res	Type	Atoms
24	B	829	CLA	C11-C10-C8-C9
24	k	303	CLA	O1A-CGA-O2A-C1
24	A	808	CLA	O1A-CGA-O2A-C1
24	B	802	CLA	O1A-CGA-O2A-C1
24	6	604	CLA	C2A-CAA-CBA-CGA
24	A	847	CLA	C2A-CAA-CBA-CGA
24	B	827	CLA	O1A-CGA-O2A-C1
25	2	211	BCR	C21-C22-C23-C24
24	6	606	CLA	C4C-C3C-CAC-CBC
24	1	302	CLA	C1A-C2A-CAA-CBA
24	1	303	CLA	C1A-C2A-CAA-CBA
24	1	308	CLA	C1A-C2A-CAA-CBA
24	8	206	CLA	C1A-C2A-CAA-CBA
24	B	810	CLA	C1A-C2A-CAA-CBA
24	B	816	CLA	C1A-C2A-CAA-CBA
24	B	825	CLA	C1A-C2A-CAA-CBA
24	A	817	CLA	CBA-CGA-O2A-C1
28	4	619	LHG	C3-O3-P-O6
24	3	308	CLA	O1D-CGD-O2D-CED
28	1	318	LHG	C4-O6-P-O5
28	3	315	LHG	C3-O3-P-O4
28	4	619	LHG	C4-O6-P-O4
28	8	213	LHG	C3-O3-P-O5
28	A	841	LHG	C3-O3-P-O5
28	A	849	LHG	C3-O3-P-O5
28	A	849	LHG	C4-O6-P-O4
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	I	103	LHG	C3-O3-P-O4
28	A	841	LHG	C13-C14-C15-C16
24	B	836	CLA	C8-C10-C11-C12
24	A	808	CLA	CBA-CGA-O2A-C1
24	A	824	CLA	CBD-CGD-O2D-CED
27	1	315	LMT	C4B-C5B-C6B-O6B
24	A	816	CLA	C2A-CAA-CBA-CGA
24	B	822	CLA	C3-C5-C6-C7
24	A	817	CLA	O1D-CGD-O2D-CED
27	3	314	LMT	C3-C4-C5-C6
24	9	305	CLA	O1A-CGA-O2A-C1
24	1	306	CLA	CAD-CBD-CGD-O1D
24	2	203	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	7	607	CLA	CAD-CBD-CGD-O1D
24	9	306	CLA	CAD-CBD-CGD-O1D
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	A	811	CLA	CAD-CBD-CGD-O1D
24	A	813	CLA	CAD-CBD-CGD-O1D
24	A	831	CLA	CAD-CBD-CGD-O1D
24	A	847	CLA	CAD-CBD-CGD-O1D
24	B	813	CLA	CAD-CBD-CGD-O1D
24	B	817	CLA	CAD-CBD-CGD-O1D
24	B	834	CLA	CAD-CBD-CGD-O1D
24	F	202	CLA	CAD-CBD-CGD-O1D
29	3	310	A1L1G	C45-C2-C44-C42
24	h	607	CLA	CBA-CGA-O2A-C1
24	B	824	CLA	C13-C15-C16-C17
28	3	315	LHG	C19-C20-C21-C22
24	3	306	CLA	CBD-CGD-O2D-CED
24	c	604	CLA	O1A-CGA-O2A-C1
27	3	314	LMT	C5'-C4'-O1B-C1B
24	A	822	CLA	C6-C7-C8-C10
24	A	831	CLA	C16-C17-C18-C20
24	c	608	CLA	C12-C13-C15-C16
24	A	802	CLA	C11-C10-C8-C7
24	B	802	CLA	C11-C10-C8-C7
24	B	803	CLA	C12-C13-C15-C16
24	B	806	CLA	C12-C13-C15-C16
24	B	823	CLA	C6-C7-C8-C10
24	B	836	CLA	C11-C12-C13-C15
28	A	841	LHG	C7-C8-C9-C10
24	A	817	CLA	O1A-CGA-O2A-C1
28	B	844	LHG	C15-C16-C17-C18
24	R	104	CLA	C2A-CAA-CBA-CGA
24	L	204	CLA	C2C-C3C-CAC-CBC
24	6	611	CLA	CAD-CBD-CGD-O1D
28	J	105	LHG	O7-C5-C6-O8
24	A	860	CLA	C15-C16-C17-C18
24	h	606	CLA	CAA-CBA-CGA-O2A
28	A	852	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	c	608	CLA	C13-C15-C16-C17
24	A	822	CLA	C5-C6-C7-C8
24	t	303	CLA	C11-C10-C8-C9
24	A	812	CLA	C14-C13-C15-C16
24	A	838	CLA	C6-C7-C8-C9
24	B	801	CLA	C11-C10-C8-C9
24	B	812	CLA	C14-C13-C15-C16
24	B	816	CLA	C6-C7-C8-C9
24	B	817	CLA	C11-C10-C8-C9
24	B	818	CLA	C14-C13-C15-C16
24	B	824	CLA	C6-C7-C8-C9
24	F	201	CLA	C14-C13-C15-C16
24	A	801	CLA	C16-C17-C18-C20
24	A	826	CLA	C16-C17-C18-C19
24	2	204	CLA	C5-C6-C7-C8
24	c	606	CLA	C2A-CAA-CBA-CGA
28	8	213	LHG	O1-C1-C2-O2
25	M	101	BCR	C13-C14-C15-C16
24	A	857	CLA	C8-C10-C11-C12
24	k	306	CLA	CAA-CBA-CGA-O2A
24	A	817	CLA	CAA-CBA-CGA-O2A
24	B	837	CLA	C2-C3-C5-C6
24	A	810	CLA	C10-C11-C12-C13
24	B	834	CLA	C15-C16-C17-C18
24	B	802	CLA	C8-C10-C11-C12
24	A	821	CLA	C1-C2-C3-C4
24	A	805	CLA	C3-C5-C6-C7
24	7	612	CLA	C2A-CAA-CBA-CGA
24	h	604	CLA	C2A-CAA-CBA-CGA
24	A	820	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	1	317	CLA	C2-C1-O2A-CGA
24	B	801	CLA	C2-C1-O2A-CGA
24	B	812	CLA	C2-C1-O2A-CGA
24	7	606	CLA	C4C-C3C-CAC-CBC
24	B	831	CLA	C8-C10-C11-C12
24	A	823	CLA	O1D-CGD-O2D-CED
24	A	823	CLA	CBD-CGD-O2D-CED
24	t	302	CLA	CAA-CBA-CGA-O2A
25	A	843	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	856	CLA	C2-C3-C5-C6
27	3	314	LMT	C3'-C4'-O1B-C1B
28	A	841	LHG	O2-C2-C3-O3
24	5	602	CLA	C6-C7-C8-C9
24	A	824	CLA	O1D-CGD-O2D-CED
27	1	316	LMT	C4'-C5'-C6'-O6'
24	A	827	CLA	O1A-CGA-O2A-C1
24	A	811	CLA	CAA-CBA-CGA-O2A
28	2	215	LHG	C4-O6-P-O3
28	8	213	LHG	C4-O6-P-O3
28	A	841	LHG	C4-O6-P-O3
28	A	852	LHG	C3-O3-P-O6
28	I	103	LHG	C4-O6-P-O3
28	J	105	LHG	C4-O6-P-O3
28	L	201	LHG	C4-O6-P-O3
24	2	202	CLA	C6-C7-C8-C10
27	A	854	LMT	C7-C8-C9-C10
24	B	807	CLA	C4-C3-C5-C6
24	B	818	CLA	C5-C6-C7-C8
24	A	818	CLA	C11-C12-C13-C15
24	A	833	CLA	C11-C12-C13-C15
24	A	847	CLA	C2-C3-C5-C6
24	B	807	CLA	C12-C13-C15-C16
24	B	817	CLA	C12-C13-C15-C16
24	7	606	CLA	CAA-CBA-CGA-O2A
24	4	602	CLA	C6-C7-C8-C9
24	B	806	CLA	C14-C13-C15-C16
24	B	809	CLA	C11-C12-C13-C14
29	2	213	A1L1G	C30-C31-C32-C33
29	7	614	A1L1G	C30-C31-C32-C33
24	A	831	CLA	C16-C17-C18-C19
24	B	815	CLA	C6-C7-C8-C9
28	8	213	LHG	C9-C10-C11-C12
24	A	816	CLA	C8-C10-C11-C12
24	B	803	CLA	C10-C11-C12-C13
24	B	804	CLA	C10-C11-C12-C13
24	B	817	CLA	C13-C15-C16-C17
24	9	305	CLA	C2A-CAA-CBA-CGA
27	1	315	LMT	C6-C7-C8-C9
24	B	802	CLA	C3-C5-C6-C7
24	L	205	CLA	C2C-C3C-CAC-CBC
24	A	822	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	2	215	LHG	C2-C3-O3-P
28	B	844	LHG	C2-C3-O3-P
28	1	318	LHG	C11-C12-C13-C14
25	A	844	BCR	C7-C8-C9-C10
24	A	827	CLA	CBA-CGA-O2A-C1
24	h	604	CLA	O1A-CGA-O2A-C1
24	7	609	CLA	O1A-CGA-O2A-C1
28	I	103	LHG	C24-C23-O8-C6
24	2	204	CLA	C2A-CAA-CBA-CGA
24	B	834	CLA	C16-C17-C18-C20
25	A	844	BCR	C9-C10-C11-C12
25	B	842	BCR	C19-C20-C21-C22
28	1	318	LHG	O6-C4-C5-C6
28	A	841	LHG	O6-C4-C5-C6
28	1	318	LHG	O6-C4-C5-O7
24	B	802	CLA	CAA-CBA-CGA-O2A
24	B	822	CLA	C4-C3-C5-C6
24	B	818	CLA	C15-C16-C17-C18
24	A	824	CLA	C2-C3-C5-C6
24	A	808	CLA	C8-C10-C11-C12
27	A	850	LMT	C9-C10-C11-C12
24	4	602	CLA	C2-C1-O2A-CGA
27	A	854	LMT	C3-C4-C5-C6
24	A	816	CLA	C15-C16-C17-C18
24	3	303	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	k	303	CLA	C2A-CAA-CBA-CGA
28	4	619	LHG	O7-C5-C6-O8
24	9	305	CLA	CAA-CBA-CGA-O1A
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	A	853	CLA	C6-C7-C8-C10
27	1	316	LMT	O5'-C5'-C6'-O6'
24	A	824	CLA	C4-C3-C5-C6
26	6	615	DD6	C27-C29-C30-C31
26	c	614	DD6	C27-C29-C30-C31
24	3	301	CLA	C6-C7-C8-C9
24	A	820	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	823	CLA	C11-C12-C13-C14
24	B	827	CLA	C11-C12-C13-C14
24	B	837	CLA	C6-C7-C8-C9
24	A	801	CLA	C16-C17-C18-C19
28	A	841	LHG	C11-C12-C13-C14
24	c	608	CLA	C10-C11-C12-C13
24	A	804	CLA	C15-C16-C17-C18
28	A	841	LHG	C29-C30-C31-C32
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
28	A	841	LHG	C4-C5-C6-O8
24	5	607	CLA	CAA-CBA-CGA-O2A
24	c	608	CLA	O2A-C1-C2-C3
27	1	316	LMT	C5'-C4'-O1B-C1B
24	5	607	CLA	CAA-CBA-CGA-O1A
25	1	310	BCR	C11-C12-C13-C35
24	7	610	CLA	CAA-CBA-CGA-O1A
28	4	619	LHG	C6-C5-O7-C7
28	L	201	LHG	C6-C5-O7-C7
24	7	601	CLA	C1A-C2A-CAA-CBA
24	A	856	CLA	C1A-C2A-CAA-CBA
24	B	812	CLA	C1A-C2A-CAA-CBA
24	3	301	CLA	C12-C13-C15-C16
24	A	810	CLA	C11-C10-C8-C7
24	A	826	CLA	C6-C7-C8-C10
24	A	831	CLA	C11-C10-C8-C7
24	A	840	CLA	C6-C7-C8-C10
24	B	831	CLA	C11-C10-C8-C7
24	B	838	CLA	C11-C12-C13-C15
24	B	836	CLA	C5-C6-C7-C8
24	3	307	CLA	CAA-CBA-CGA-O1A
24	c	605	CLA	C4C-C3C-CAC-CBC
24	7	601	CLA	C2A-CAA-CBA-CGA
24	h	612	CLA	C2A-CAA-CBA-CGA
24	F	203	CLA	C2A-CAA-CBA-CGA
24	B	803	CLA	C15-C16-C17-C18
24	B	806	CLA	C8-C10-C11-C12
24	B	833	CLA	C8-C10-C11-C12
31	A	839	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	B	847	CLA	CBA-CGA-O2A-C1
28	A	841	LHG	C10-C11-C12-C13
24	A	824	CLA	C16-C17-C18-C19
28	1	318	LHG	C10-C11-C12-C13
28	A	841	LHG	C28-C29-C30-C31
24	B	847	CLA	O1A-CGA-O2A-C1
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	1	307	CLA	CAA-CBA-CGA-O2A
24	6	601	CLA	CAA-CBA-CGA-O2A
25	k	316	BCR	C19-C20-C21-C22
24	5	603	CLA	CAA-CBA-CGA-O1A
24	5	606	CLA	O1A-CGA-O2A-C1
24	1	307	CLA	CAA-CBA-CGA-O1A
24	t	306	CLA	CAA-CBA-CGA-O1A
24	t	306	CLA	CAA-CBA-CGA-O2A
28	A	841	LHG	C12-C13-C14-C15
24	3	306	CLA	O1D-CGD-O2D-CED
24	h	602	CLA	C4-C3-C5-C6
24	B	810	CLA	CAA-CBA-CGA-O1A
24	A	806	CLA	C2-C1-O2A-CGA
24	A	808	CLA	C2-C1-O2A-CGA
24	A	814	CLA	C2-C1-O2A-CGA
24	B	828	CLA	C2-C1-O2A-CGA
24	1	317	CLA	C16-C17-C18-C19
24	c	609	CLA	C6-C7-C8-C9
24	A	805	CLA	C11-C10-C8-C9
24	A	836	CLA	C11-C12-C13-C14
31	B	839	PQN	C19-C18-C20-C21
24	4	601	CLA	C2C-C3C-CAC-CBC
24	3	307	CLA	CAA-CBA-CGA-O2A
29	7	614	A1L1G	C14-C29-C30-C26
24	5	602	CLA	CAA-CBA-CGA-O2A
24	A	832	CLA	C5-C6-C7-C8
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	t	303	CLA	C16-C17-C18-C20
24	A	812	CLA	C16-C17-C18-C19
24	3	305	CLA	O1A-CGA-O2A-C1
25	A	859	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	1	306	CLA	O1D-CGD-O2D-CED
24	1	306	CLA	CAA-CBA-CGA-O2A
24	1	317	CLA	CAA-CBA-CGA-O2A
24	4	604	CLA	CAA-CBA-CGA-O2A
24	t	309	CLA	CAA-CBA-CGA-O2A
28	J	105	LHG	C4-C5-C6-O8
24	8	208	CLA	CAA-CBA-CGA-O2A
24	A	836	CLA	C5-C6-C7-C8
29	2	213	A1L1G	C34-C35-C36-C37
24	B	825	CLA	C6-C7-C8-C10
24	A	823	CLA	C15-C16-C17-C18
24	B	807	CLA	C2-C3-C5-C6
24	7	608	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	C13-C15-C16-C17
24	5	603	CLA	CAA-CBA-CGA-O2A
24	h	612	CLA	CAA-CBA-CGA-O2A
24	9	311	CLA	CAA-CBA-CGA-O2A
24	h	601	CLA	CAA-CBA-CGA-O2A
24	8	202	CLA	C2A-CAA-CBA-CGA
24	9	306	CLA	C2A-CAA-CBA-CGA
24	t	310	CLA	C2A-CAA-CBA-CGA
24	B	802	CLA	C2A-CAA-CBA-CGA
24	c	602	CLA	C3-C5-C6-C7
24	6	601	CLA	CAA-CBA-CGA-O1A
24	B	829	CLA	CAA-CBA-CGA-O2A
28	I	103	LHG	O10-C23-O8-C6
24	1	317	CLA	C11-C12-C13-C15
24	A	838	CLA	C6-C7-C8-C10
24	B	812	CLA	C11-C10-C8-C7
24	B	817	CLA	C11-C10-C8-C7
24	B	818	CLA	C12-C13-C15-C16
24	B	829	CLA	C12-C13-C15-C16
24	F	201	CLA	C12-C13-C15-C16
24	B	805	CLA	C16-C17-C18-C19
24	B	834	CLA	C16-C17-C18-C19
28	A	852	LHG	C5-C4-O6-P
24	3	305	CLA	CBA-CGA-O2A-C1
24	A	821	CLA	O2A-C1-C2-C3
24	9	306	CLA	CAA-CBA-CGA-O2A
24	k	307	CLA	CAA-CBA-CGA-O2A
24	A	801	CLA	CAA-CBA-CGA-O2A
24	B	831	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	A	828	CLA	C8-C10-C11-C12
24	F	202	CLA	CBA-CGA-O2A-C1
26	9	315	DD6	C9-C10-C11-C12
24	A	807	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	C4-C3-C5-C6
24	B	825	CLA	C4-C3-C5-C6
24	B	831	CLA	C4-C3-C5-C6
24	A	815	CLA	CAA-CBA-CGA-O2A
24	k	305	CLA	CAA-CBA-CGA-O2A
24	c	608	CLA	C14-C13-C15-C16
24	A	802	CLA	C11-C10-C8-C9
24	A	818	CLA	C6-C7-C8-C9
24	B	831	CLA	C11-C10-C8-C9
24	B	825	CLA	C3-C5-C6-C7
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	k	302	CLA	CAA-CBA-CGA-O2A
24	B	828	CLA	CAA-CBA-CGA-O2A
24	7	603	CLA	CAA-CBA-CGA-O2A
24	9	311	CLA	CAA-CBA-CGA-O1A
24	4	604	CLA	CAD-CBD-CGD-O2D
24	4	608	CLA	CAD-CBD-CGD-O2D
24	5	607	CLA	CAD-CBD-CGD-O2D
24	6	604	CLA	CAD-CBD-CGD-O2D
24	6	606	CLA	CAD-CBD-CGD-O2D
24	6	609	CLA	CAD-CBD-CGD-O2D
24	7	604	CLA	CAD-CBD-CGD-O2D
24	7	609	CLA	CAD-CBD-CGD-O2D
24	7	612	CLA	CAD-CBD-CGD-O2D
24	8	203	CLA	CAD-CBD-CGD-O2D
24	8	209	CLA	CAD-CBD-CGD-O2D
24	h	602	CLA	CAD-CBD-CGD-O2D
24	h	610	CLA	CAD-CBD-CGD-O2D
24	c	609	CLA	CAD-CBD-CGD-O2D
24	t	303	CLA	CAD-CBD-CGD-O2D
24	k	302	CLA	CAD-CBD-CGD-O2D
24	k	311	CLA	CAD-CBD-CGD-O2D
24	A	806	CLA	CAD-CBD-CGD-O2D
24	A	808	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	810	CLA	CAD-CBD-CGD-O2D
24	A	825	CLA	CAD-CBD-CGD-O2D
24	A	827	CLA	CAD-CBD-CGD-O2D
24	A	856	CLA	CAD-CBD-CGD-O2D
24	B	815	CLA	CAD-CBD-CGD-O2D
24	B	824	CLA	CAD-CBD-CGD-O2D
24	B	838	CLA	CAD-CBD-CGD-O2D
29	7	614	A1L1G	C45-C2-C44-C43
24	B	805	CLA	C16-C17-C18-C20
24	A	831	CLA	C2A-CAA-CBA-CGA
24	B	825	CLA	C2A-CAA-CBA-CGA
24	F	201	CLA	C15-C16-C17-C18
24	3	302	CLA	CAA-CBA-CGA-O2A
24	7	610	CLA	CAA-CBA-CGA-O2A
24	6	603	CLA	CAA-CBA-CGA-O2A
24	7	602	CLA	CAA-CBA-CGA-O2A
24	A	806	CLA	CAA-CBA-CGA-O2A
24	B	804	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	CAA-CBA-CGA-O2A
24	B	847	CLA	CAA-CBA-CGA-O2A
24	A	837	CLA	C4-C3-C5-C6
24	7	604	CLA	CAA-CBA-CGA-O2A
24	h	601	CLA	CAA-CBA-CGA-O1A
24	A	837	CLA	C2-C3-C5-C6
24	c	605	CLA	CAA-CBA-CGA-O2A
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
28	A	841	LHG	C14-C15-C16-C17
26	3	312	DD6	C13-C14-C15-O1
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	7	601	CLA	CAA-CBA-CGA-O2A
24	h	612	CLA	CAA-CBA-CGA-O1A
24	B	833	CLA	O1A-CGA-O2A-C1
24	t	307	CLA	CAA-CBA-CGA-O2A
24	h	607	CLA	O1A-CGA-O2A-C1
24	3	302	CLA	CAA-CBA-CGA-O1A
24	7	603	CLA	CAA-CBA-CGA-O1A
24	7	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	8	207	CLA	CAA-CBA-CGA-O2A
24	8	208	CLA	CAA-CBA-CGA-O1A
24	1	317	CLA	O2A-C1-C2-C3
24	A	824	CLA	O2A-C1-C2-C3
24	A	825	CLA	O2A-C1-C2-C3
24	B	815	CLA	O2A-C1-C2-C3
24	B	847	CLA	O2A-C1-C2-C3
28	I	103	LHG	C27-C28-C29-C30
24	4	609	CLA	CAA-CBA-CGA-O1A
24	7	608	CLA	CAA-CBA-CGA-O1A
24	A	824	CLA	C16-C17-C18-C20
24	A	847	CLA	C6-C7-C8-C9
24	1	317	CLA	CHA-CBD-CGD-O1D
24	1	317	CLA	CHA-CBD-CGD-O2D
24	3	302	CLA	CHA-CBD-CGD-O1D
24	3	309	CLA	CHA-CBD-CGD-O1D
24	3	309	CLA	CHA-CBD-CGD-O2D
24	4	607	CLA	CHA-CBD-CGD-O1D
24	4	607	CLA	CHA-CBD-CGD-O2D
24	4	613	CLA	CHA-CBD-CGD-O1D
24	4	613	CLA	CHA-CBD-CGD-O2D
24	5	605	CLA	CHA-CBD-CGD-O1D
24	5	605	CLA	CHA-CBD-CGD-O2D
24	6	608	CLA	CHA-CBD-CGD-O1D
24	6	608	CLA	CHA-CBD-CGD-O2D
24	7	601	CLA	CHA-CBD-CGD-O1D
24	7	607	CLA	CHA-CBD-CGD-O2D
24	7	611	CLA	CHA-CBD-CGD-O2D
24	8	202	CLA	CHA-CBD-CGD-O1D
24	8	202	CLA	CHA-CBD-CGD-O2D
24	8	203	CLA	CHA-CBD-CGD-O2D
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	305	CLA	CHA-CBD-CGD-O2D
24	9	309	CLA	CHA-CBD-CGD-O1D
24	9	311	CLA	CHA-CBD-CGD-O1D
24	9	311	CLA	CHA-CBD-CGD-O2D
24	h	612	CLA	CHA-CBD-CGD-O1D
24	h	612	CLA	CHA-CBD-CGD-O2D
24	c	603	CLA	CHA-CBD-CGD-O2D
24	c	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	t	302	CLA	CHA-CBD-CGD-O1D
24	t	302	CLA	CHA-CBD-CGD-O2D
24	t	310	CLA	CHA-CBD-CGD-O1D
24	k	304	CLA	CHA-CBD-CGD-O2D
24	k	307	CLA	CHA-CBD-CGD-O2D
24	k	308	CLA	CHA-CBD-CGD-O1D
24	k	308	CLA	CHA-CBD-CGD-O2D
24	A	802	CLA	CHA-CBD-CGD-O1D
24	A	802	CLA	CHA-CBD-CGD-O2D
24	A	804	CLA	CHA-CBD-CGD-O1D
24	A	816	CLA	CHA-CBD-CGD-O1D
24	A	823	CLA	CHA-CBD-CGD-O1D
24	A	824	CLA	CHA-CBD-CGD-O1D
24	A	830	CLA	CHA-CBD-CGD-O2D
24	A	833	CLA	CHA-CBD-CGD-O1D
24	A	833	CLA	CHA-CBD-CGD-O2D
24	A	834	CLA	CHA-CBD-CGD-O2D
24	A	836	CLA	CHA-CBD-CGD-O2D
24	B	816	CLA	CHA-CBD-CGD-O2D
24	B	837	CLA	CHA-CBD-CGD-O1D
24	B	837	CLA	CHA-CBD-CGD-O2D
24	B	846	CLA	CHA-CBD-CGD-O1D
26	8	210	DD6	C11-C10-C9-C8
24	A	815	CLA	CAA-CBA-CGA-O1A
24	B	831	CLA	C2-C3-C5-C6
24	c	602	CLA	C10-C11-C12-C13
24	B	847	CLA	C2C-C3C-CAC-CBC
26	9	314	DD6	C9-C10-C11-C13
24	7	612	CLA	CAA-CBA-CGA-O2A
24	9	309	CLA	CAA-CBA-CGA-O2A
28	L	201	LHG	O8-C23-C24-C25
28	A	852	LHG	C25-C26-C27-C28
24	8	207	CLA	CAA-CBA-CGA-O1A
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	836	CLA	C2A-CAA-CBA-CGA
28	3	315	LHG	O1-C1-C2-O2
24	A	804	CLA	CAA-CBA-CGA-O2A
24	B	848	CLA	CAA-CBA-CGA-O2A
24	B	816	CLA	C2-C3-C5-C6
24	B	824	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	808	CLA	C16-C17-C18-C19
26	1	313	DD6	C27-C29-C30-C31
26	3	311	DD6	C27-C29-C30-C31
26	4	615	DD6	C27-C29-C30-C31
26	4	616	DD6	C27-C29-C30-C31
26	5	608	DD6	C27-C29-C30-C31
26	h	613	DD6	C27-C29-C30-C31
29	k	312	A1L1G	C14-C29-C30-C31
24	A	808	CLA	CAA-CBA-CGA-O2A
24	B	831	CLA	CAA-CBA-CGA-O2A
24	c	608	CLA	C6-C7-C8-C9
24	A	804	CLA	C11-C12-C13-C14
24	A	828	CLA	C6-C7-C8-C9
24	A	840	CLA	C6-C7-C8-C9
24	B	812	CLA	C11-C10-C8-C9
24	B	817	CLA	C14-C13-C15-C16
24	A	807	CLA	CAA-CBA-CGA-O1A
25	A	844	BCR	C19-C20-C21-C22
28	A	849	LHG	C10-C11-C12-C13
24	A	812	CLA	C16-C17-C18-C20
24	A	860	CLA	C2A-CAA-CBA-CGA
24	4	613	CLA	CAA-CBA-CGA-O2A
24	k	311	CLA	CAA-CBA-CGA-O2A
24	A	832	CLA	CAA-CBA-CGA-O2A
24	7	601	CLA	CAA-CBA-CGA-O1A
24	A	806	CLA	CAA-CBA-CGA-O1A
24	B	828	CLA	CAA-CBA-CGA-O1A
24	B	825	CLA	C6-C7-C8-C9
24	B	825	CLA	C2-C3-C5-C6
24	6	603	CLA	CAA-CBA-CGA-O1A
24	k	307	CLA	CAA-CBA-CGA-O1A
24	2	209	CLA	C1A-C2A-CAA-CBA
24	4	612	CLA	C1A-C2A-CAA-CBA
24	4	613	CLA	C1A-C2A-CAA-CBA
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	c	603	CLA	C1A-C2A-CAA-CBA
24	c	610	CLA	CHA-CBD-CGD-O2D
24	A	804	CLA	C1A-C2A-CAA-CBA
24	A	814	CLA	C1A-C2A-CAA-CBA
24	A	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	A	835	CLA	C1A-C2A-CAA-CBA
24	B	809	CLA	C1A-C2A-CAA-CBA
24	L	203	CLA	C1A-C2A-CAA-CBA
24	6	602	CLA	C2-C1-O2A-CGA
24	4	607	CLA	CAA-CBA-CGA-O1A
24	7	602	CLA	CAA-CBA-CGA-O1A
24	B	847	CLA	CAA-CBA-CGA-O1A
24	k	302	CLA	C2C-C3C-CAC-CBC
24	A	801	CLA	CAA-CBA-CGA-O1A
28	I	103	LHG	C29-C30-C31-C32
24	1	304	CLA	C2A-CAA-CBA-CGA
24	t	303	CLA	C2A-CAA-CBA-CGA
24	1	306	CLA	CBD-CGD-O2D-CED
24	B	836	CLA	C16-C17-C18-C20
24	k	305	CLA	CAA-CBA-CGA-O1A
24	1	302	CLA	CAA-CBA-CGA-O2A
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	3	301	CLA	C5-C6-C7-C8
24	B	832	CLA	CAA-CBA-CGA-O2A
28	2	215	LHG	C4-O6-P-O5
28	8	213	LHG	C4-O6-P-O5
28	J	105	LHG	C4-O6-P-O5
24	7	612	CLA	CAA-CBA-CGA-O1A
24	9	301	CLA	CAA-CBA-CGA-O1A
24	h	603	CLA	CAA-CBA-CGA-O1A
24	c	605	CLA	CAA-CBA-CGA-O1A
24	t	307	CLA	CAA-CBA-CGA-O1A
24	B	831	CLA	CAA-CBA-CGA-O1A
28	B	844	LHG	C27-C28-C29-C30
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	9	309	CLA	CAA-CBA-CGA-O1A
24	B	804	CLA	CAA-CBA-CGA-O1A
24	3	308	CLA	CAA-CBA-CGA-O2A
24	6	610	CLA	CAA-CBA-CGA-O2A
24	A	817	CLA	C2A-CAA-CBA-CGA
24	t	308	CLA	CAA-CBA-CGA-O1A
24	B	848	CLA	CAA-CBA-CGA-O1A
24	A	824	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	831	CLA	C13-C15-C16-C17
24	F	202	CLA	CAA-CBA-CGA-O2A
28	A	849	LHG	O7-C7-C8-C9
24	3	306	CLA	C13-C15-C16-C17
24	A	804	CLA	CAA-CBA-CGA-O1A
24	2	204	CLA	C11-C12-C13-C14
24	B	808	CLA	C16-C17-C18-C20
24	5	605	CLA	CAD-CBD-CGD-O1D
24	9	308	CLA	CAD-CBD-CGD-O1D
24	t	307	CLA	CAD-CBD-CGD-O1D
24	A	801	CLA	CAD-CBD-CGD-O1D
24	A	804	CLA	CAD-CBD-CGD-O1D
24	A	823	CLA	CAD-CBD-CGD-O1D
24	A	836	CLA	CAD-CBD-CGD-O1D
24	B	810	CLA	CAD-CBD-CGD-O1D
24	B	832	CLA	CAD-CBD-CGD-O1D
24	B	836	CLA	CAD-CBD-CGD-O1D
24	B	847	CLA	CAD-CBD-CGD-O1D
24	L	204	CLA	O1A-CGA-O2A-C1
28	L	201	LHG	O10-C23-C24-C25
24	B	801	CLA	C8-C10-C11-C12
24	3	305	CLA	C11-C10-C8-C9
24	A	802	CLA	C11-C12-C13-C14
24	A	813	CLA	C11-C10-C8-C9
24	A	818	CLA	C11-C10-C8-C9
24	A	825	CLA	C11-C12-C13-C14
24	A	829	CLA	C11-C10-C8-C9
24	B	805	CLA	C11-C12-C13-C14
24	B	838	CLA	C11-C12-C13-C14
24	1	302	CLA	CAA-CBA-CGA-O1A
24	8	205	CLA	CAA-CBA-CGA-O2A
24	B	833	CLA	CBA-CGA-O2A-C1
24	3	301	CLA	CAA-CBA-CGA-O2A
24	6	606	CLA	CAA-CBA-CGA-O2A
24	9	302	CLA	CAA-CBA-CGA-O2A
24	t	303	CLA	CAA-CBA-CGA-O2A
24	A	822	CLA	CAA-CBA-CGA-O2A
24	B	809	CLA	CAA-CBA-CGA-O2A
24	A	801	CLA	C8-C10-C11-C12
24	A	806	CLA	C8-C10-C11-C12
24	B	846	CLA	C2A-CAA-CBA-CGA
24	2	209	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	9	303	CLA	CAA-CBA-CGA-O2A
24	c	603	CLA	CAA-CBA-CGA-O2A
28	B	844	LHG	C1-C2-C3-O3
24	k	311	CLA	CAA-CBA-CGA-O1A
24	A	832	CLA	CAA-CBA-CGA-O1A
24	c	602	CLA	C13-C15-C16-C17
24	3	301	CLA	C11-C10-C8-C7
24	6	611	CLA	CAD-CBD-CGD-O2D
24	7	602	CLA	C3A-C2A-CAA-CBA
24	c	609	CLA	C6-C7-C8-C10
24	A	801	CLA	C12-C13-C15-C16
24	A	804	CLA	C11-C10-C8-C7
24	A	804	CLA	C11-C12-C13-C15
24	A	818	CLA	C6-C7-C8-C10
24	A	828	CLA	C6-C7-C8-C10
24	A	856	CLA	C3A-C2A-CAA-CBA
24	B	805	CLA	C11-C12-C13-C15
24	B	813	CLA	C3A-C2A-CAA-CBA
24	F	201	CLA	C11-C10-C8-C7
24	F	201	CLA	C11-C12-C13-C15
24	5	606	CLA	CAA-CBA-CGA-O1A
24	t	303	CLA	CAA-CBA-CGA-O1A
24	A	808	CLA	CAA-CBA-CGA-O1A
24	B	809	CLA	CAA-CBA-CGA-O1A
24	2	206	CLA	CAA-CBA-CGA-O2A
24	2	207	CLA	CAA-CBA-CGA-O2A
24	9	308	CLA	CAA-CBA-CGA-O2A
28	J	105	LHG	O8-C23-C24-C25
24	1	304	CLA	C3-C5-C6-C7
24	L	204	CLA	C3-C5-C6-C7
24	2	207	CLA	CAA-CBA-CGA-O1A
24	3	308	CLA	CAA-CBA-CGA-O1A
24	9	302	CLA	CAA-CBA-CGA-O1A
24	B	821	CLA	CAA-CBA-CGA-O1A
24	3	306	CLA	CAA-CBA-CGA-O2A
24	A	816	CLA	CAA-CBA-CGA-O2A
24	B	835	CLA	CAA-CBA-CGA-O2A
24	L	205	CLA	CAA-CBA-CGA-O2A
24	4	613	CLA	CAA-CBA-CGA-O1A
24	c	603	CLA	CAA-CBA-CGA-O1A
24	B	832	CLA	CAA-CBA-CGA-O1A
24	7	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	1	308	CLA	CAA-CBA-CGA-O2A
24	4	603	CLA	CAA-CBA-CGA-O2A
24	A	820	CLA	CAA-CBA-CGA-O2A
24	B	811	CLA	CAA-CBA-CGA-O2A
24	8	202	CLA	CAA-CBA-CGA-O1A
24	A	816	CLA	CAA-CBA-CGA-O1A
24	A	822	CLA	CAA-CBA-CGA-O1A
24	8	205	CLA	CAA-CBA-CGA-O1A
24	B	812	CLA	C10-C11-C12-C13
24	9	303	CLA	CAA-CBA-CGA-O1A
24	t	304	CLA	CAA-CBA-CGA-O2A
24	A	830	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

205 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	301	CLA	2	0
25	B	841	BCR	2	0
25	I	102	BCR	2	0
24	B	804	CLA	6	0
26	c	613	DD6	1	0
26	5	608	DD6	2	0
26	7	618	DD6	1	0
24	4	602	CLA	3	0
24	5	607	CLA	2	0
24	4	607	CLA	4	0
29	3	310	A1L1G	2	0
28	3	315	LHG	1	0
24	J	103	CLA	1	0
27	1	316	LMT	2	0
24	3	305	CLA	1	0
24	B	838	CLA	2	0
24	B	824	CLA	2	0
24	L	205	CLA	5	0
26	h	614	DD6	1	0
24	9	302	CLA	2	0
24	A	819	CLA	1	0
24	B	803	CLA	4	0
24	B	829	CLA	4	0
24	A	805	CLA	1	0
24	2	207	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	k	309	CLA	1	0
28	I	103	LHG	1	0
24	B	810	CLA	1	0
24	A	817	CLA	2	0
24	6	606	CLA	1	0
24	3	308	CLA	2	0
24	c	603	CLA	1	0
24	2	201	CLA	3	0
25	B	843	BCR	5	0
24	4	608	CLA	4	0
24	A	812	CLA	1	0
24	5	606	CLA	1	0
24	3	304	CLA	5	0
24	2	206	CLA	2	0
26	k	315	DD6	3	0
25	k	316	BCR	2	0
24	A	826	CLA	2	0
28	J	105	LHG	1	0
24	B	817	CLA	2	0
26	1	313	DD6	1	0
24	7	612	CLA	2	0
24	B	833	CLA	2	0
24	c	602	CLA	2	0
24	t	302	CLA	1	0
26	6	615	DD6	1	0
29	9	312	A1L1G	1	0
25	1	314	BCR	3	0
24	B	830	CLA	7	0
24	A	804	CLA	1	0
24	A	801	CLA	1	0
25	7	617	BCR	2	0
25	B	840	BCR	1	0
25	1	310	BCR	4	0
24	B	848	CLA	1	0
24	1	305	CLA	4	0
24	A	802	CLA	2	0
24	9	305	CLA	3	0
26	5	609	DD6	1	0
24	6	603	CLA	3	0
24	8	204	CLA	2	0
26	9	313	DD6	2	0
25	F	204	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	824	CLA	1	0
24	1	302	CLA	1	0
24	2	204	CLA	1	0
24	B	828	CLA	1	0
24	6	608	CLA	1	0
25	R	102	BCR	2	0
27	3	314	LMT	1	0
24	9	301	CLA	8	0
25	B	849	BCR	1	0
24	B	847	CLA	1	0
24	6	601	CLA	3	0
24	7	606	CLA	4	0
24	7	607	CLA	4	0
24	9	308	CLA	2	0
24	A	840	CLA	1	0
24	B	846	CLA	1	0
28	L	201	LHG	4	0
24	A	816	CLA	1	0
24	1	304	CLA	3	0
24	8	203	CLA	2	0
25	2	211	BCR	4	0
24	A	823	CLA	1	0
25	A	846	BCR	2	0
24	B	832	CLA	3	0
24	c	610	CLA	1	0
25	A	843	BCR	2	0
24	B	835	CLA	1	0
24	t	306	CLA	1	0
24	B	825	CLA	1	0
24	c	607	CLA	1	0
30	2	214	LMG	1	0
26	4	615	DD6	1	0
24	h	610	CLA	1	0
24	1	317	CLA	2	0
29	k	312	A1L1G	2	0
24	1	307	CLA	2	0
26	9	317	DD6	1	0
25	L	202	BCR	2	0
24	B	806	CLA	1	0
24	4	611	CLA	10	0
25	J	104	BCR	1	0
26	k	313	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	8	209	CLA	1	0
24	h	608	CLA	2	0
24	B	801	CLA	1	0
25	t	312	BCR	2	0
25	J	101	BCR	4	0
27	h	617	LMT	1	0
24	B	815	CLA	1	0
24	B	834	CLA	2	0
24	6	602	CLA	2	0
24	h	612	CLA	2	0
24	A	832	CLA	1	0
26	2	210	DD6	1	0
24	5	604	CLA	2	0
24	L	204	CLA	1	0
24	B	827	CLA	1	0
24	t	305	CLA	3	0
24	k	305	CLA	1	0
24	7	611	CLA	2	0
24	A	838	CLA	1	0
26	1	311	DD6	5	0
24	1	303	CLA	1	0
26	3	312	DD6	1	0
24	B	805	CLA	3	0
24	c	601	CLA	2	0
26	c	612	DD6	2	0
24	7	610	CLA	2	0
24	A	853	CLA	2	0
26	2	212	DD6	1	0
24	A	829	CLA	2	0
24	A	847	CLA	1	0
25	I	101	BCR	1	0
24	B	802	CLA	2	0
24	B	811	CLA	1	0
24	4	609	CLA	2	0
24	A	830	CLA	6	0
24	9	311	CLA	1	0
25	c	615	BCR	7	0
24	9	303	CLA	1	0
24	A	810	CLA	1	0
25	A	859	BCR	1	0
28	4	619	LHG	1	0
24	2	202	CLA	1	0

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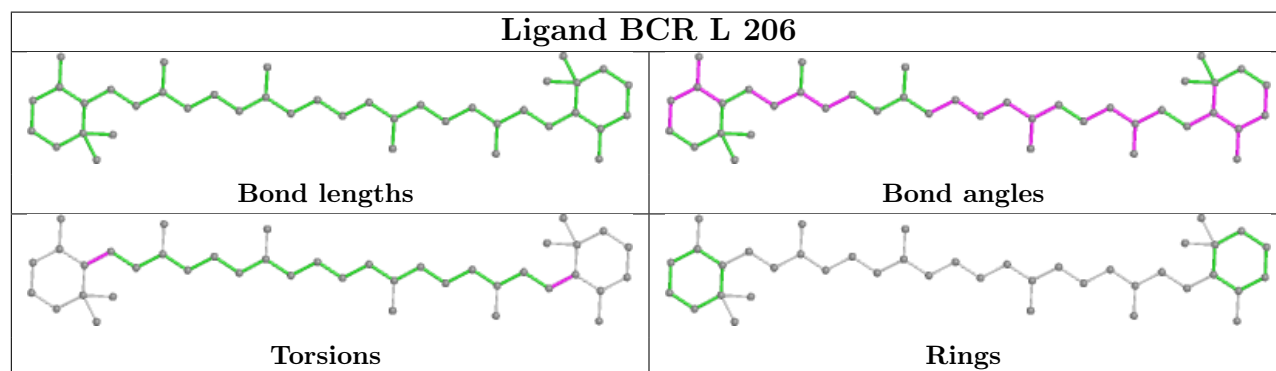
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	2	205	CLA	1	0
24	2	209	CLA	4	0
25	B	842	BCR	2	0
24	A	818	CLA	3	0
24	k	301	CLA	4	0
24	6	611	CLA	1	0
24	5	605	CLA	2	0
24	9	310	CLA	2	0
24	B	808	CLA	2	0
24	k	304	CLA	2	0
24	R	103	CLA	1	0
27	A	851	LMT	1	0
24	B	831	CLA	3	0
24	t	308	CLA	1	0
24	k	308	CLA	2	0
27	A	854	LMT	3	0
24	6	607	CLA	2	0
25	A	845	BCR	1	0
25	A	844	BCR	3	0
24	A	814	CLA	1	0
24	7	602	CLA	9	0
28	A	842	LHG	2	0
26	9	315	DD6	3	0
28	1	318	LHG	2	0
25	9	316	BCR	9	0
26	4	614	DD6	1	0
24	4	605	CLA	1	0
31	A	839	PQN	1	0
24	A	835	CLA	1	0
24	4	612	CLA	2	0
26	1	312	DD6	1	0
28	8	213	LHG	1	0
24	1	306	CLA	1	0
24	B	822	CLA	1	0
24	8	206	CLA	2	0
24	B	807	CLA	1	0
26	8	211	DD6	1	0
24	A	834	CLA	1	0
26	8	212	DD6	1	0
24	7	601	CLA	1	0
24	8	201	CLA	2	0
24	B	812	CLA	3	0

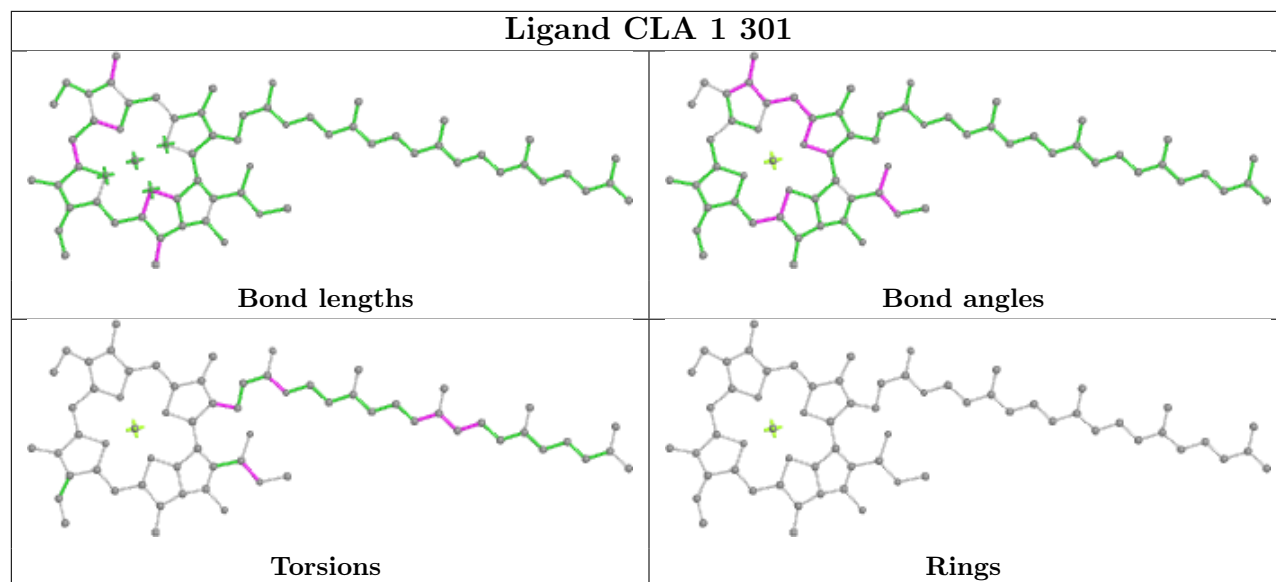
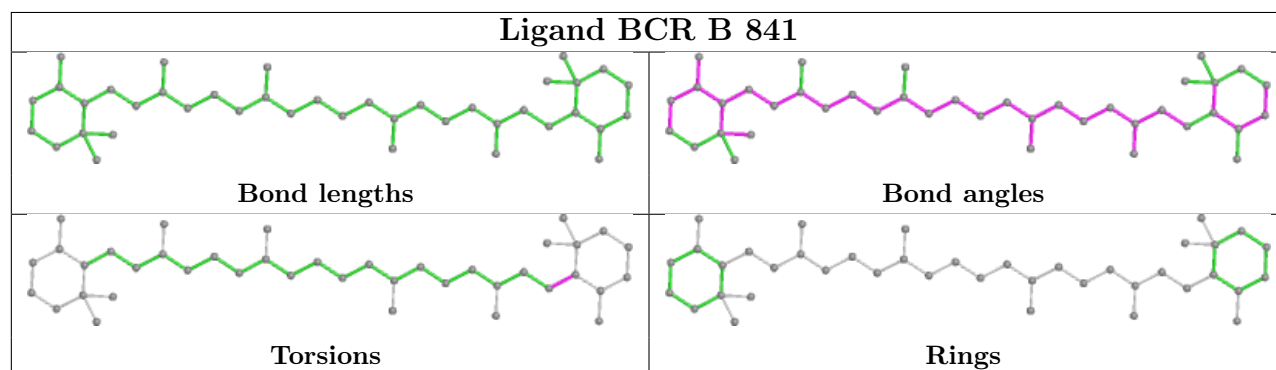
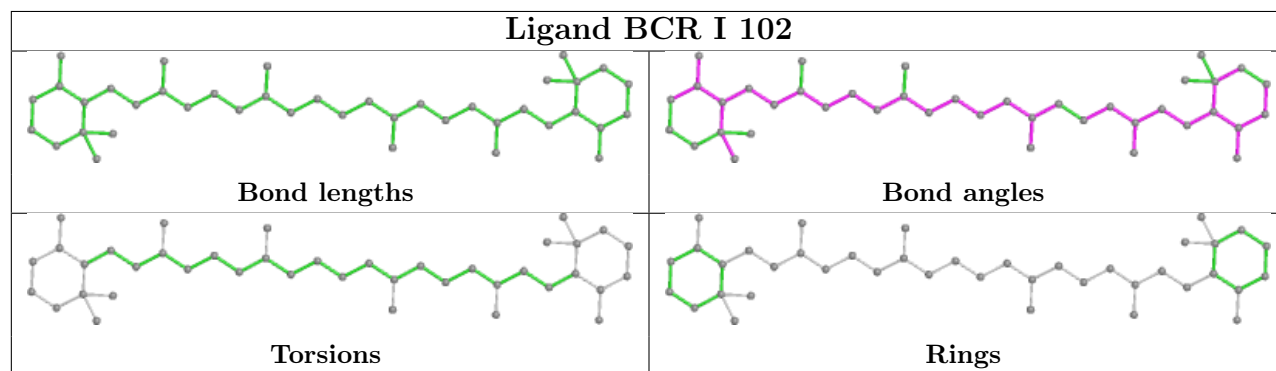
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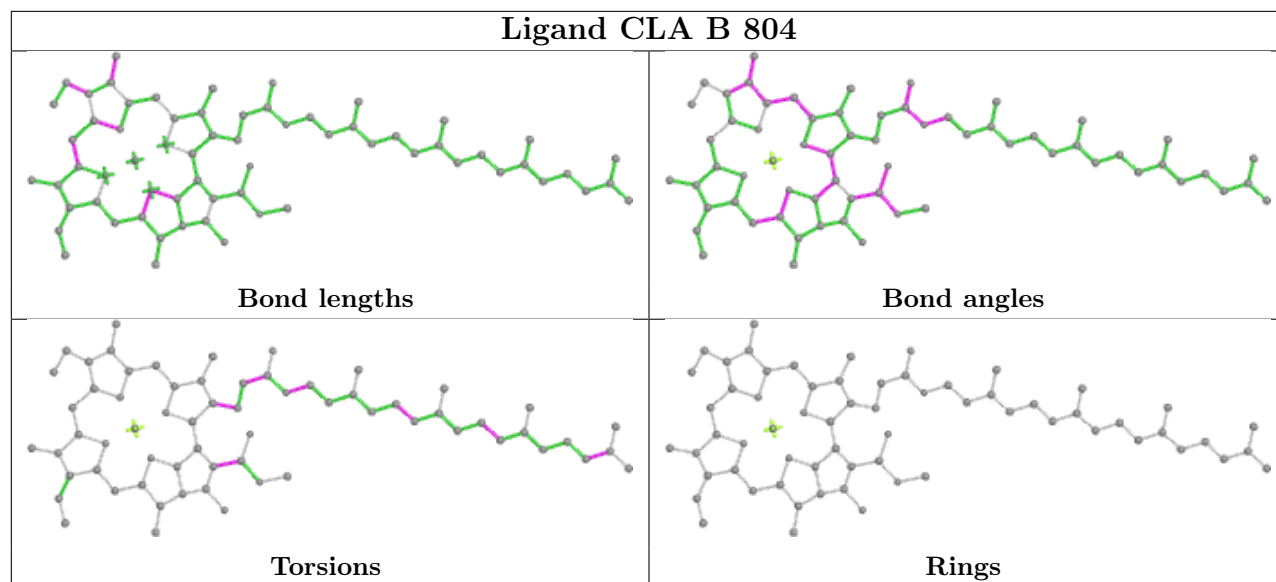
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	615	DD6	1	0
24	t	307	CLA	2	0
24	k	307	CLA	1	0
24	B	821	CLA	1	0
24	4	613	CLA	2	0
25	M	101	BCR	2	0
26	6	613	DD6	1	0
24	F	202	CLA	1	0
24	B	823	CLA	1	0
25	4	618	BCR	7	0
24	4	606	CLA	1	0
26	7	613	DD6	1	0

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

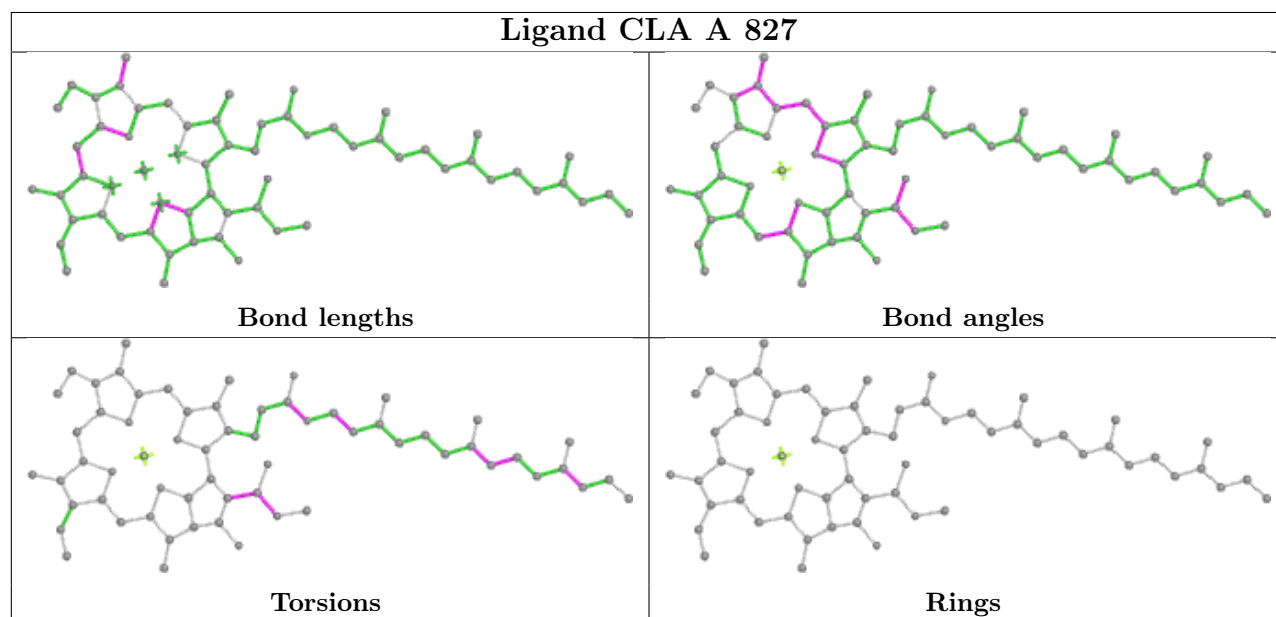


Ligand CLA 1 301**Ligand BCR B 841****Ligand BCR I 102**

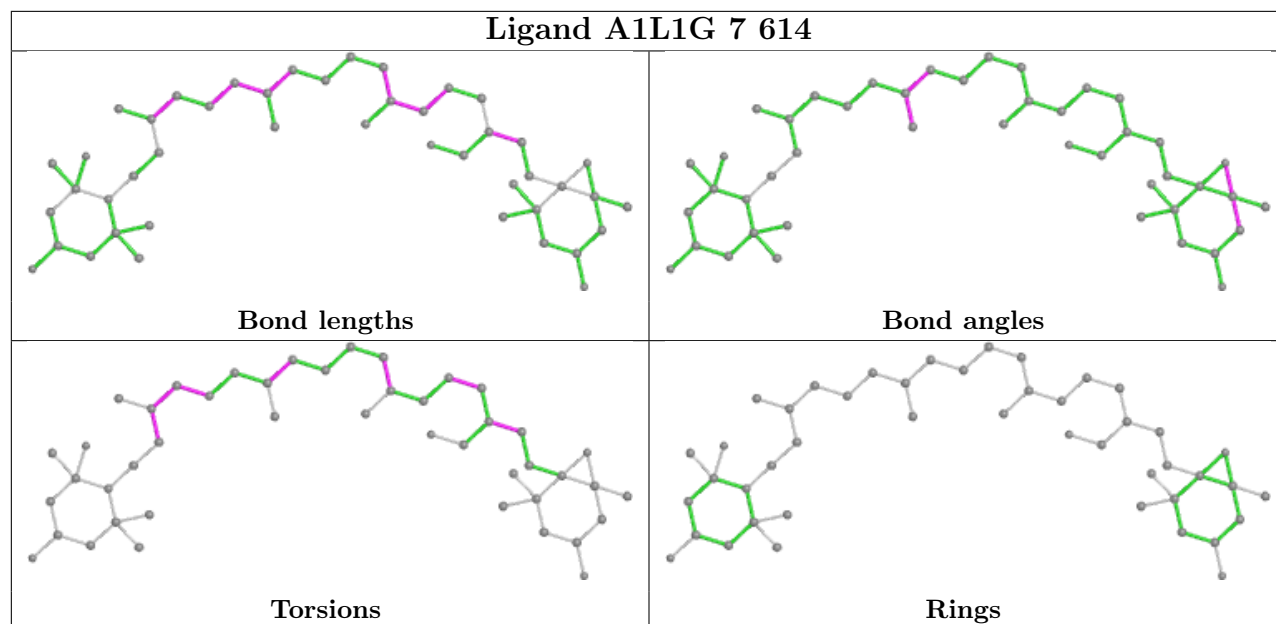
Ligand CLA B 804



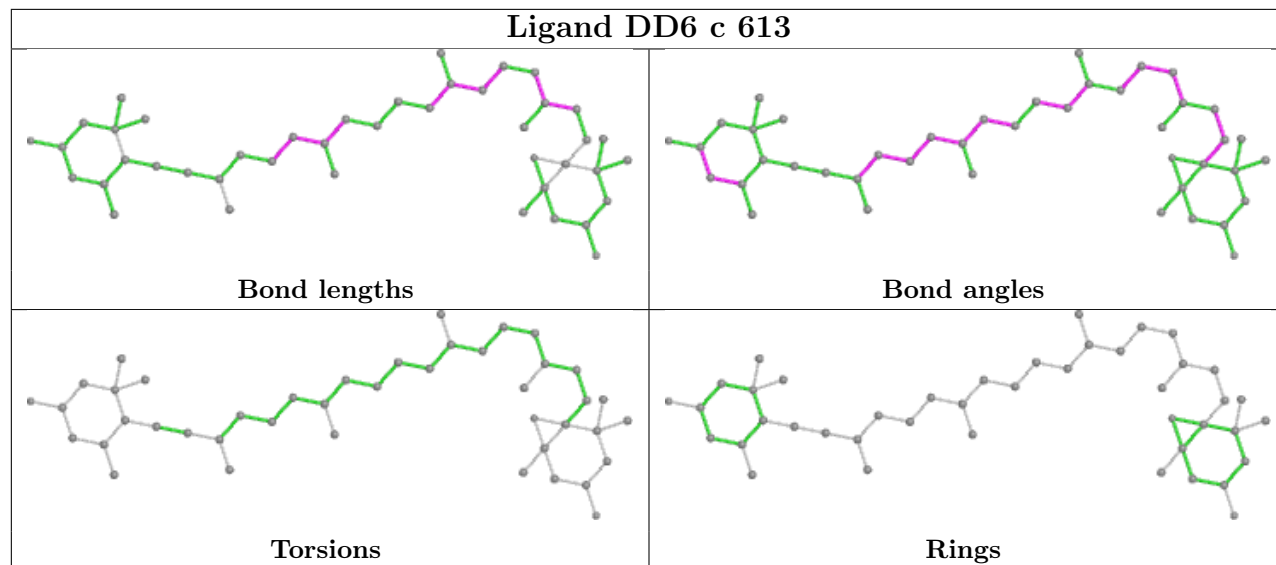
Ligand CLA A 827



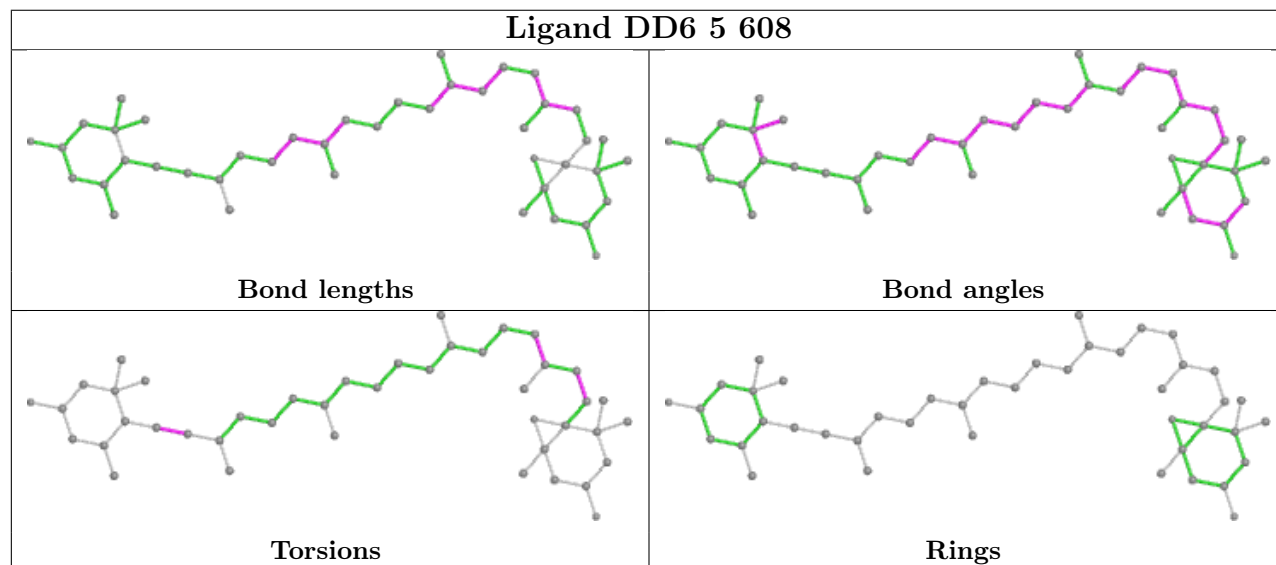
Ligand A1L1G 7 614



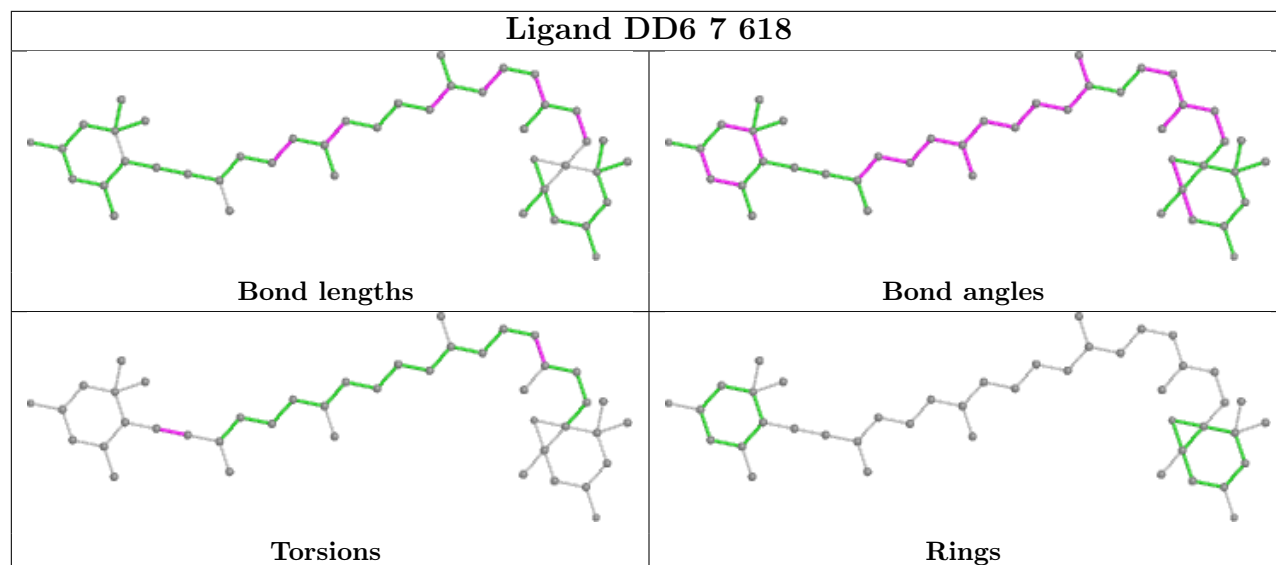
Ligand DD6 c 613



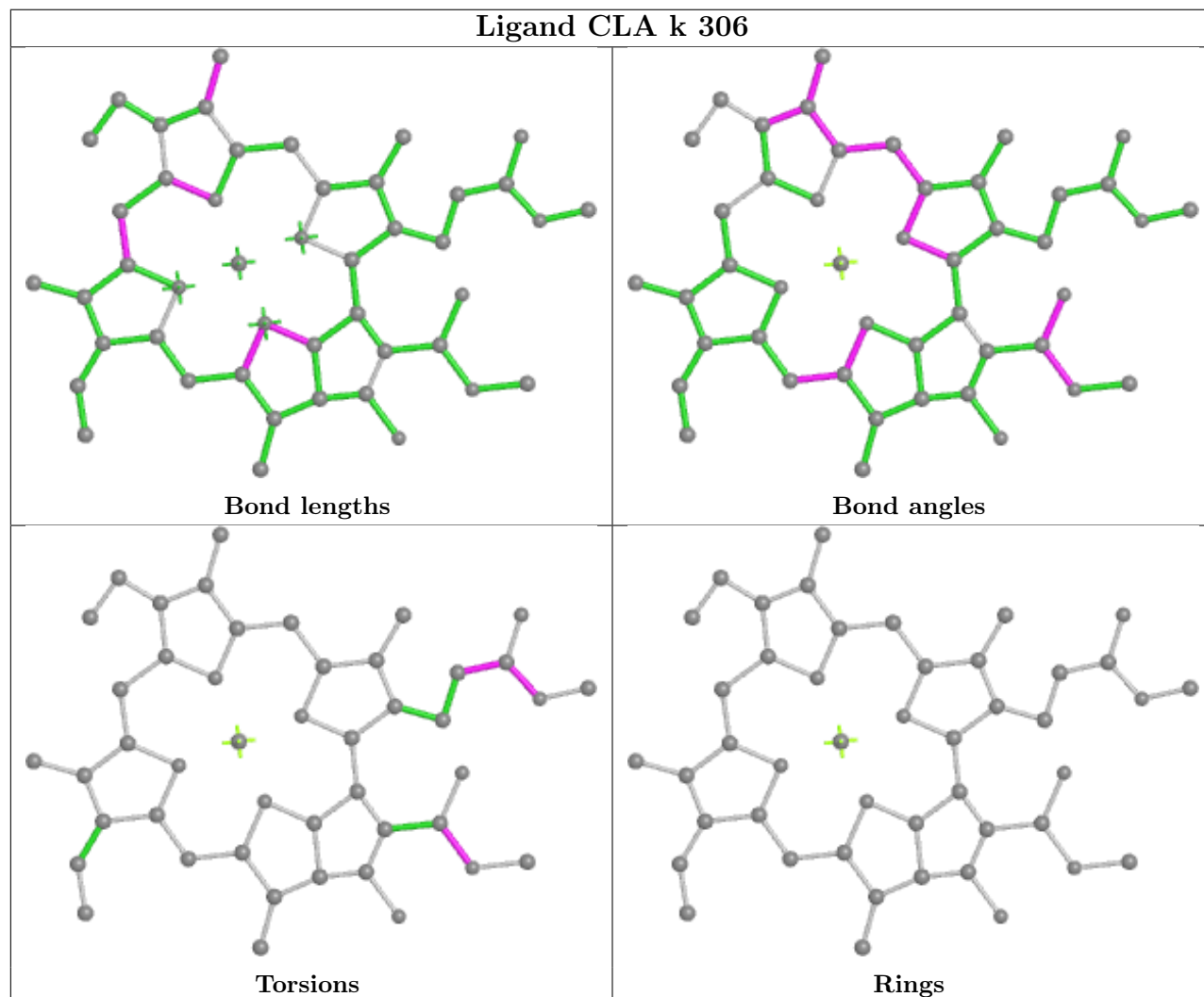
Ligand DD6 5 608



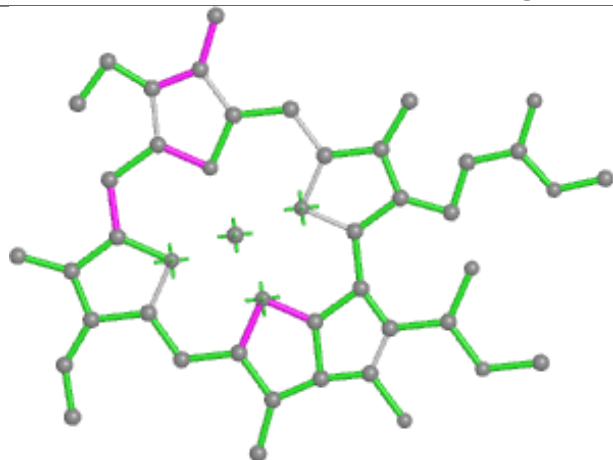
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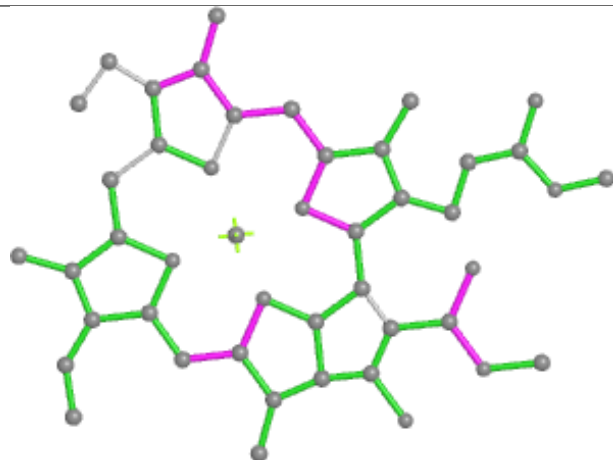
Ligand CLA k 306



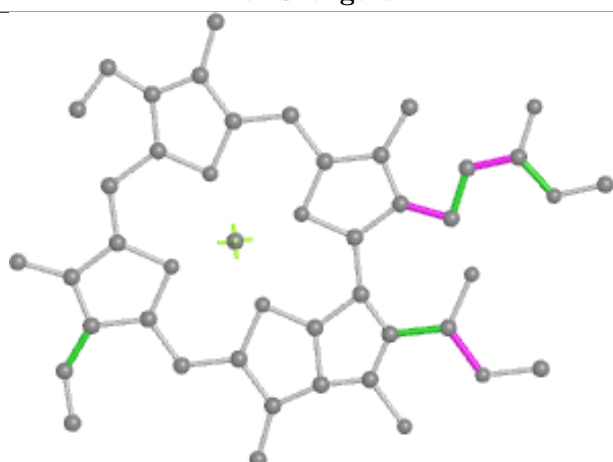
Ligand CLA 1 308



Bond lengths



Bond angles

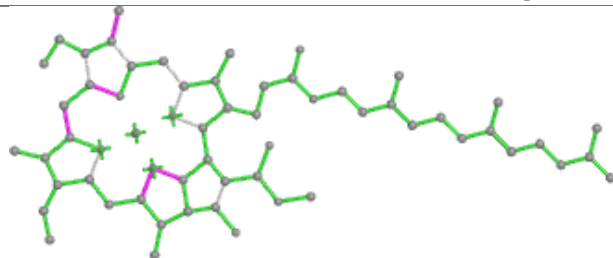


Torsions

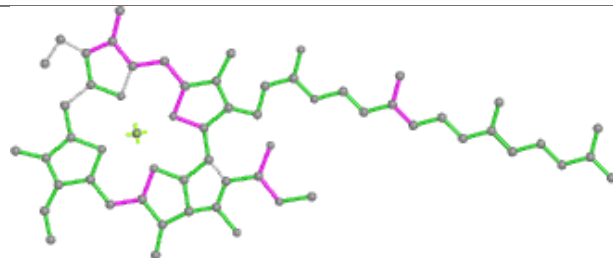


Rings

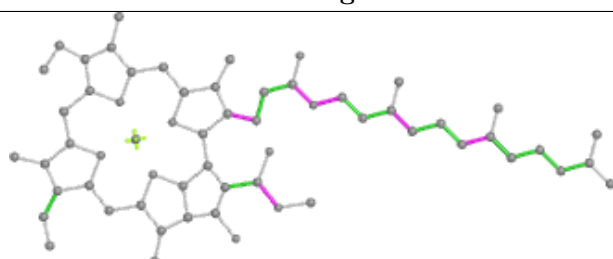
Ligand CLA 4 602



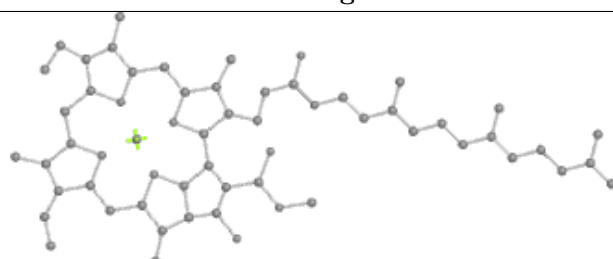
Bond lengths



Bond angles

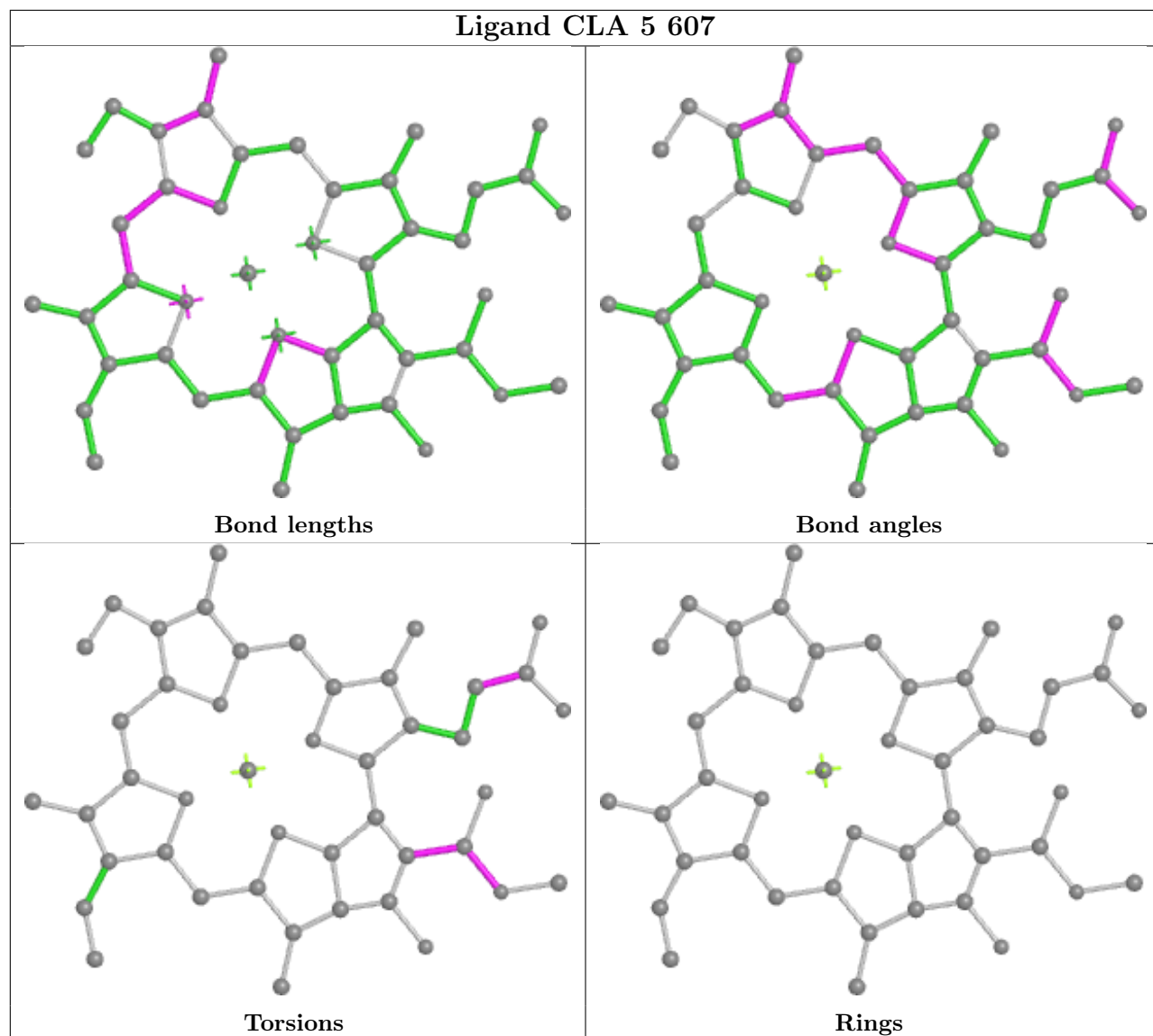


Torsions

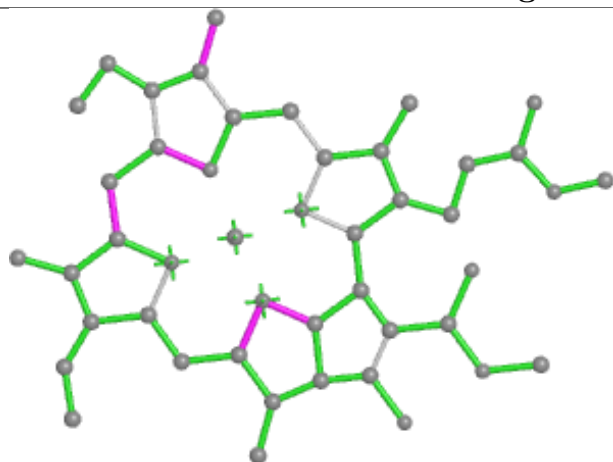


Rings

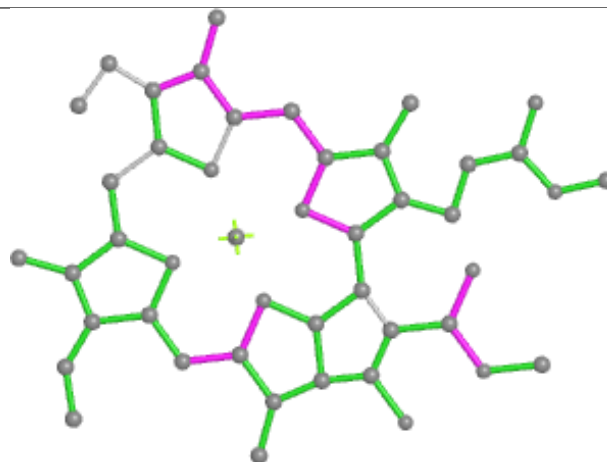
Ligand CLA 5 607



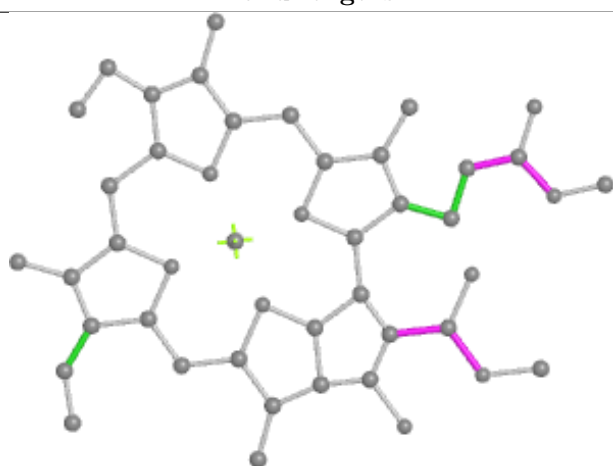
Ligand CLA 4 607



Bond lengths



Bond angles

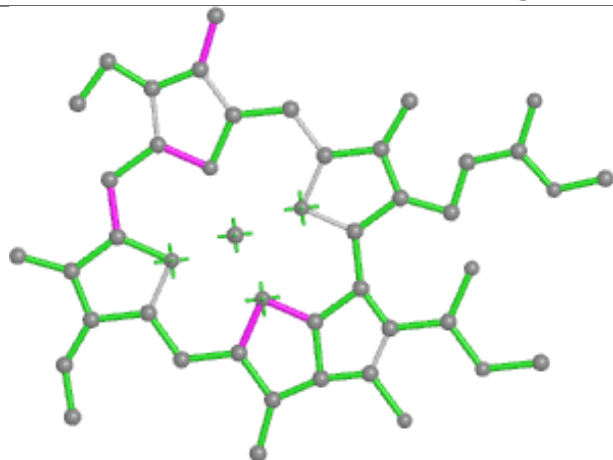


Torsions

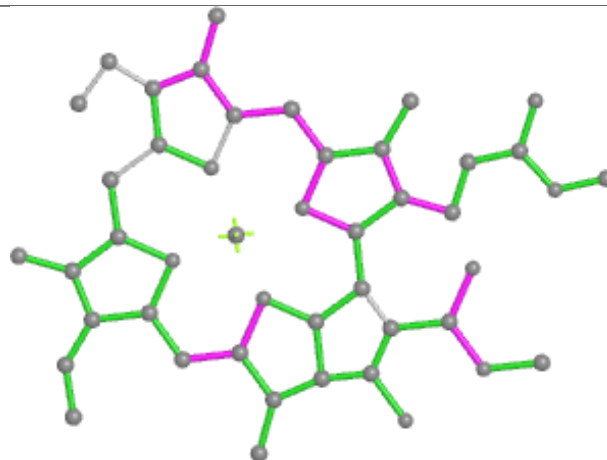


Rings

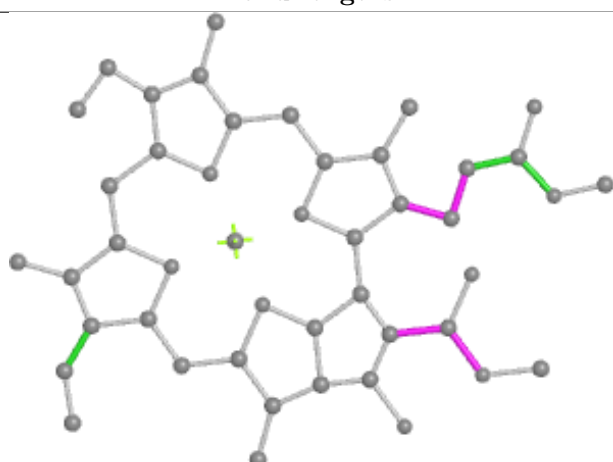
Ligand CLA B 813



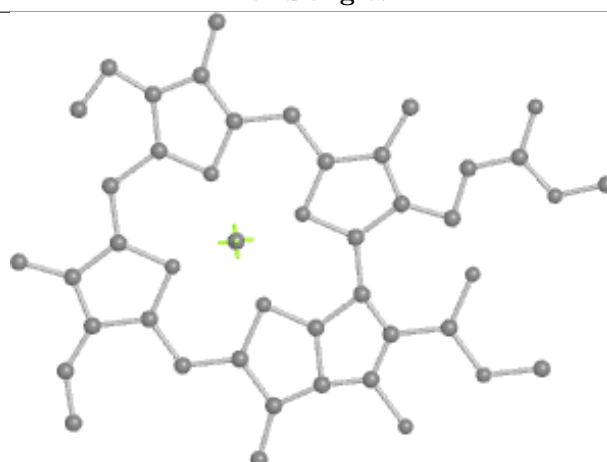
Bond lengths



Bond angles

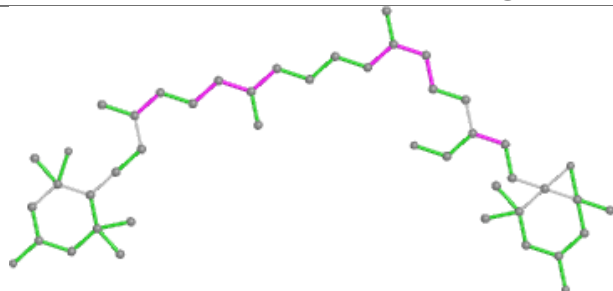


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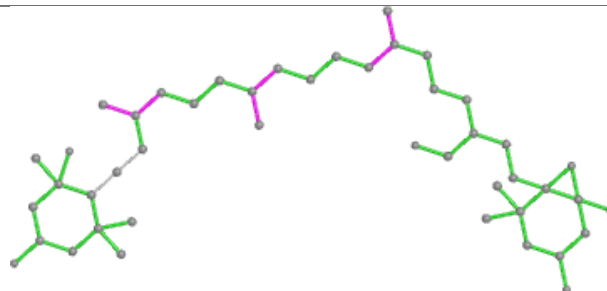


Rings

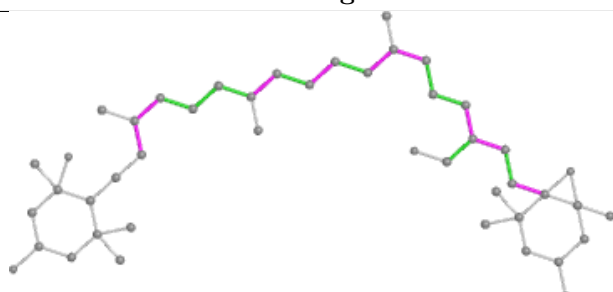
Ligand A1L1G 3 310



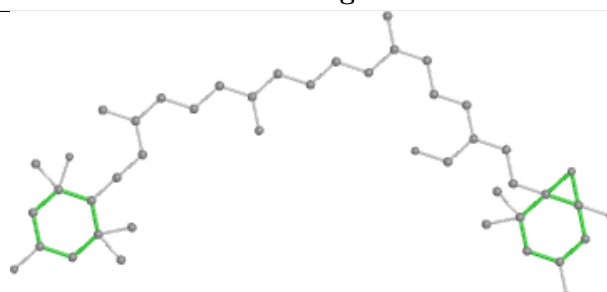
Bond lengths



Bond angles

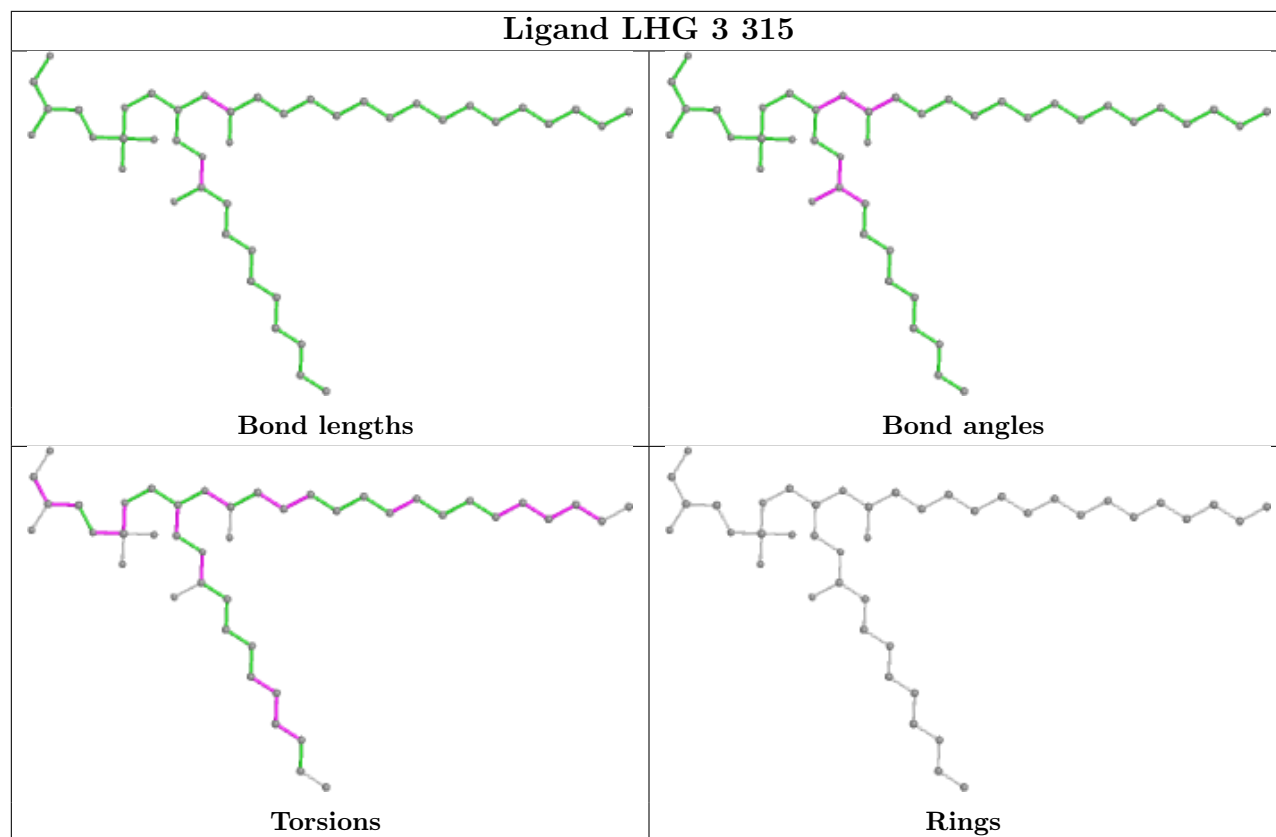


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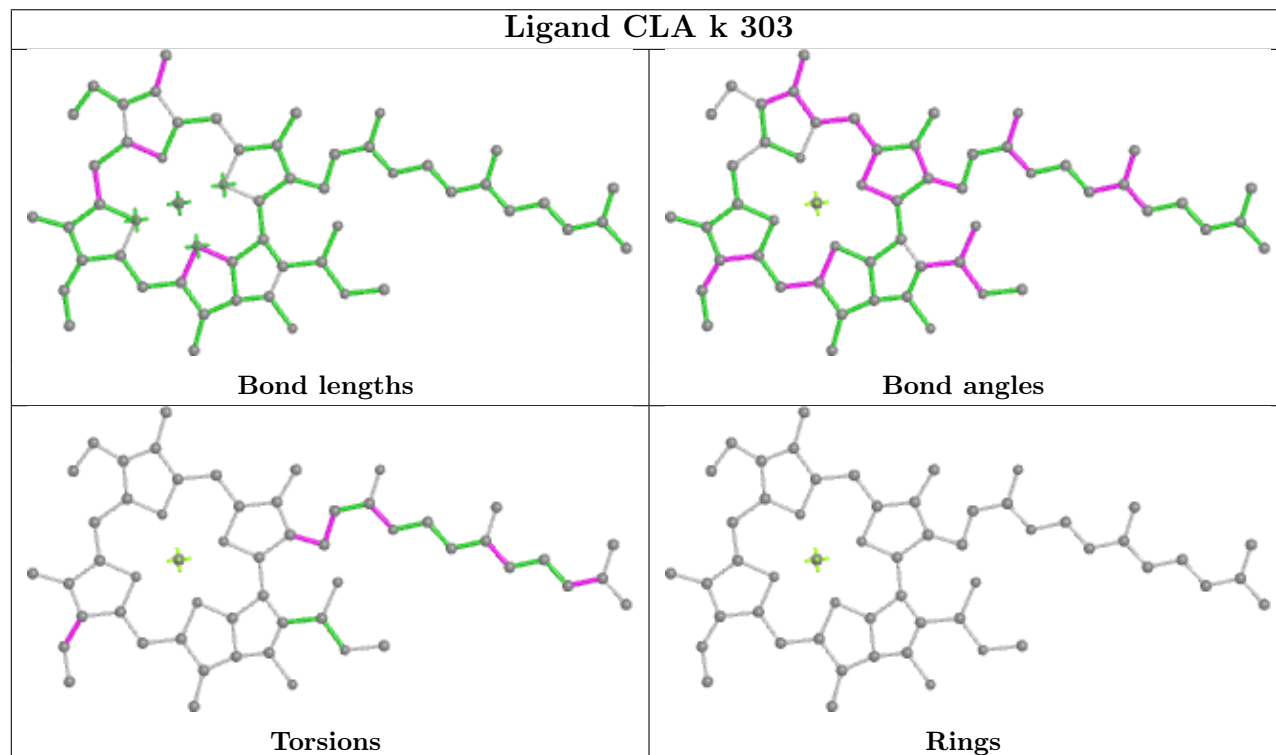


Rings

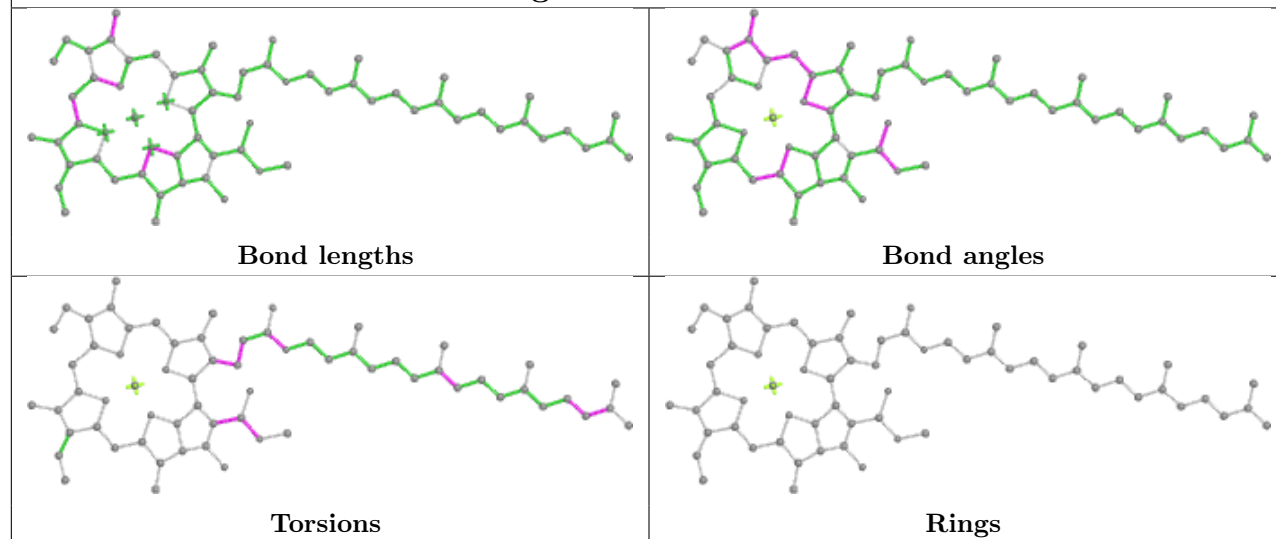
Ligand LHG 3 315



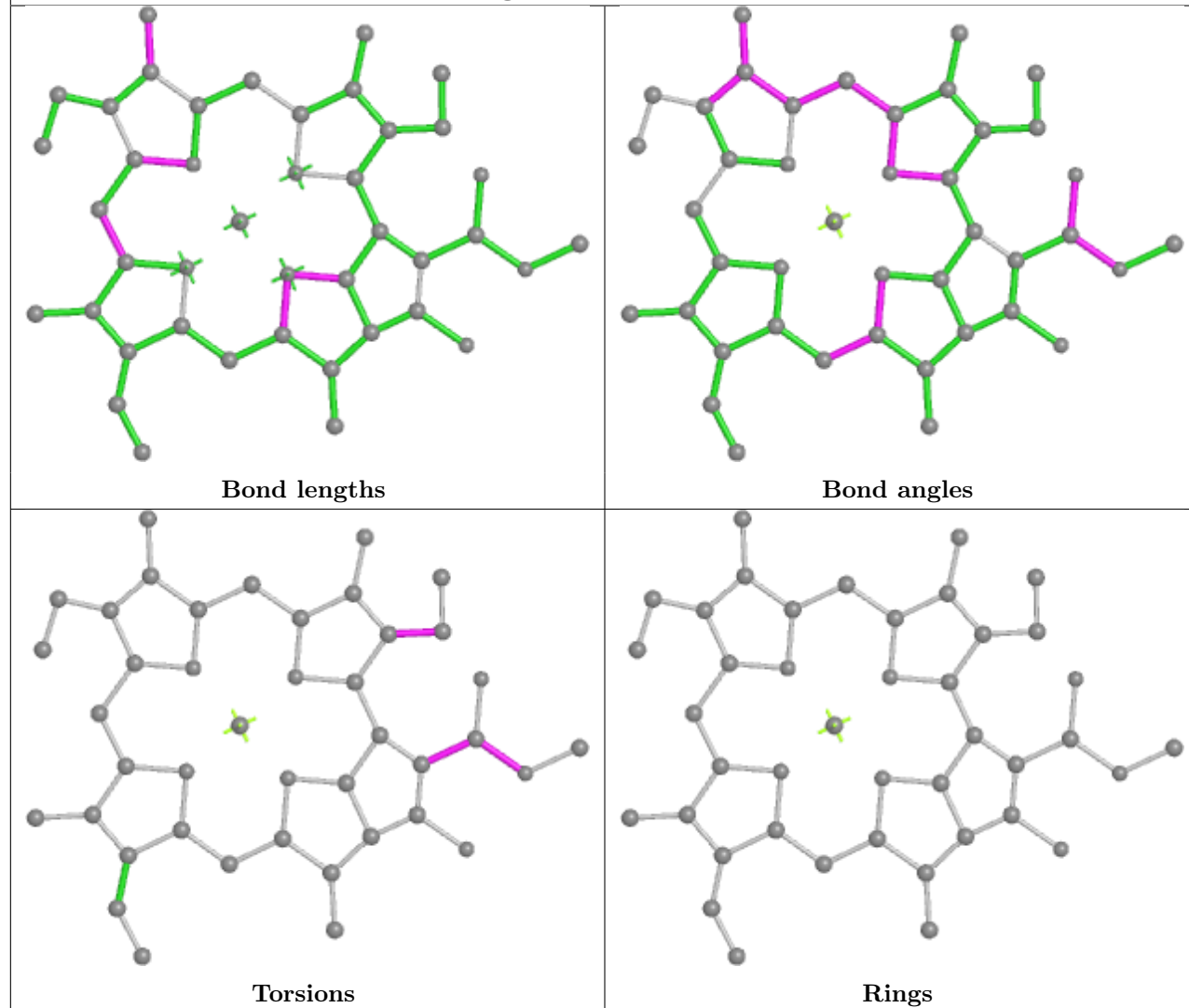
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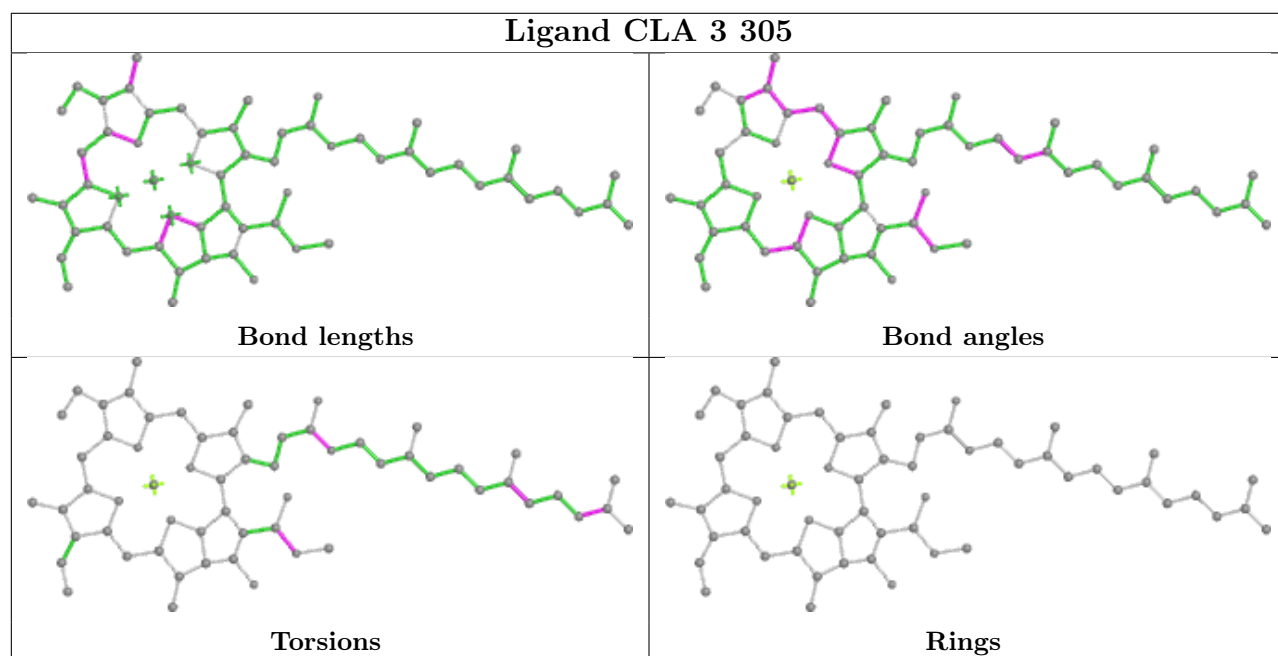
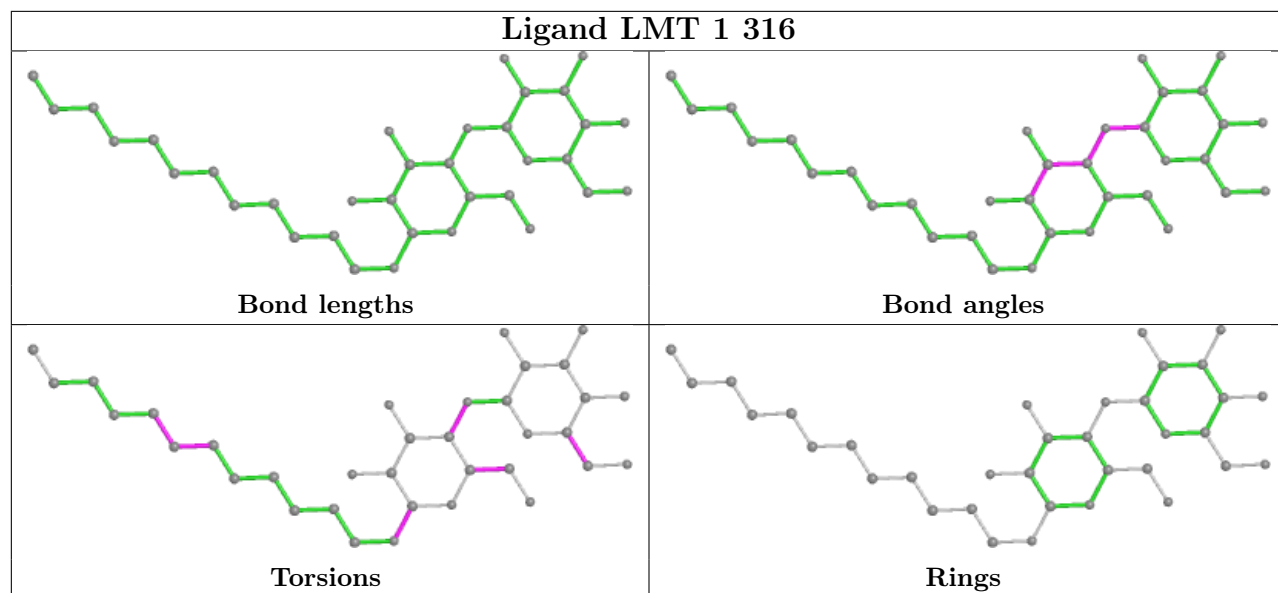


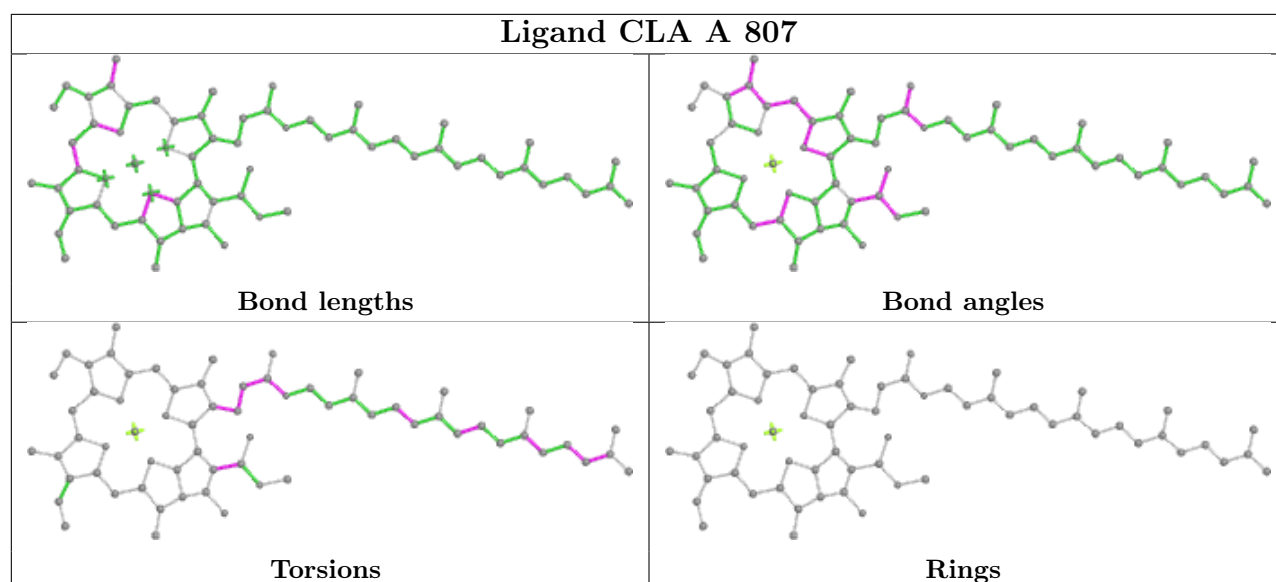
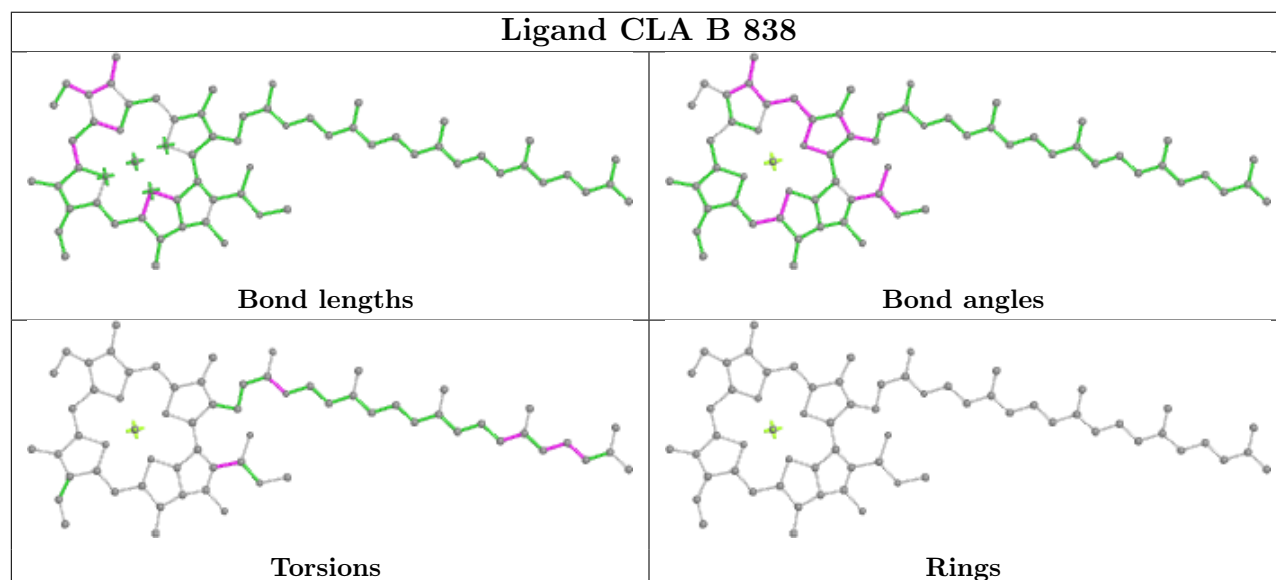
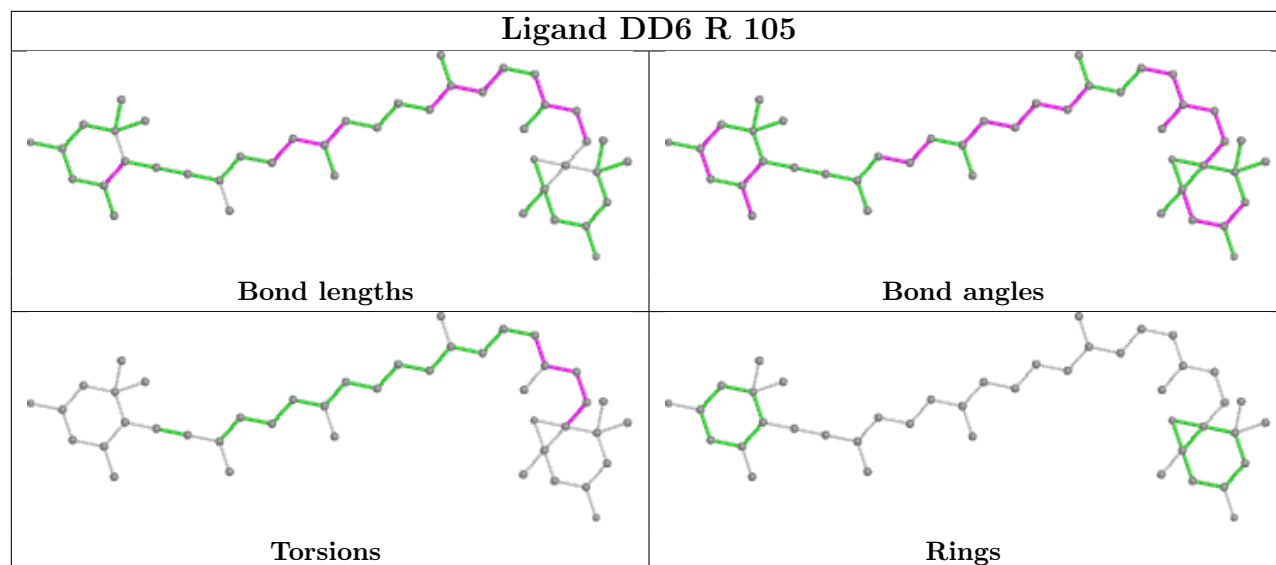
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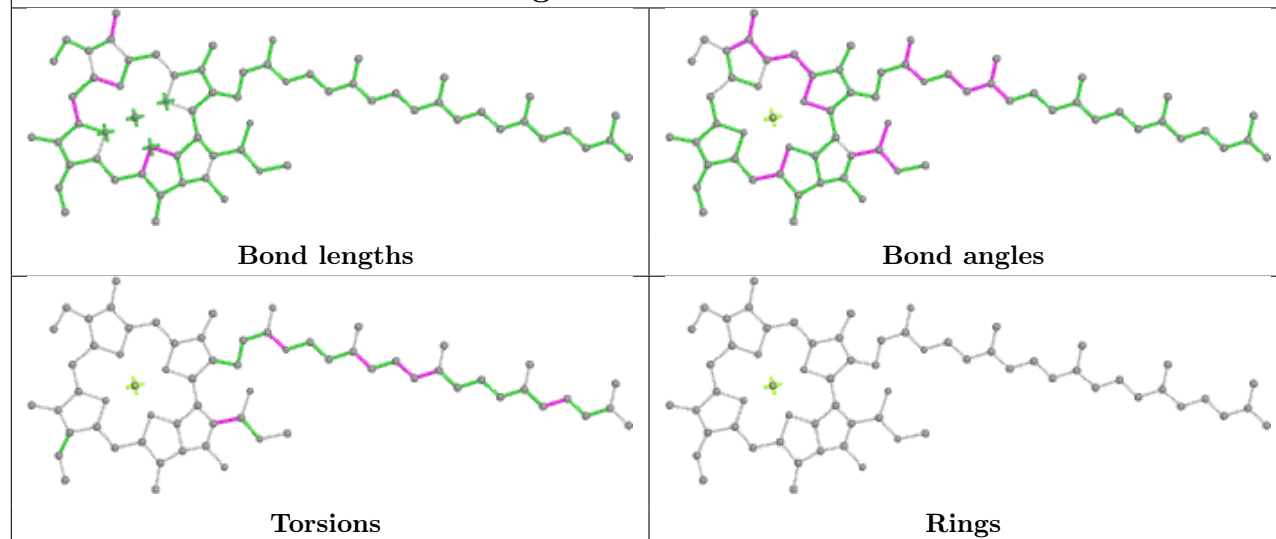
Ligand CLA J 103



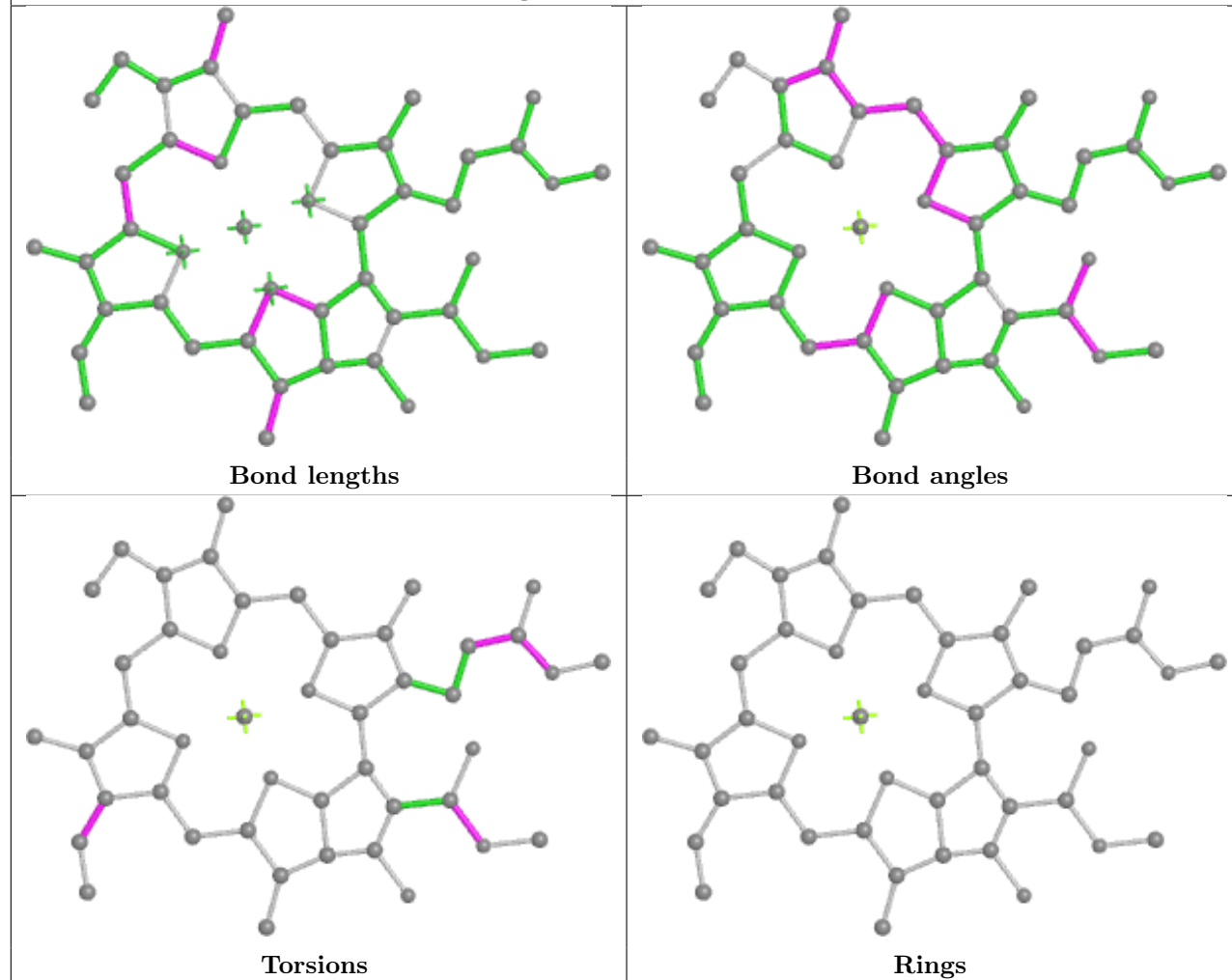


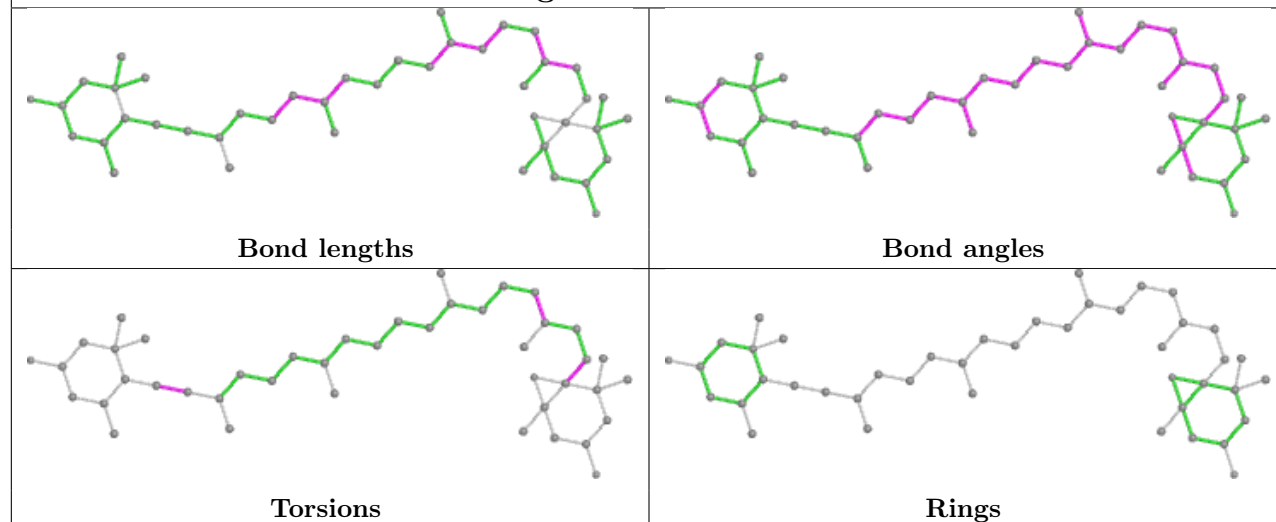
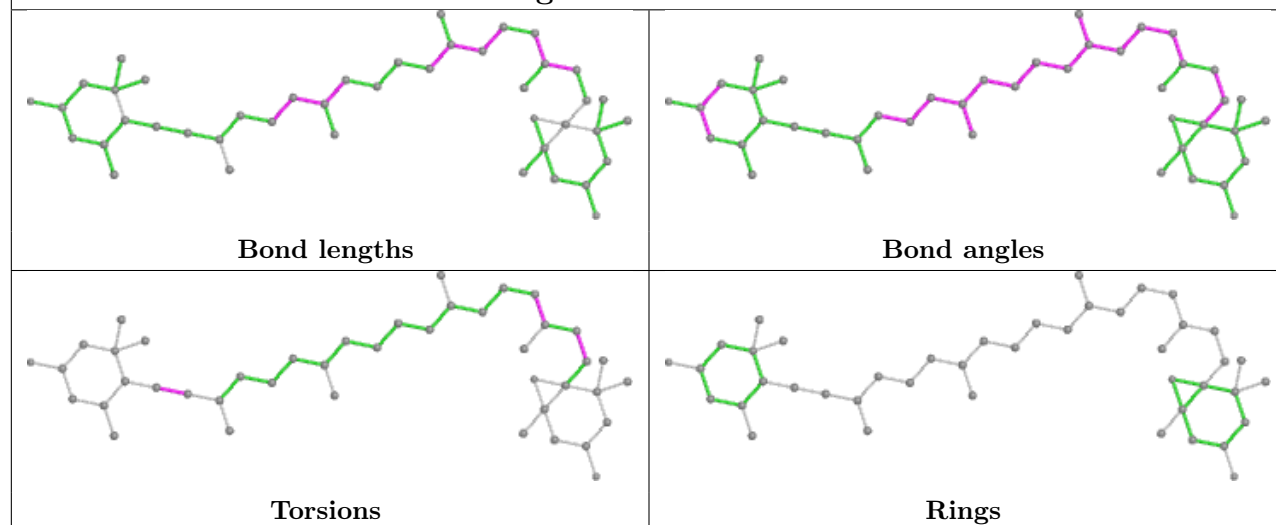


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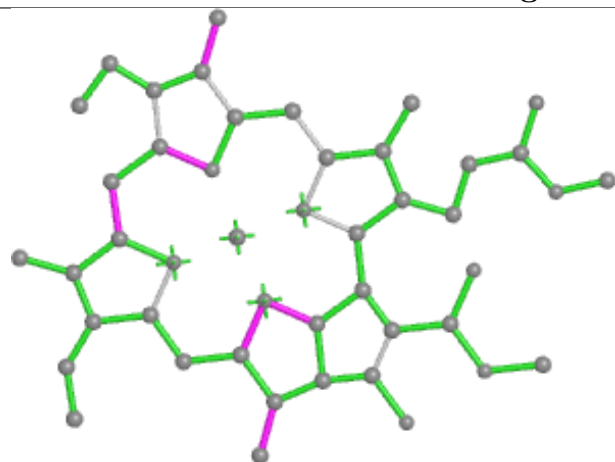


Ligand CLA L 205

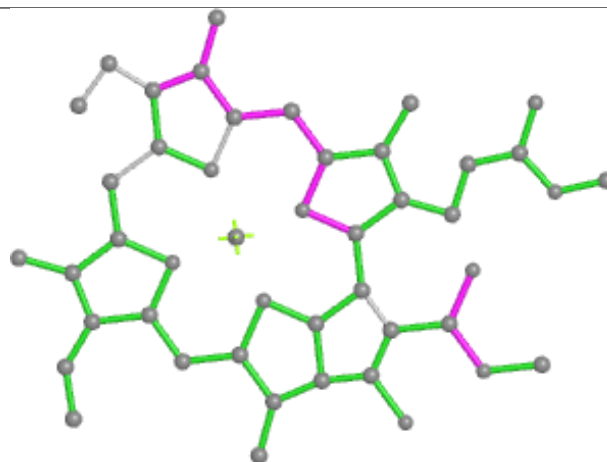


Ligand DD6 4 616**Ligand DD6 h 614**

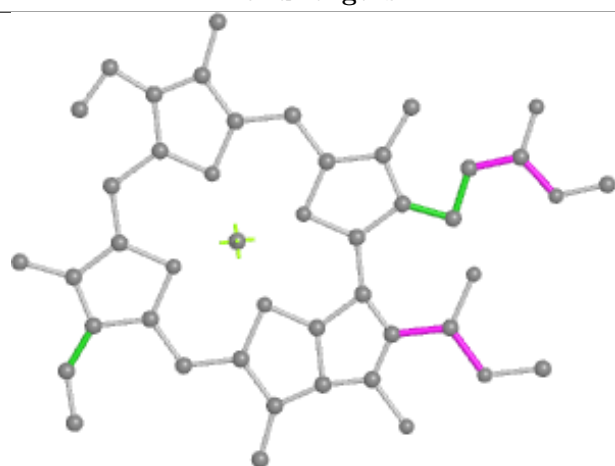
Ligand CLA 9 302



Bond lengths



Bond angles

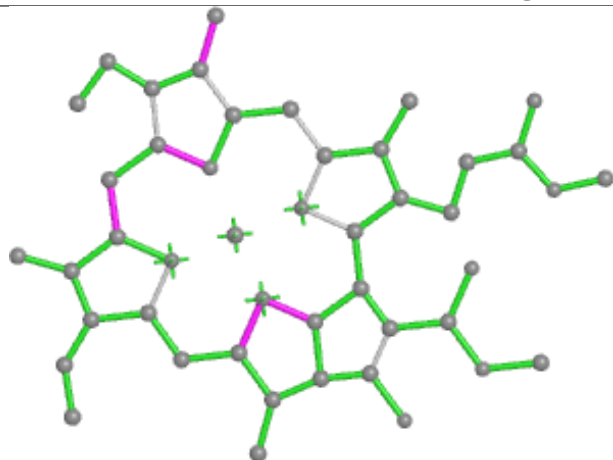


Torsions

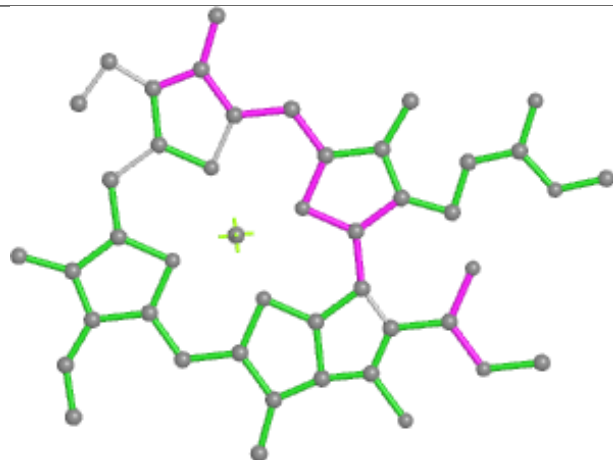


Rings

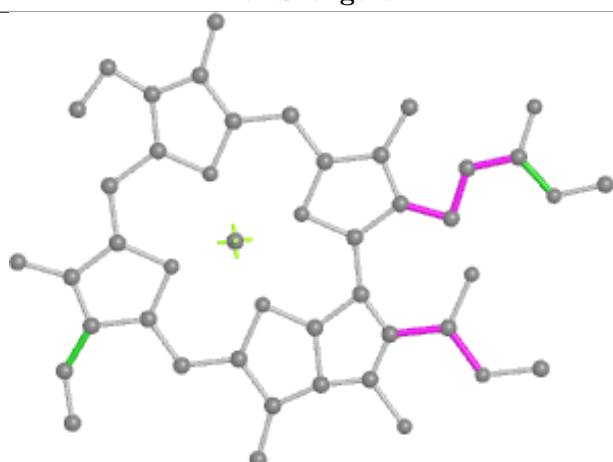
Ligand CLA 8 202



Bond lengths



Bond angles

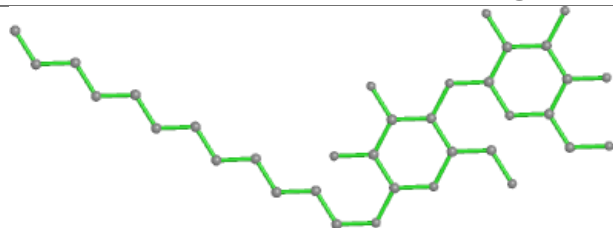


Torsions

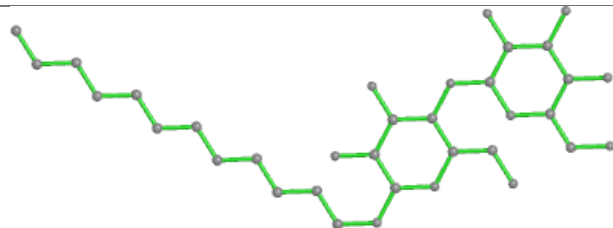


Rings

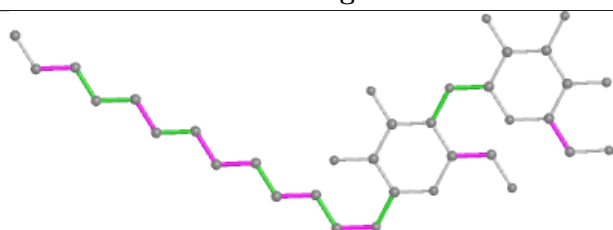
Ligand LMT A 850



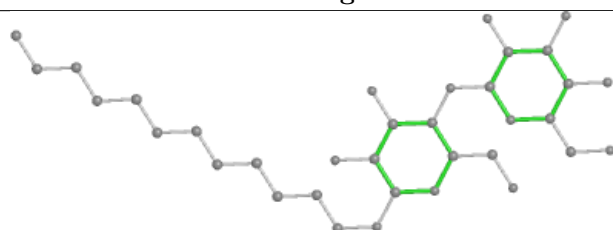
Bond lengths



Bond angles

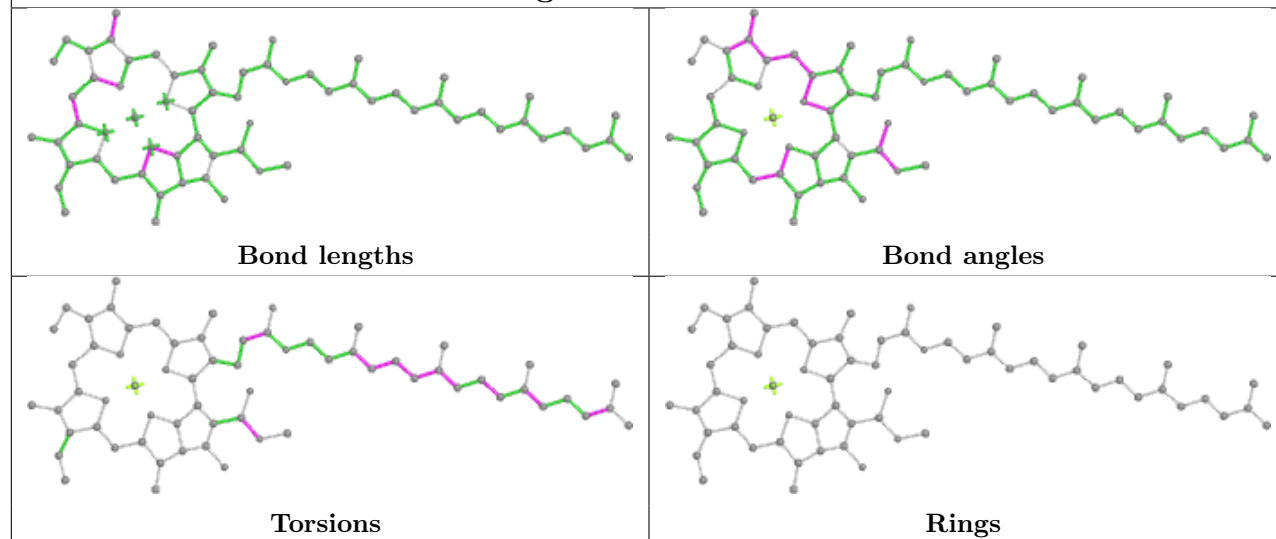


Torsions

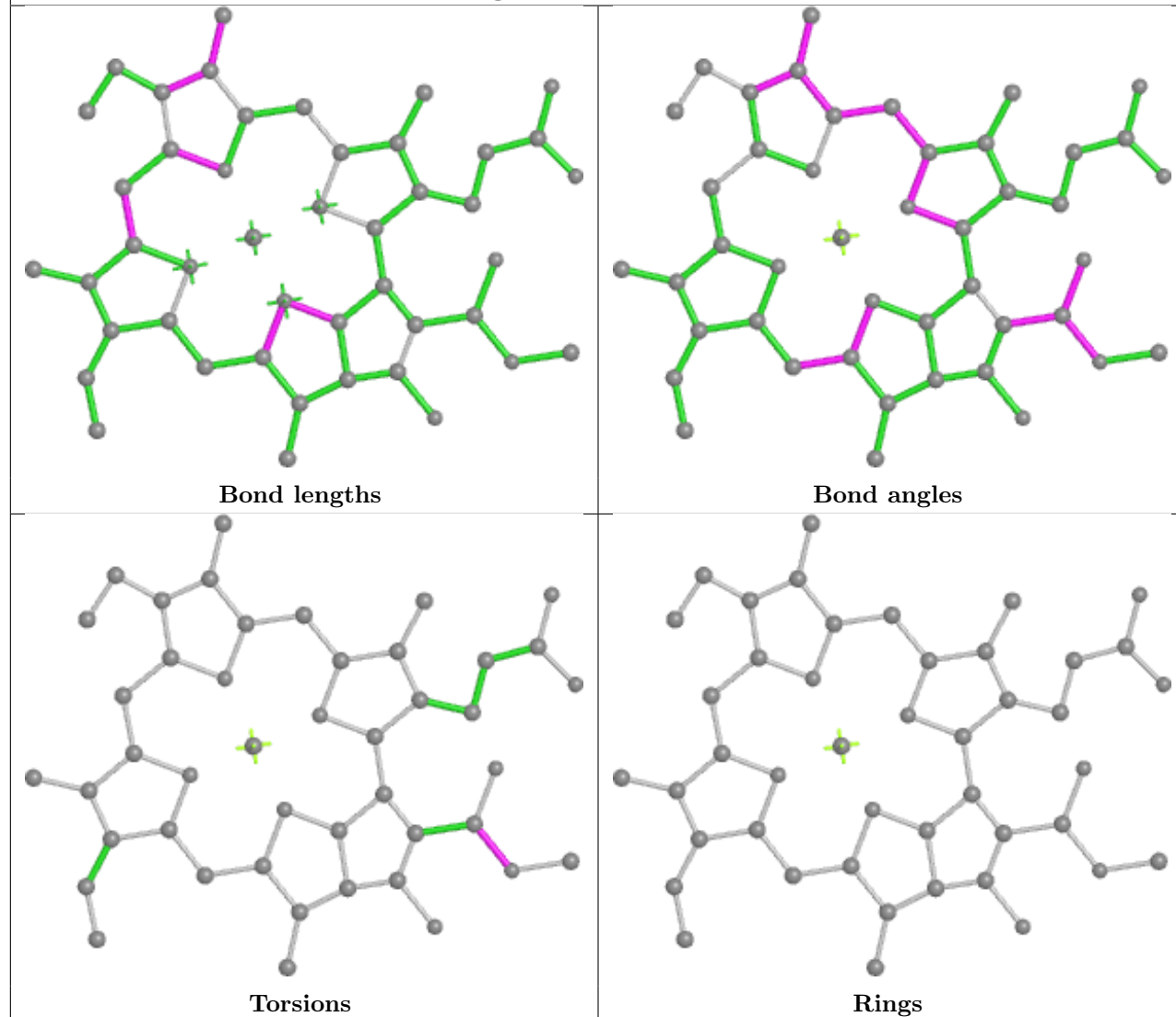


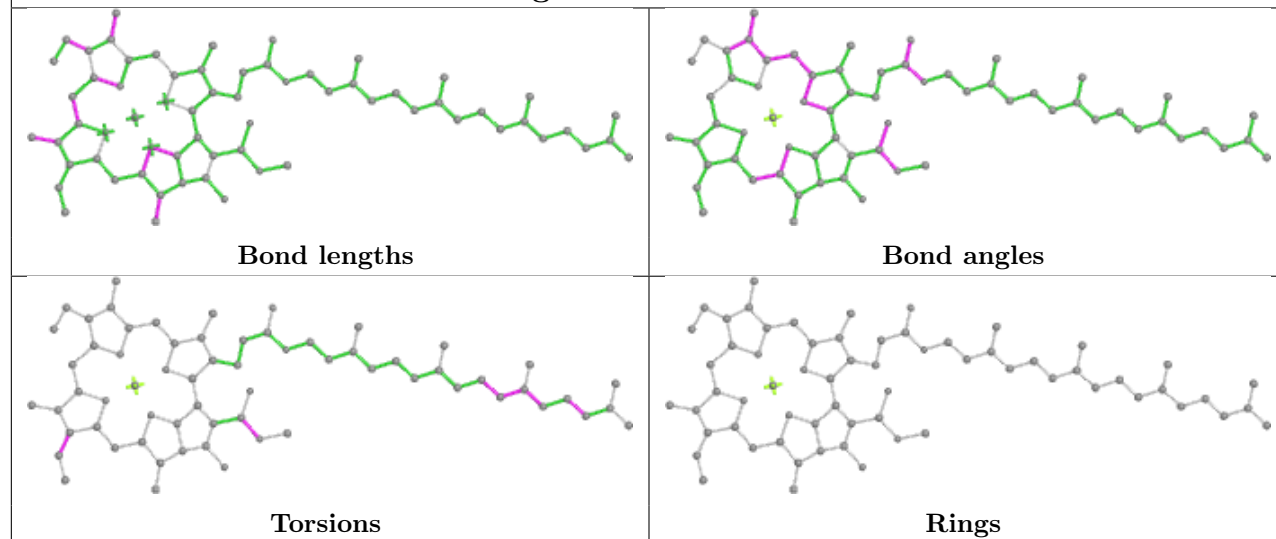
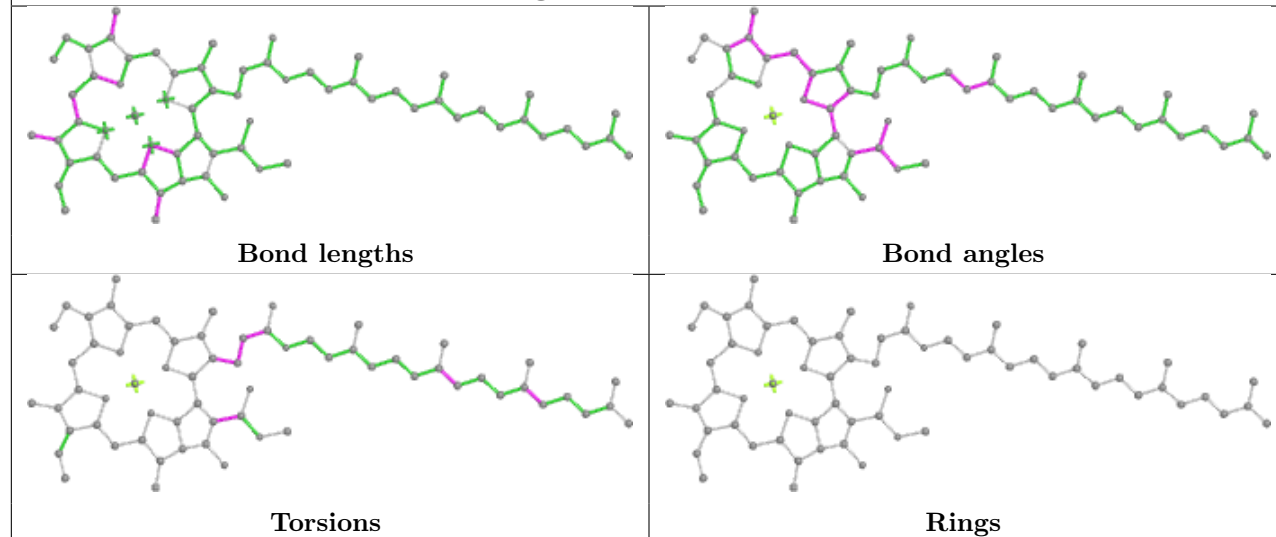
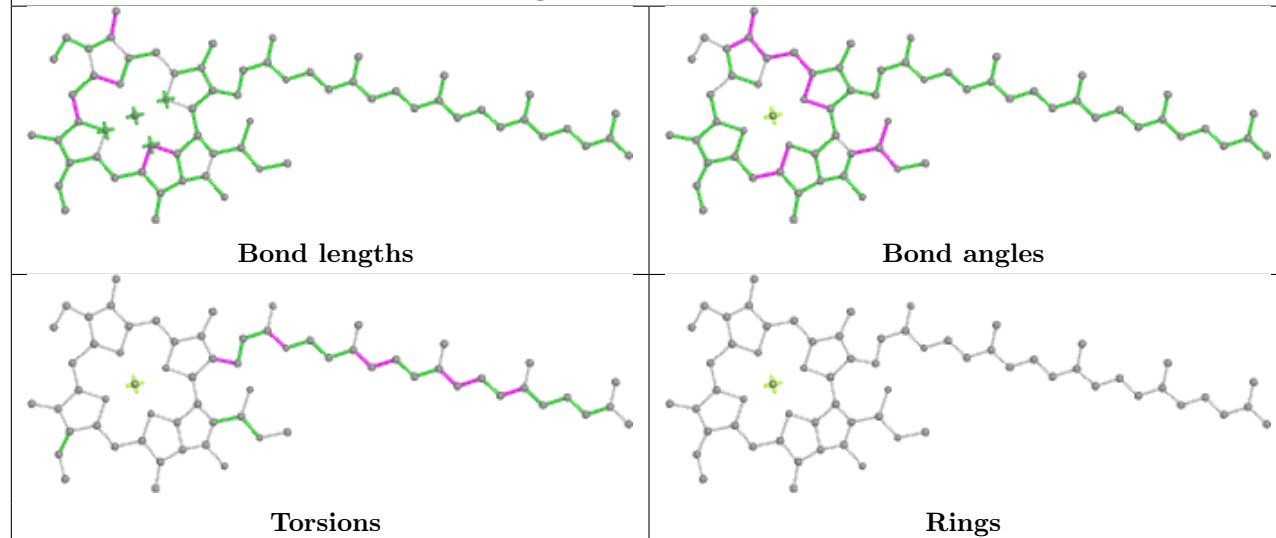
Rings

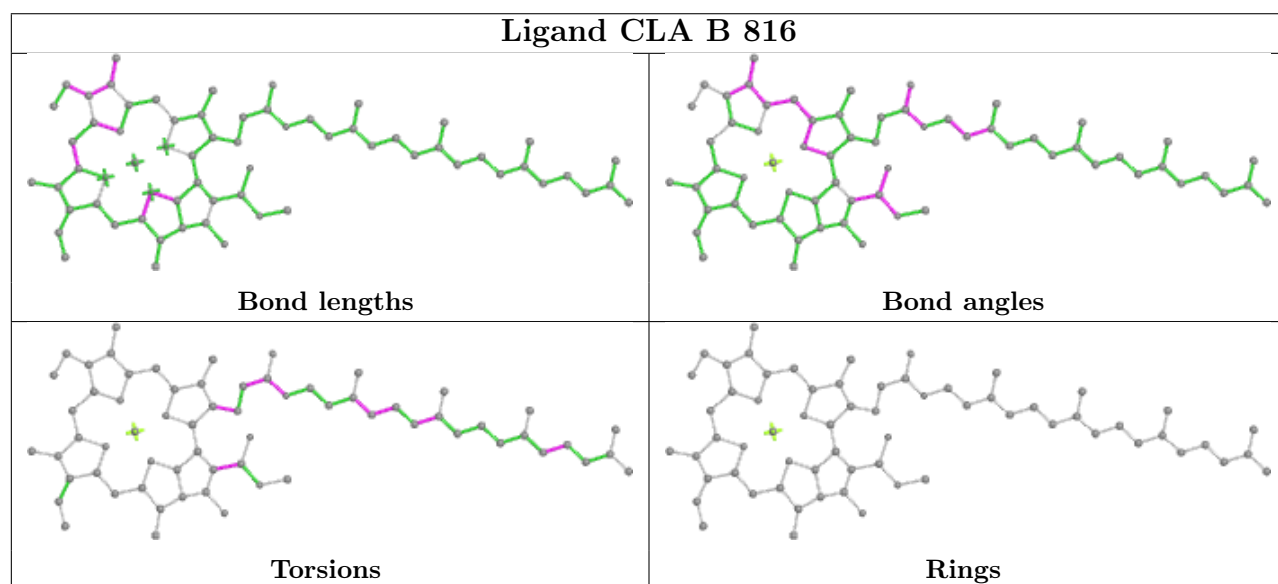
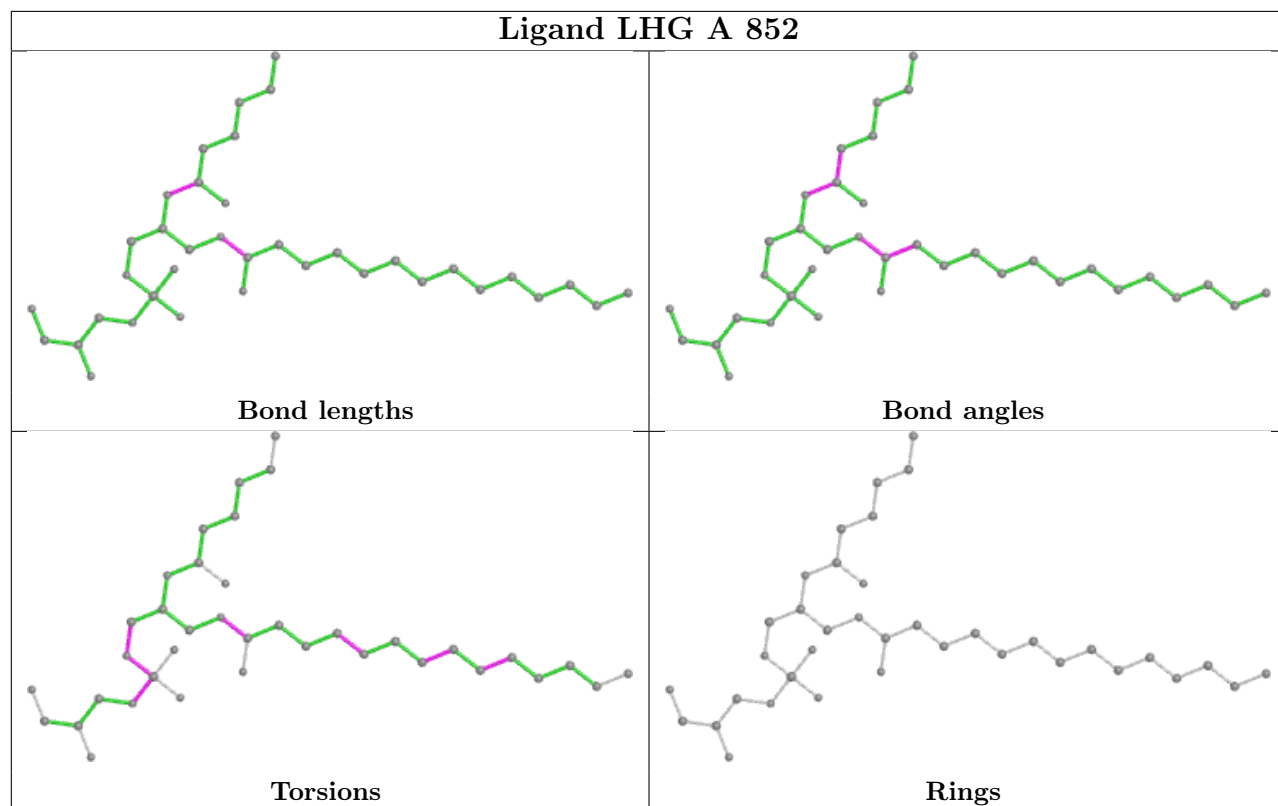
Ligand CLA 3 301



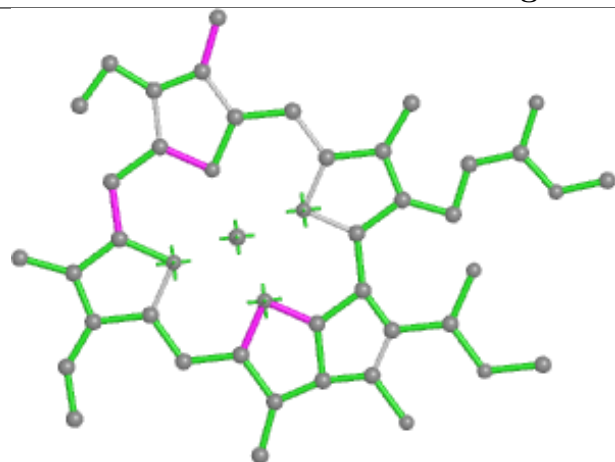
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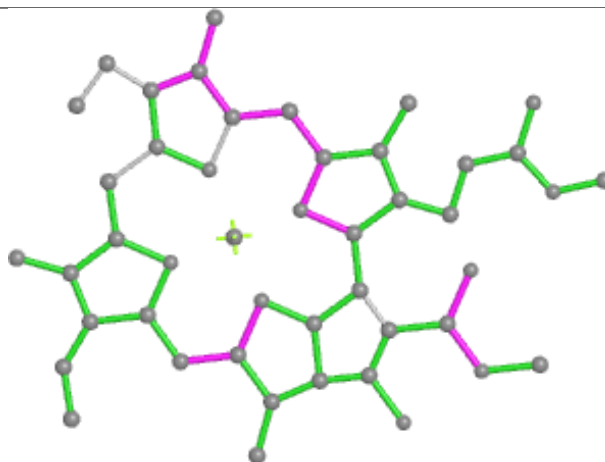
Ligand CLA B 803**Ligand CLA B 829****Ligand CLA A 805**



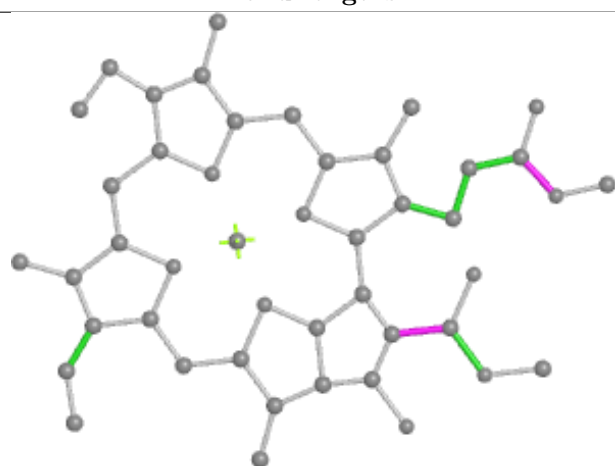
Ligand CLA 7 605



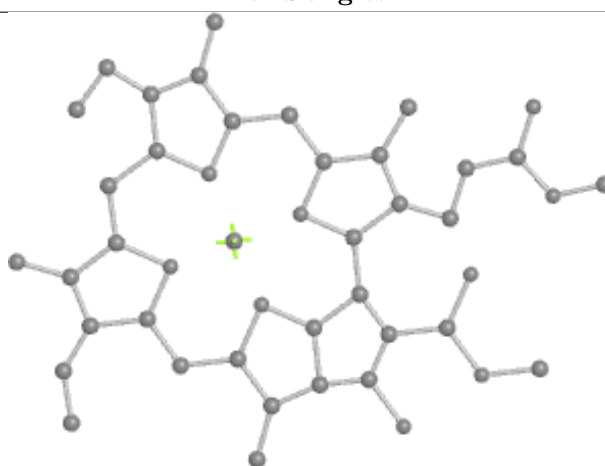
Bond lengths



Bond angles

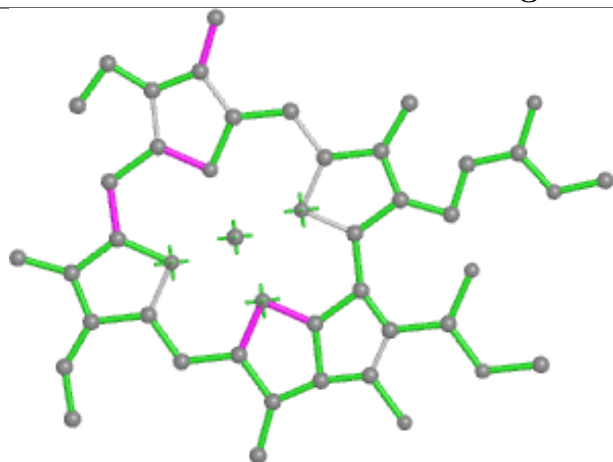


Torsions

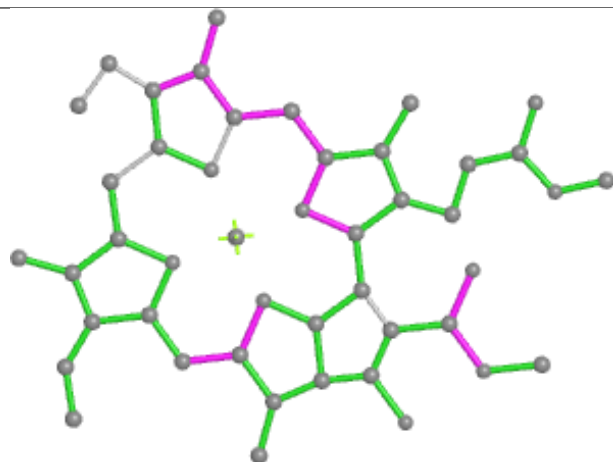


Rings

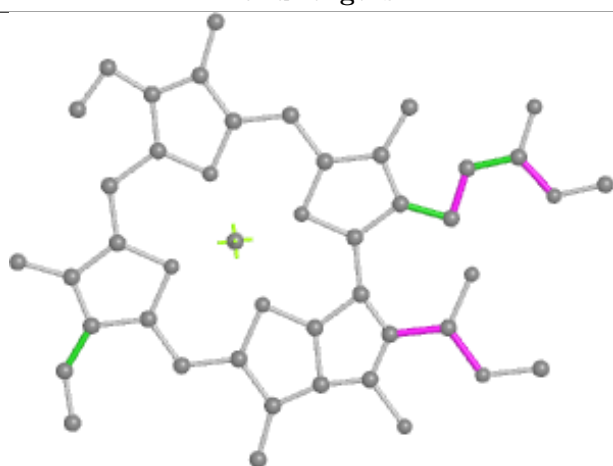
Ligand CLA t 310



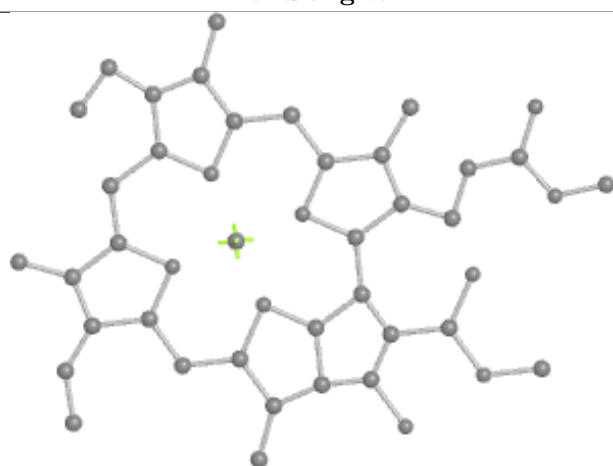
Bond lengths



Bond angles

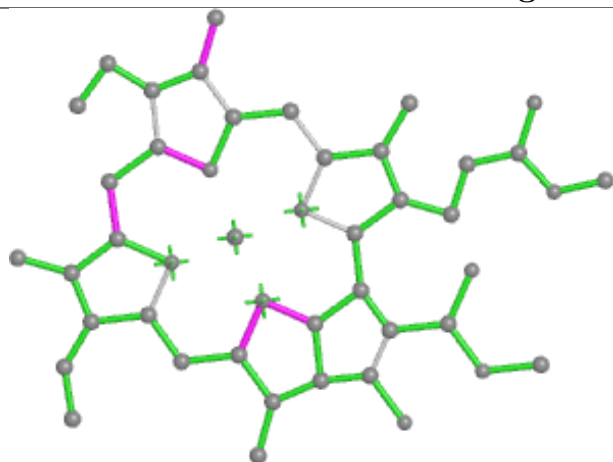


Torsions

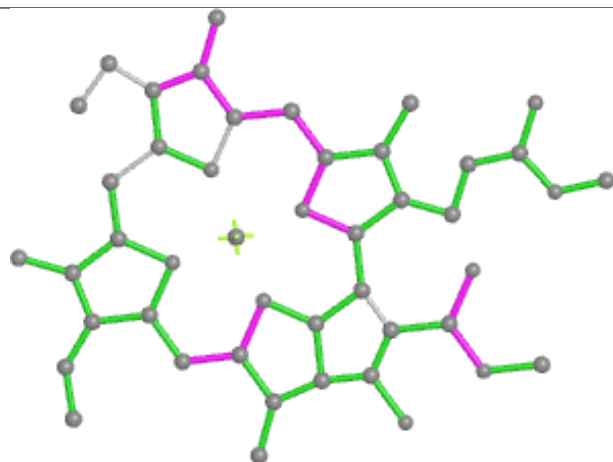


Rings

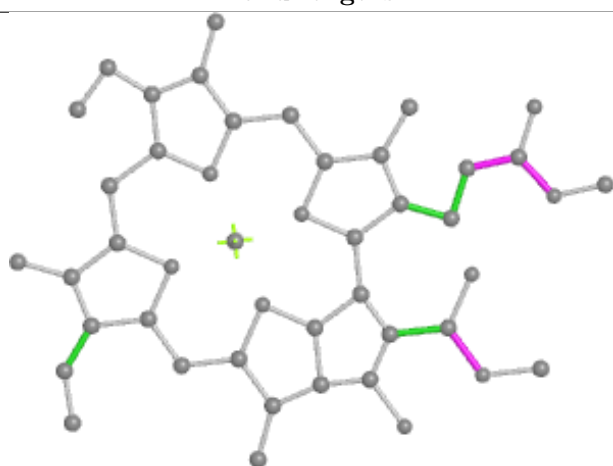
Ligand CLA 2 207



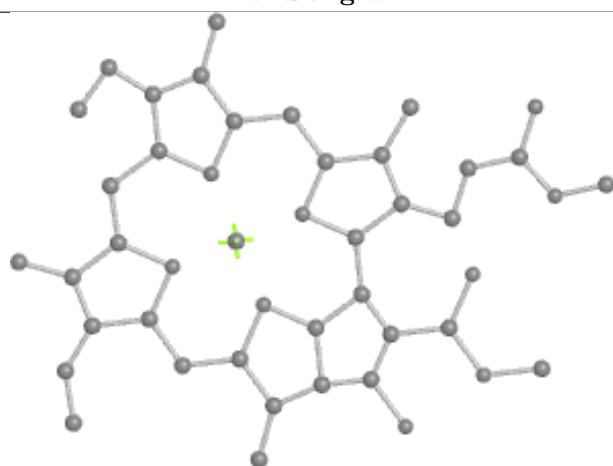
Bond lengths



Bond angles

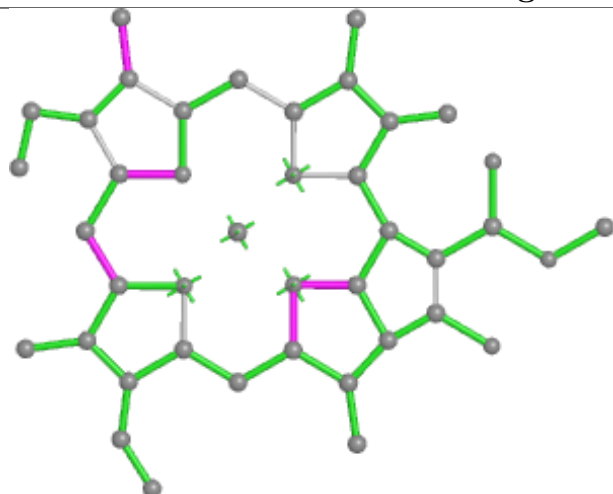


Torsions

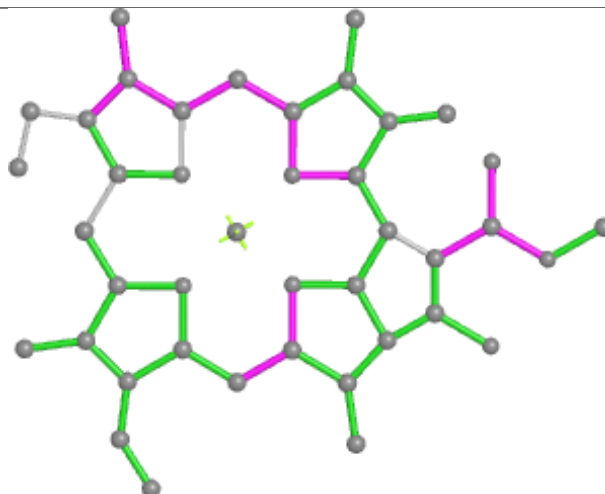


Rings

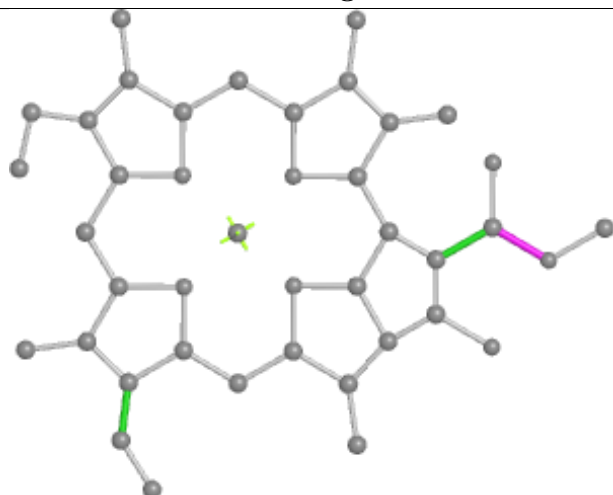
Ligand CLA k 310



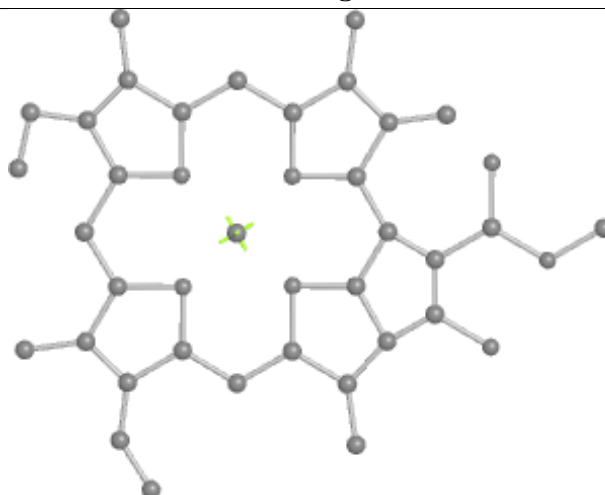
Bond lengths



Bond angles

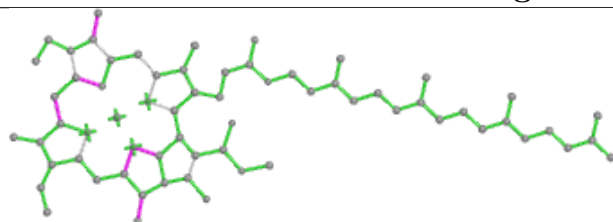


Torsions

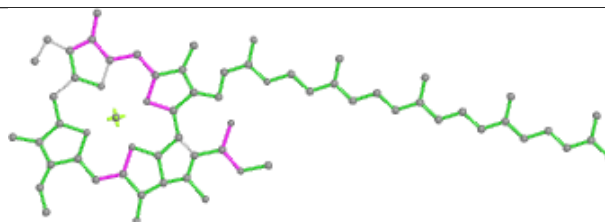


Rings

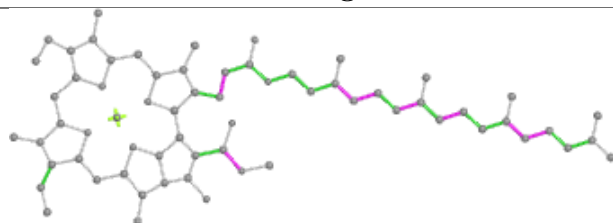
Ligand CLA A 828



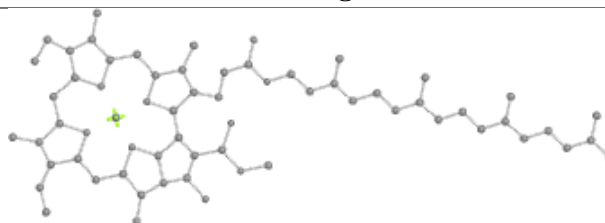
Bond lengths



Bond angles

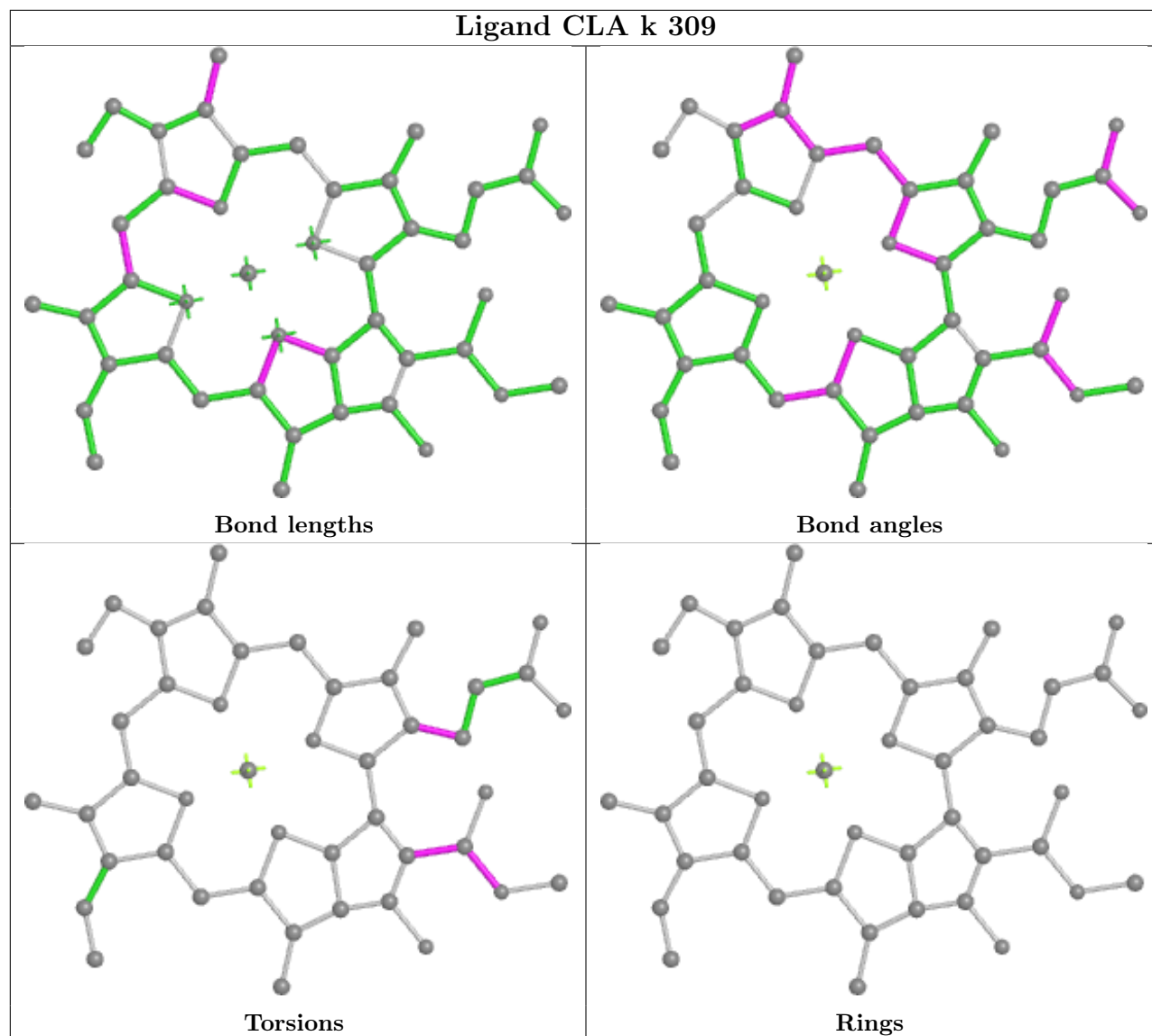


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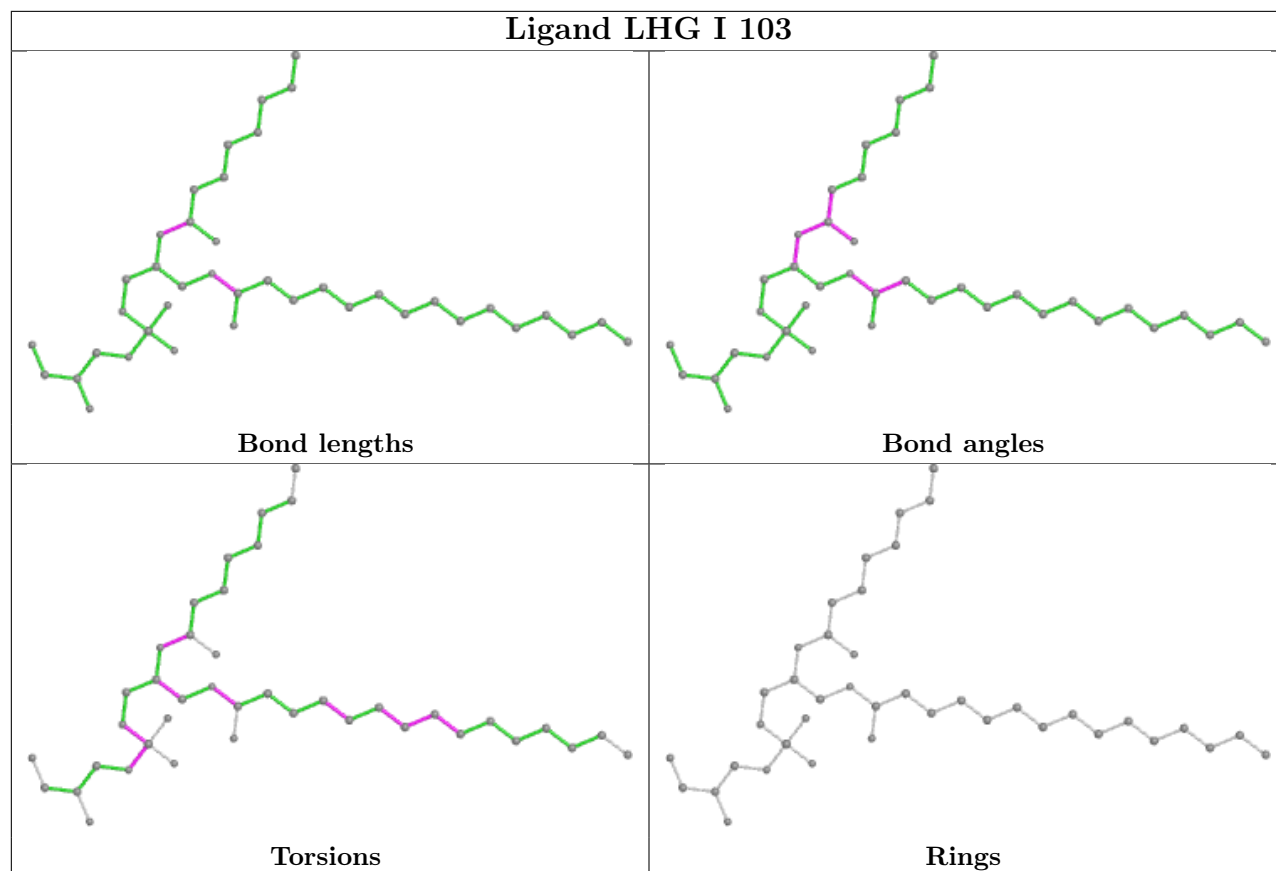


Rings

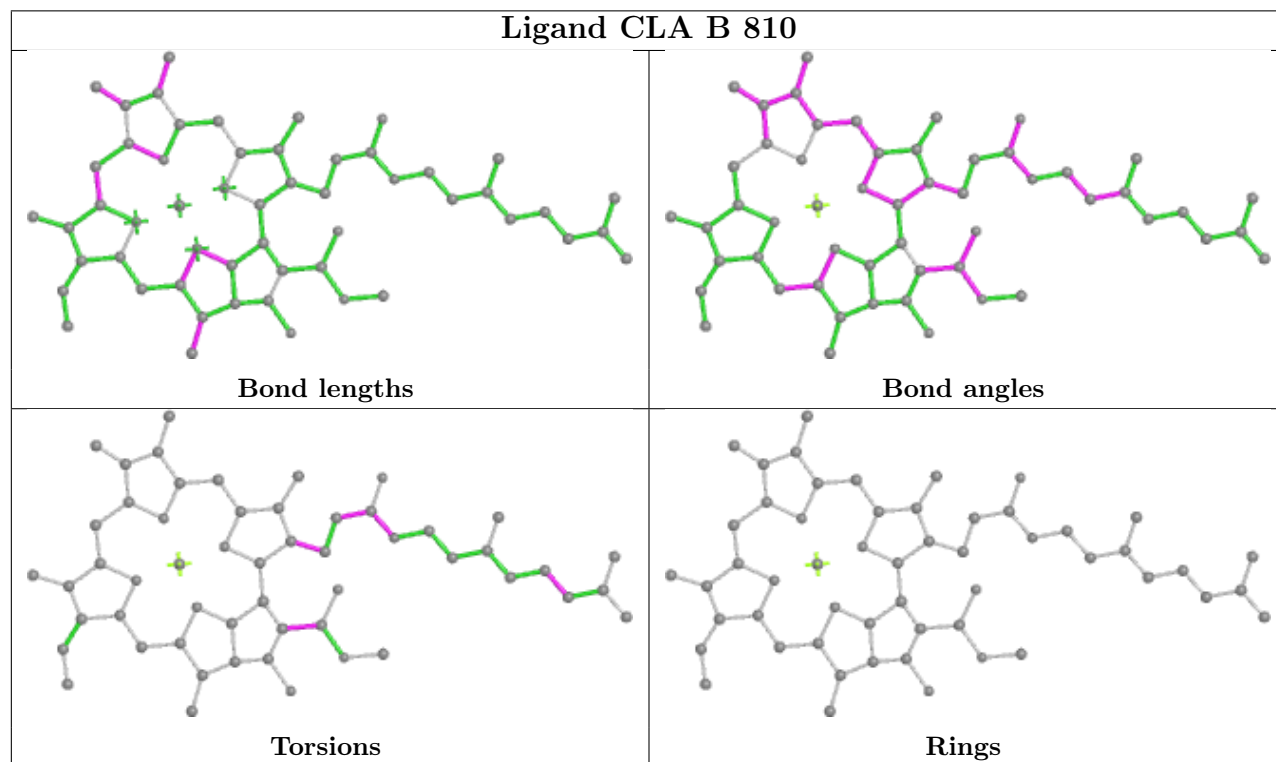
Ligand CLA k 309

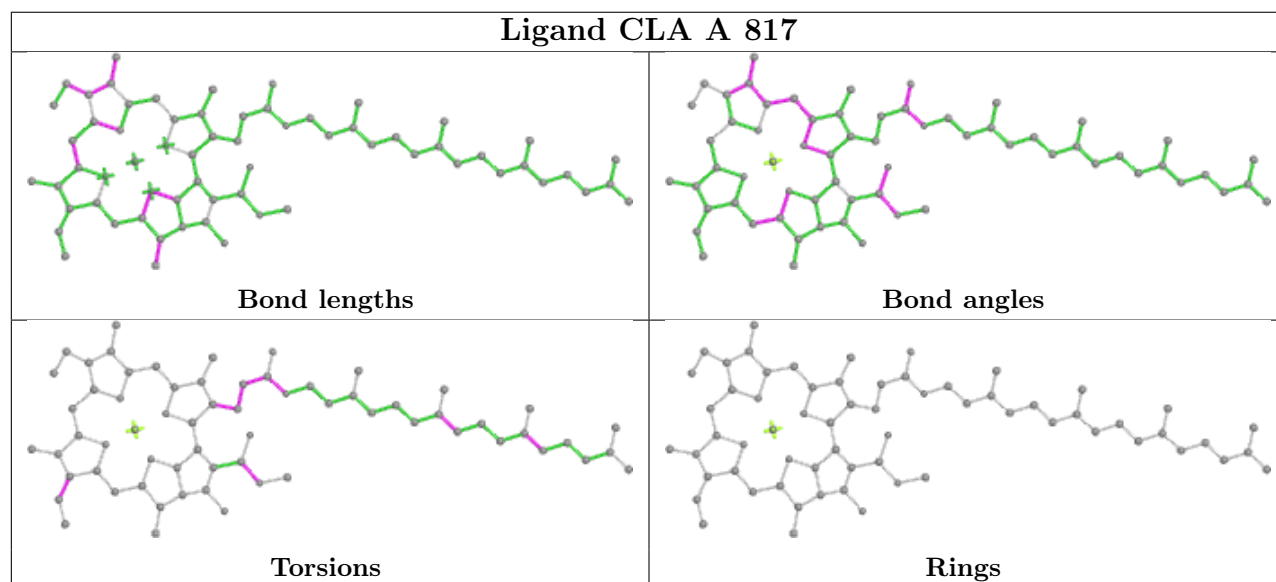
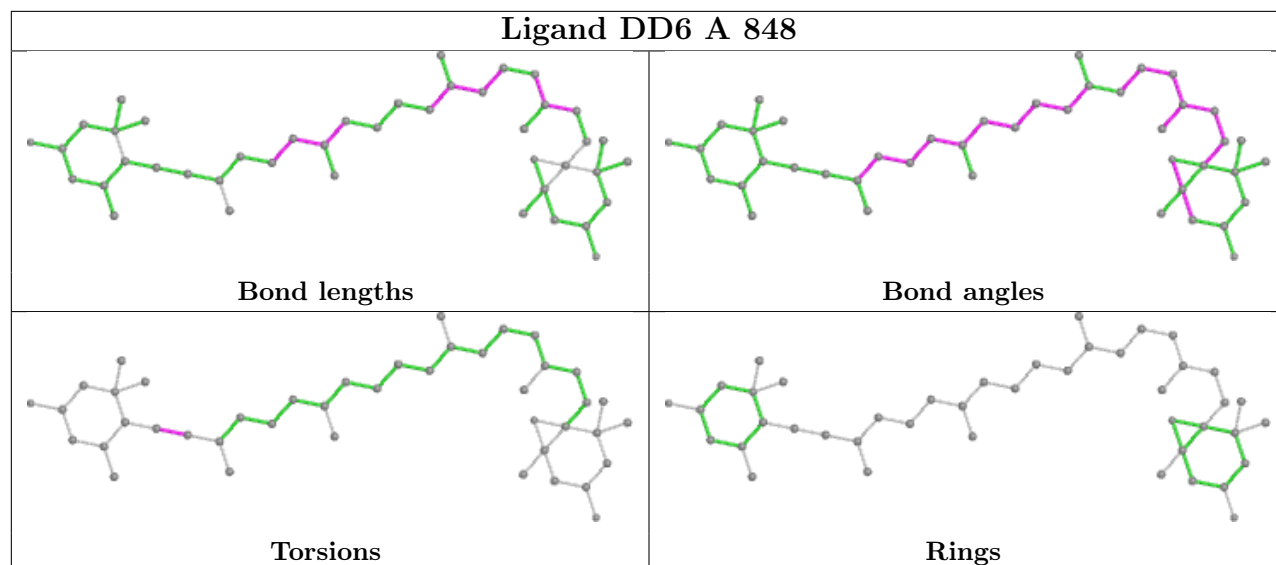


Ligand LHG I 103

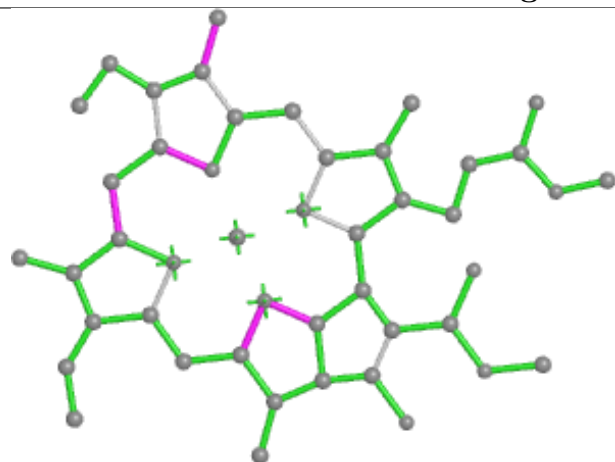


Ligand CLA B 810

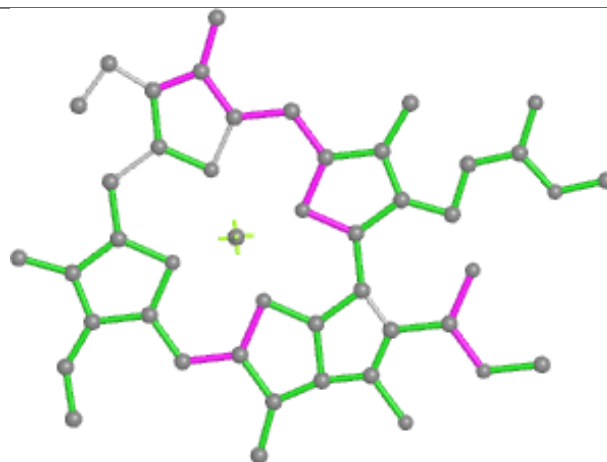




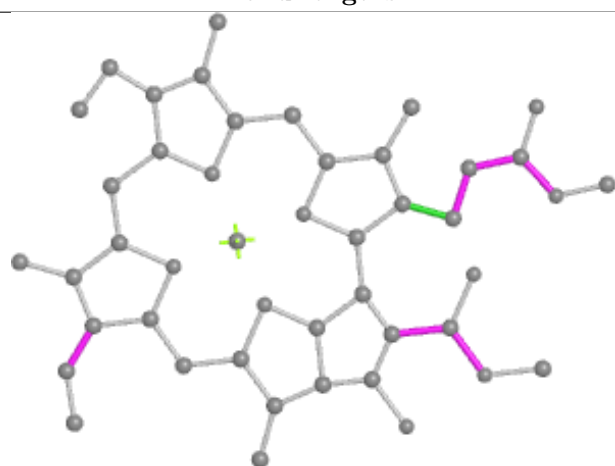
Ligand CLA 6 606



Bond lengths



Bond angles

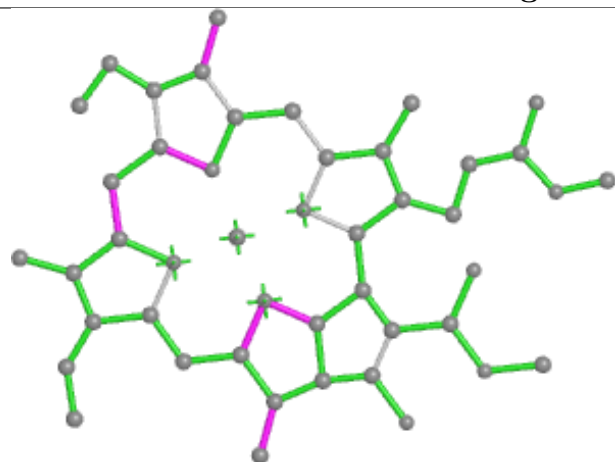


Torsions

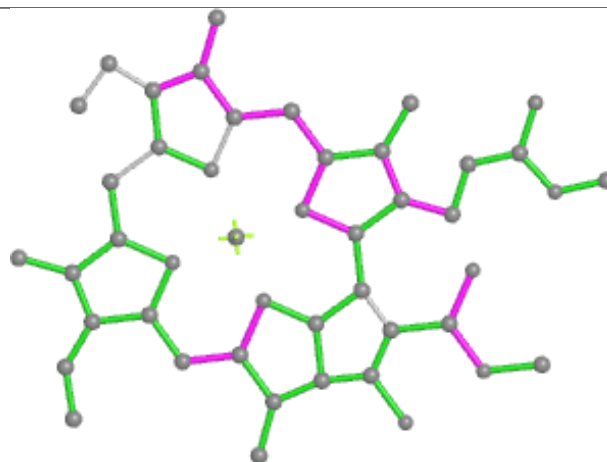


Rings

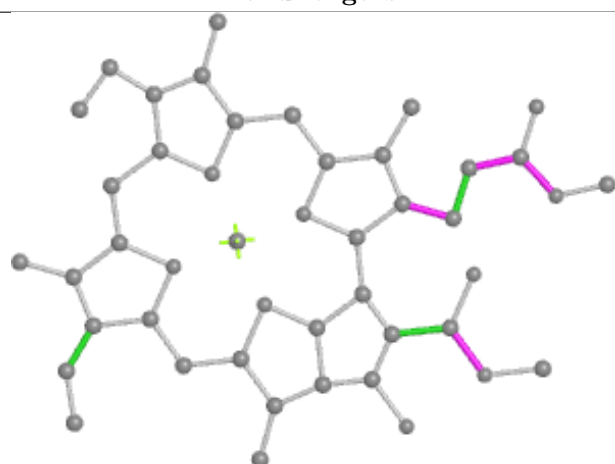
Ligand CLA 3 308



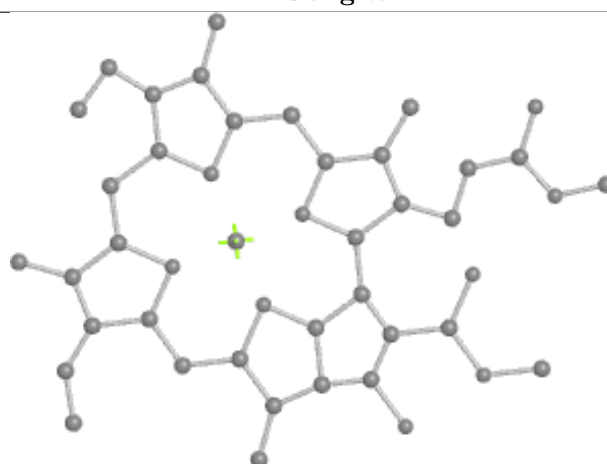
Bond lengths



Bond angles

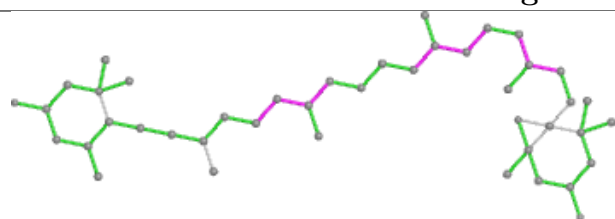


Torsions

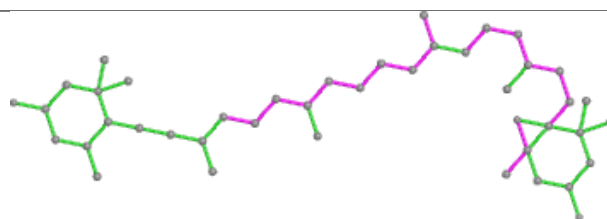


Rings

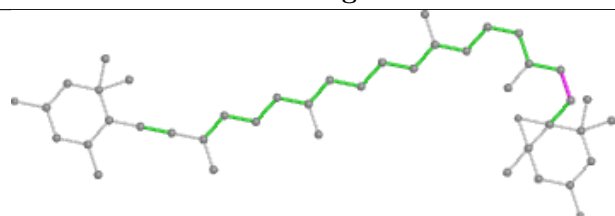
Ligand DD6 4 617



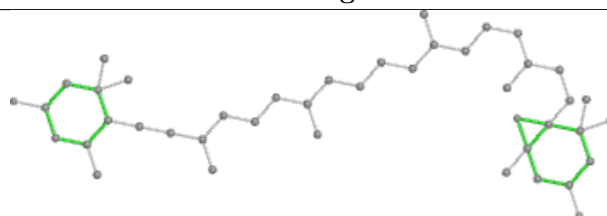
Bond lengths



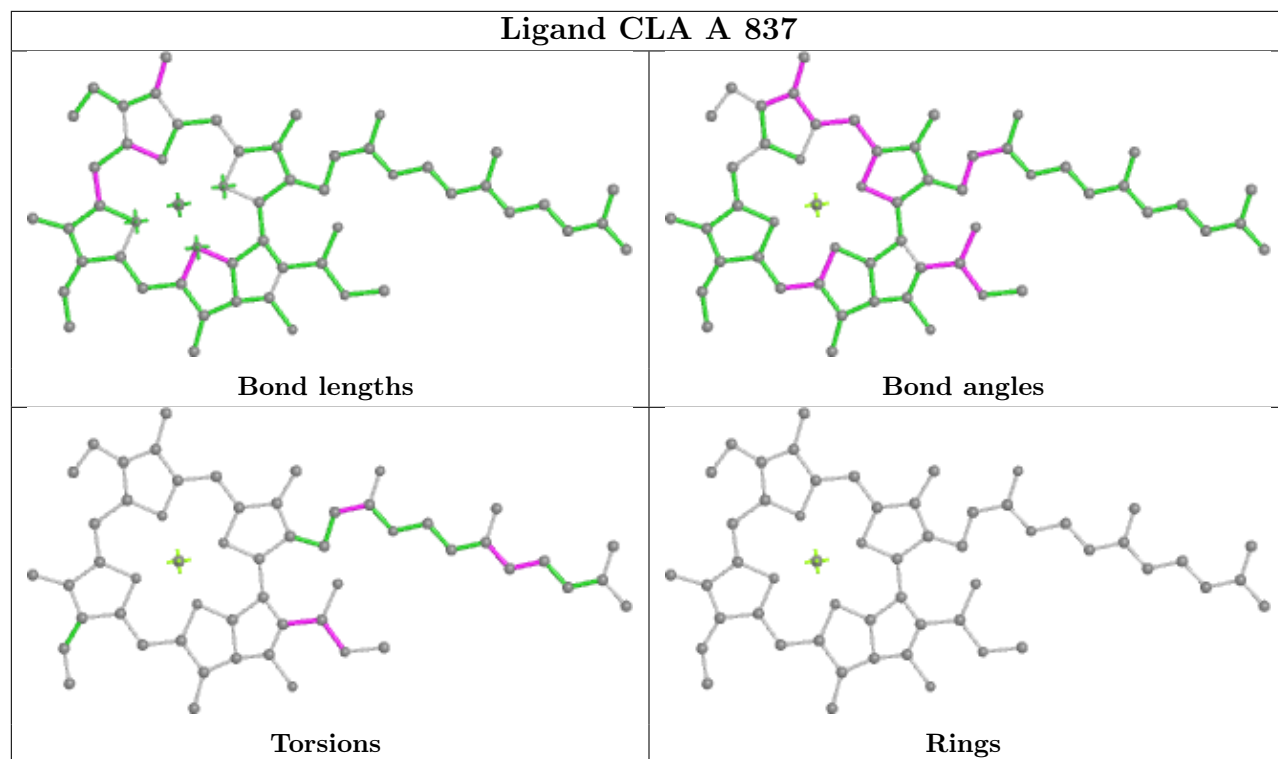
Bond angles



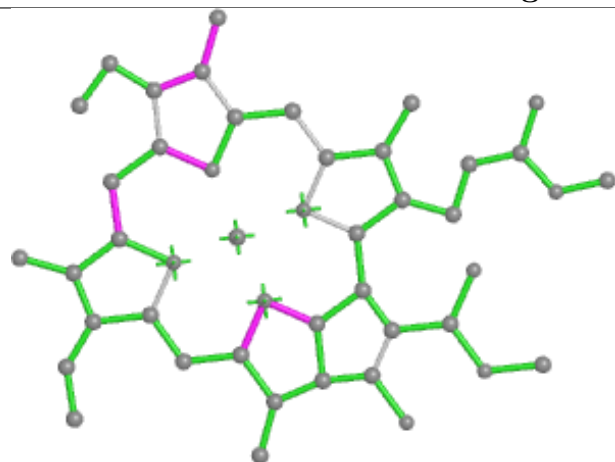
Torsions



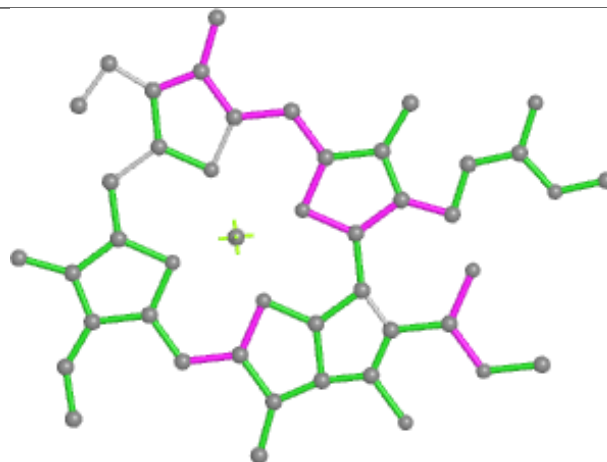
Rings



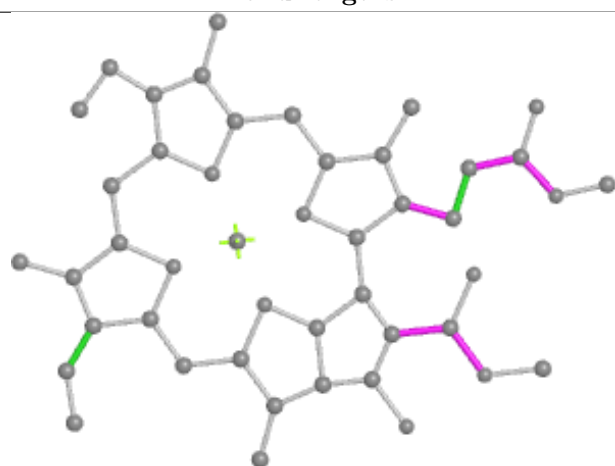
Ligand CLA c 603



Bond lengths



Bond angles

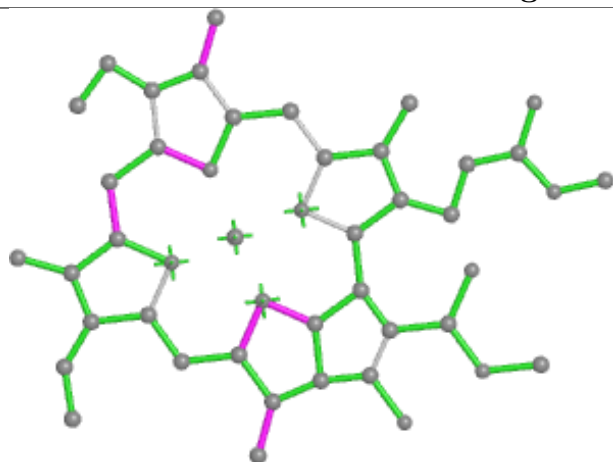


Torsions

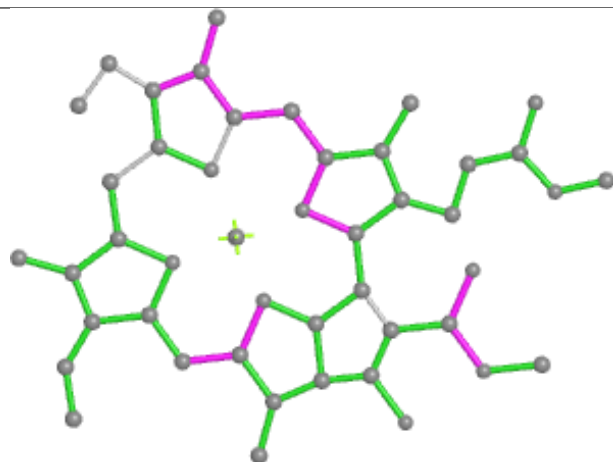


Rings

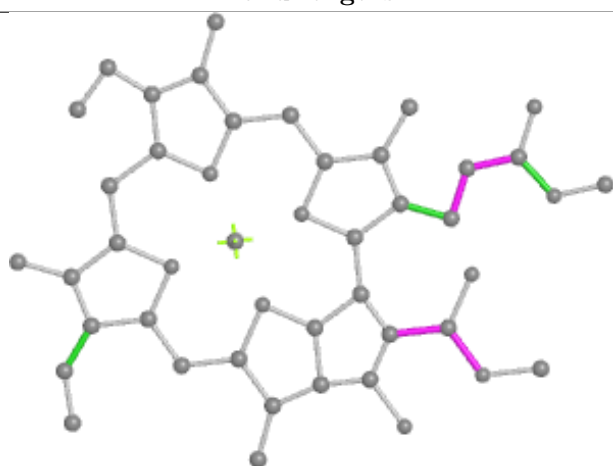
Ligand CLA t 304



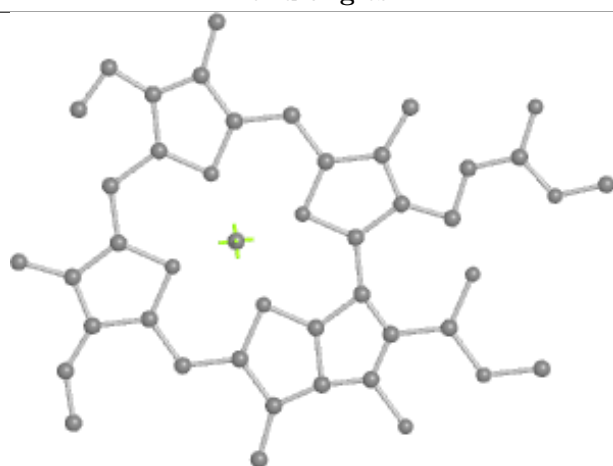
Bond lengths



Bond angles

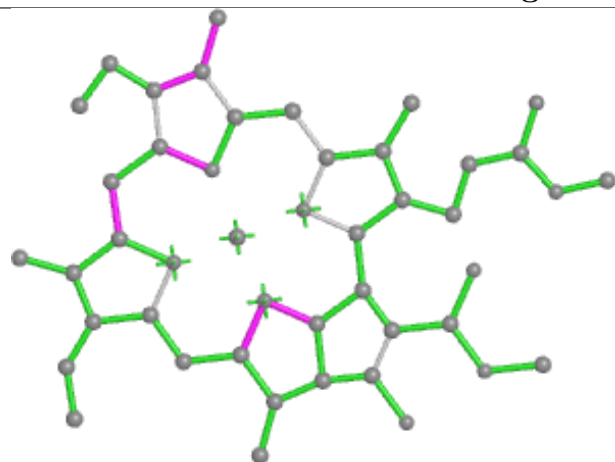


Torsions

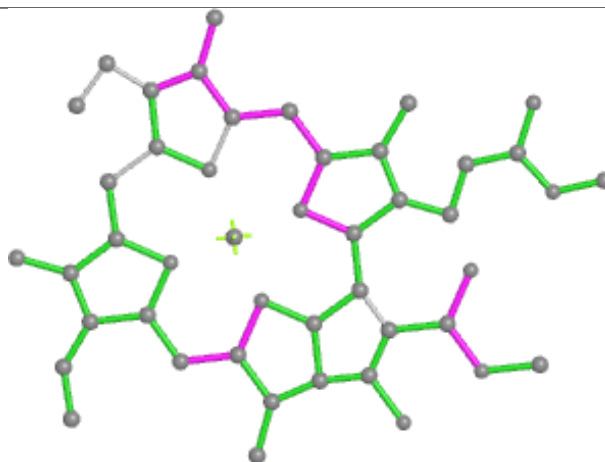


Rings

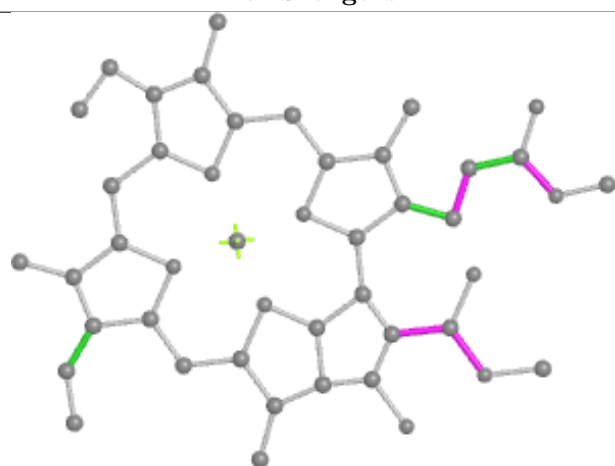
Ligand CLA c 604



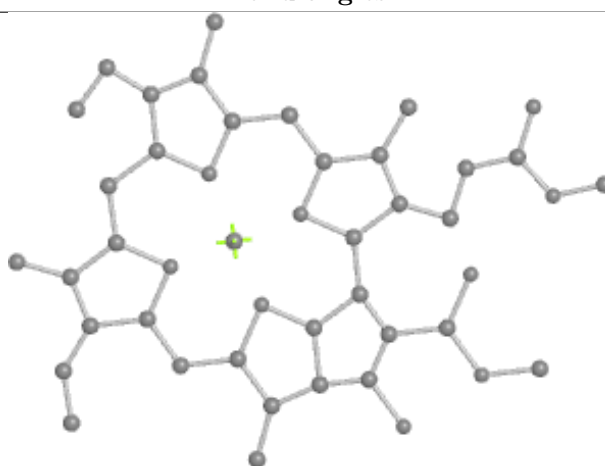
Bond lengths



Bond angles

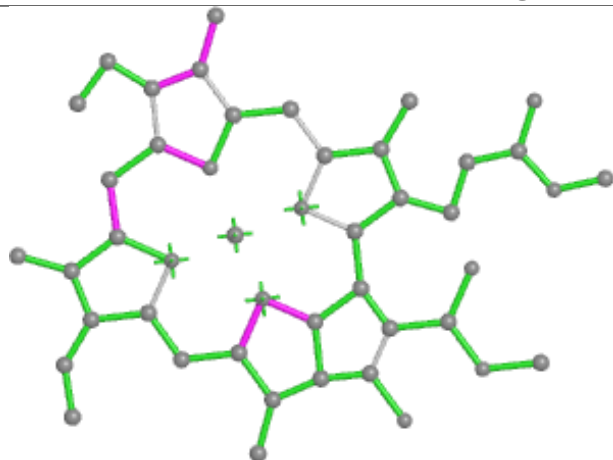


Torsions

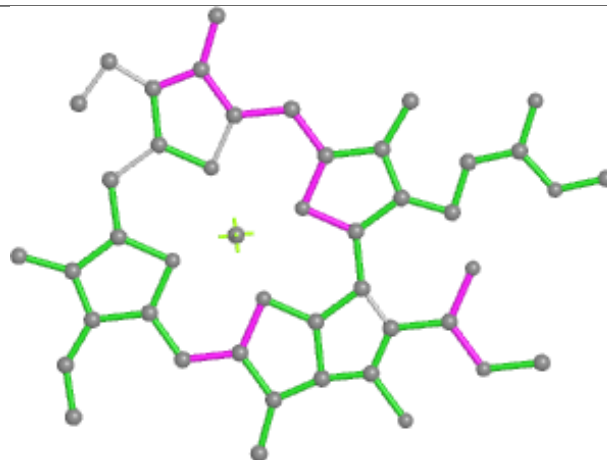


Rings

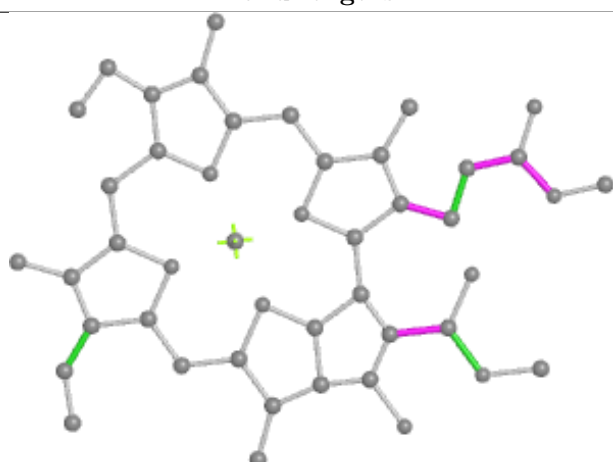
Ligand CLA A 811



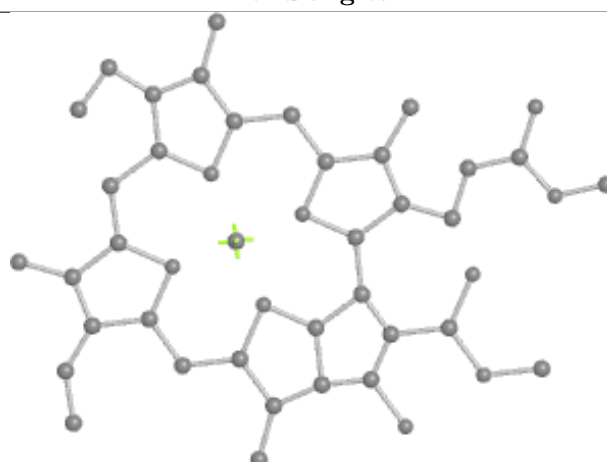
Bond lengths



Bond angles

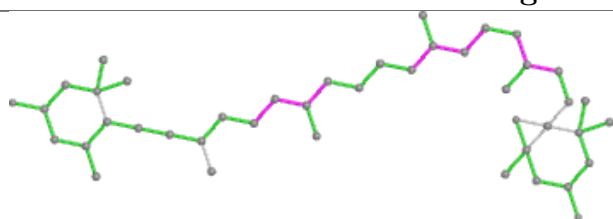


Torsions

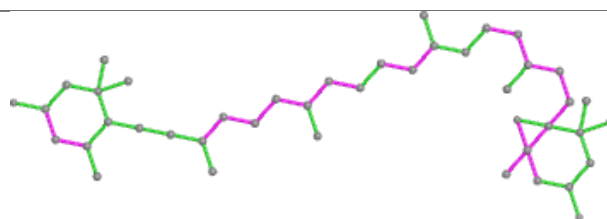


Rings

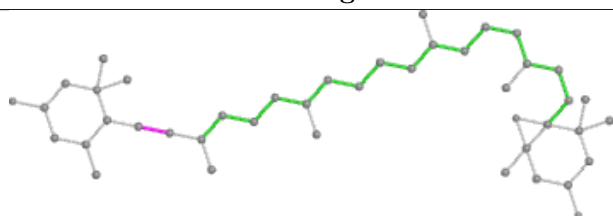
Ligand DD6 c 614



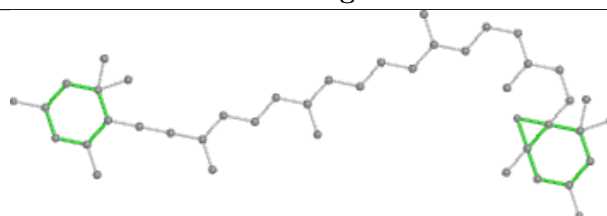
Bond lengths



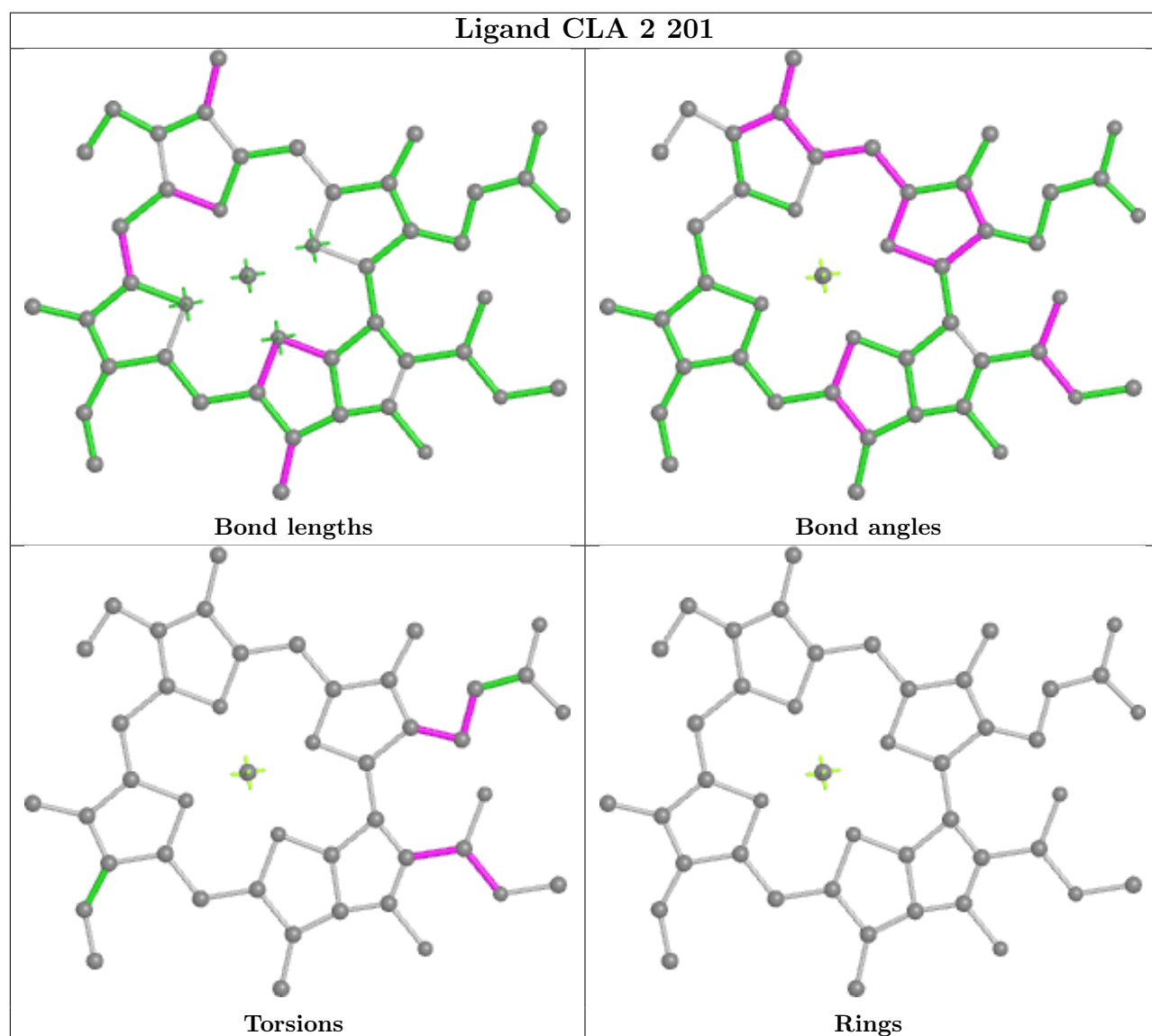
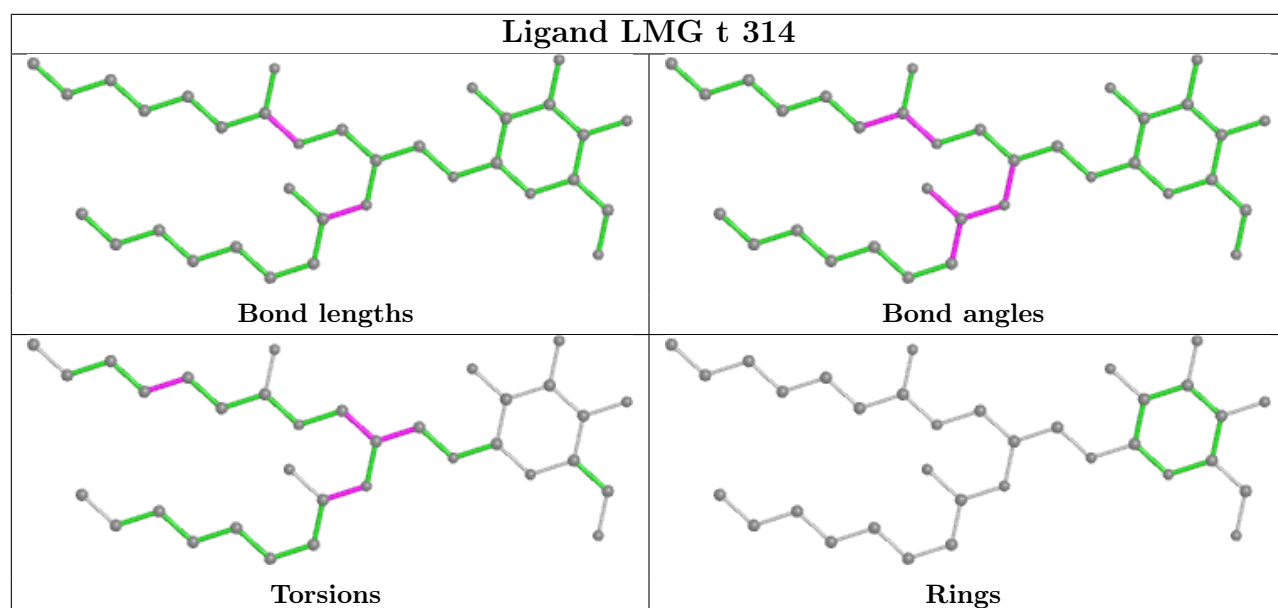
Bond angles

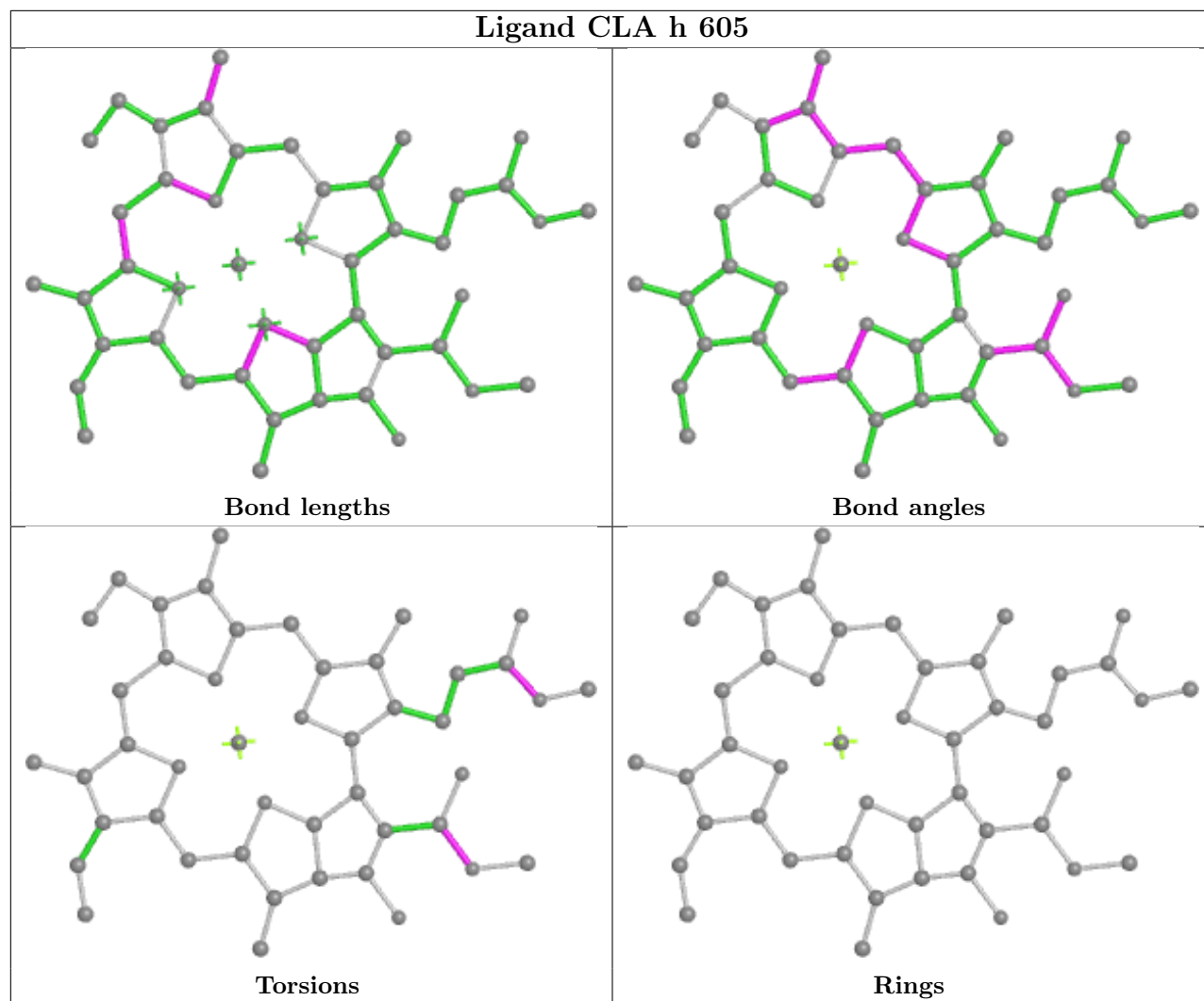
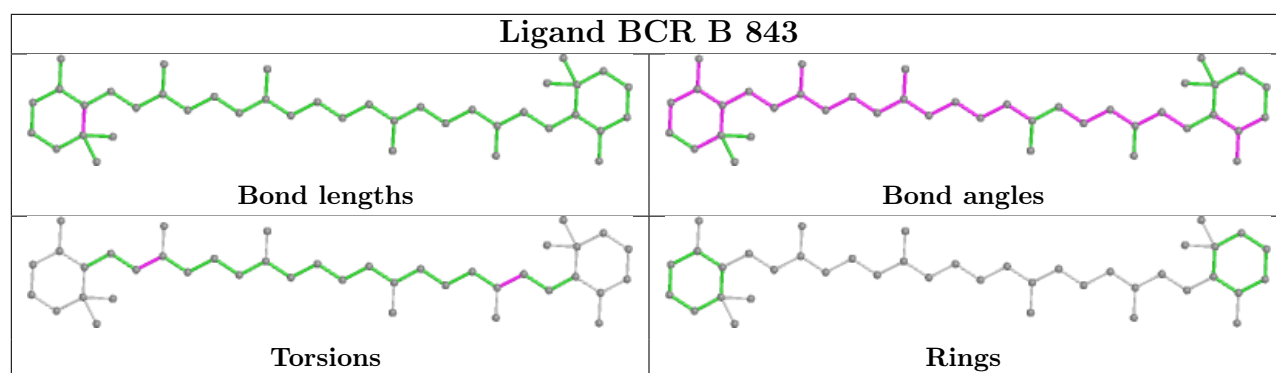


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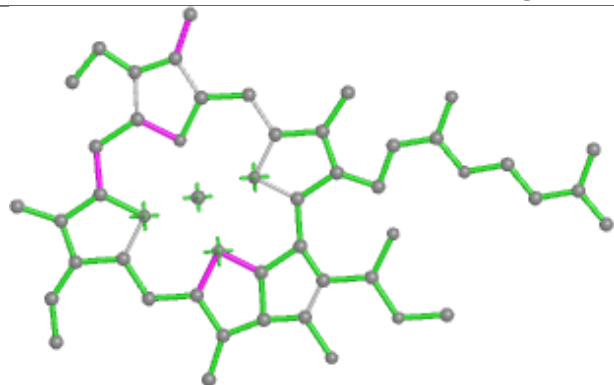


Rings

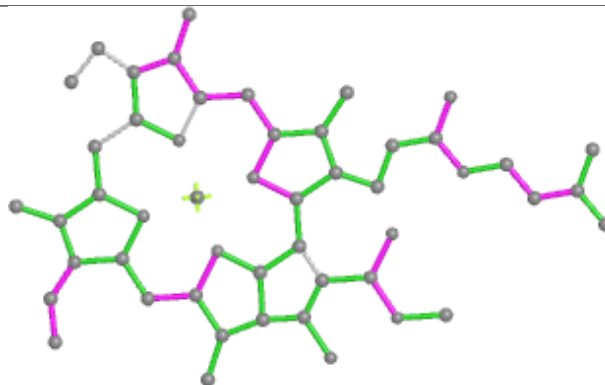




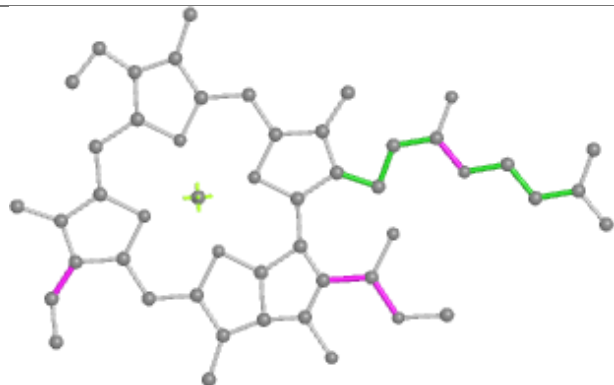
Ligand CLA 4 608



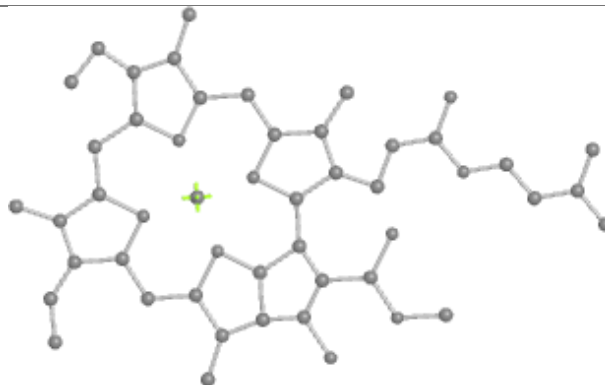
Bond lengths



Bond angles

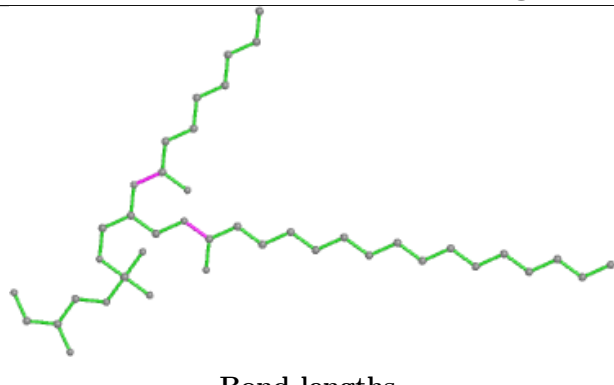


Torsions

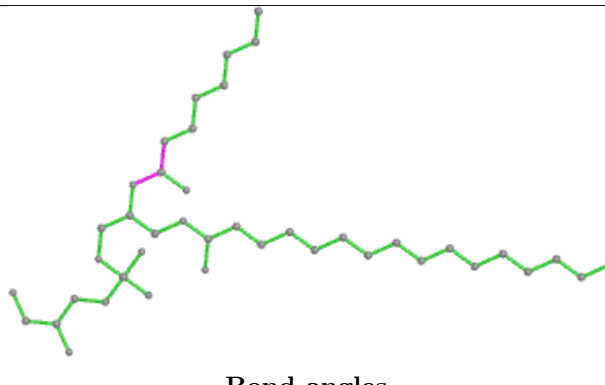


Rings

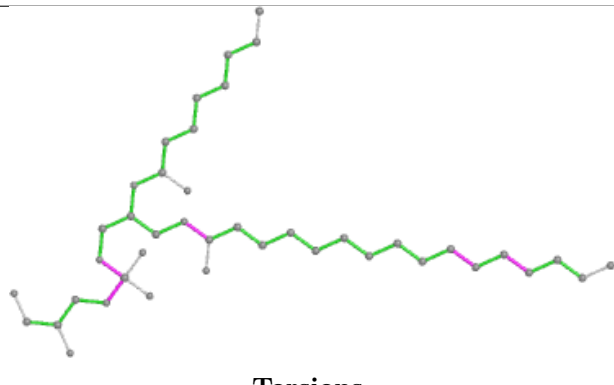
Ligand LHG B 845



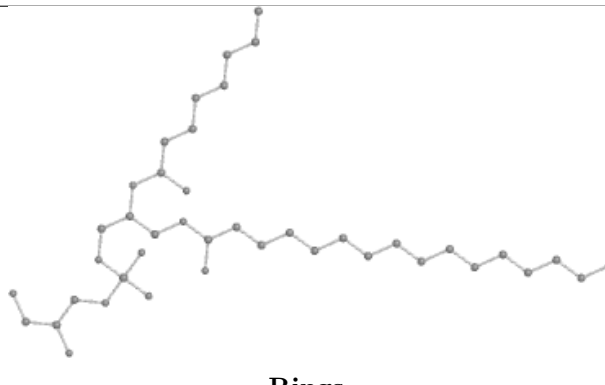
Bond lengths



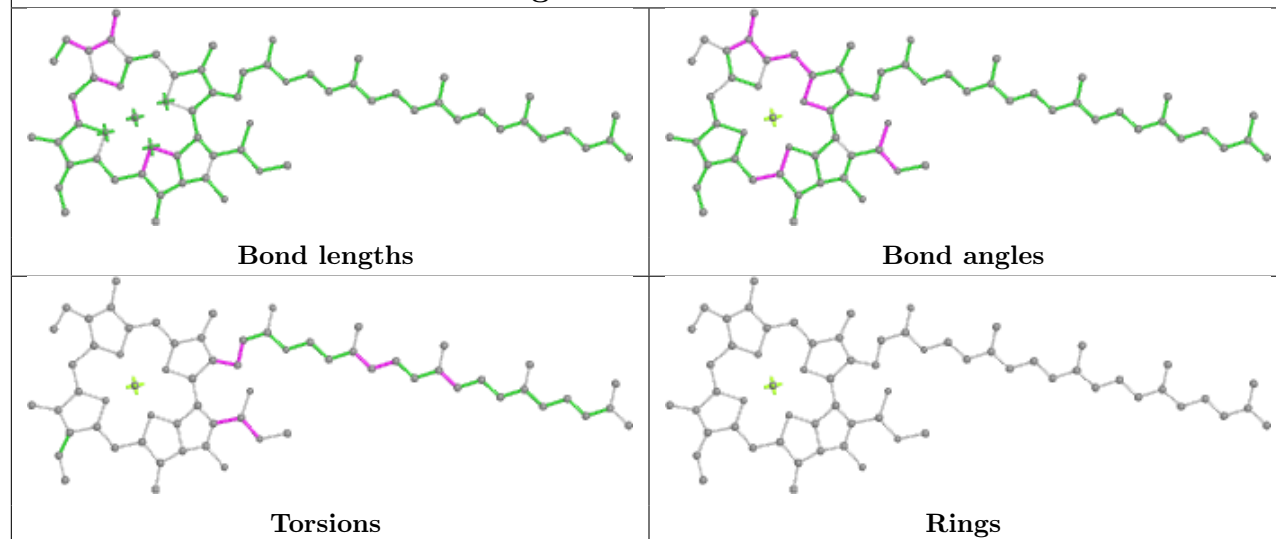
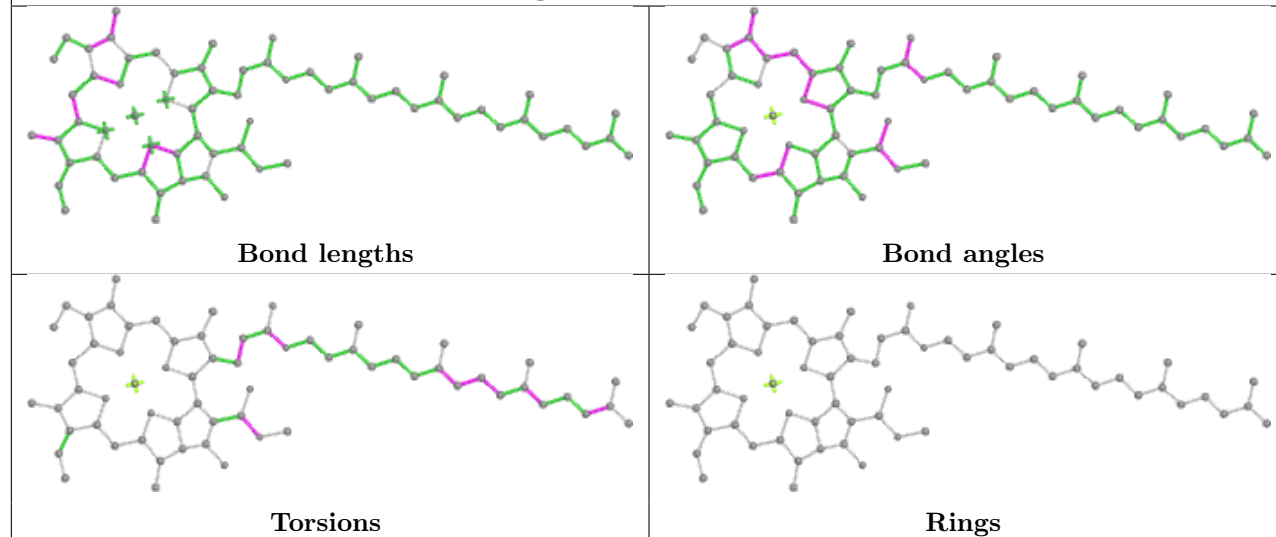
Bond angles

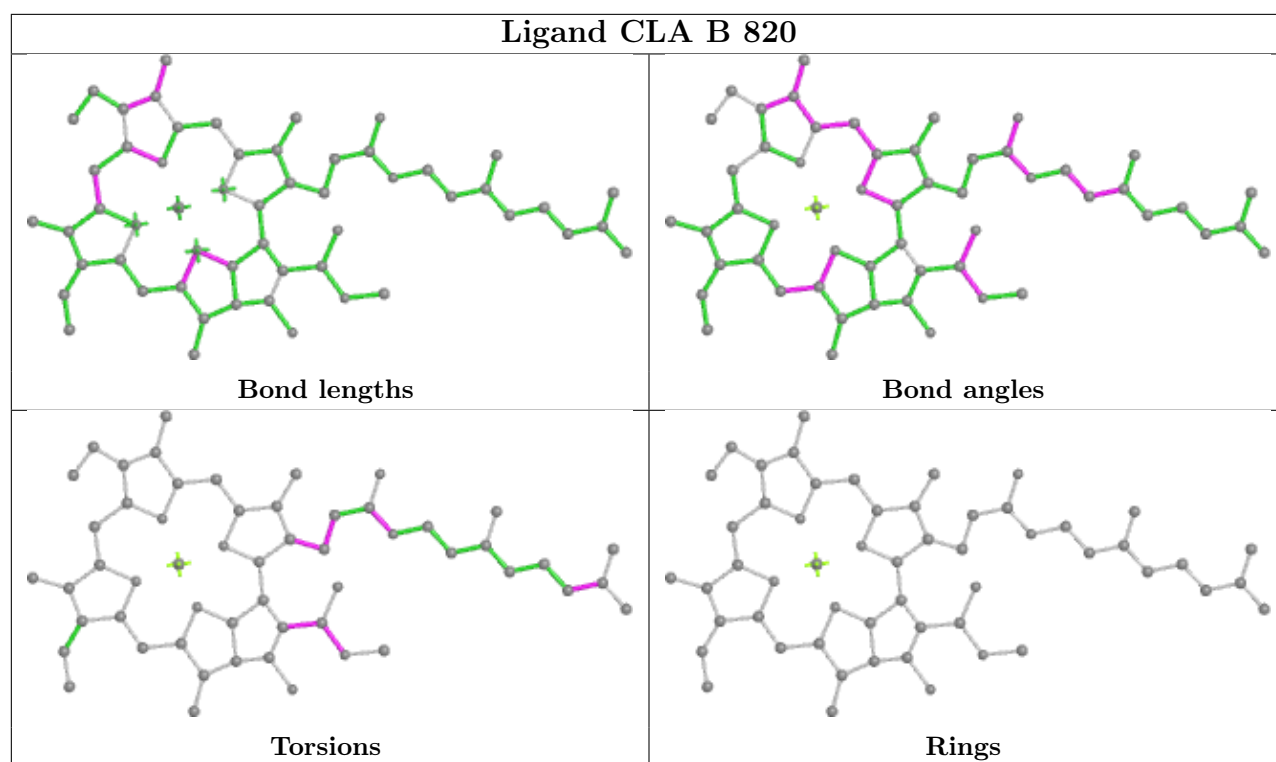


Torsions

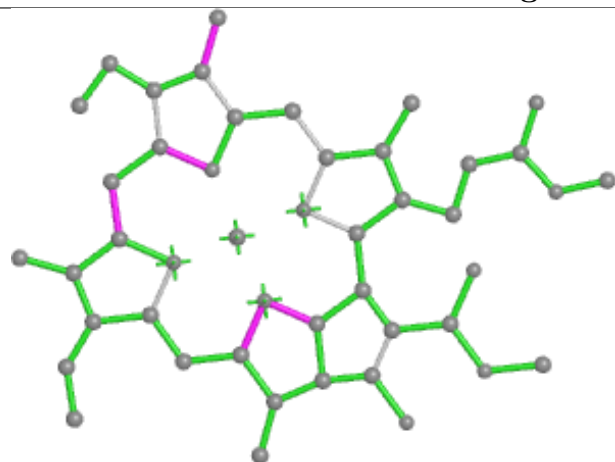


Rings

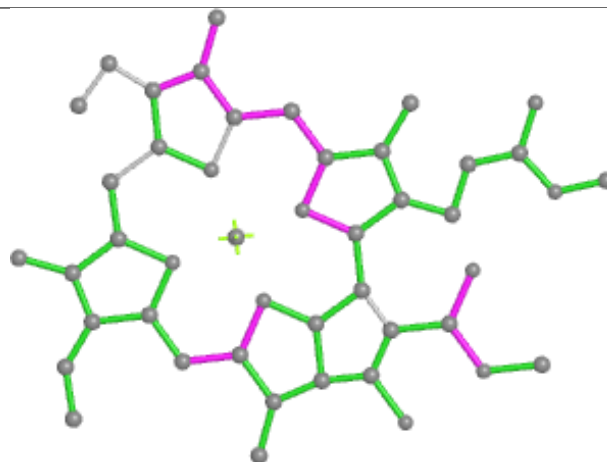
Ligand CLA A 856**Ligand CLA A 812**



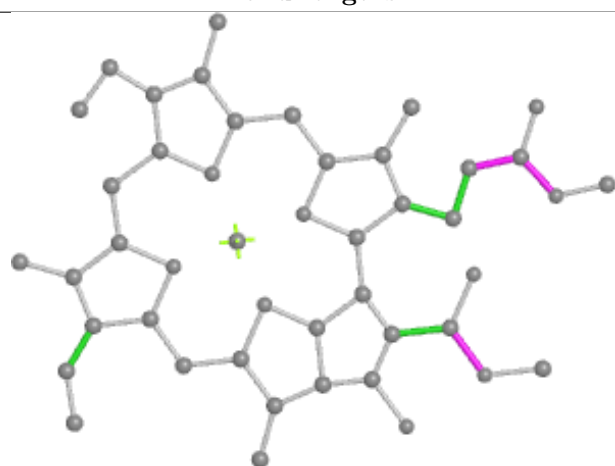
Ligand CLA 5 606



Bond lengths



Bond angles

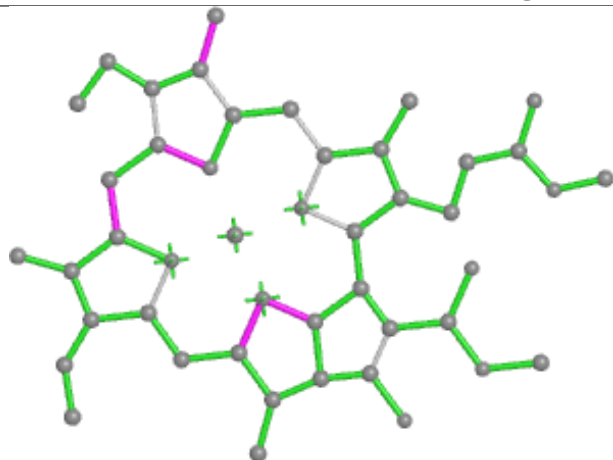


Torsions

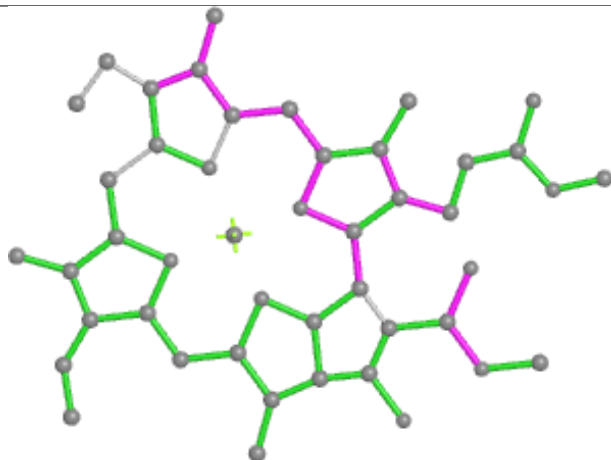


Rings

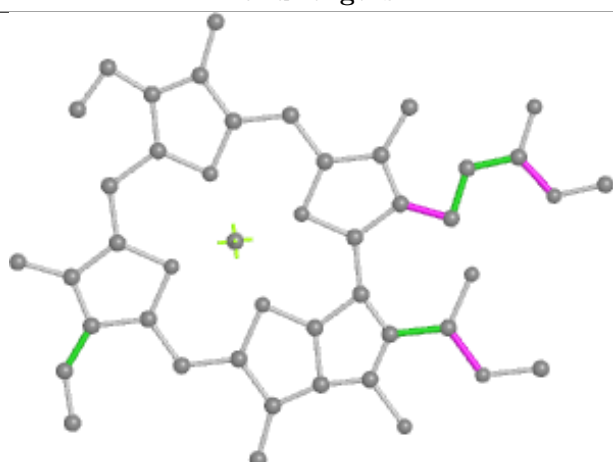
Ligand CLA 3 304



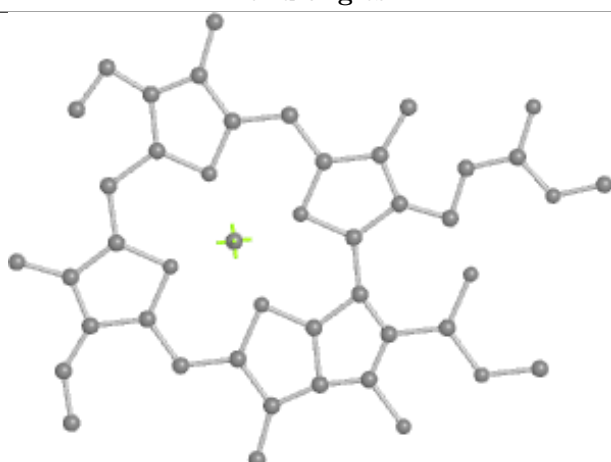
Bond lengths



Bond angles

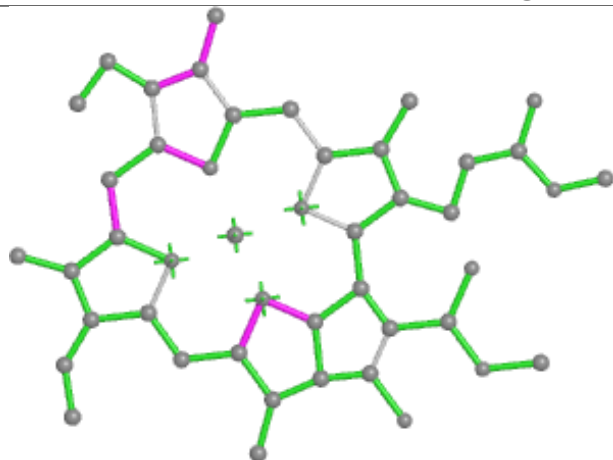


Torsions

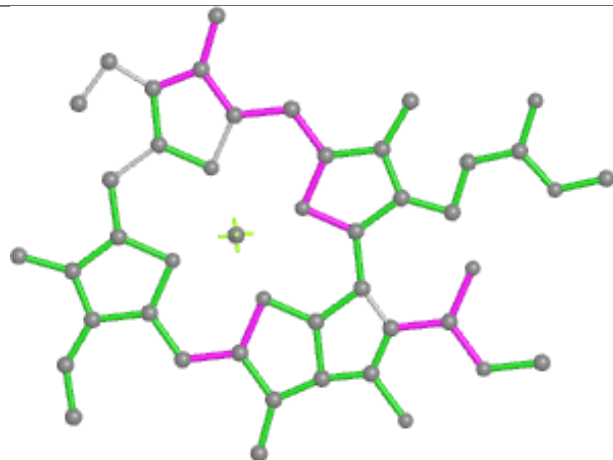


Rings

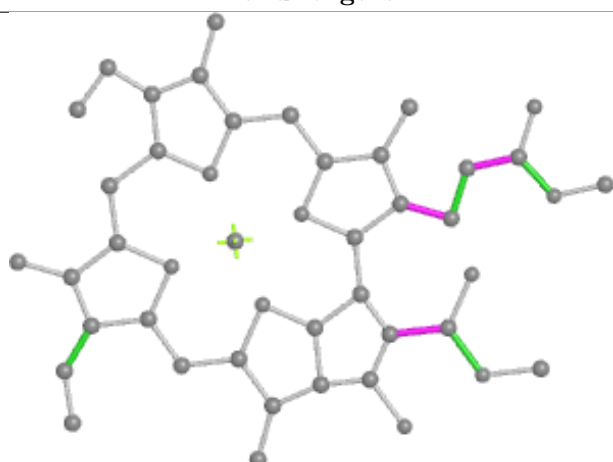
Ligand CLA 2 206



Bond lengths



Bond angles

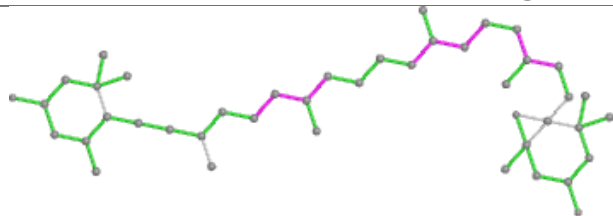


Torsions

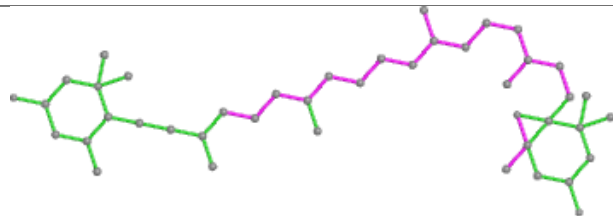


Rings

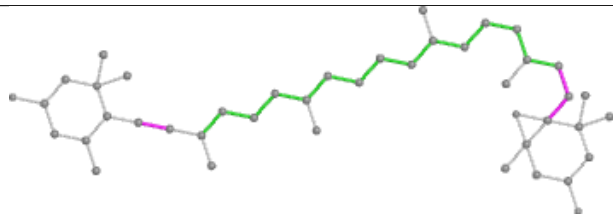
Ligand DD6 k 315



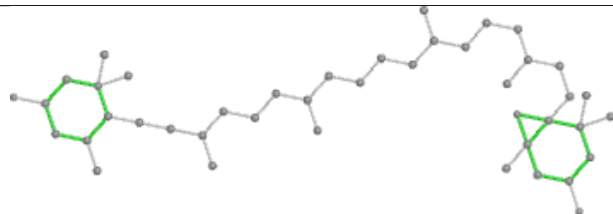
Bond lengths



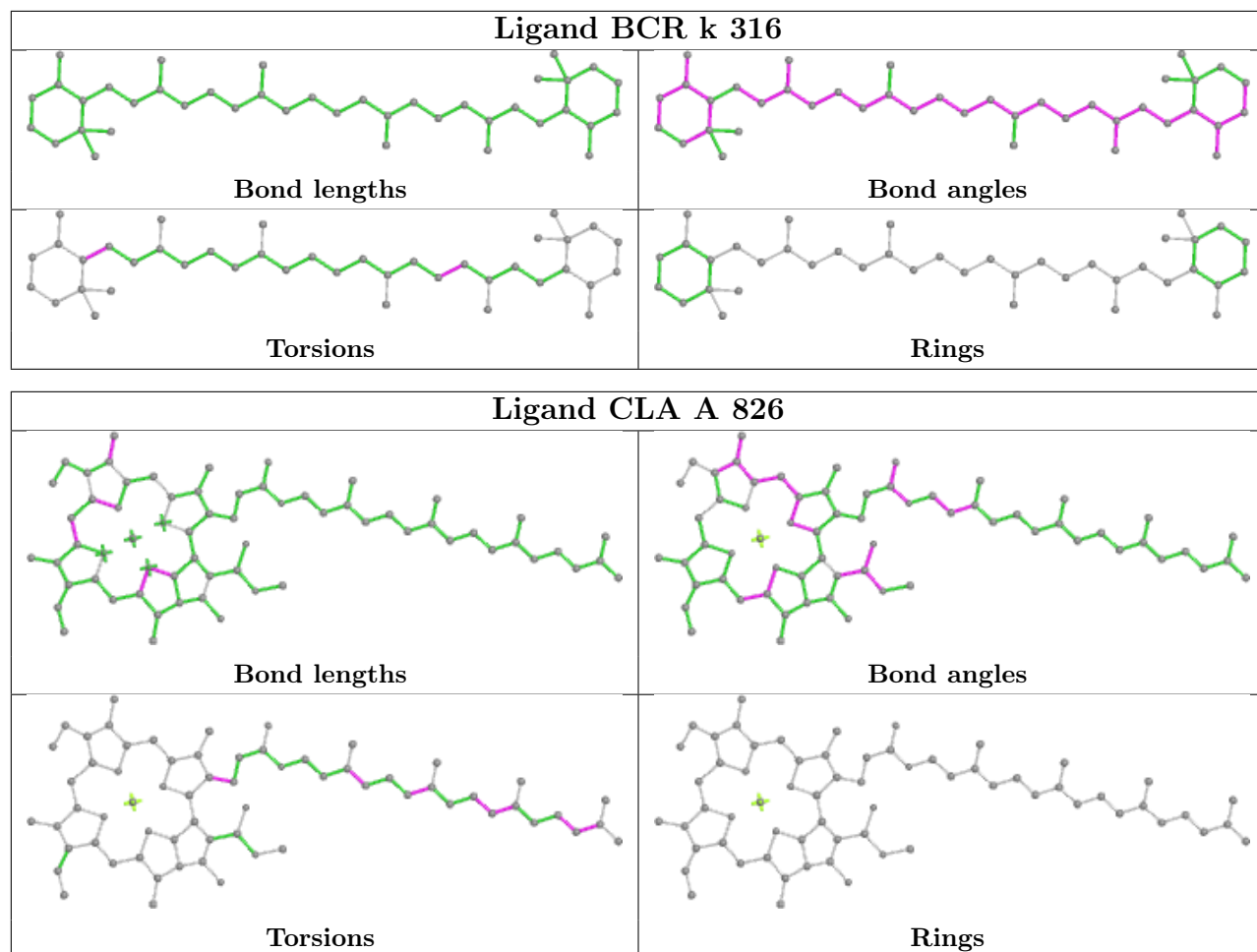
Bond angles

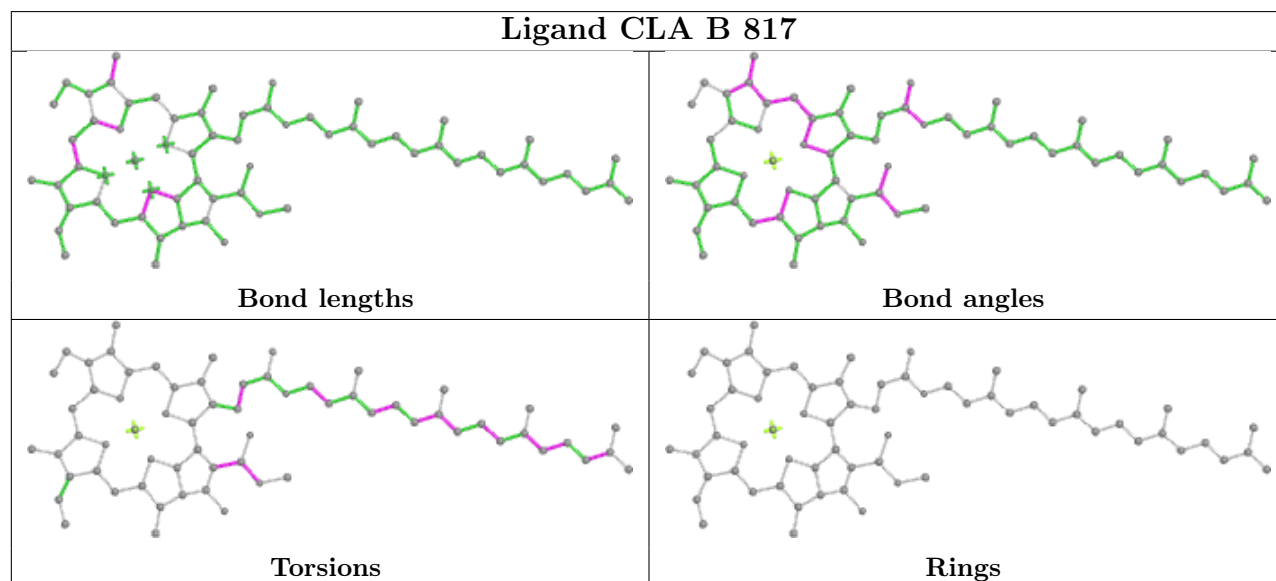
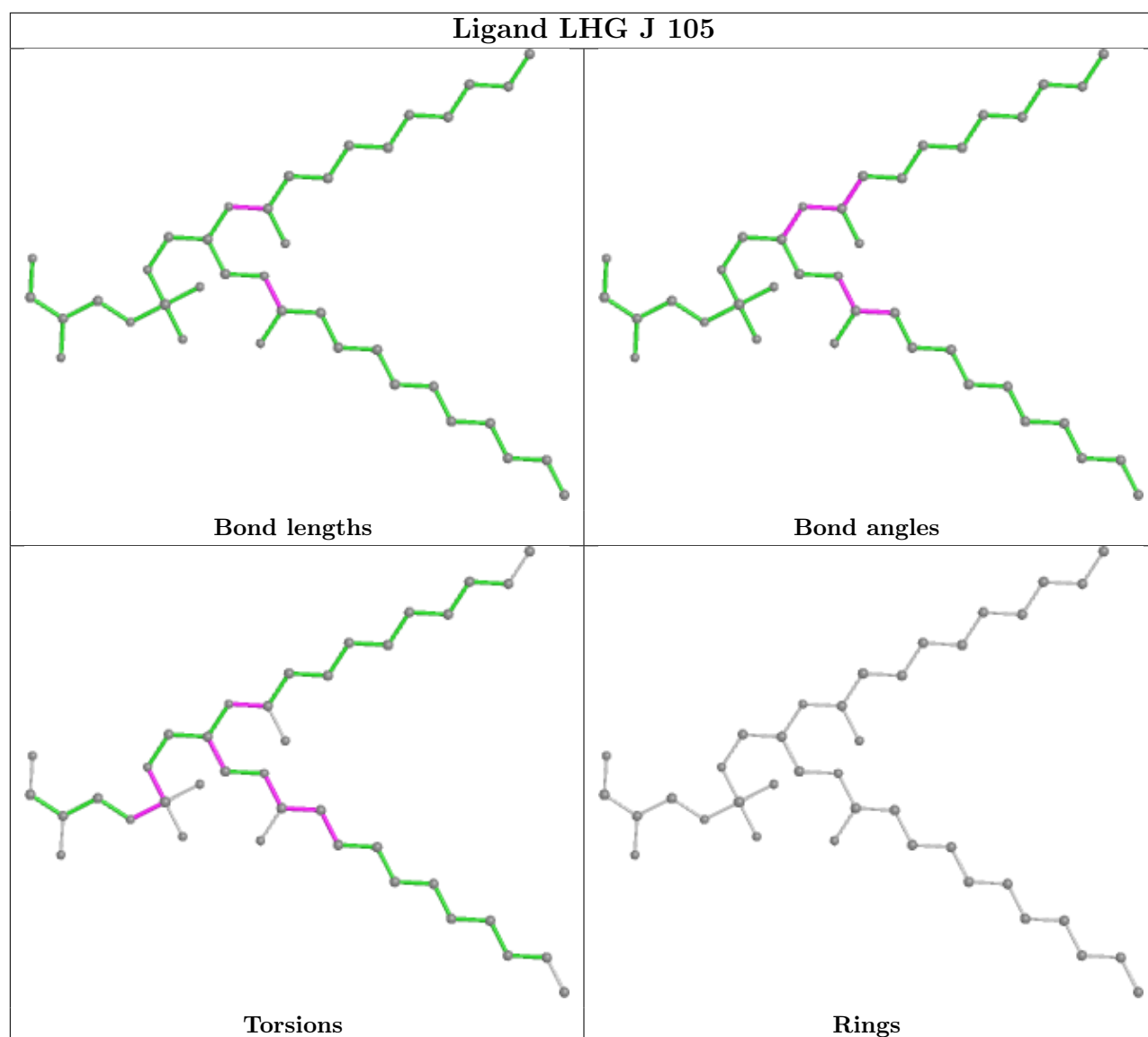


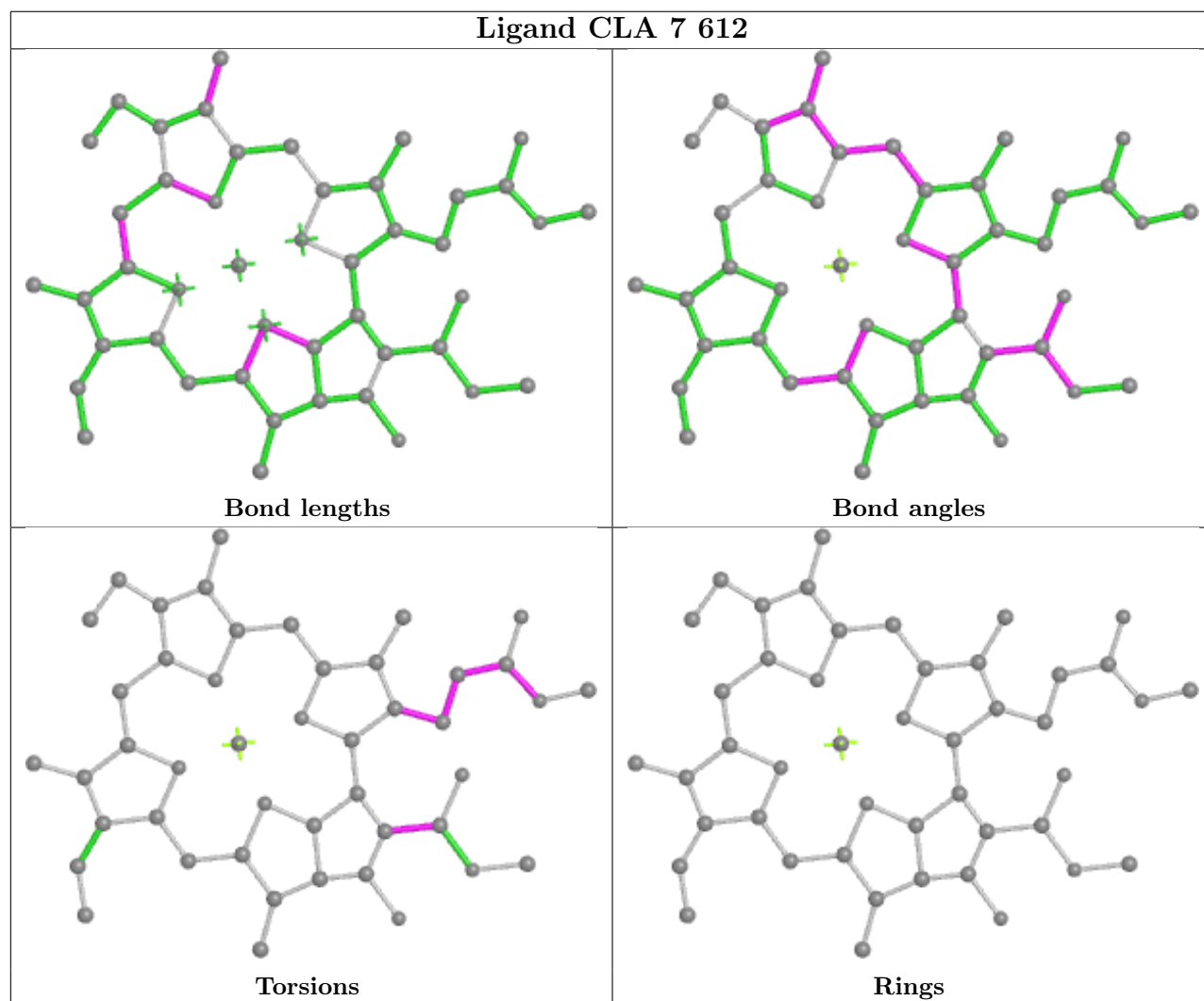
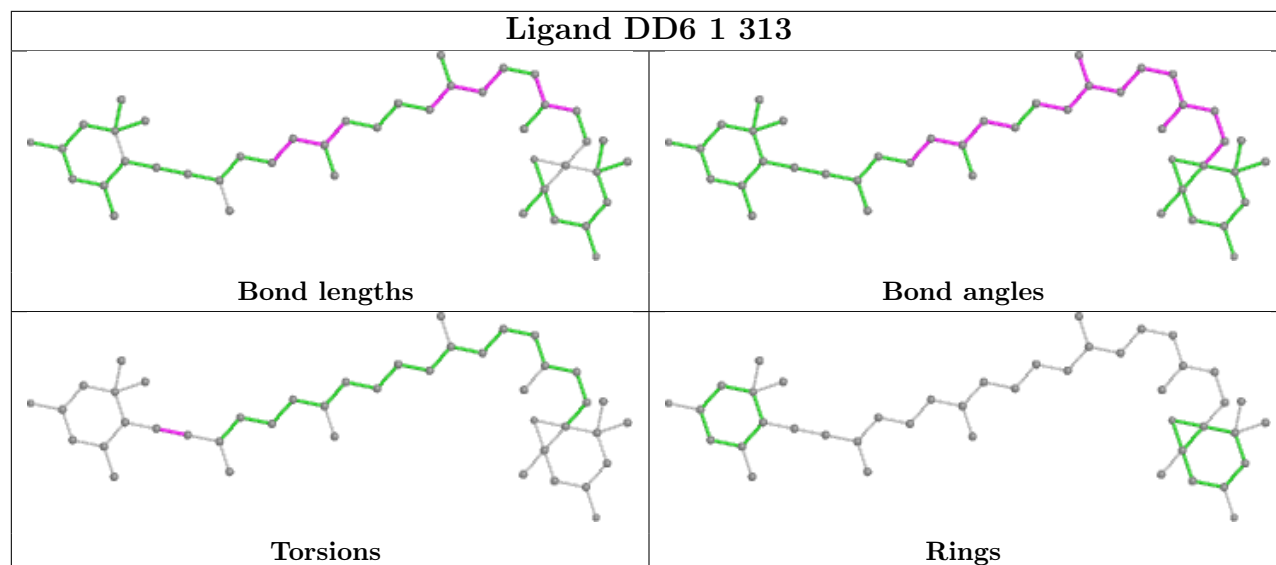
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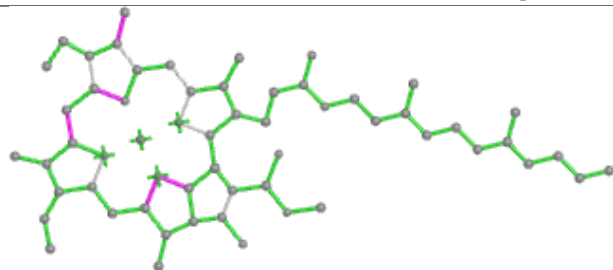
Rings



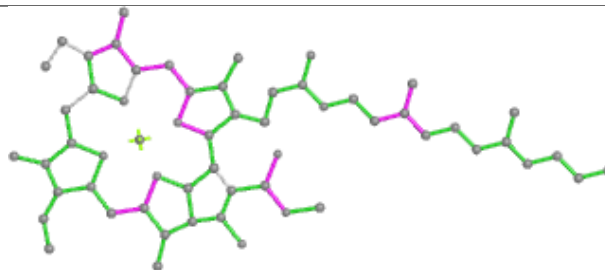




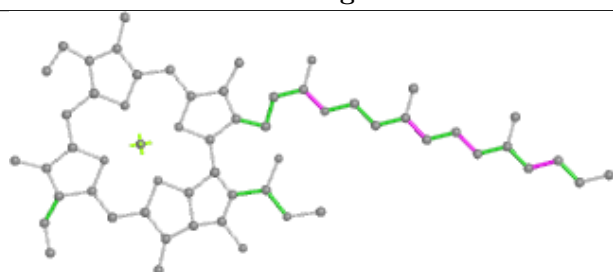
Ligand CLA B 833



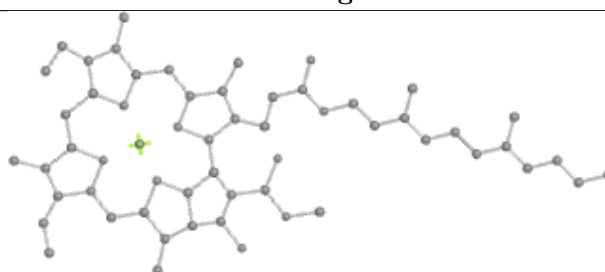
Bond lengths



Bond angles

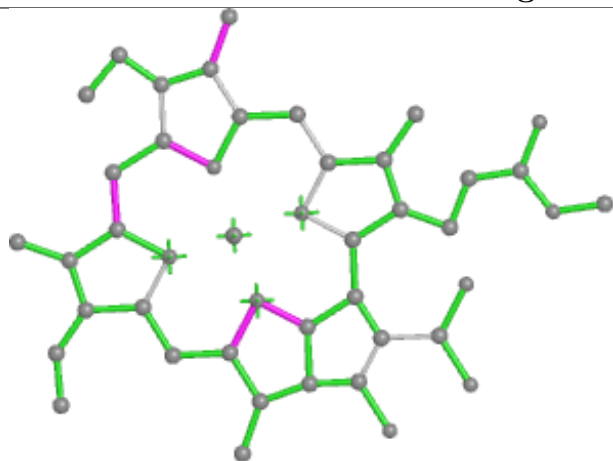


Torsions

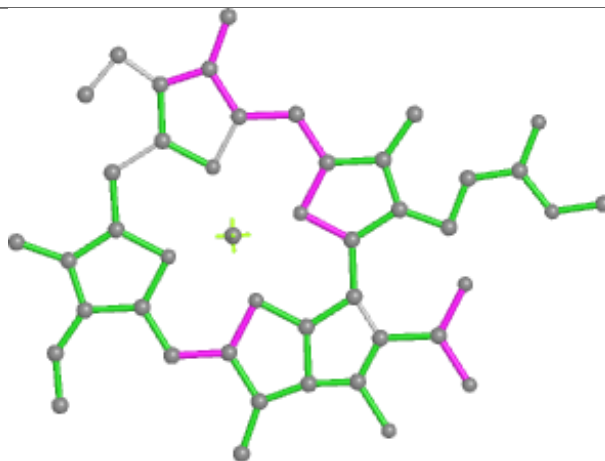


Rings

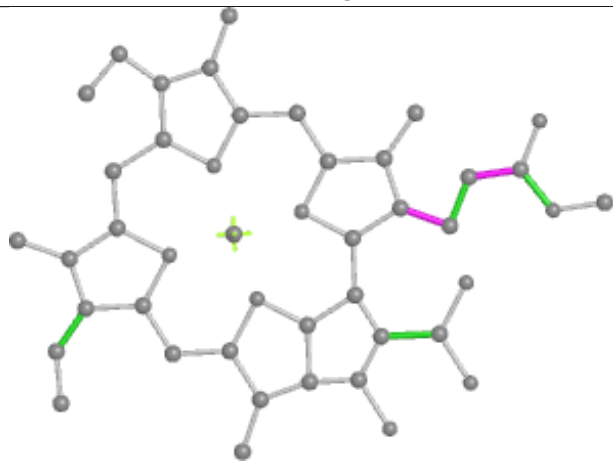
Ligand CLA h 603



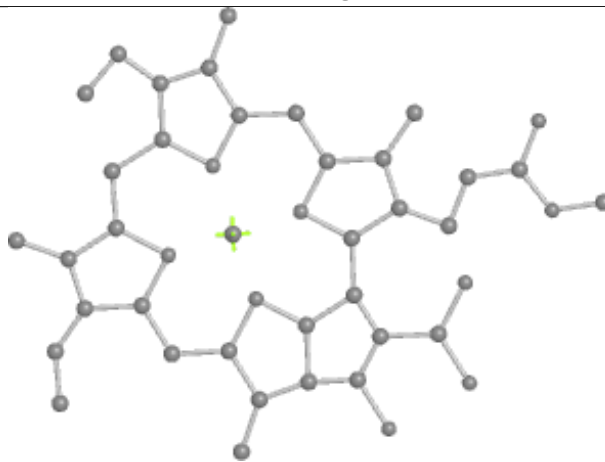
Bond lengths



Bond angles

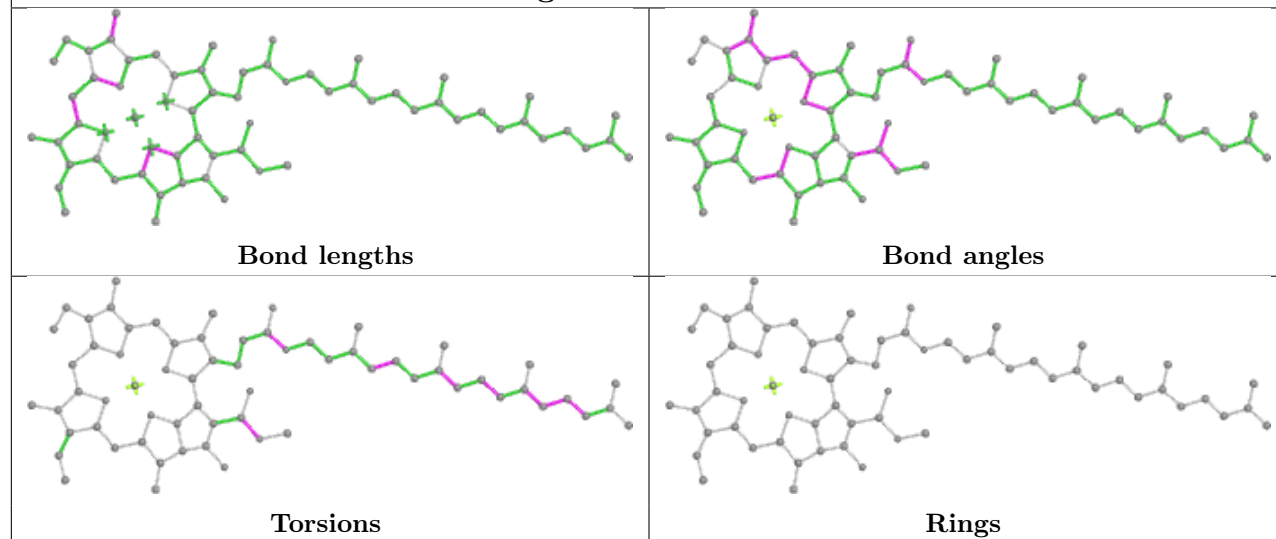


Torsions

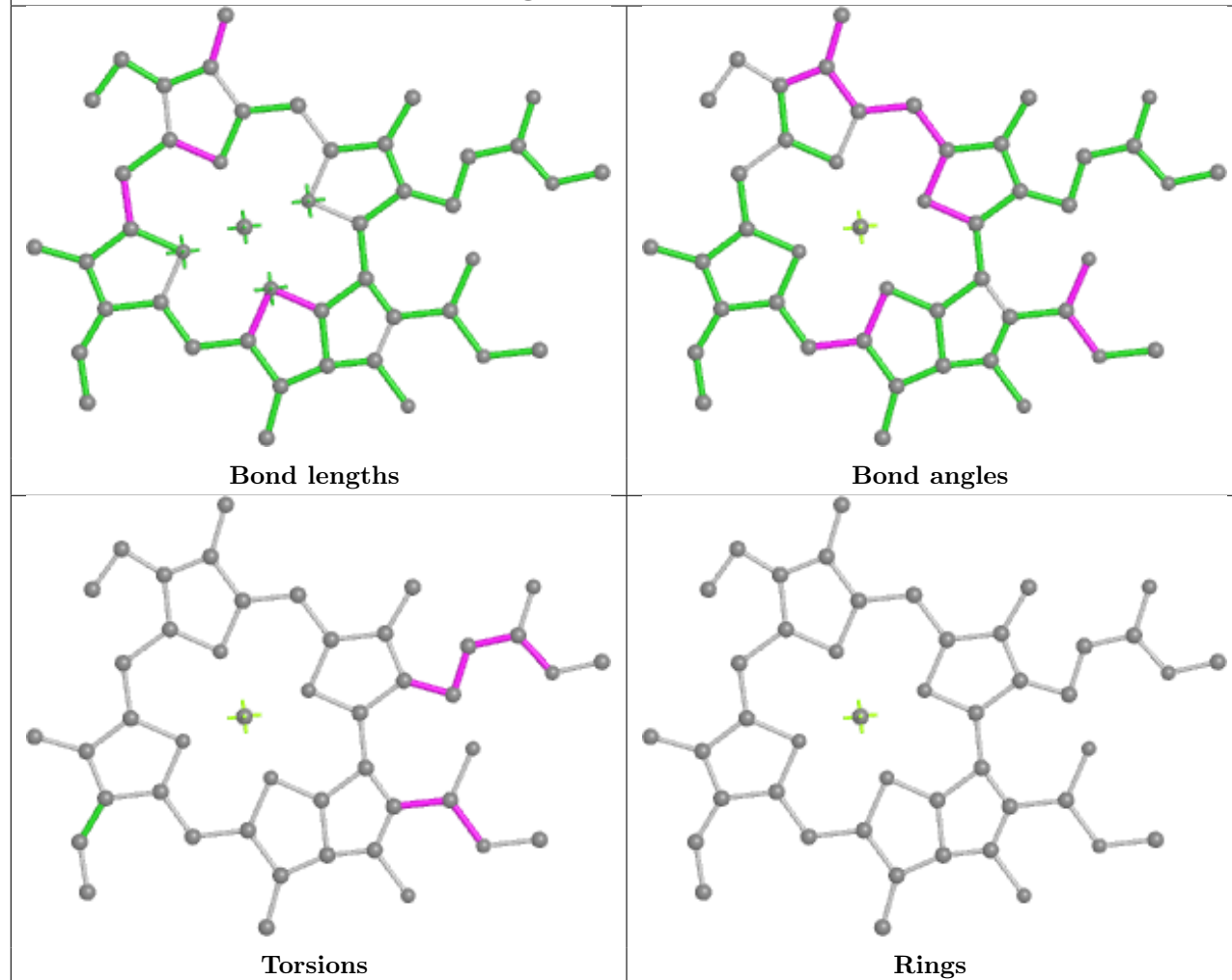


Rings

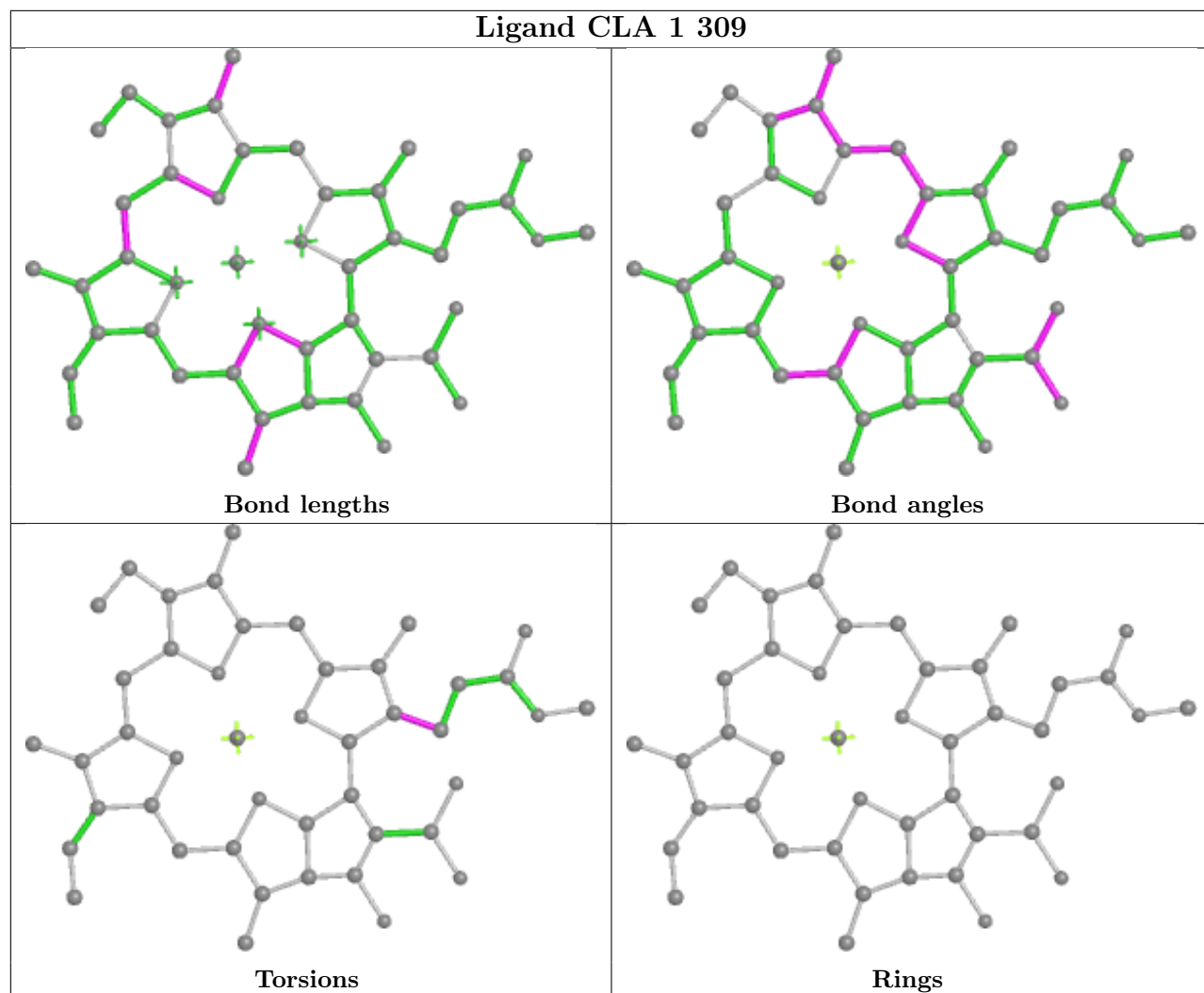
Ligand CLA c 602



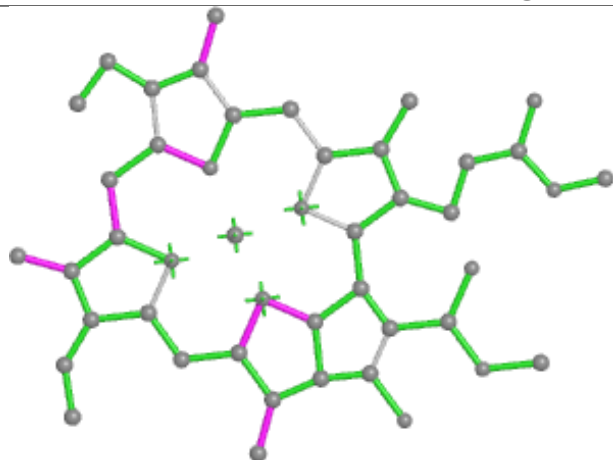
Ligand CLA t 302



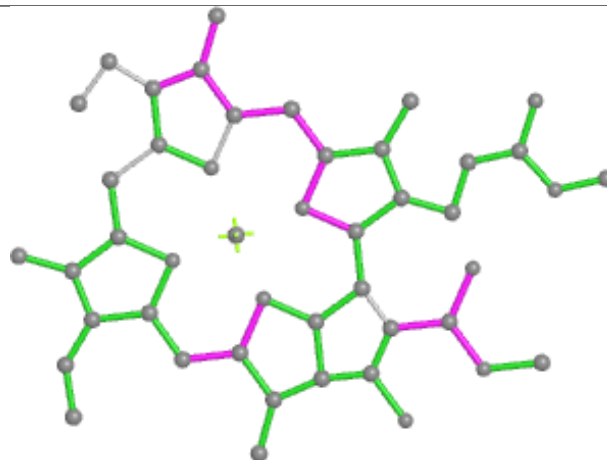
Ligand CLA 1 309



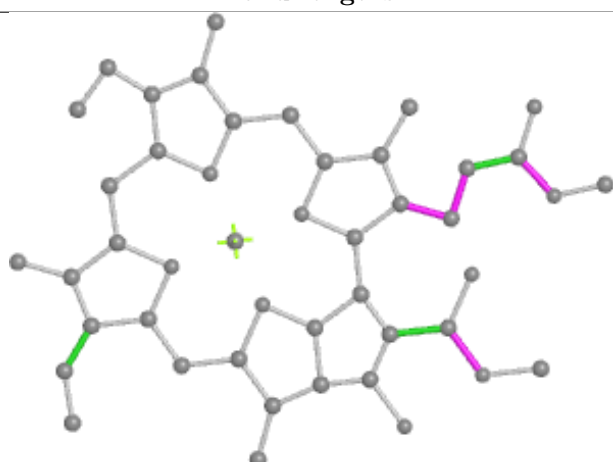
Ligand CLA 9 307



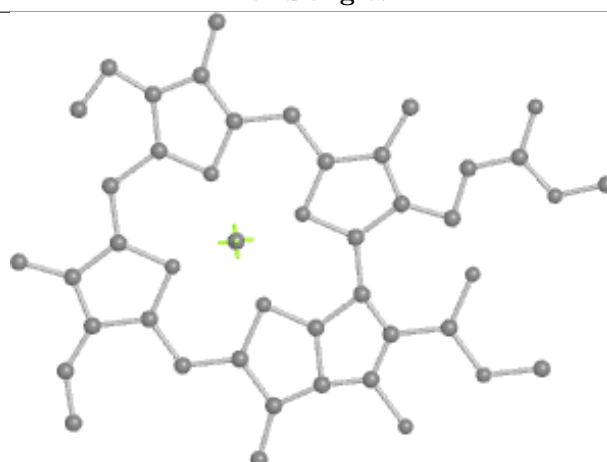
Bond lengths



Bond angles

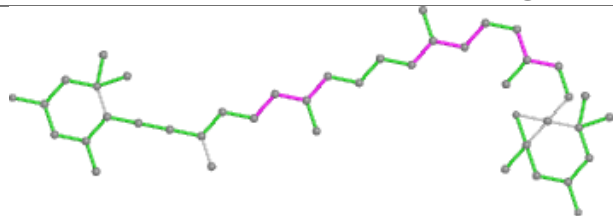


Torsions

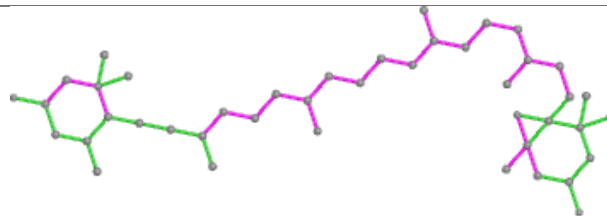


Rings

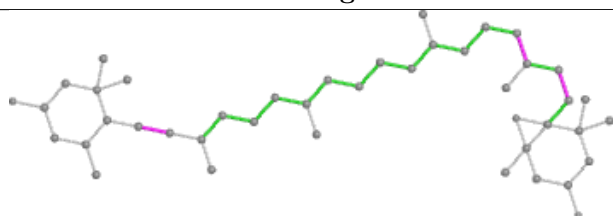
Ligand DD6 6 615



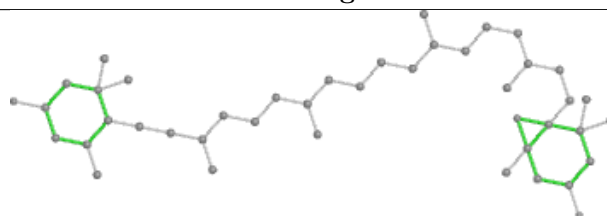
Bond lengths



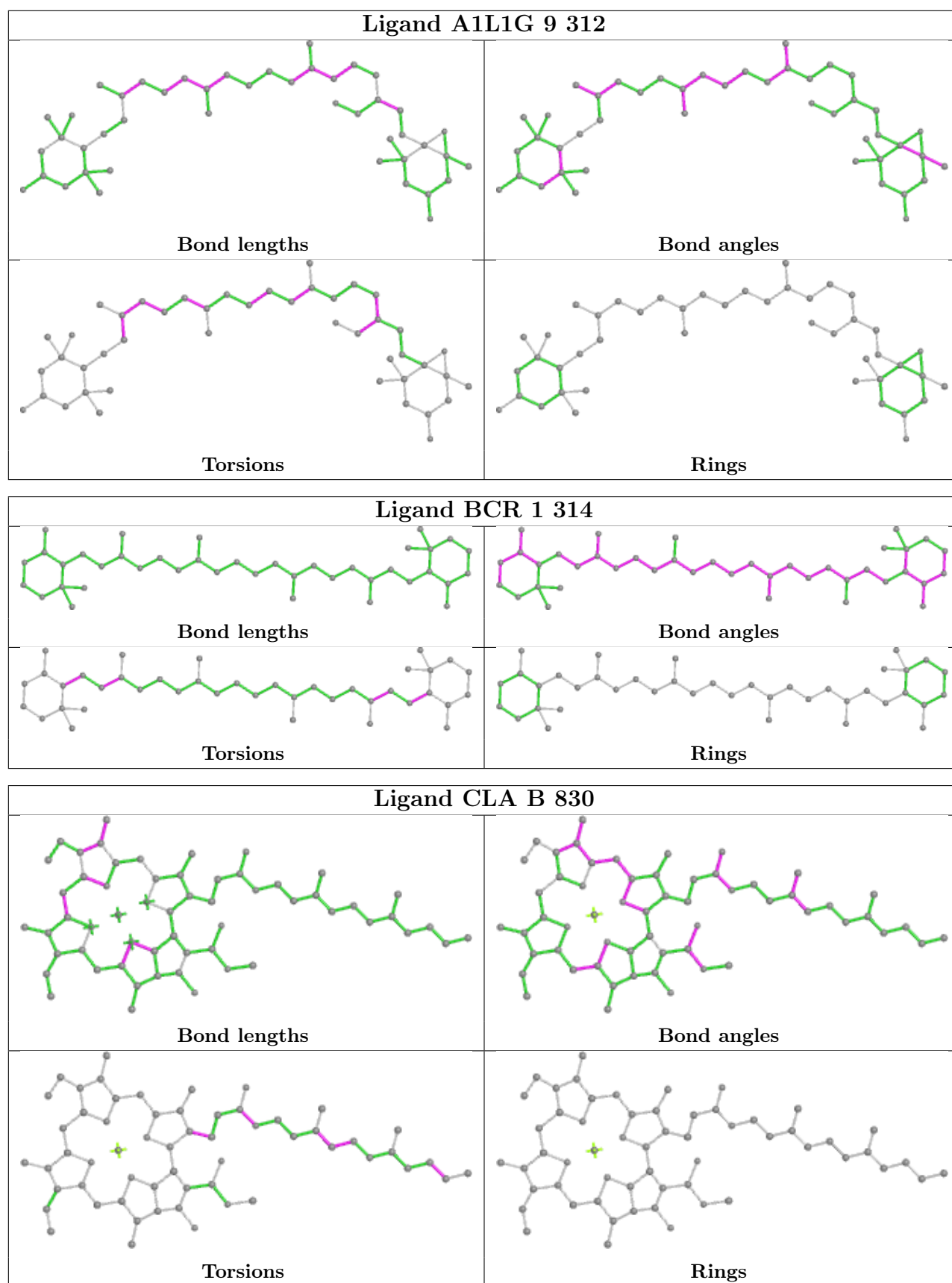
Bond angles



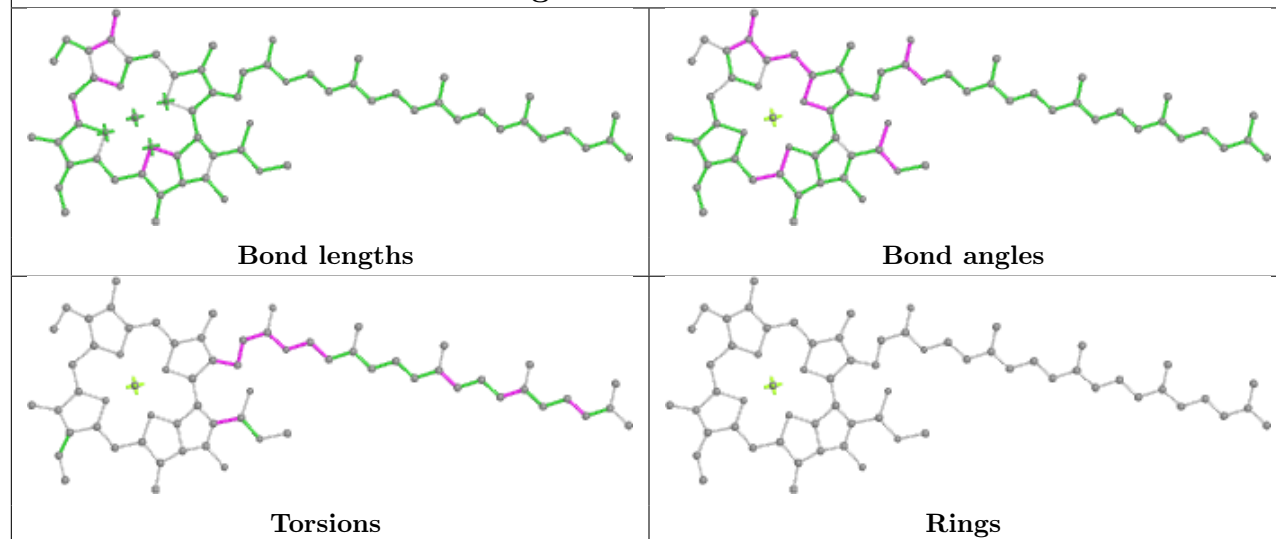
Torsions



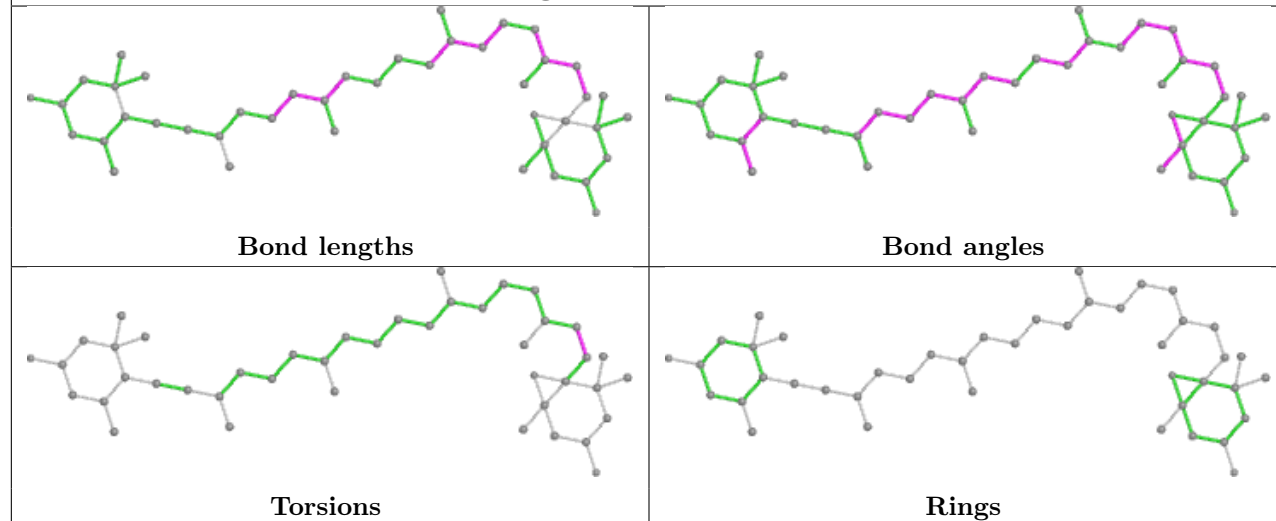
Rings



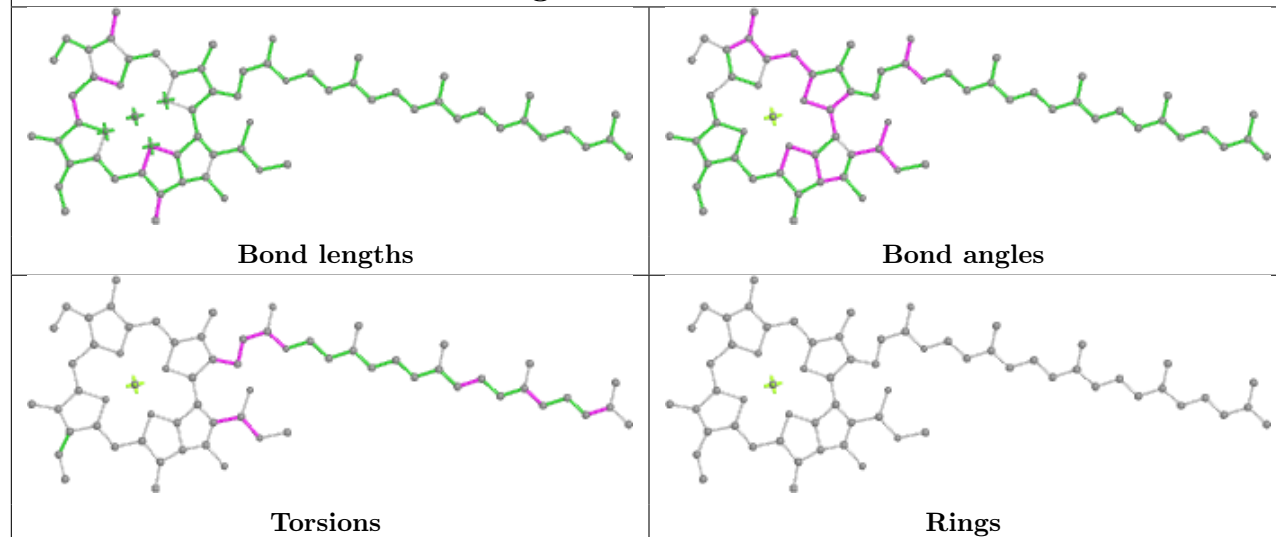
Ligand CLA A 804

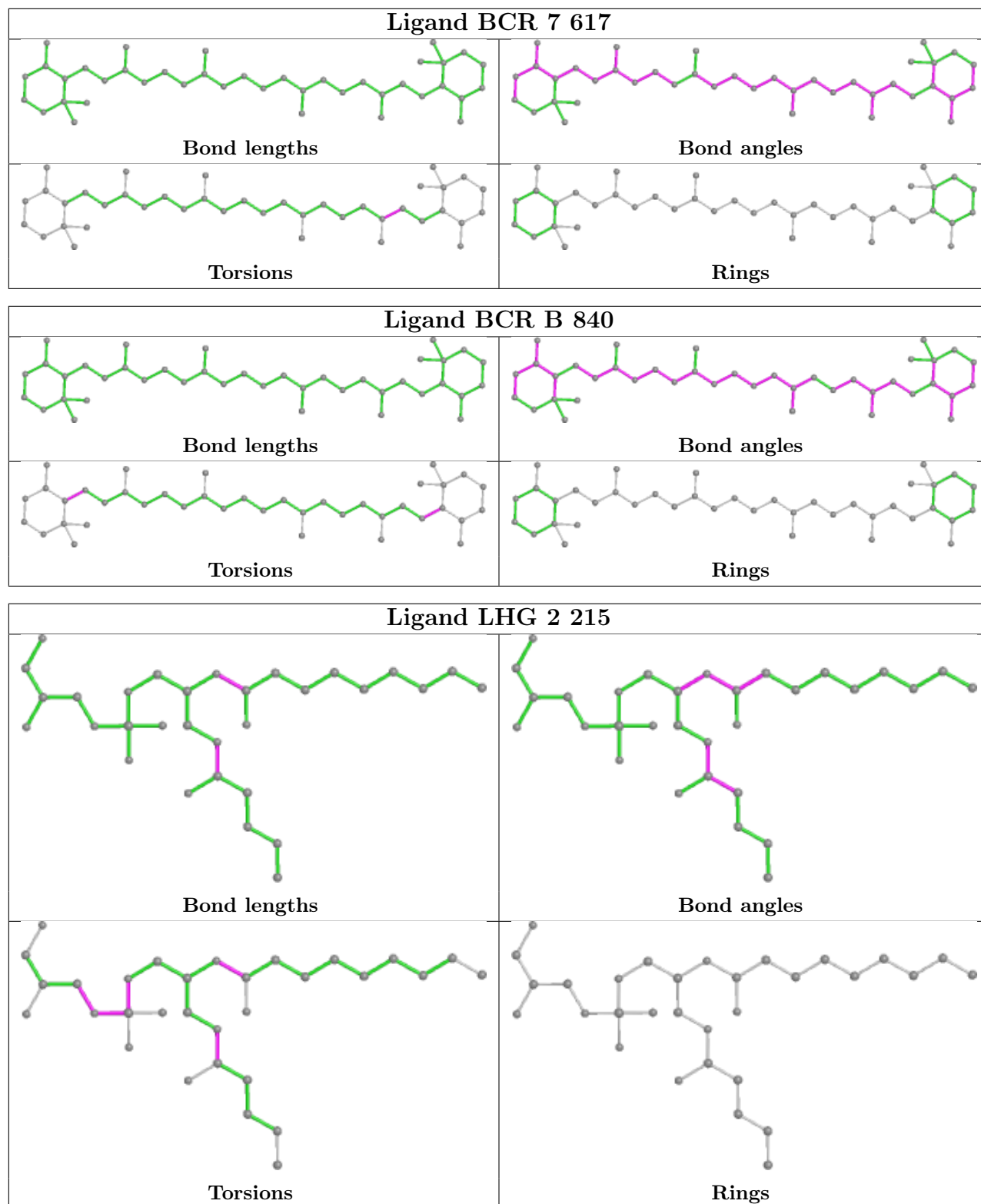


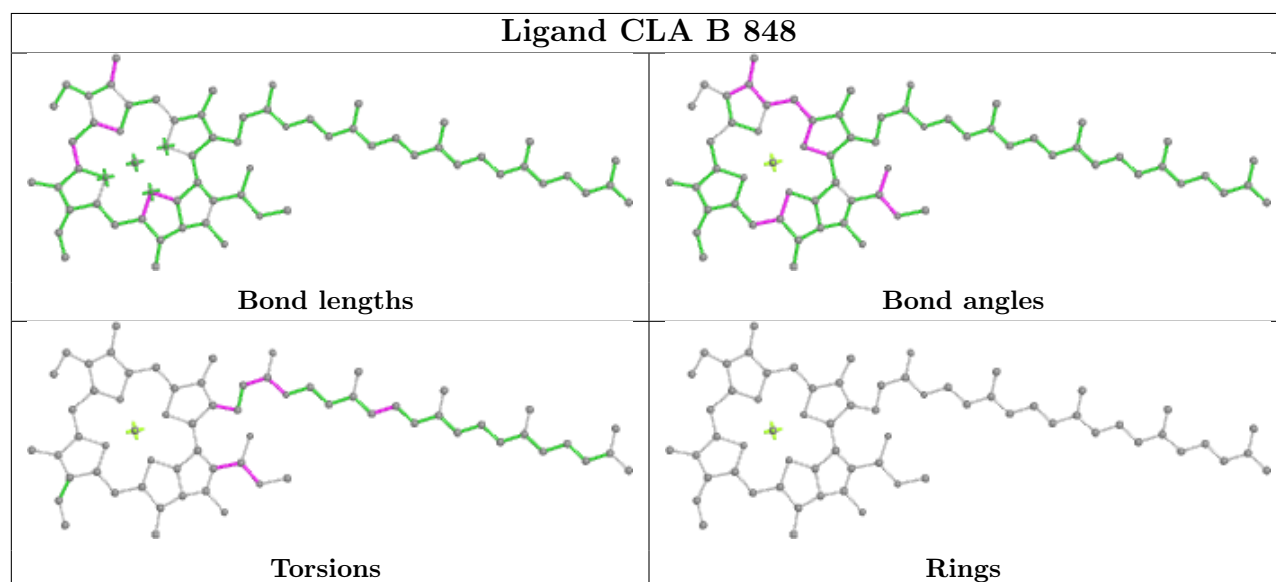
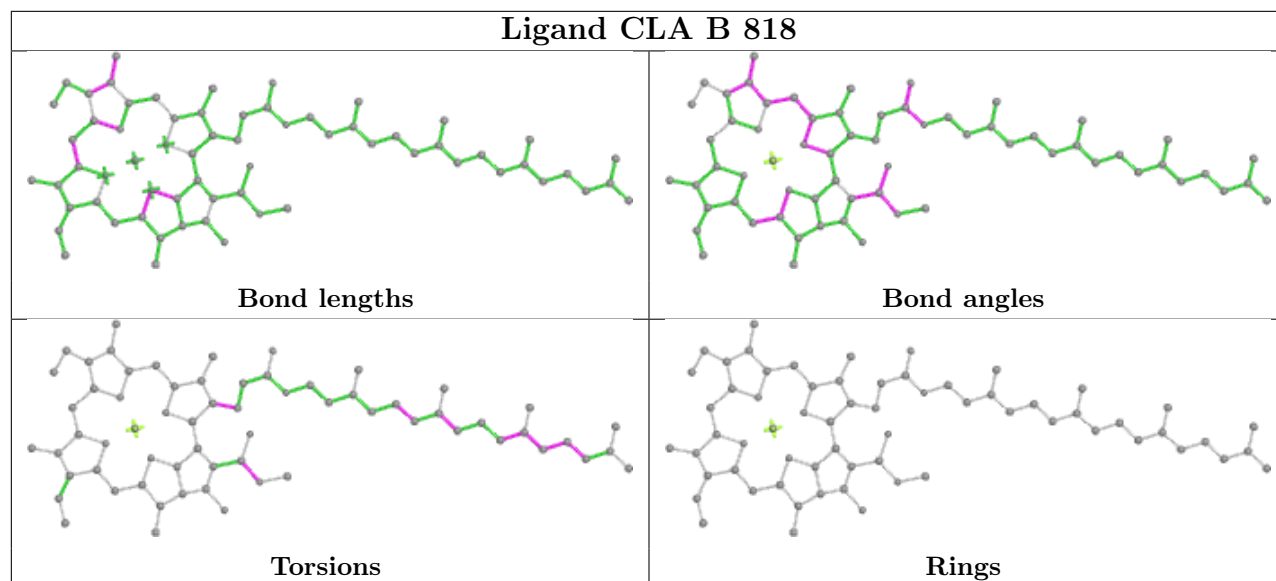
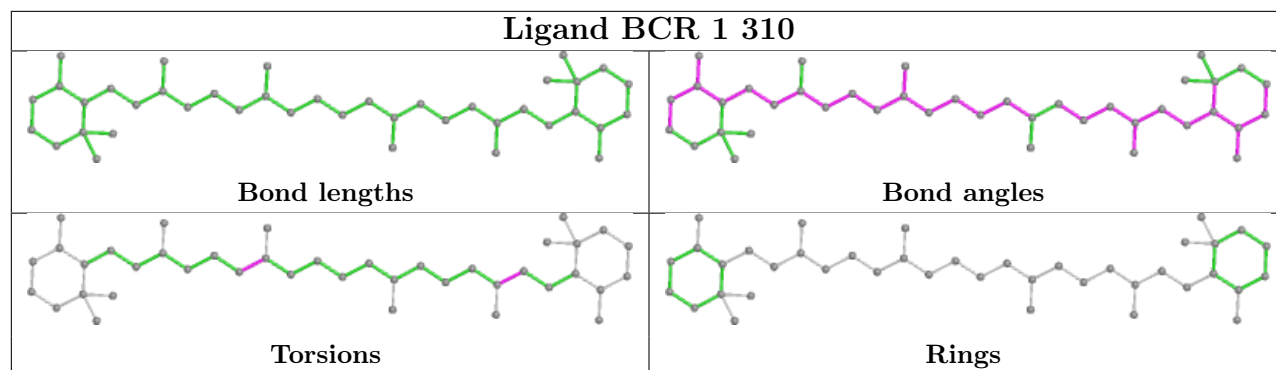
Ligand DD6 6 617



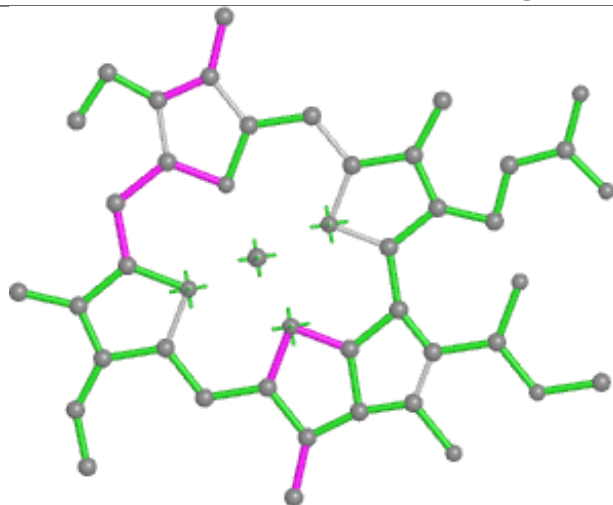
Ligand CLA A 801



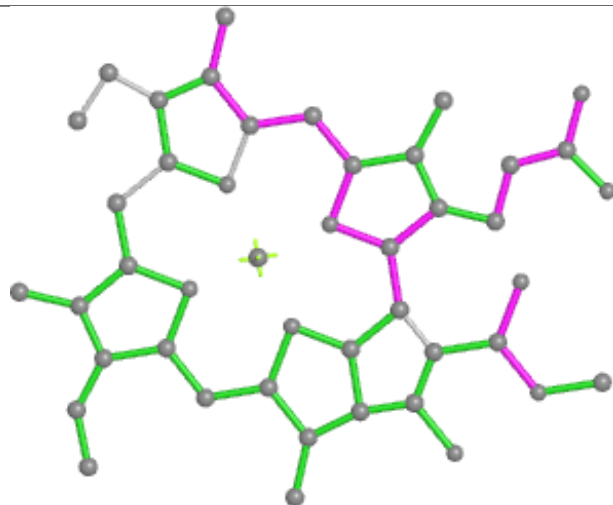




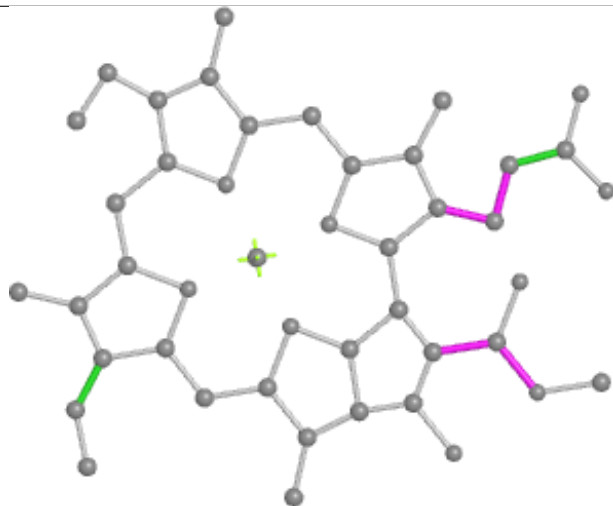
Ligand CLA 1 305



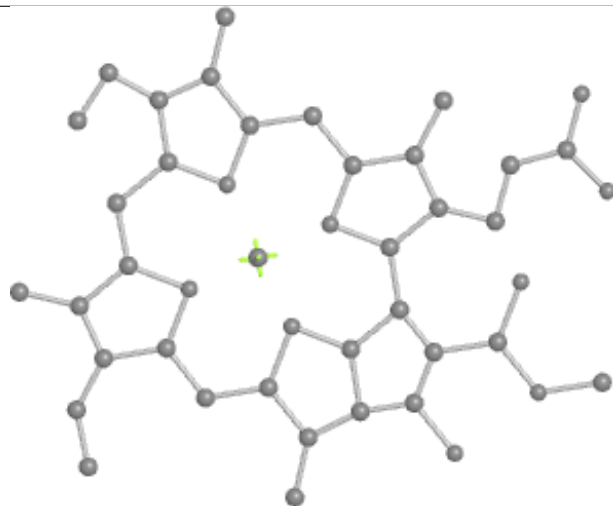
Bond lengths



Bond angles

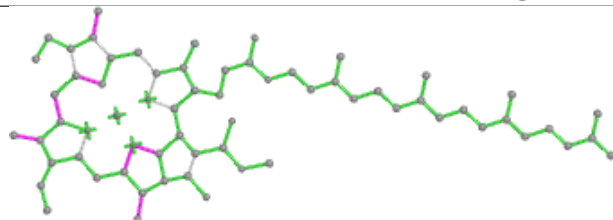


Torsions

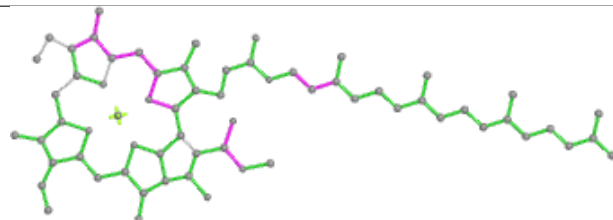


Rings

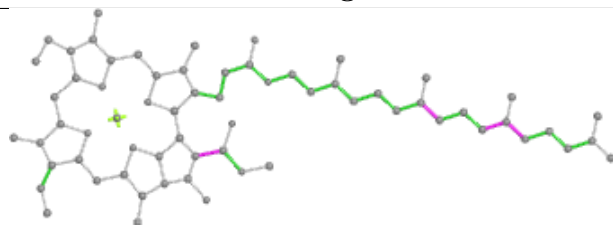
Ligand CLA A 802



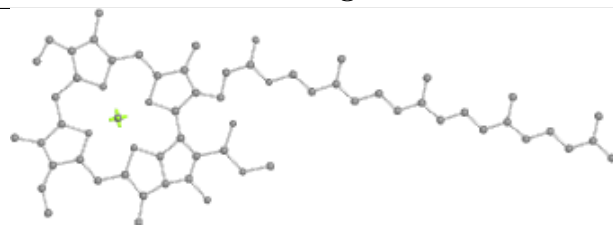
Bond lengths



Bond angles

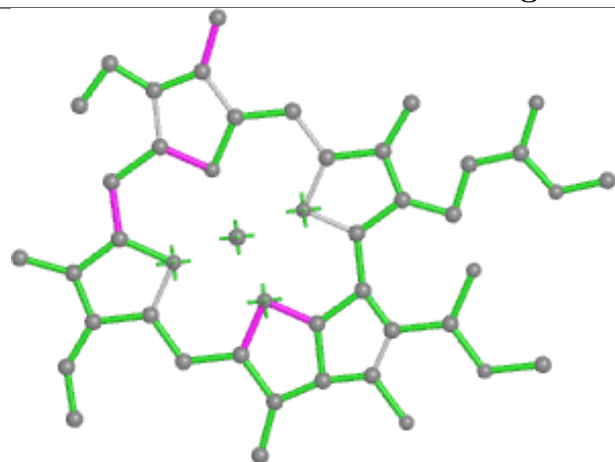


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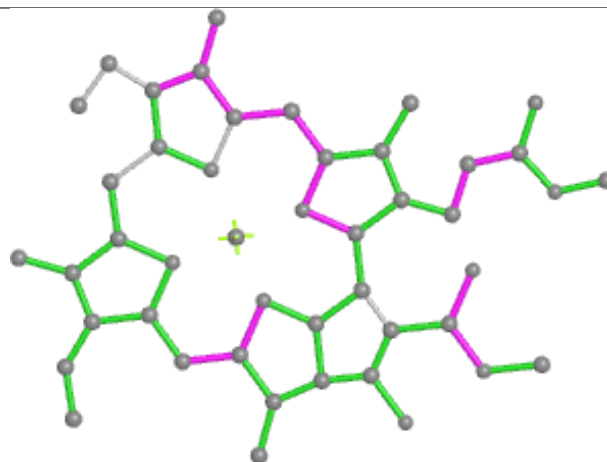


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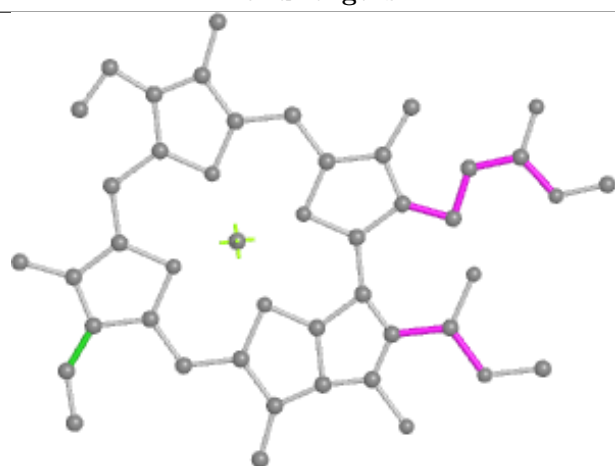
Ligand CLA 9 305



Bond lengths



Bond angles

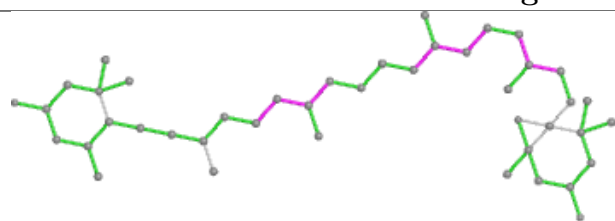


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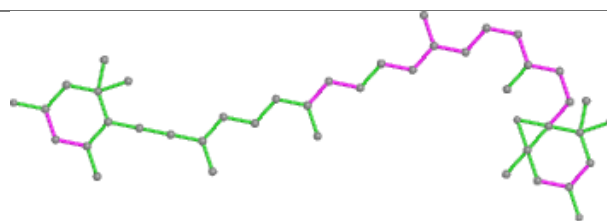


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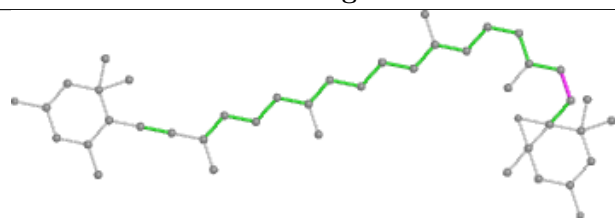
Ligand DD6 5 609



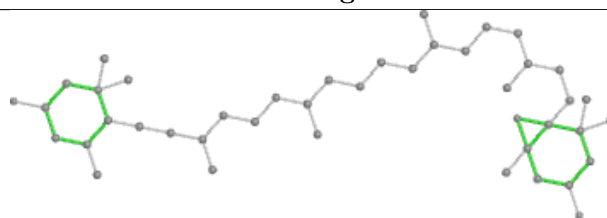
Bond lengths



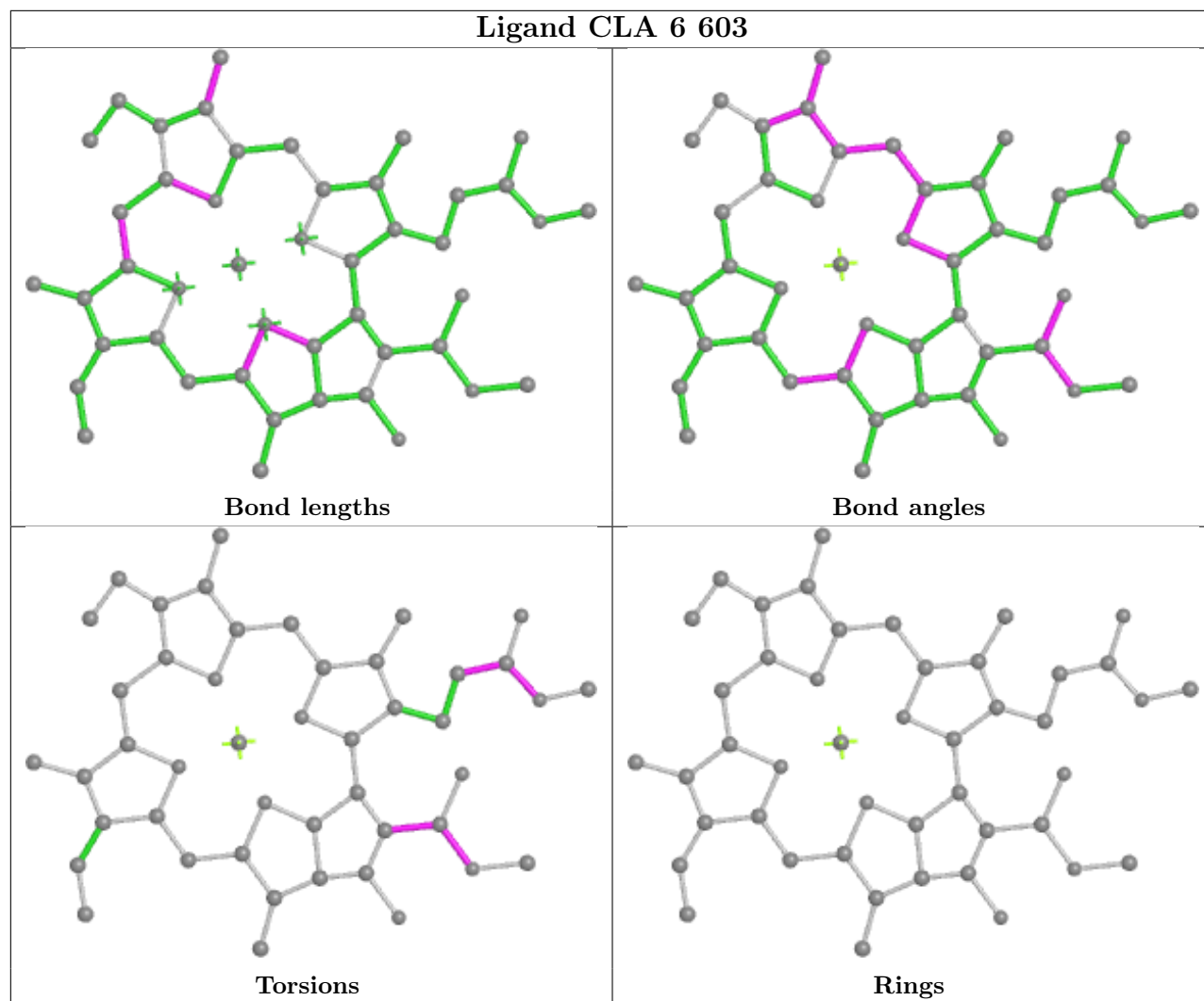
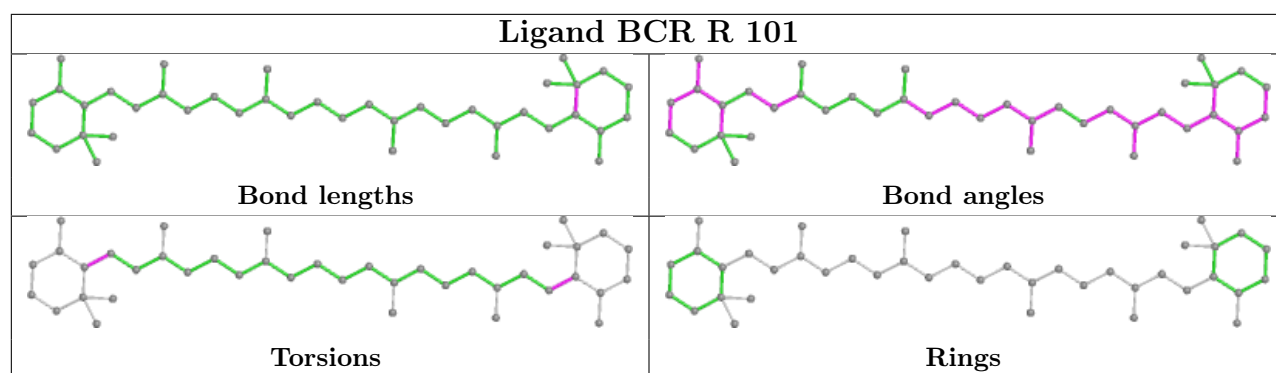
Bond angles



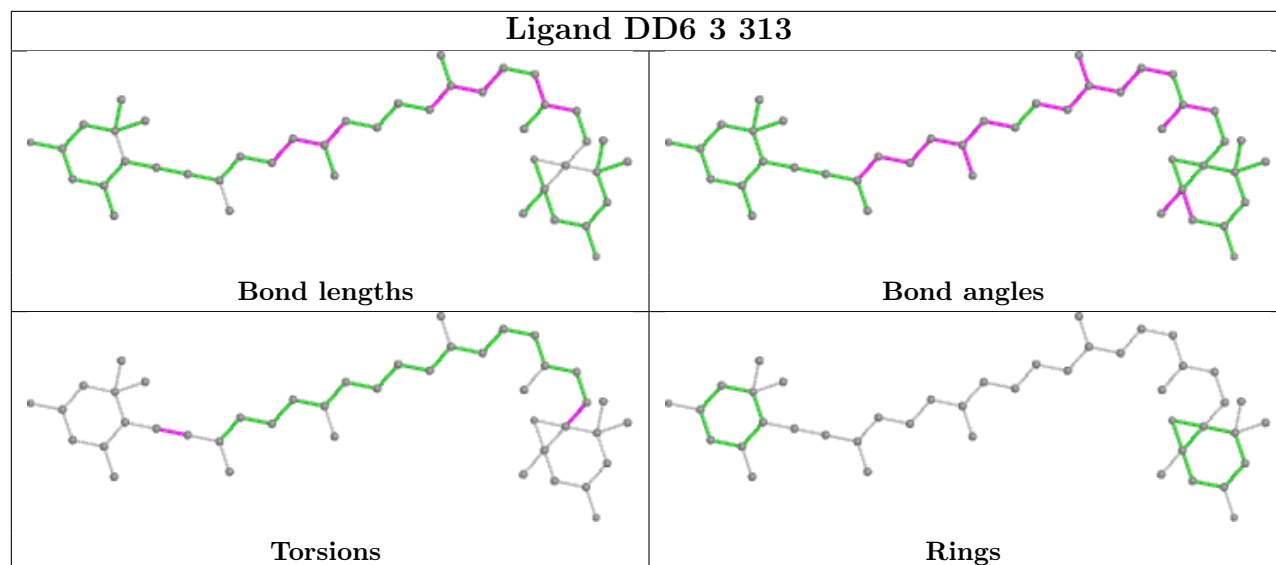
Torsions



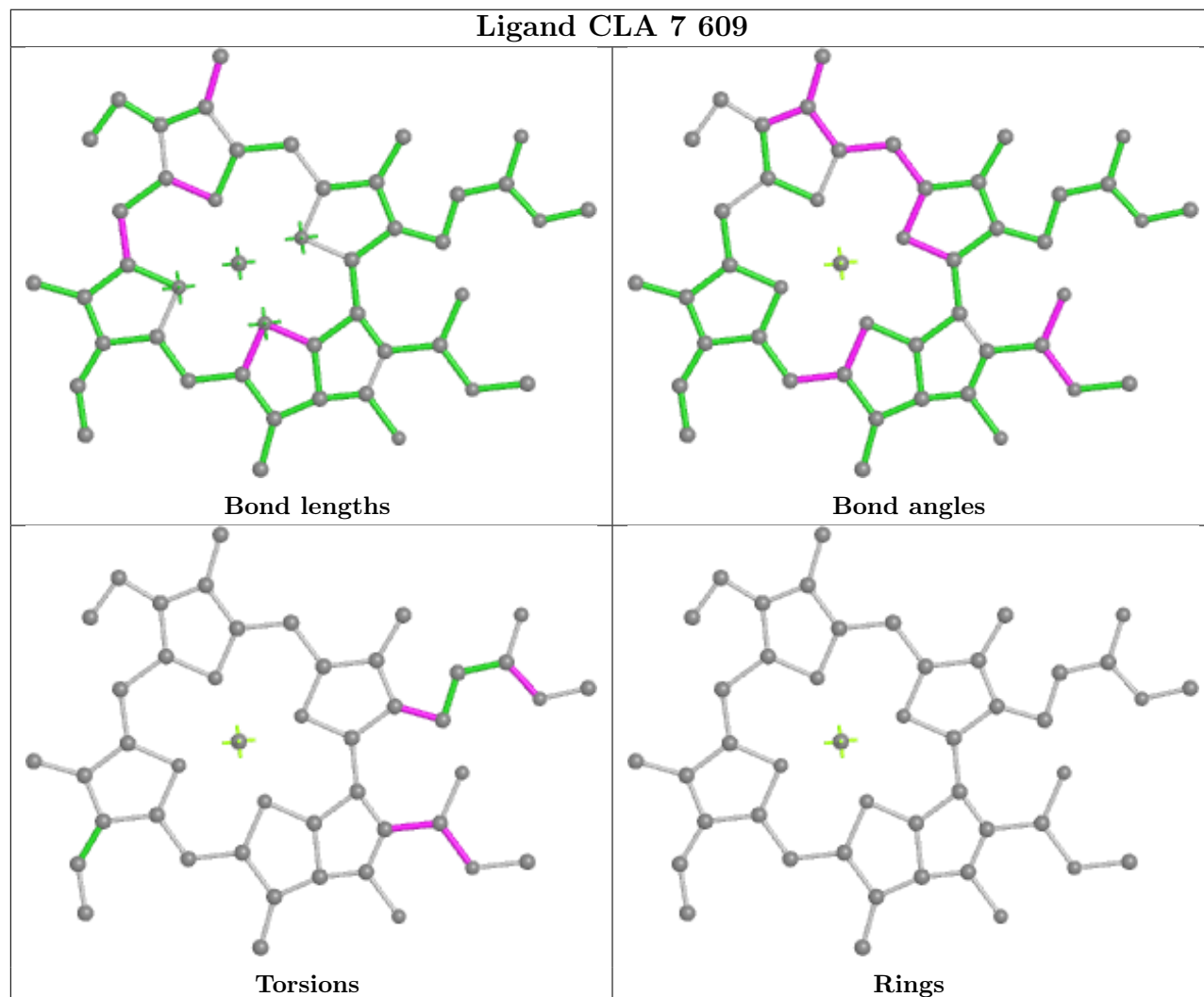
Rings



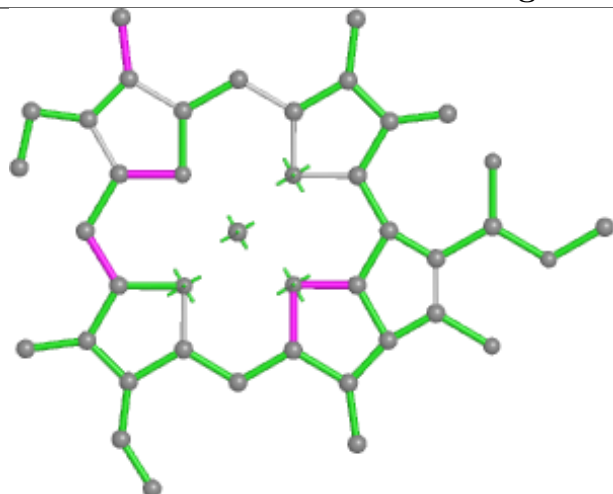
Ligand DD6 3 313



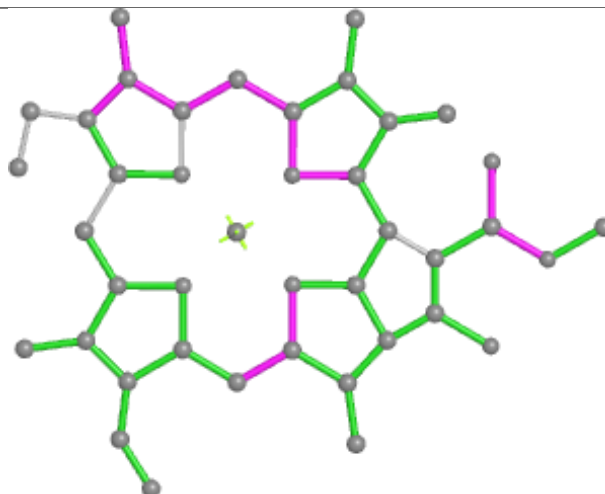
Ligand CLA 7 609



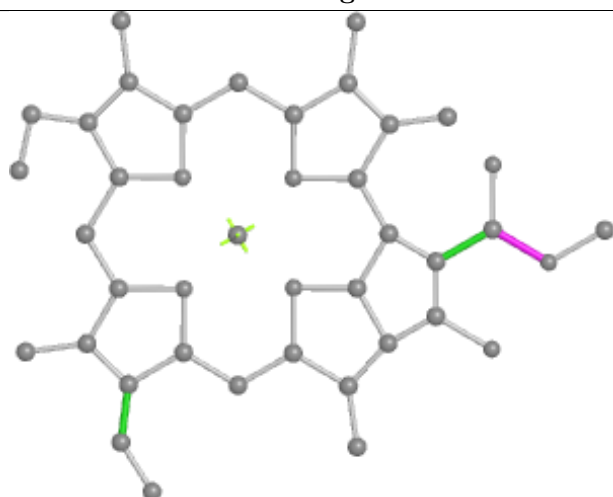
Ligand CLA 4 610



Bond lengths



Bond angles

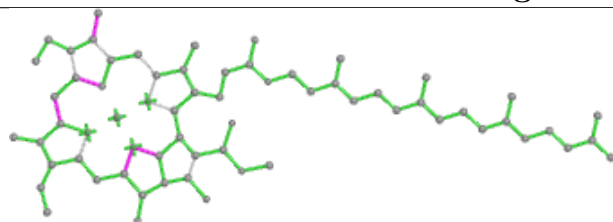


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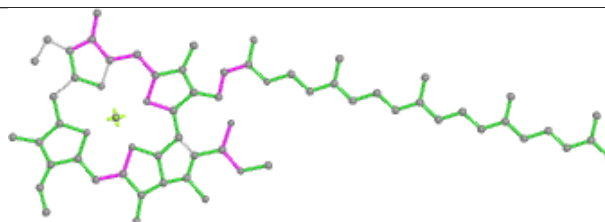


Rings

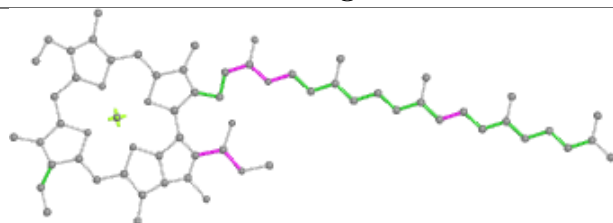
Ligand CLA A 808



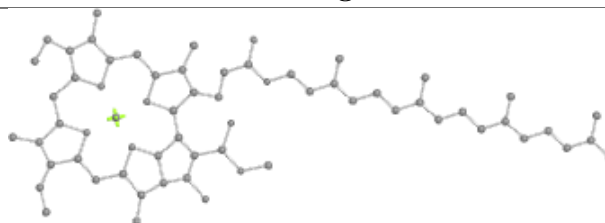
Bond lengths



Bond angles

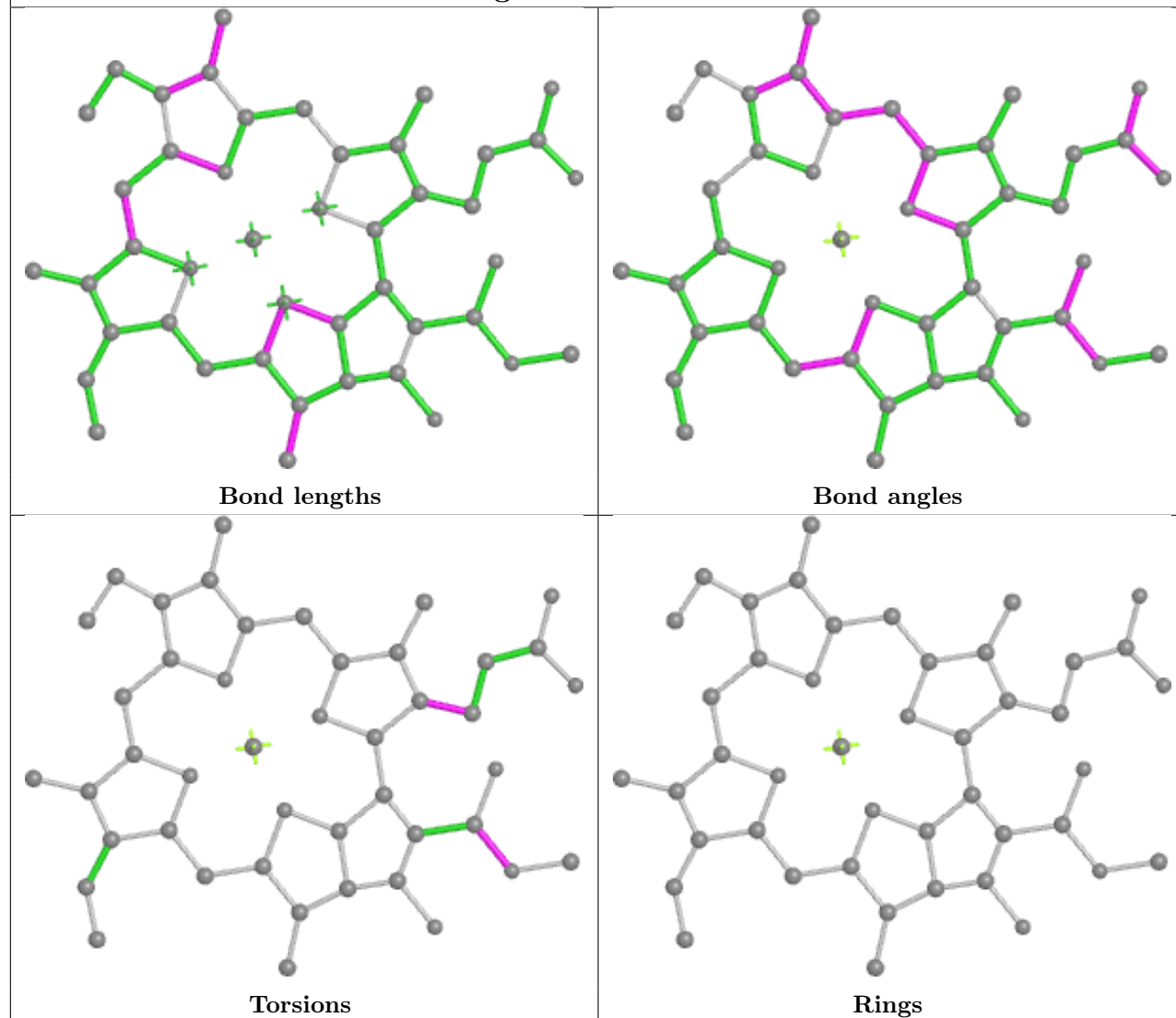


Torsions

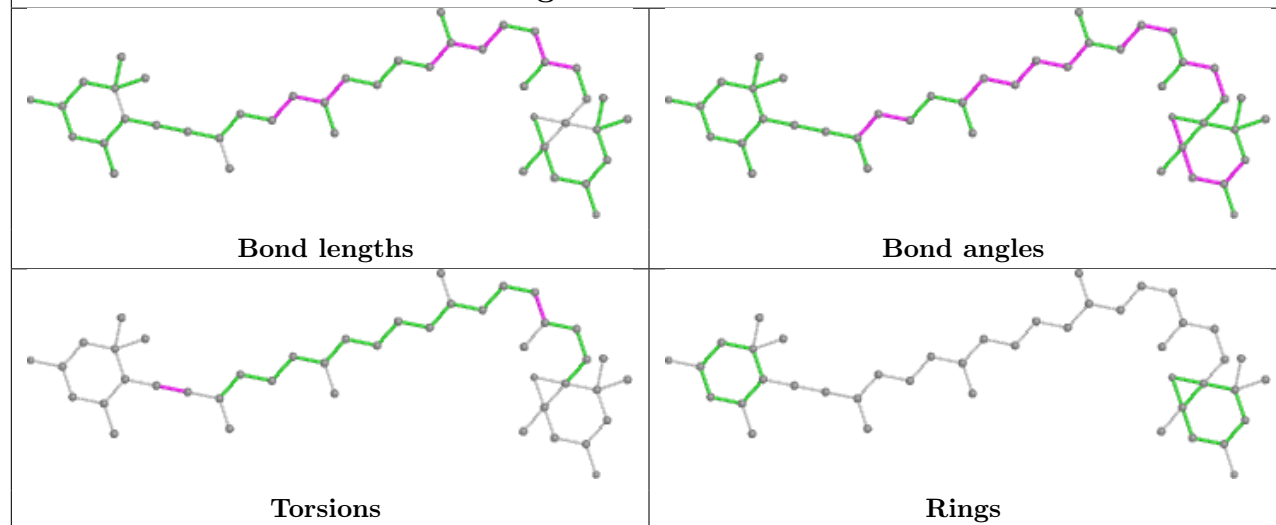


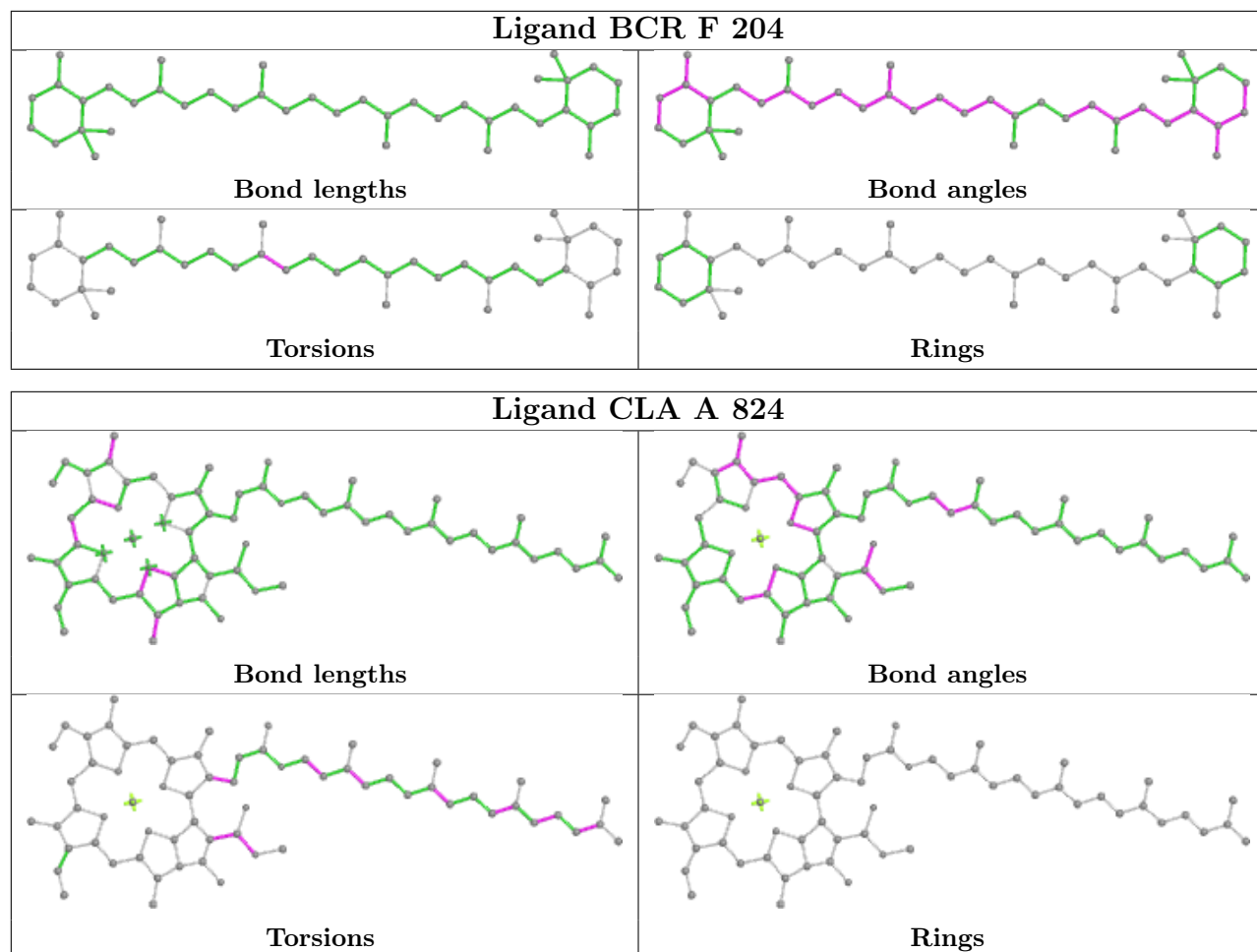
Rings

Ligand CLA 8 204

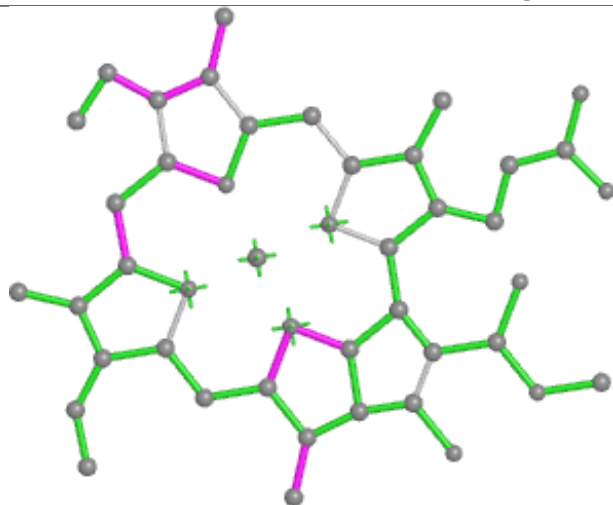


Ligand DD6 9 313

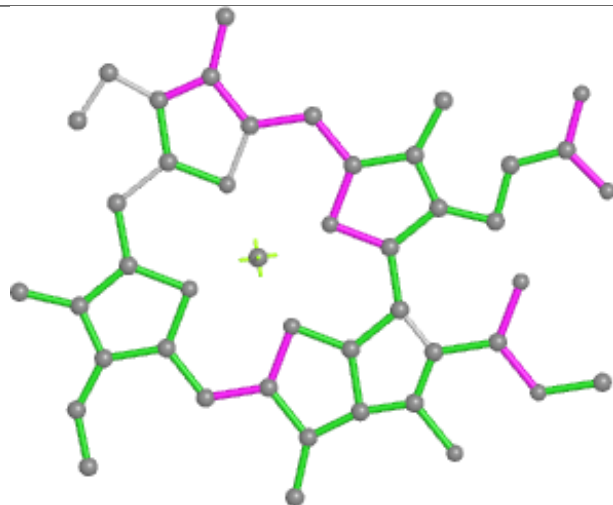




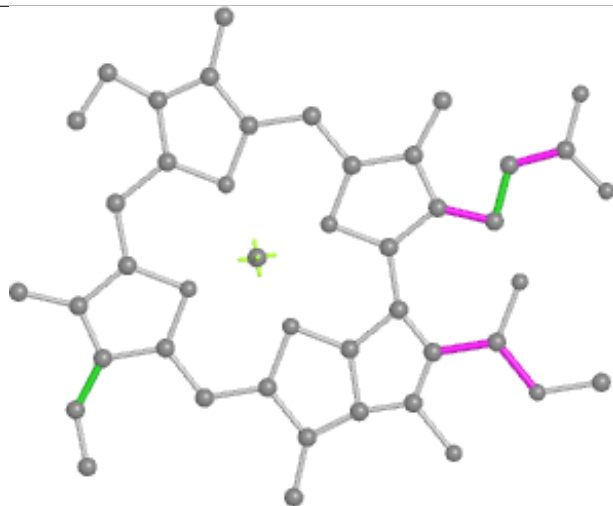
Ligand CLA 1 302



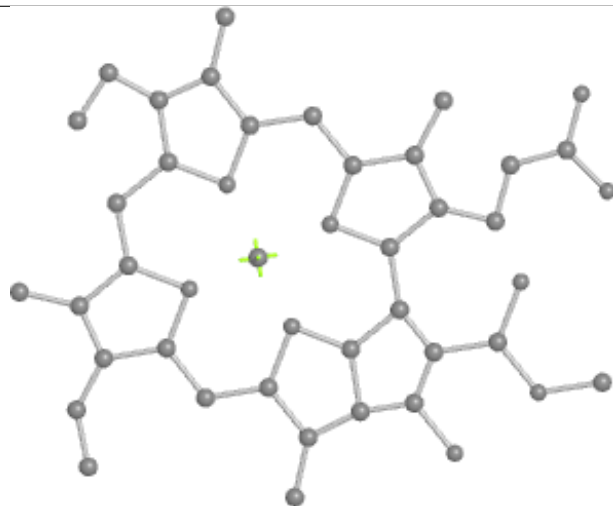
Bond lengths



Bond angles

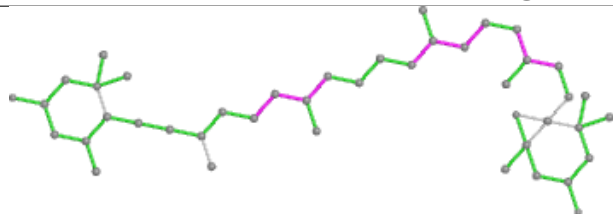


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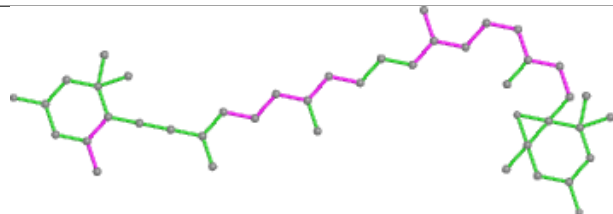


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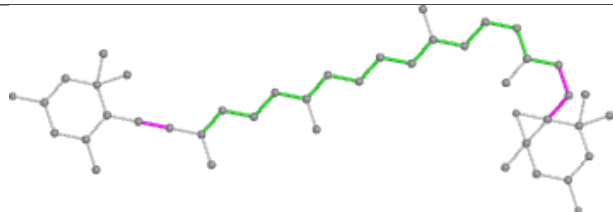
Ligand DD6 h 615



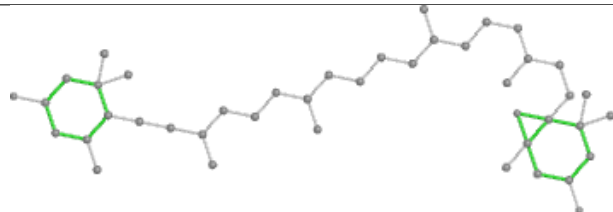
Bond lengths



Bond angles

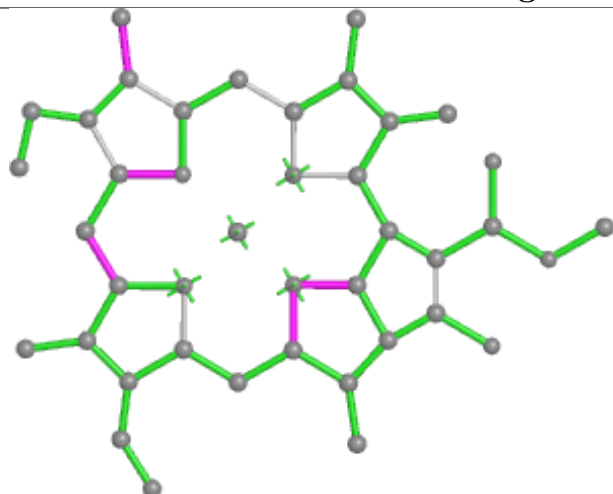


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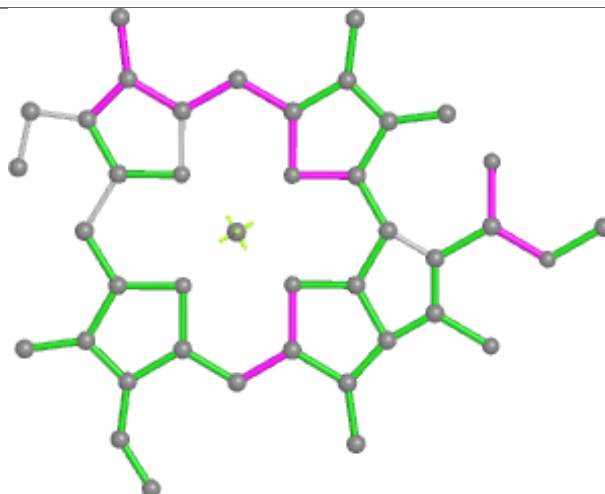


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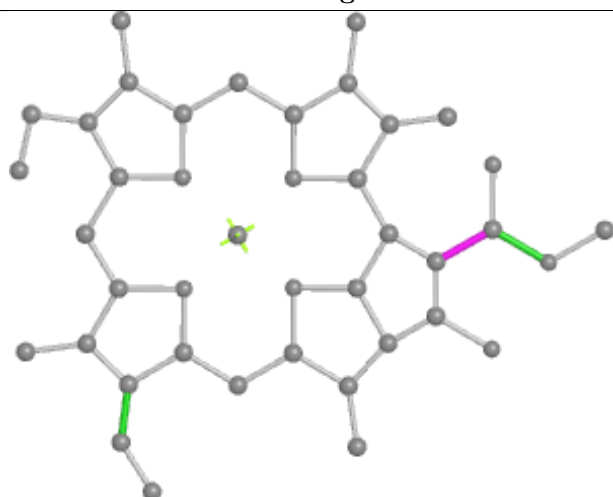
Ligand CLA 3 309



Bond lengths



Bond angles

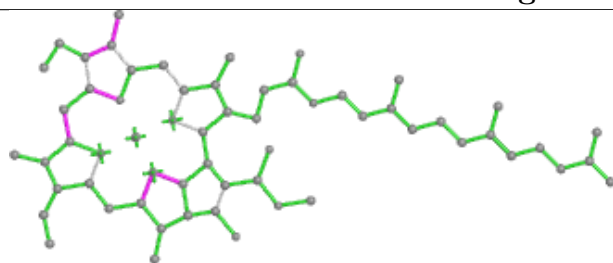


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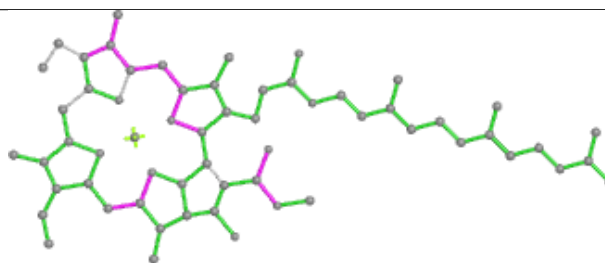


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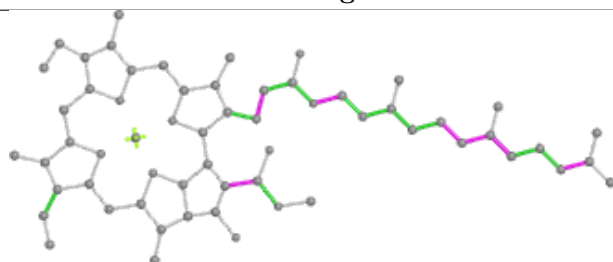
Ligand CLA 2 204



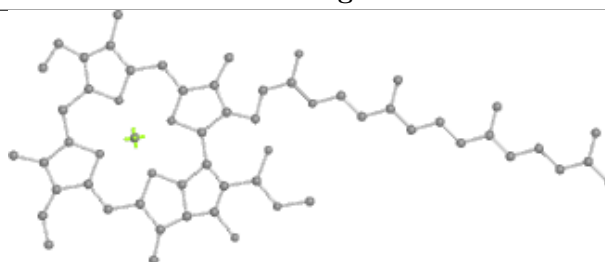
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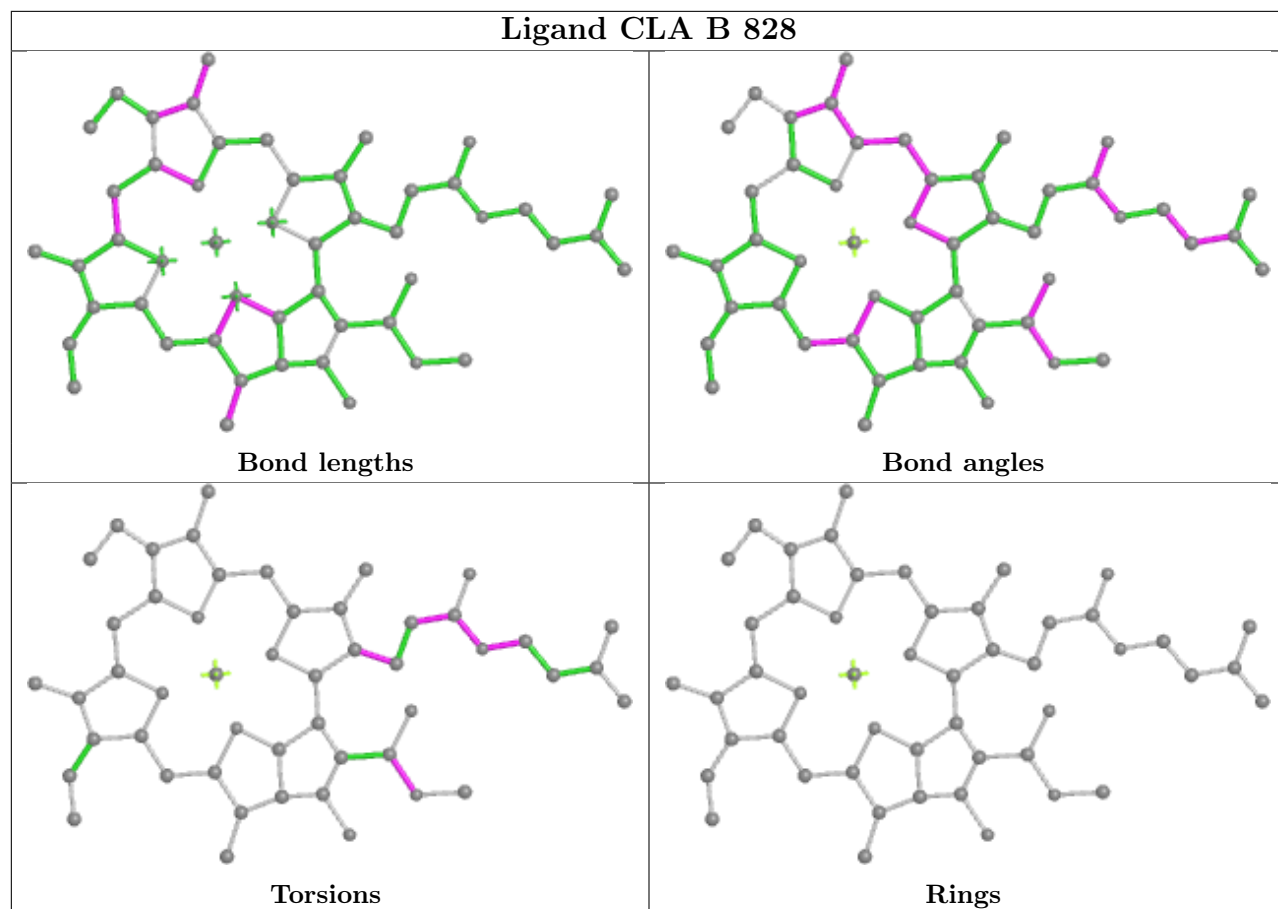
Bond angles



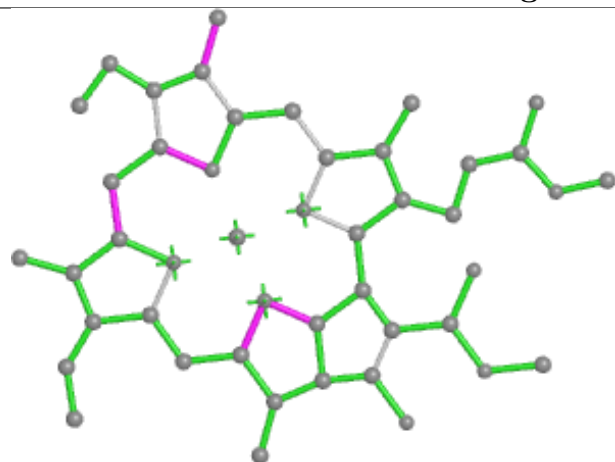
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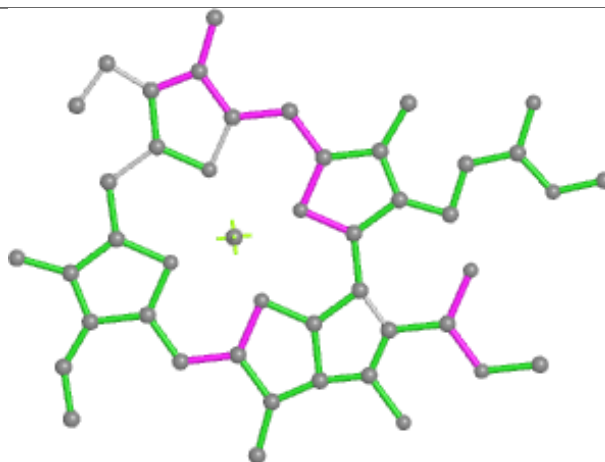
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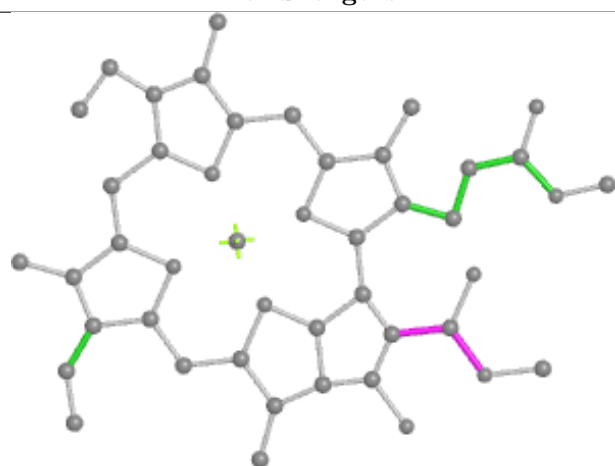
Ligand CLA 6 608



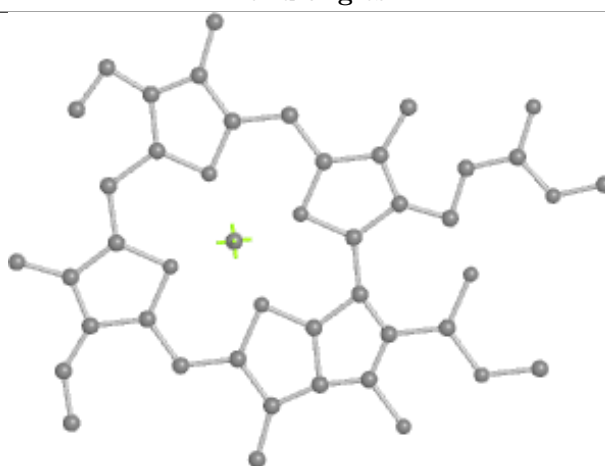
Bond lengths



Bond angles

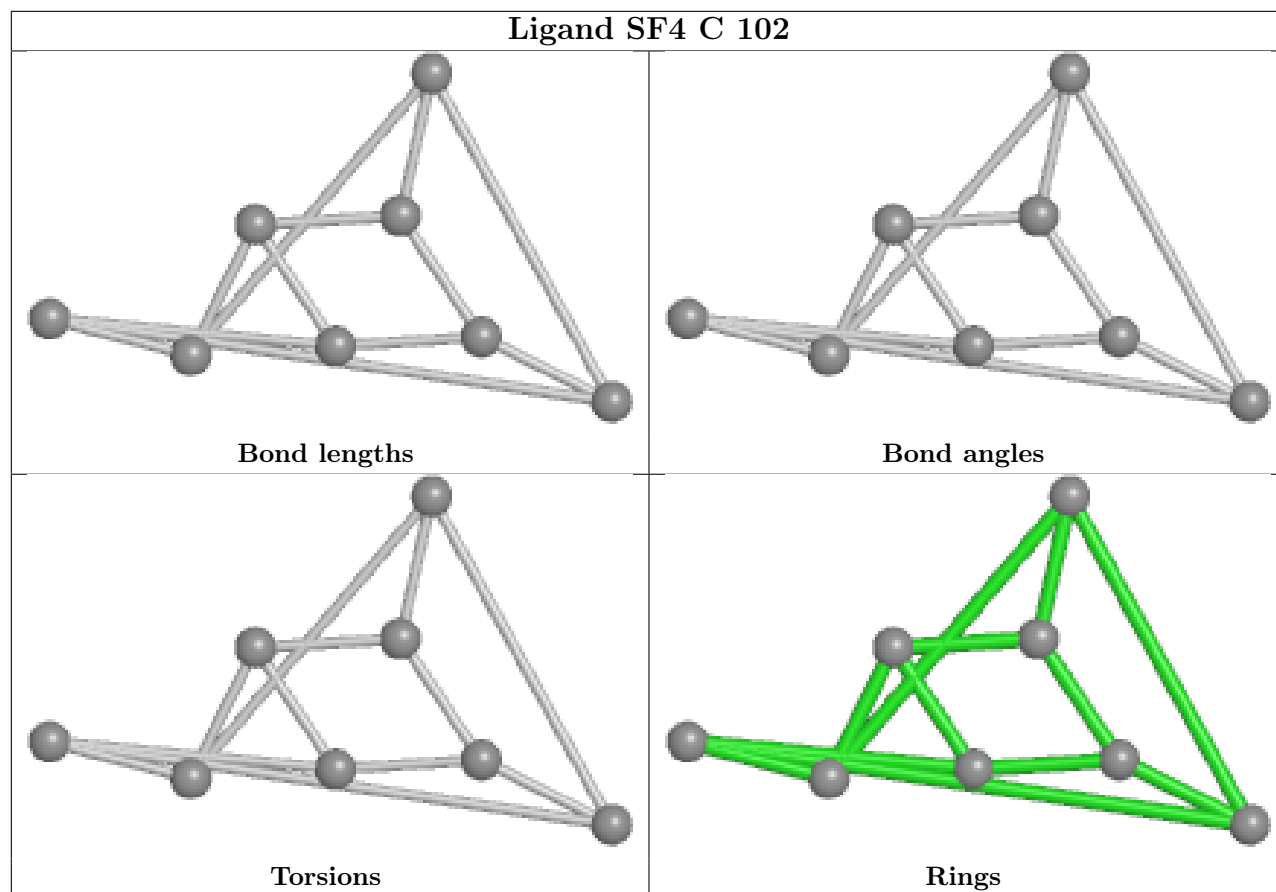


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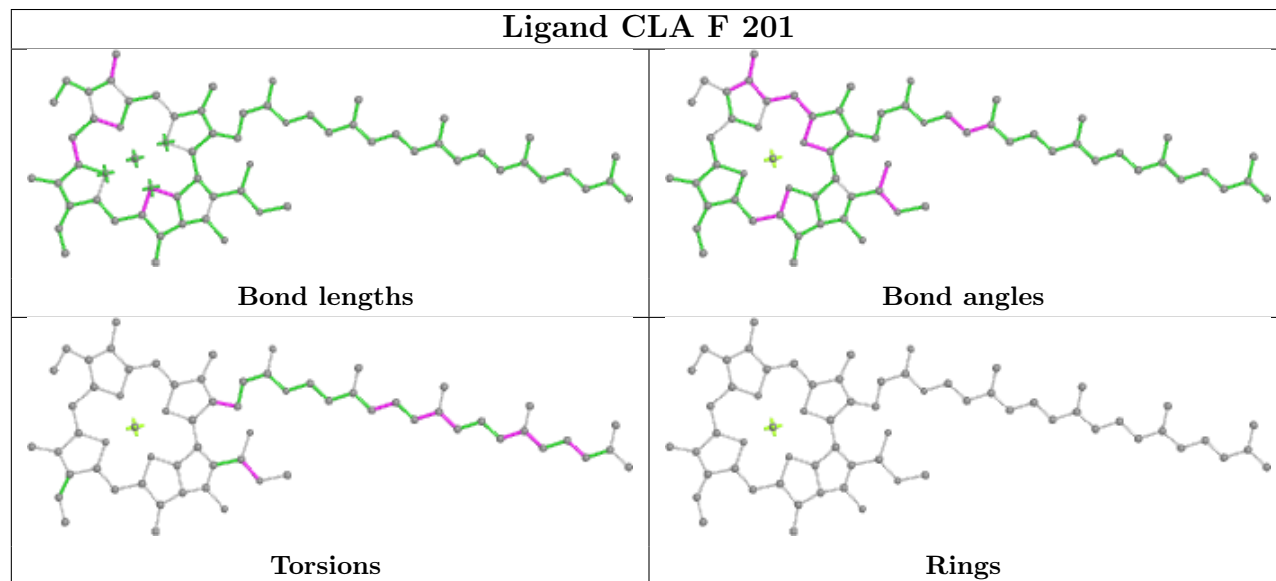


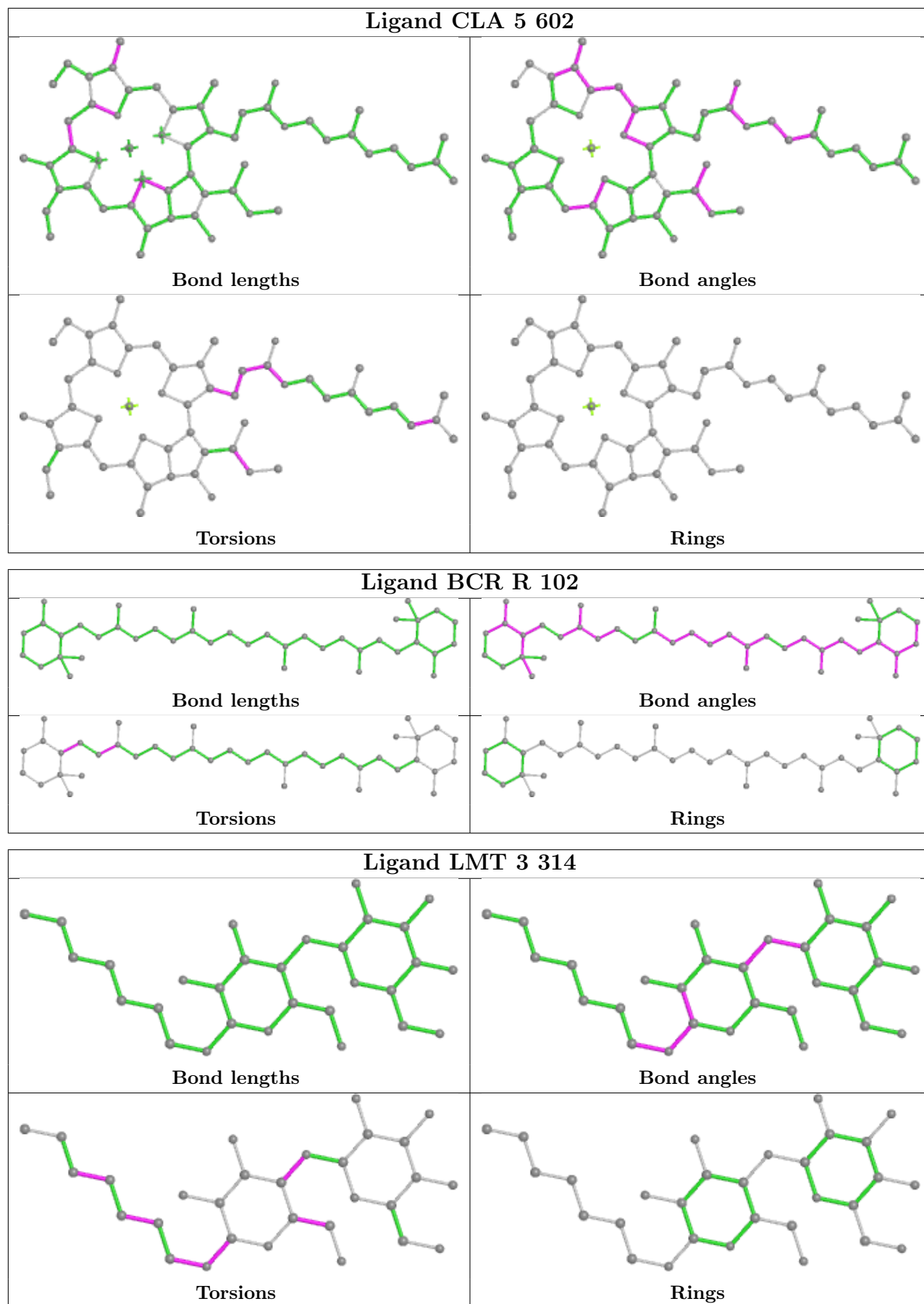
Rings

Ligand SF4 C 102

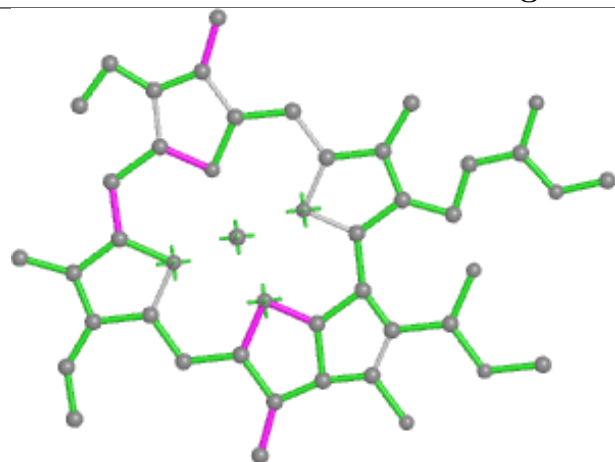


Ligand CLA F 201

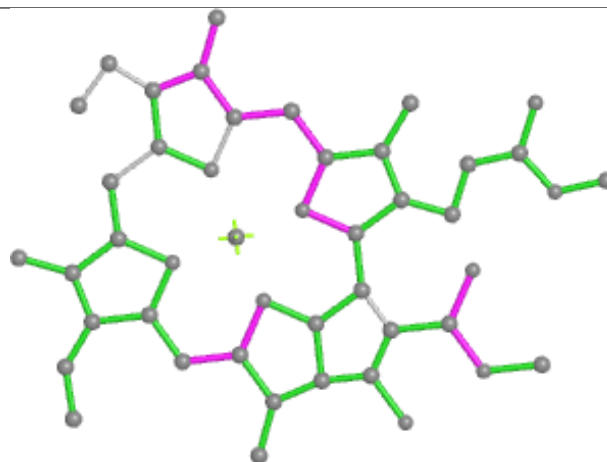




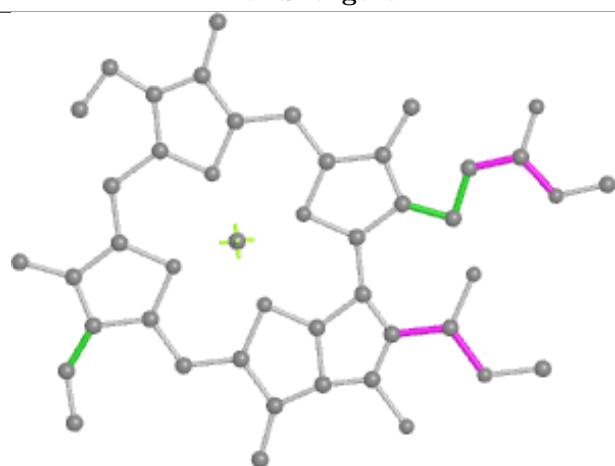
Ligand CLA 9 301



Bond lengths



Bond angles

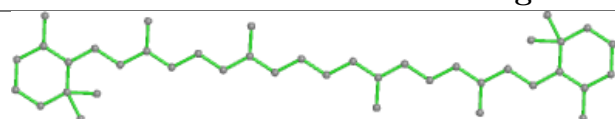


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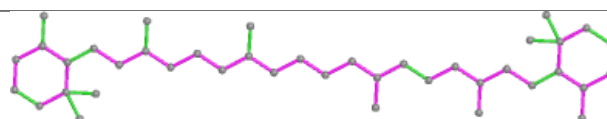


Rings

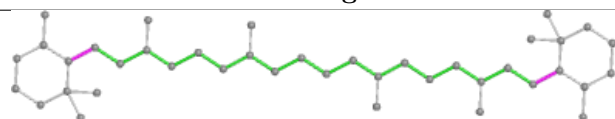
Ligand BCR B 849



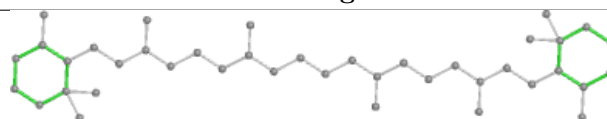
Bond lengths



Bond angles

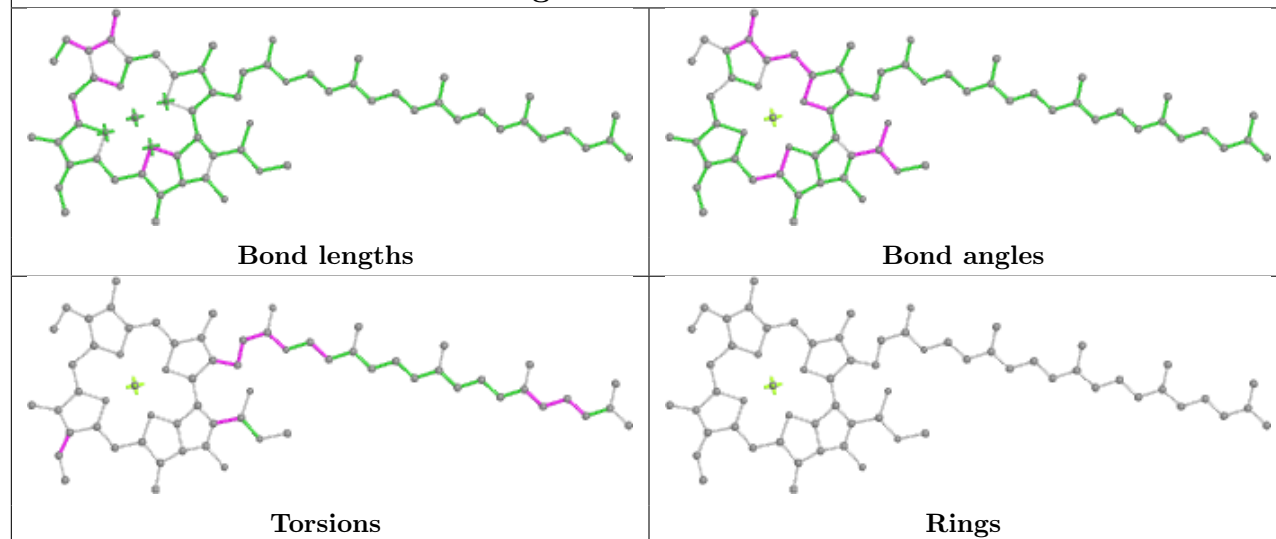


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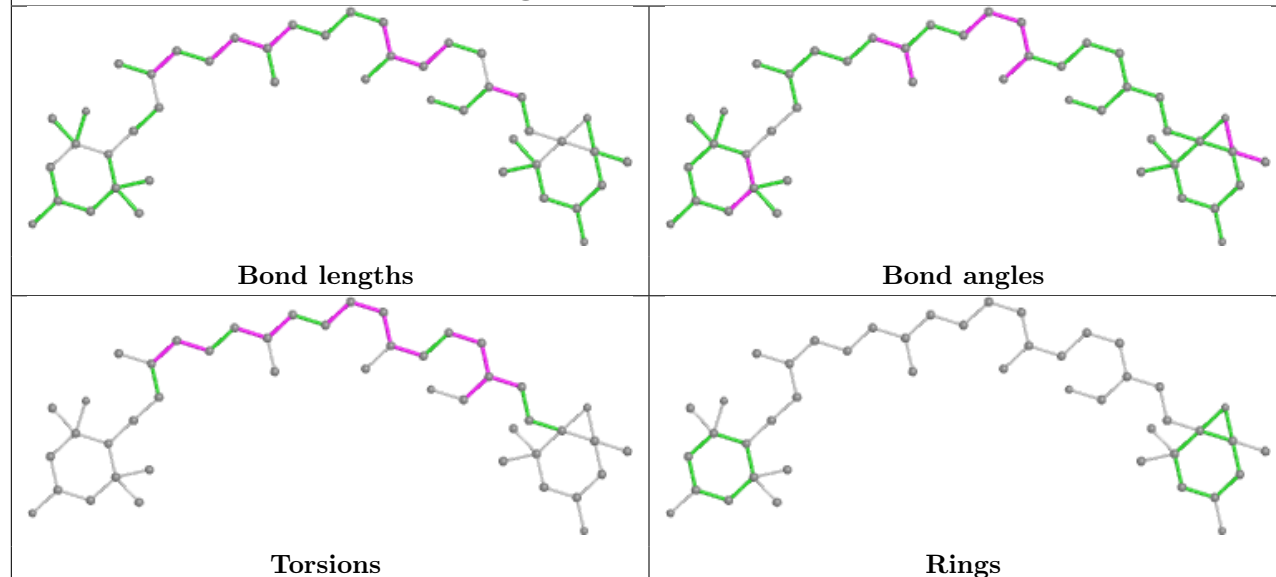


Rings

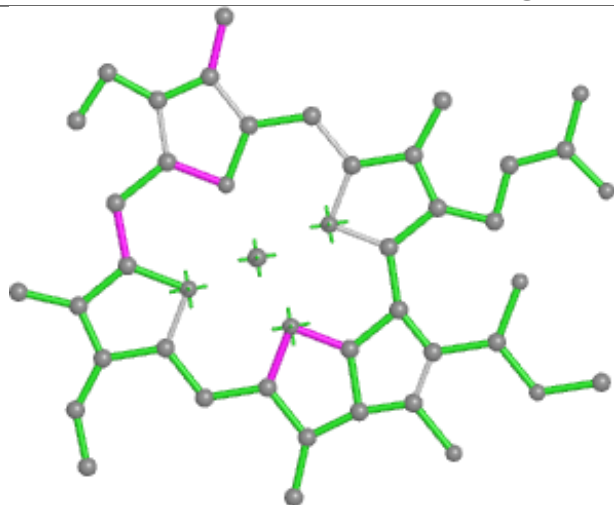
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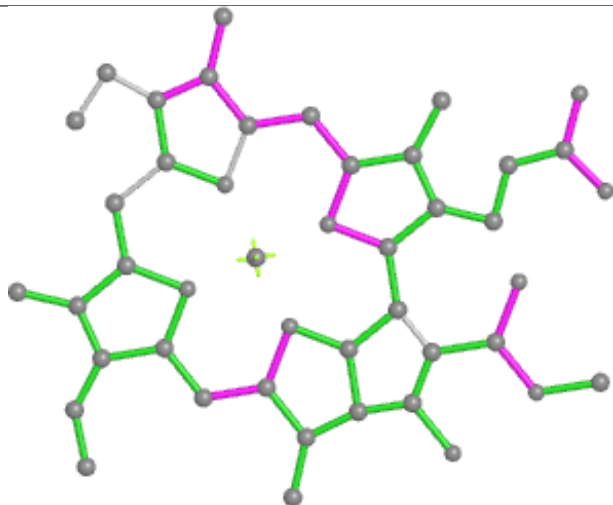
Ligand A1L1G 2 213



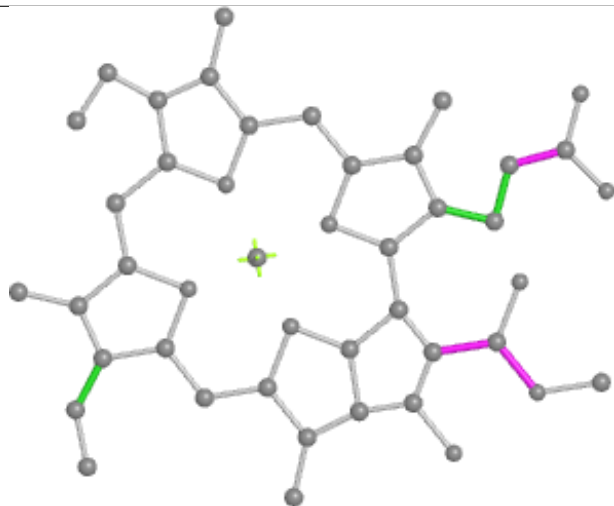
Ligand CLA 6 601



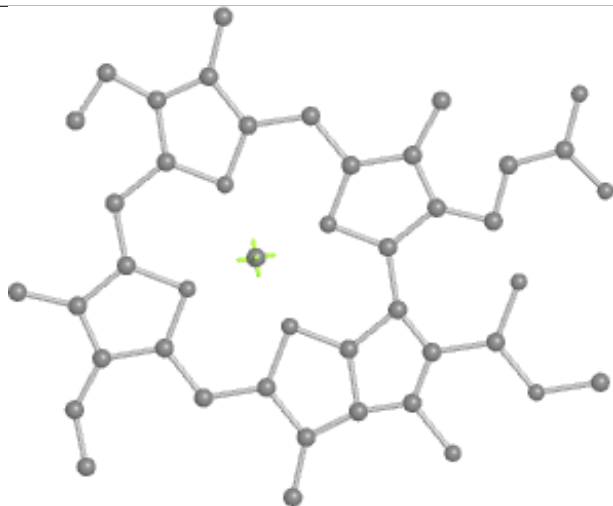
Bond lengths



Bond angles

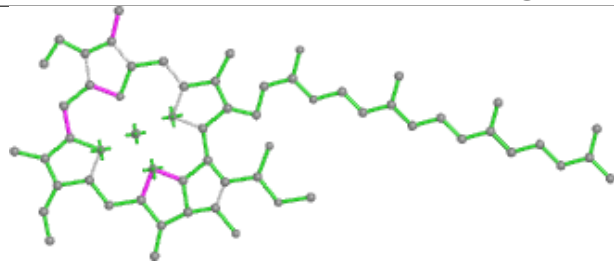


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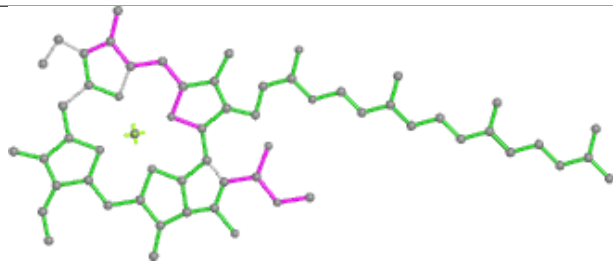


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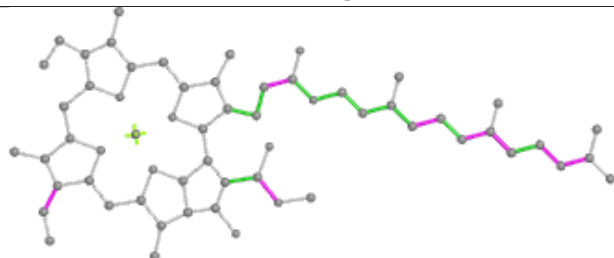
Ligand CLA 7 606



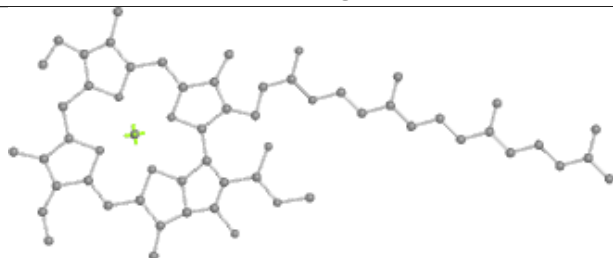
Bond lengths



Bond angles

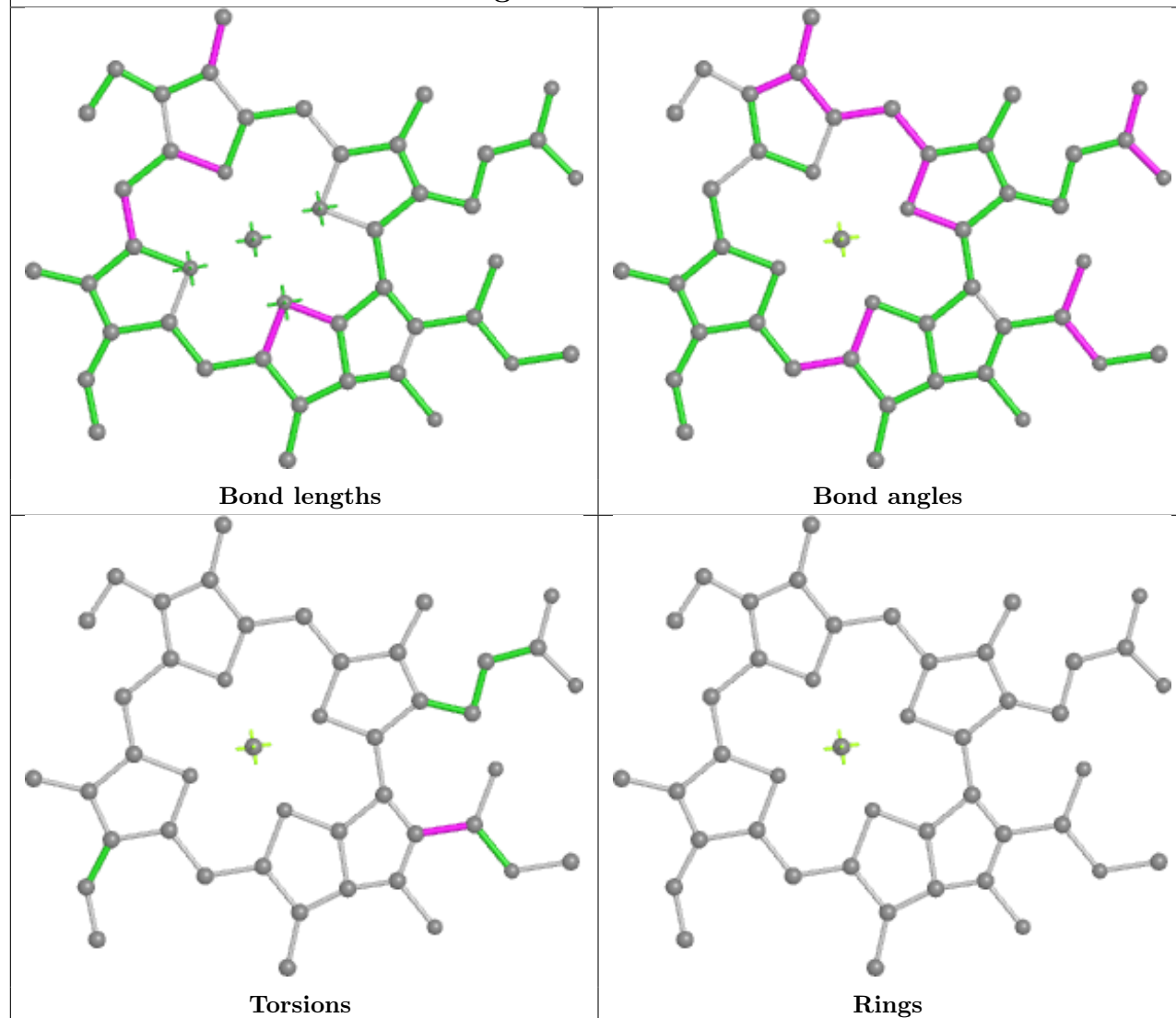


Torsions

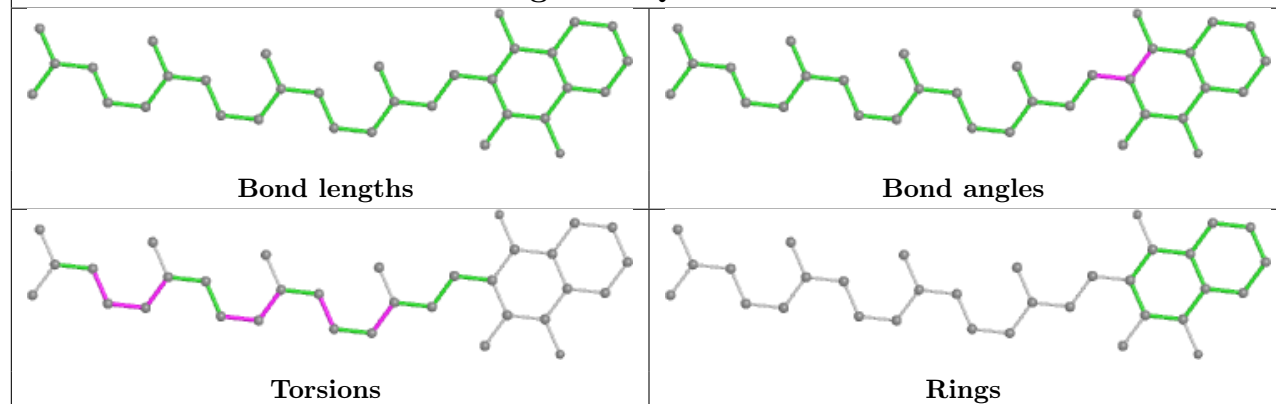


Rings

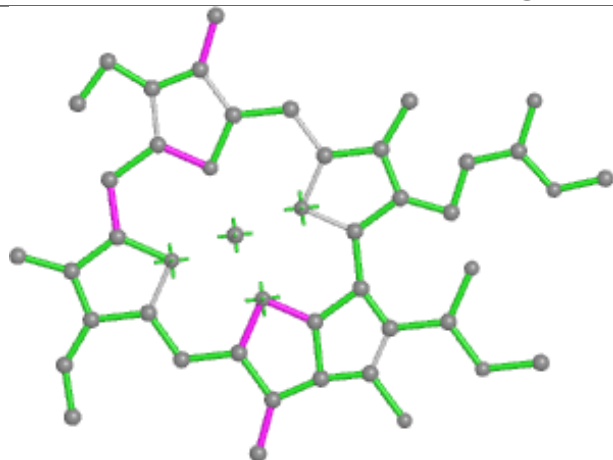
Ligand CLA 7 607



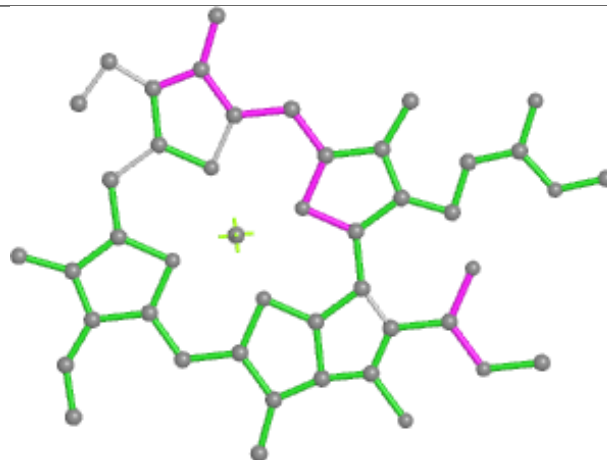
Ligand PQN B 839



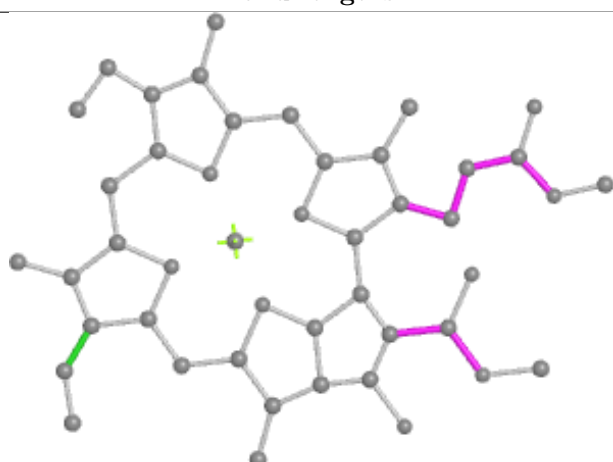
Ligand CLA 9 308



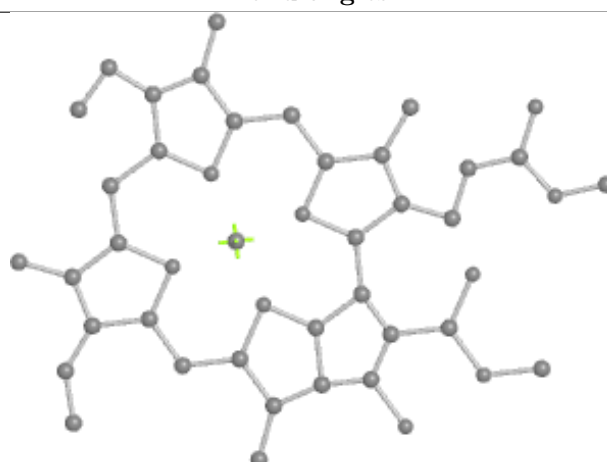
Bond lengths



Bond angles

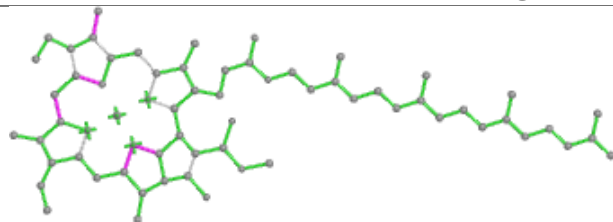


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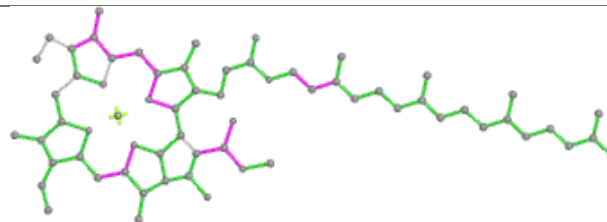


Rings

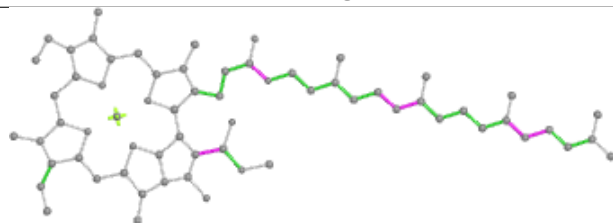
Ligand CLA A 840



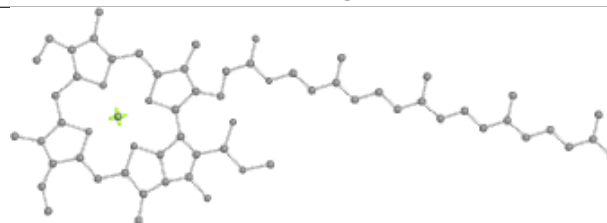
Bond lengths



Bond angles

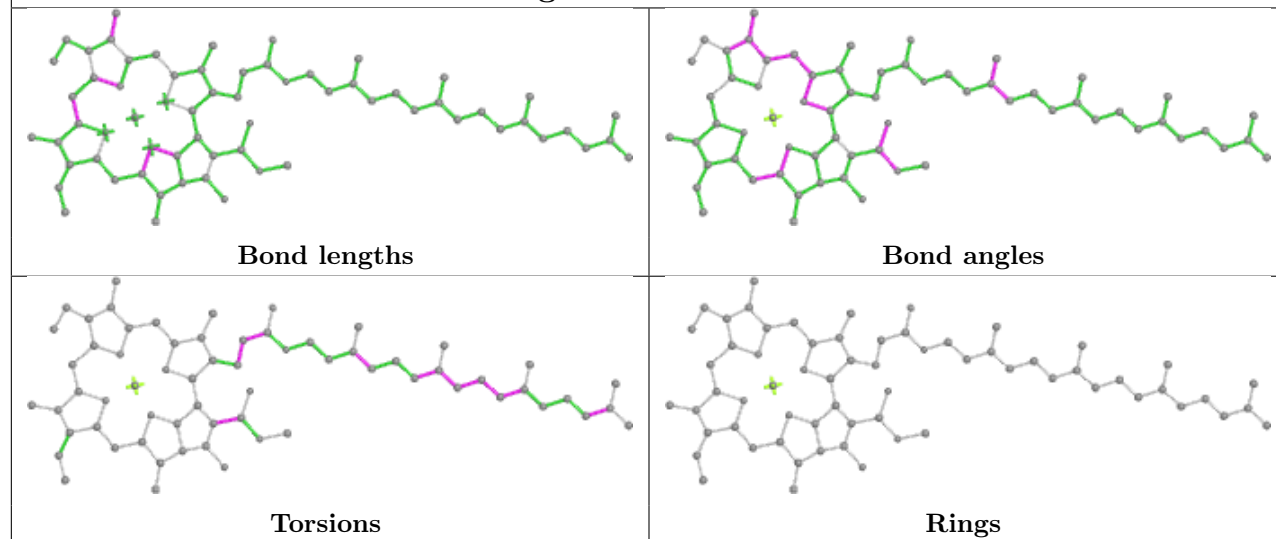


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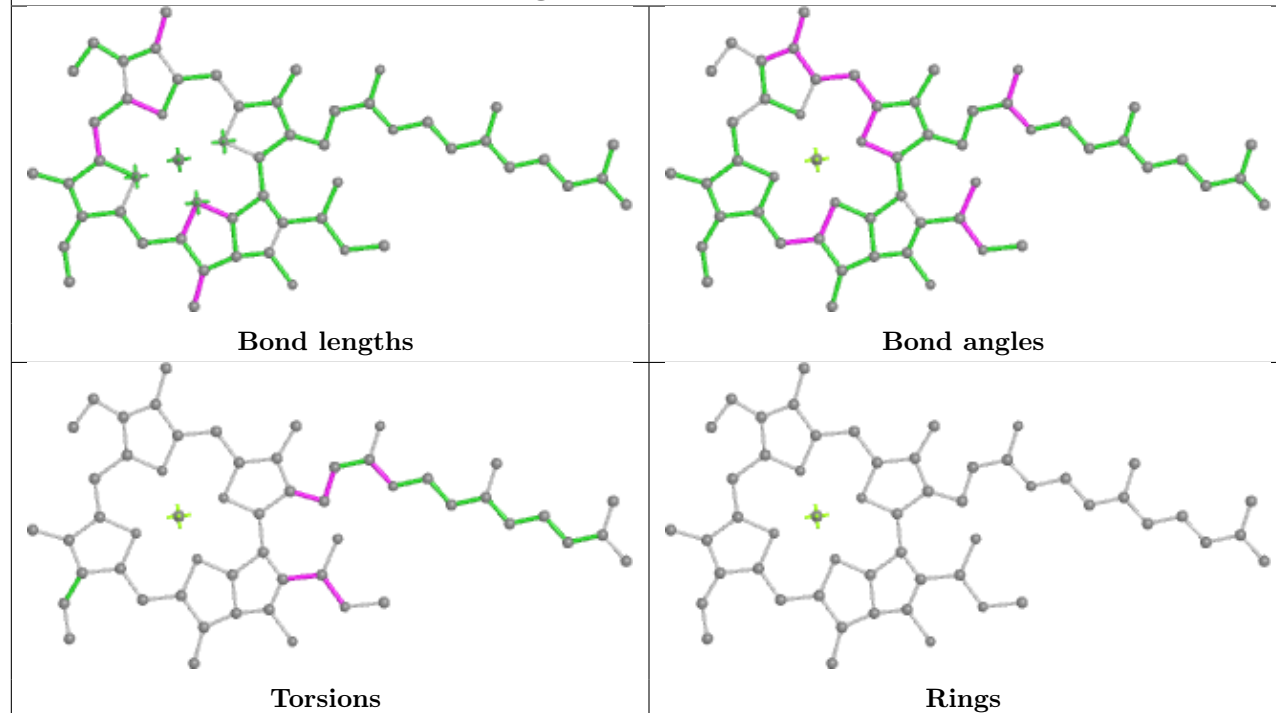


Rings

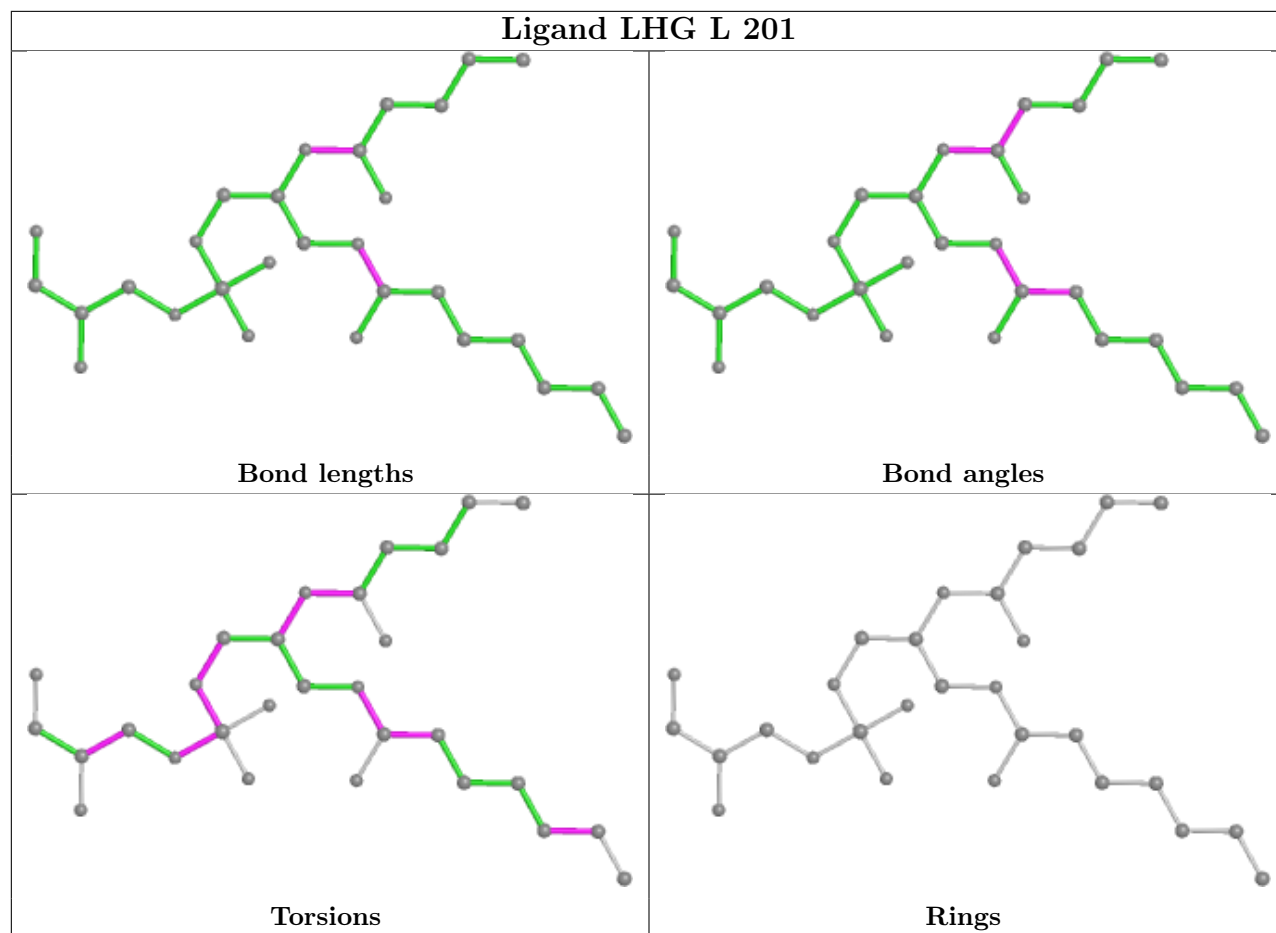
Ligand CLA t 303



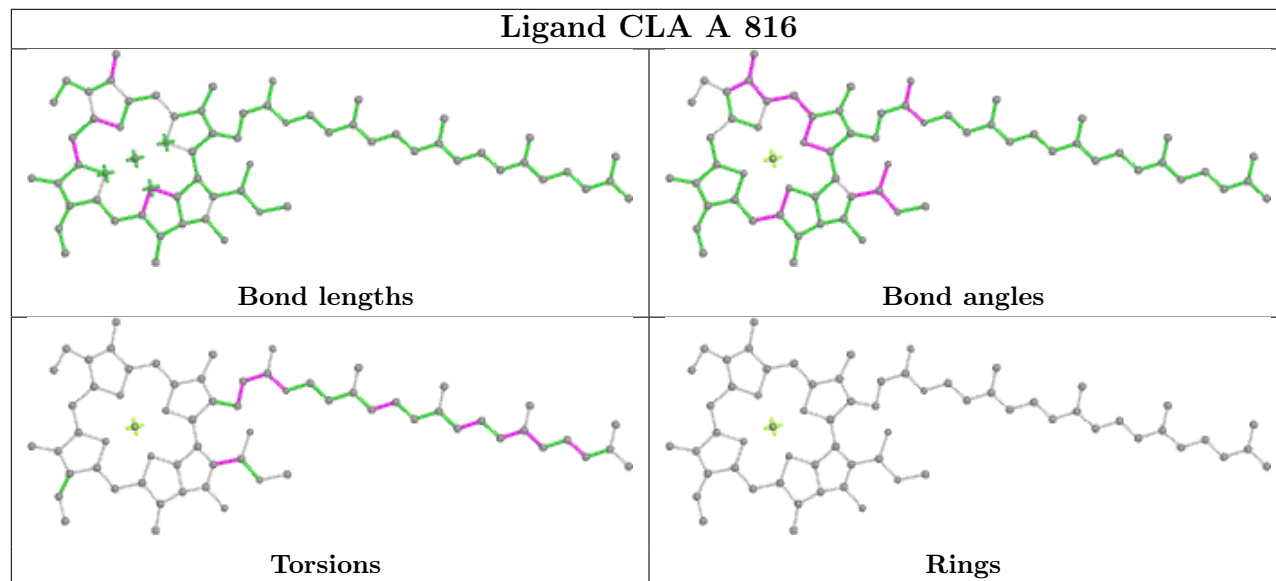
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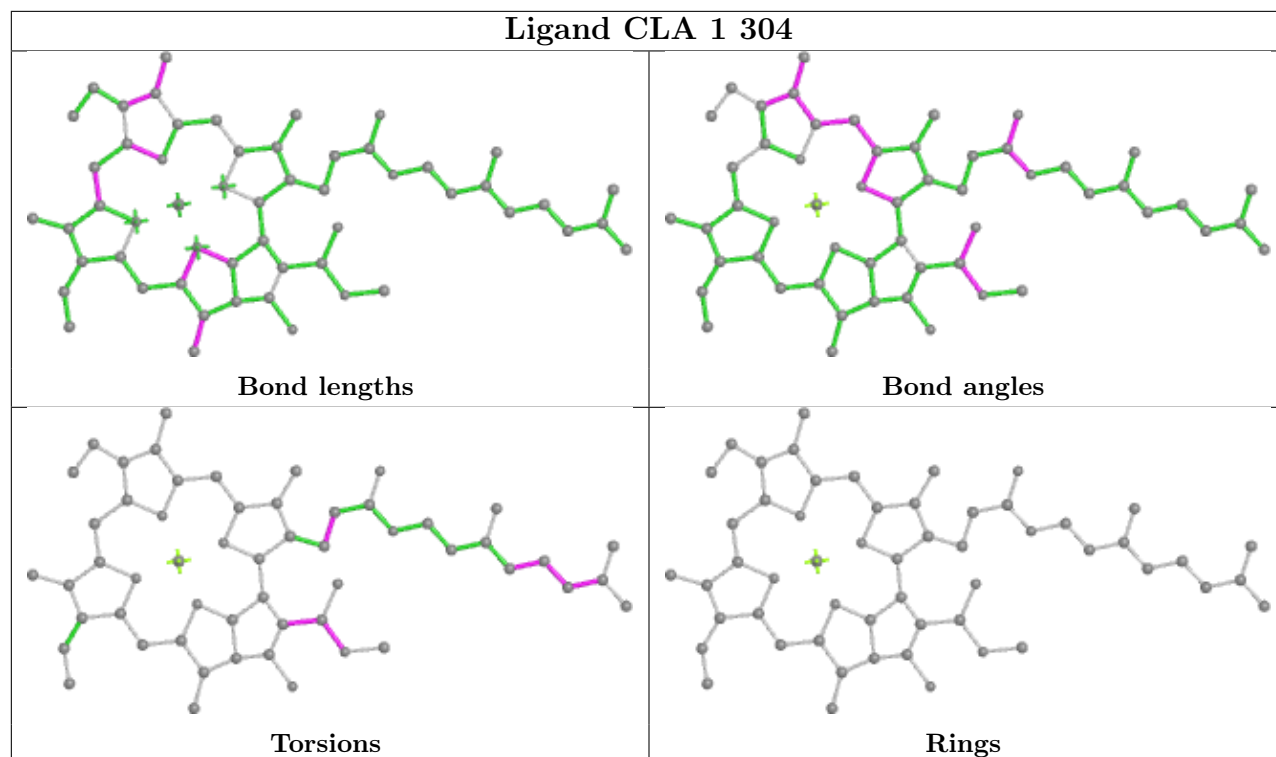
Ligand LHG L 201



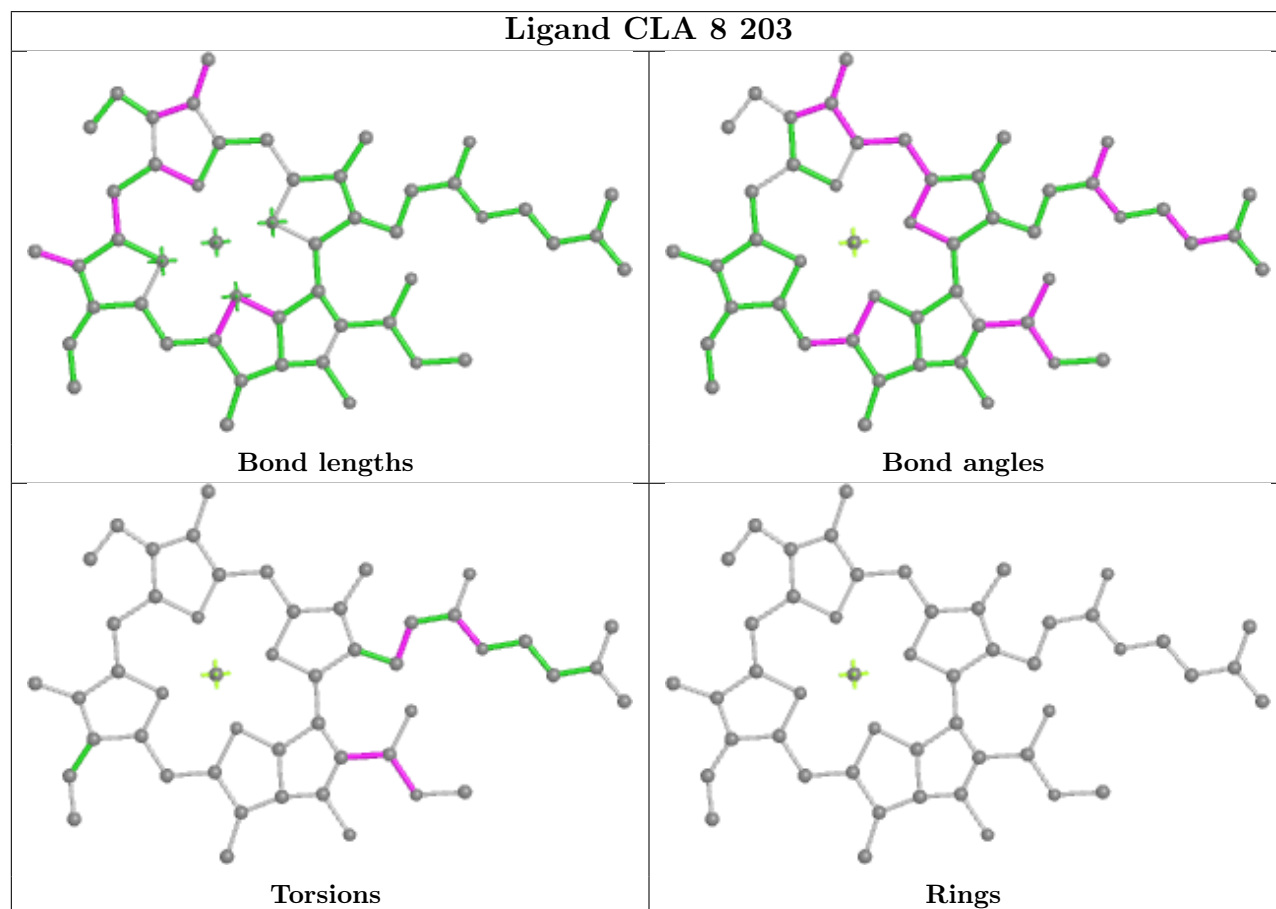
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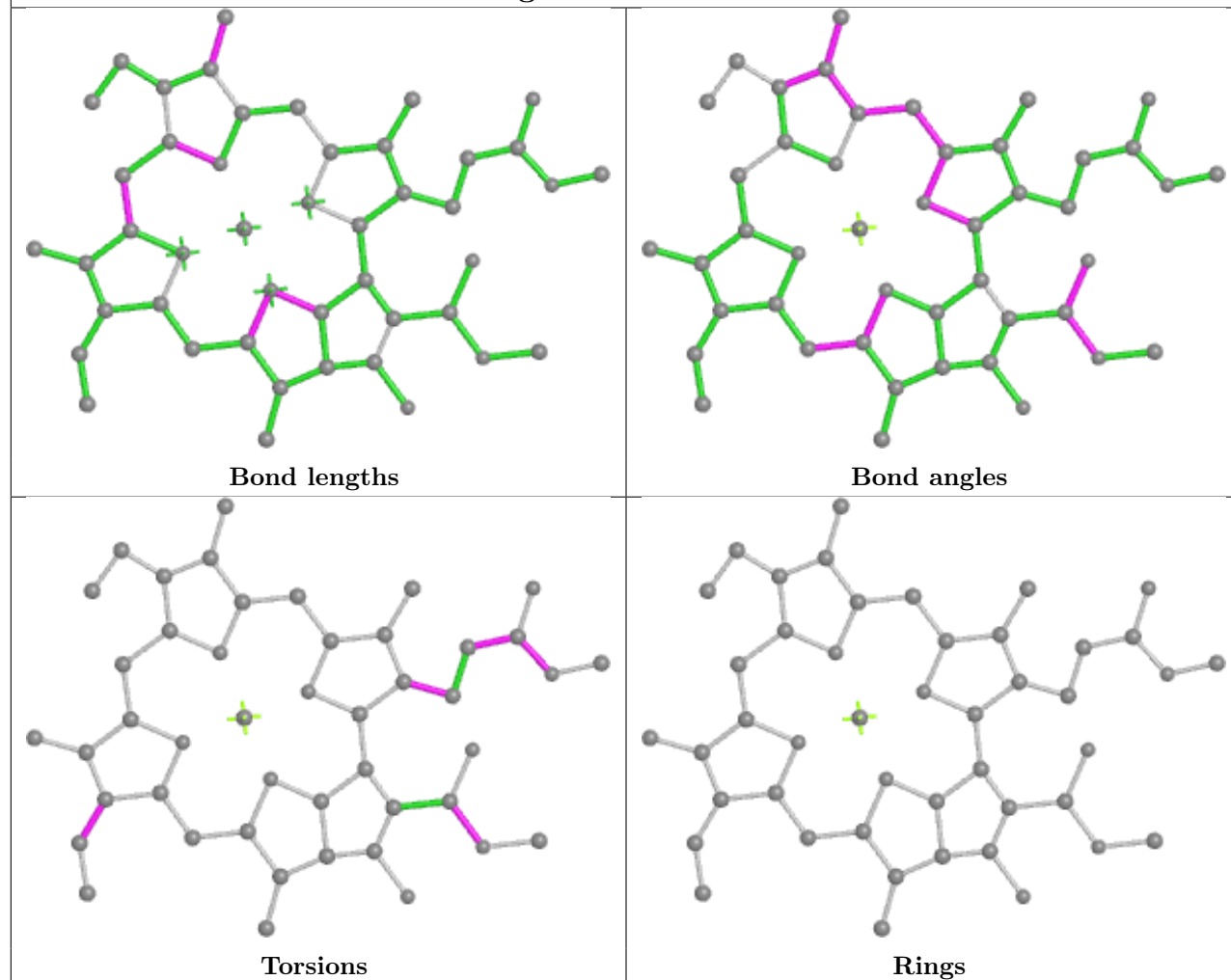
Ligand CLA 1 304



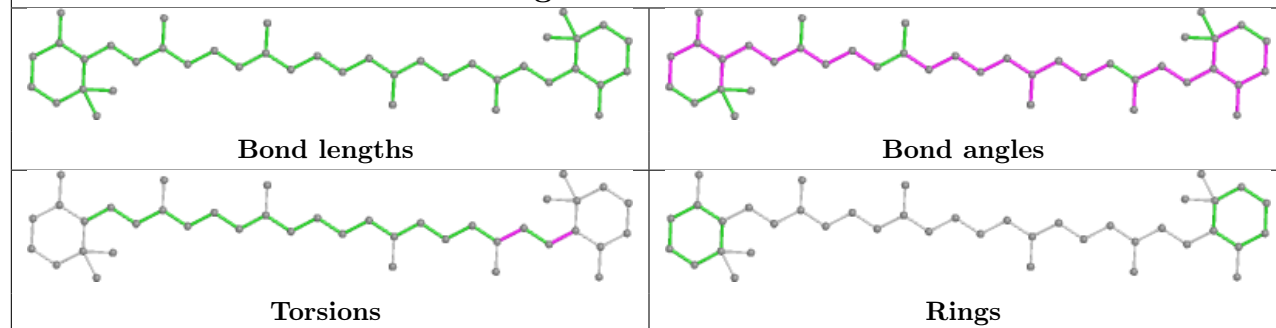
Ligand CLA 8 203

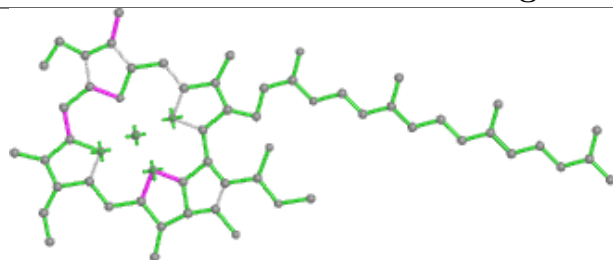


Ligand CLA c 605

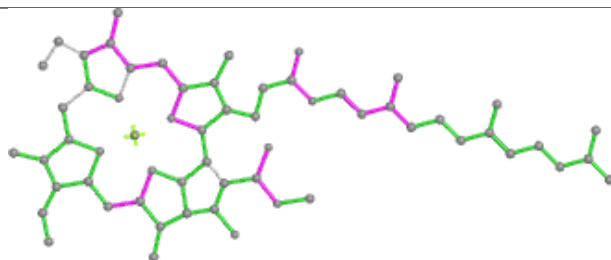


Ligand BCR 2 211

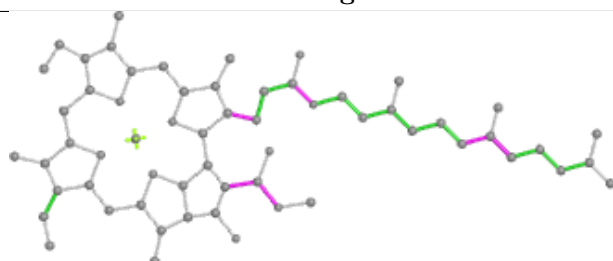


Ligand CLA c 609

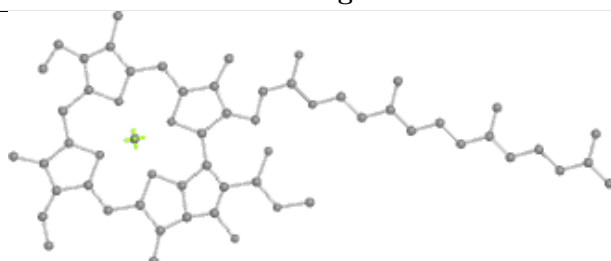
Bond lengths



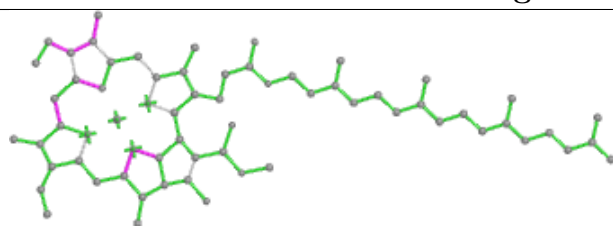
Bond angles



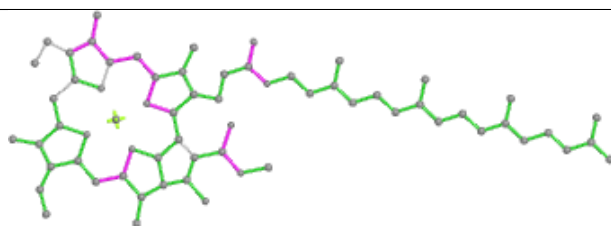
Torsions



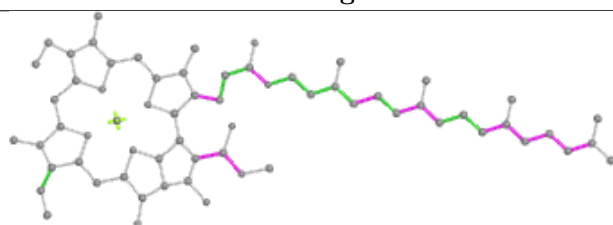
Rings

Ligand CLA A 823

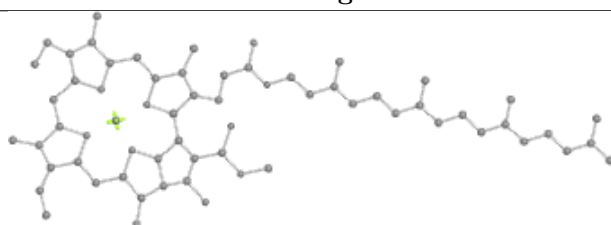
Bond lengths



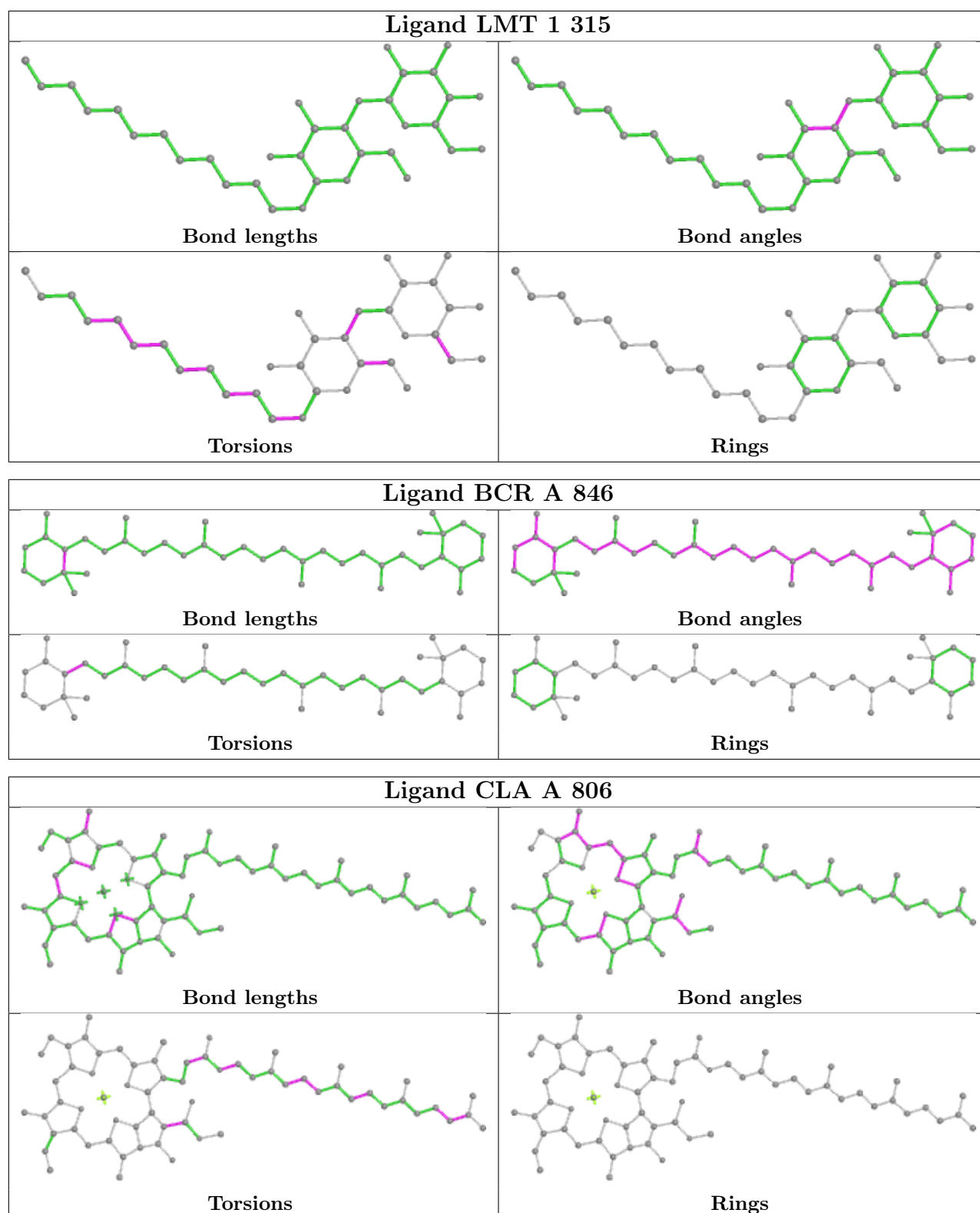
Bond angles



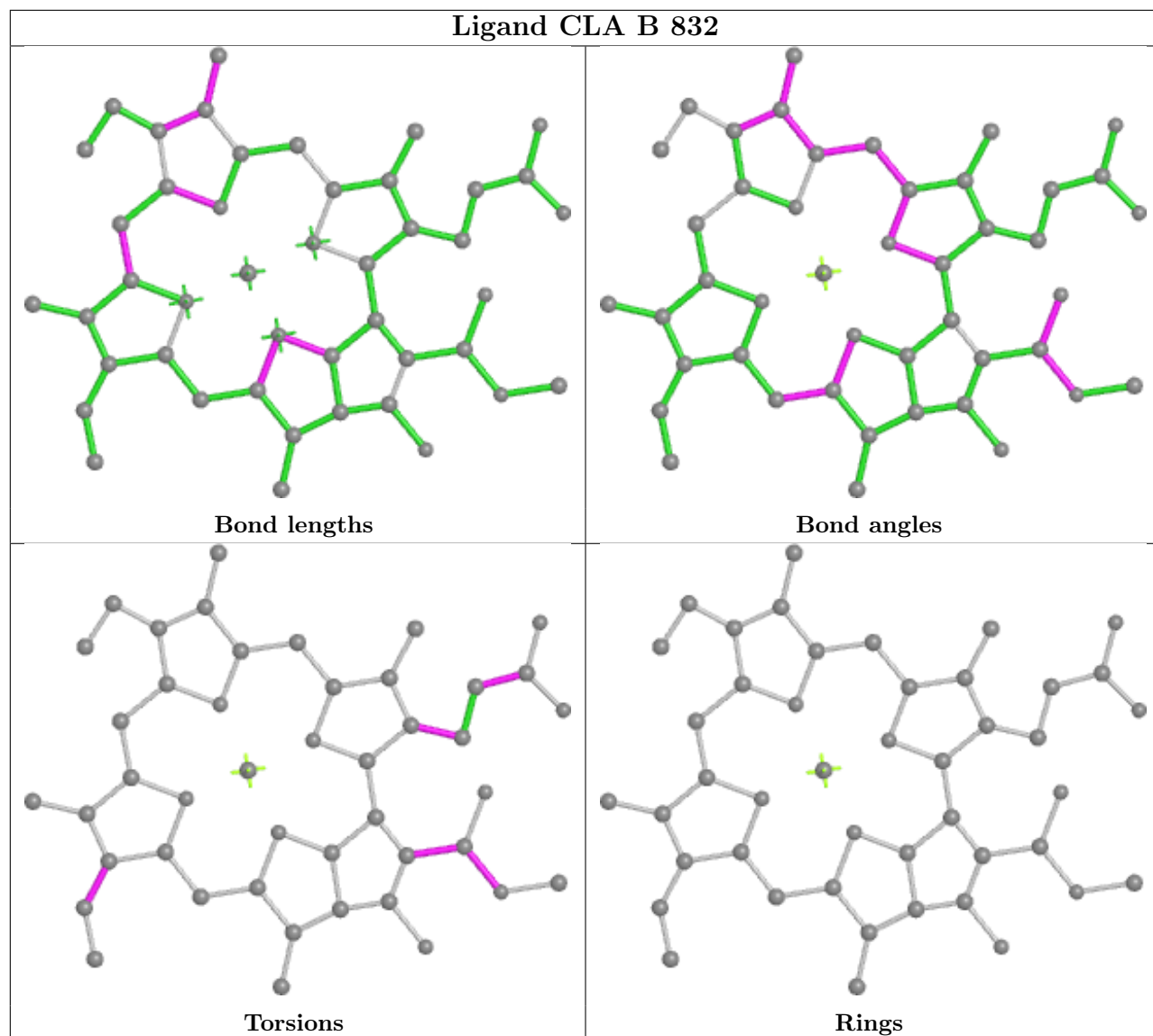
Torsions



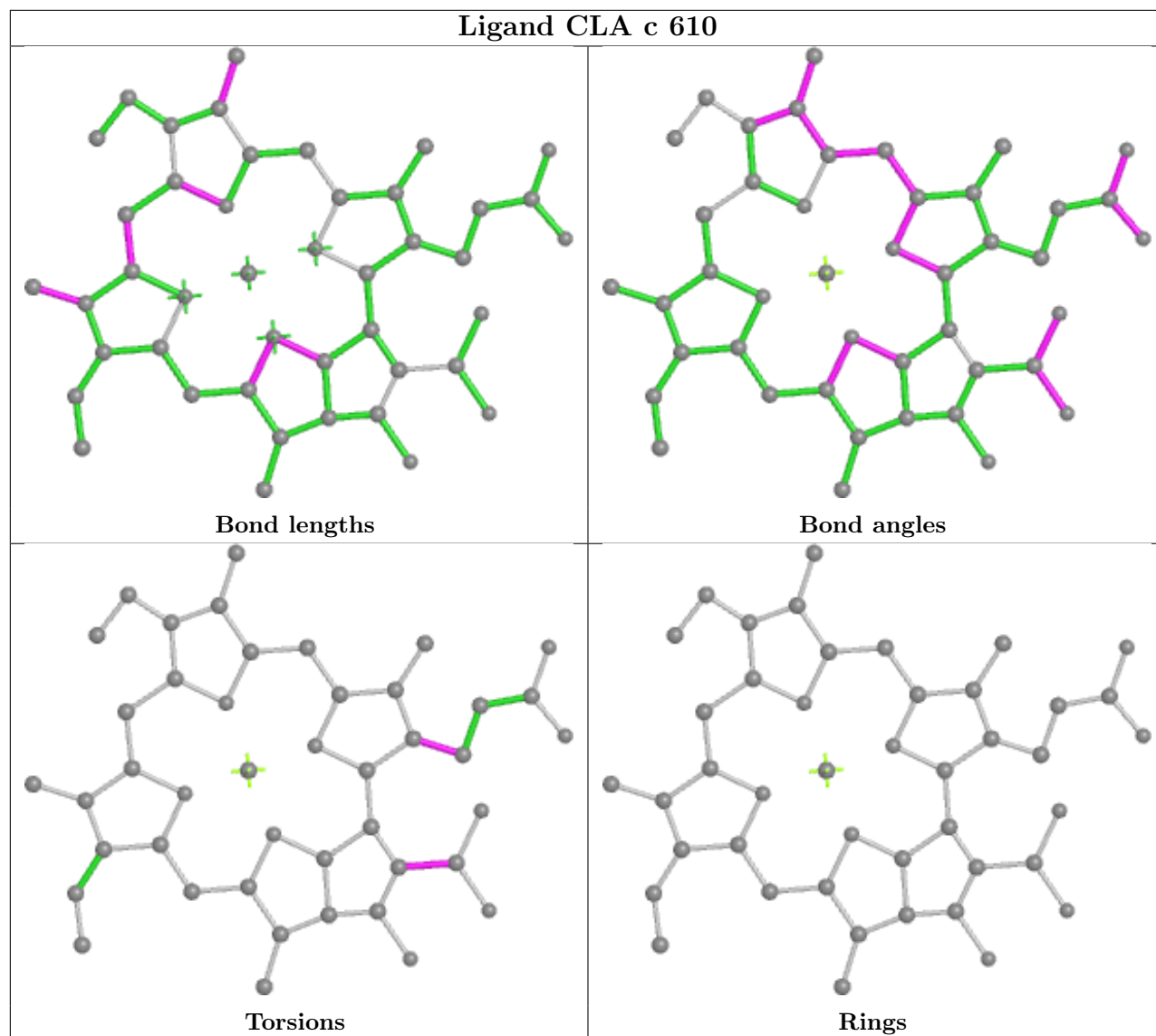
Rings



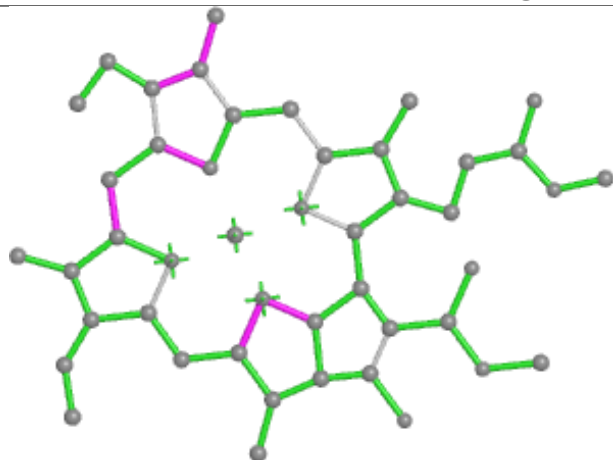
Ligand CLA B 832



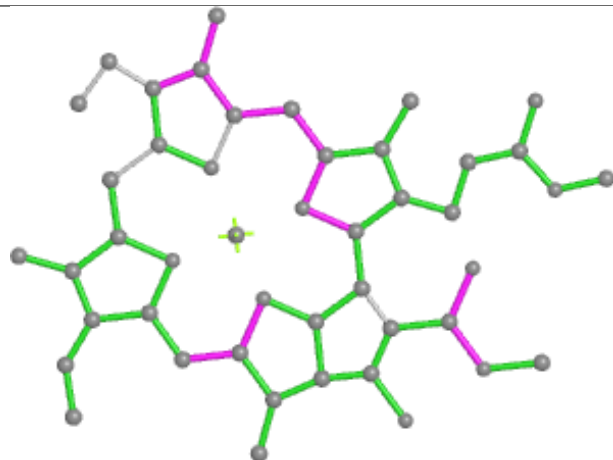
Ligand CLA c 610



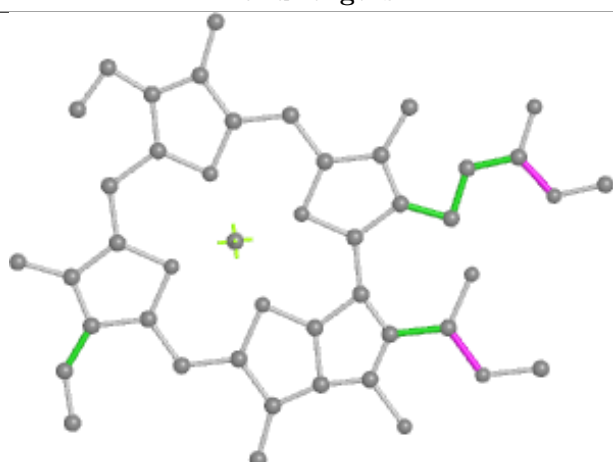
Ligand CLA h 607



Bond lengths



Bond angles

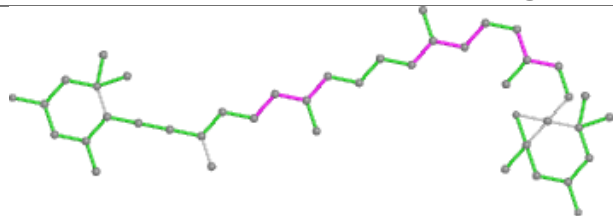


Torsions

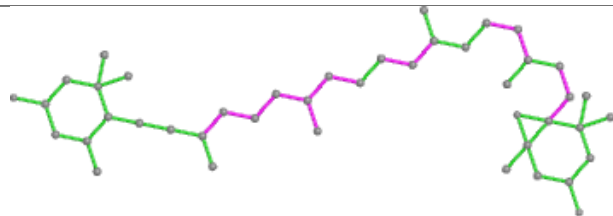


Rings

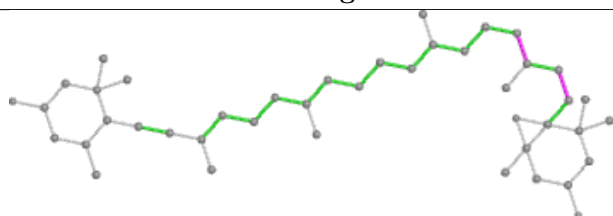
Ligand DD6 t 311



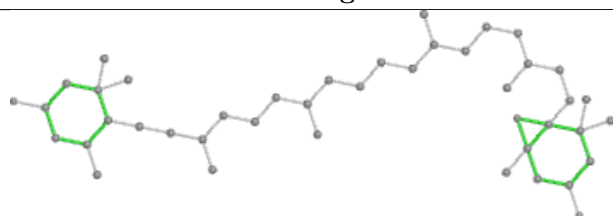
Bond lengths



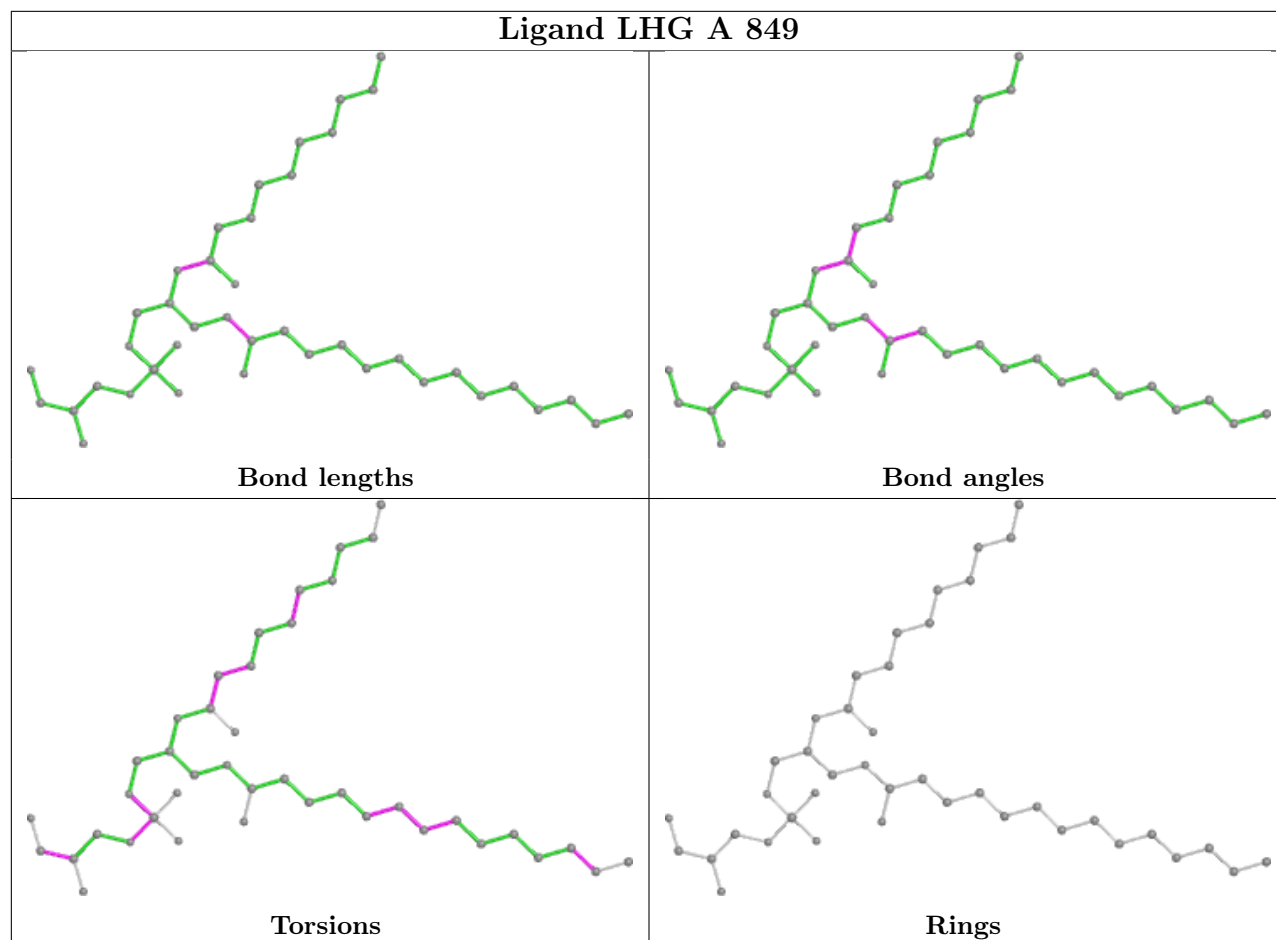
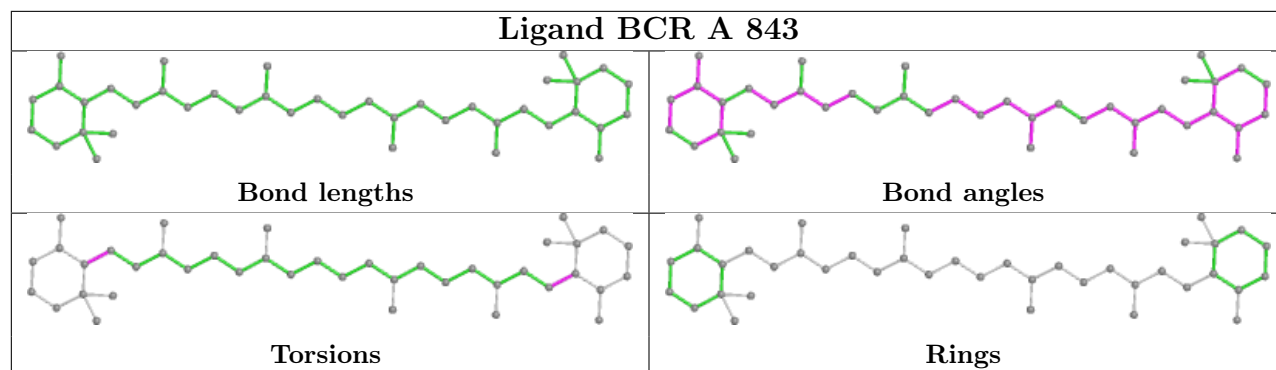
Bond angles



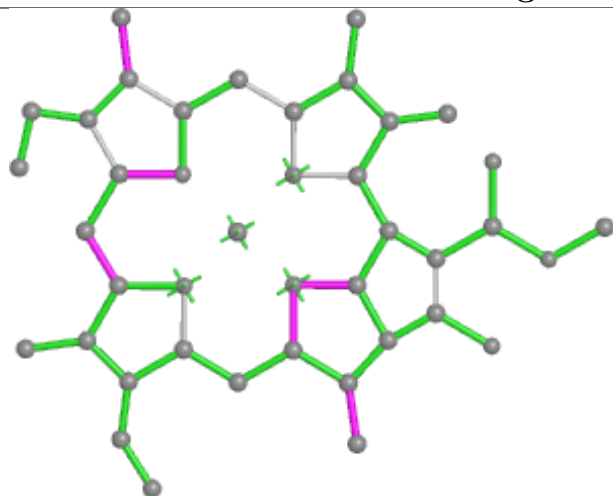
Torsions



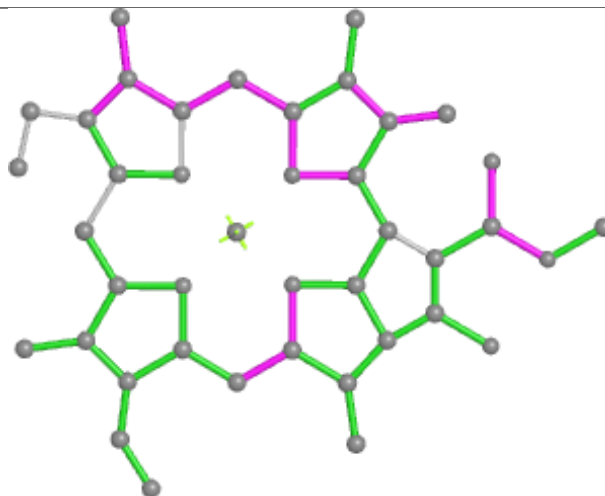
Rings



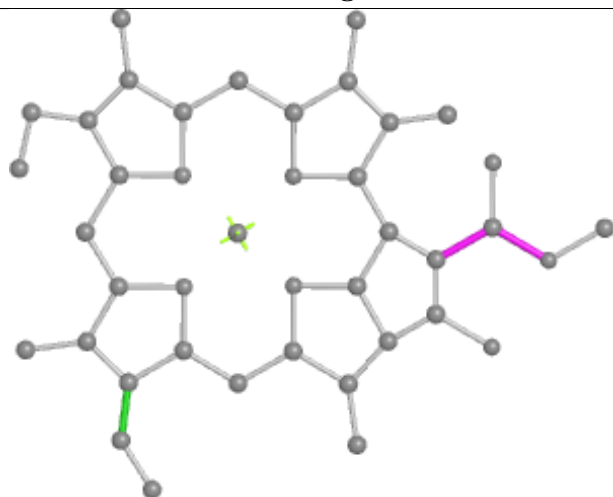
Ligand CLA h 611



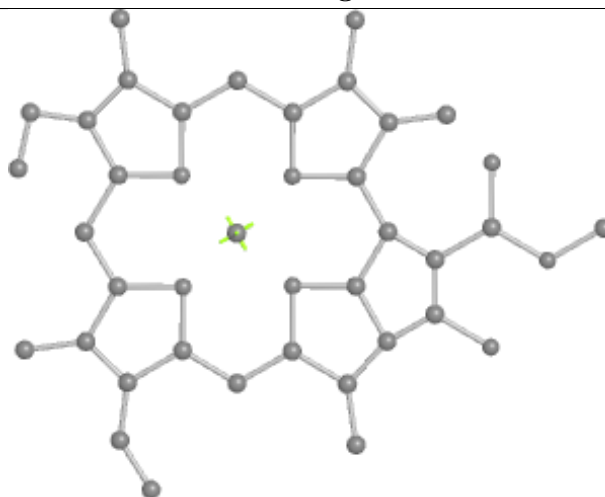
Bond lengths



Bond angles

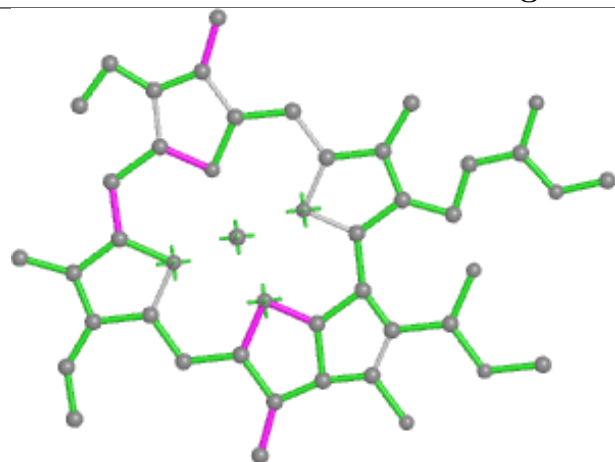


Torsions

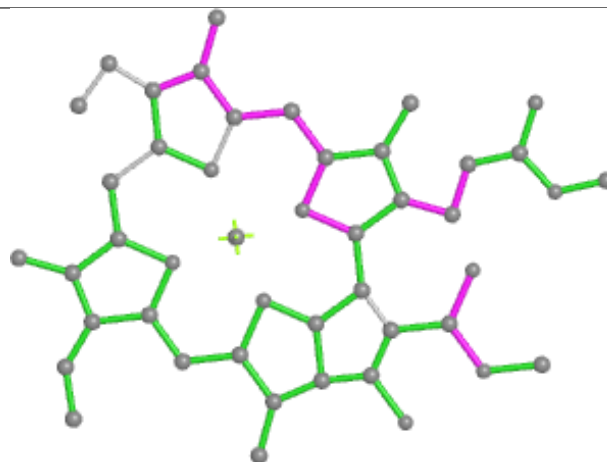


Rings

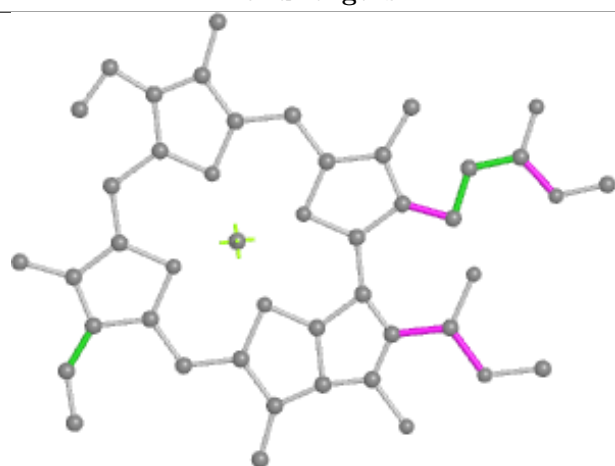
Ligand CLA 9 304



Bond lengths



Bond angles

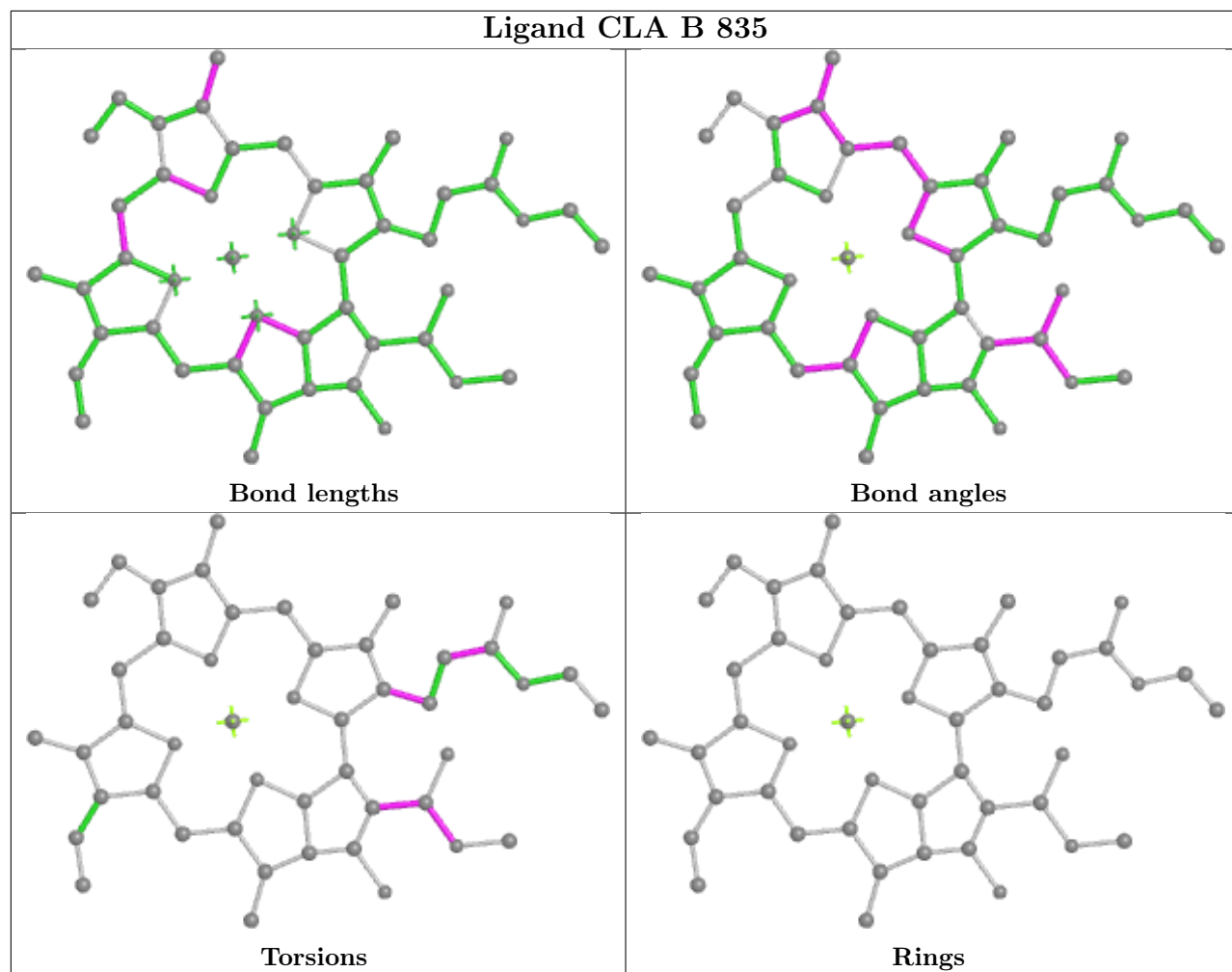


Torsions

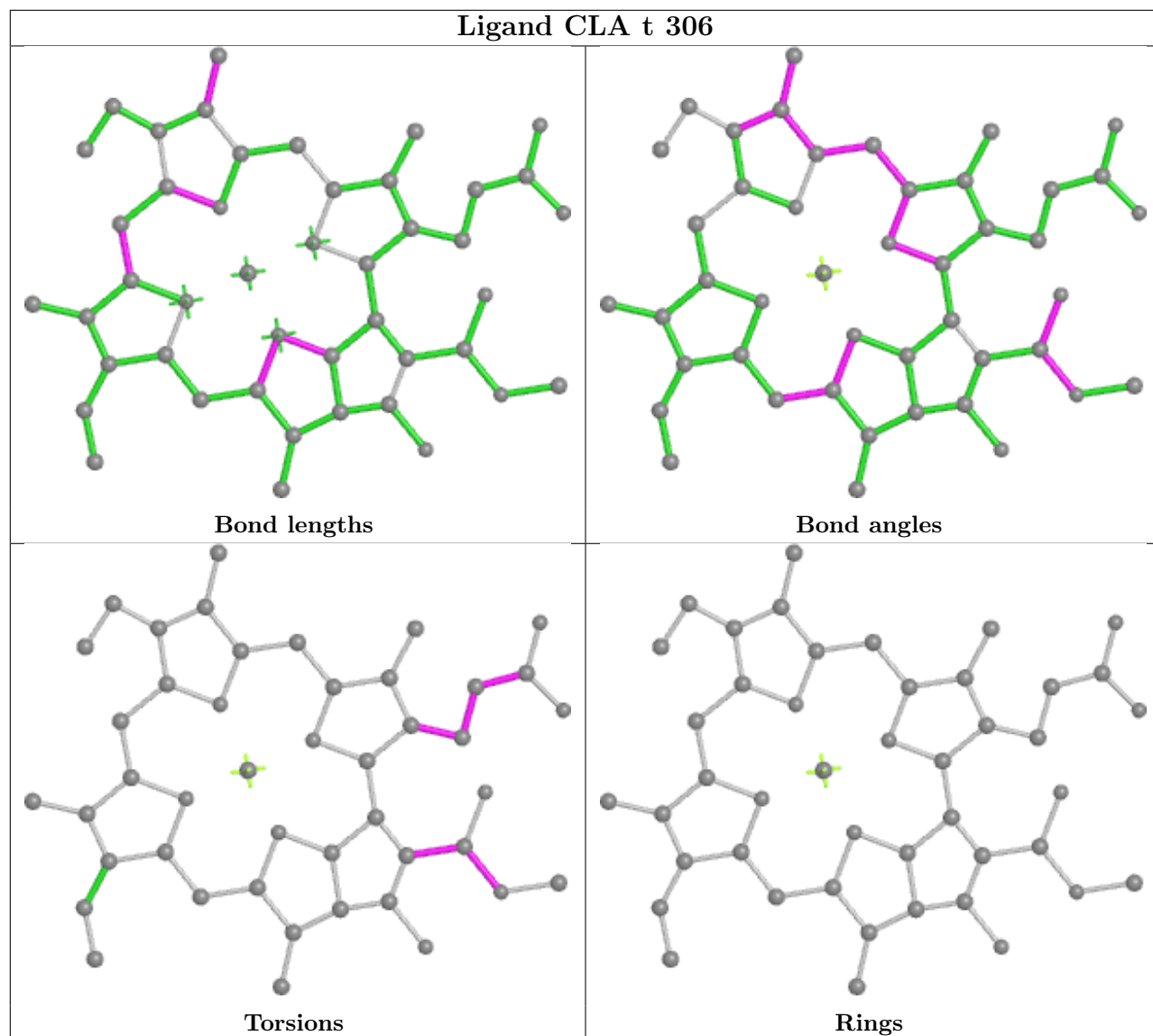


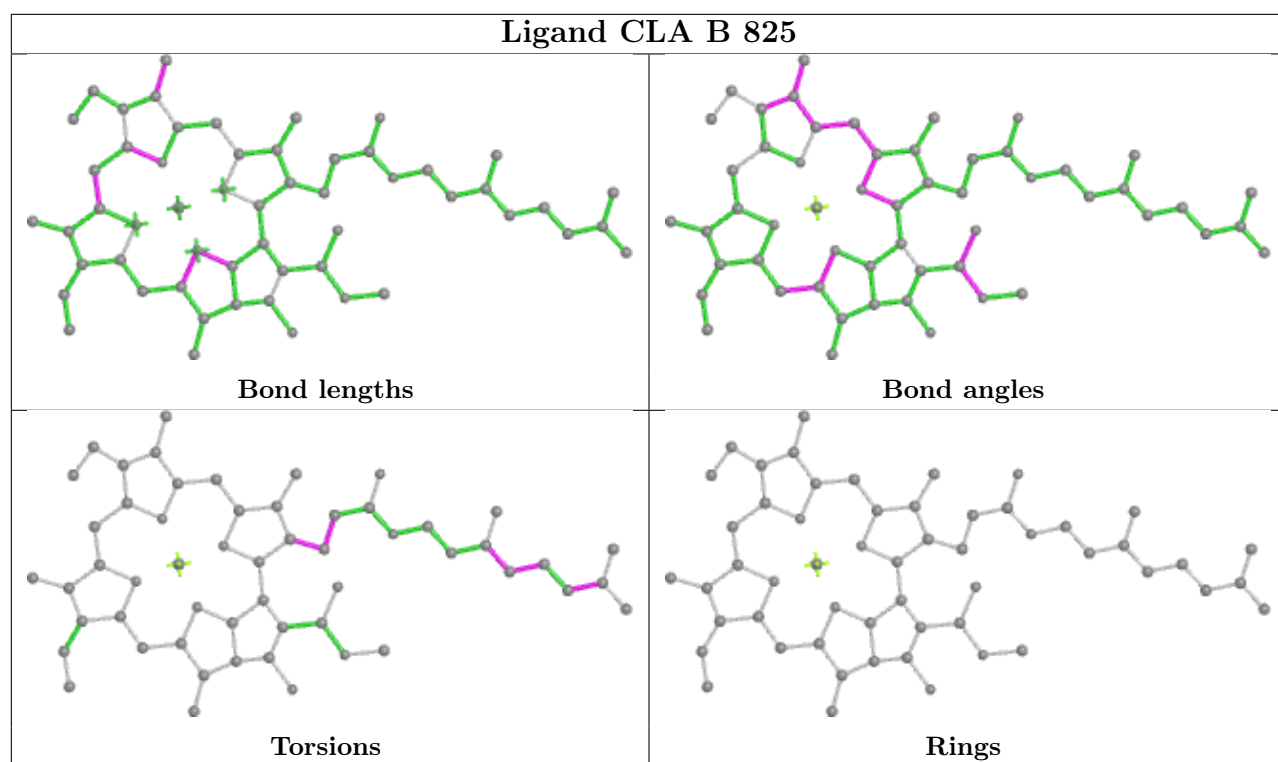
Rings

Ligand CLA B 835

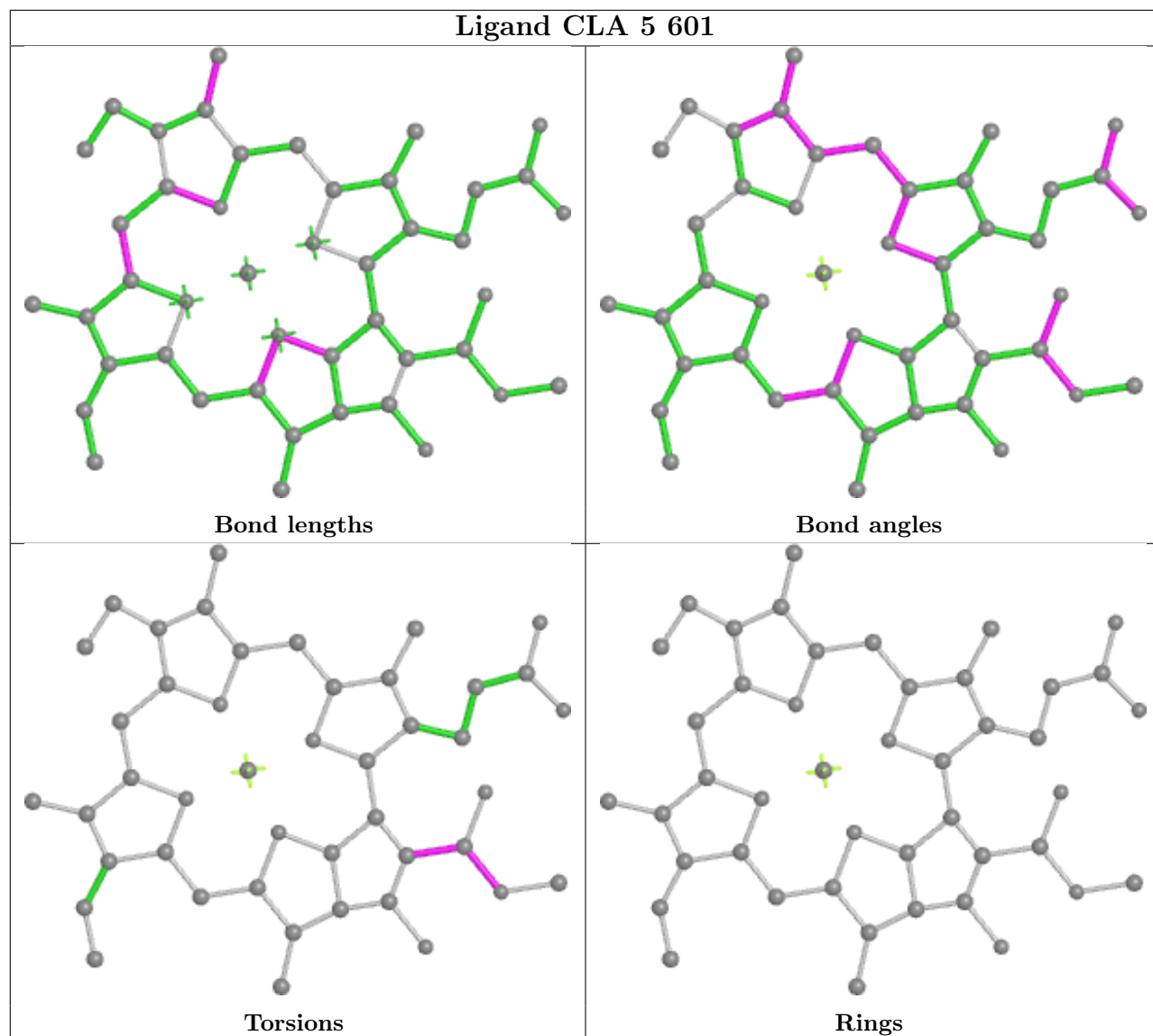


Ligand CLA t 306

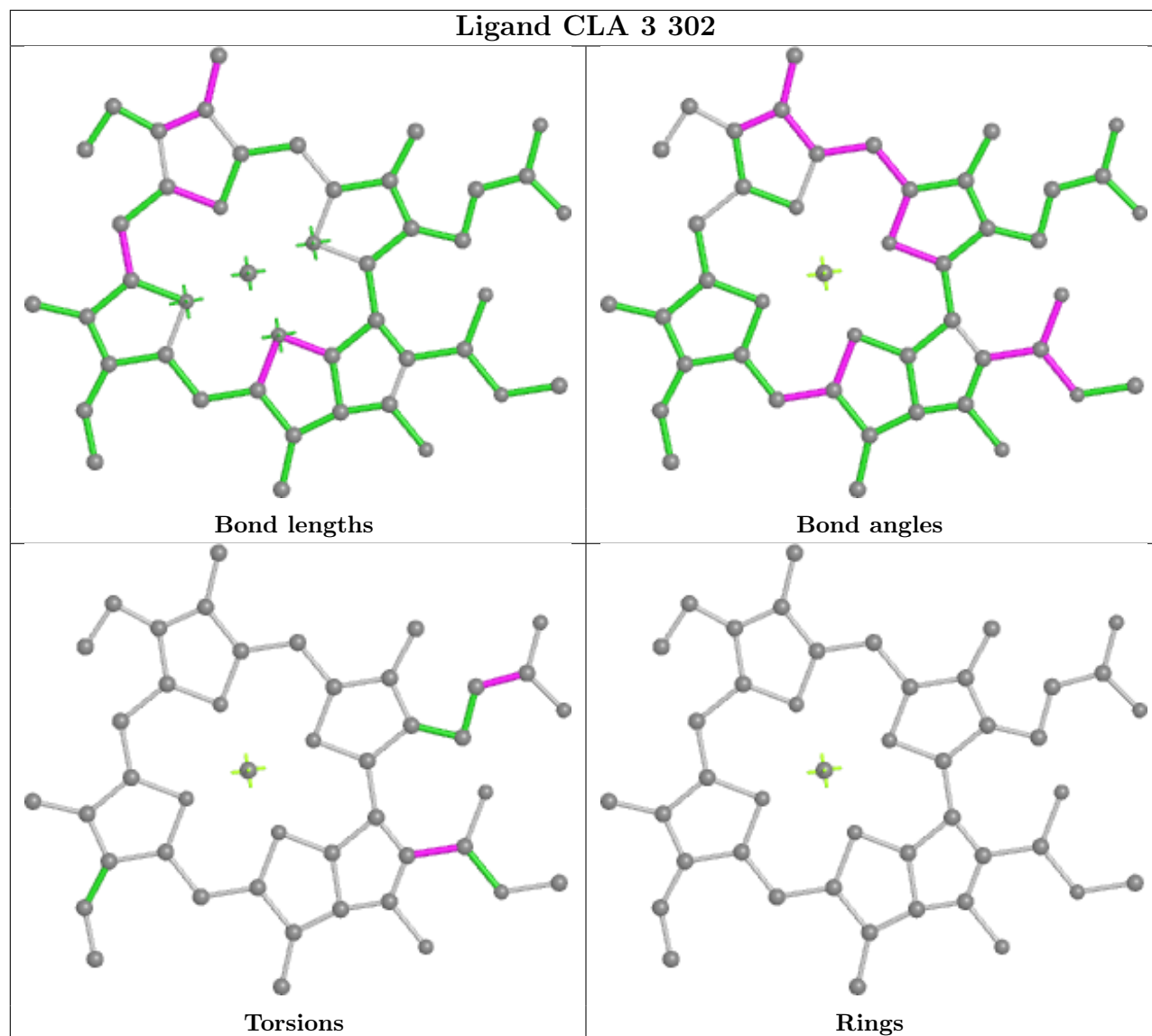




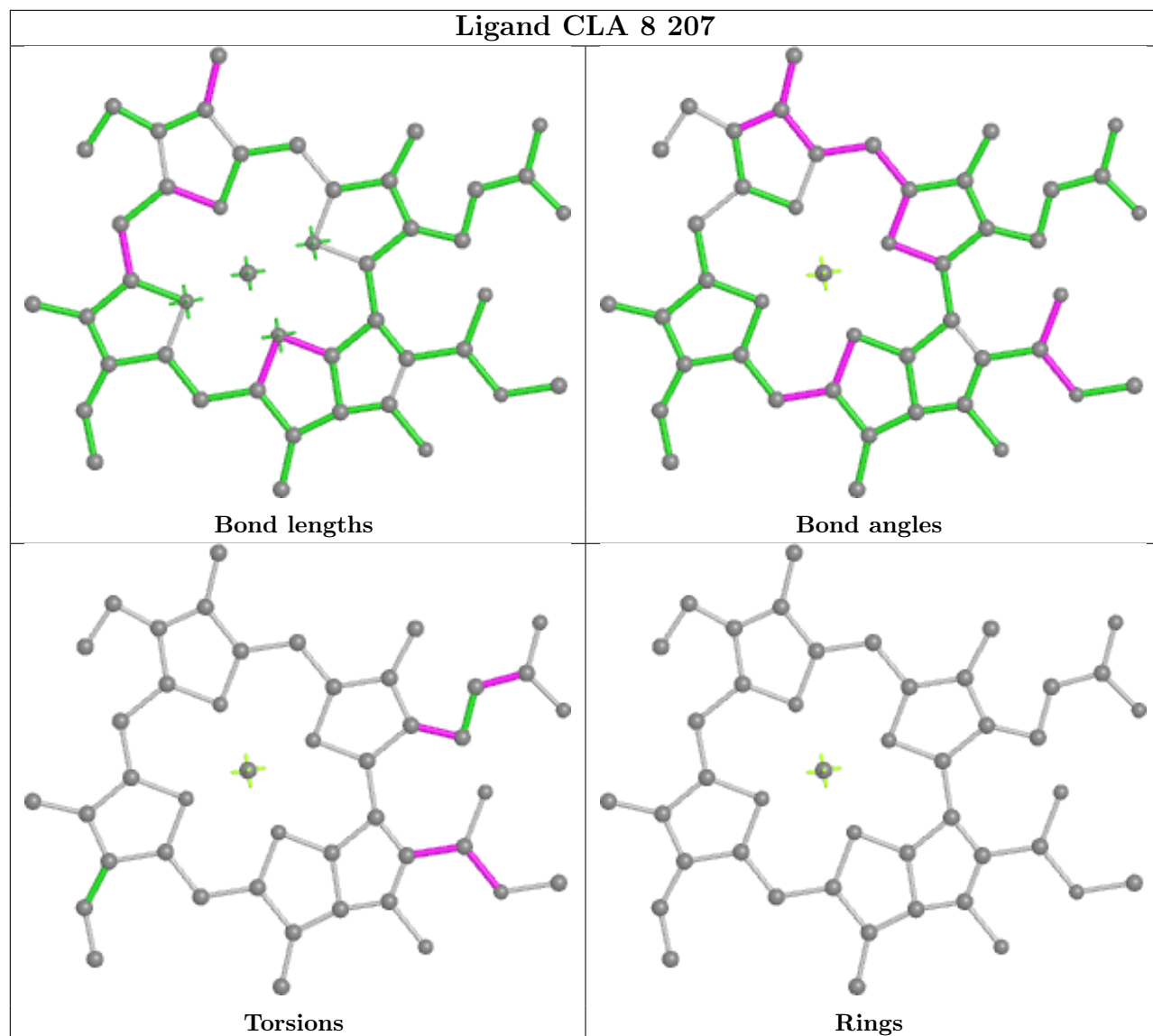
Ligand CLA 5 601



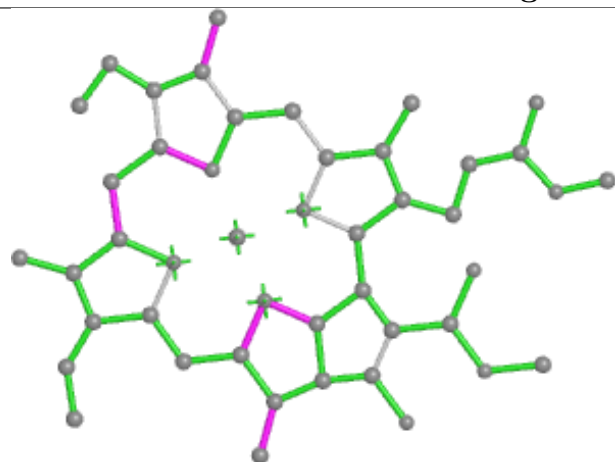
Ligand CLA 3 302



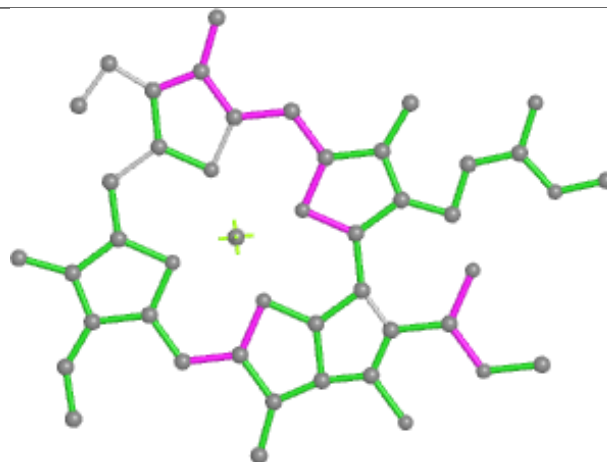
Ligand CLA 8 207



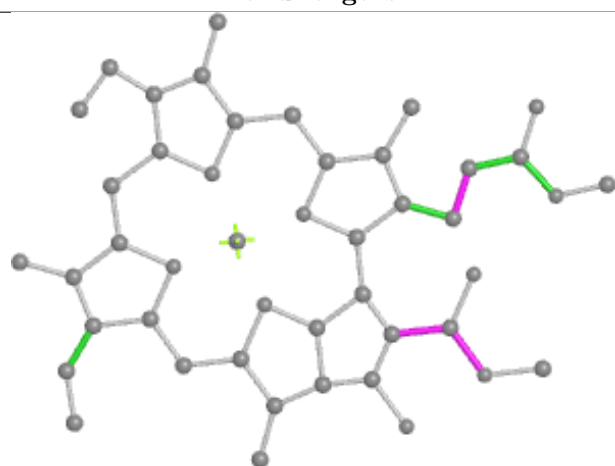
Ligand CLA 6 604



Bond lengths



Bond angles

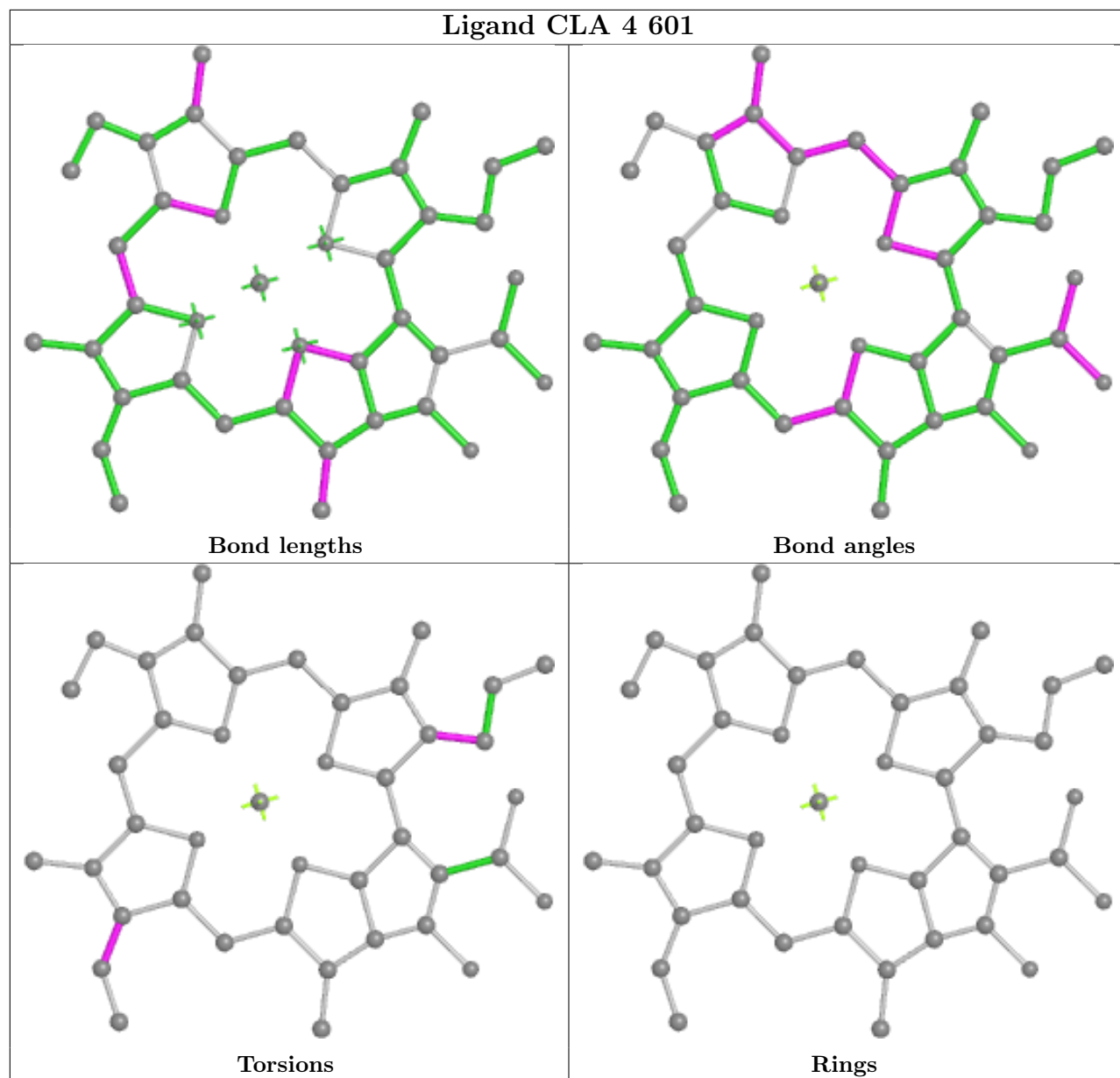


Torsions

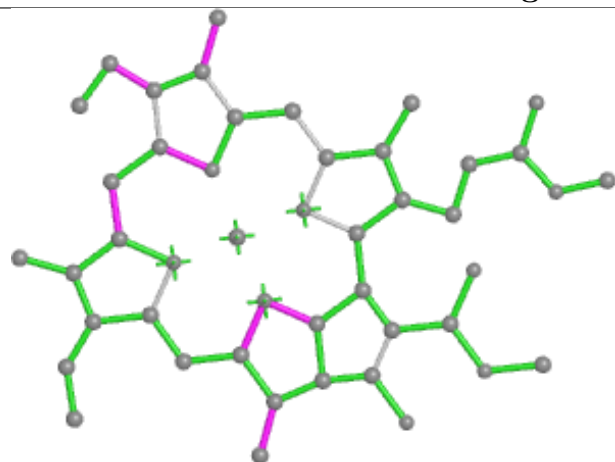


Rings

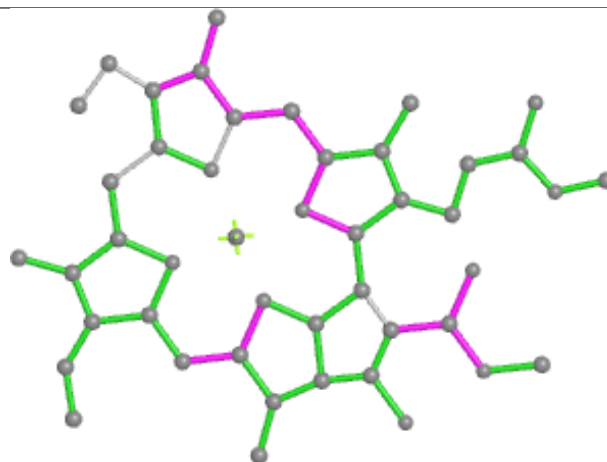
Ligand CLA 4 601



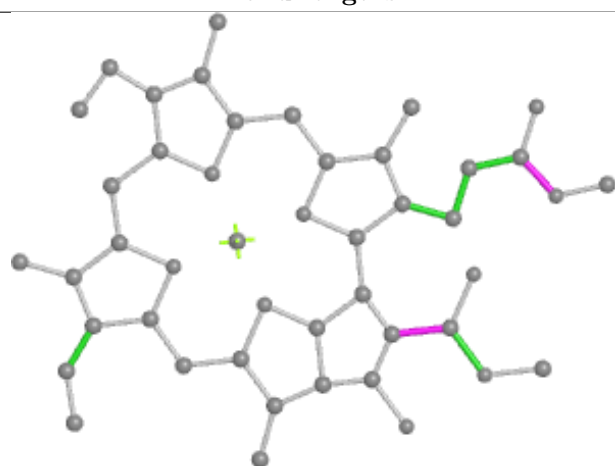
Ligand CLA c 607



Bond lengths



Bond angles

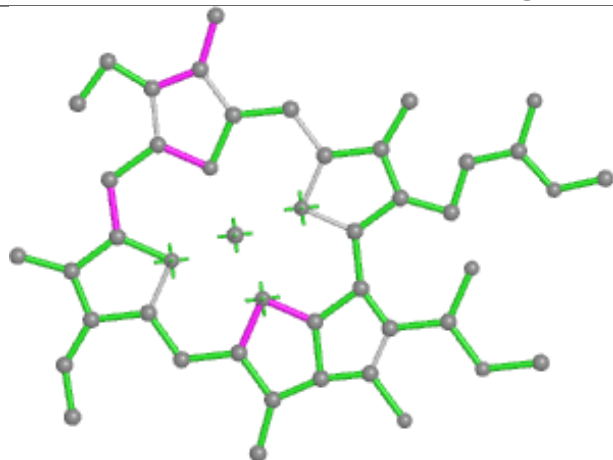


Torsions

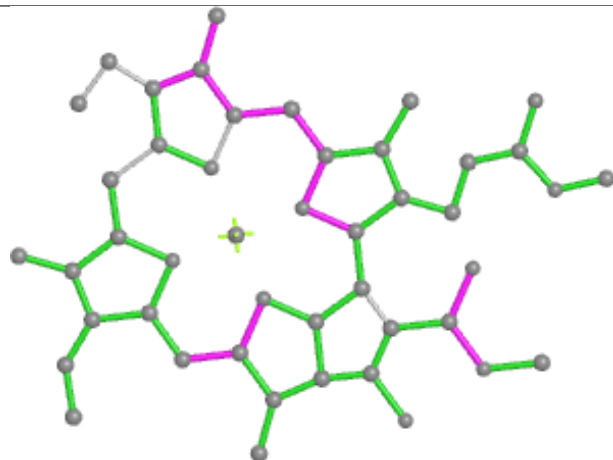


Rings

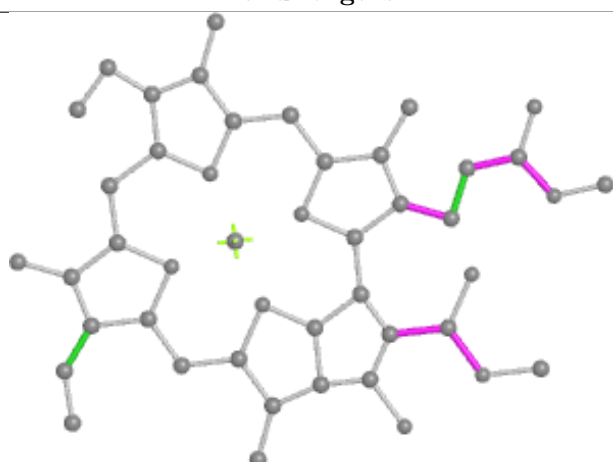
Ligand CLA 4 604



Bond lengths



Bond angles

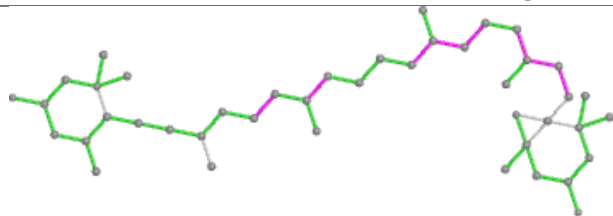


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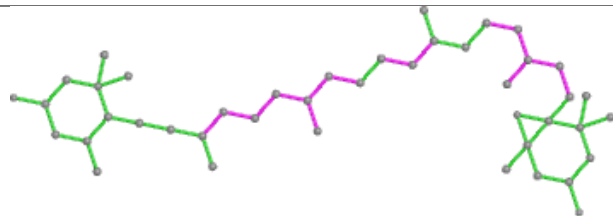


Rings

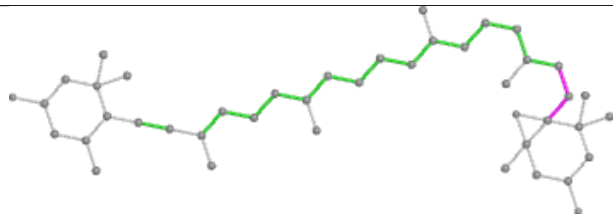
Ligand DD6 7 616



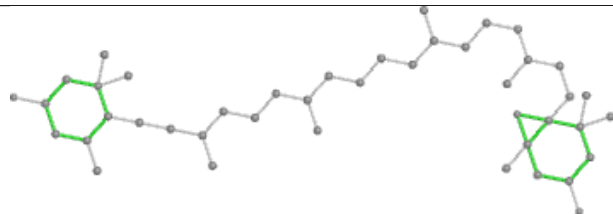
Bond lengths



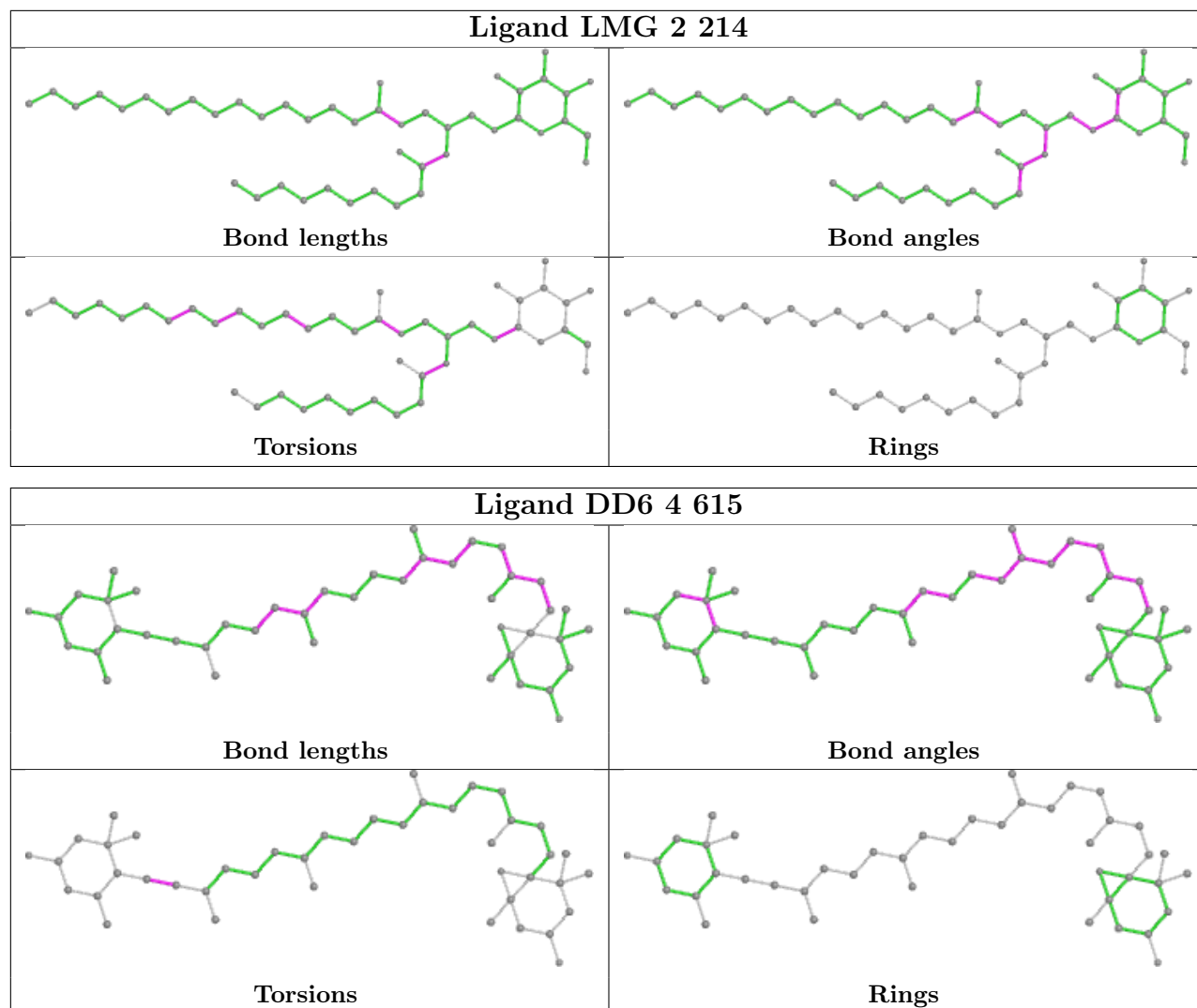
Bond angles



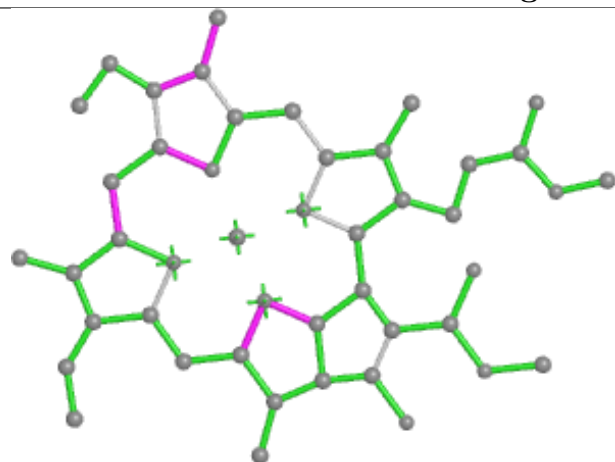
Torsions



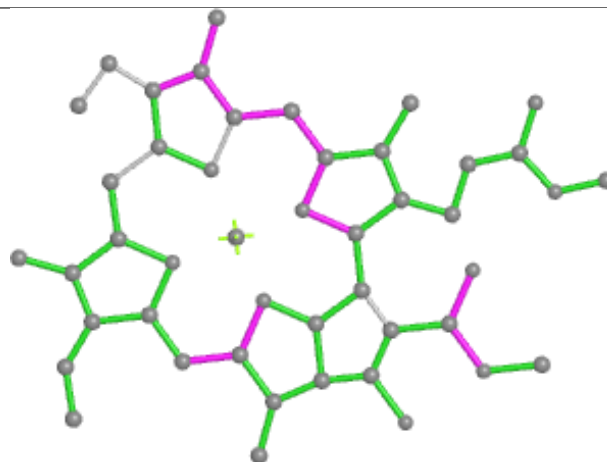
Rings



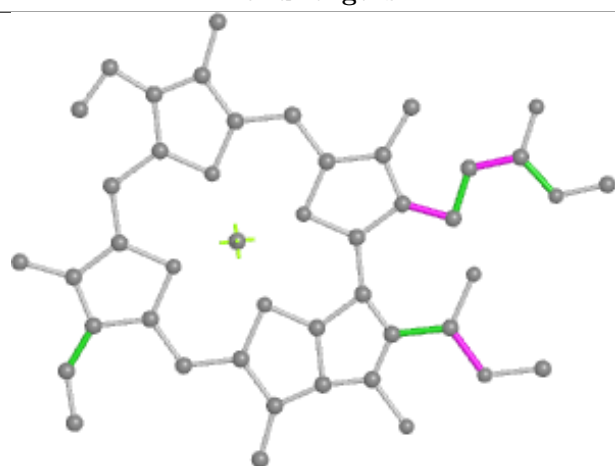
Ligand CLA 6 610



Bond lengths



Bond angles

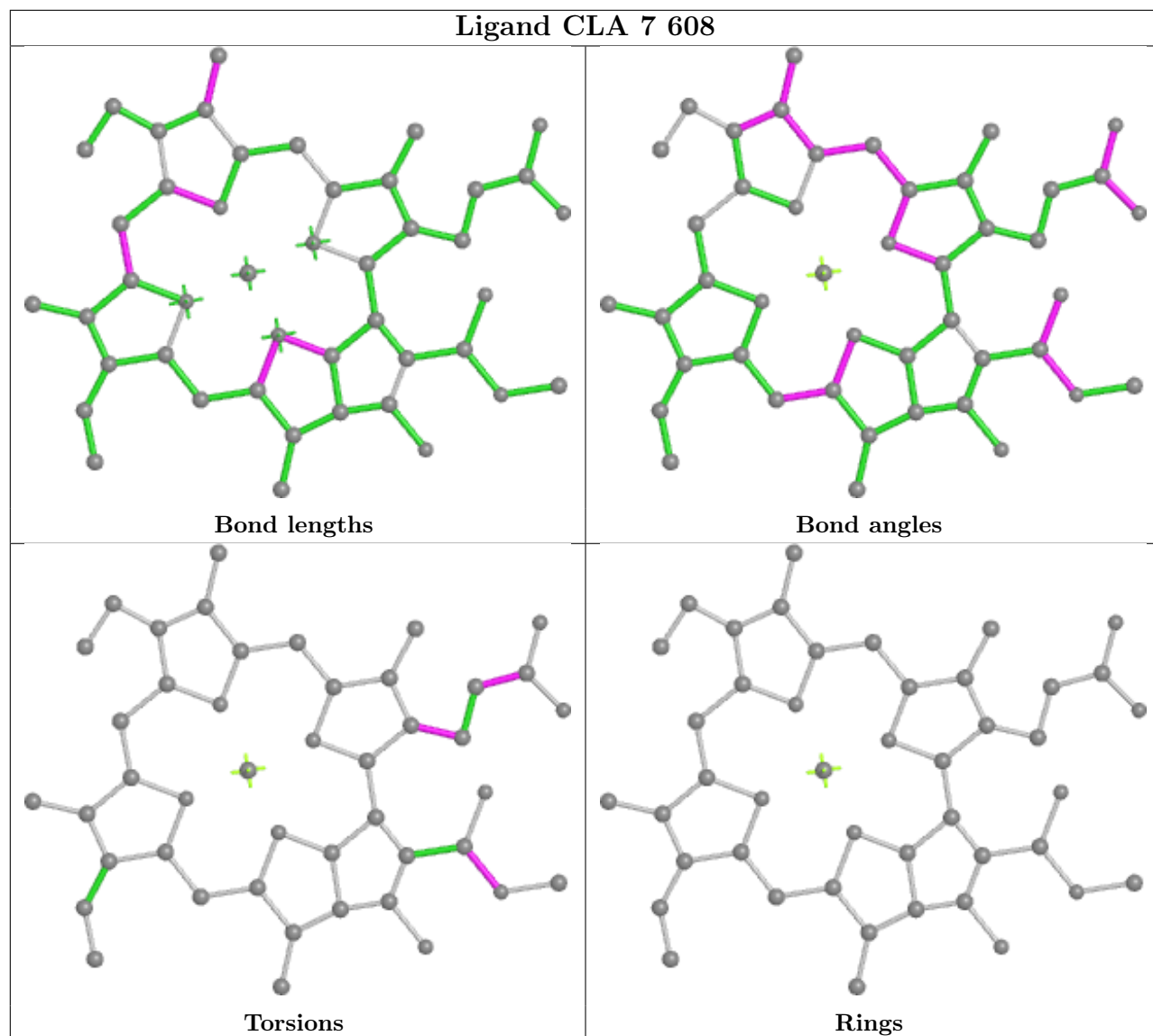


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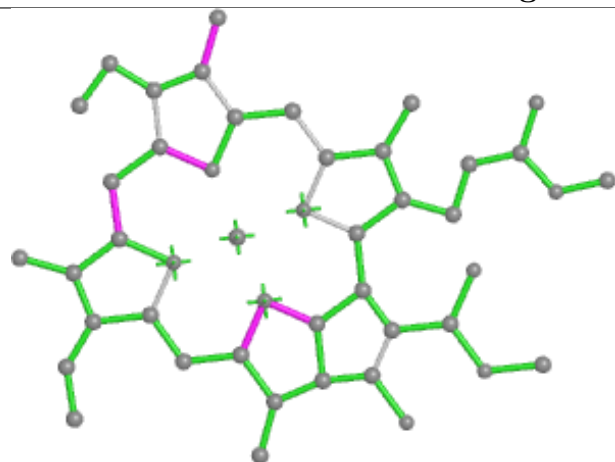


Rings

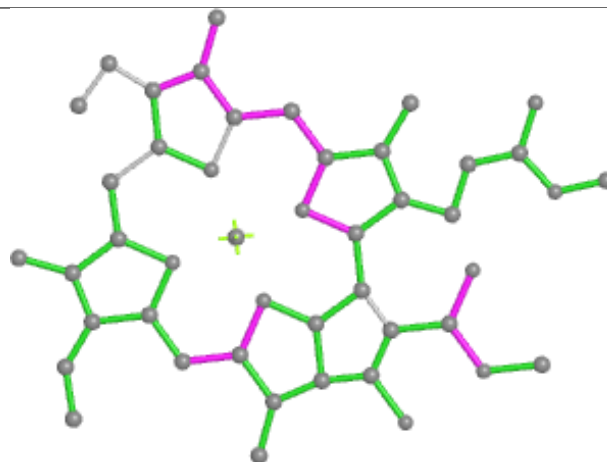
Ligand CLA 7 608



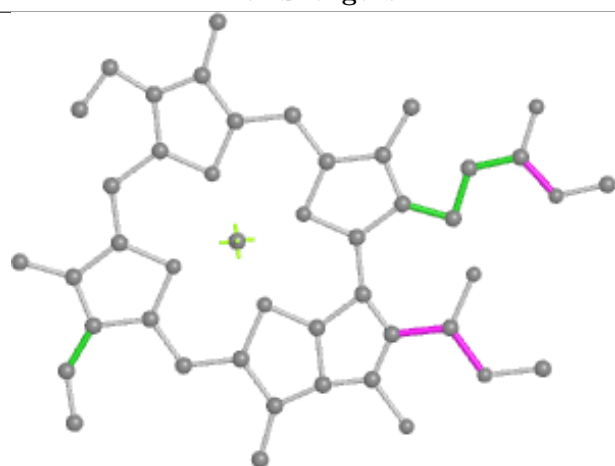
Ligand CLA h 609



Bond lengths



Bond angles

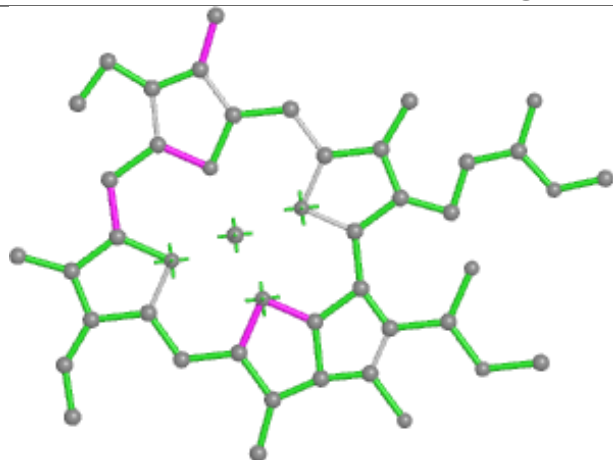


Torsions

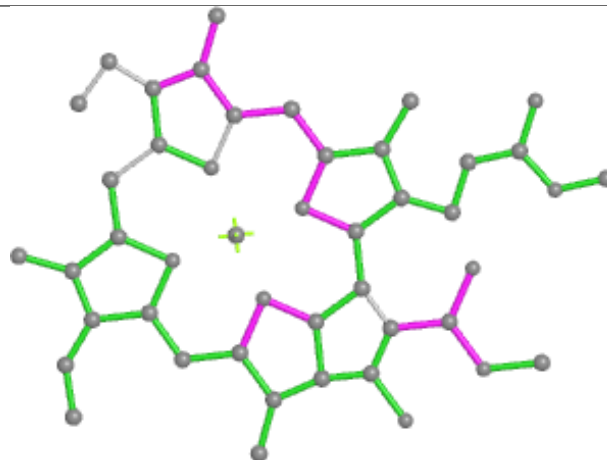


Rings

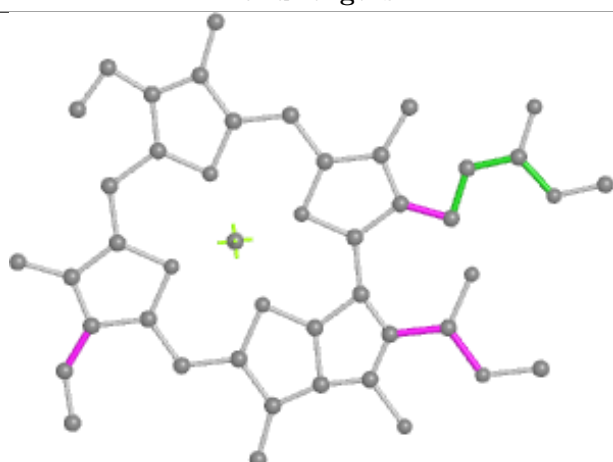
Ligand CLA h 610



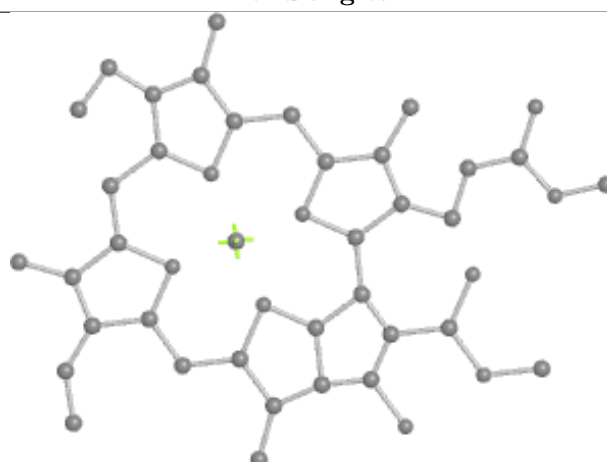
Bond lengths



Bond angles

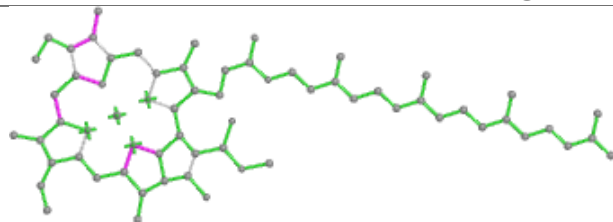


Torsions

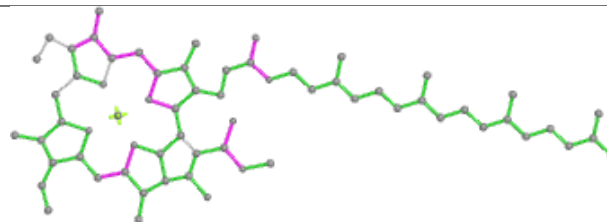


Rings

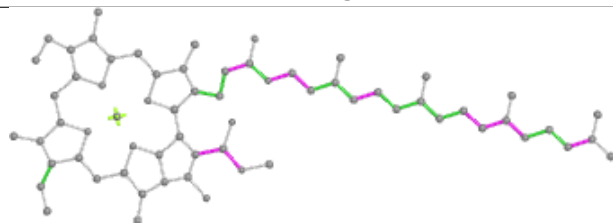
Ligand CLA 1 317



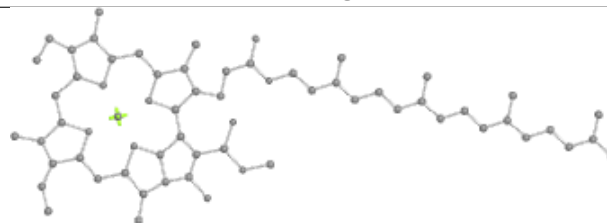
Bond lengths



Bond angles

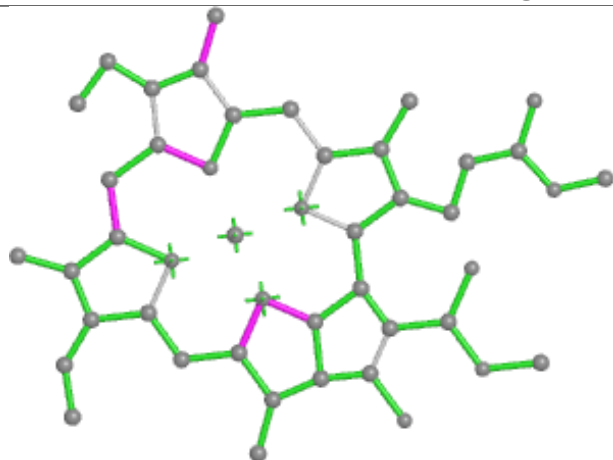


Torsions

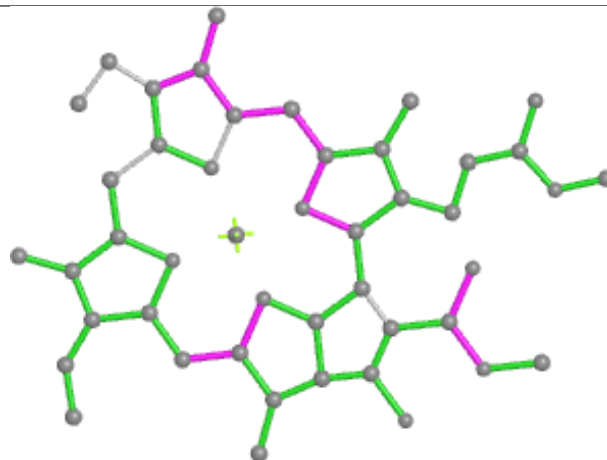


Rings

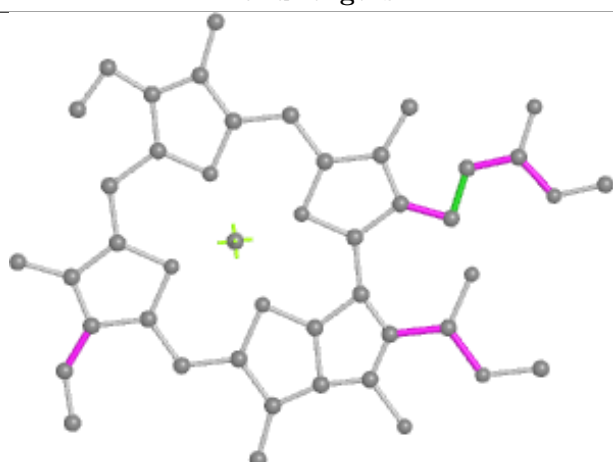
Ligand CLA k 302



Bond lengths



Bond angles

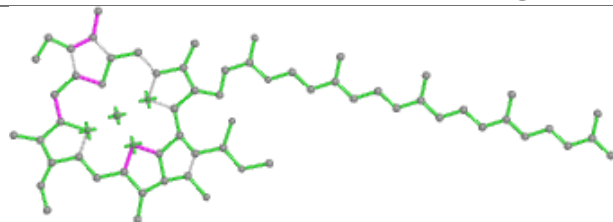


Torsions

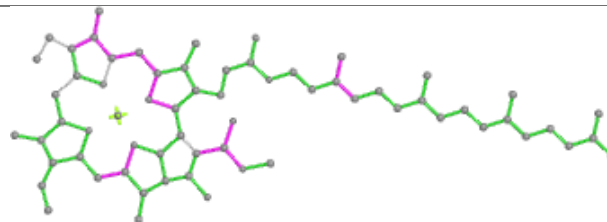


Rings

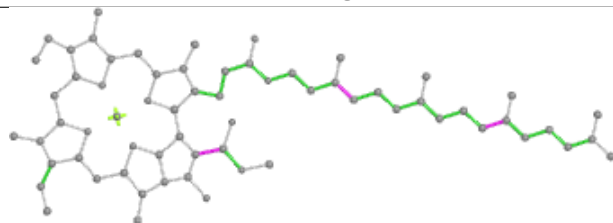
Ligand CLA A 833



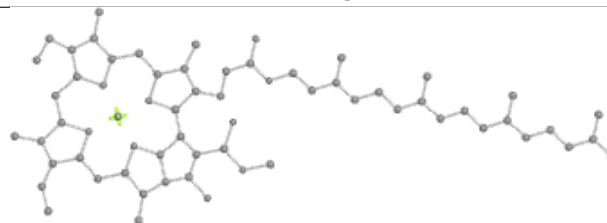
Bond lengths



Bond angles

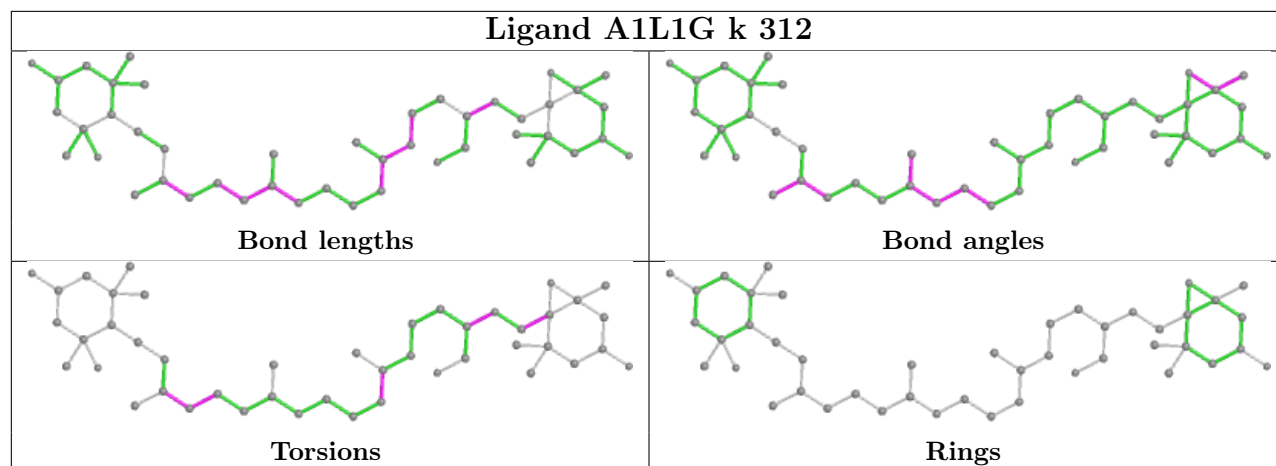


Torsions

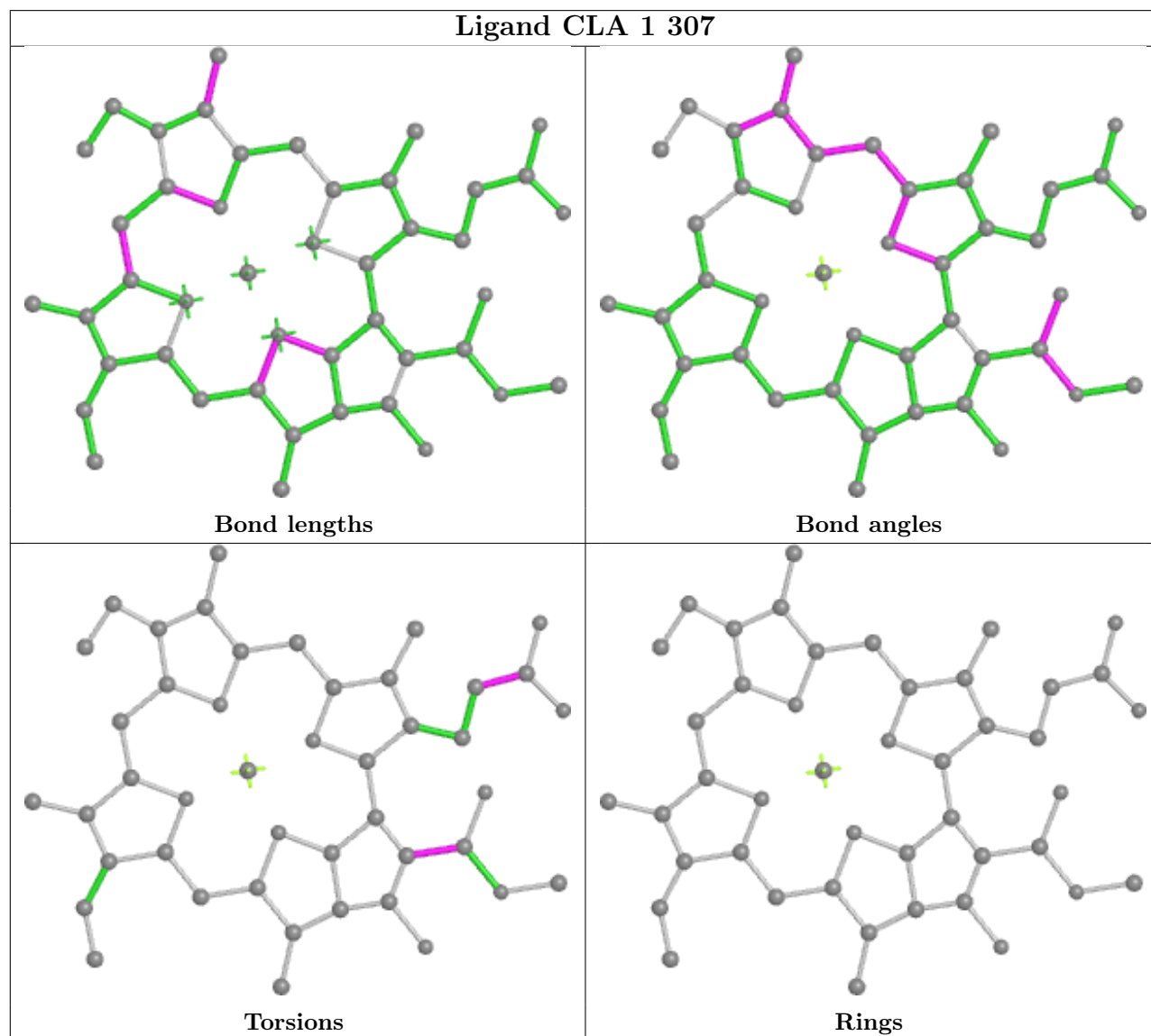


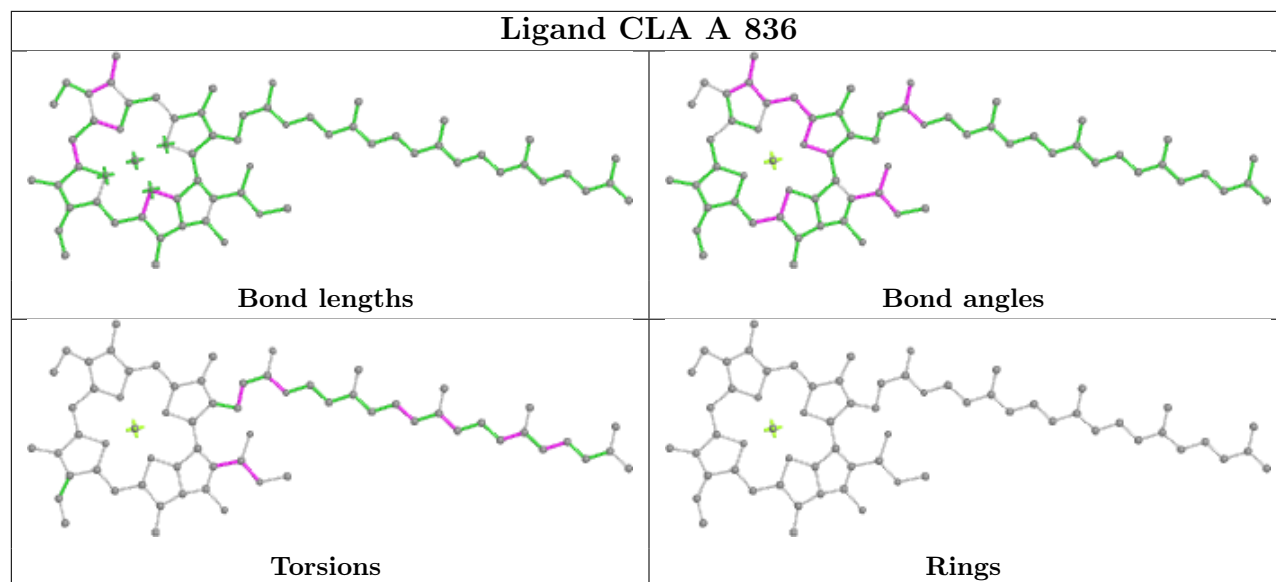
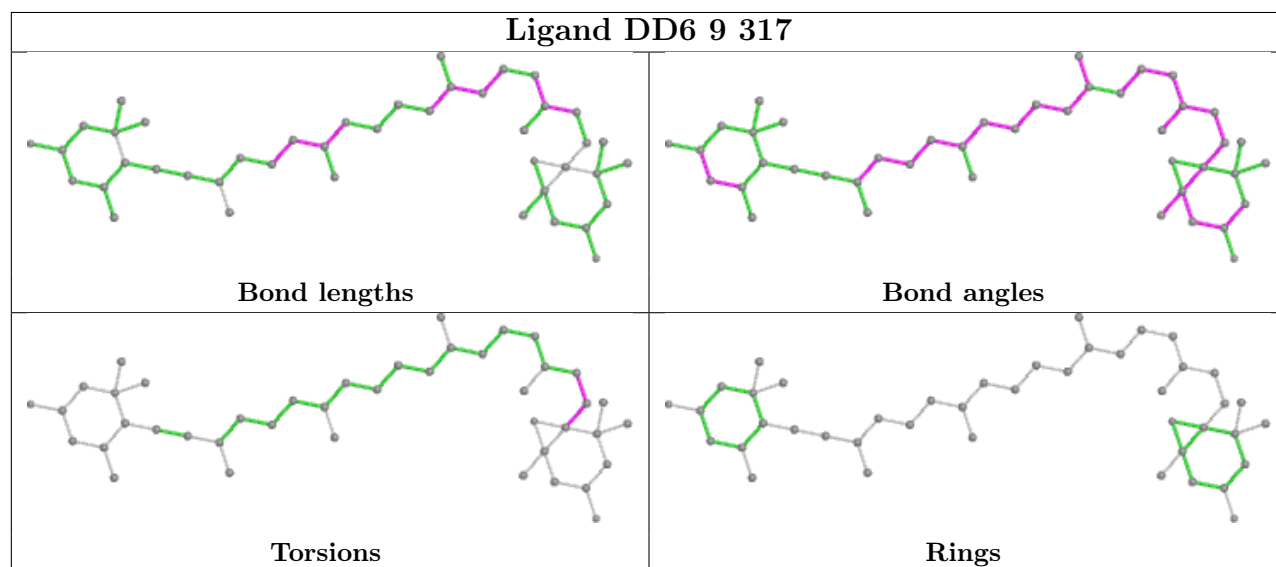
Rings

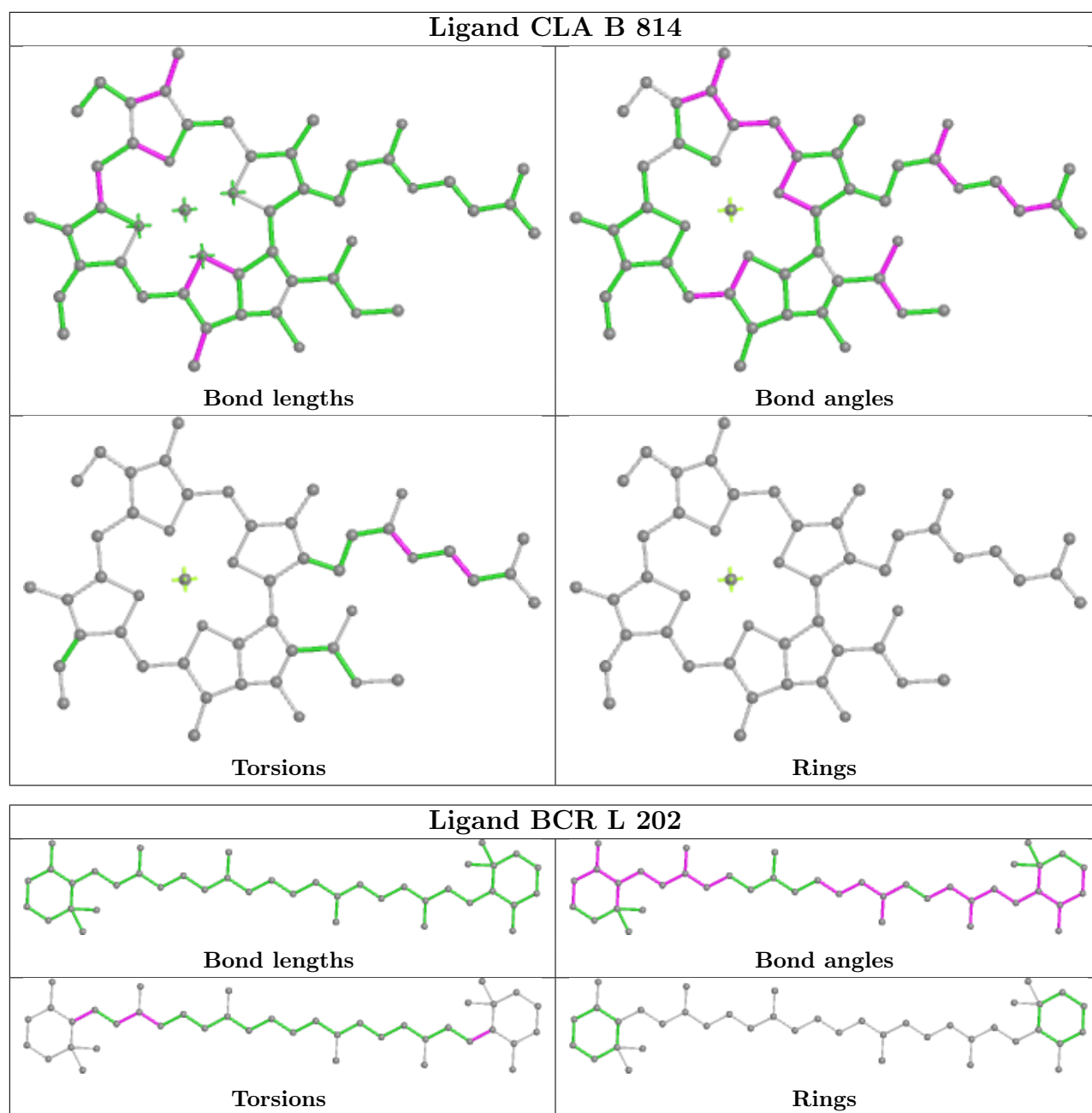
Ligand A1L1G k 312



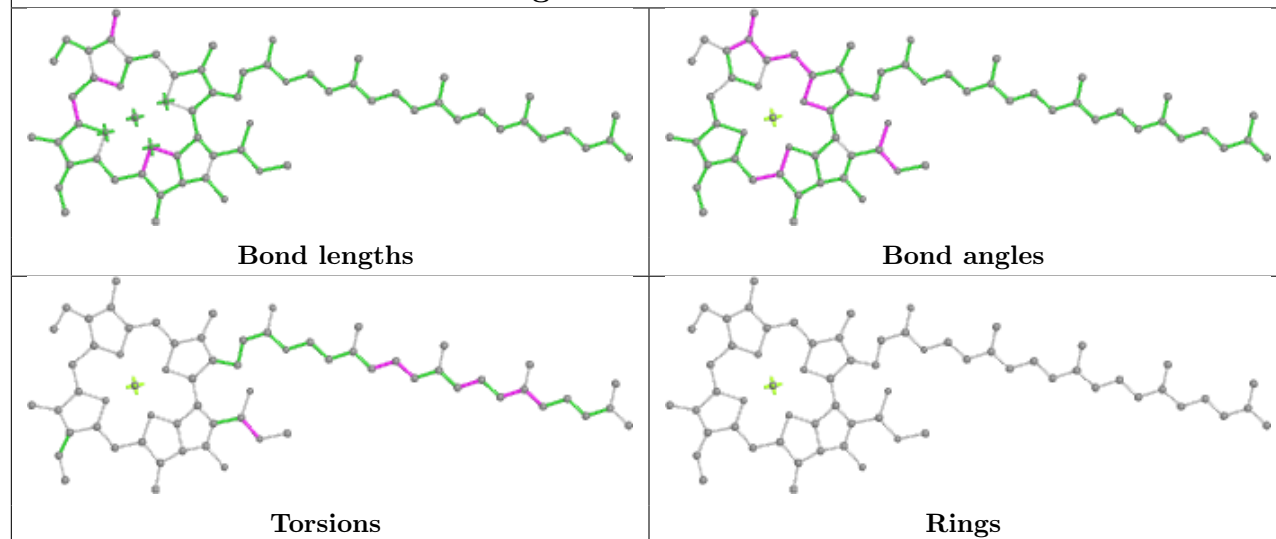
Ligand CLA 1 307



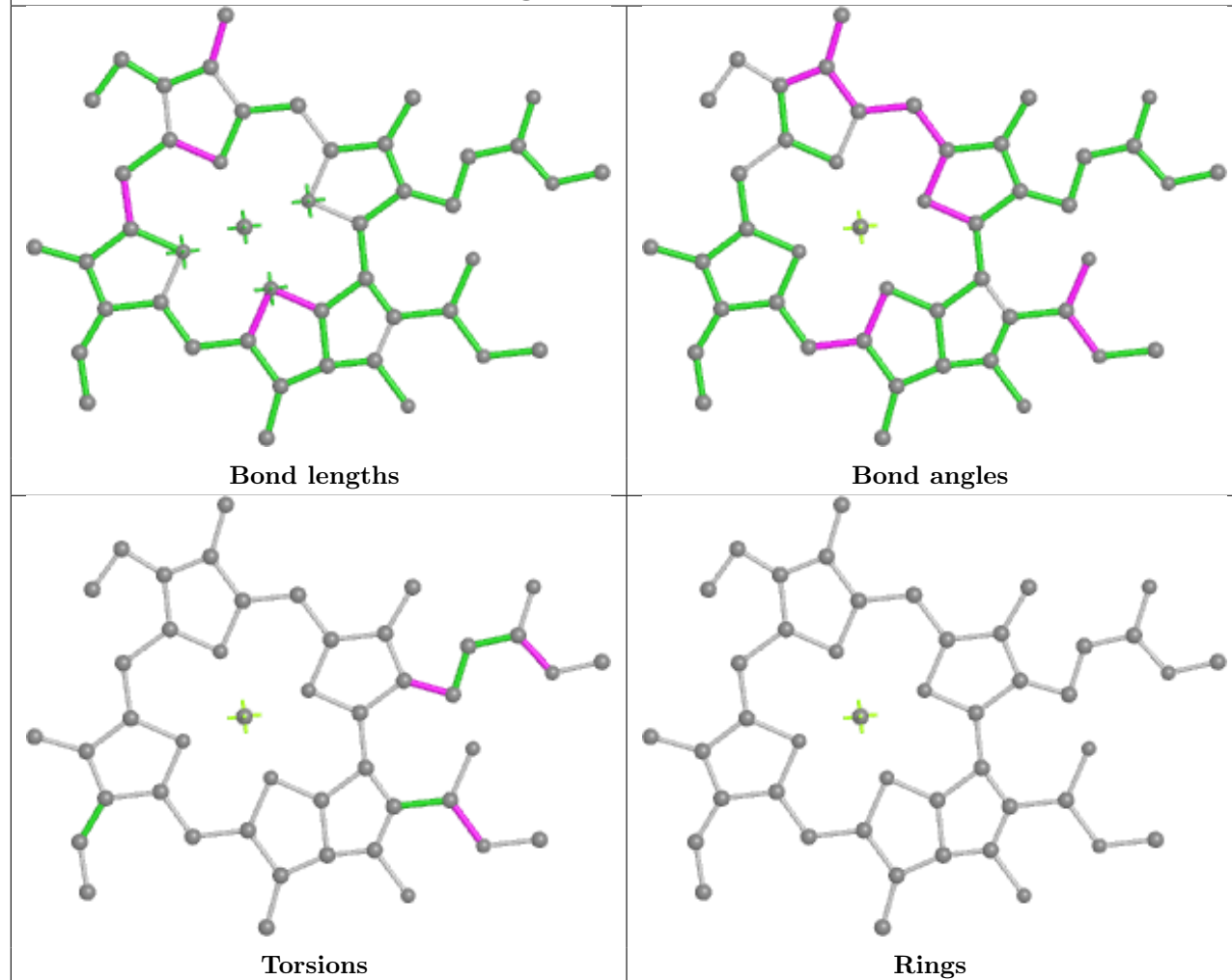
Ligand CLA A 836**Ligand DD6 9 317**

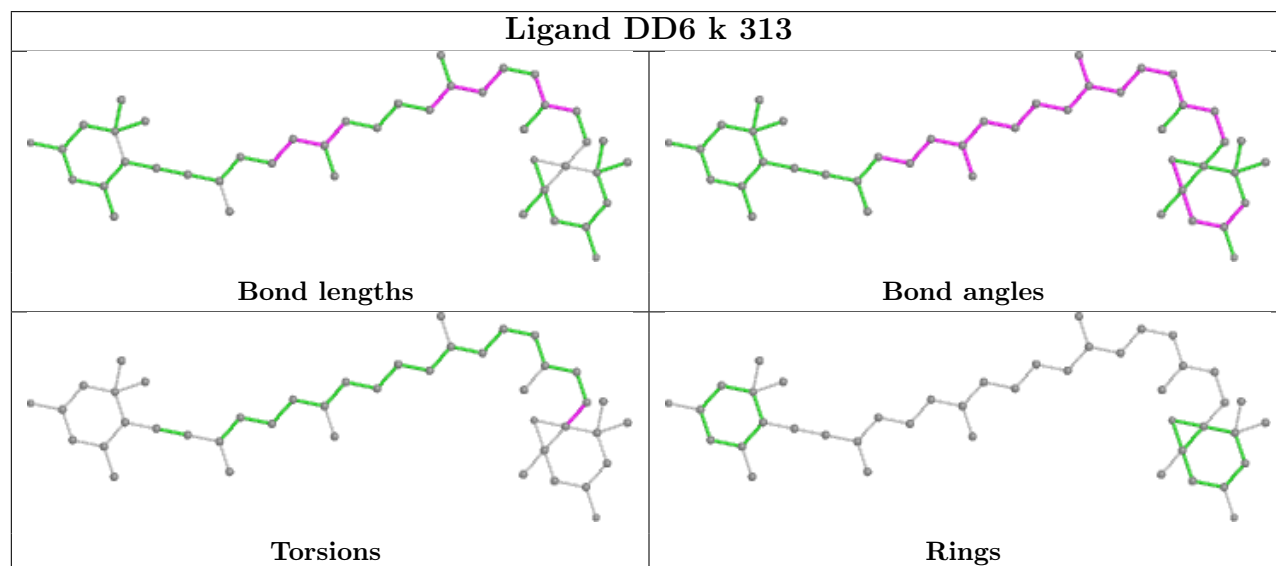
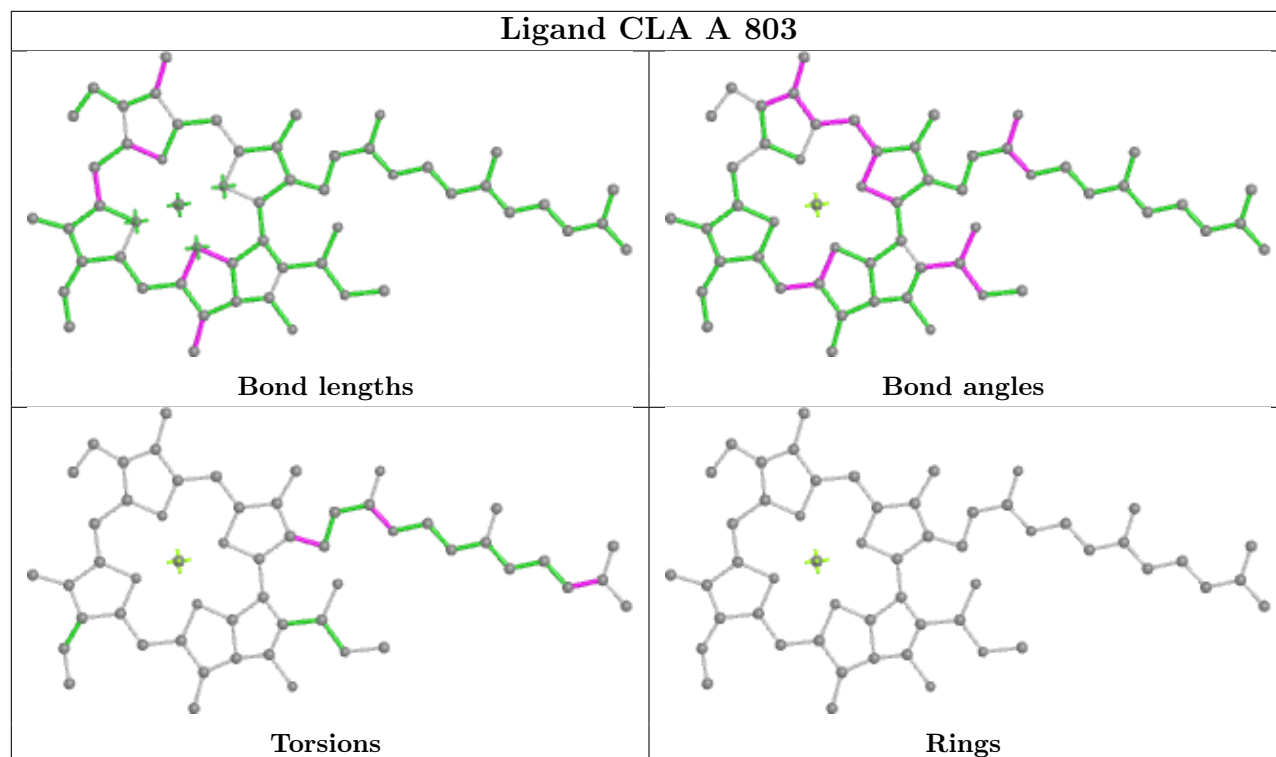
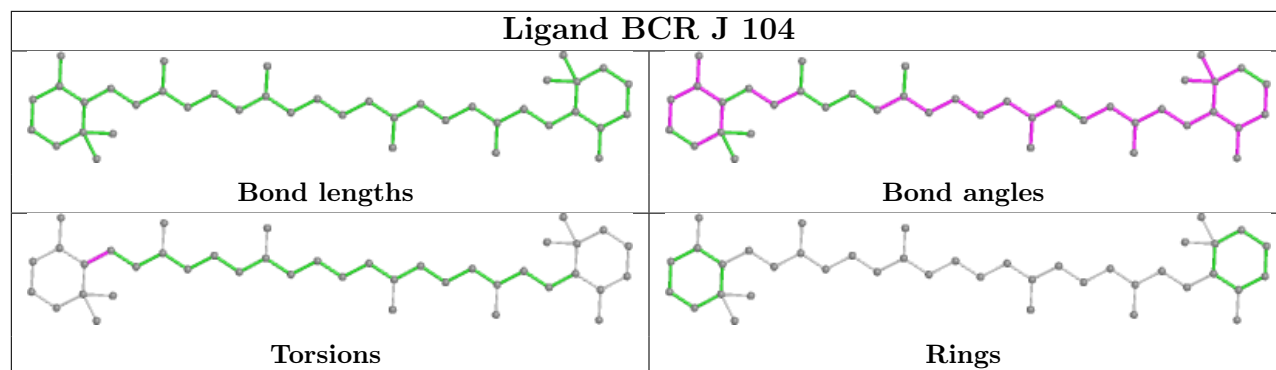


Ligand CLA B 806

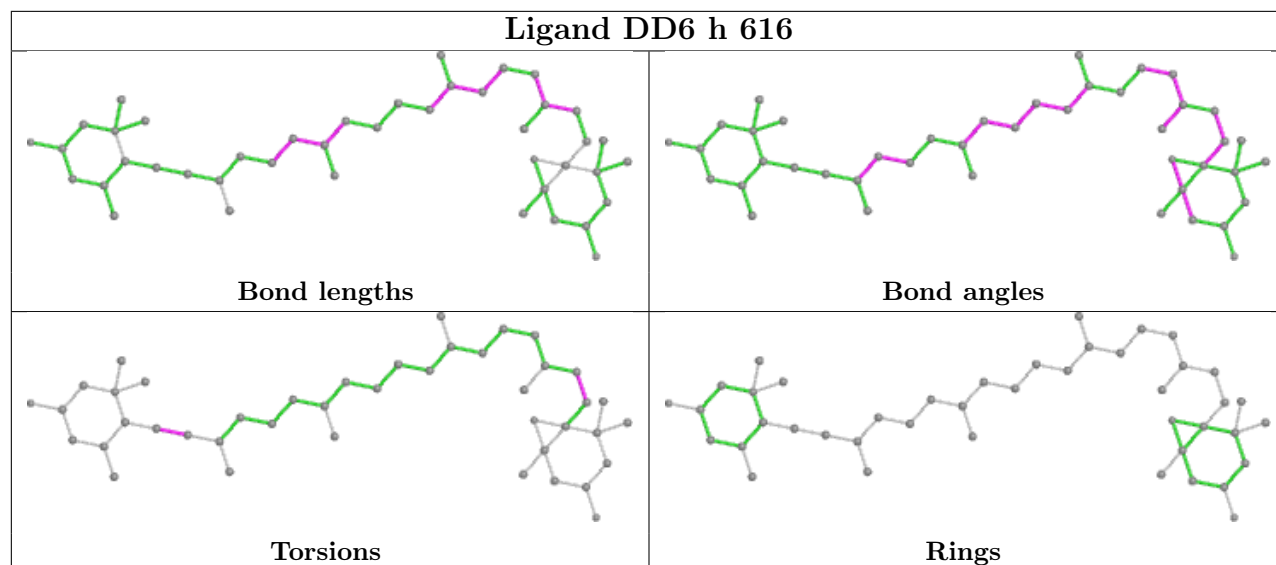


Ligand CLA 4 611

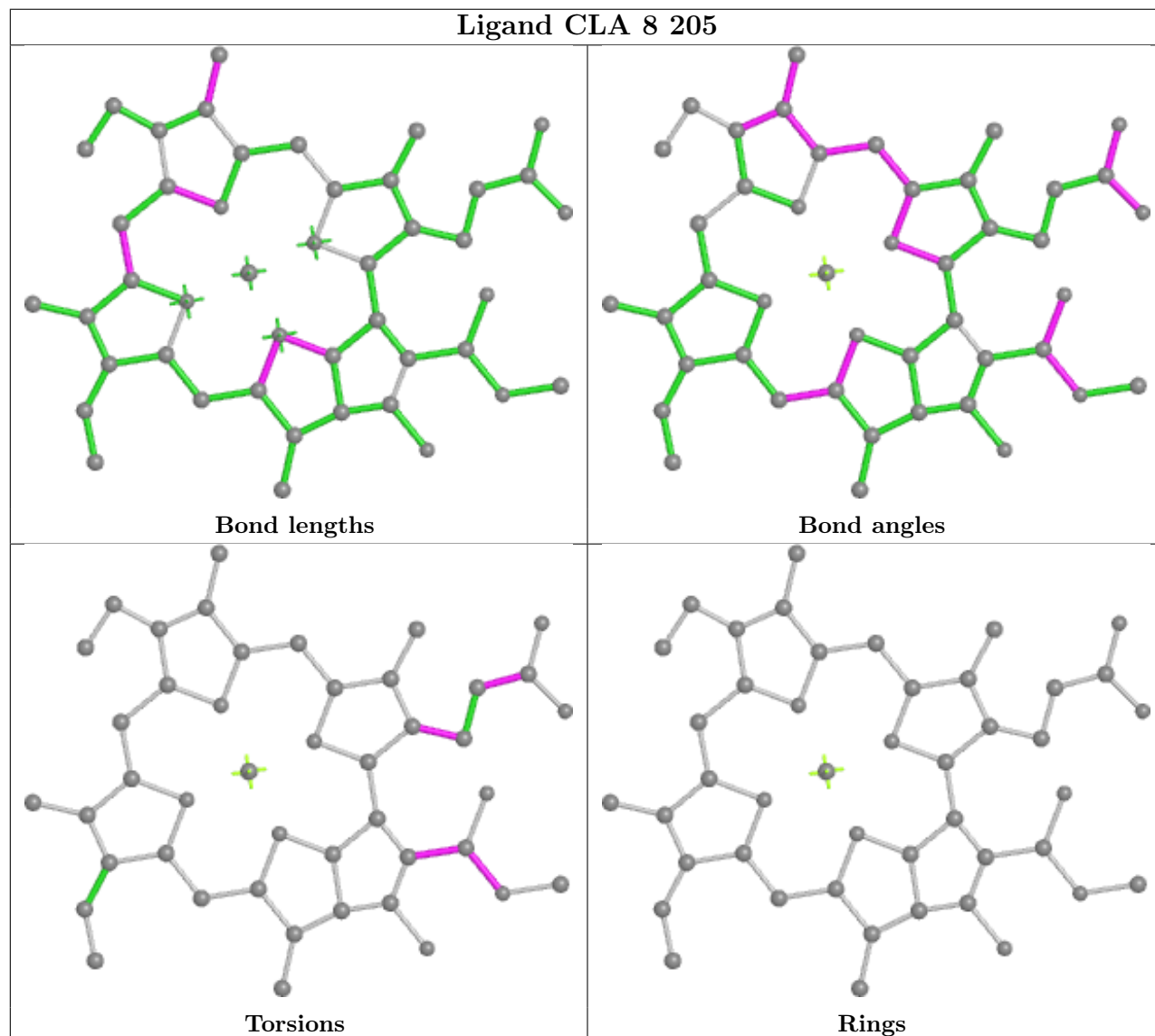




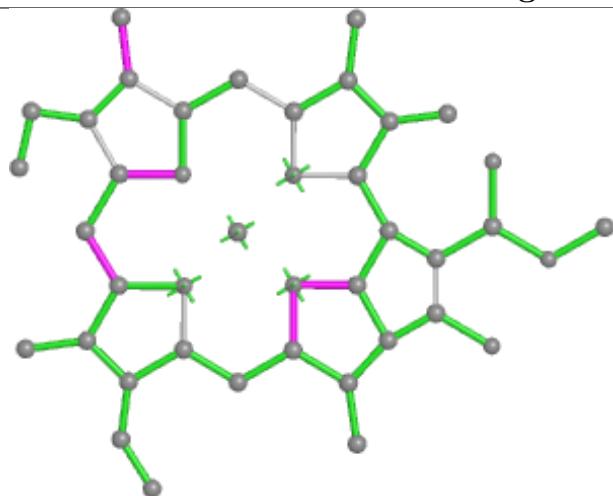
Ligand DD6 h 616



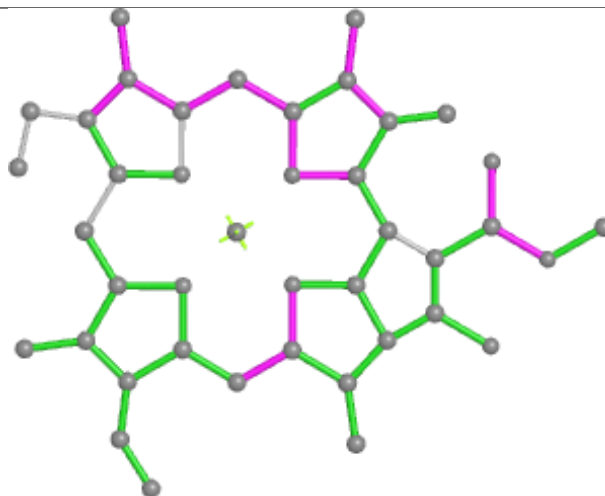
Ligand CLA 8 205



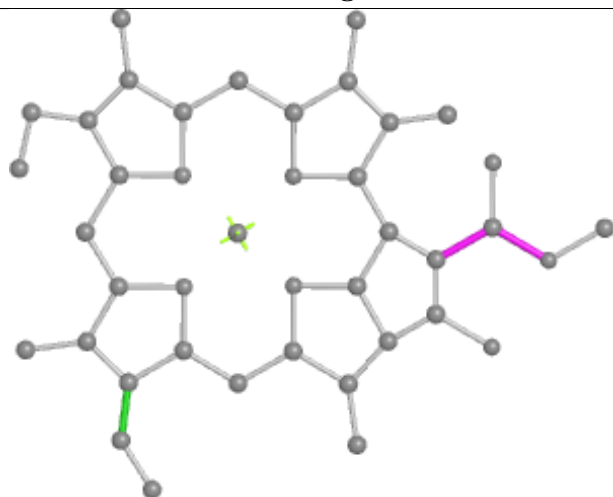
Ligand CLA 8 209



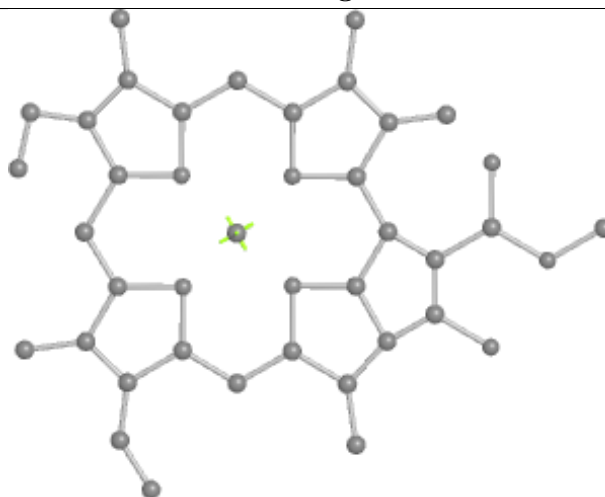
Bond lengths



Bond angles

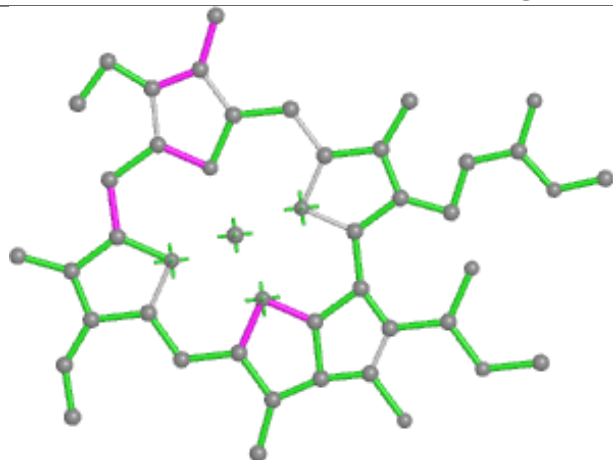


Torsions

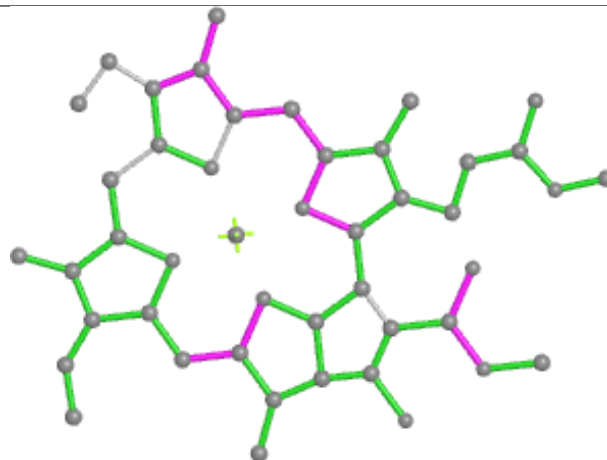


Rings

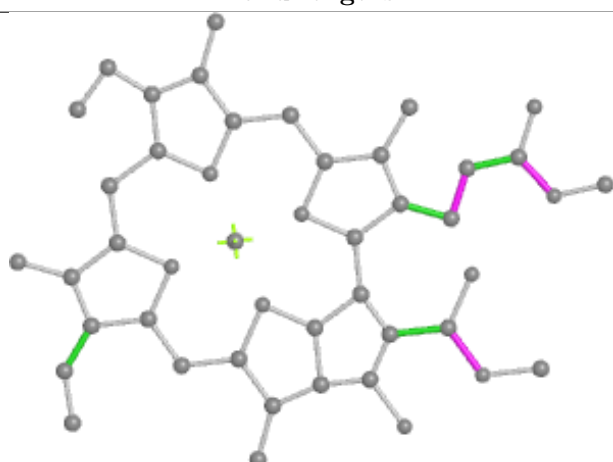
Ligand CLA h 608



Bond lengths



Bond angles

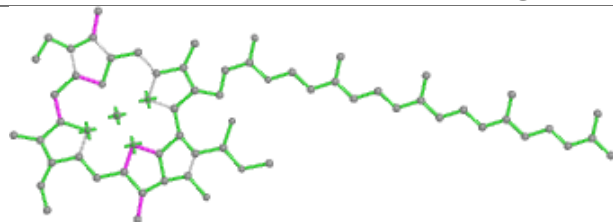


Torsions

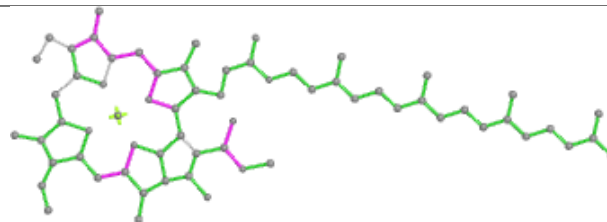


Rings

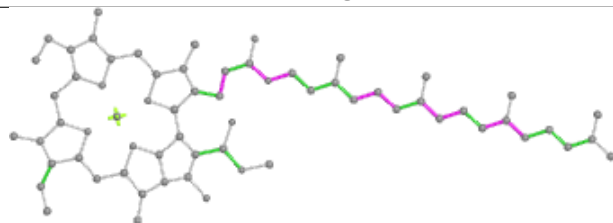
Ligand CLA B 801



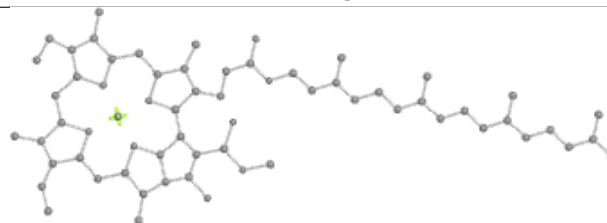
Bond lengths



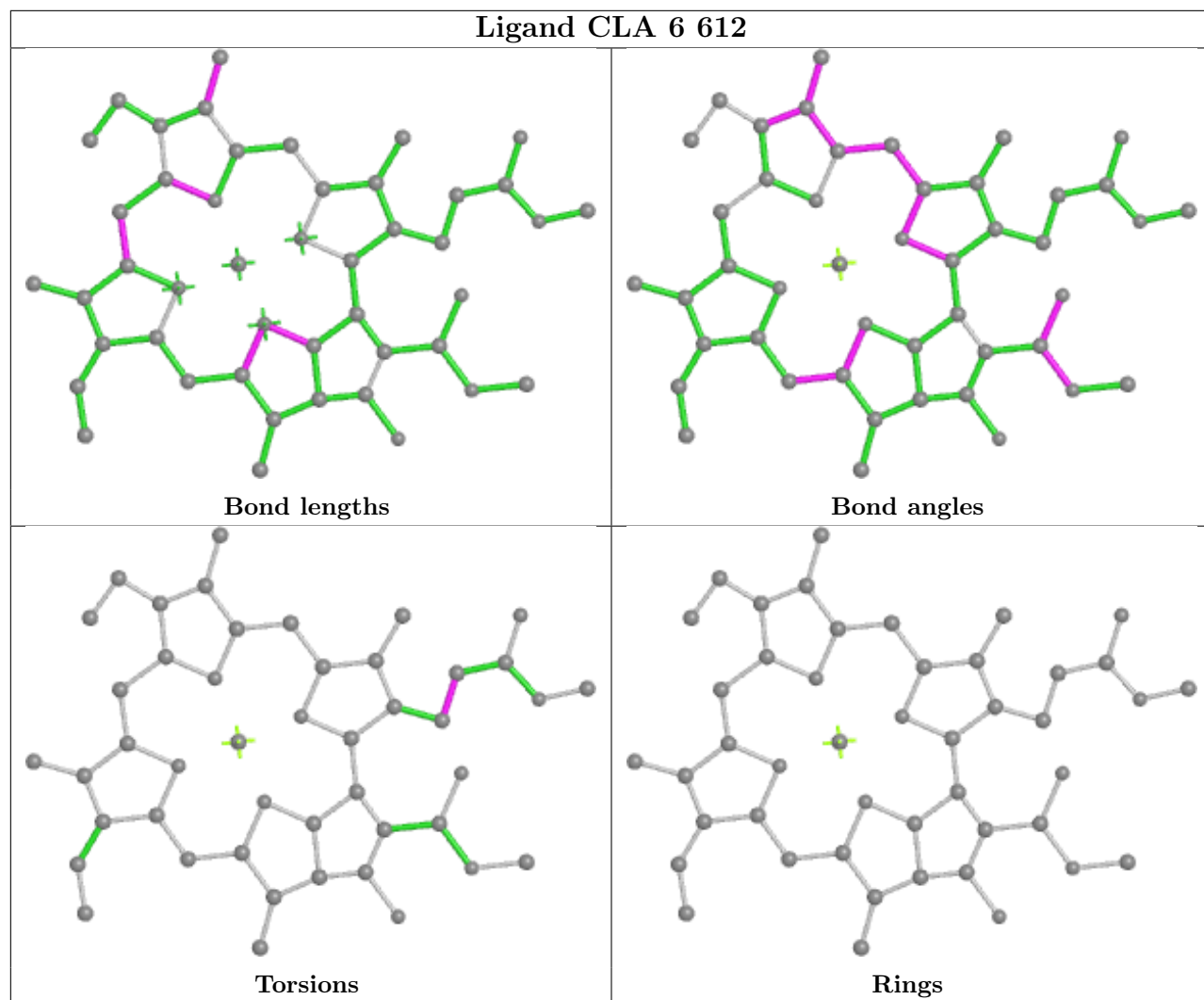
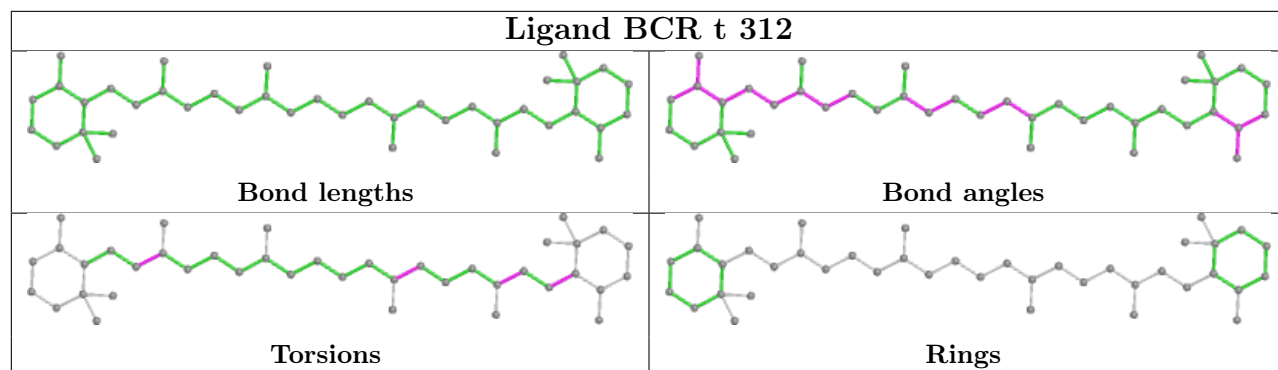
Bond angles



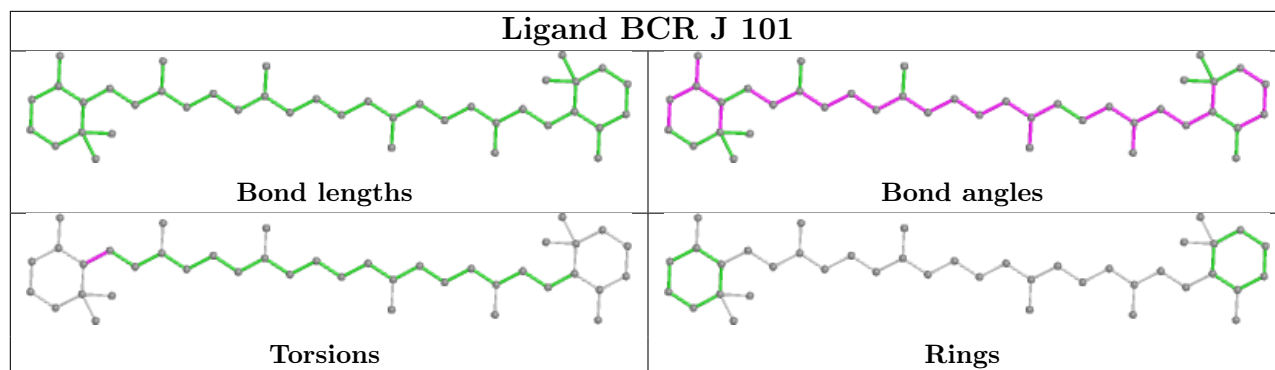
Torsions



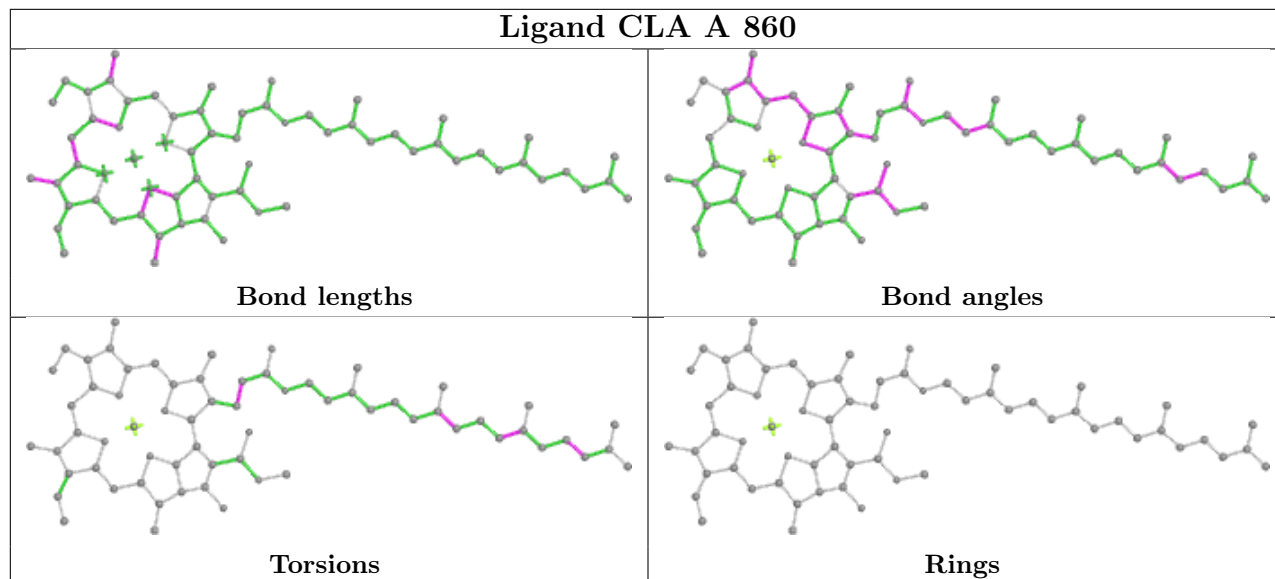
Rings



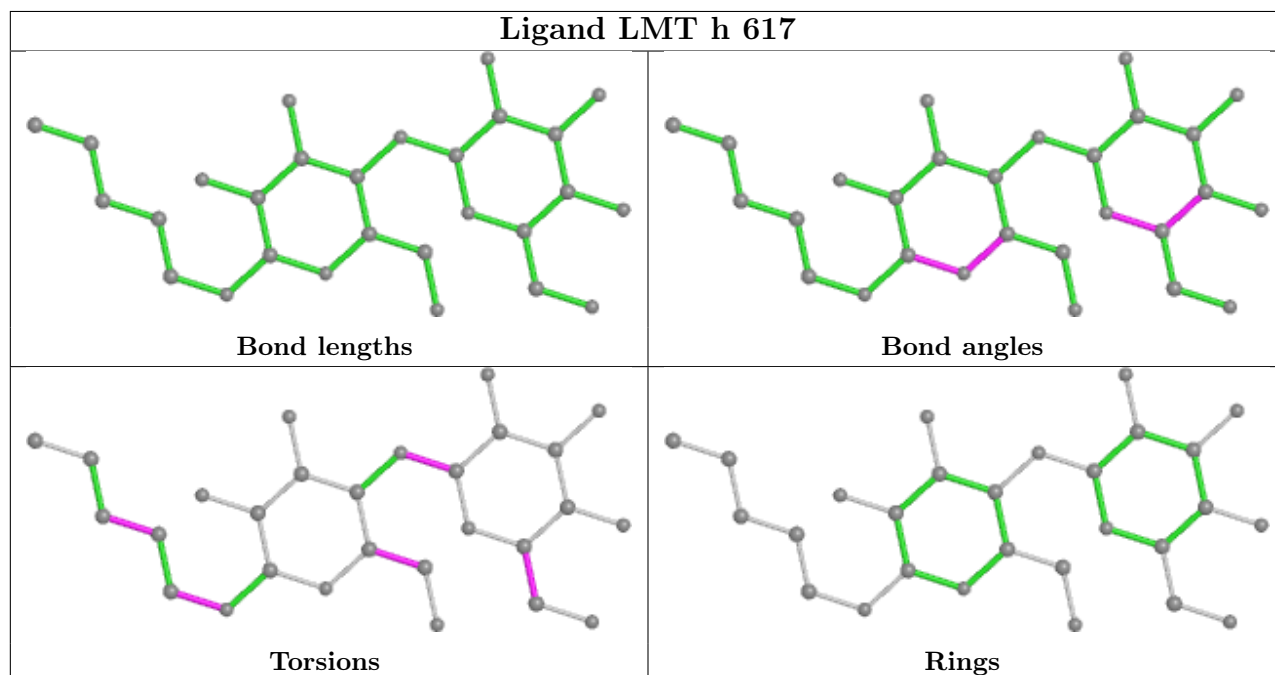
Ligand BCR J 101

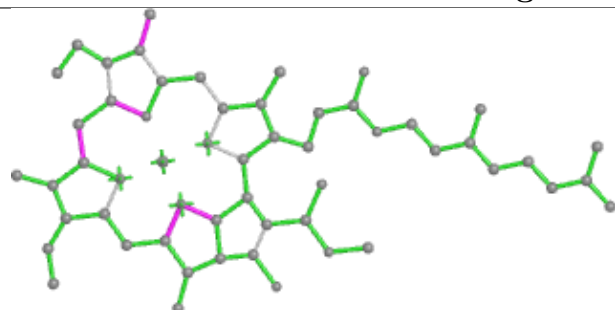
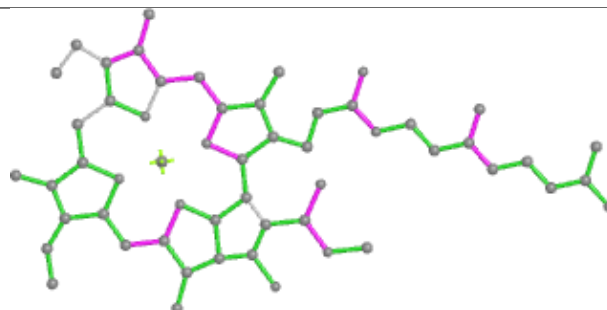
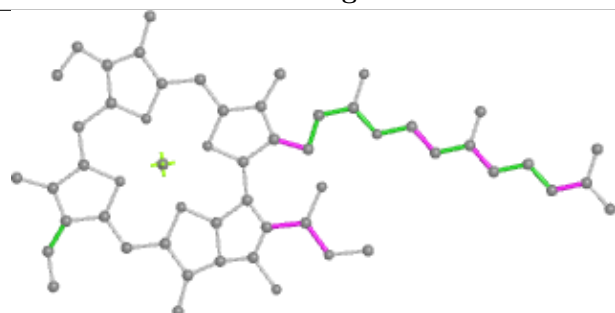
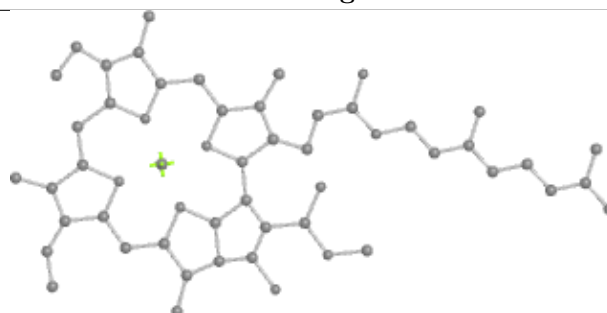
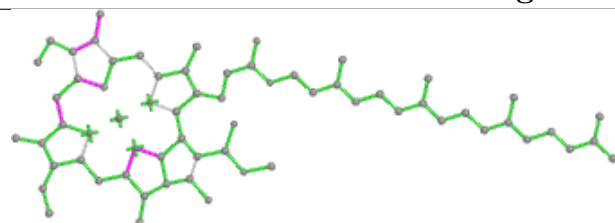
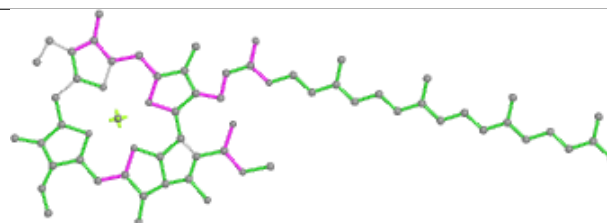
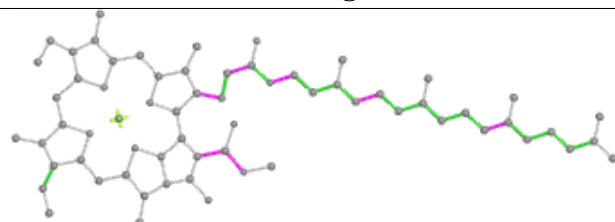
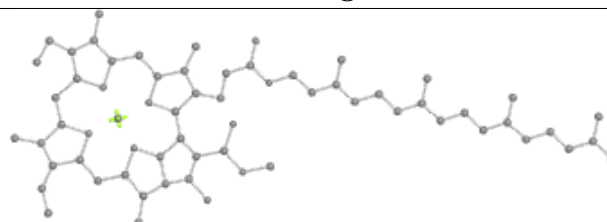


Ligand CLA A 860

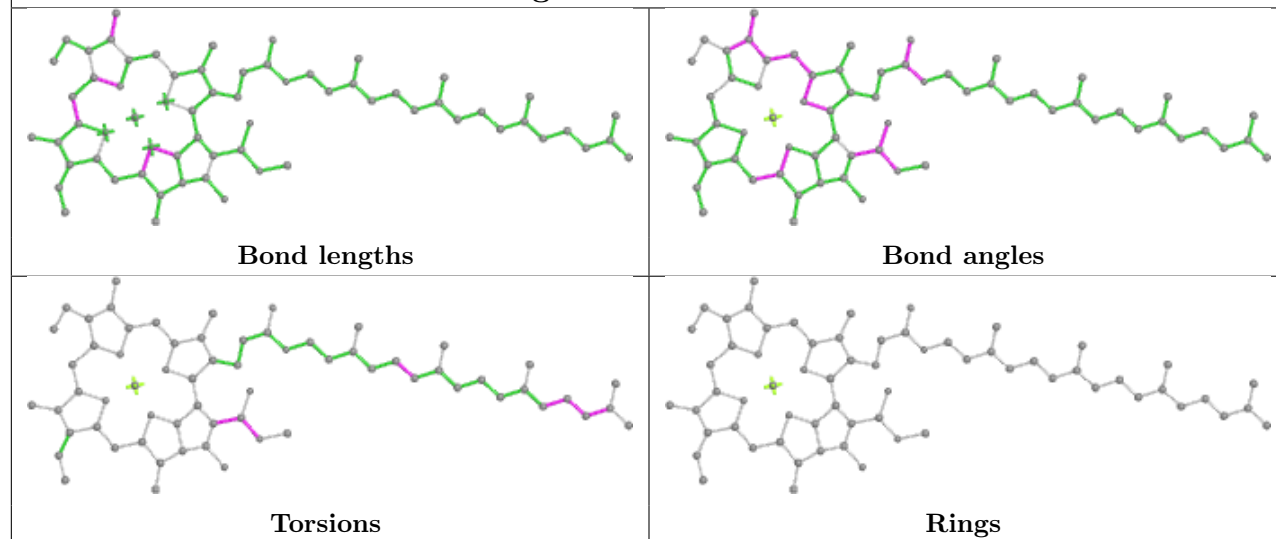


Ligand LMT h 617

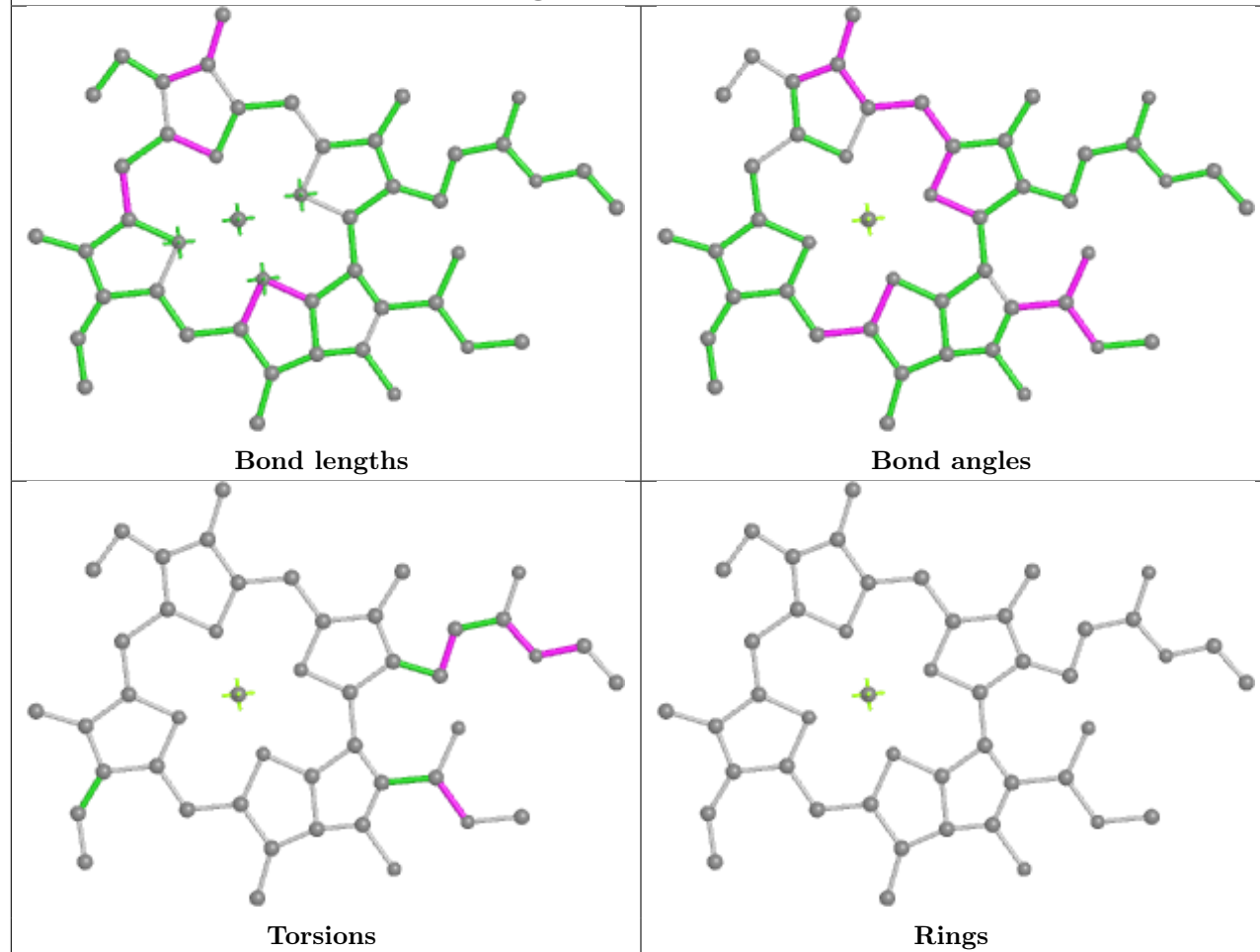


Ligand CLA B 815**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 809****Bond lengths****Bond angles****Torsions****Rings**

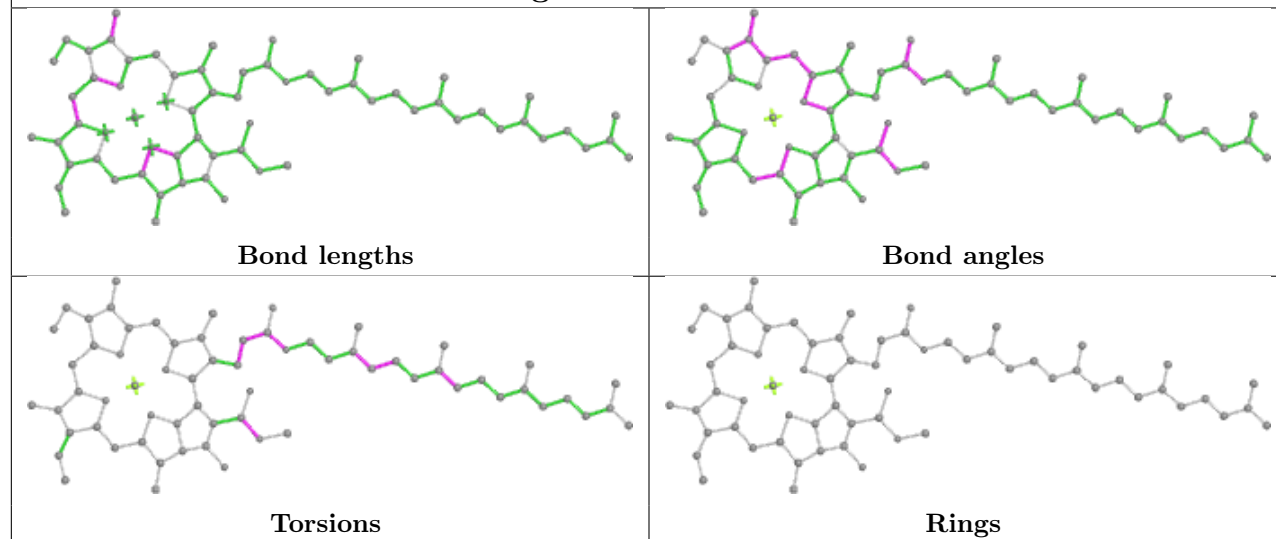
Ligand CLA B 834



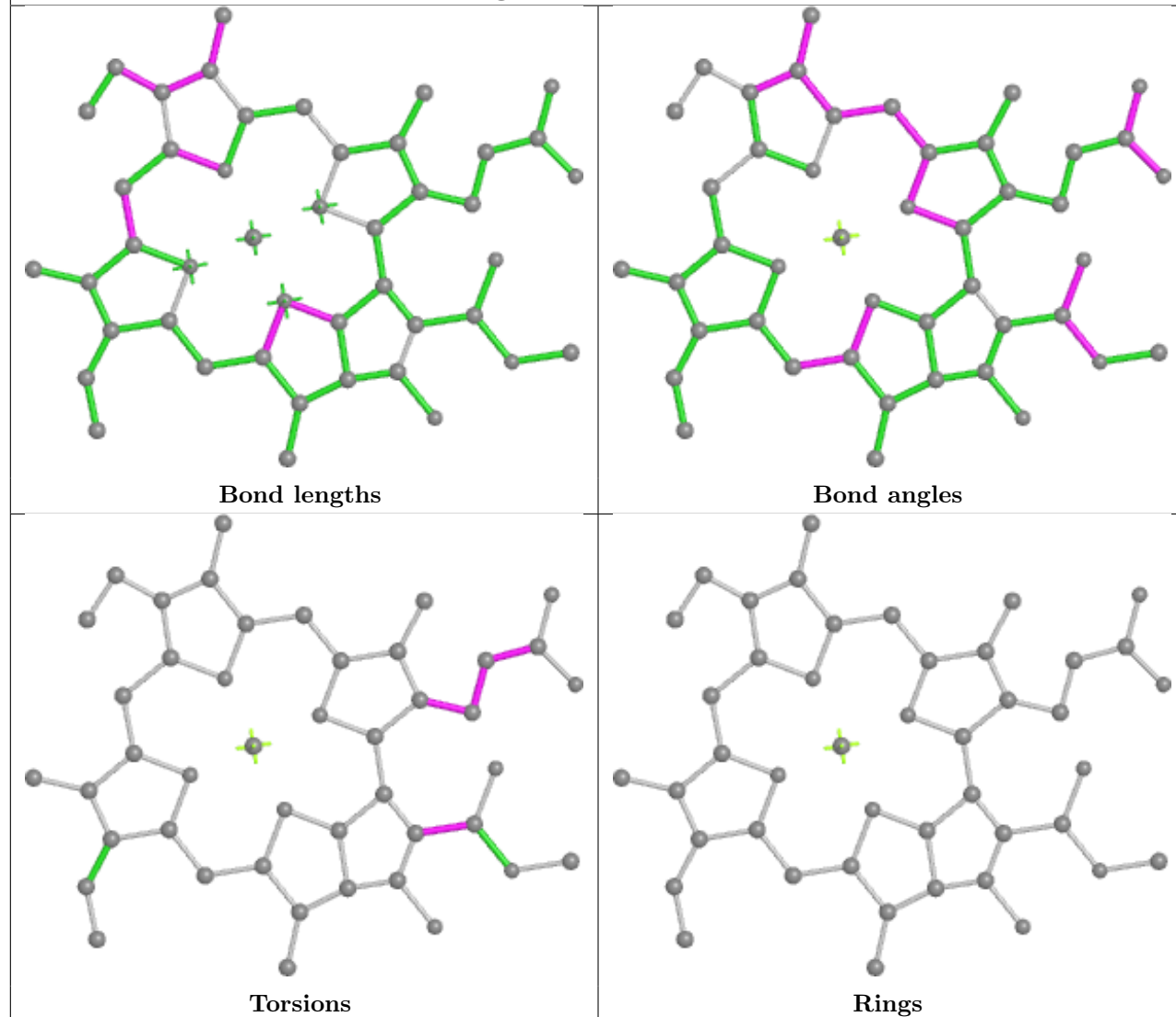
Ligand CLA 6 602

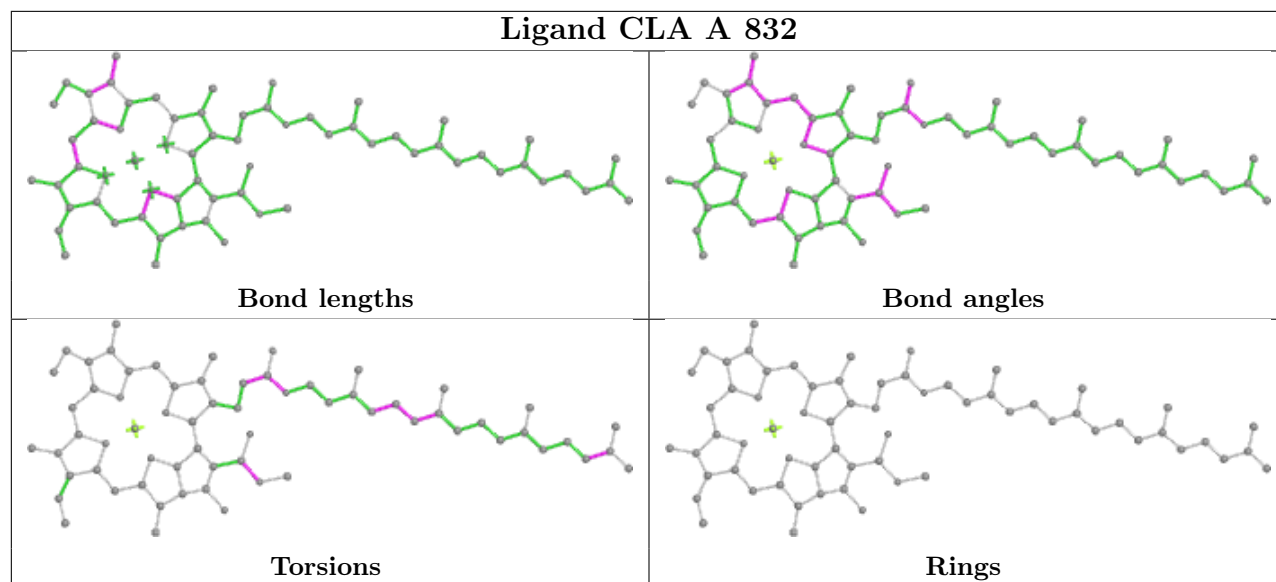
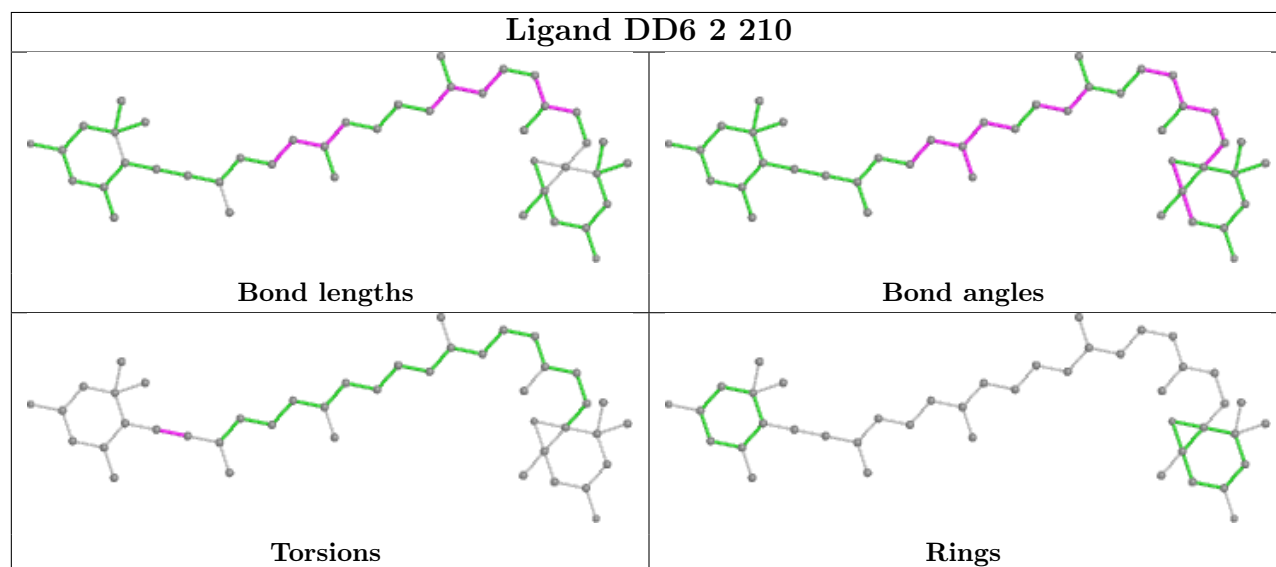


Ligand CLA A 820

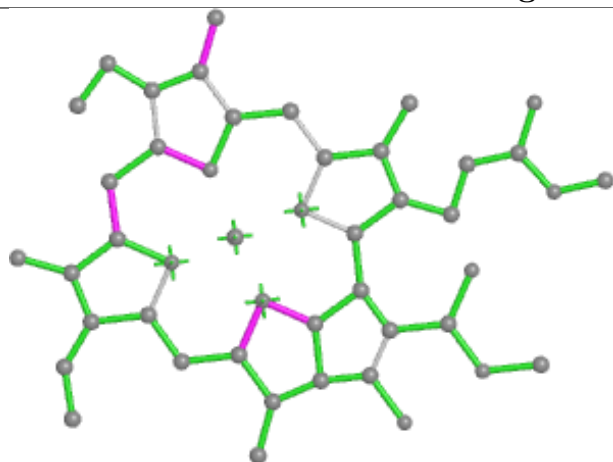


Ligand CLA h 612

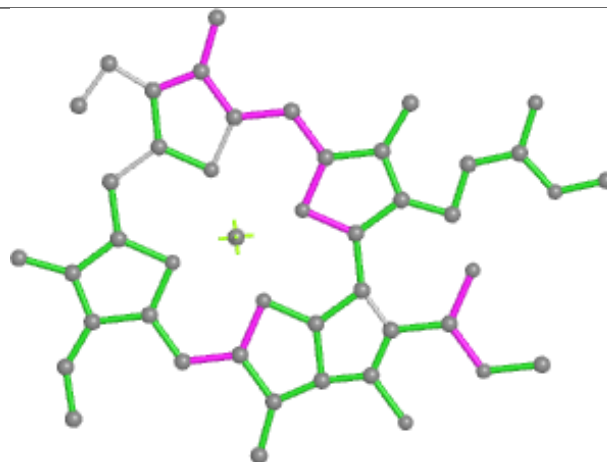


Ligand CLA A 832**Ligand DD6 2 210**

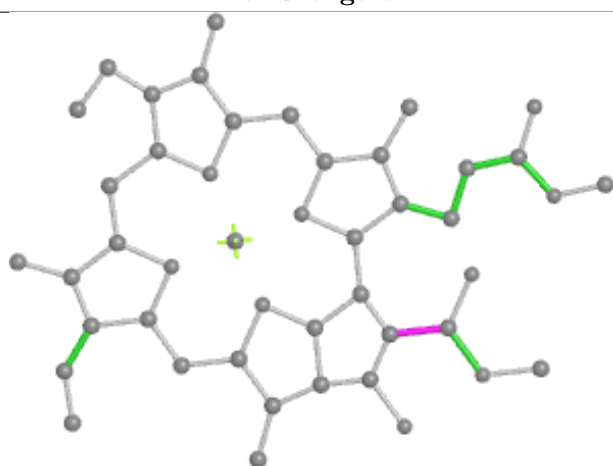
Ligand CLA 5 604



Bond lengths



Bond angles

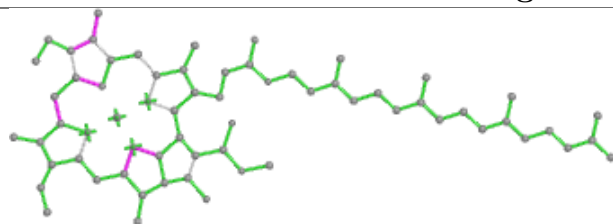


Torsions

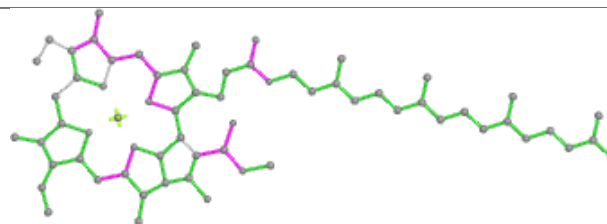


Rings

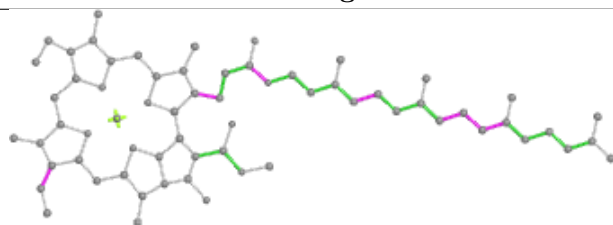
Ligand CLA L 204



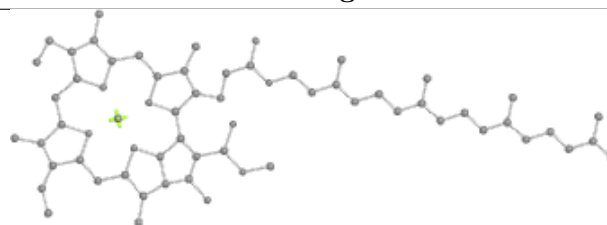
Bond lengths



Bond angles

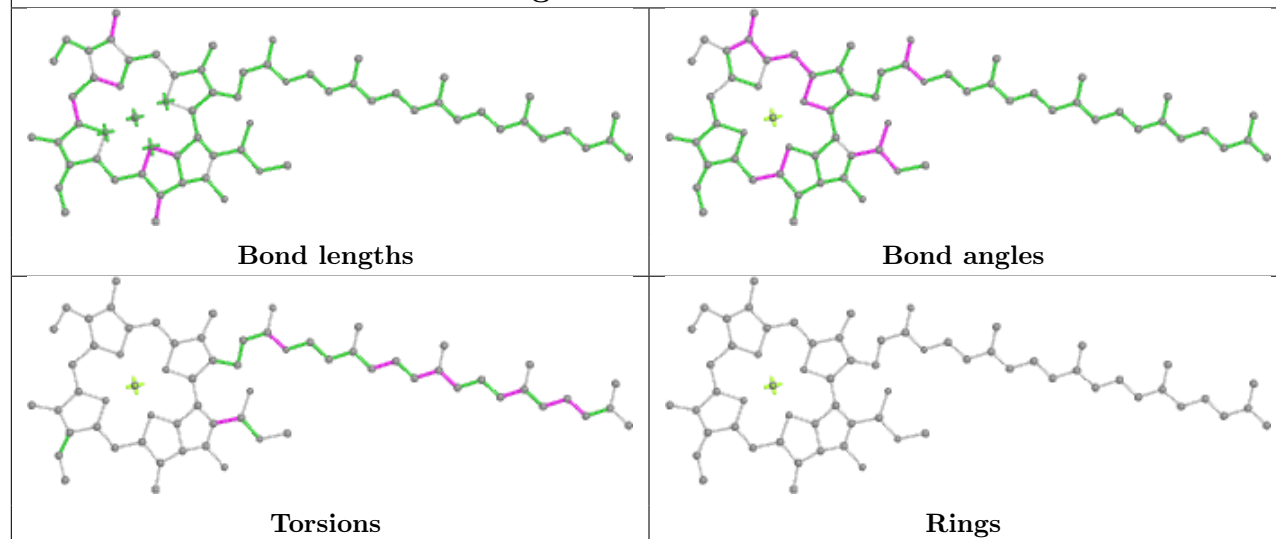


Torsions

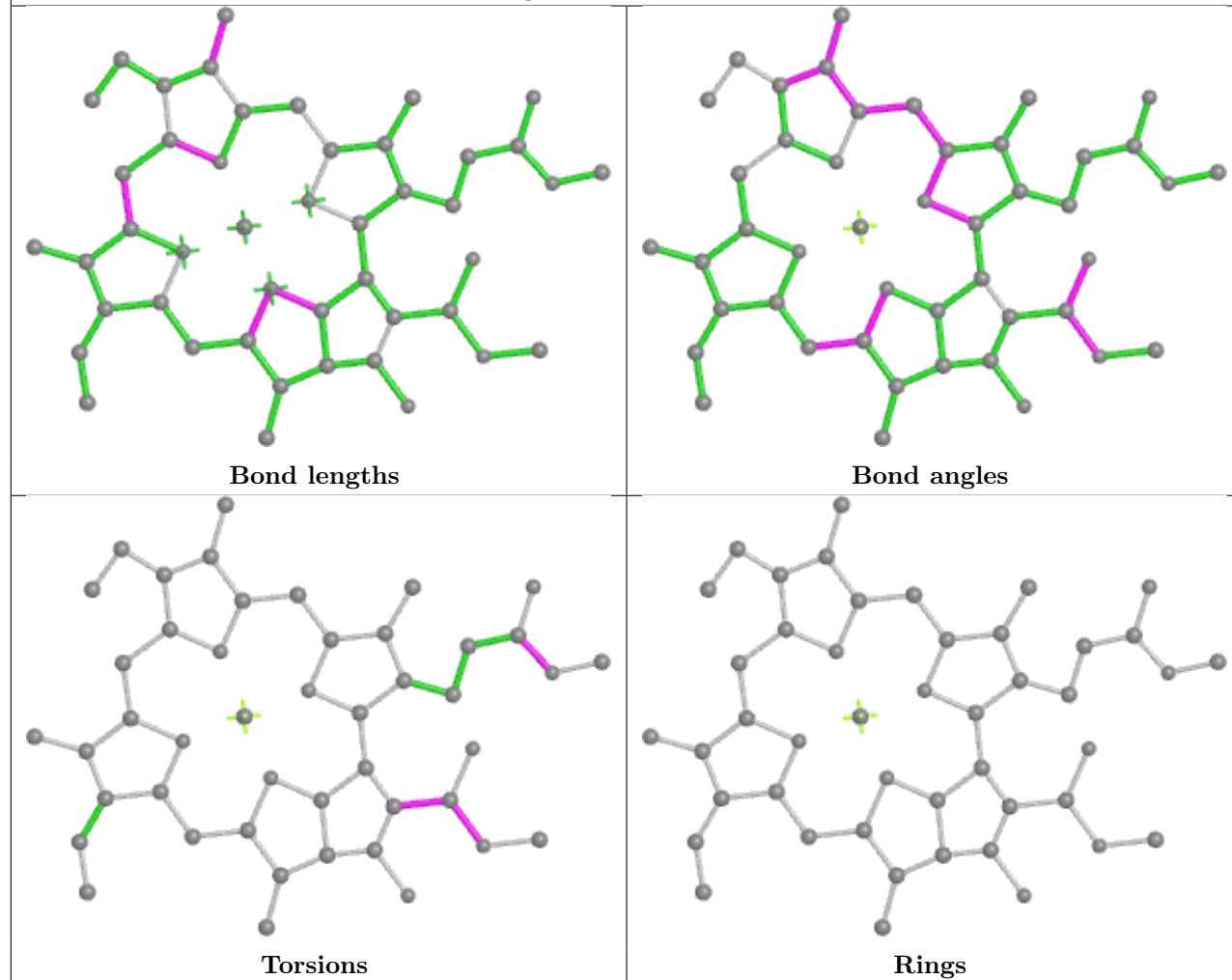


Rings

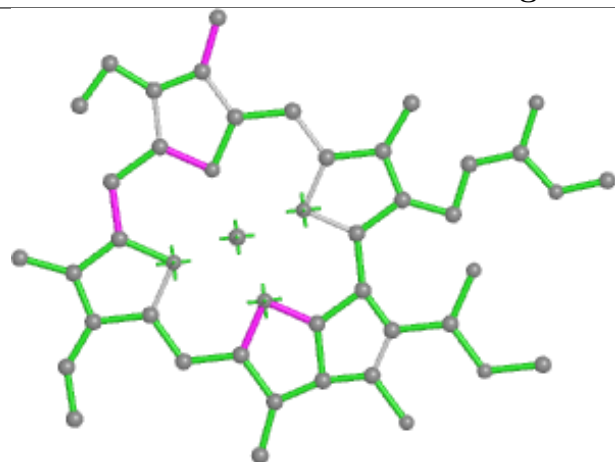
Ligand CLA B 827



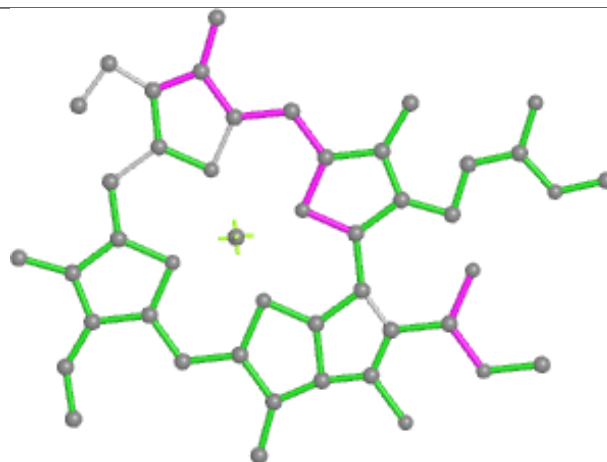
Ligand CLA t 305



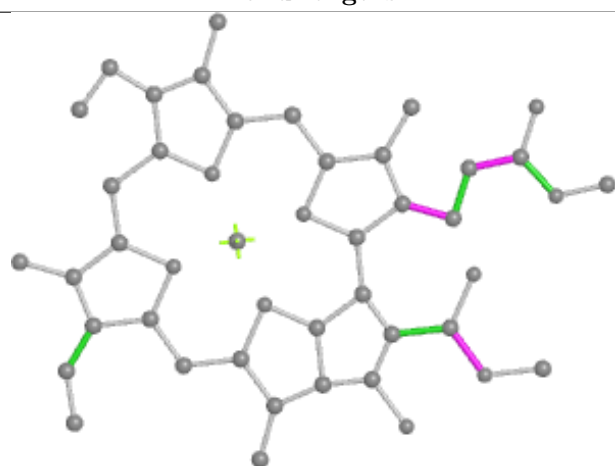
Ligand CLA k 305



Bond lengths



Bond angles

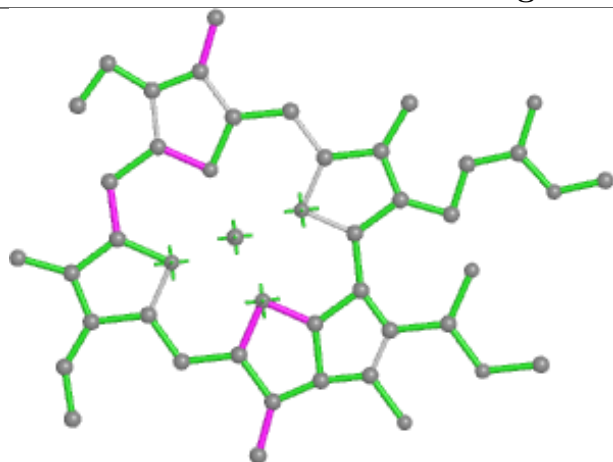


Torsions

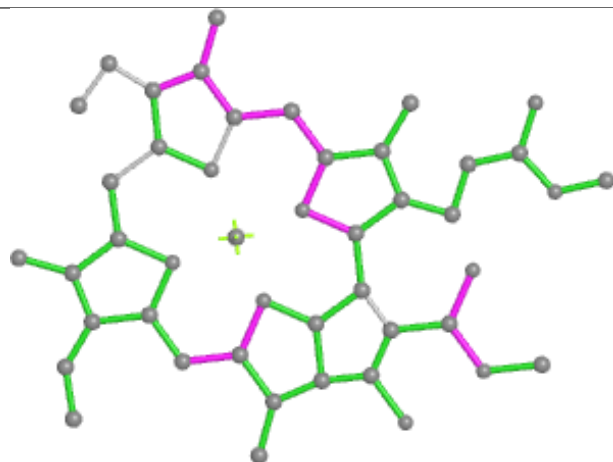


Rings

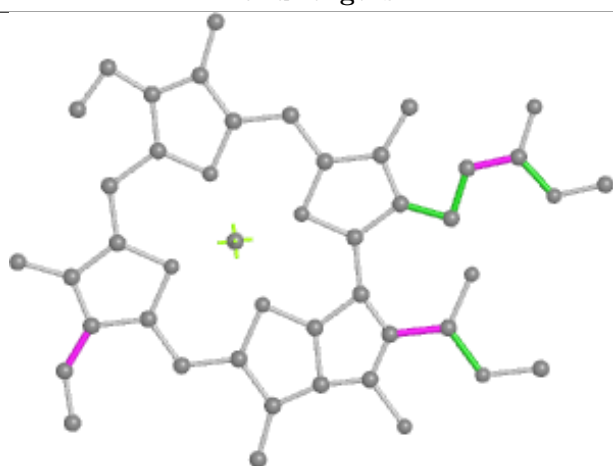
Ligand CLA h 606



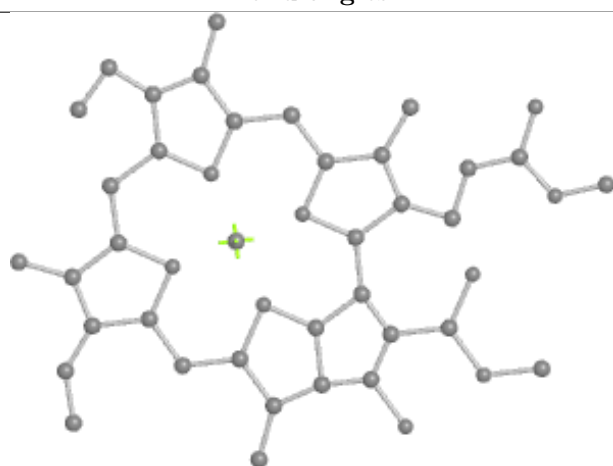
Bond lengths



Bond angles

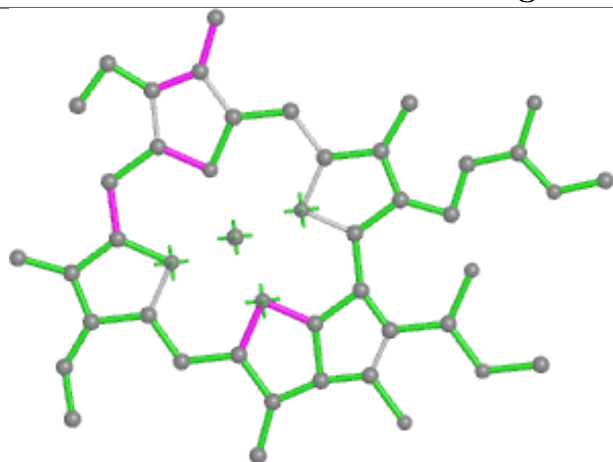


Torsions

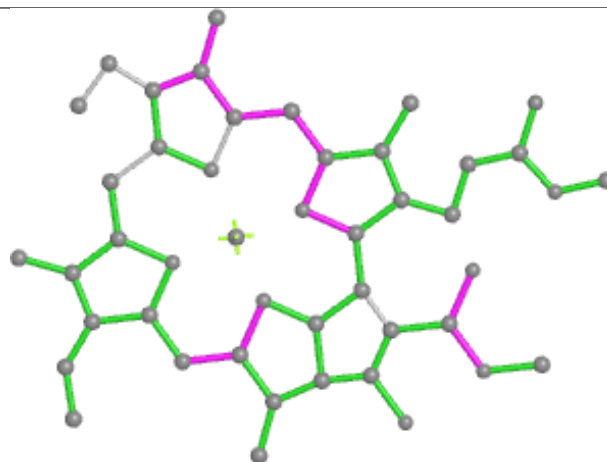


Rings

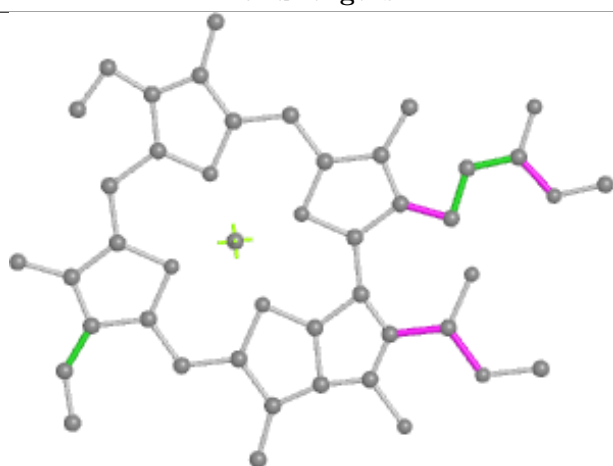
Ligand CLA 7 611



Bond lengths



Bond angles

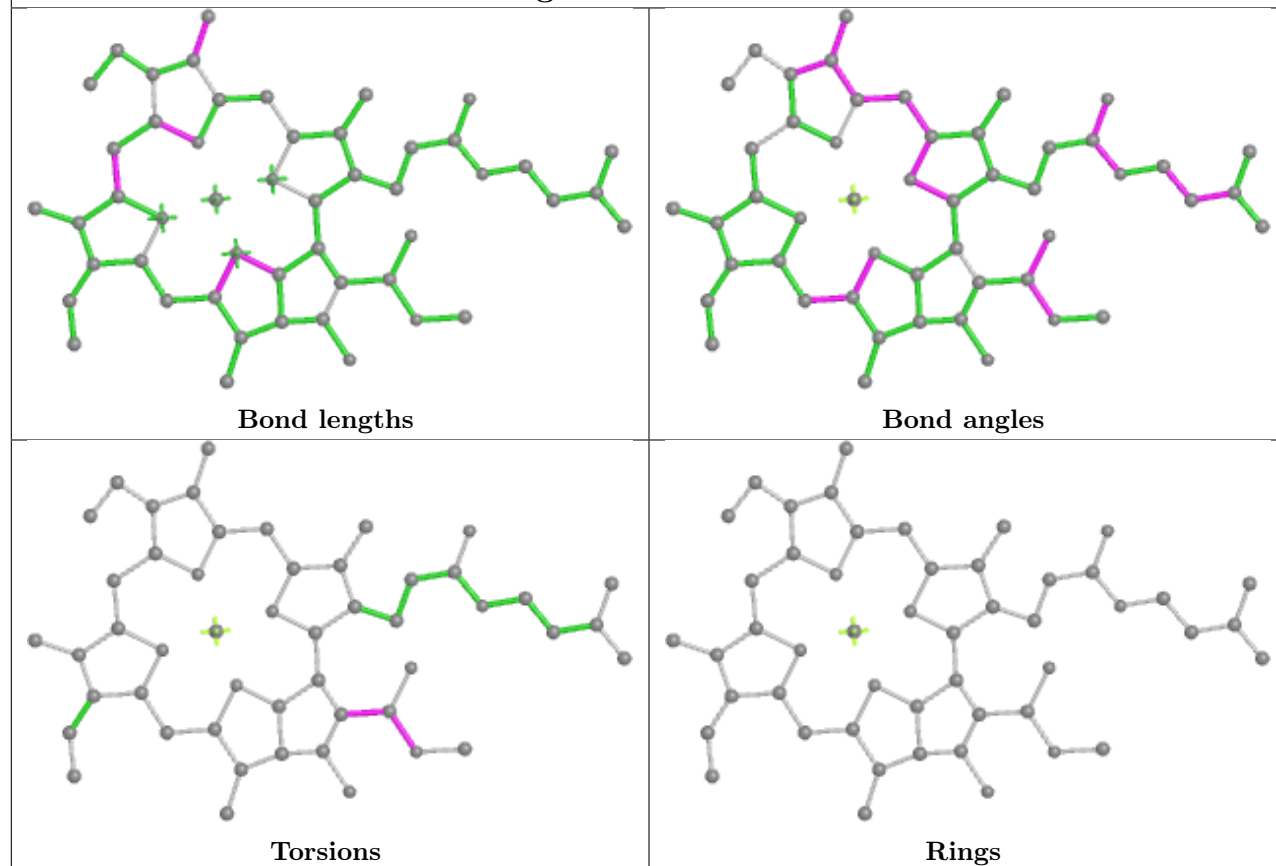


Torsions

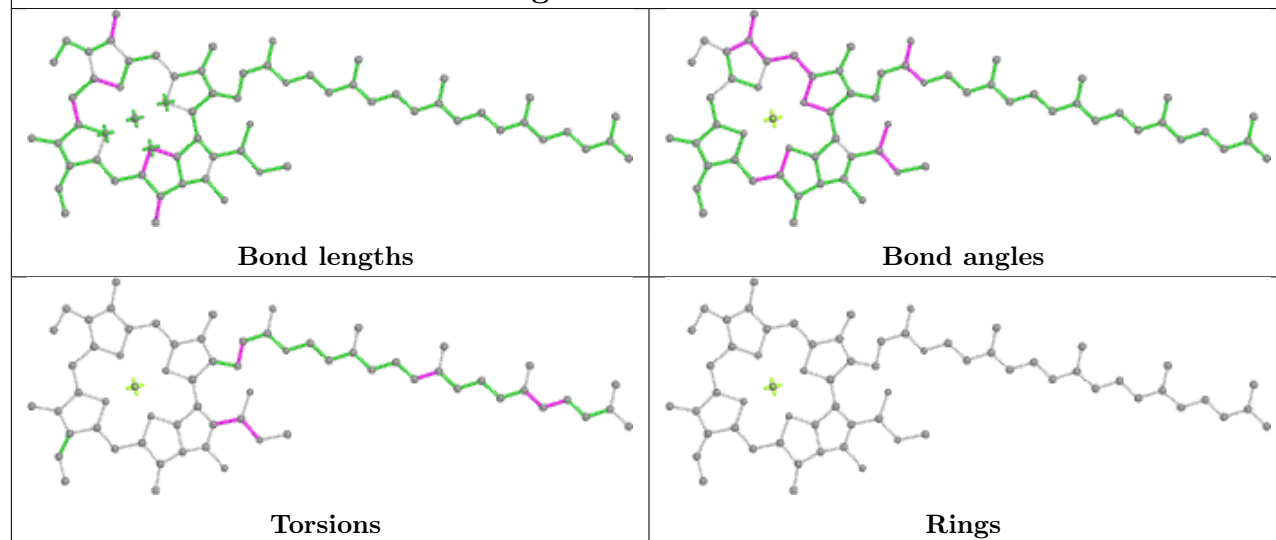


Rings

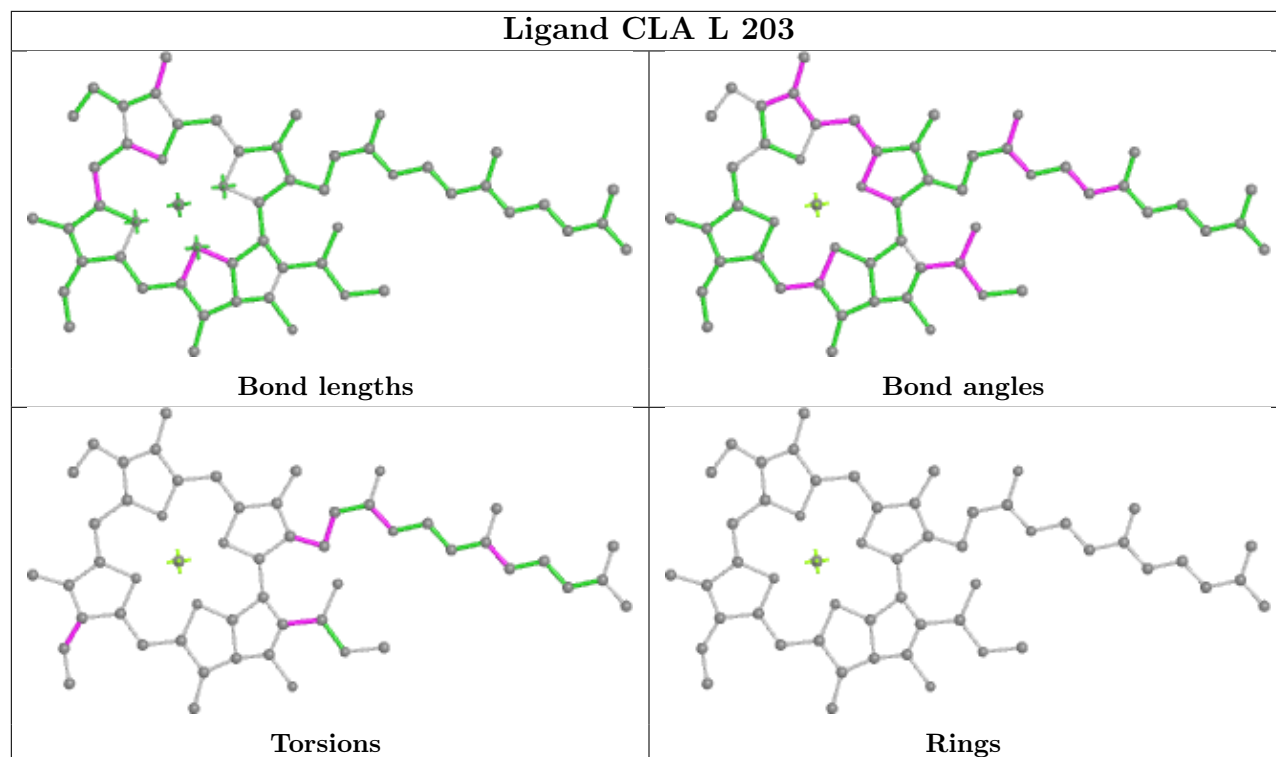
Ligand CLA 2 203



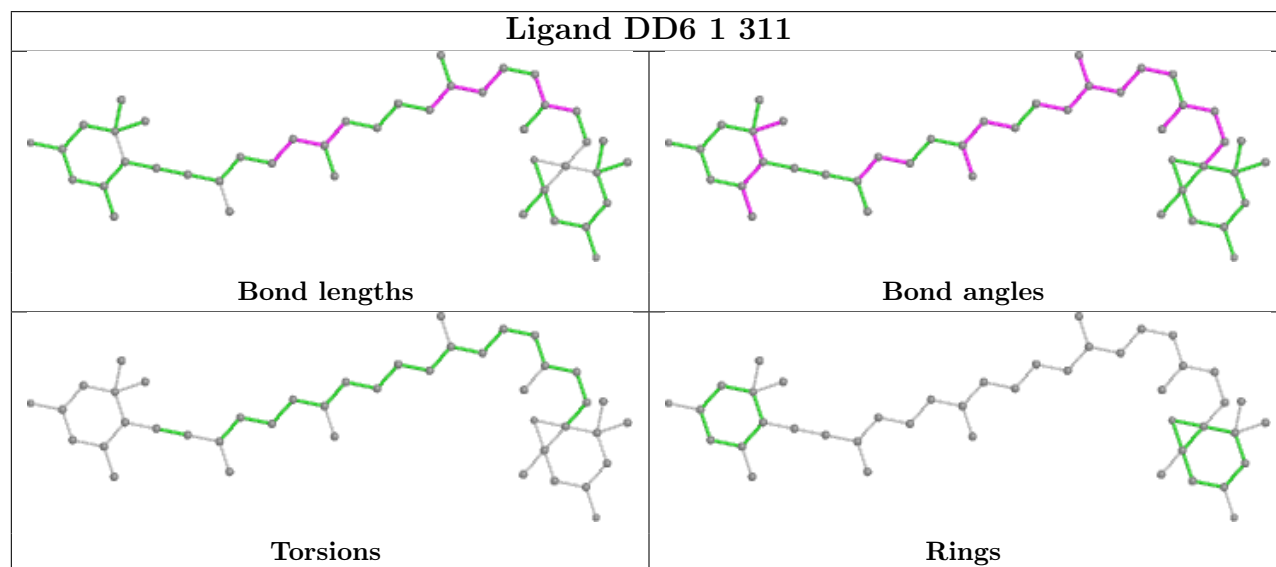
Ligand CLA A 838



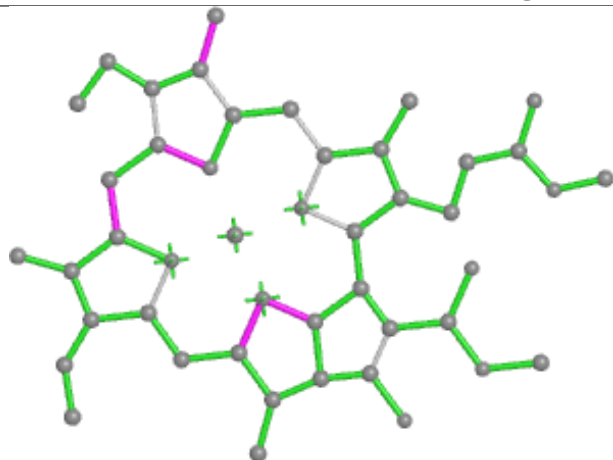
Ligand CLA L 203



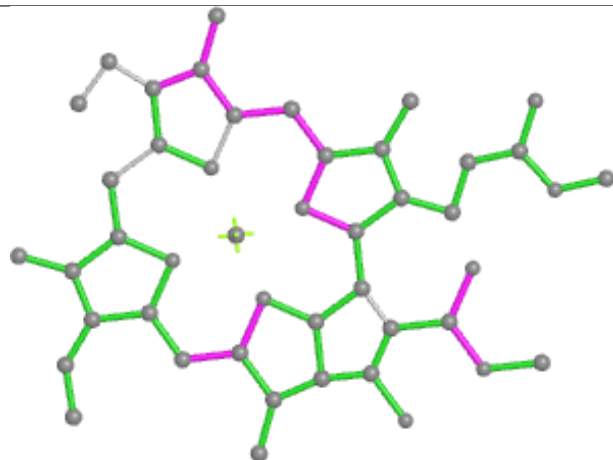
Ligand DD6 1 311



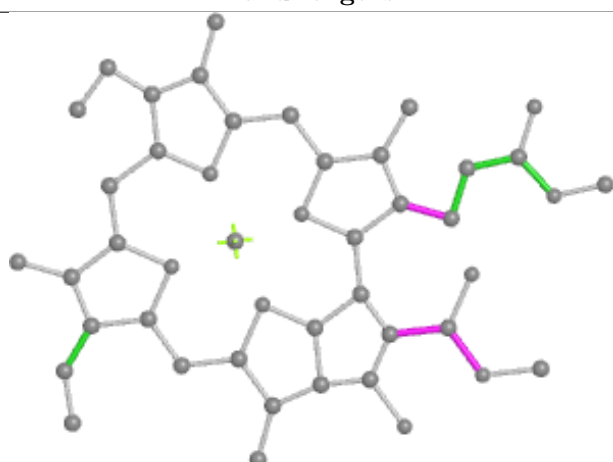
Ligand CLA 1 303



Bond lengths



Bond angles

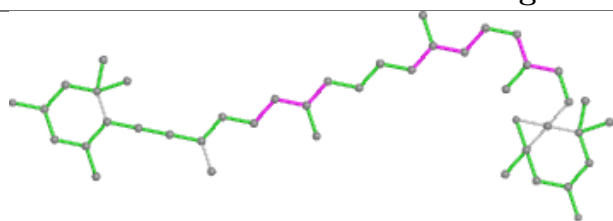


Torsions

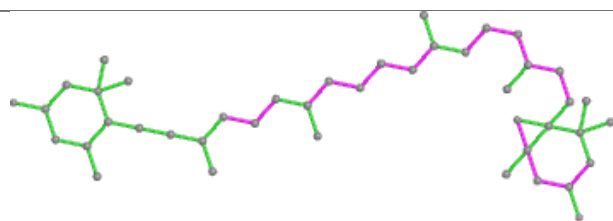


Rings

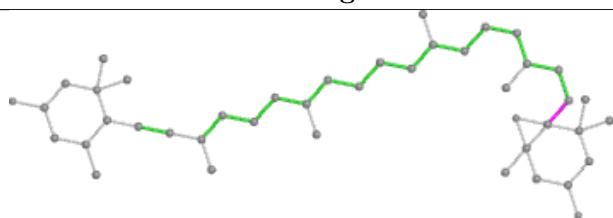
Ligand DD6 3 312



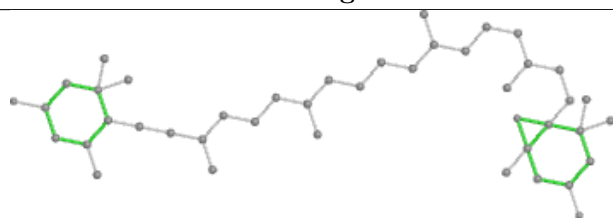
Bond lengths



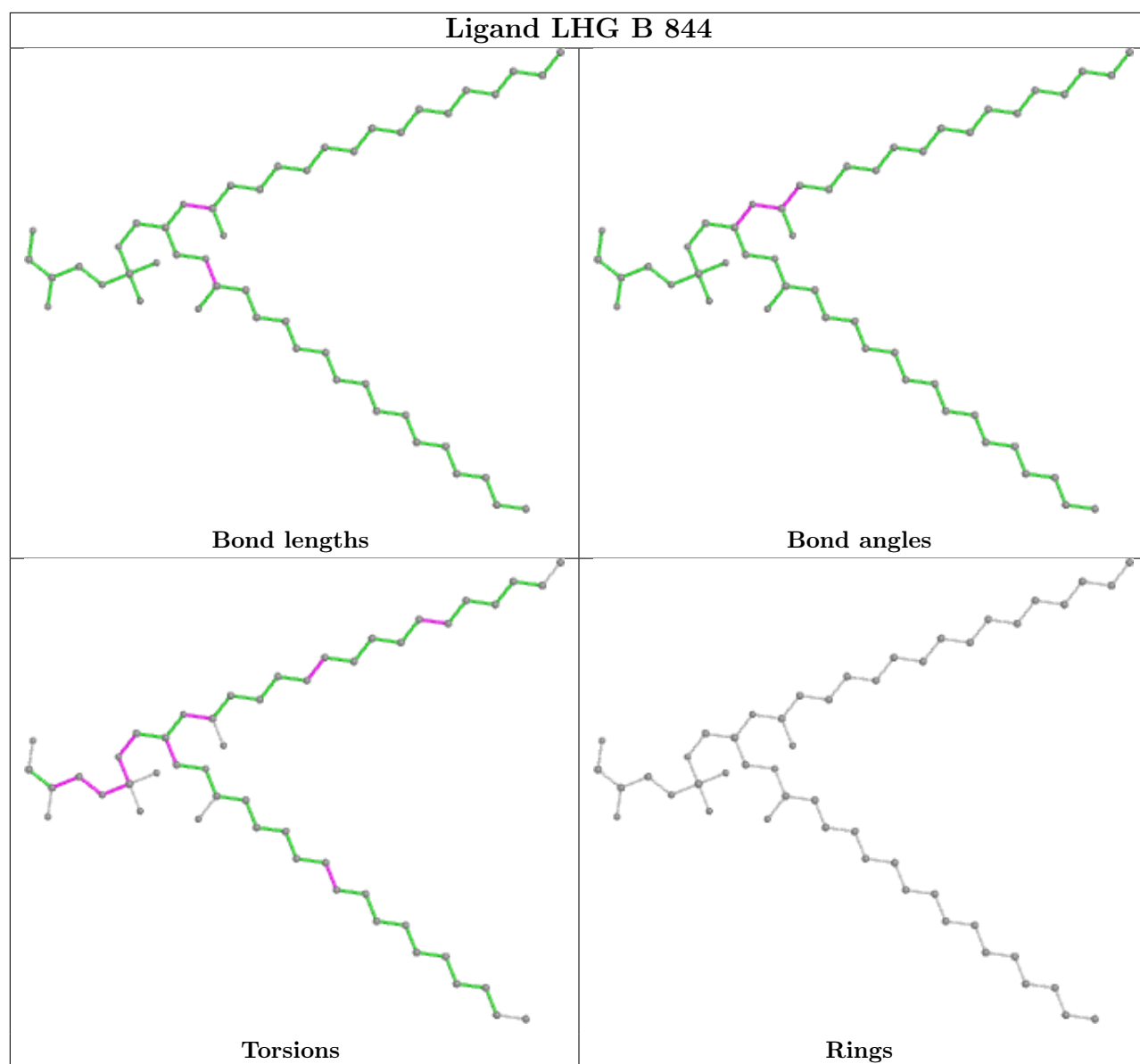
Bond angles



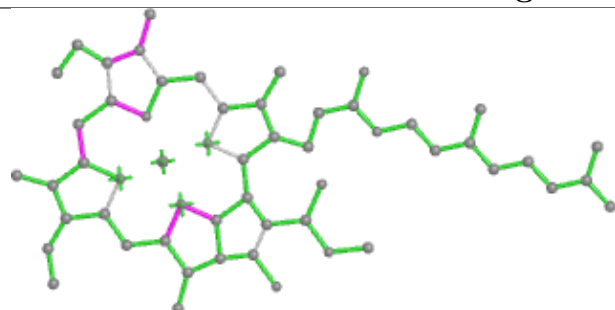
Torsions



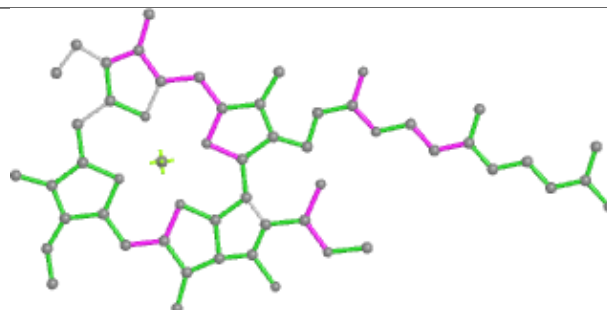
Rings



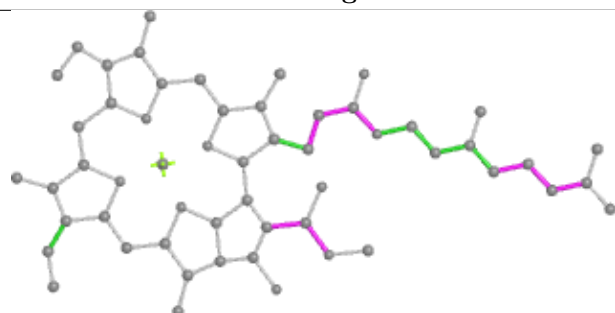
Ligand CLA A 822



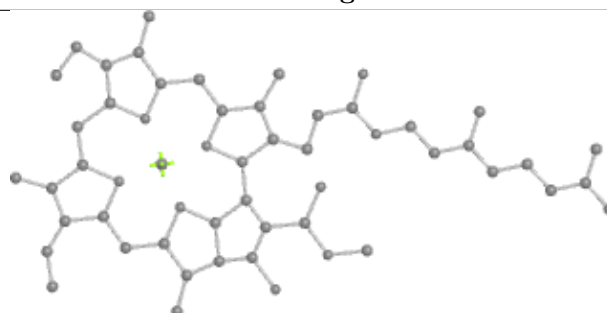
Bond lengths



Bond angles

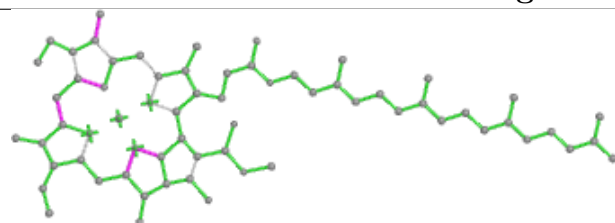


Torsions

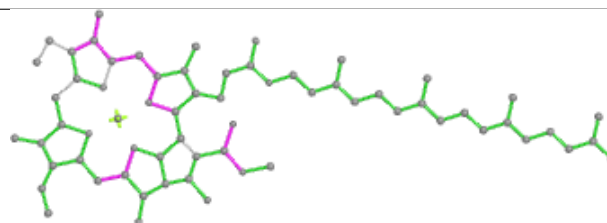


Rings

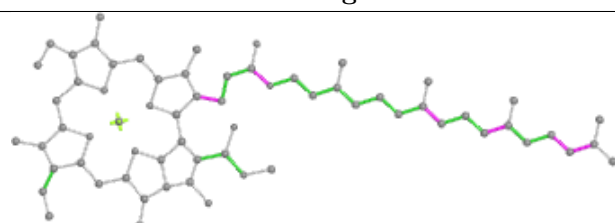
Ligand CLA B 805



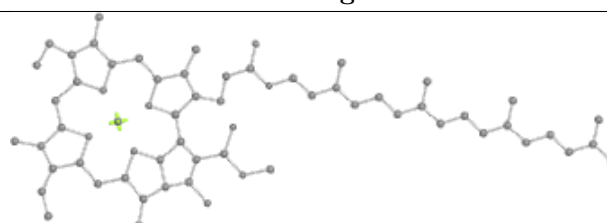
Bond lengths



Bond angles

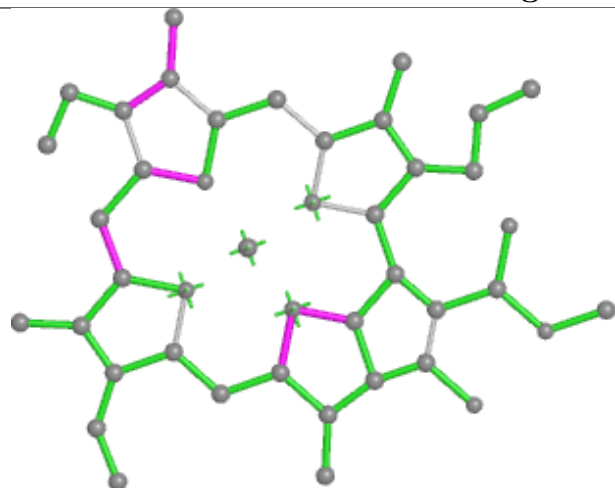


Torsions

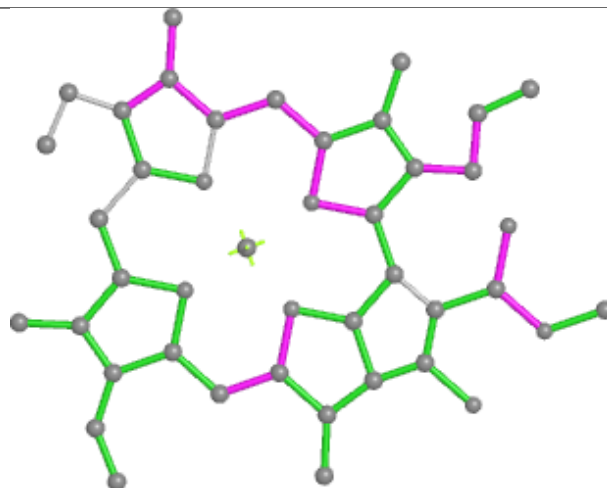


Rings

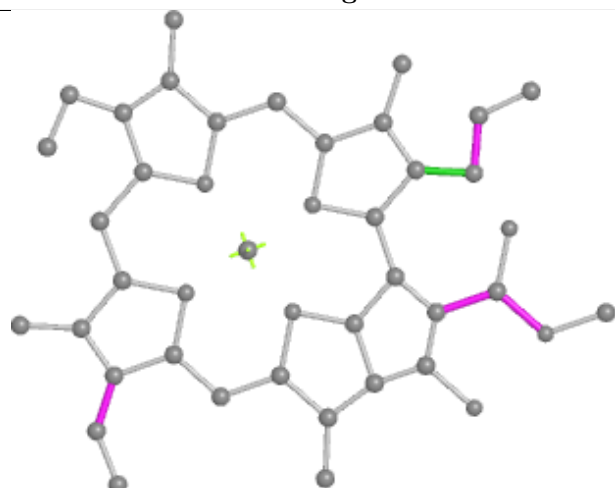
Ligand CLA c 601



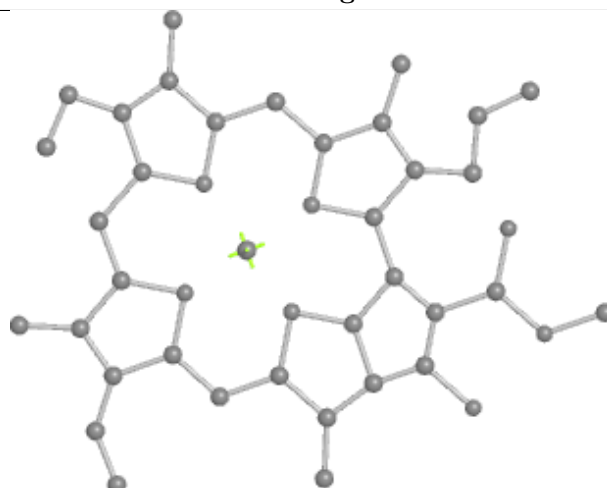
Bond lengths



Bond angles

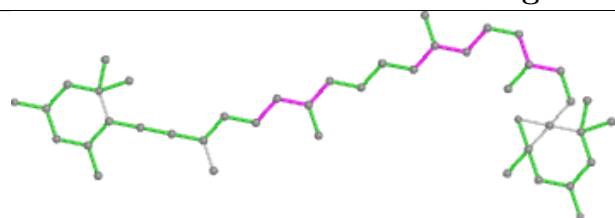


Torsions

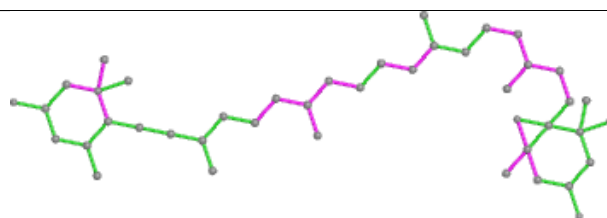


Rings

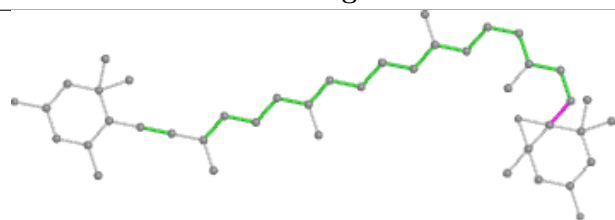
Ligand DD6 c 612



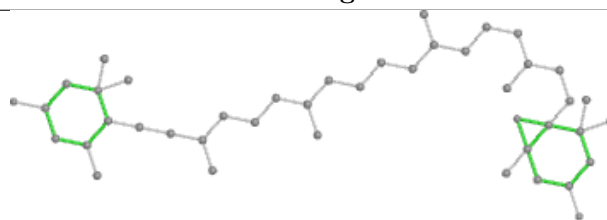
Bond lengths



Bond angles

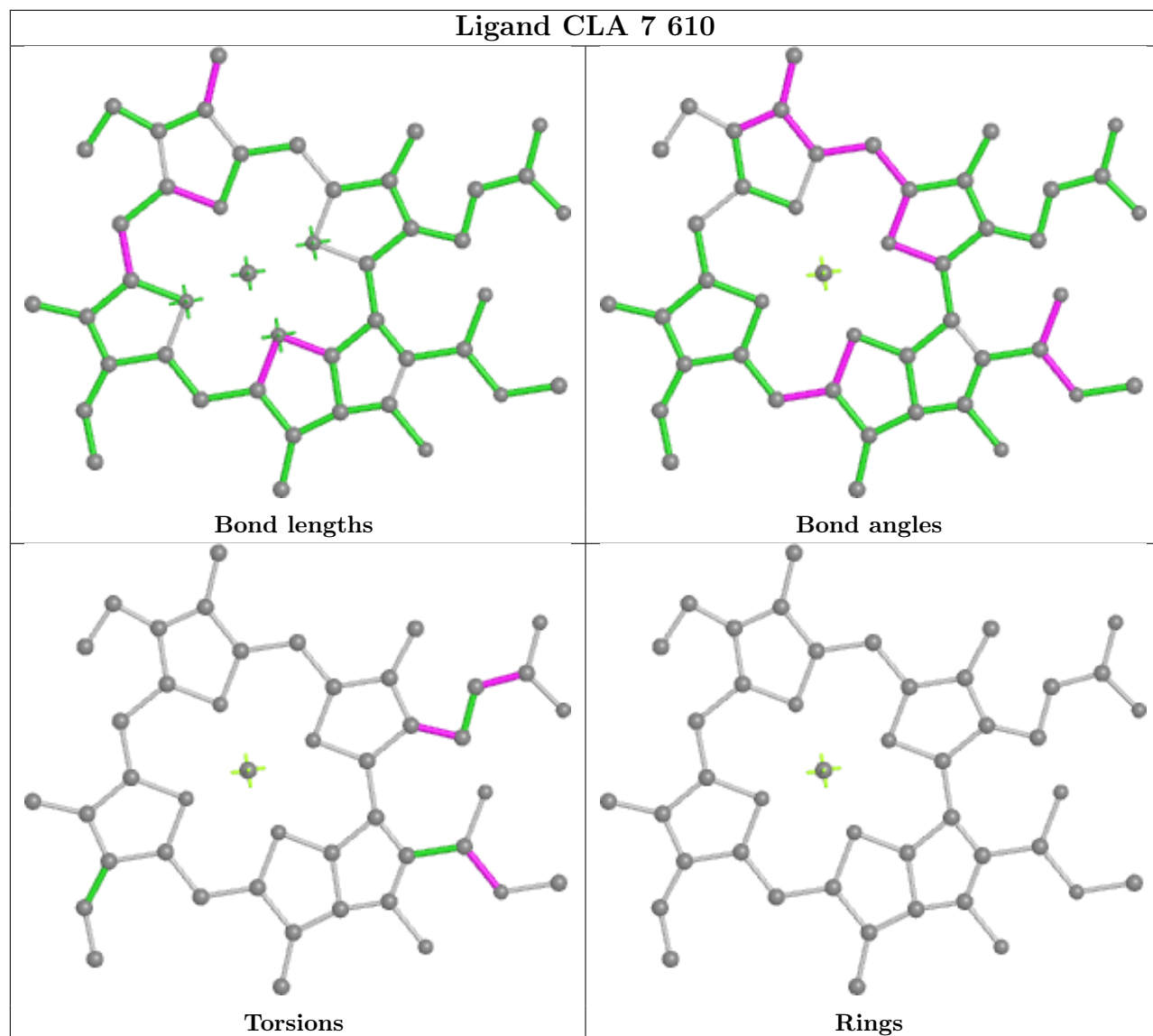


Torsions

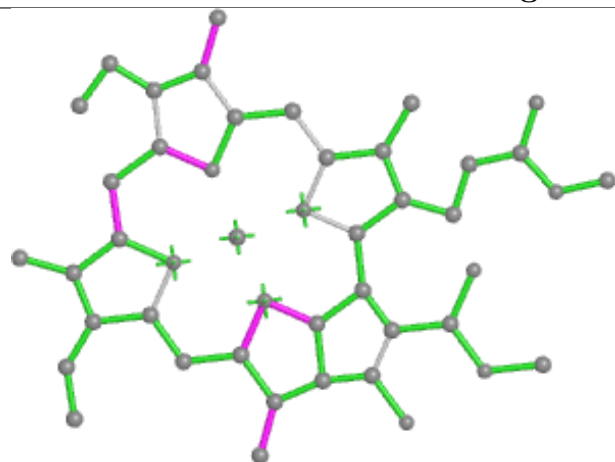


Rings

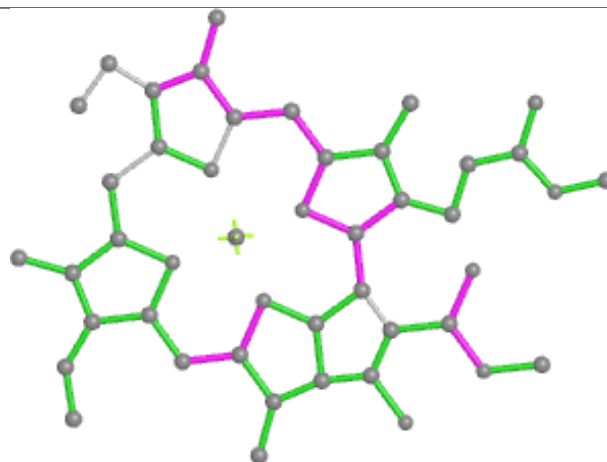
Ligand CLA 7 610



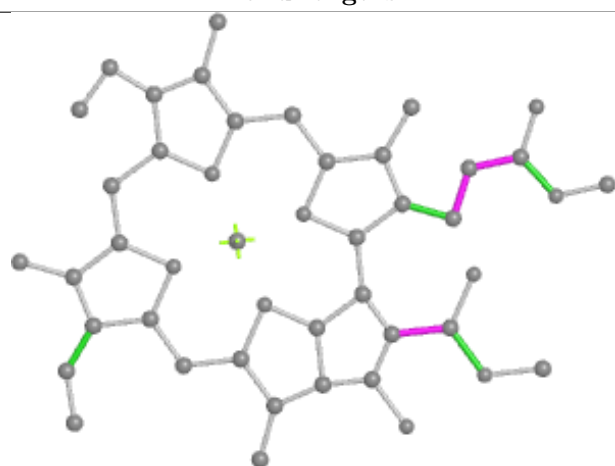
Ligand CLA 9 306



Bond lengths



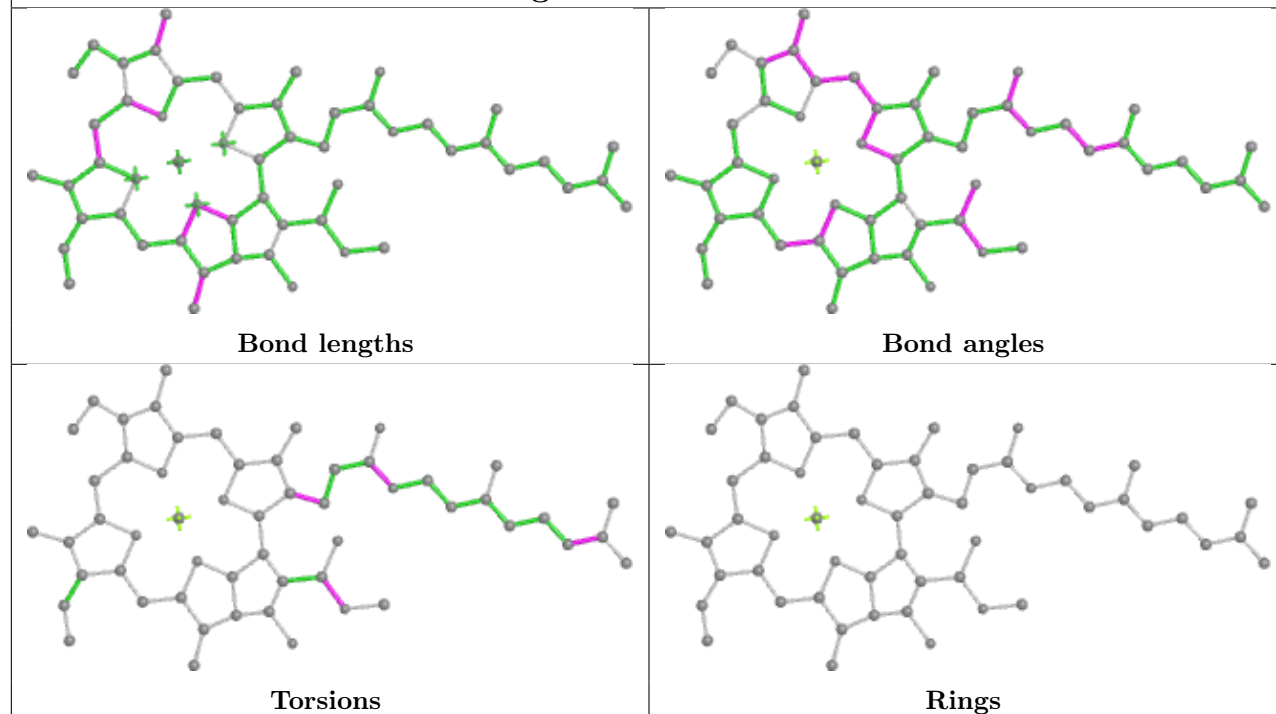
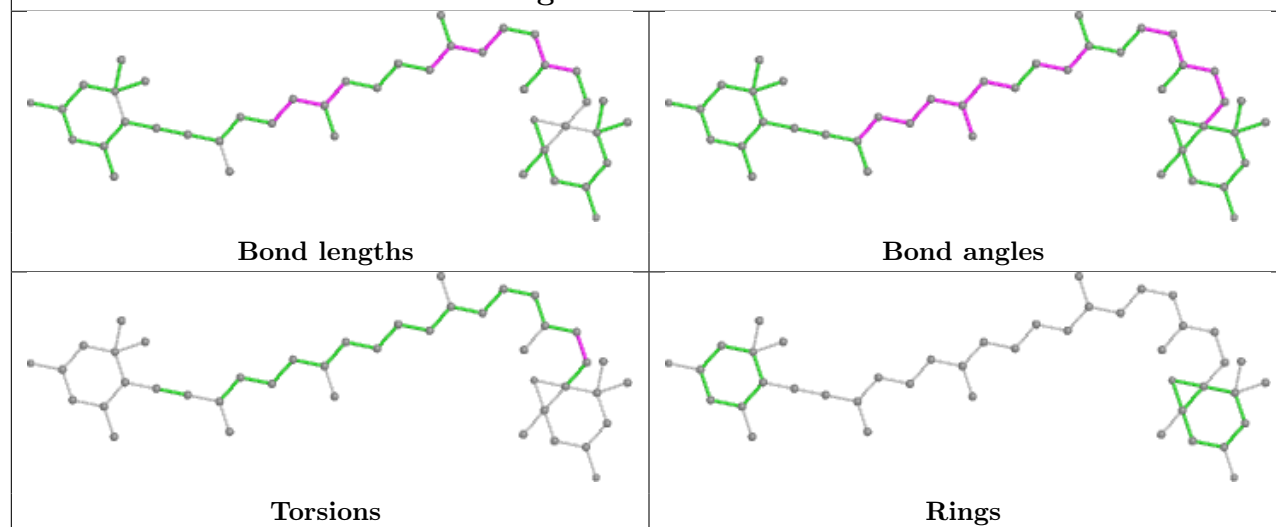
Bond angles



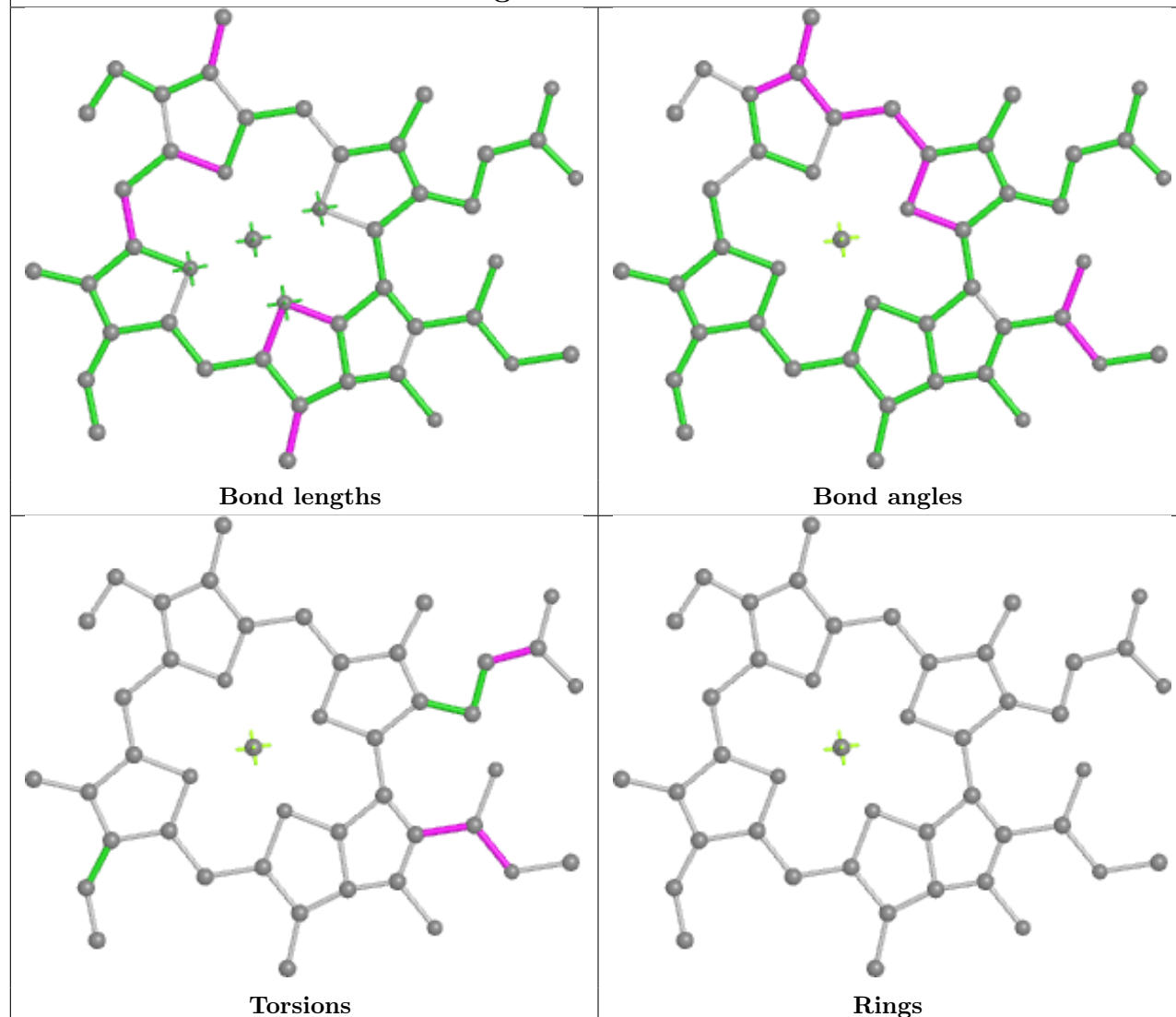
Torsions



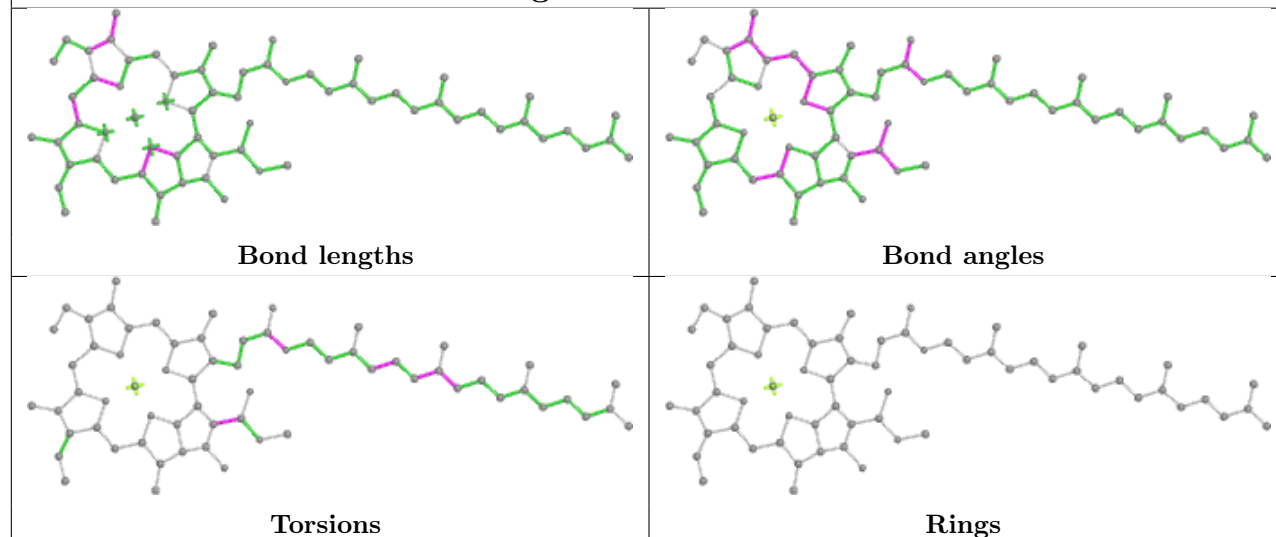
Rings

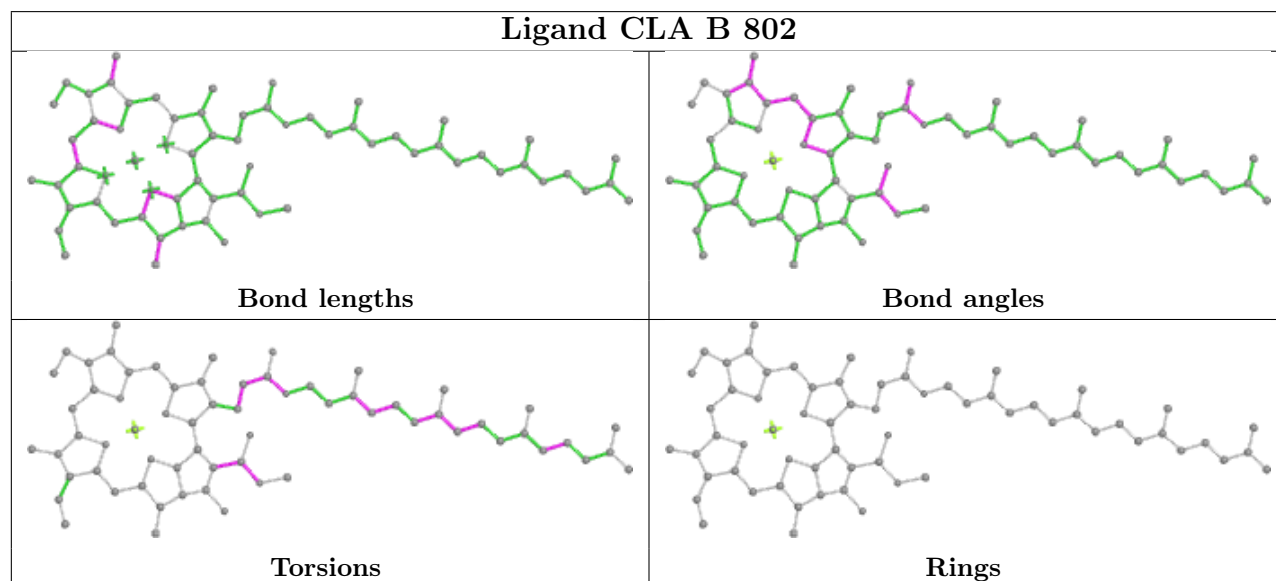
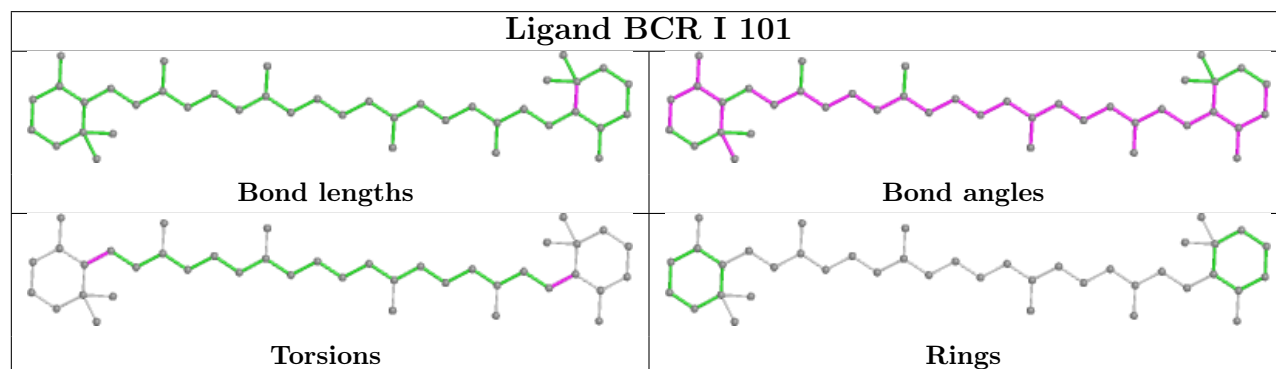
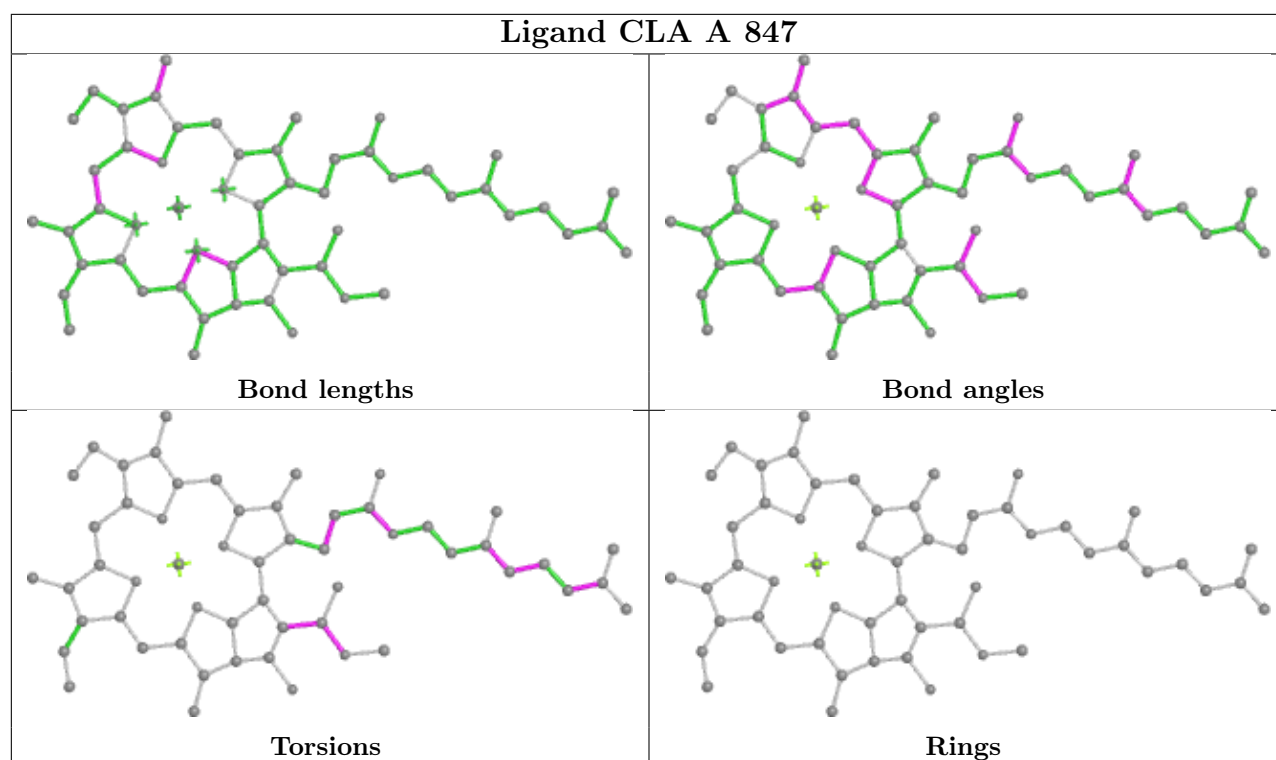
Ligand CLA A 853**Ligand DD6 2 212**

Ligand CLA 8 208

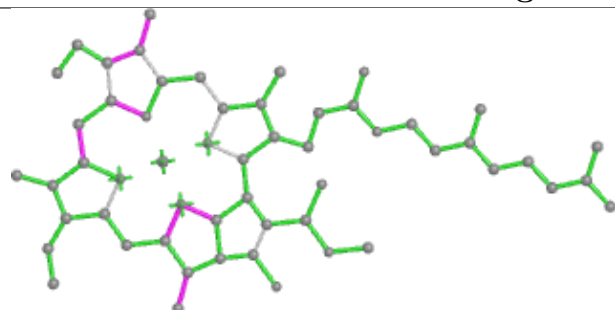


Ligand CLA A 829

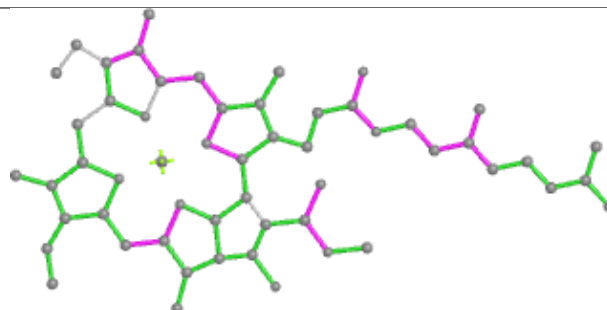




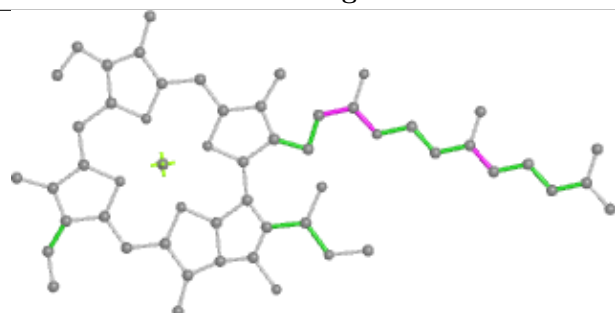
Ligand CLA B 811



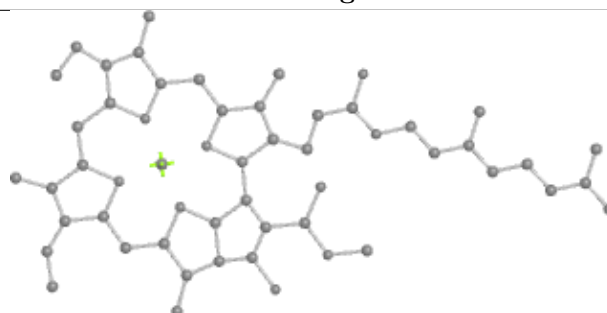
Bond lengths



Bond angles

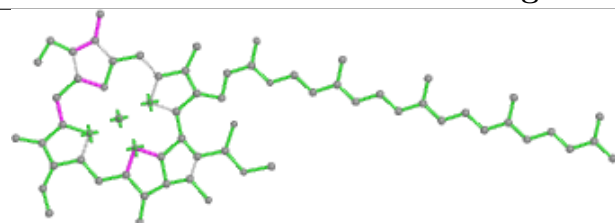


Torsions

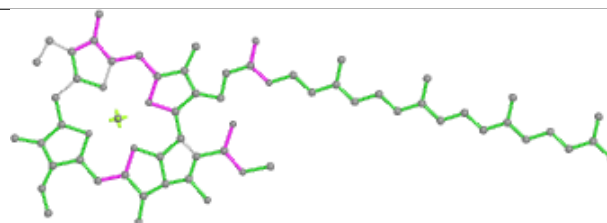


Rings

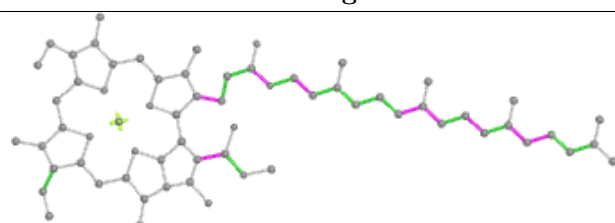
Ligand CLA c 608



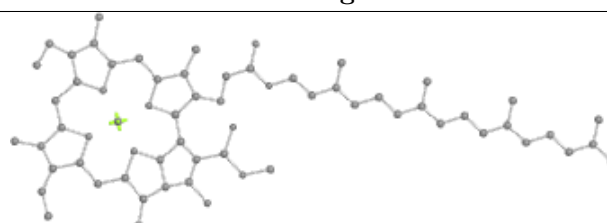
Bond lengths



Bond angles

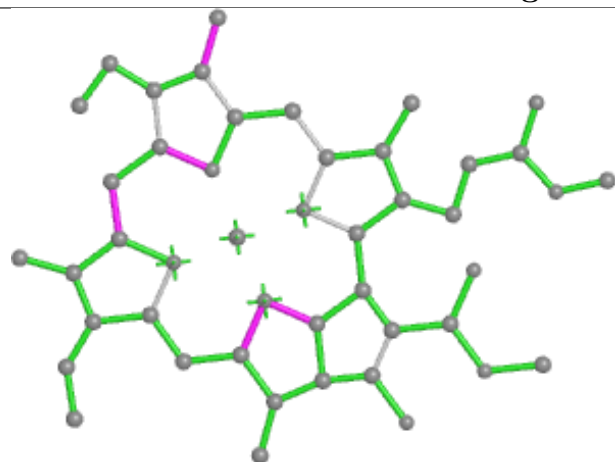


Torsions

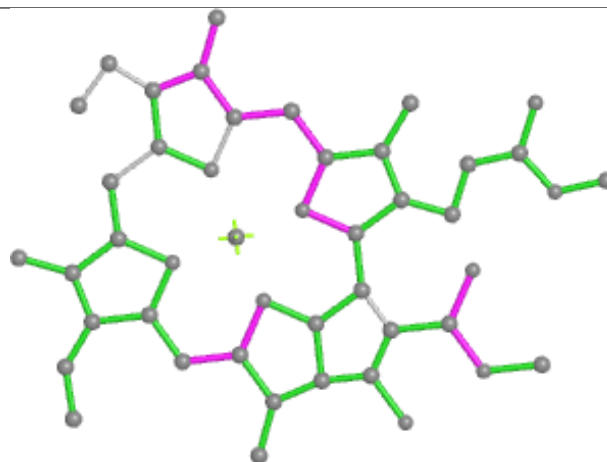


Rings

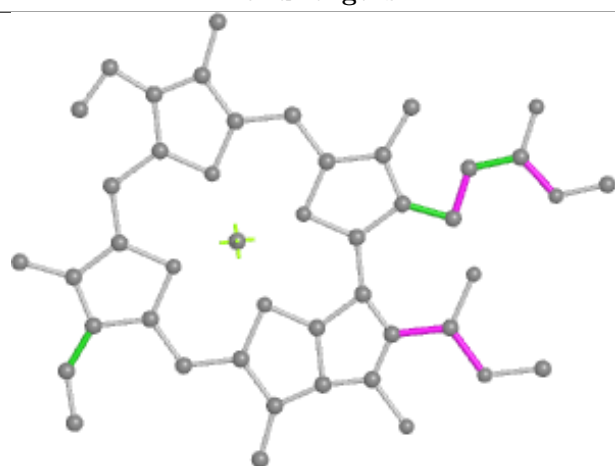
Ligand CLA c 606



Bond lengths



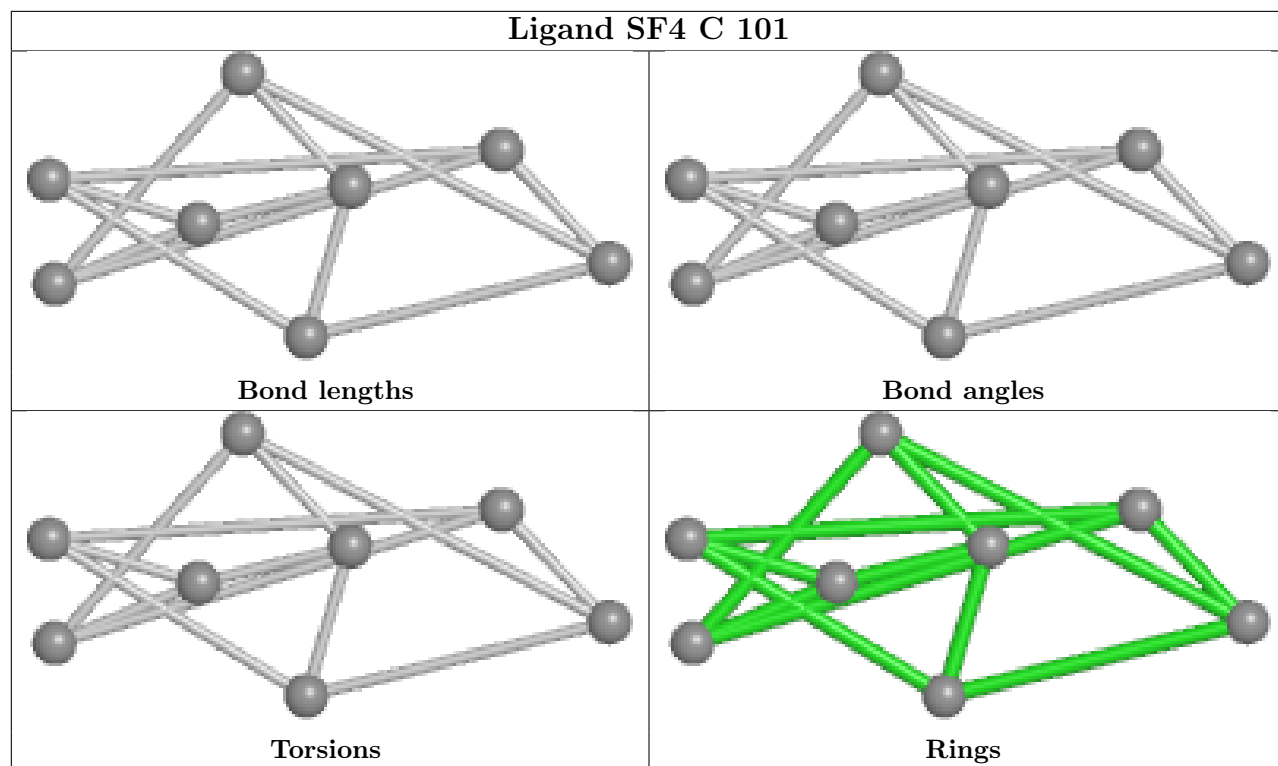
Bond angles



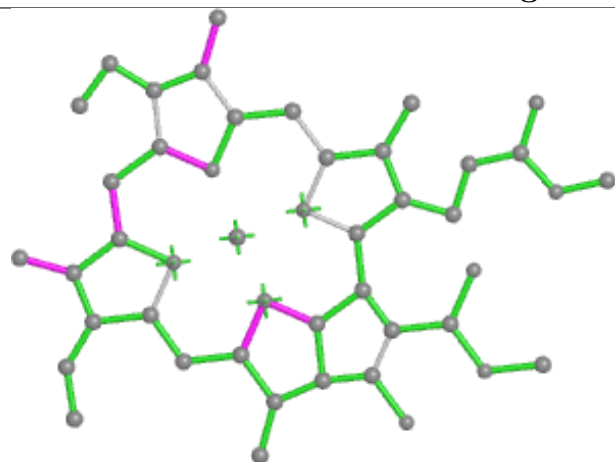
Torsions



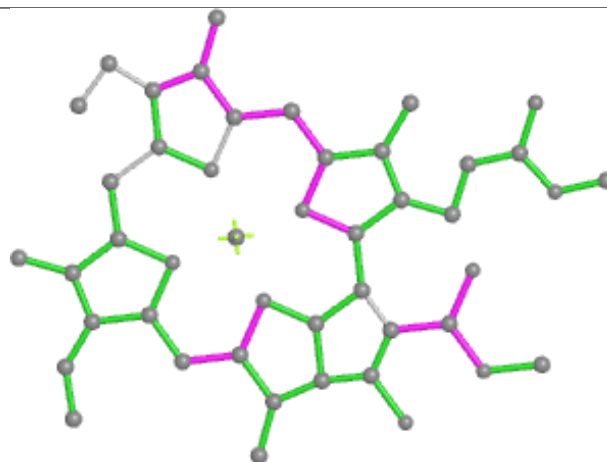
Rings



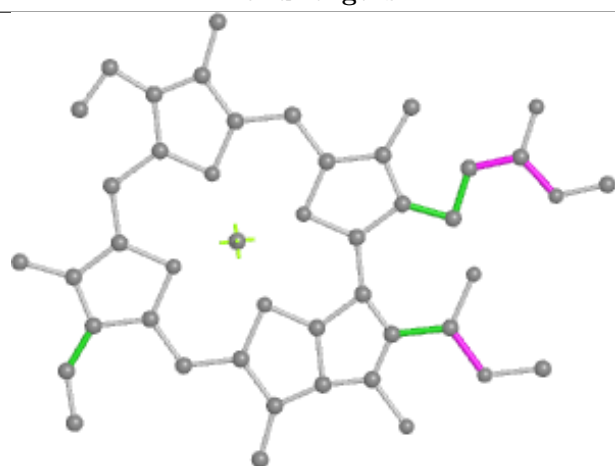
Ligand CLA 4 609



Bond lengths



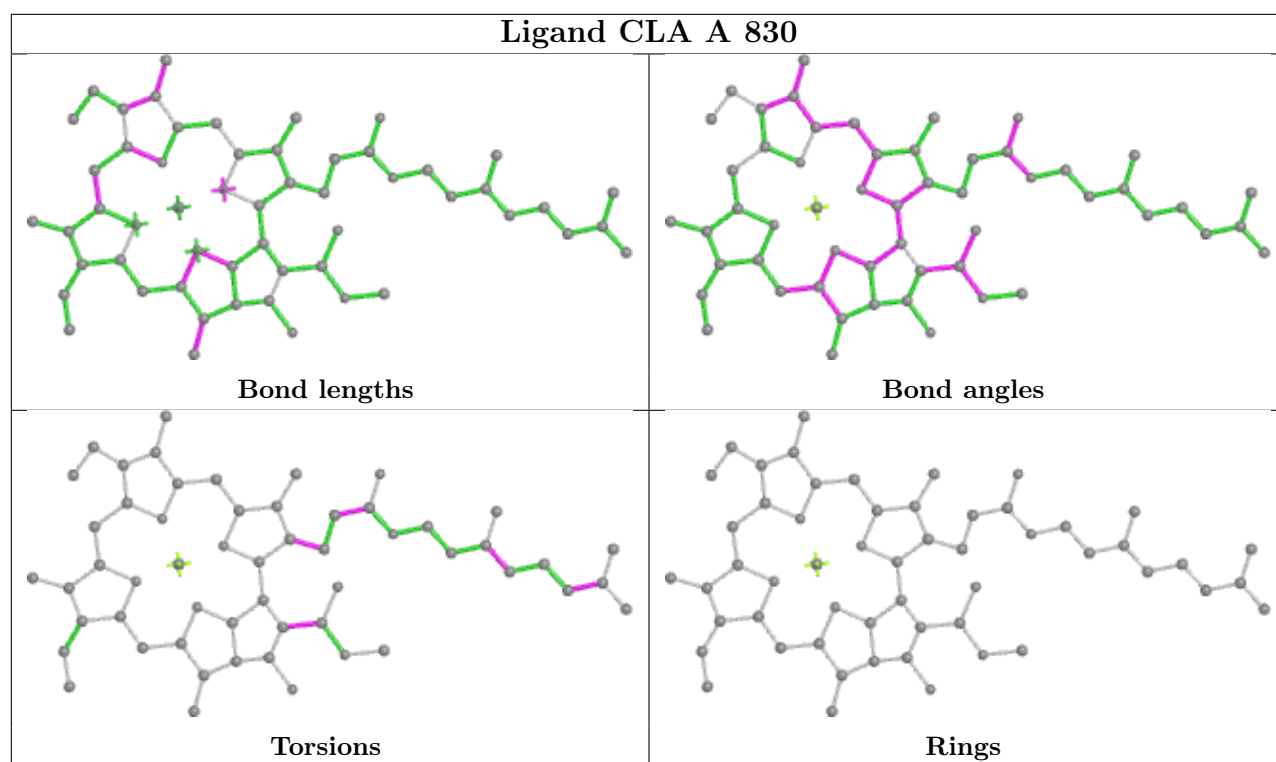
Bond angles



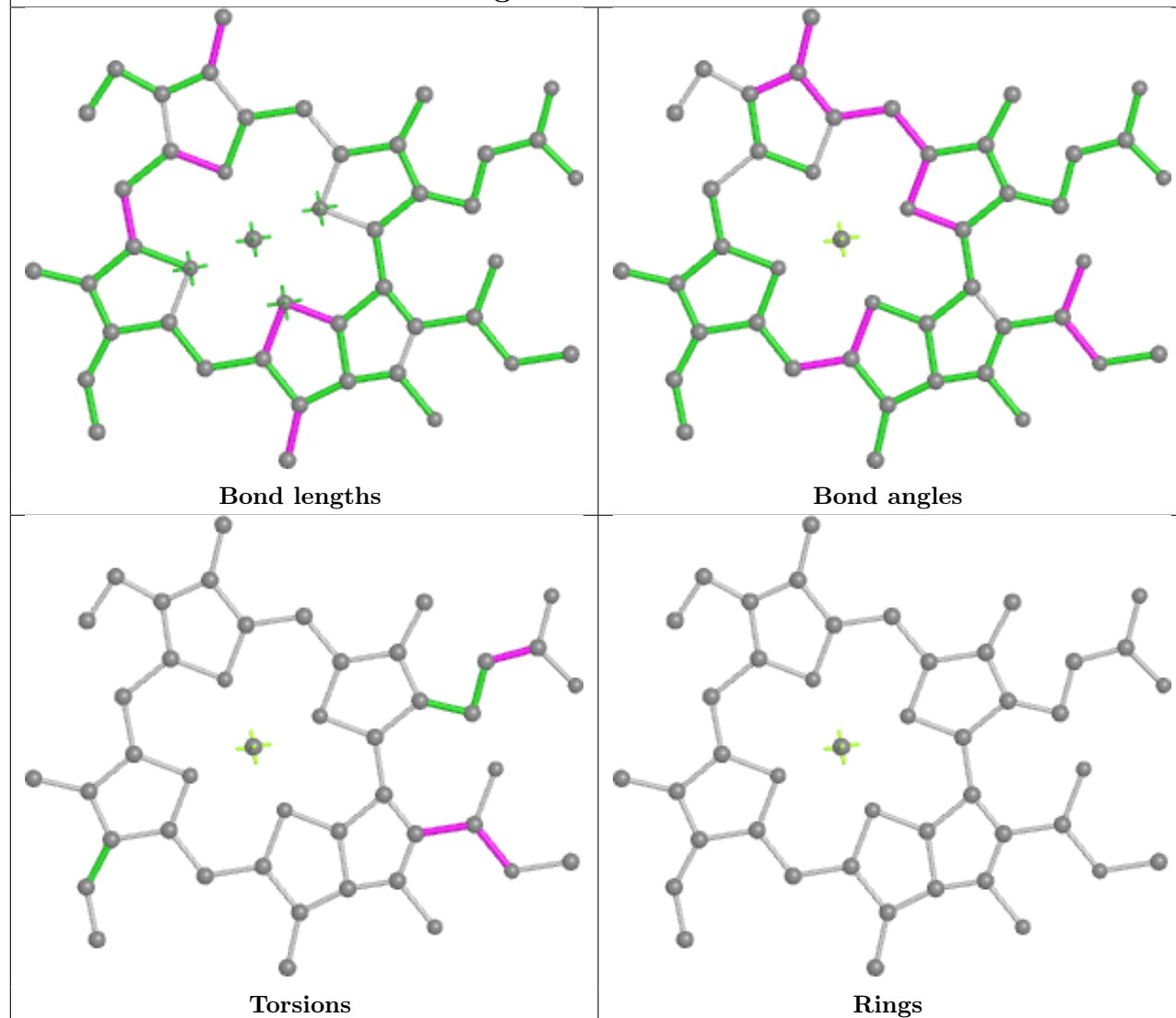
Torsions



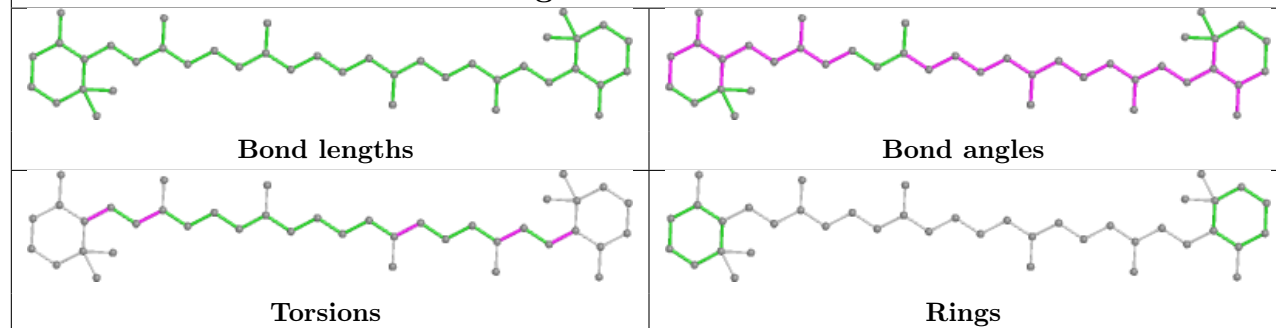
Rings



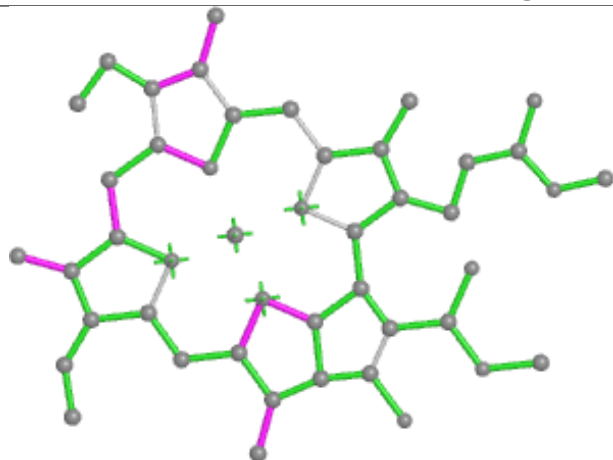
Ligand CLA 9 311



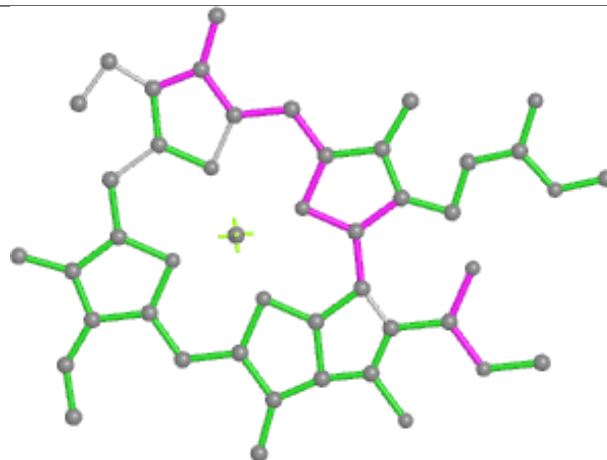
Ligand BCR c 615



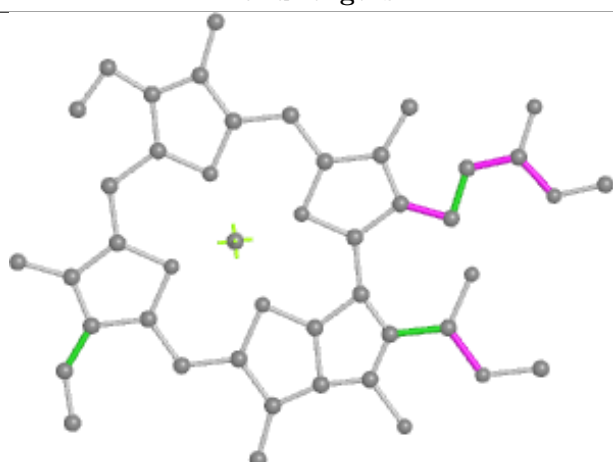
Ligand CLA 9 303



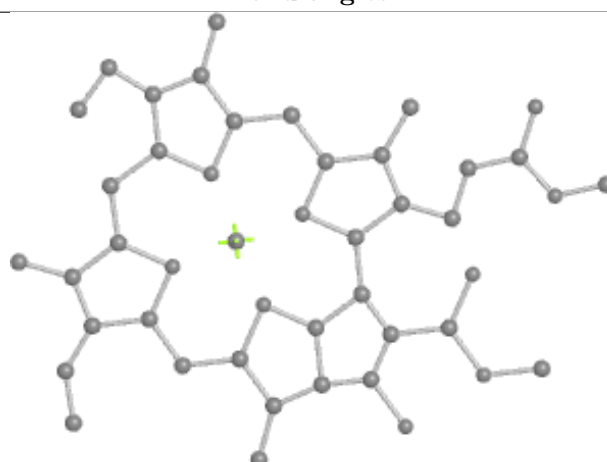
Bond lengths



Bond angles

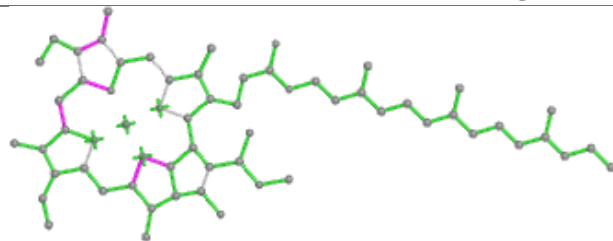


Torsions

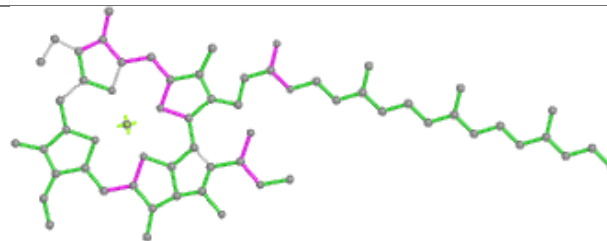


Rings

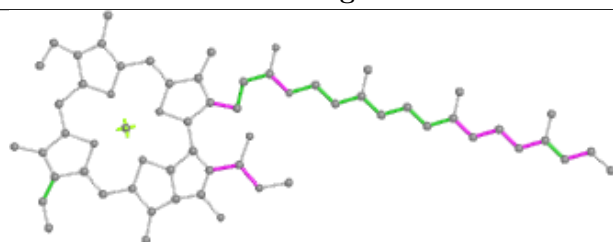
Ligand CLA A 810



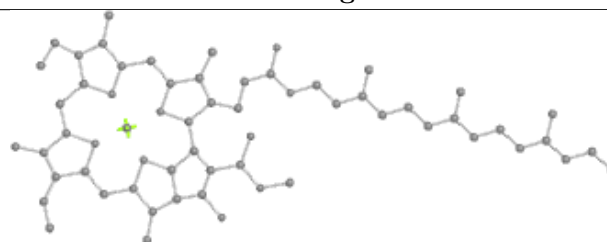
Bond lengths



Bond angles

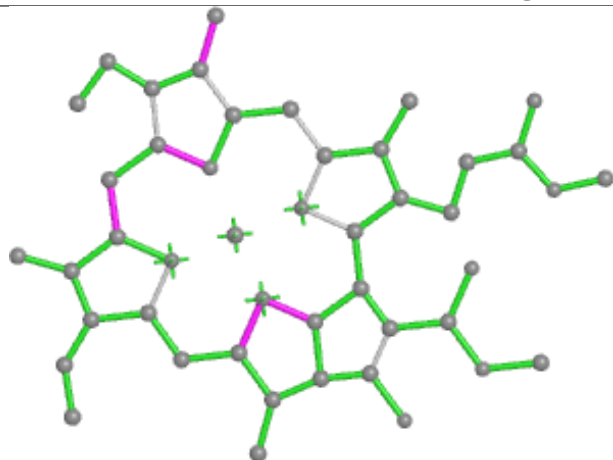


Torsions

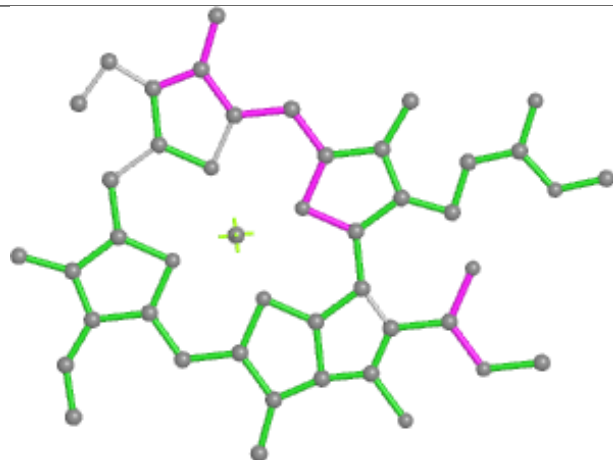


Rings

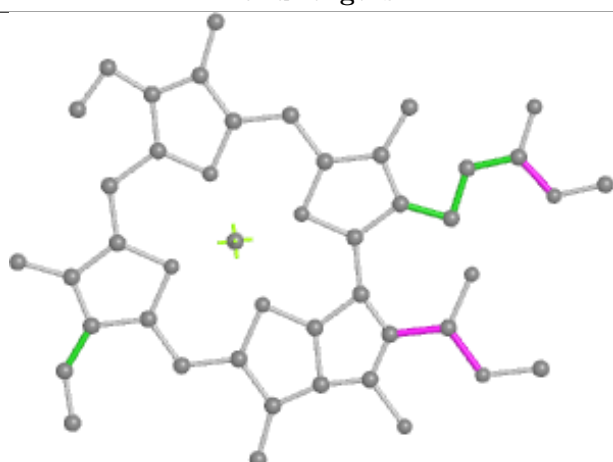
Ligand CLA 2 208



Bond lengths



Bond angles

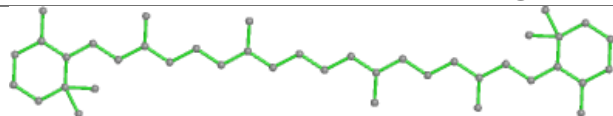


Torsions

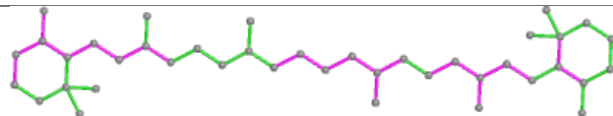


Rings

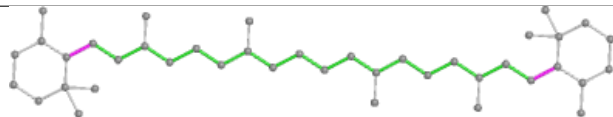
Ligand BCR A 859



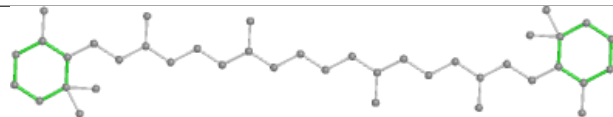
Bond lengths



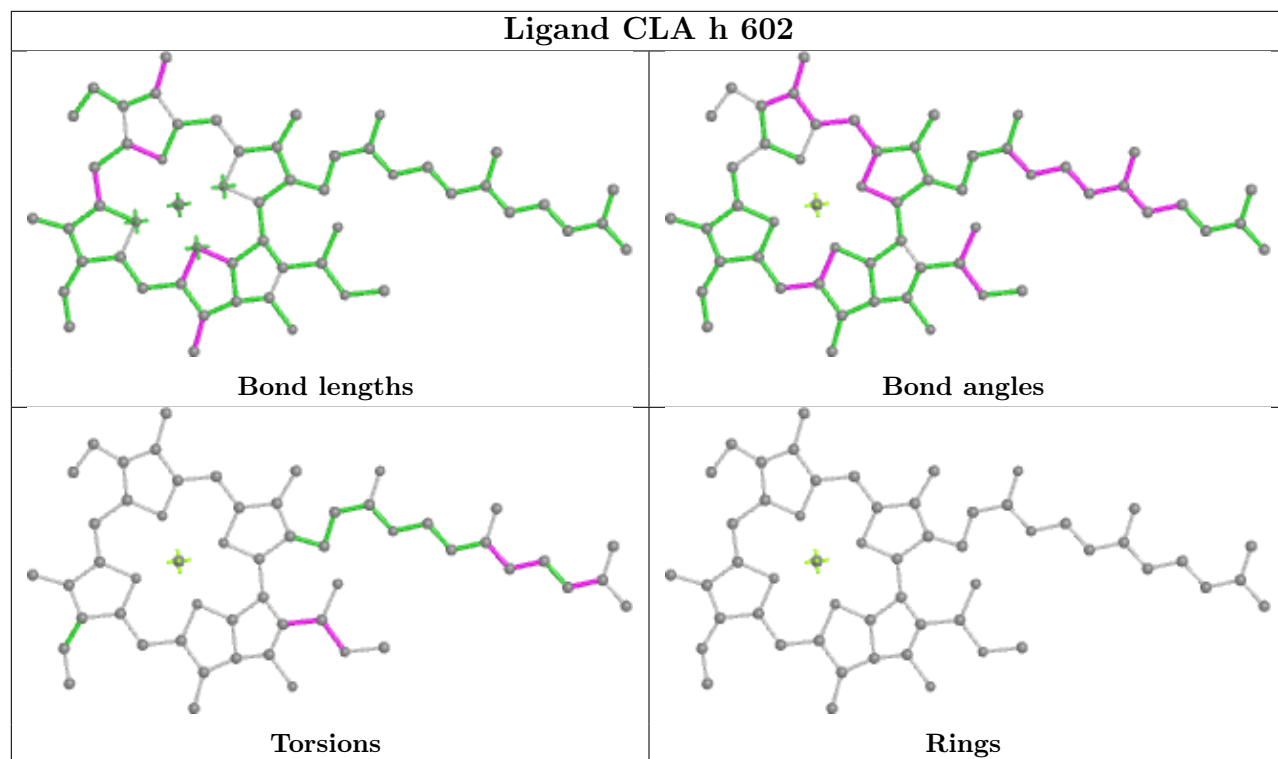
Bond angles



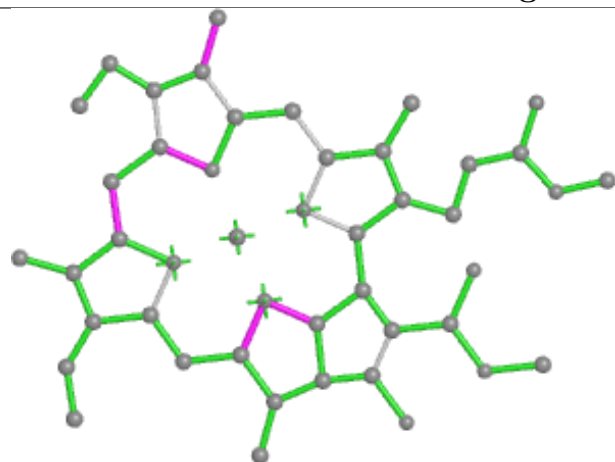
Torsions



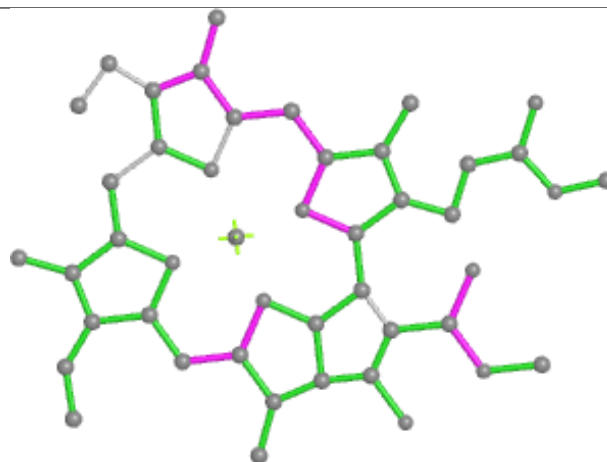
Rings



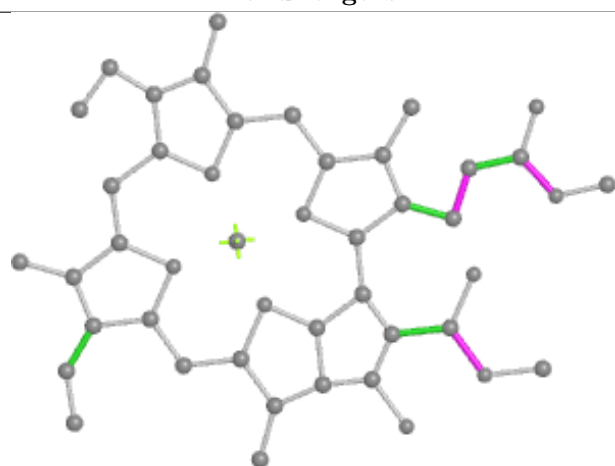
Ligand CLA h 604



Bond lengths



Bond angles

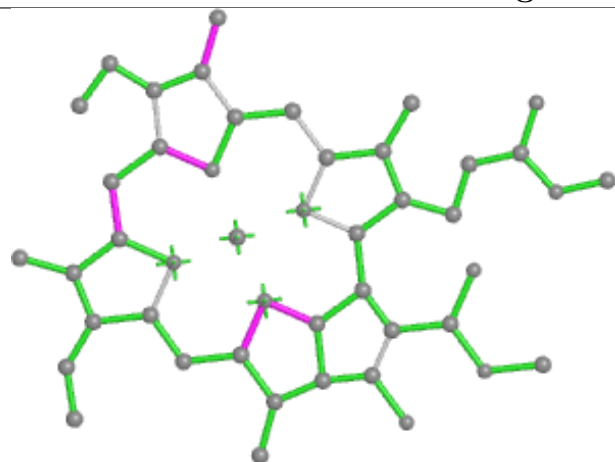


Torsions

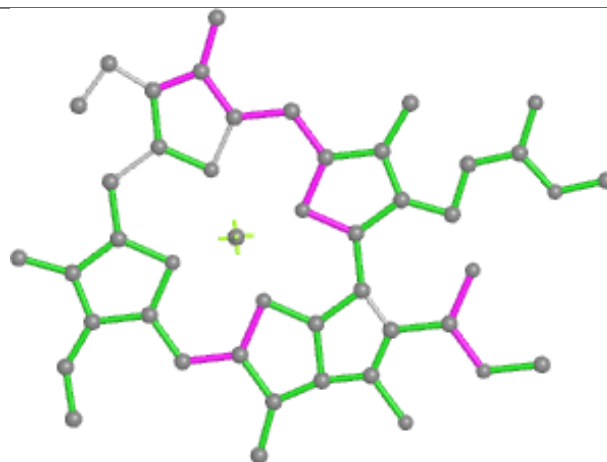


Rings

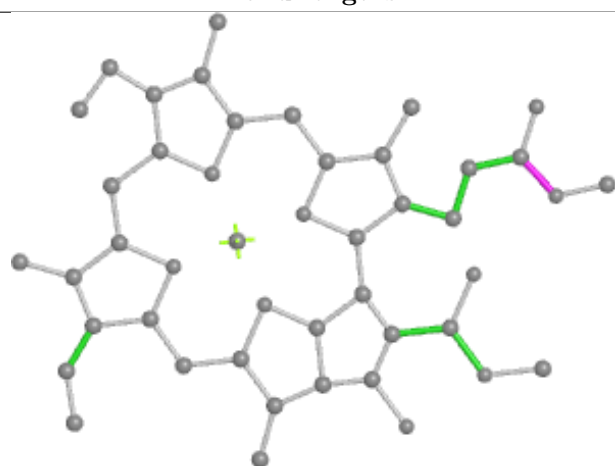
Ligand CLA B 819



Bond lengths



Bond angles

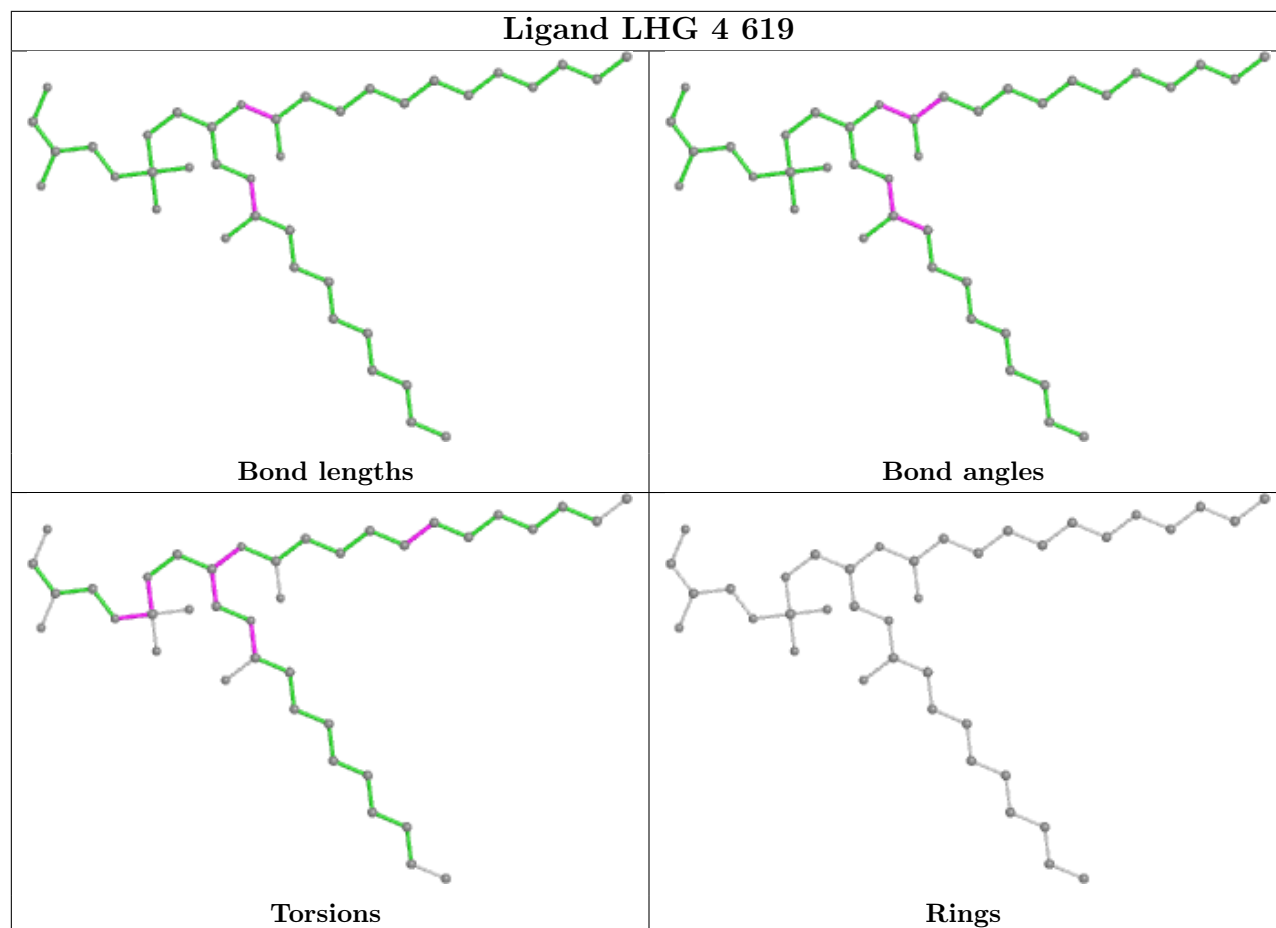


Torsions

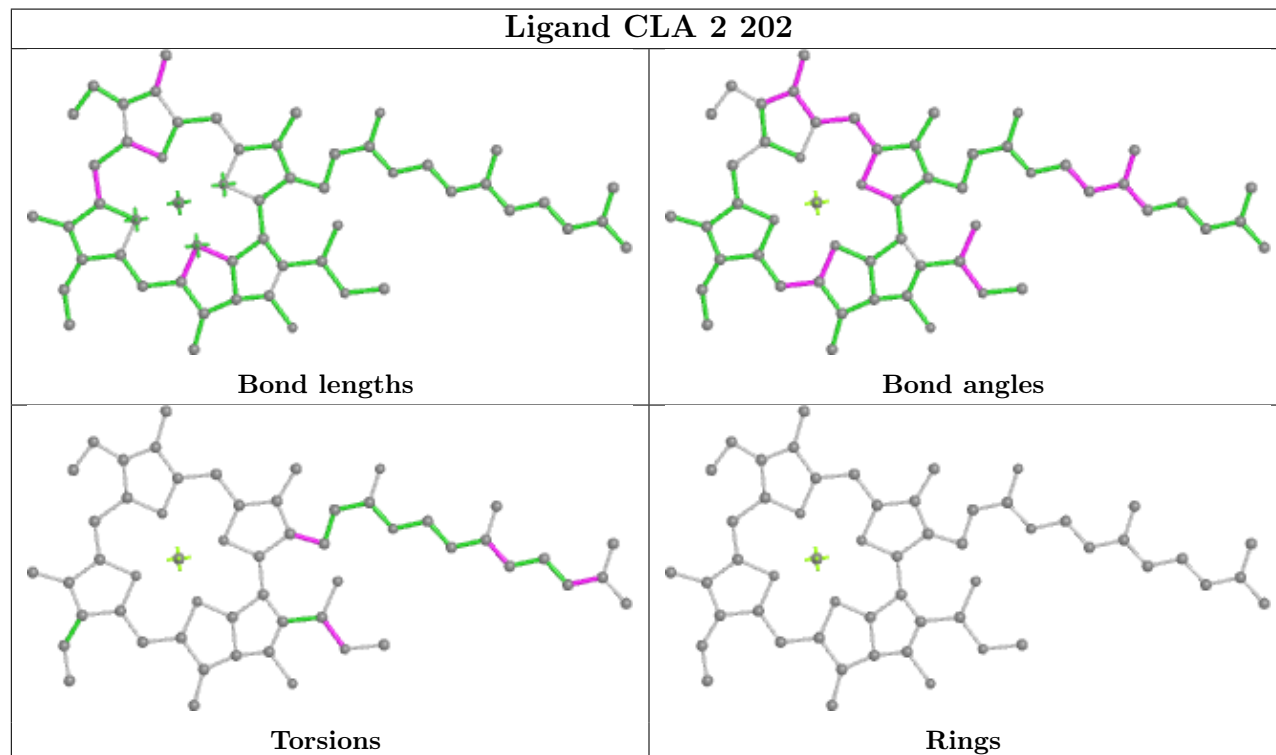


Rings

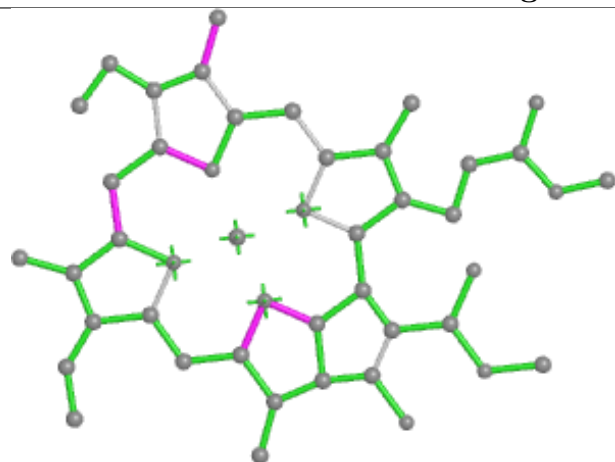
Ligand LHG 4 619



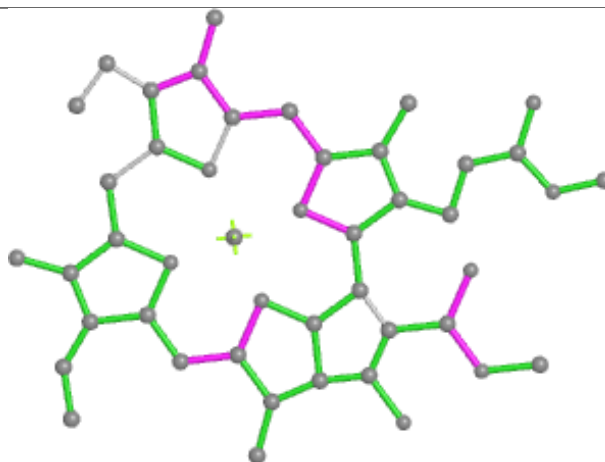
Ligand CLA 2 202



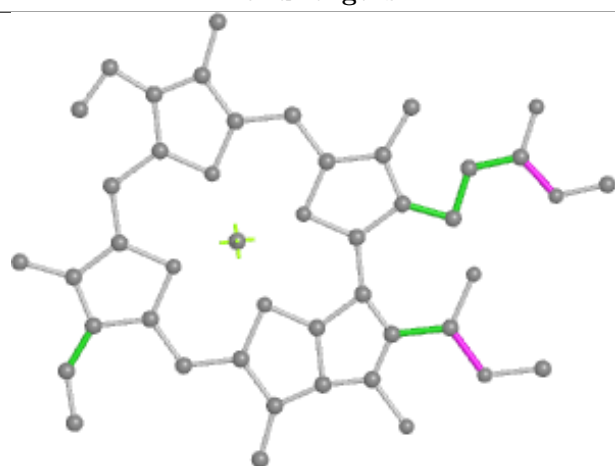
Ligand CLA 2 205



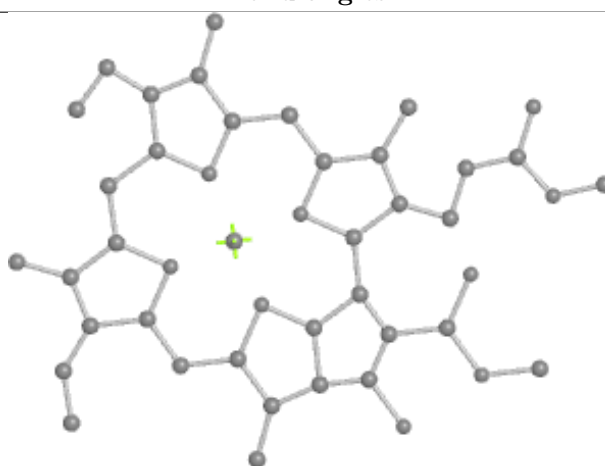
Bond lengths



Bond angles

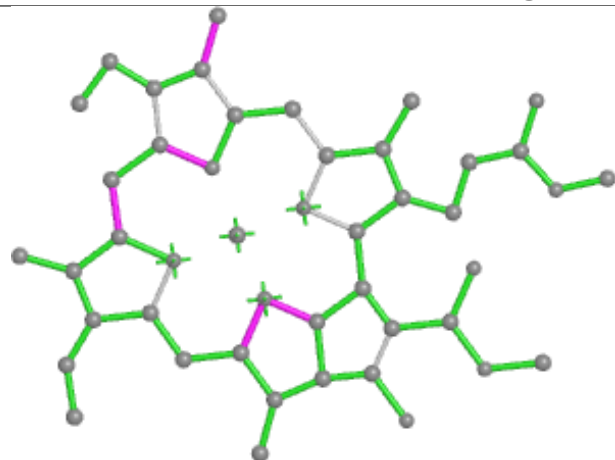


Torsions

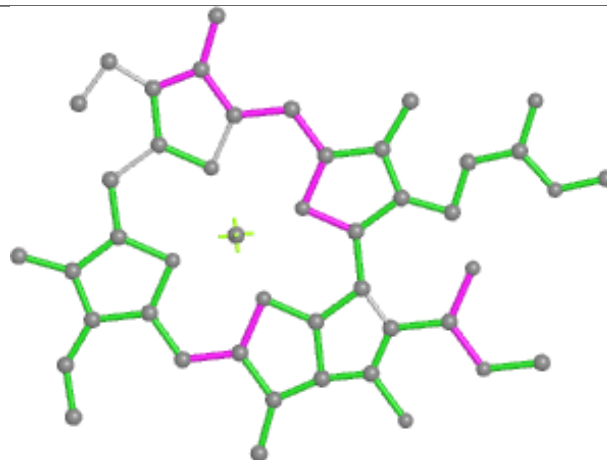


Rings

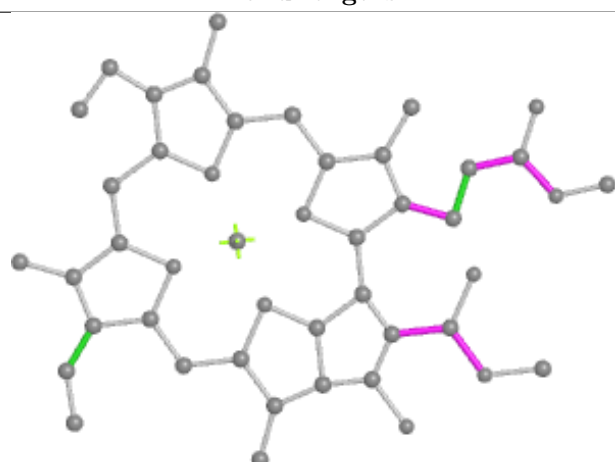
Ligand CLA 2 209



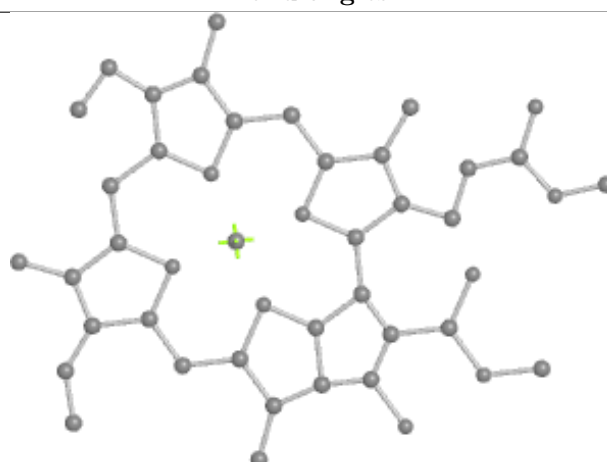
Bond lengths



Bond angles

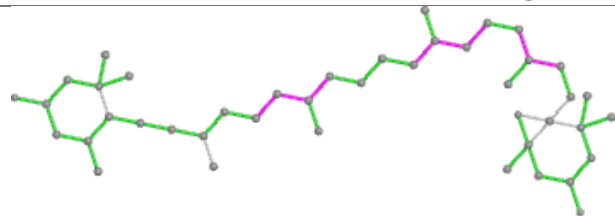


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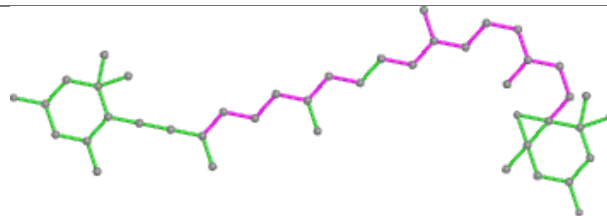


Rings

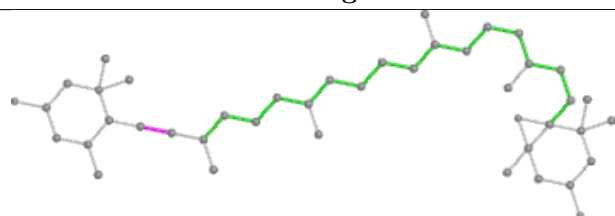
Ligand DD6 h 613



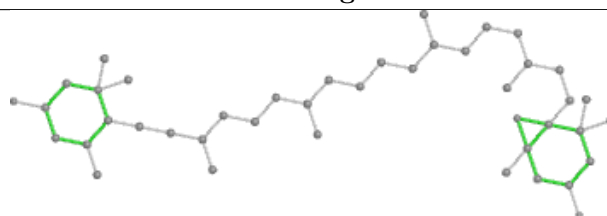
Bond lengths



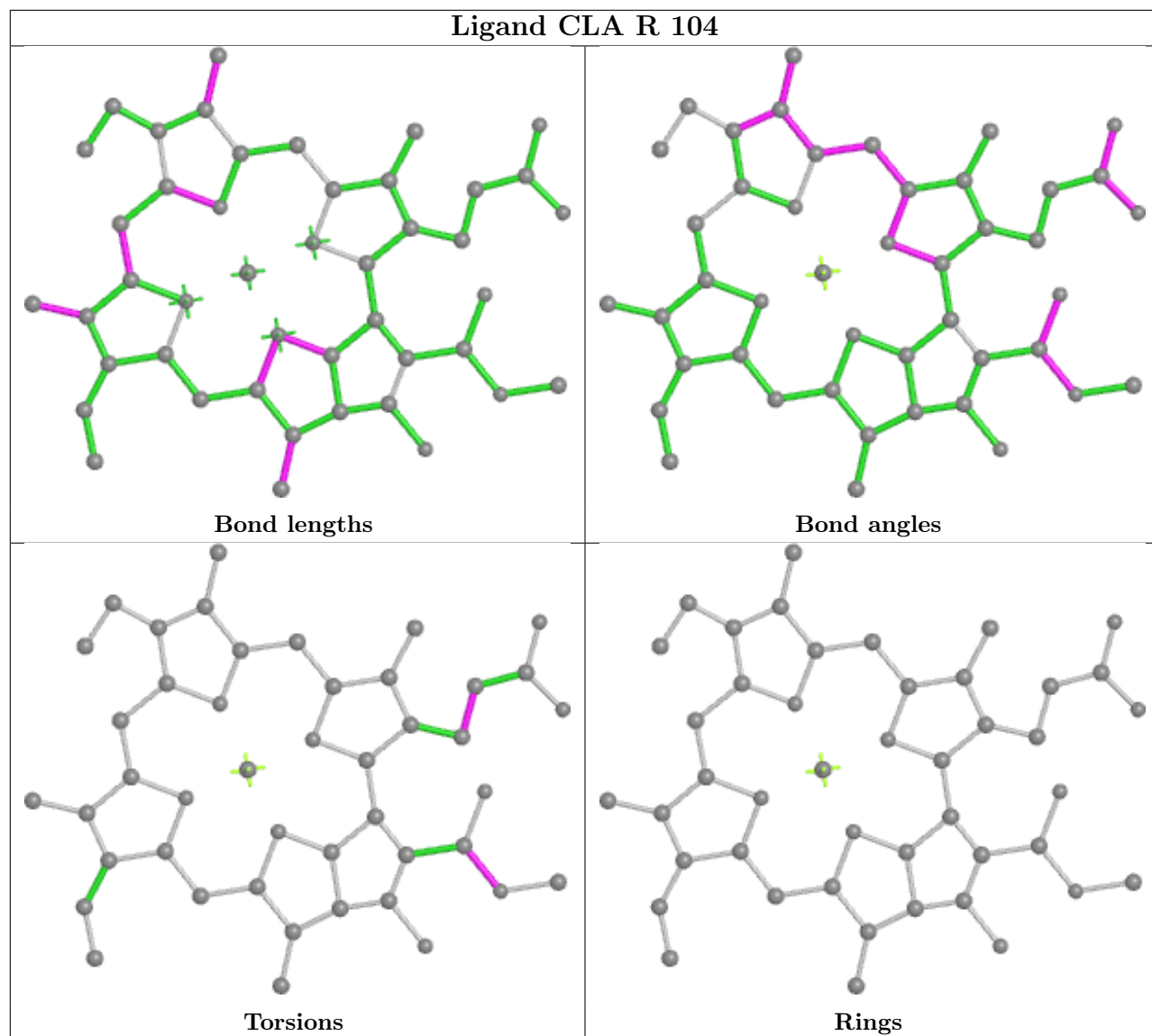
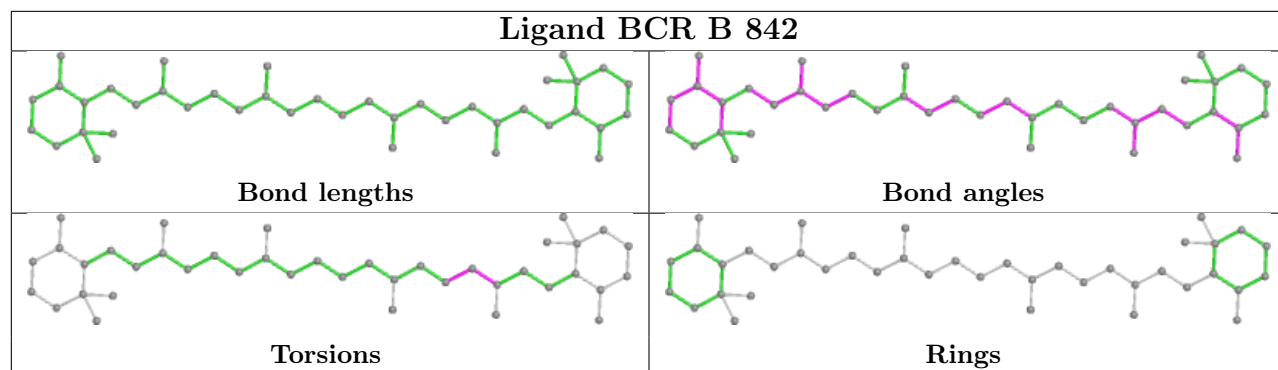
Bond angles



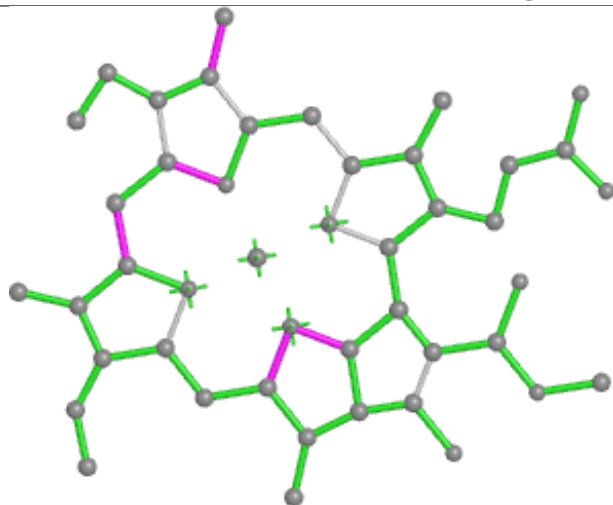
Torsions



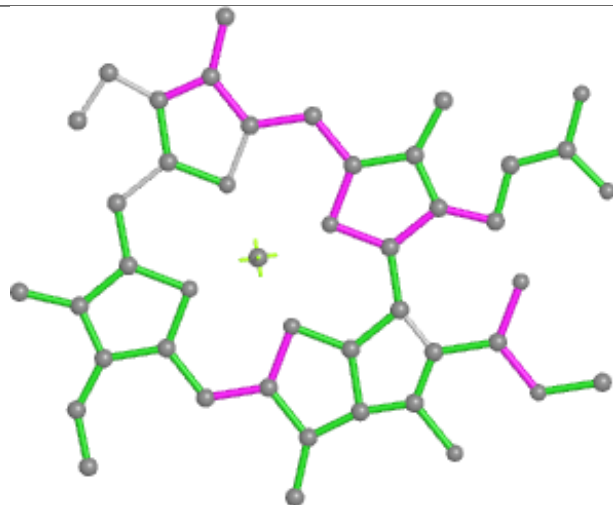
Rings



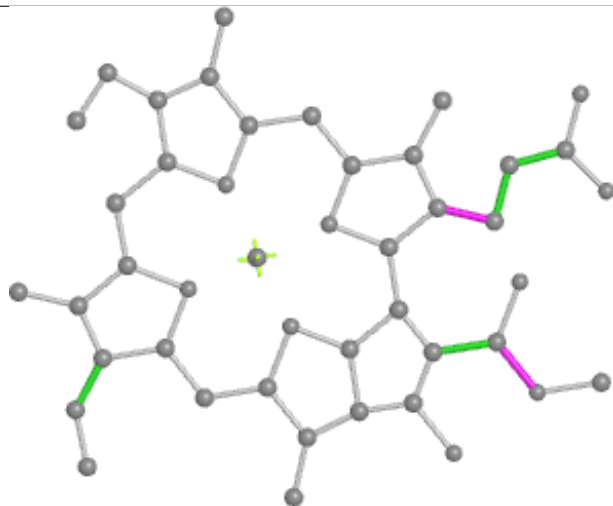
Ligand CLA t 301



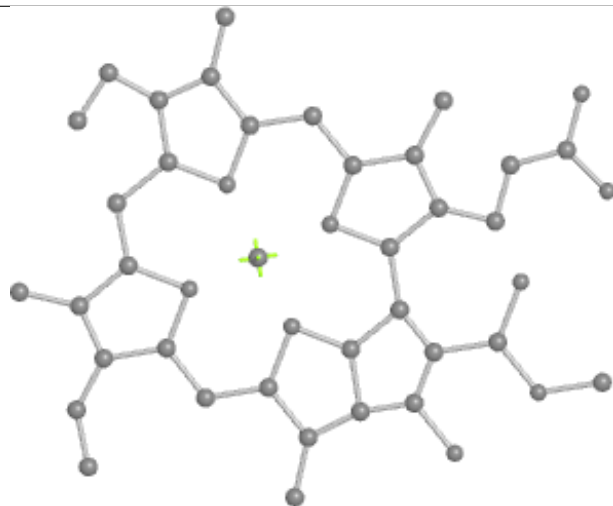
Bond lengths



Bond angles

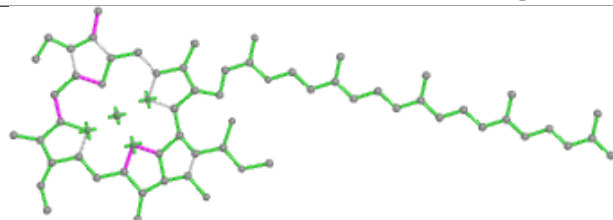


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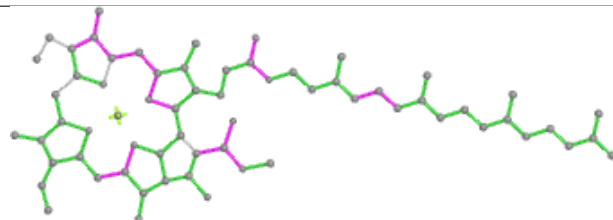


Rings

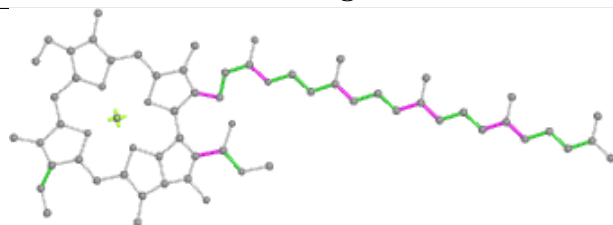
Ligand CLA A 818



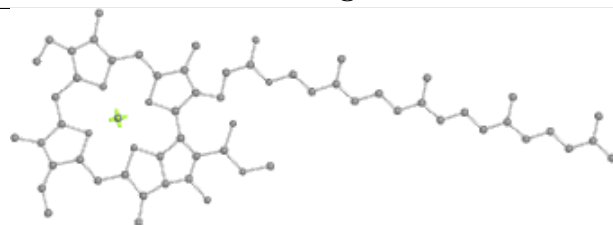
Bond lengths



Bond angles

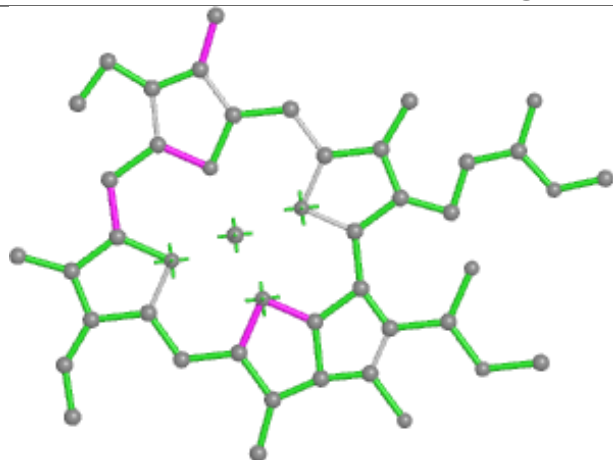


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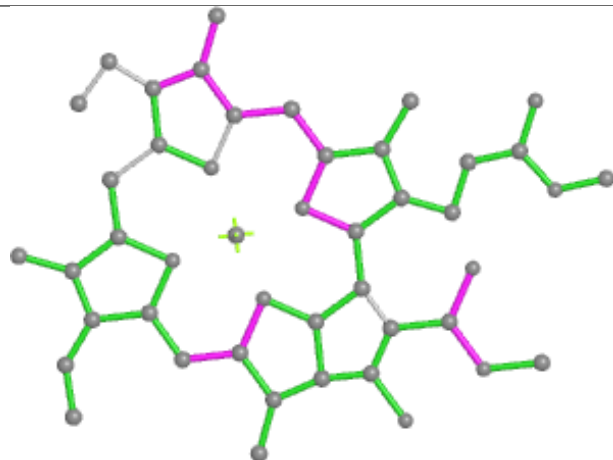


Rings

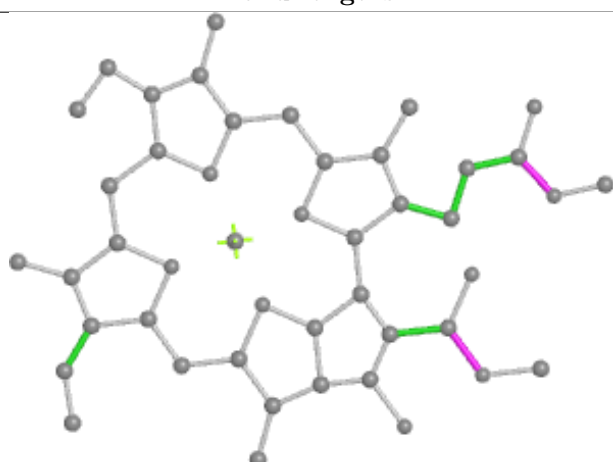
Ligand CLA k 301



Bond lengths



Bond angles

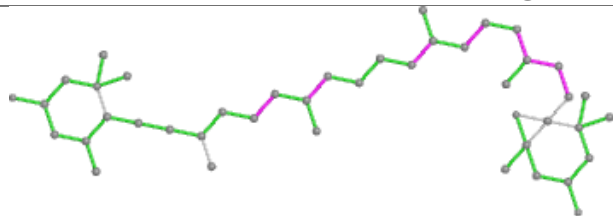


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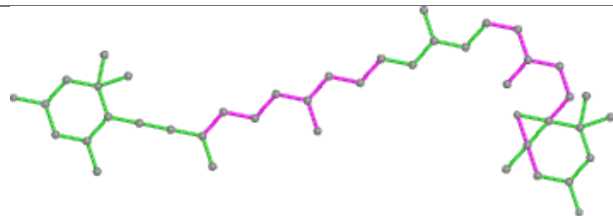


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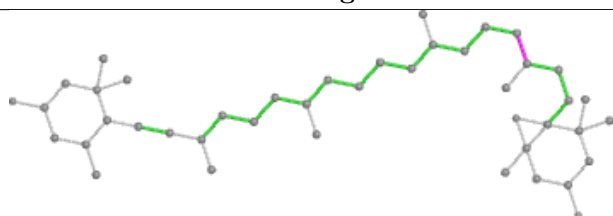
Ligand DD6 9 314



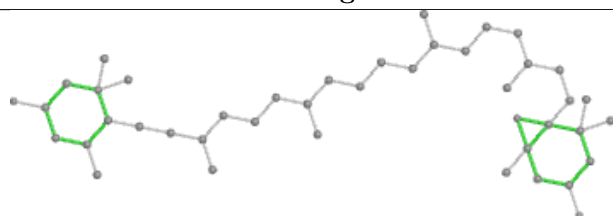
Bond lengths



Bond angles

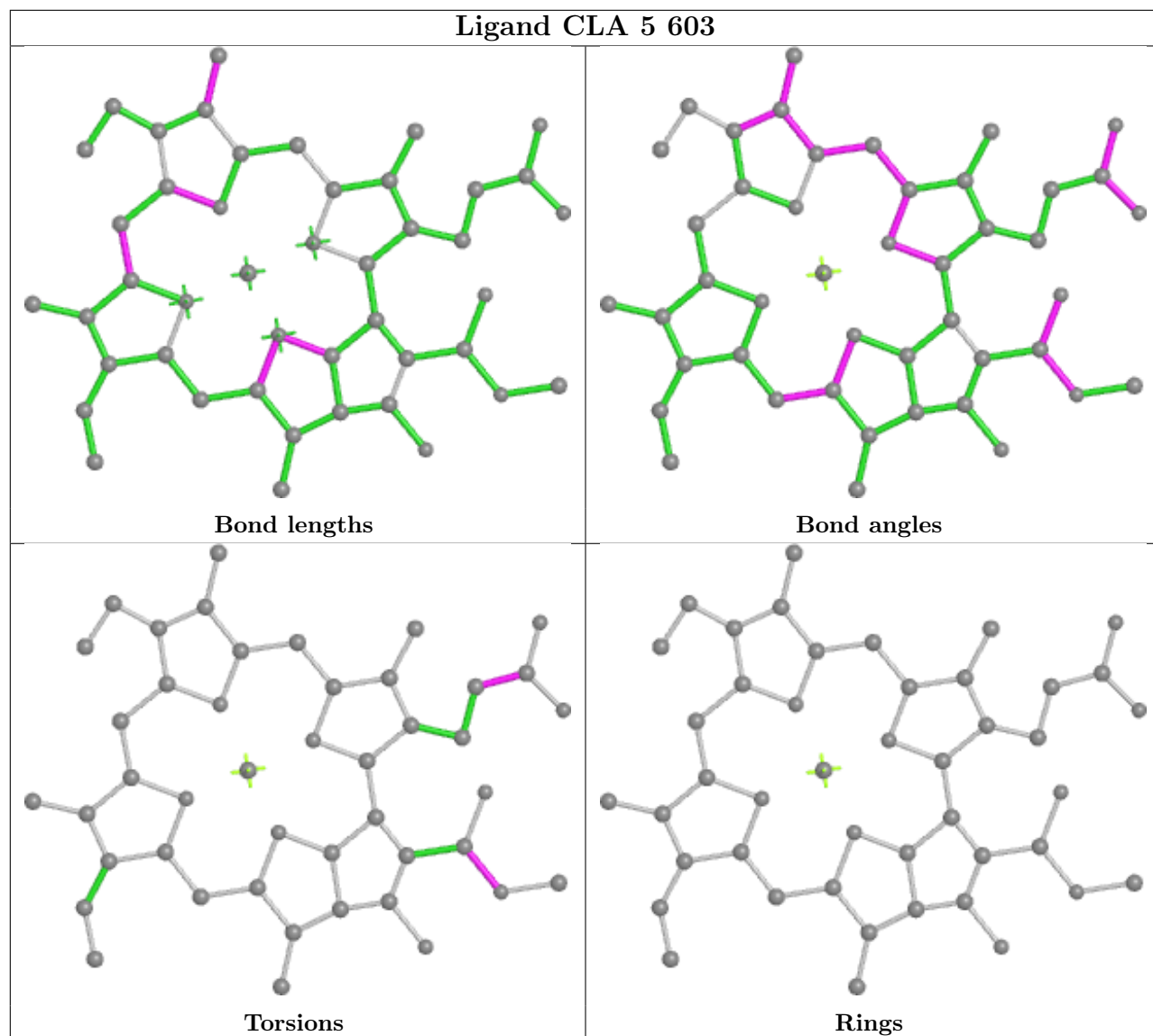


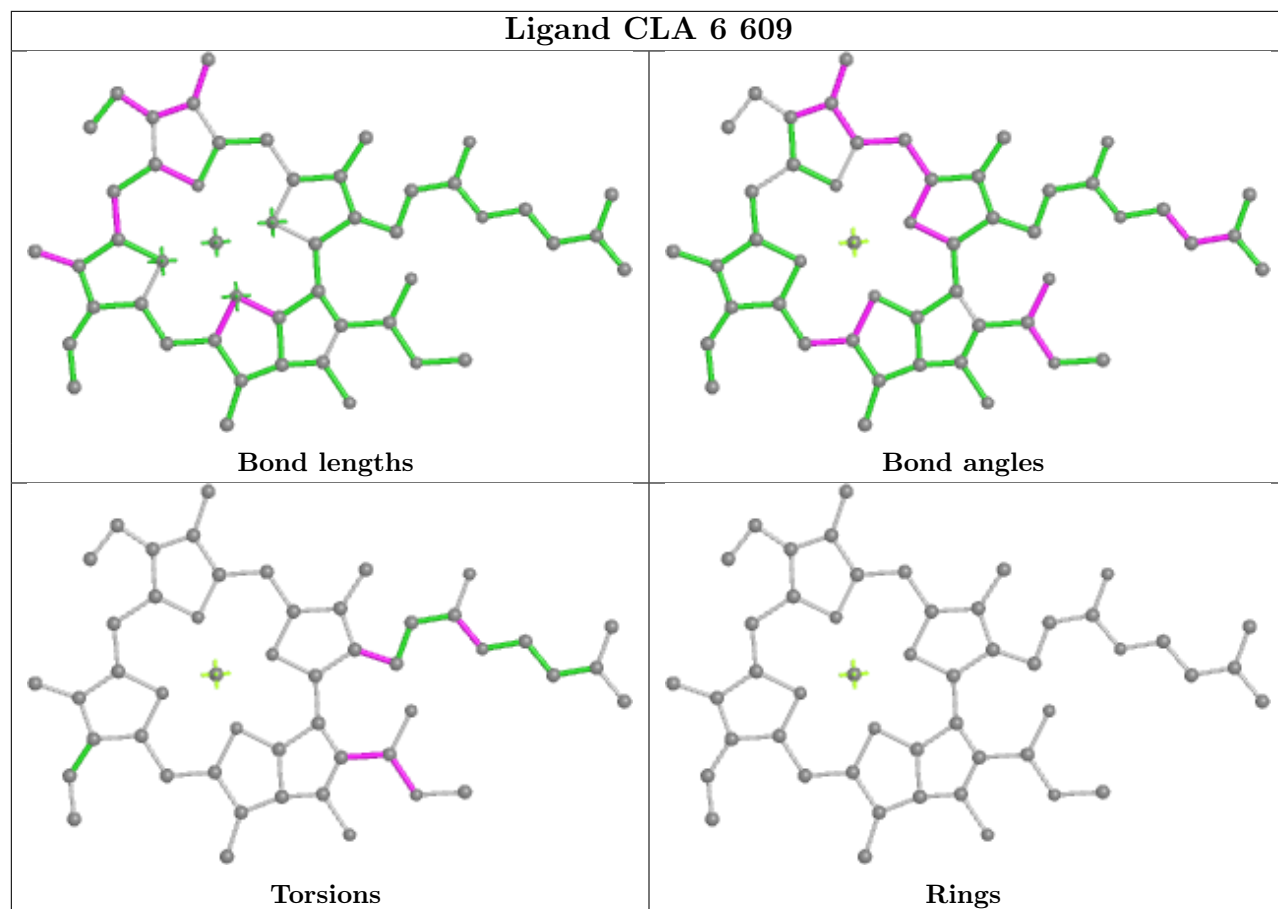
Torsions



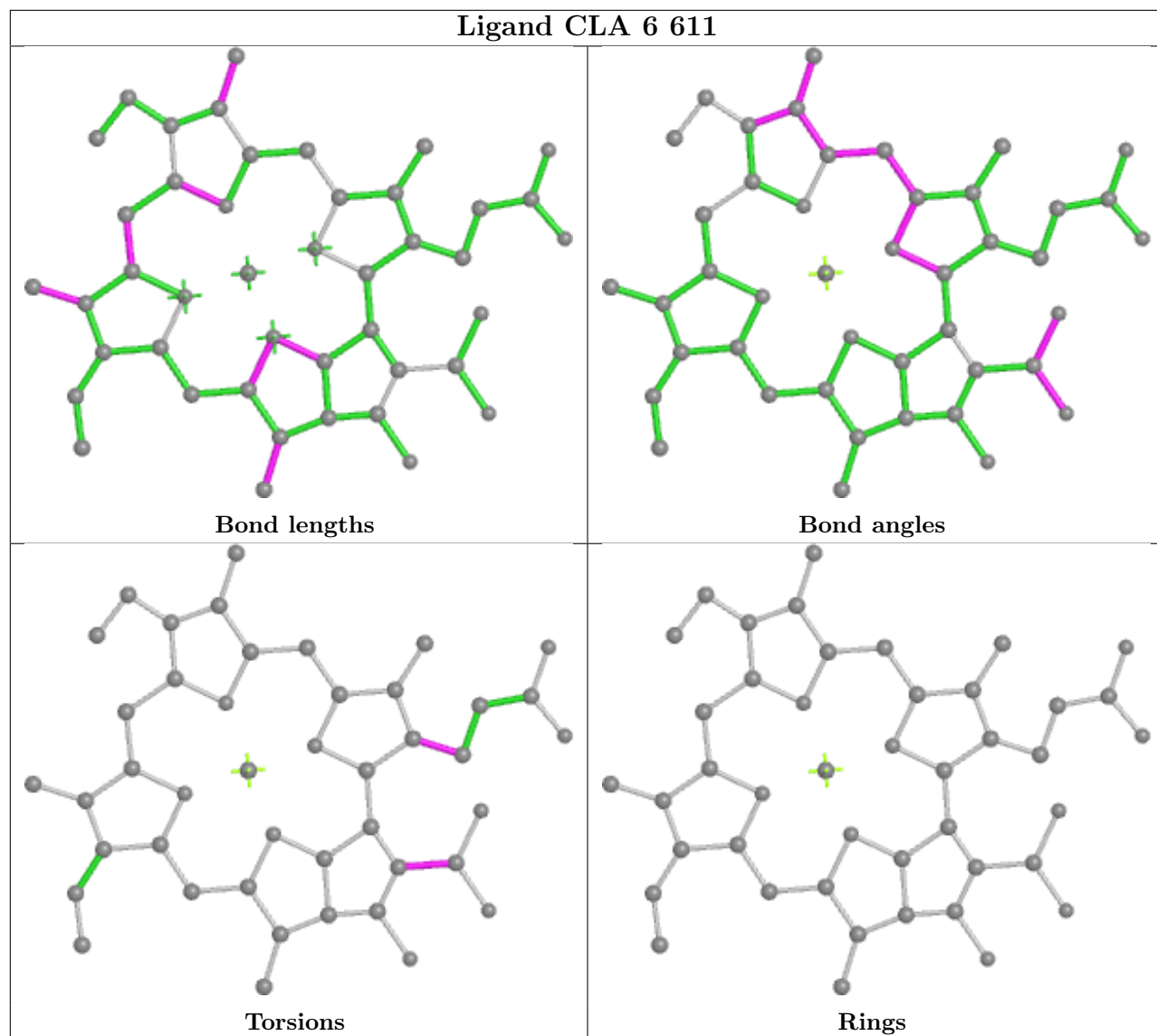
Rings

Ligand CLA 5 603

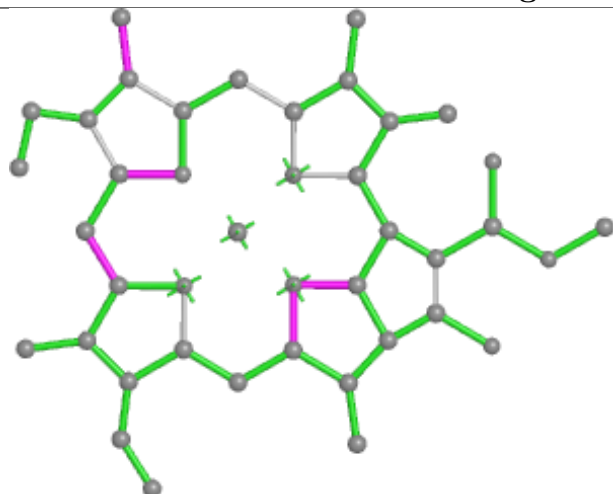




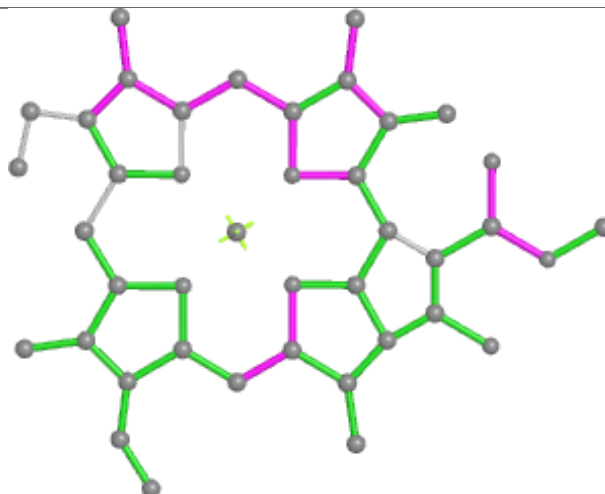
Ligand CLA 6 611



Ligand CLA c 611



Bond lengths



Bond angles

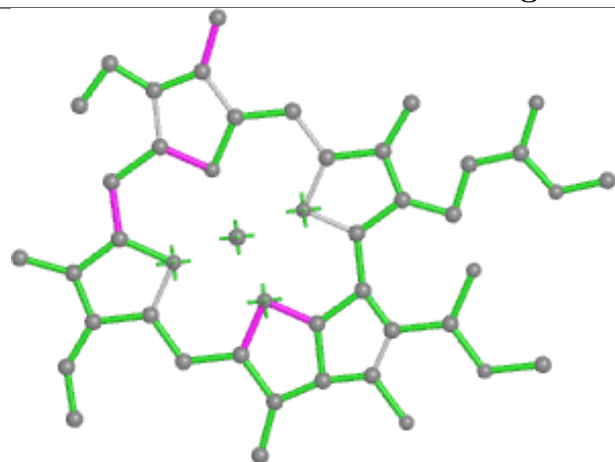


Torsions

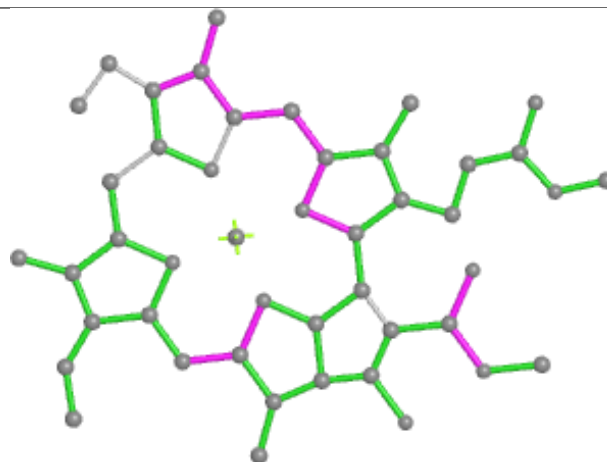


Rings

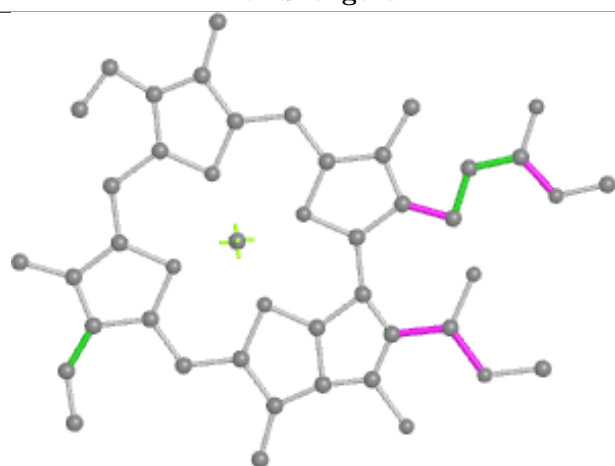
Ligand CLA 5 605



Bond lengths



Bond angles

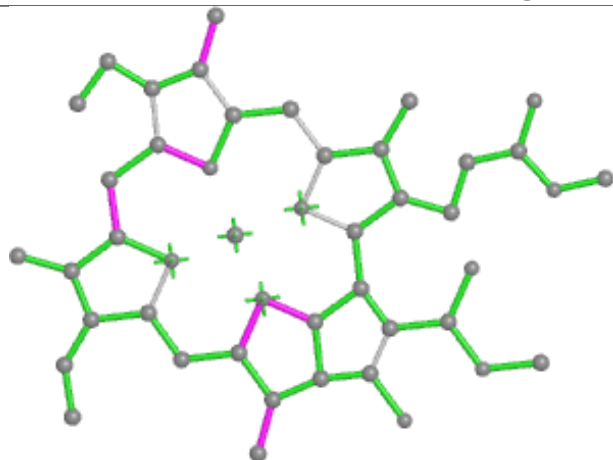


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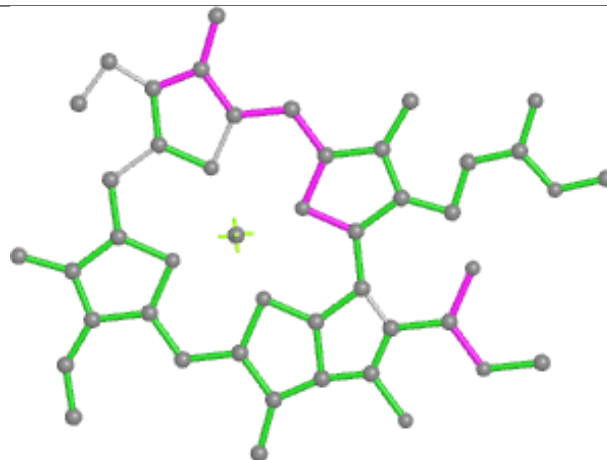


Rings

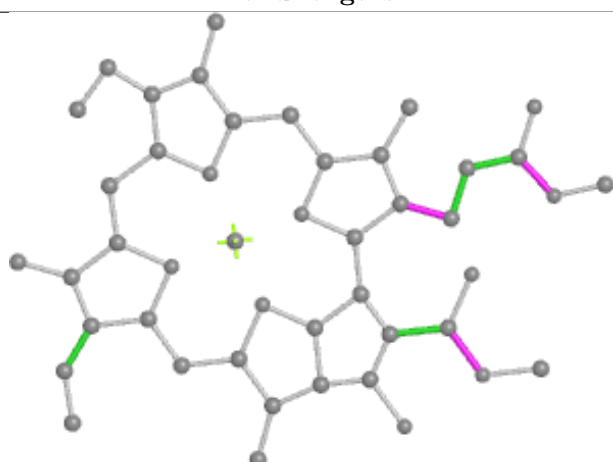
Ligand CLA 9 310



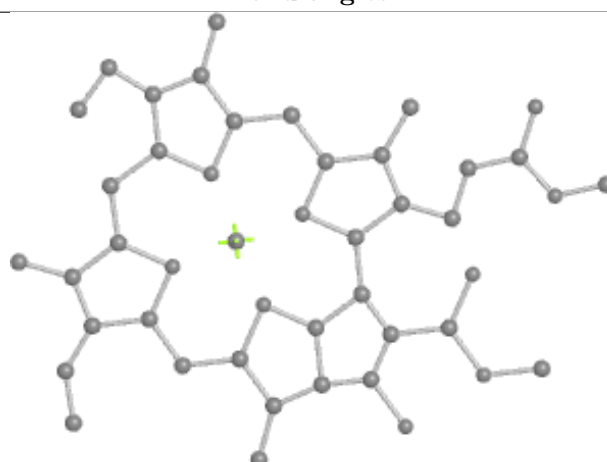
Bond lengths



Bond angles

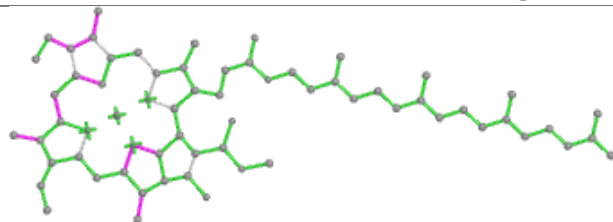


Torsions

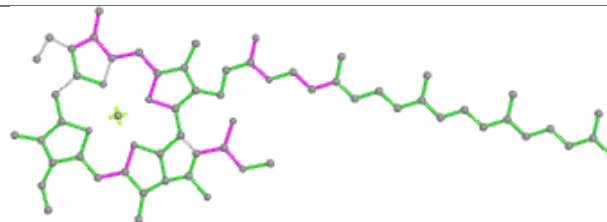


Rings

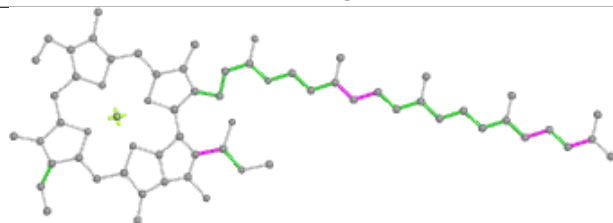
Ligand CLA B 808



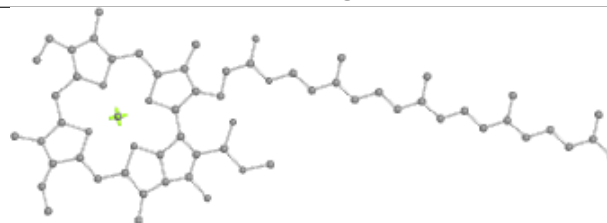
Bond lengths



Bond angles

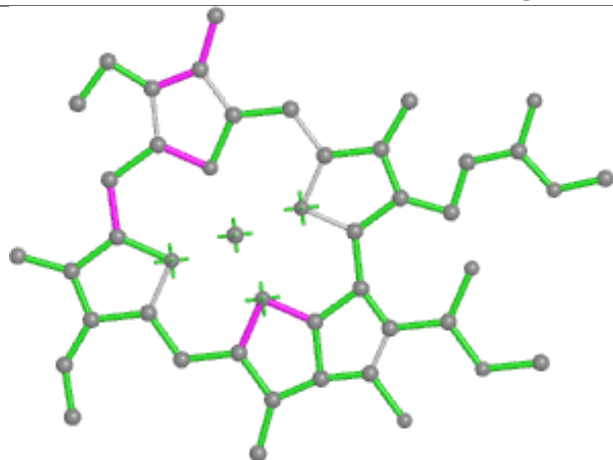


Torsions

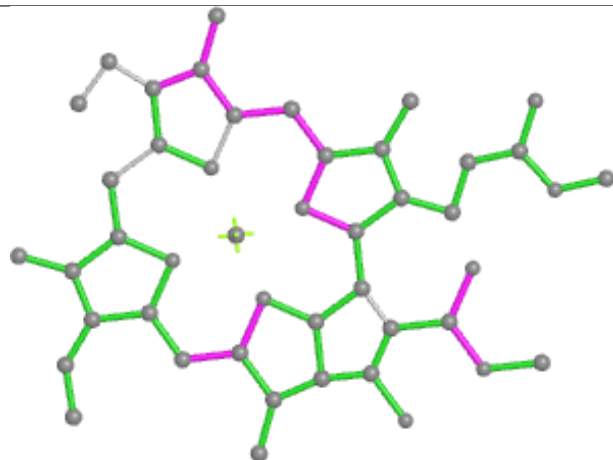


Rings

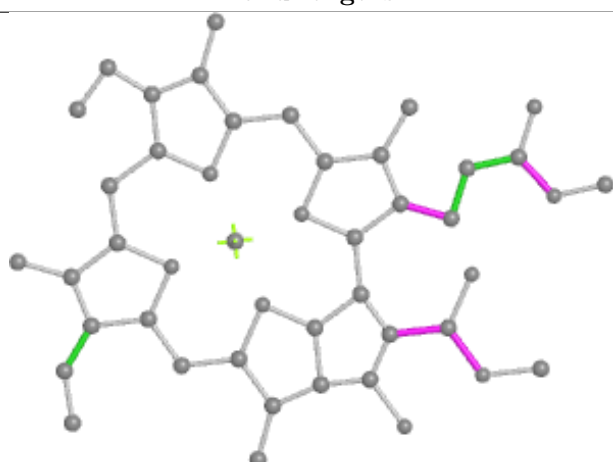
Ligand CLA k 304



Bond lengths



Bond angles

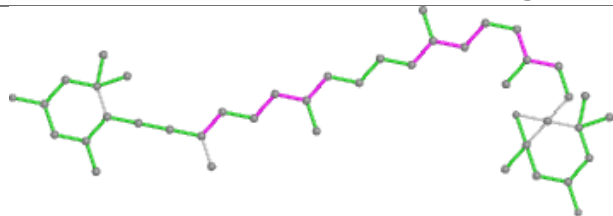


Torsions

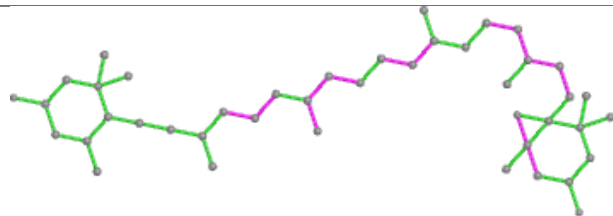


Rings

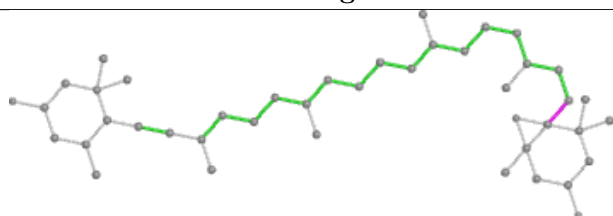
Ligand DD6 k 314



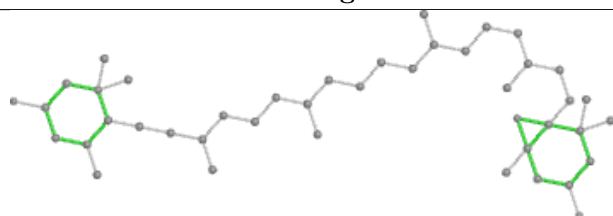
Bond lengths



Bond angles

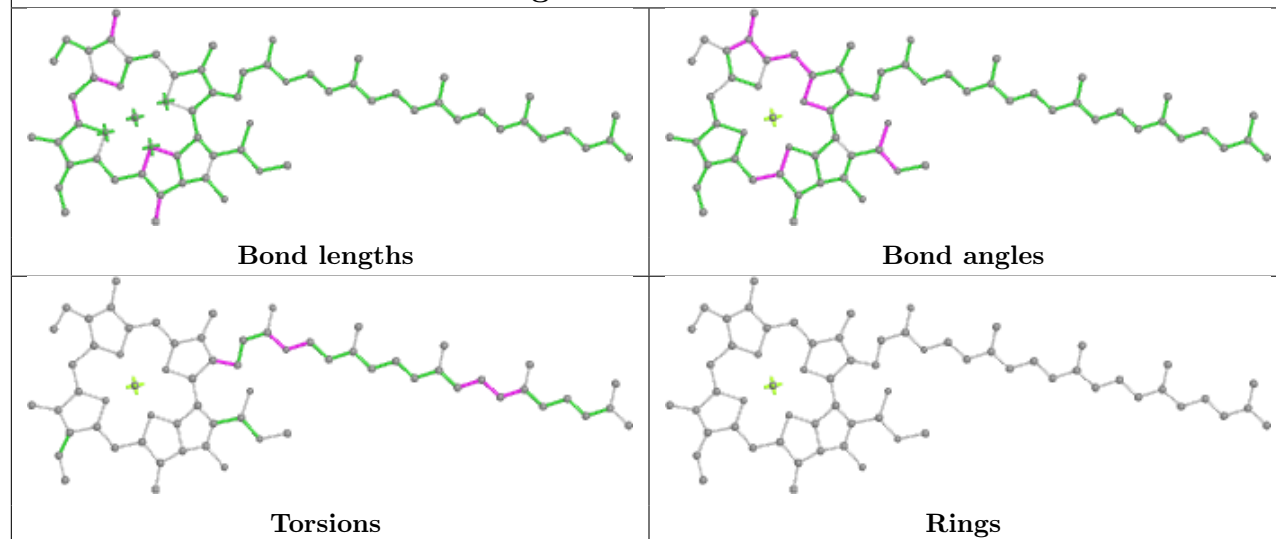


Torsions

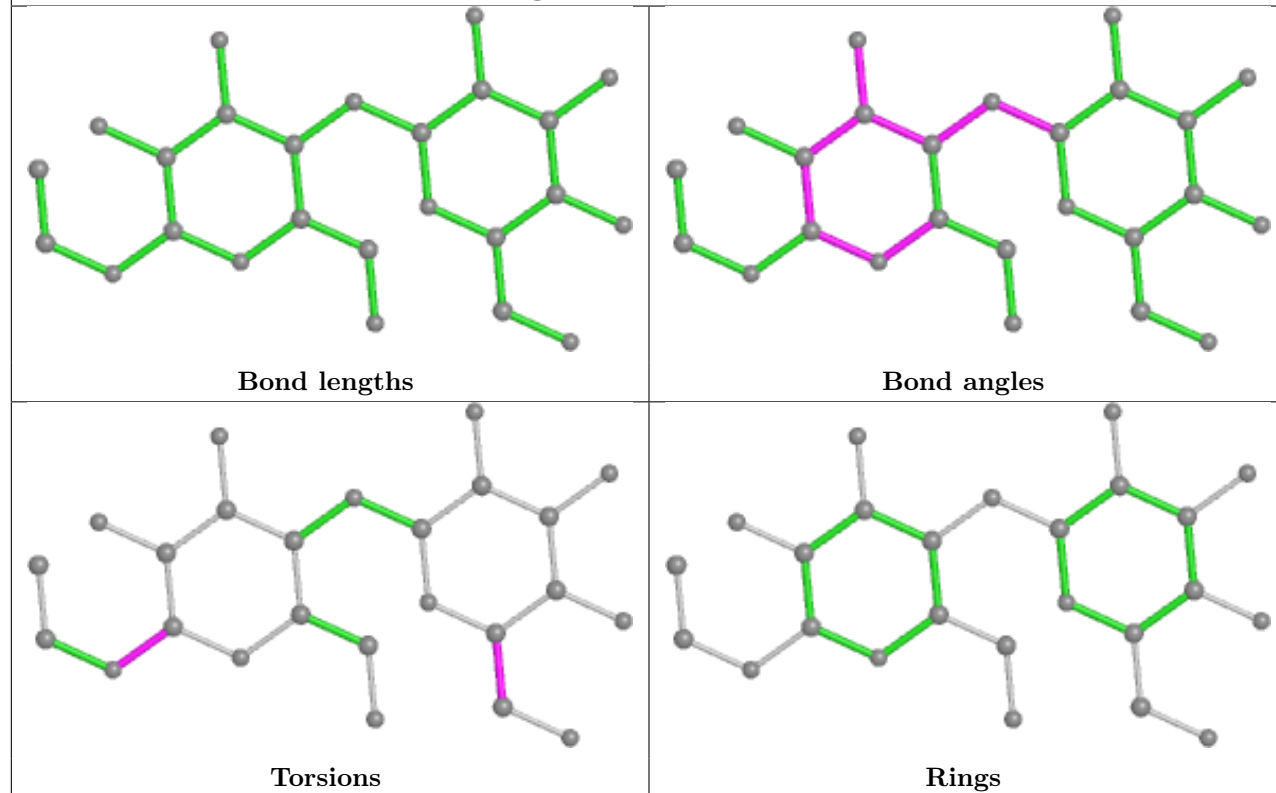


Rings

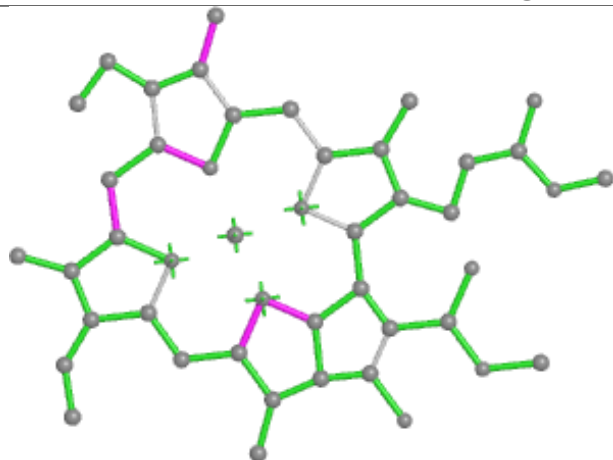
Ligand CLA R 103



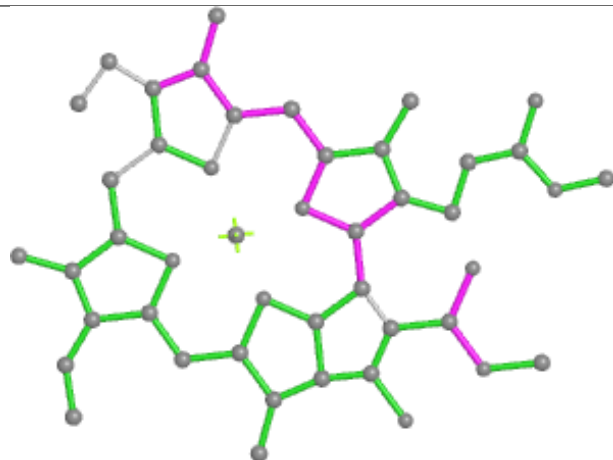
Ligand LMT A 851



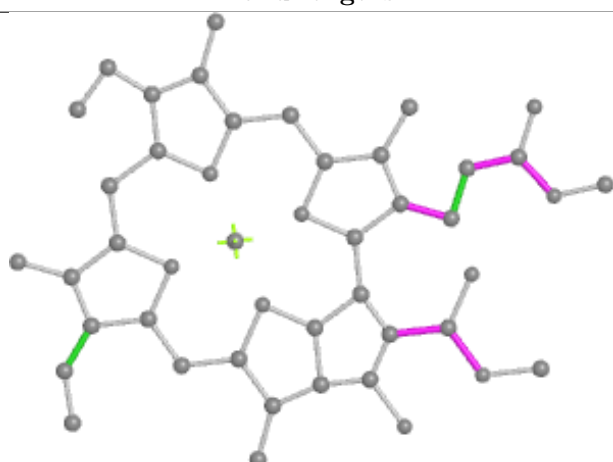
Ligand CLA 9 309



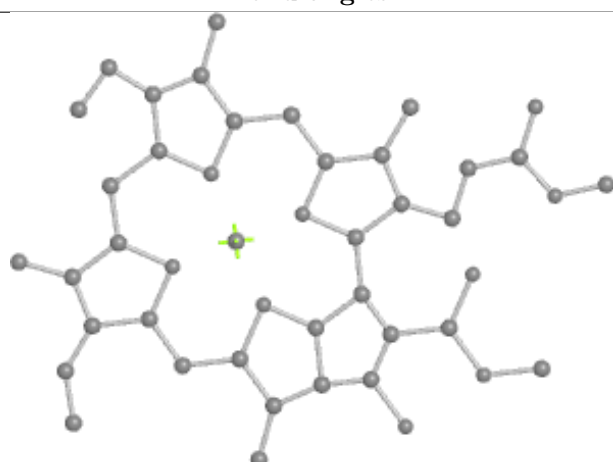
Bond lengths



Bond angles

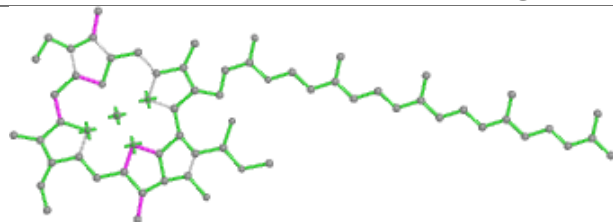


Torsions

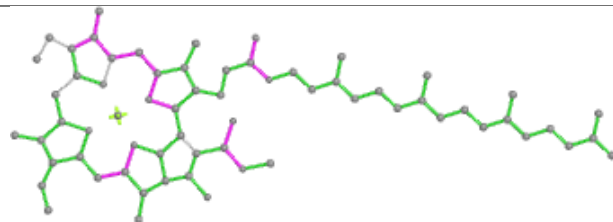


Rings

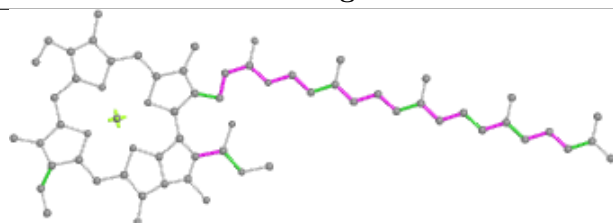
Ligand CLA B 831



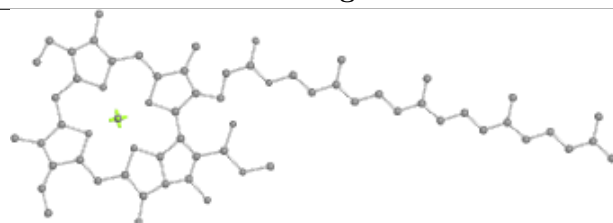
Bond lengths



Bond angles

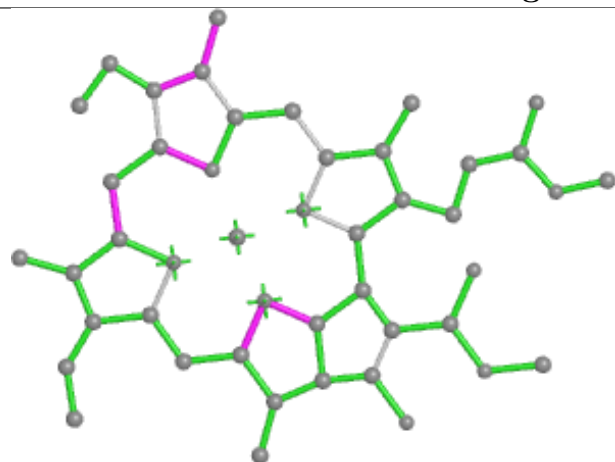


Torsions

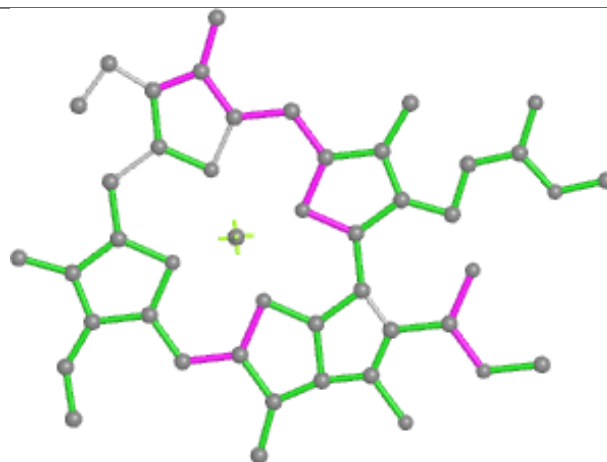


Rings

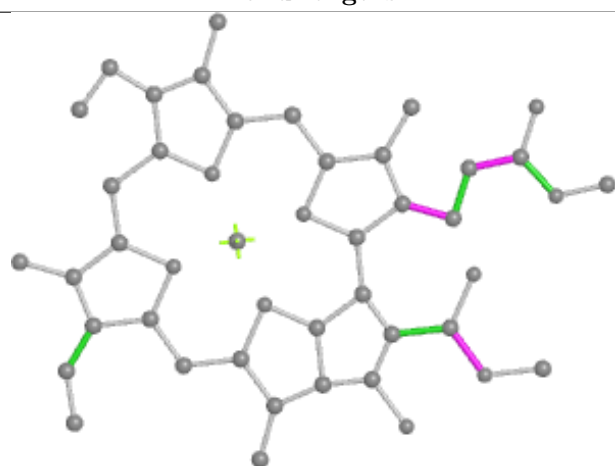
Ligand CLA t 308



Bond lengths



Bond angles

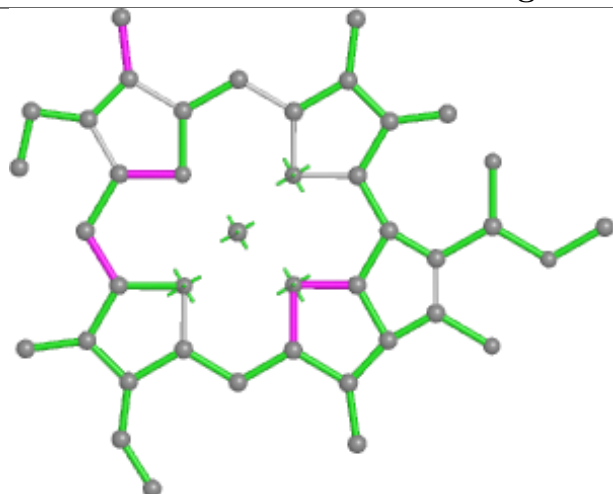


Torsions

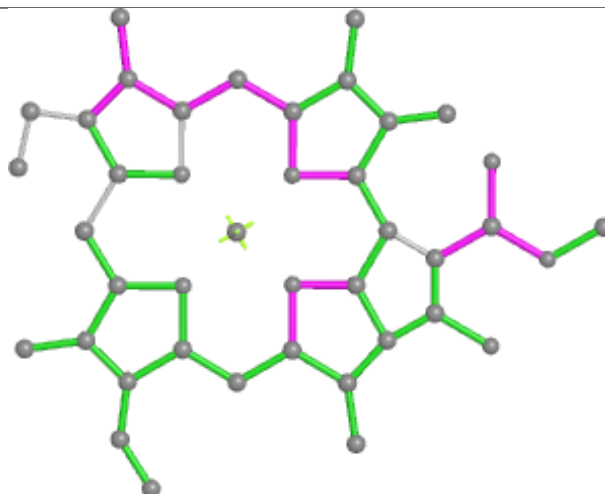


Rings

Ligand CLA k 308



Bond lengths



Bond angles

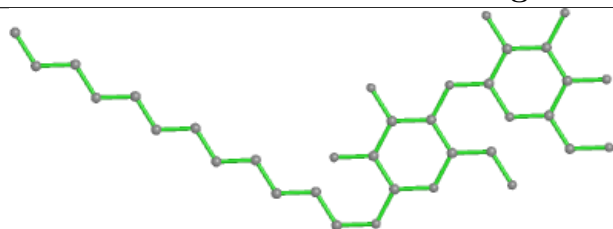


Torsions

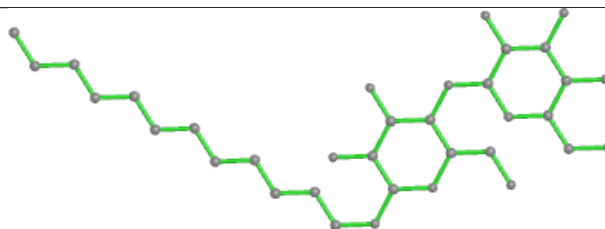


Rings

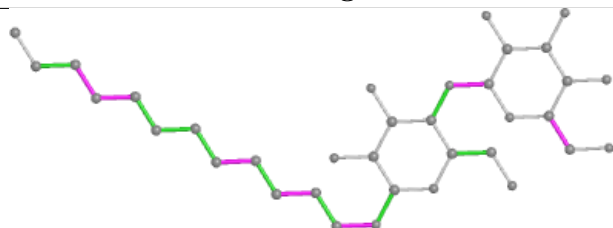
Ligand LMT A 854



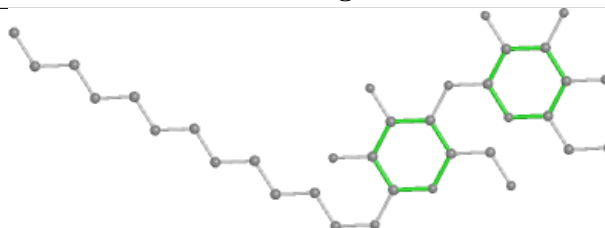
Bond lengths



Bond angles

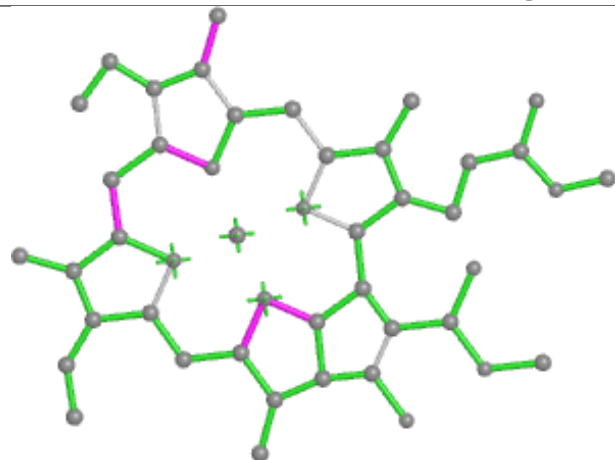


Torsions

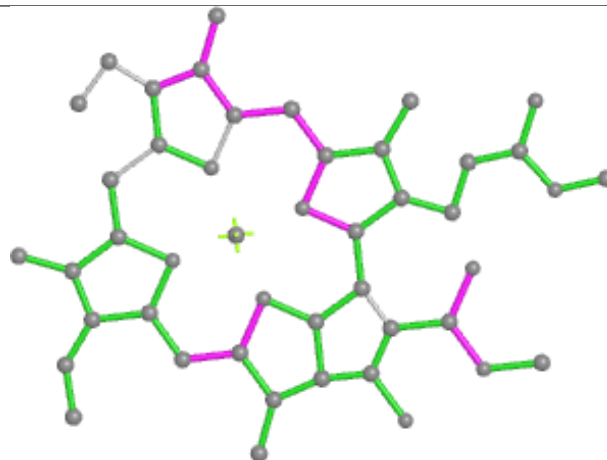


Rings

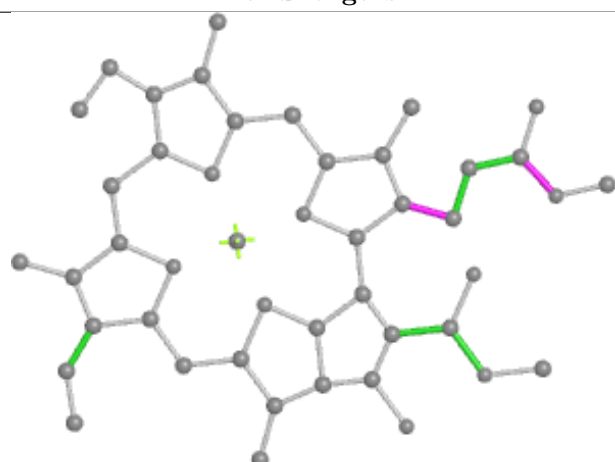
Ligand CLA 6 607



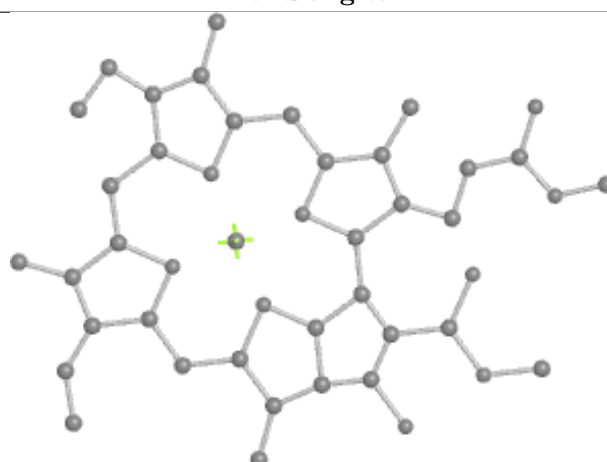
Bond lengths



Bond angles

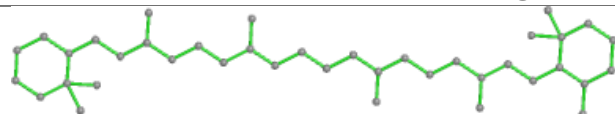


Torsions

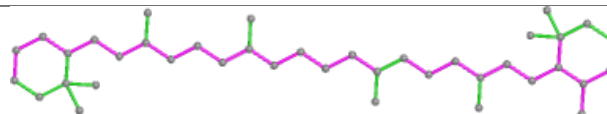


Rings

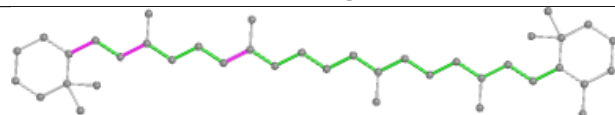
Ligand BCR A 845



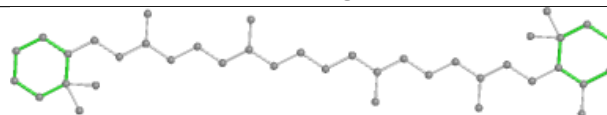
Bond lengths



Bond angles

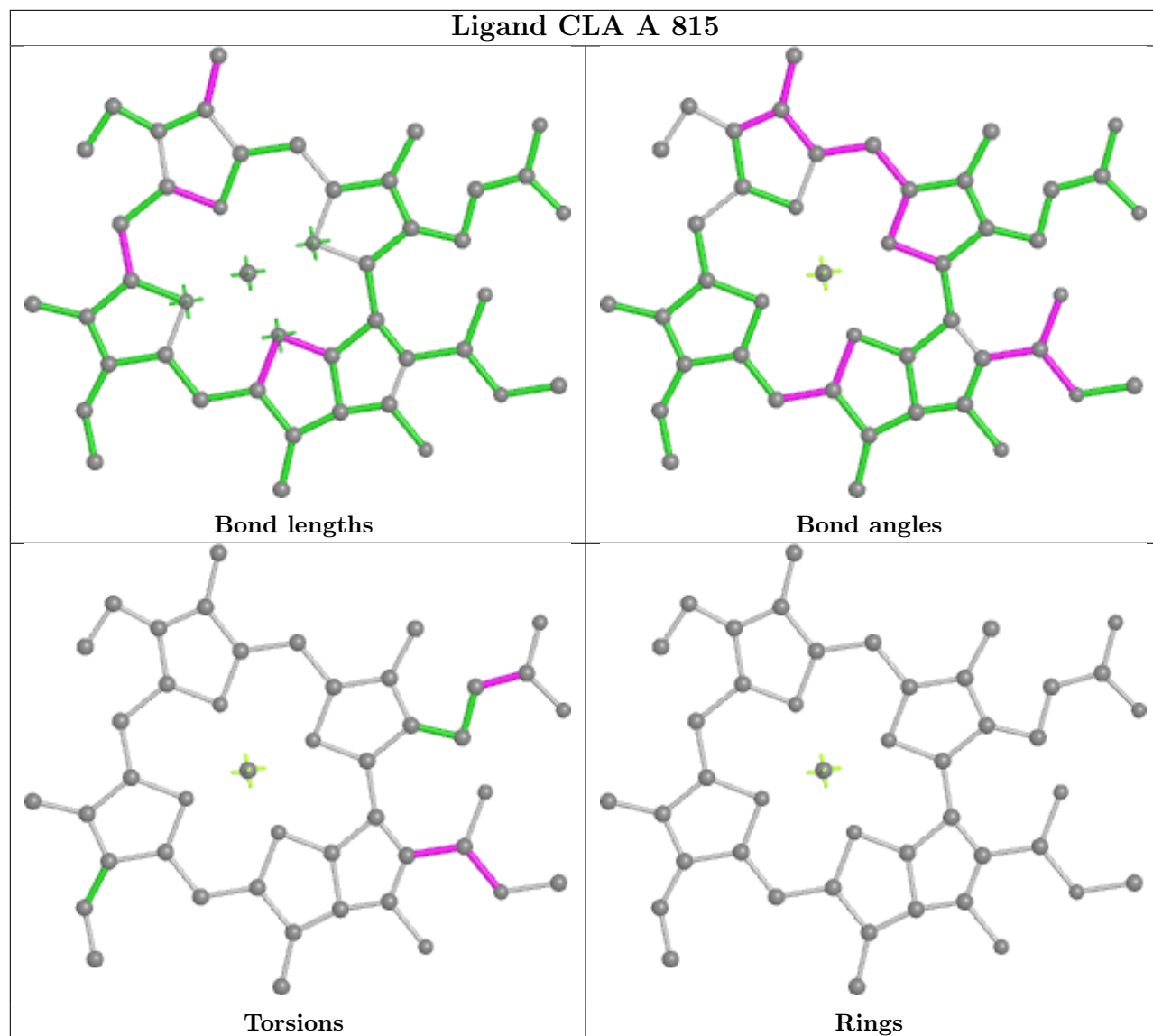


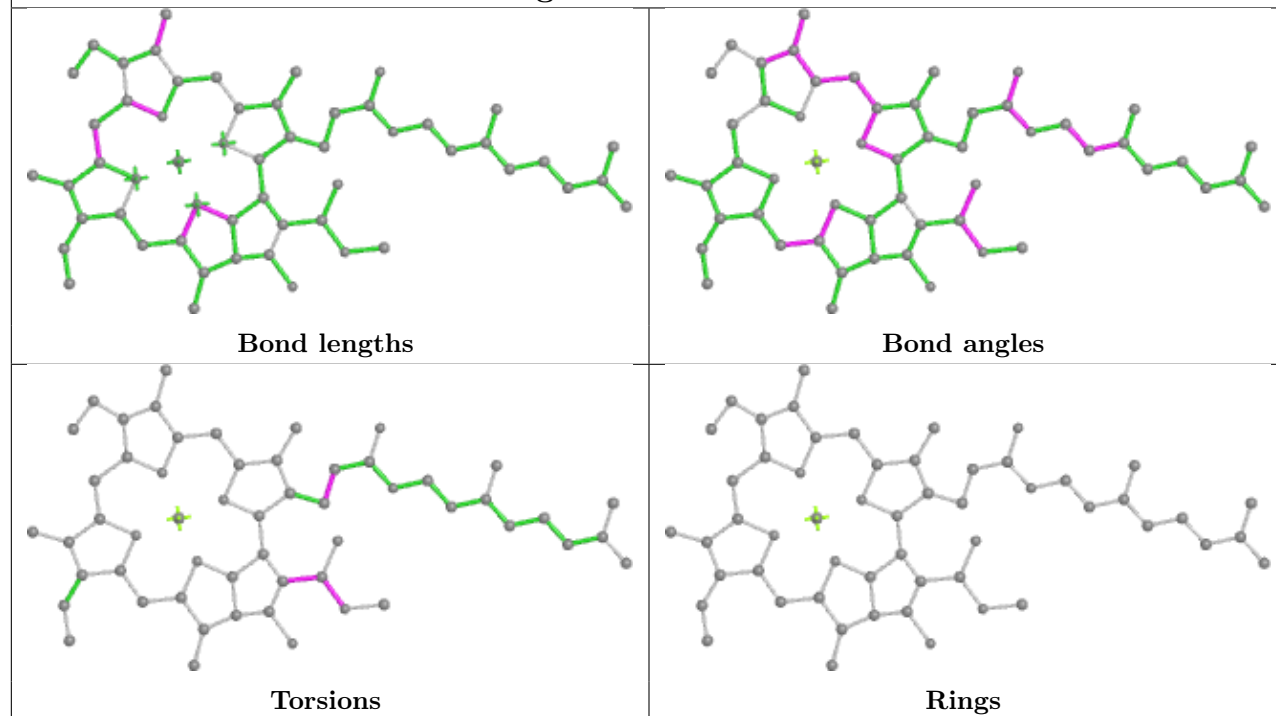
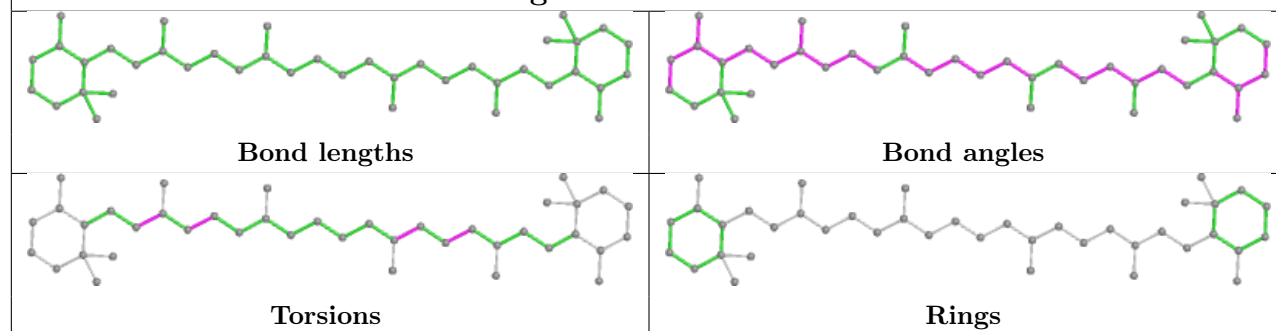
Torsions



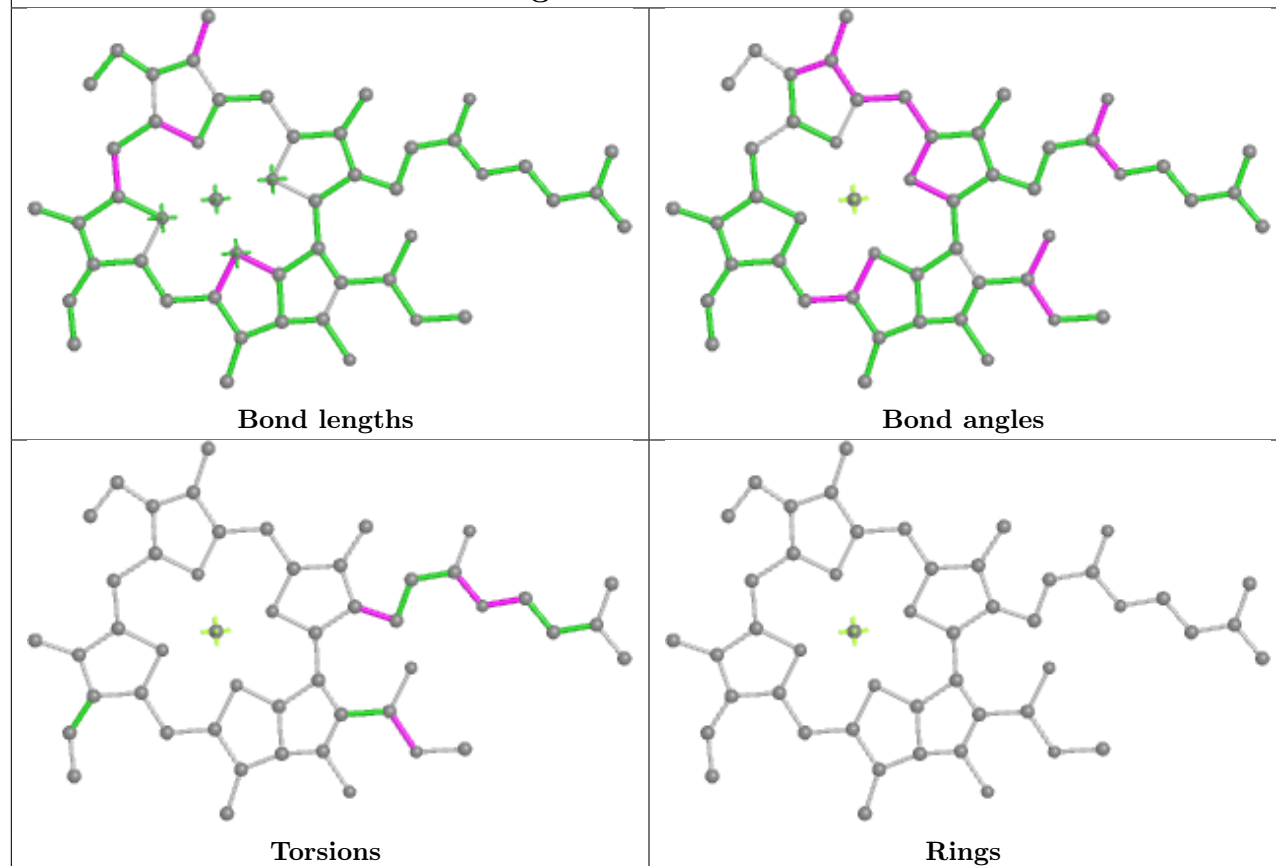
Rings

Ligand CLA A 815

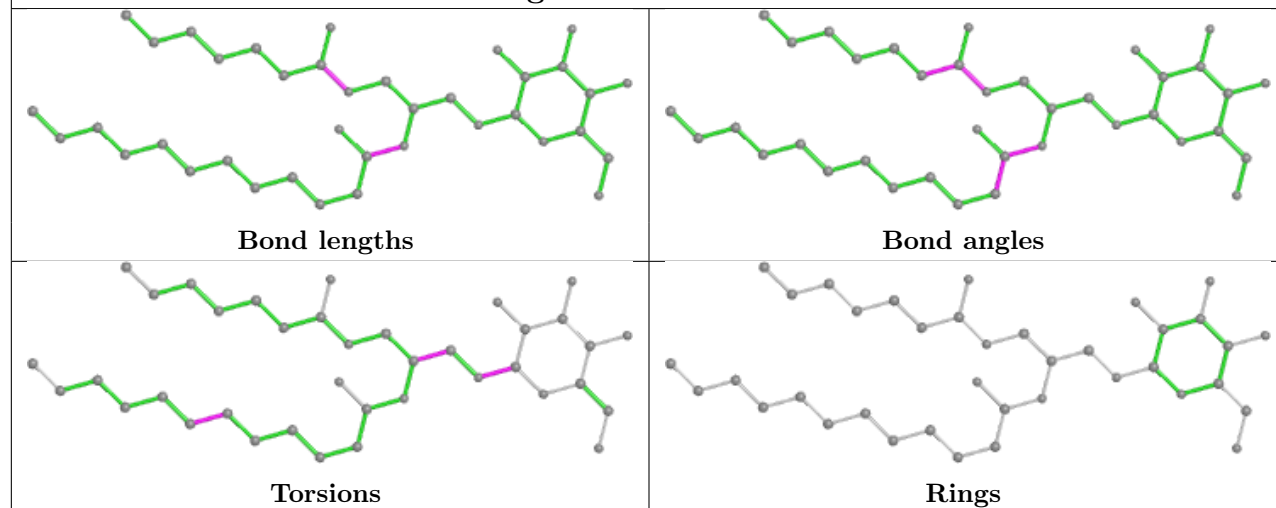


Ligand CLA 3 303**Ligand BCR A 844**

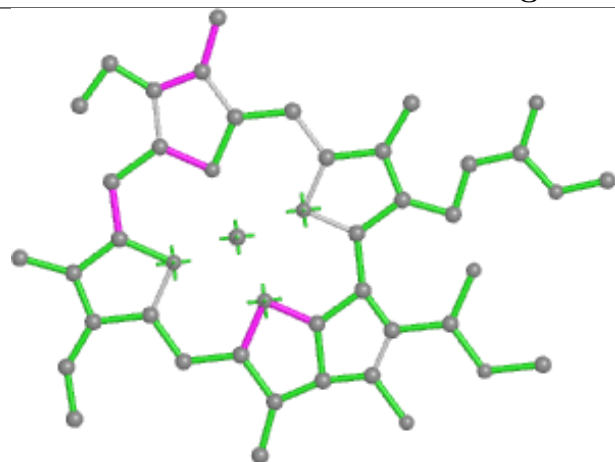
Ligand CLA A 814



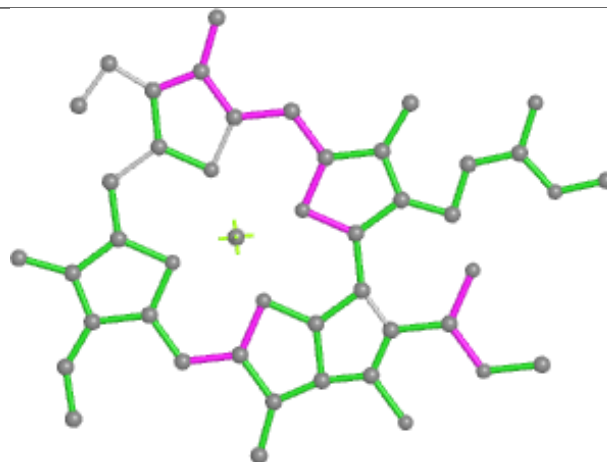
Ligand LMG A 855



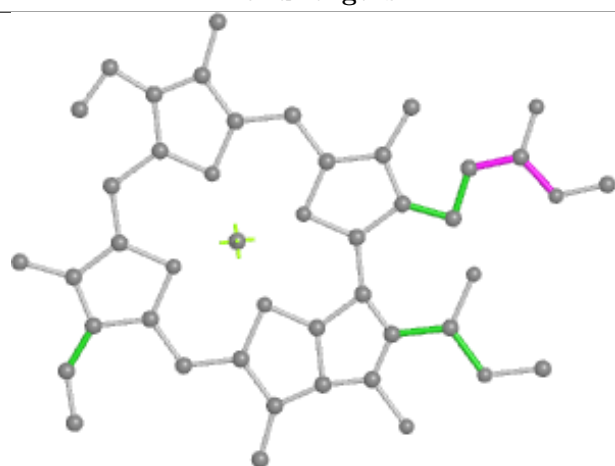
Ligand CLA 4 603



Bond lengths



Bond angles

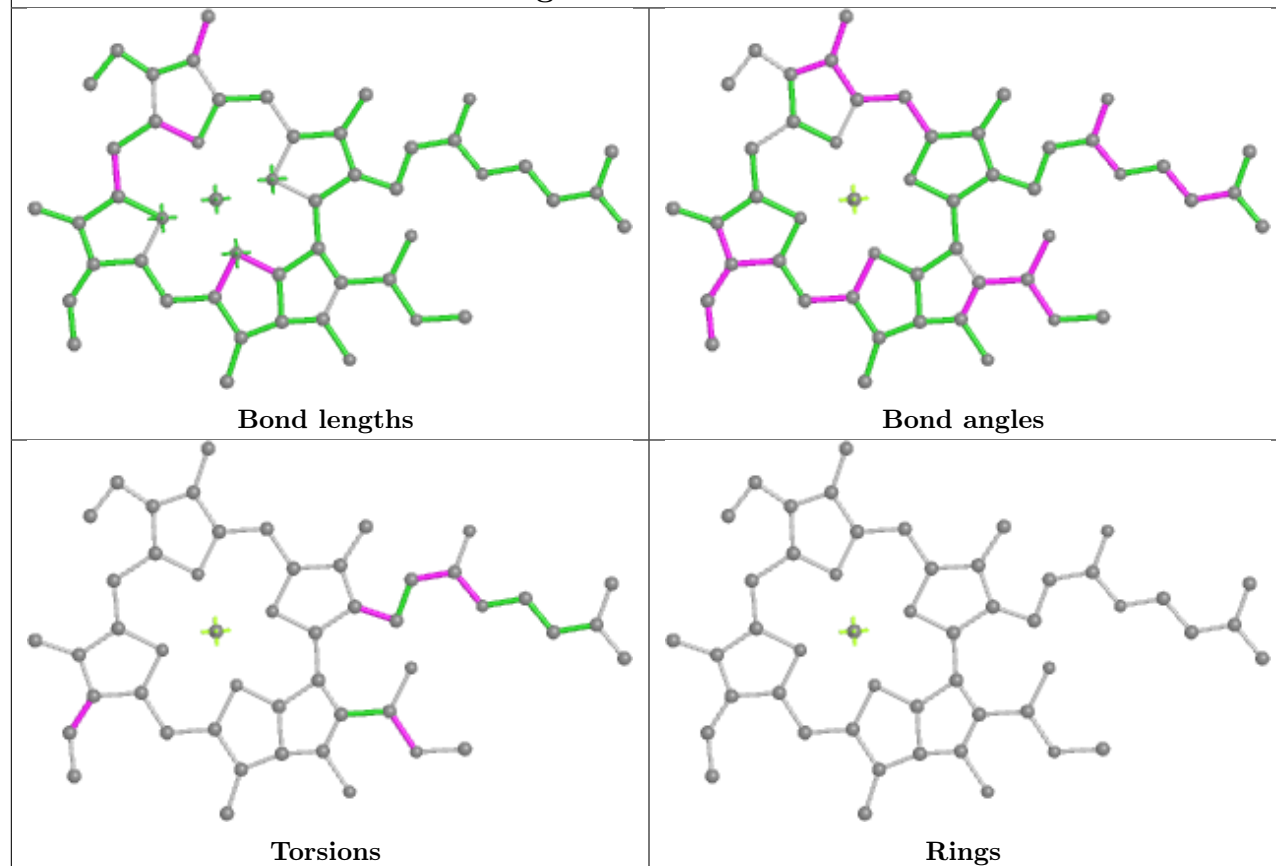


Torsions

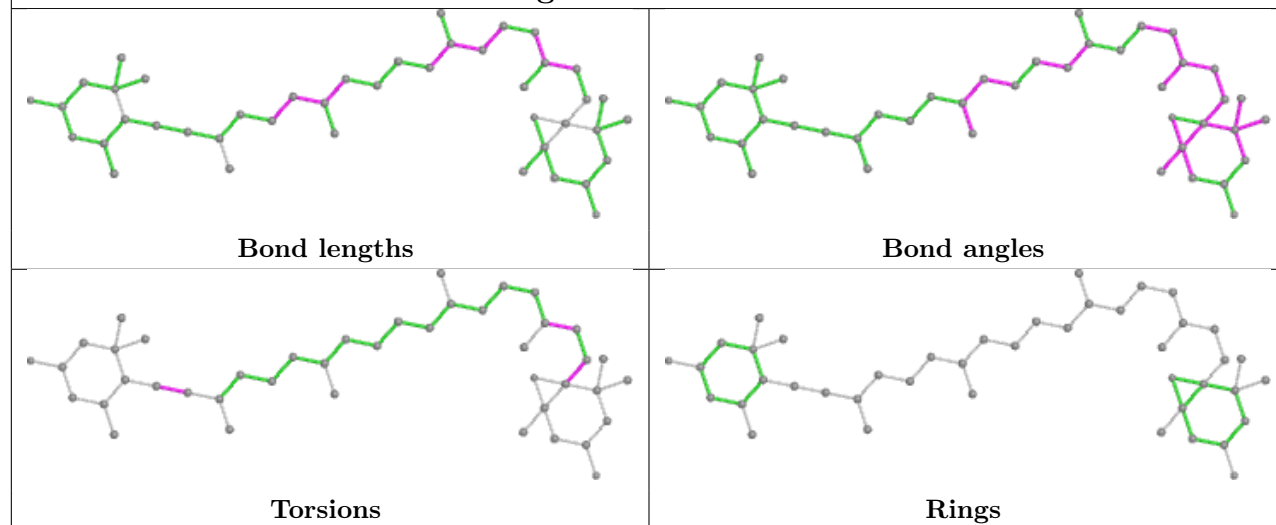


Rings

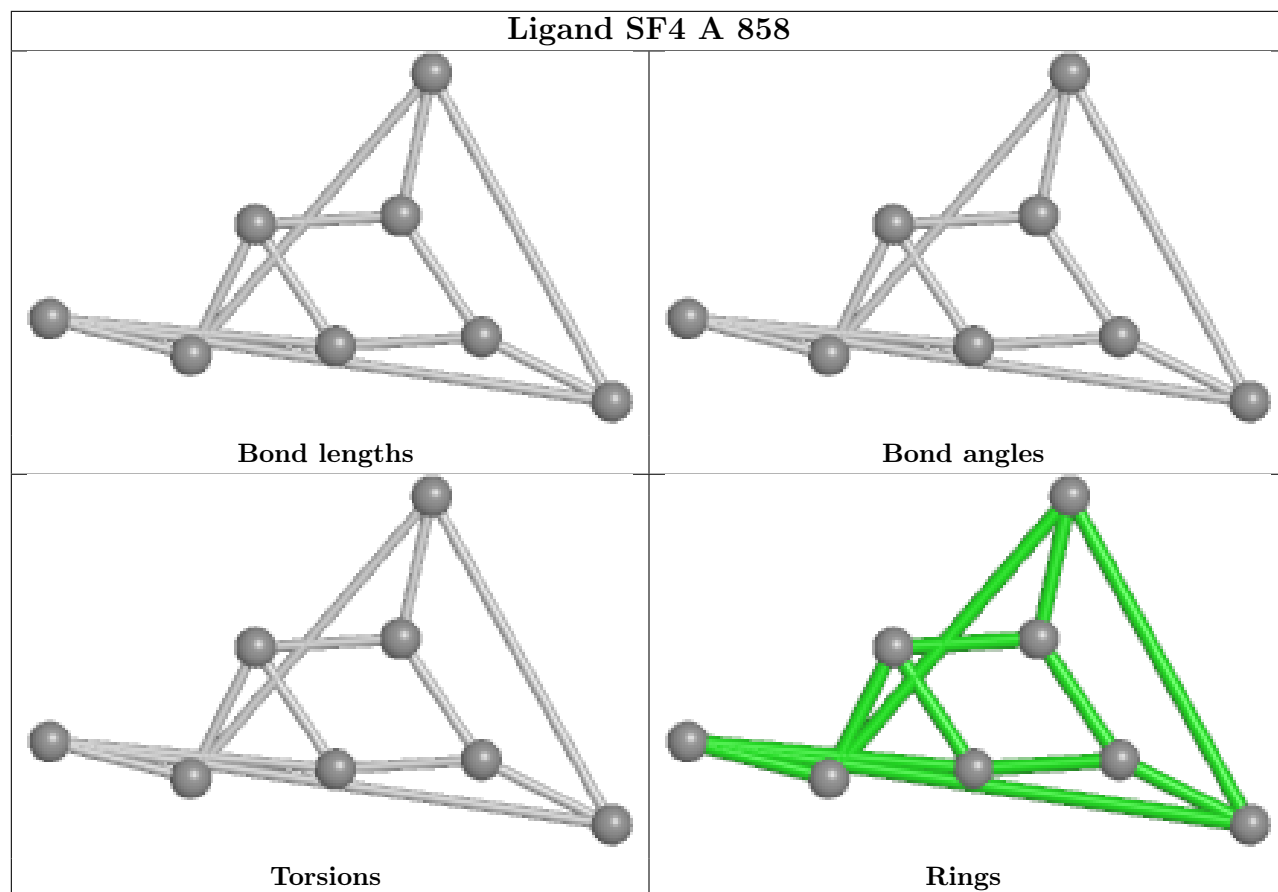
Ligand CLA 7 602



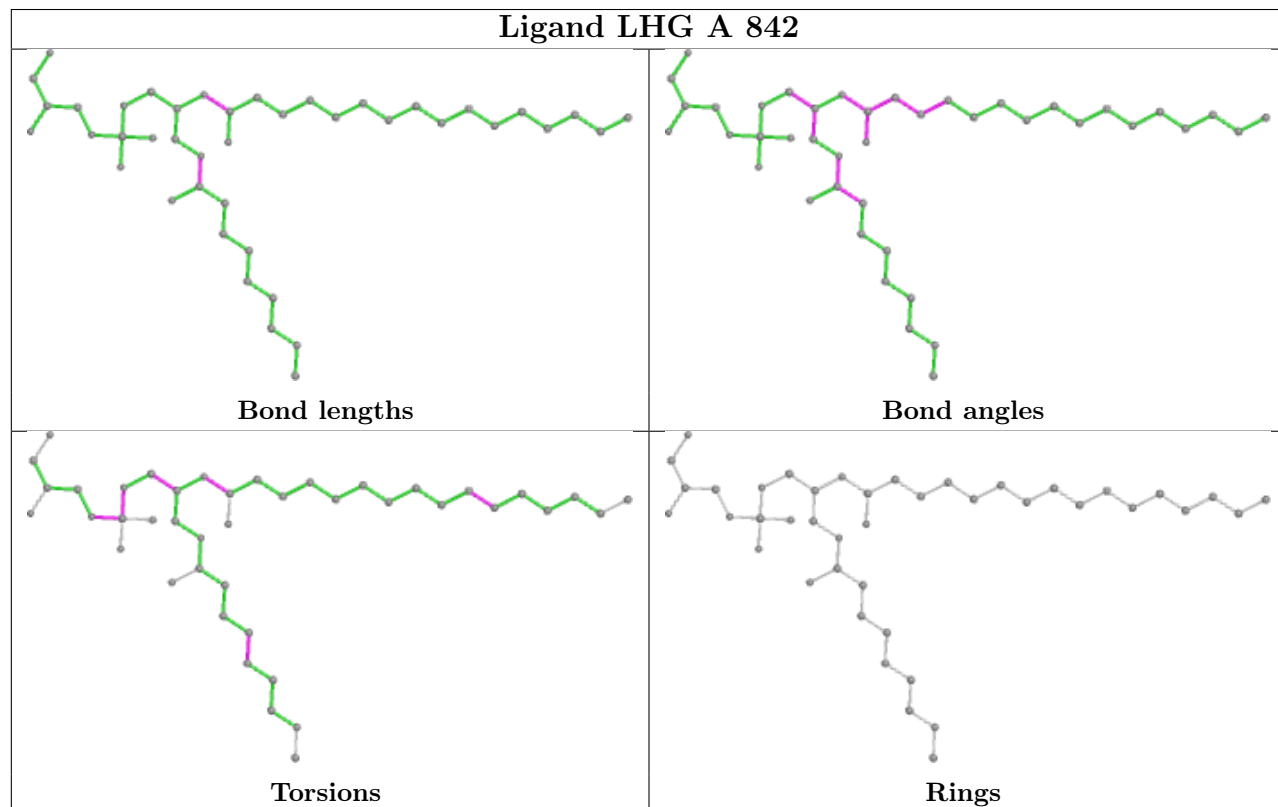
Ligand DD6 6 616

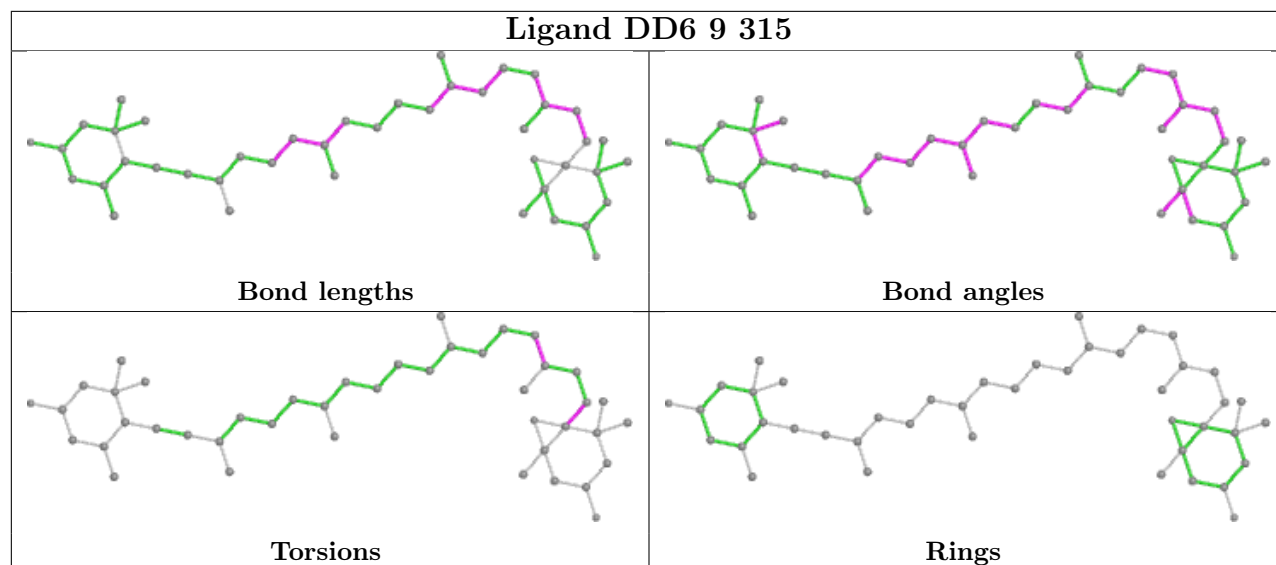
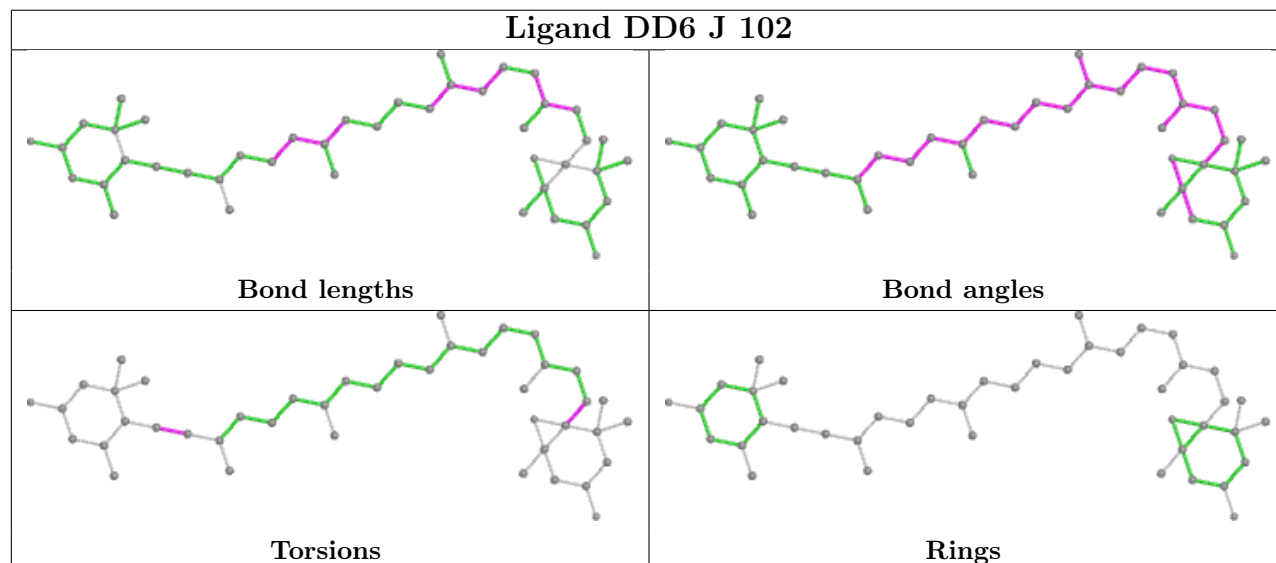
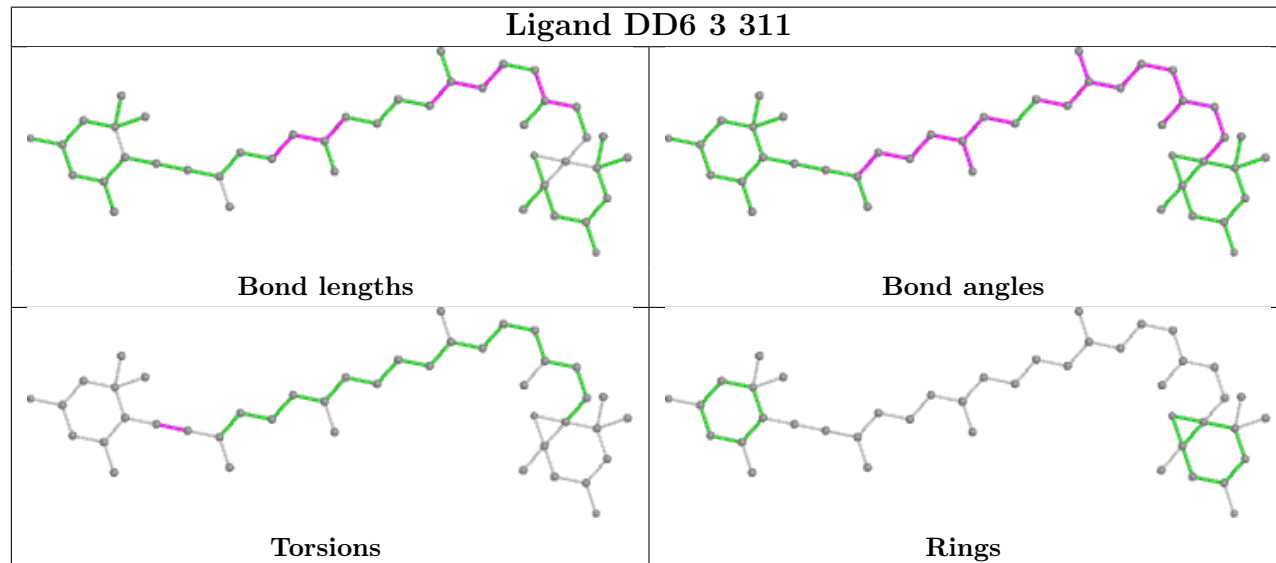


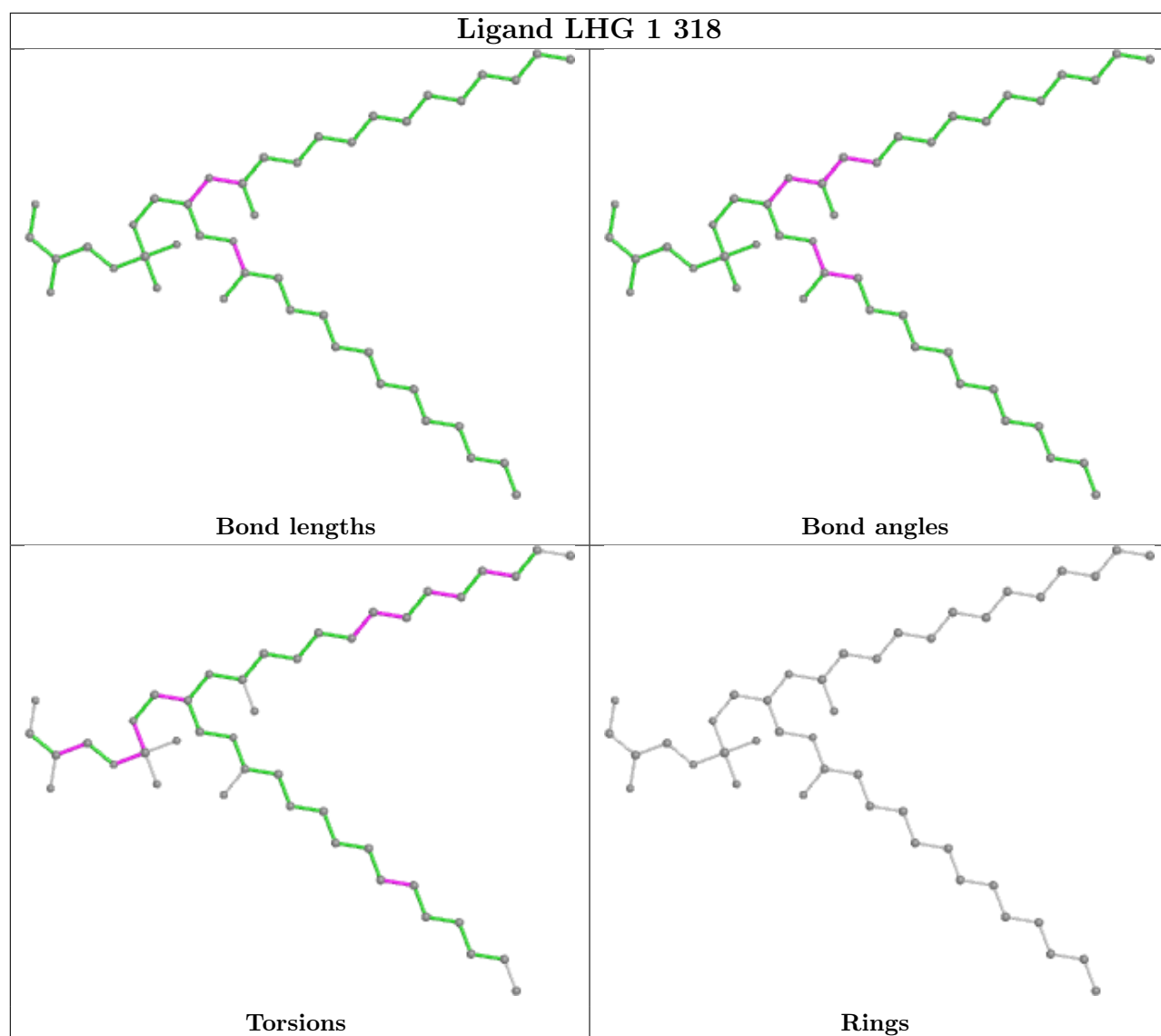
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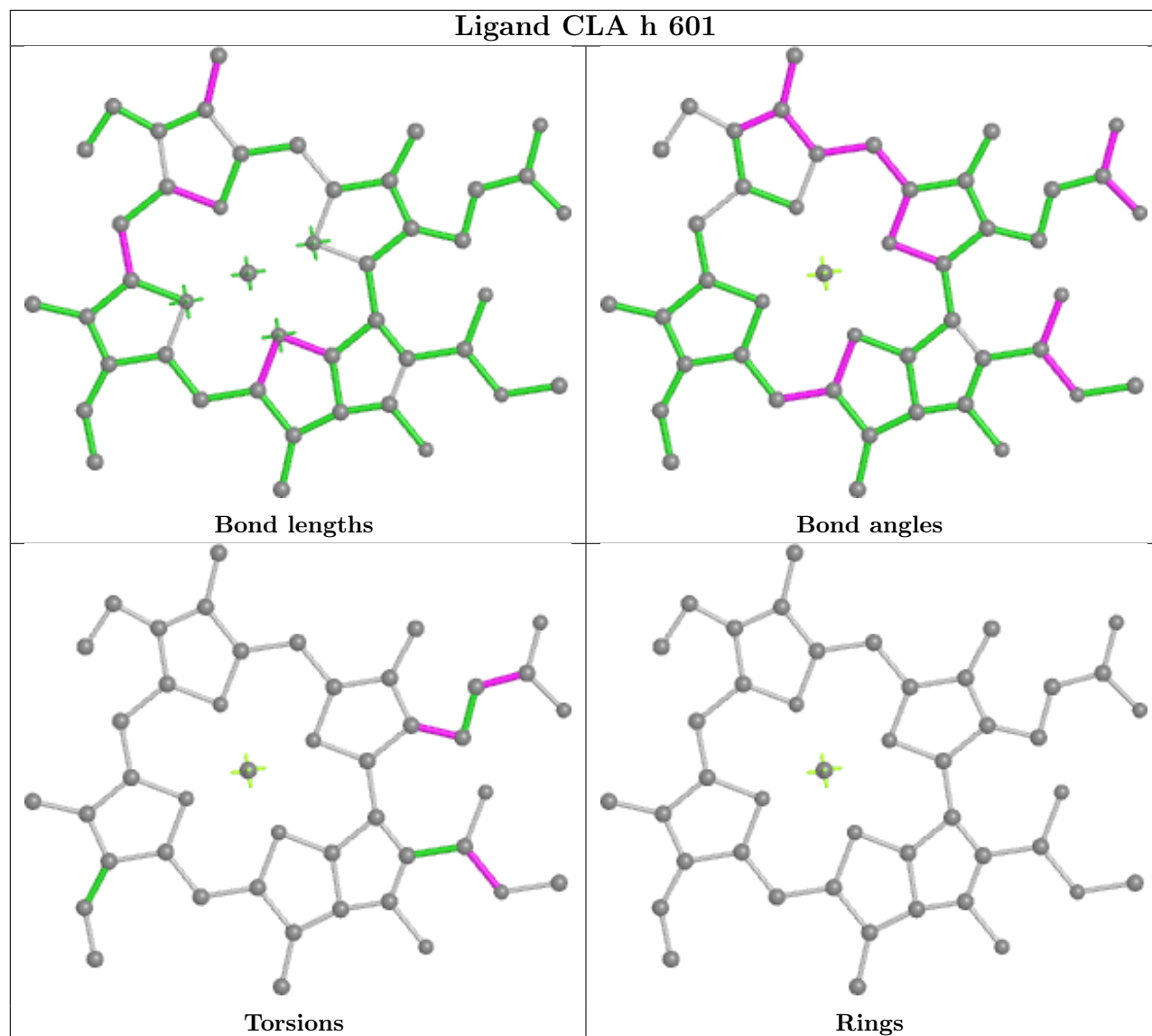
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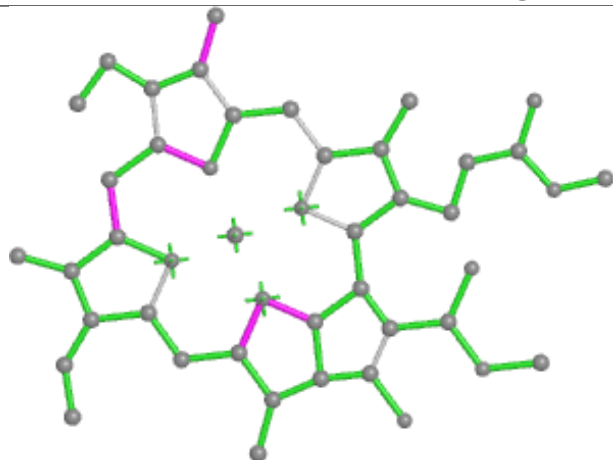
Ligand DD6 9 315**Ligand DD6 J 102****Ligand DD6 3 311**



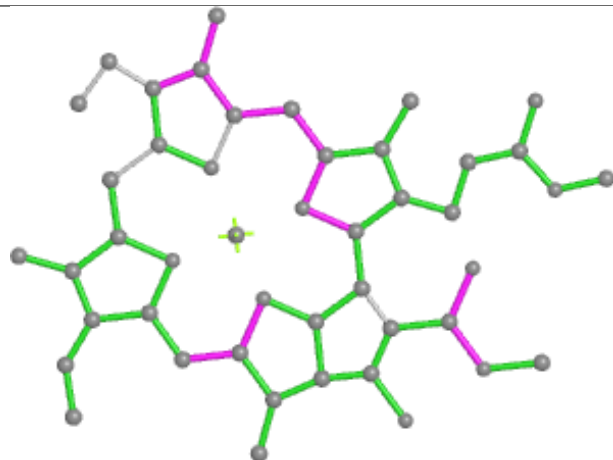
Ligand CLA h 601



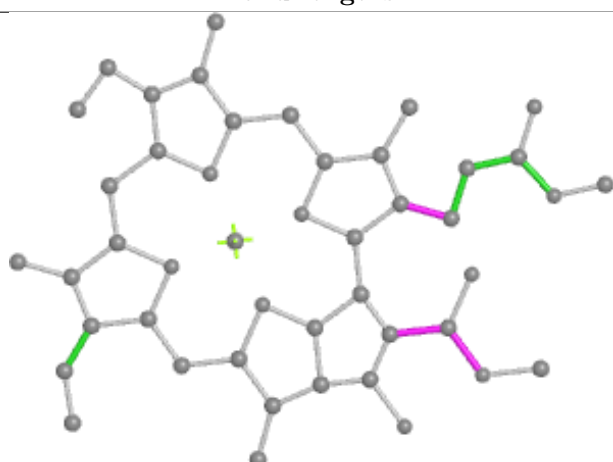
Ligand CLA A 809



Bond lengths



Bond angles

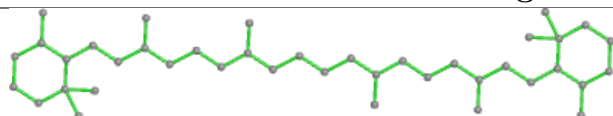


Torsions

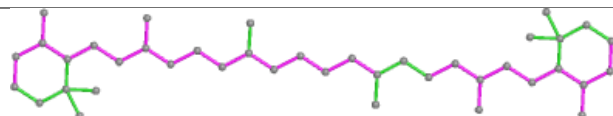


Rings

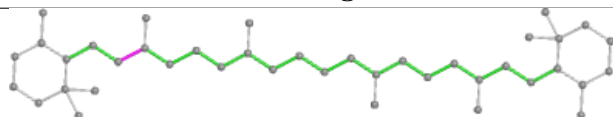
Ligand BCR 9 316



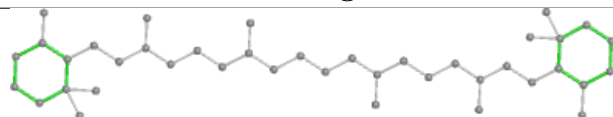
Bond lengths



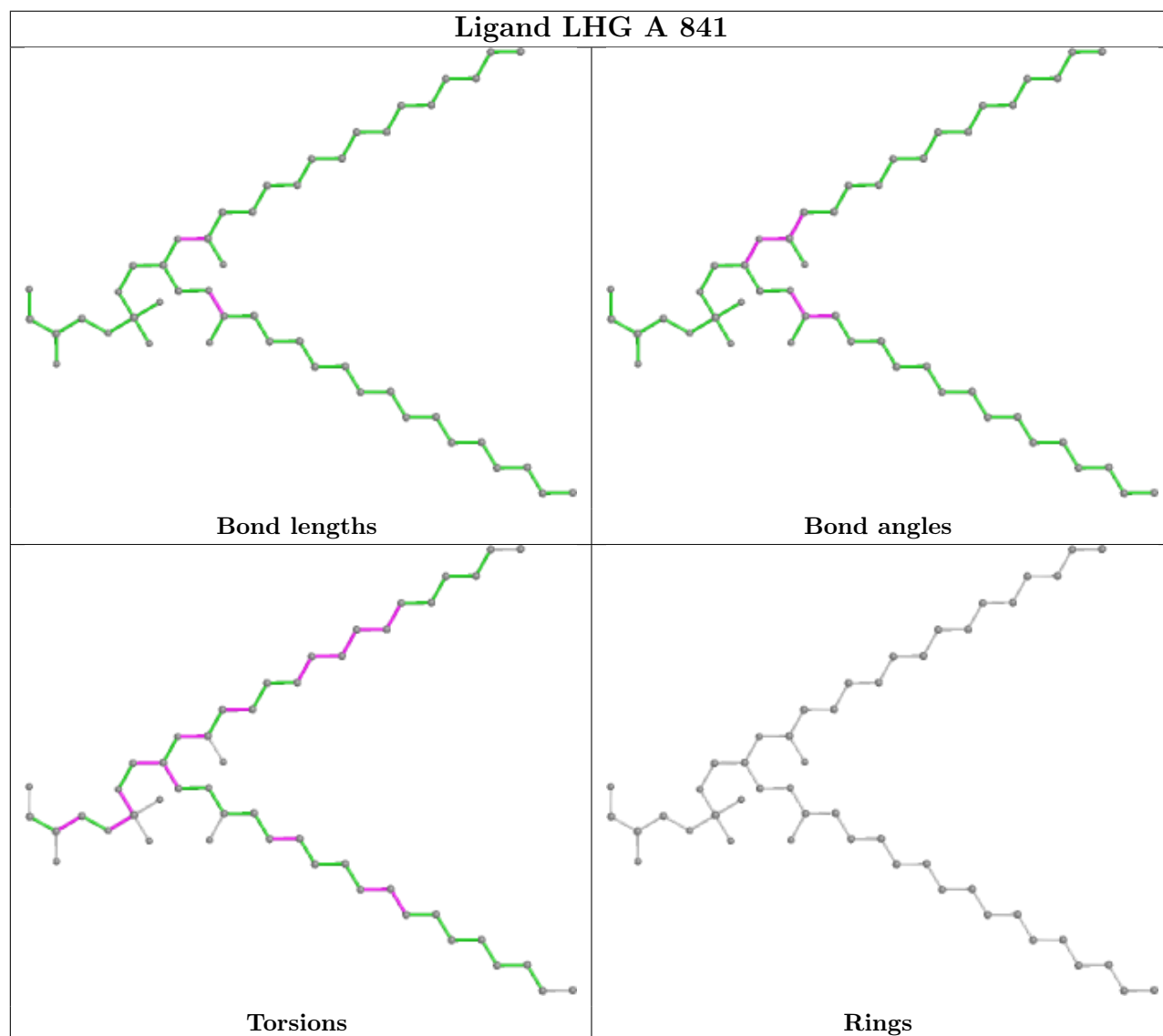
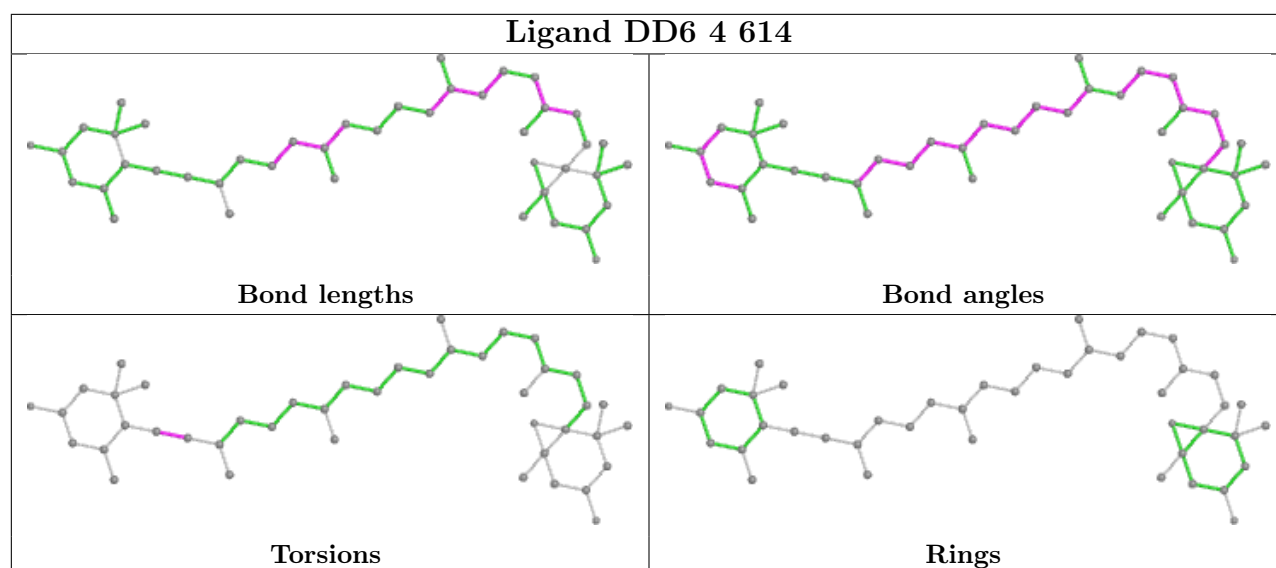
Bond angles



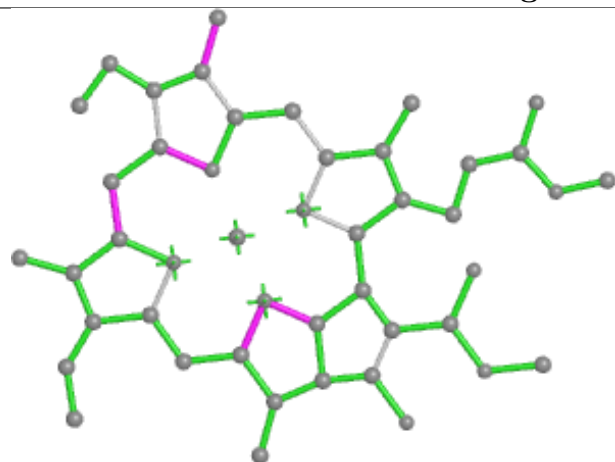
Torsions



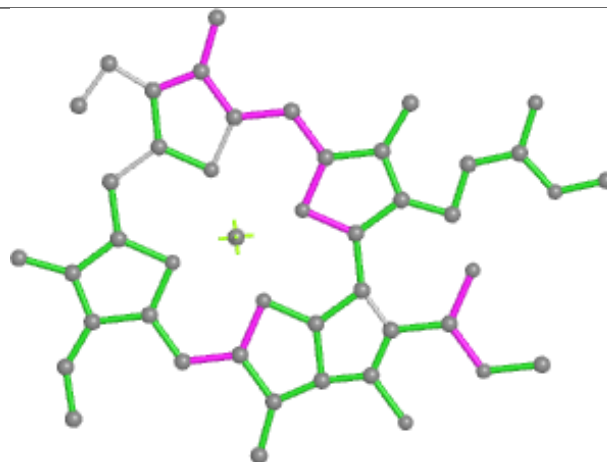
Rings



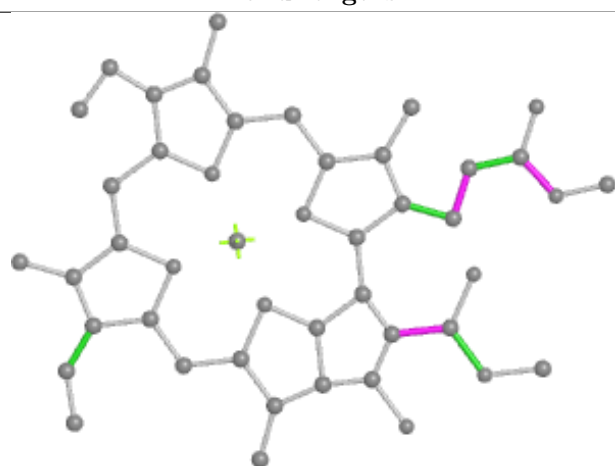
Ligand CLA 4 605



Bond lengths



Bond angles

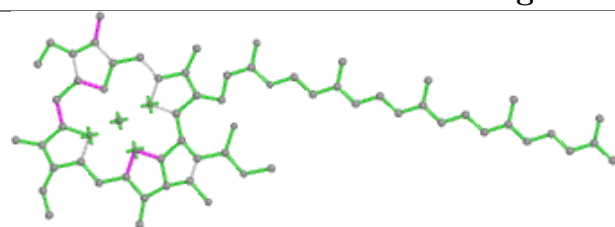


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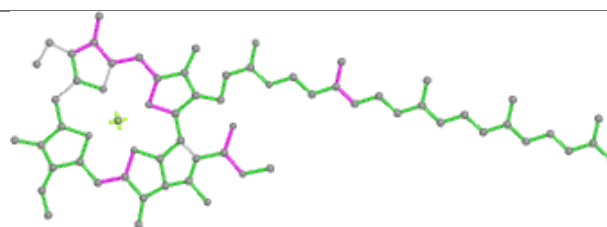


Rings

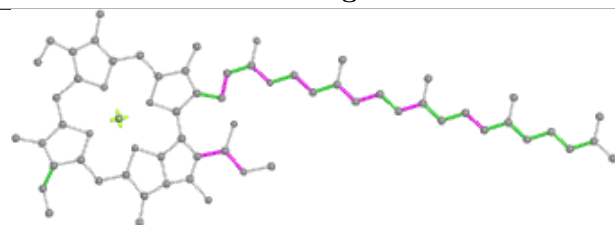
Ligand CLA B 837



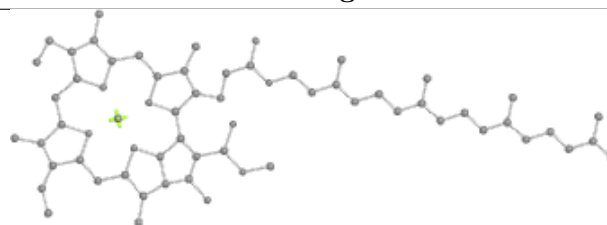
Bond lengths



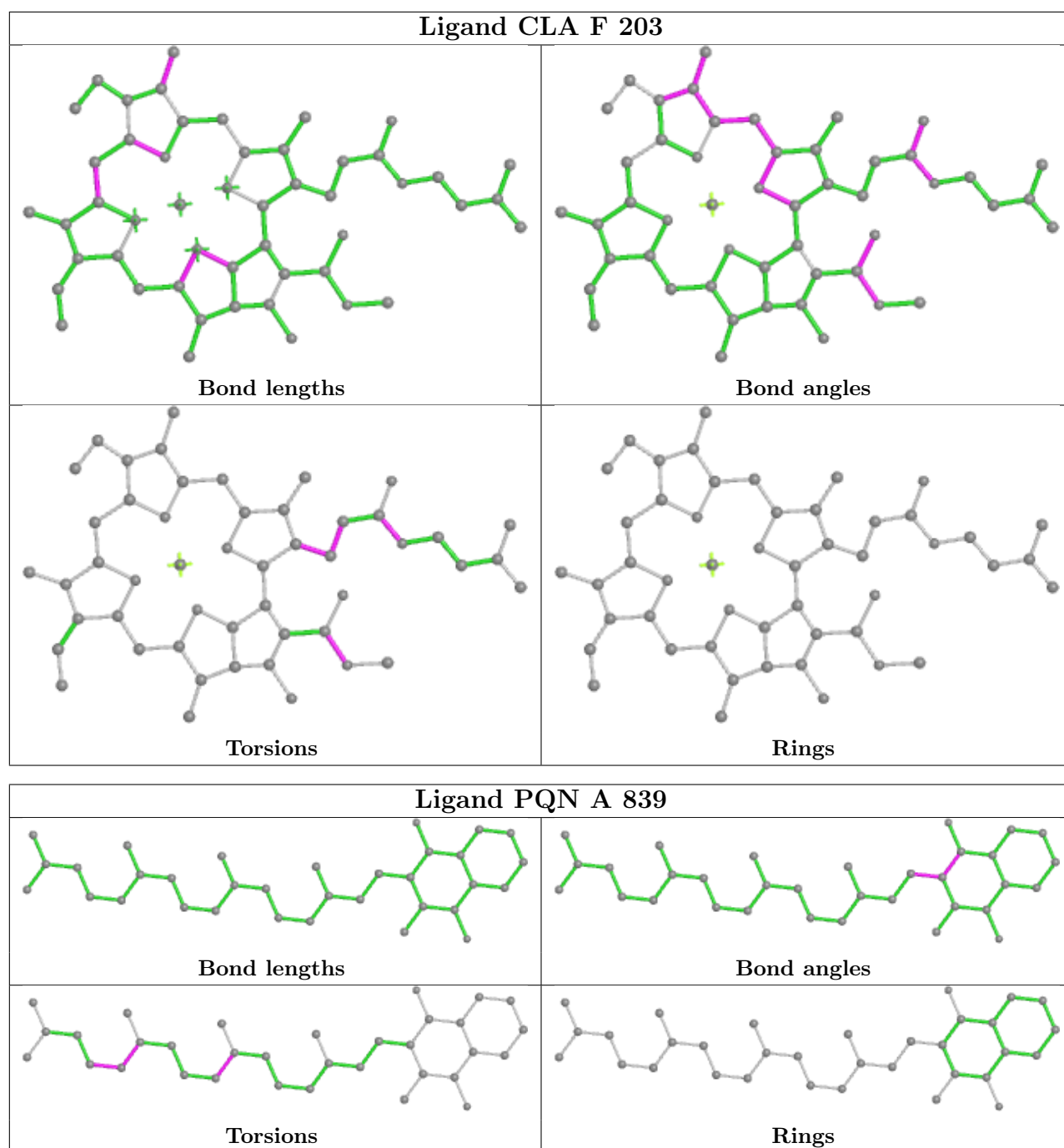
Bond angles



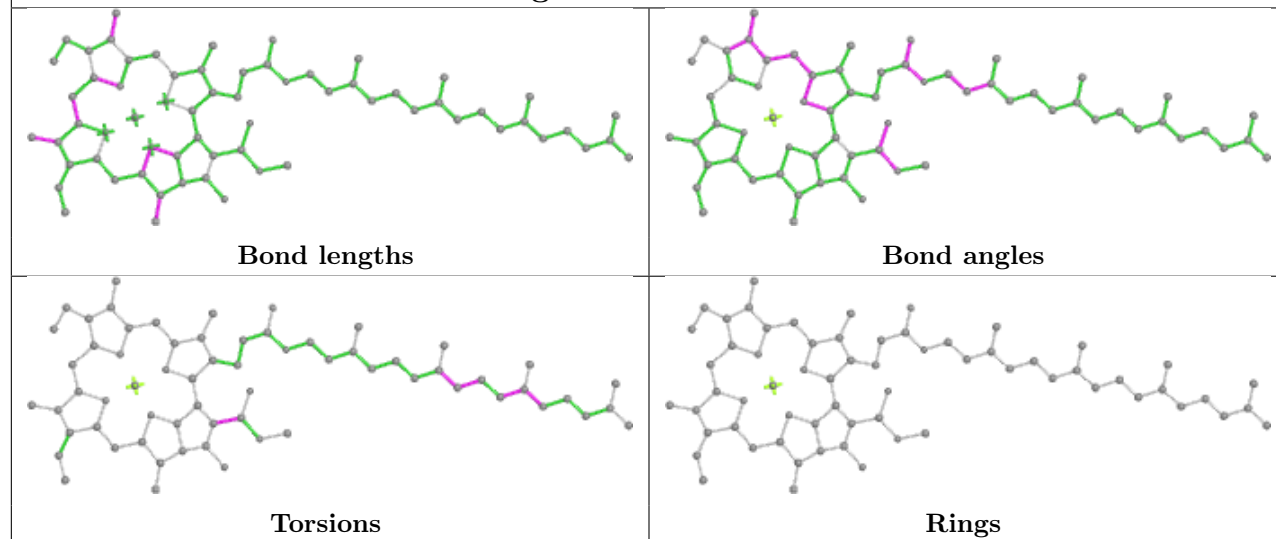
Torsions



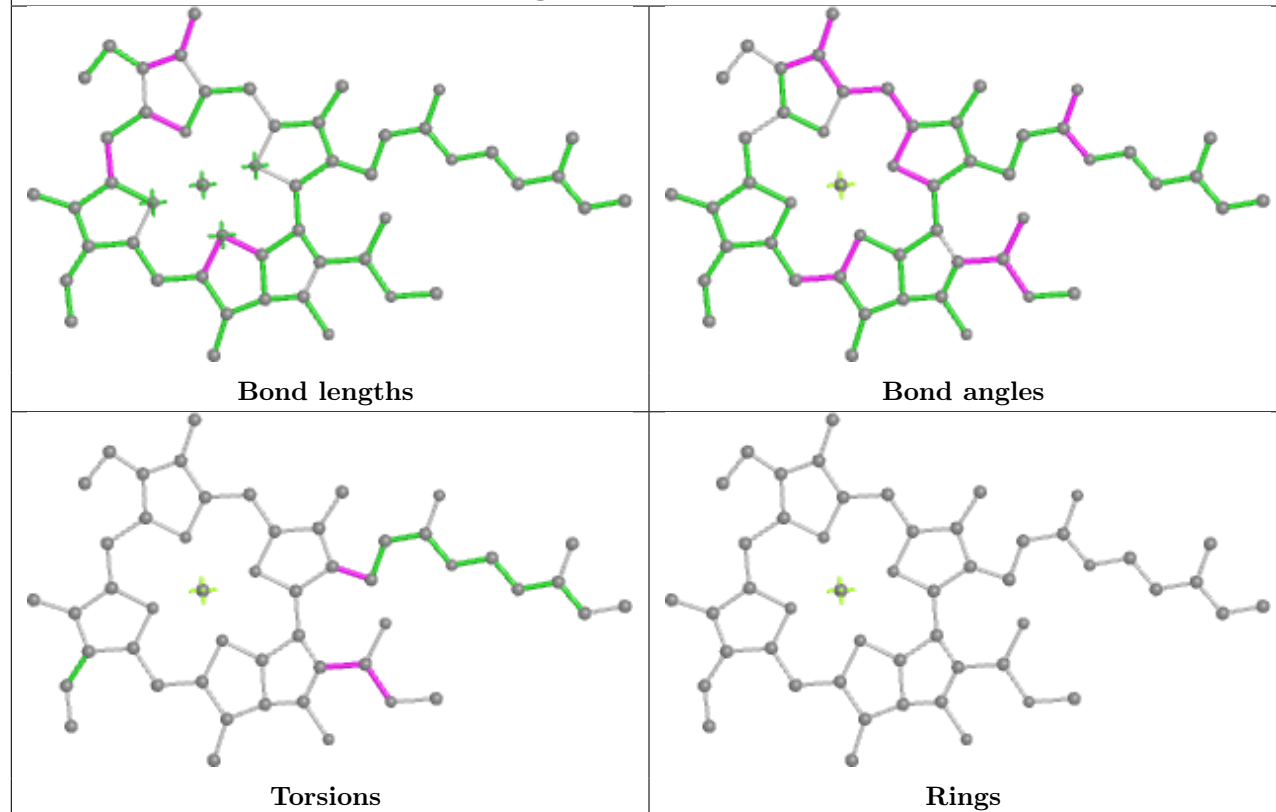
Rings



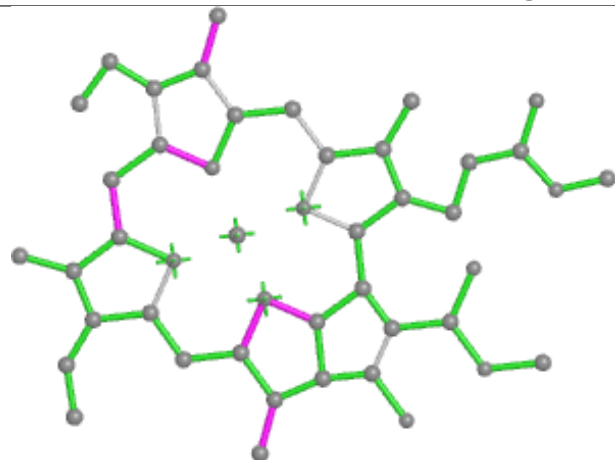
Ligand CLA A 857



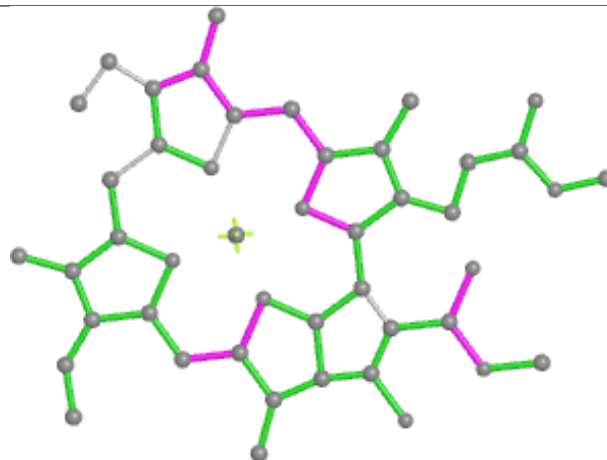
Ligand CLA A 835



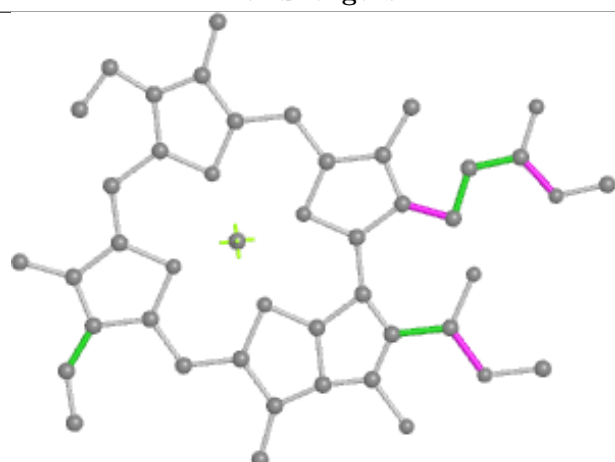
Ligand CLA 4 612



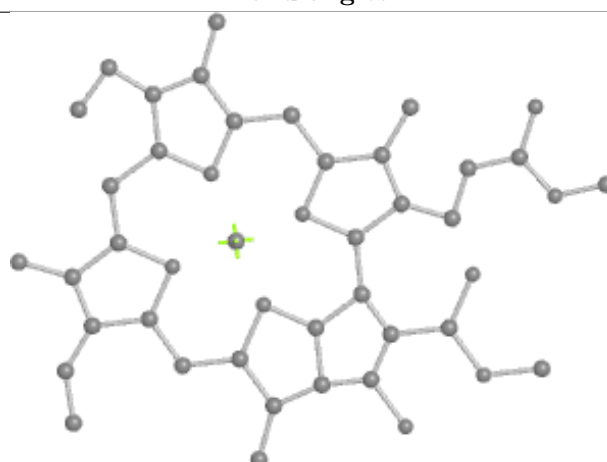
Bond lengths



Bond angles

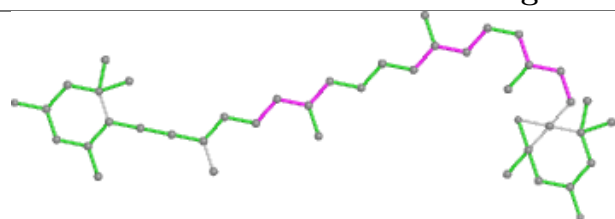


Torsions

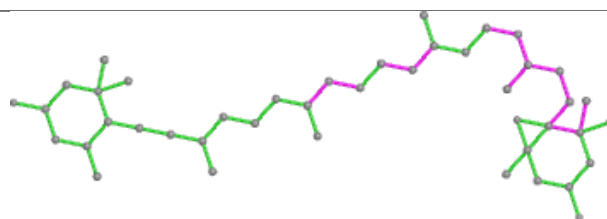


Rings

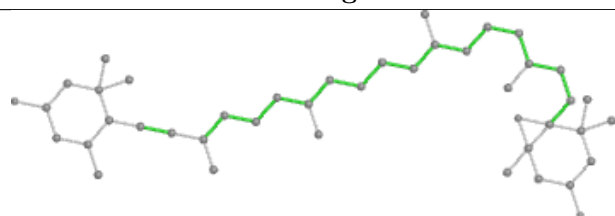
Ligand DD6 1 312



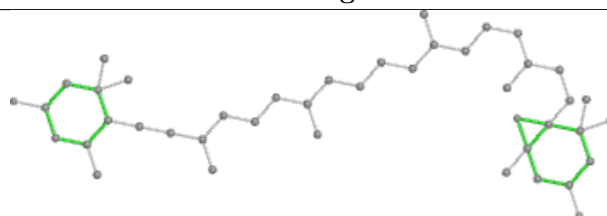
Bond lengths



Bond angles

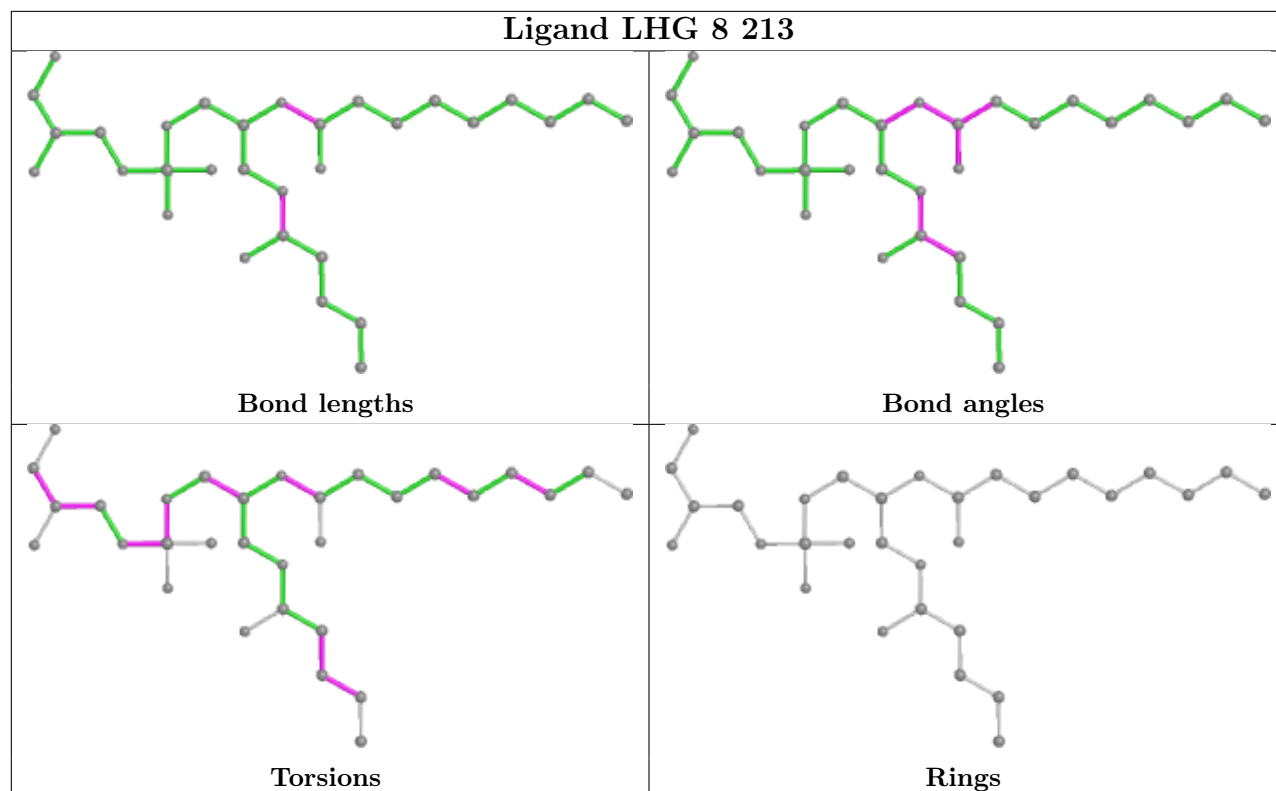


Torsions

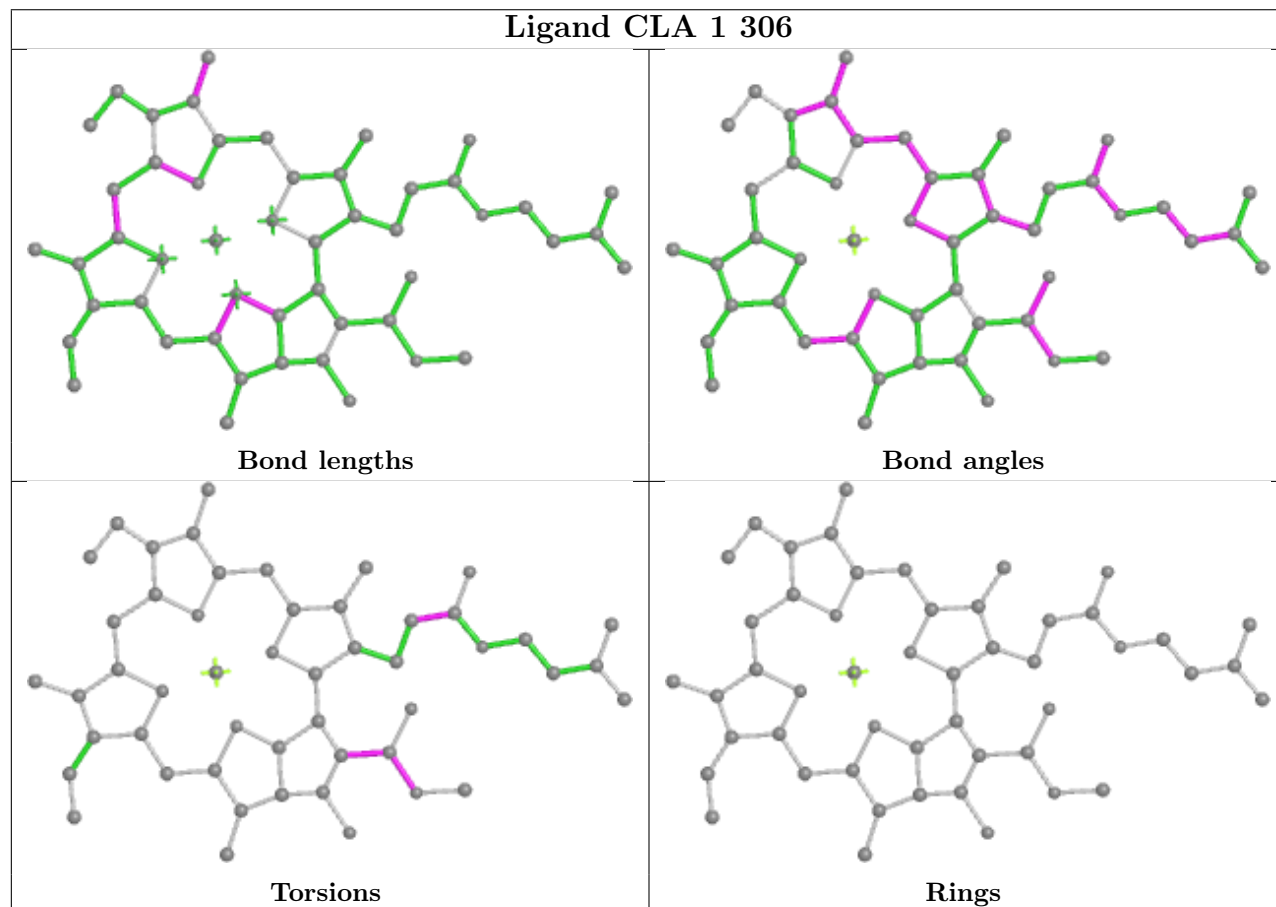


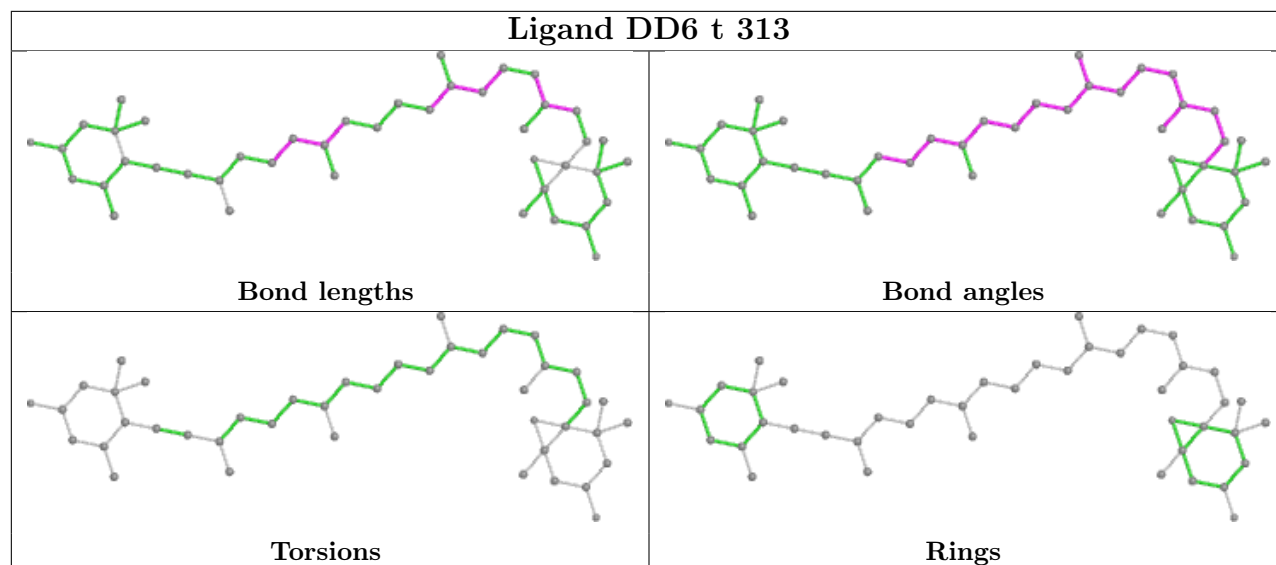
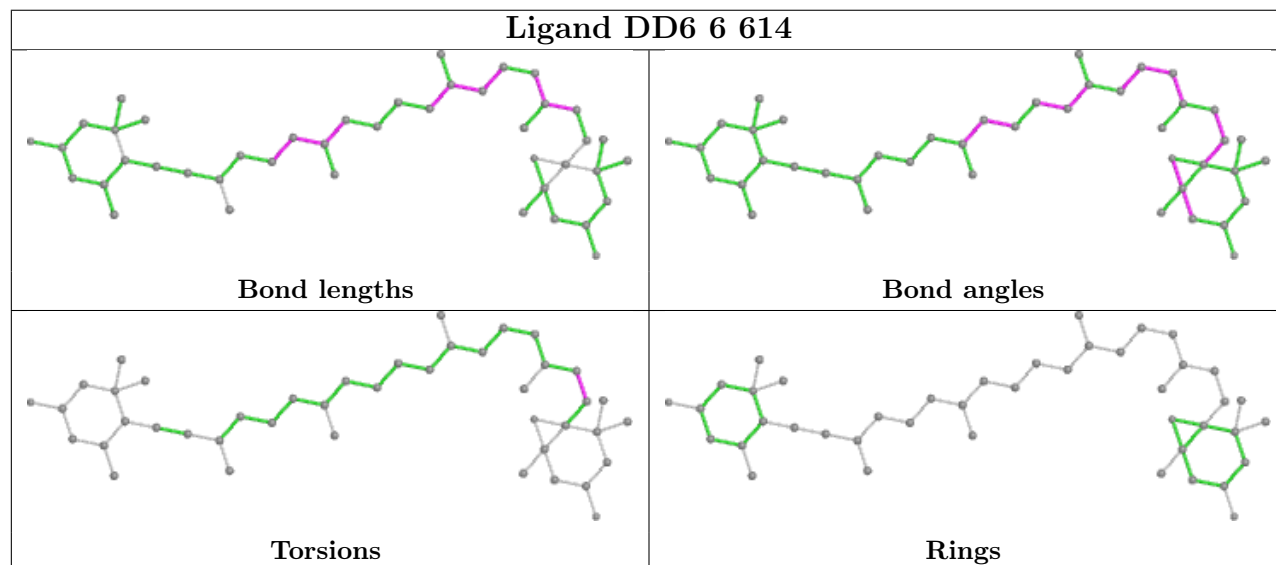
Rings

Ligand LHG 8 213

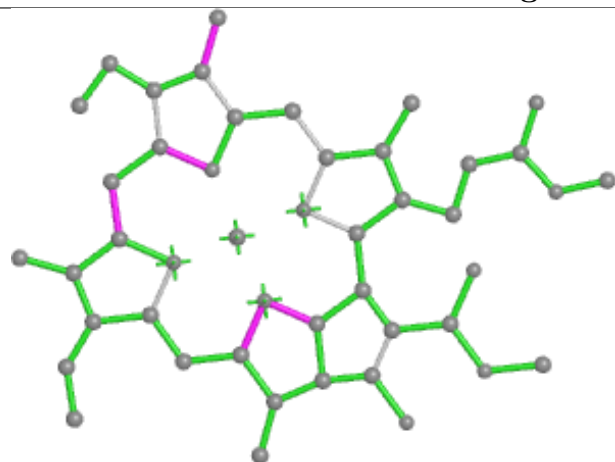


Ligand CLA 1 306

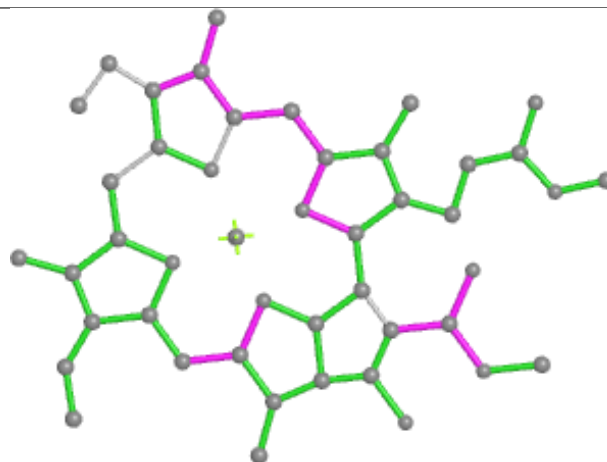


Ligand DD6 t 313**Ligand DD6 6 614**

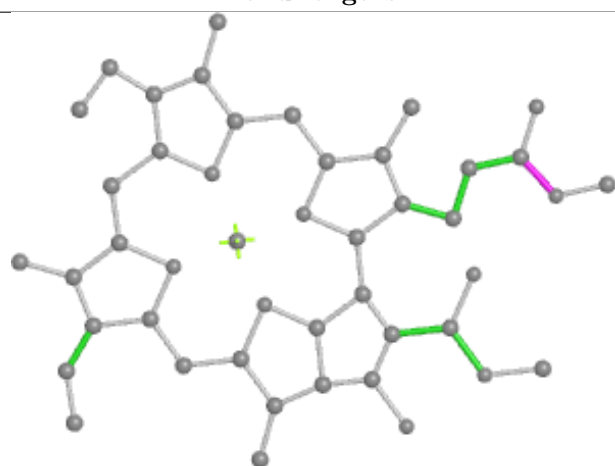
Ligand CLA 6 605



Bond lengths



Bond angles

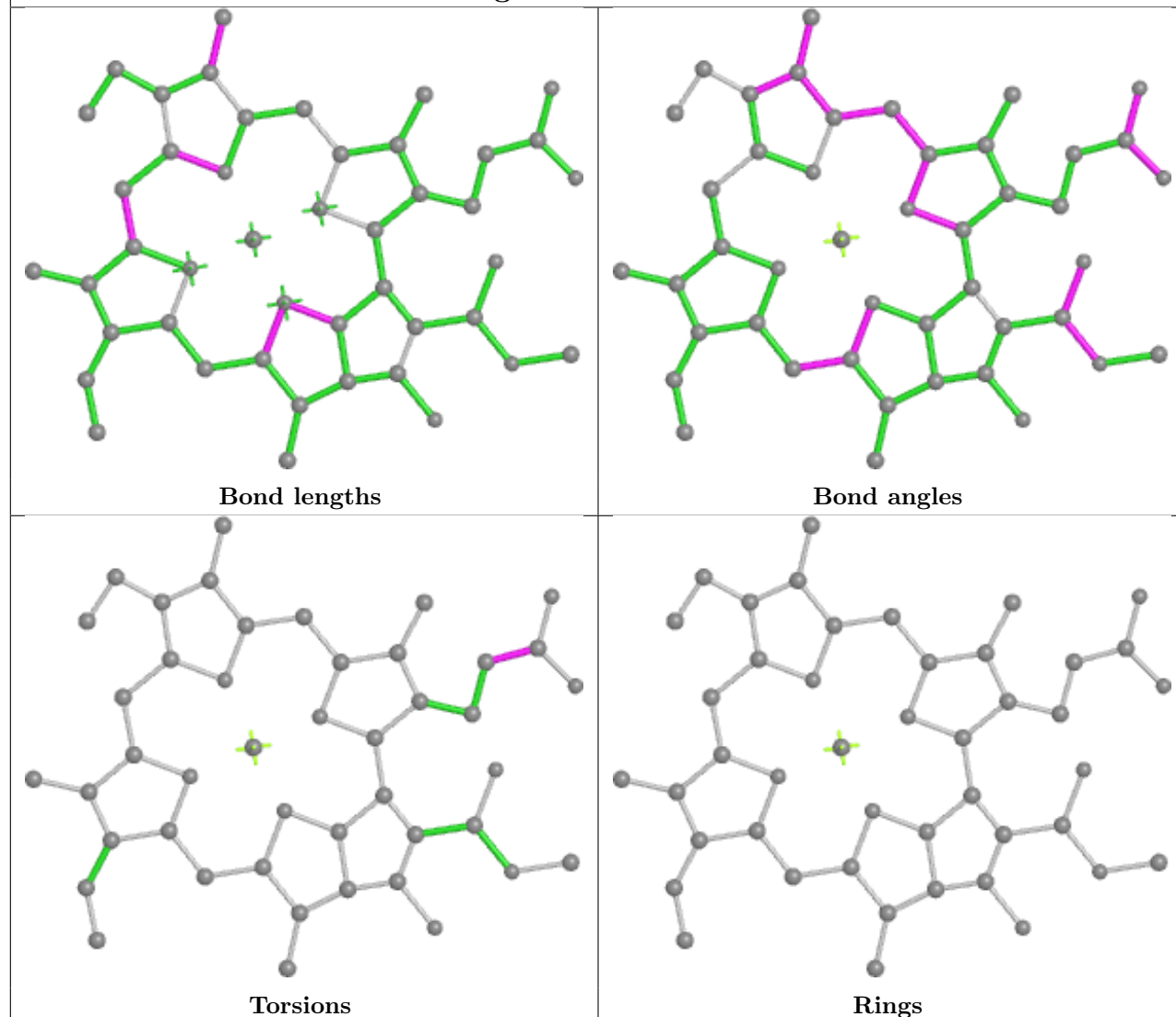


Torsions

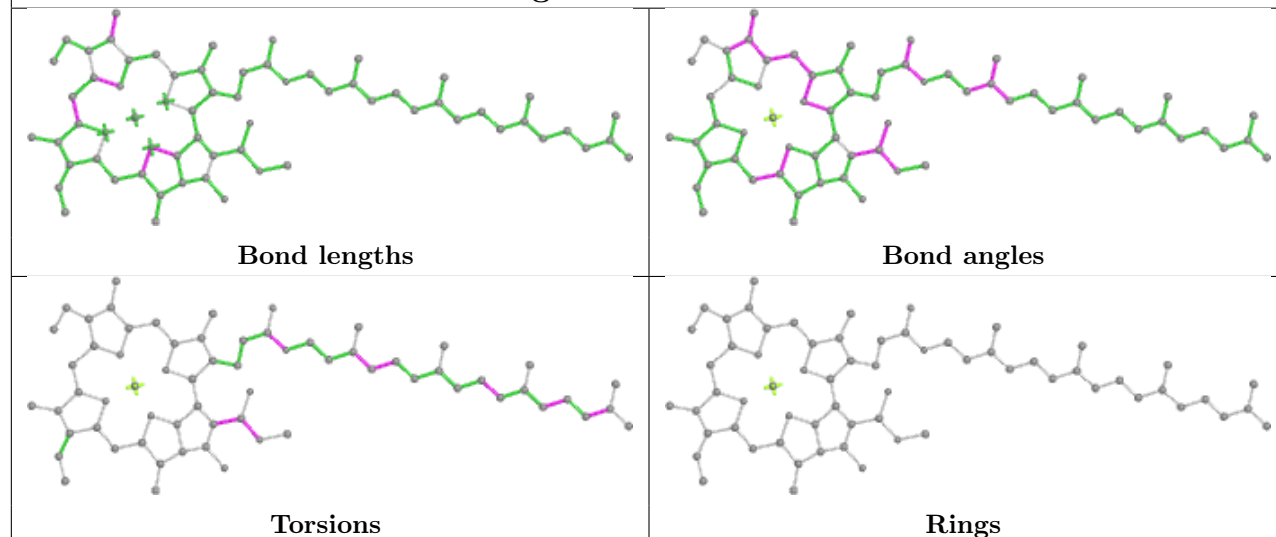


Rings

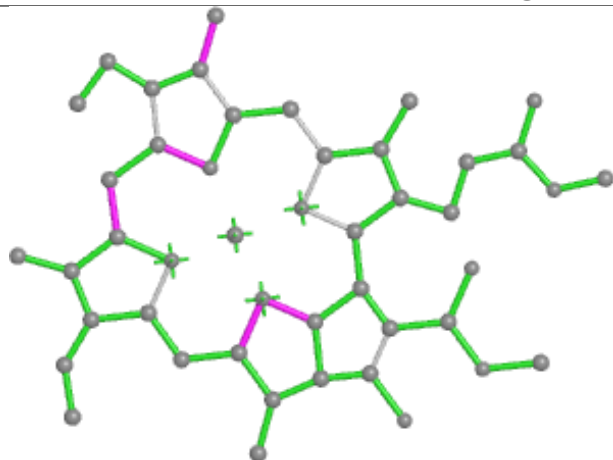
Ligand CLA 7 603



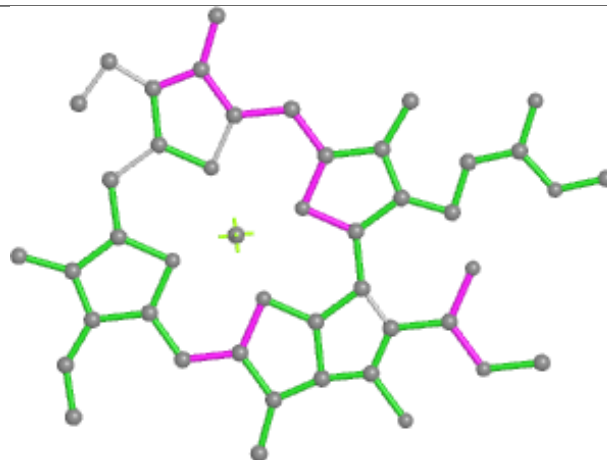
Ligand CLA B 822



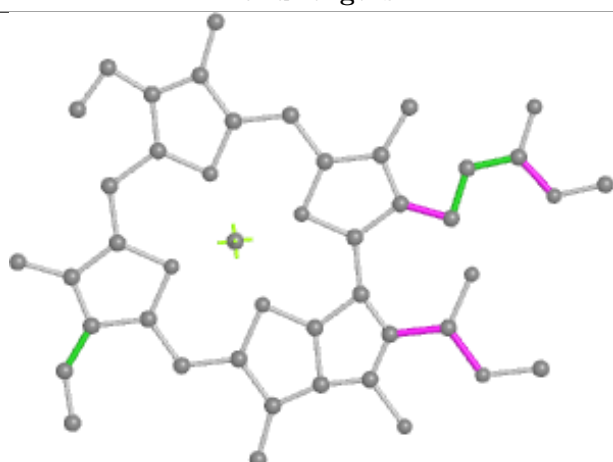
Ligand CLA 8 206



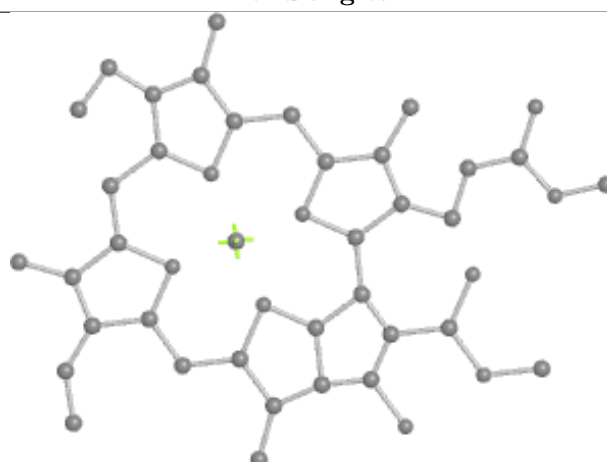
Bond lengths



Bond angles

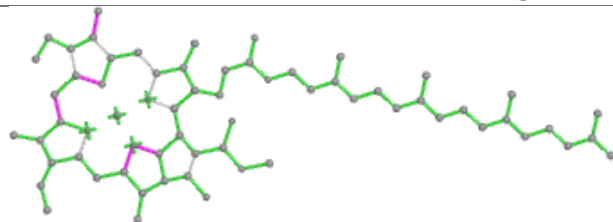


Torsions

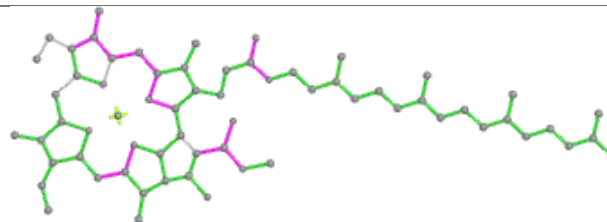


Rings

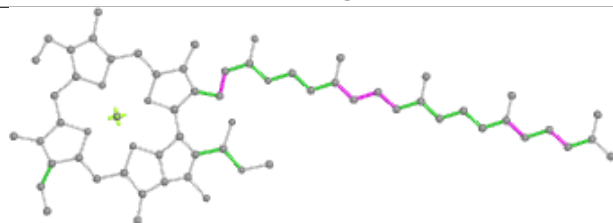
Ligand CLA B 807



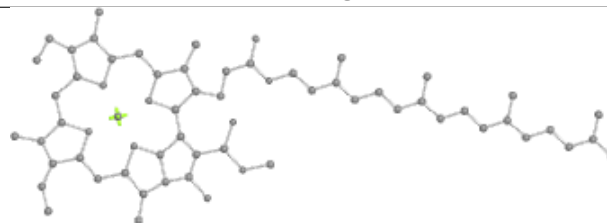
Bond lengths



Bond angles

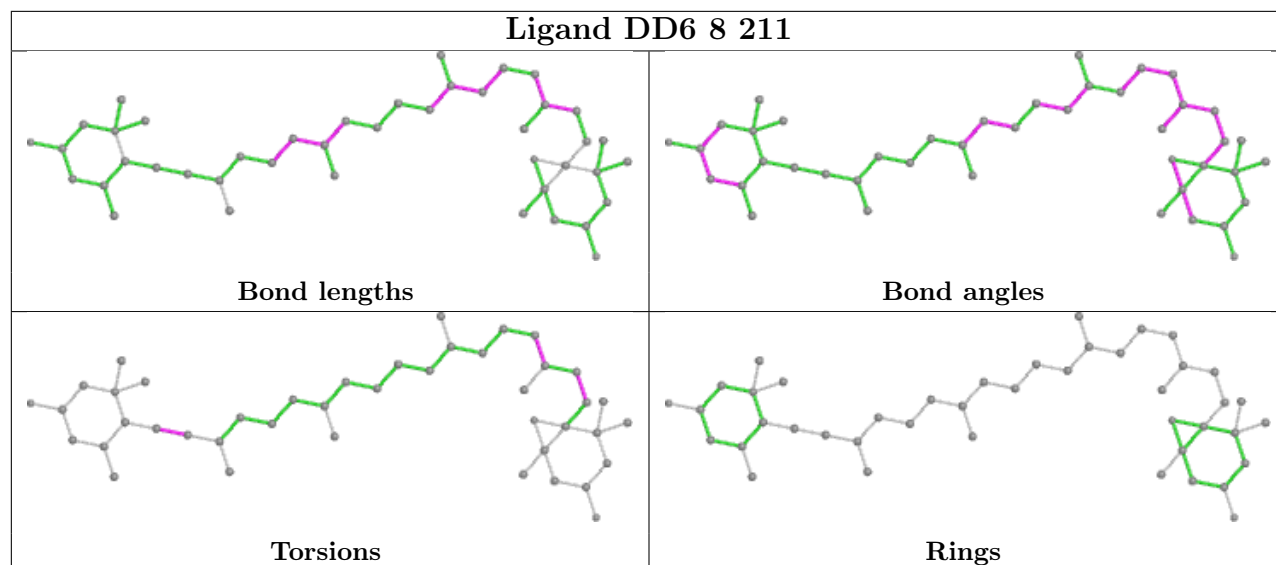


Torsions

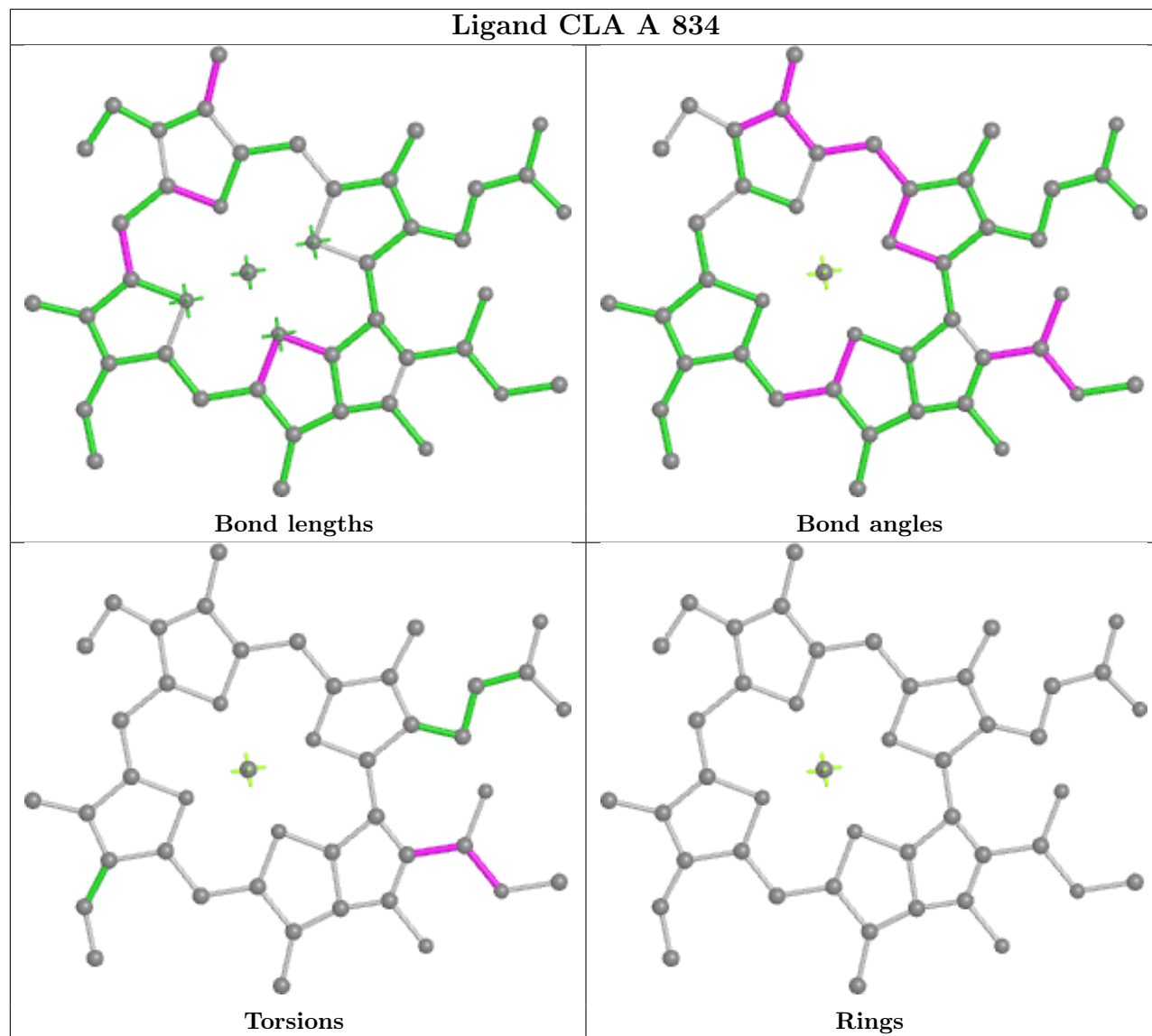


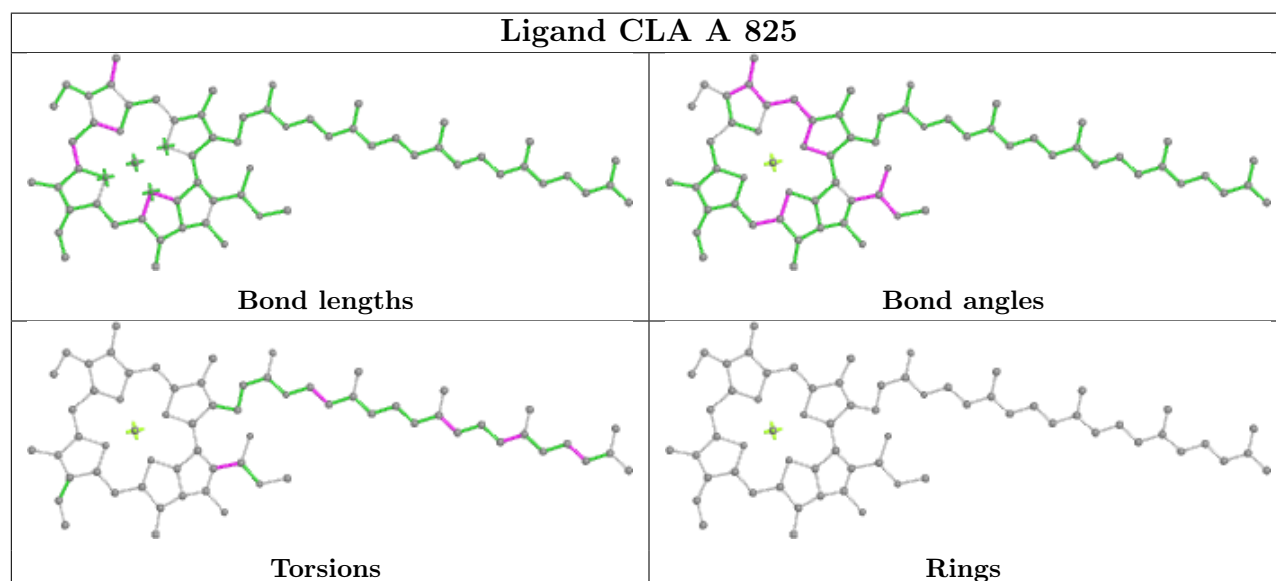
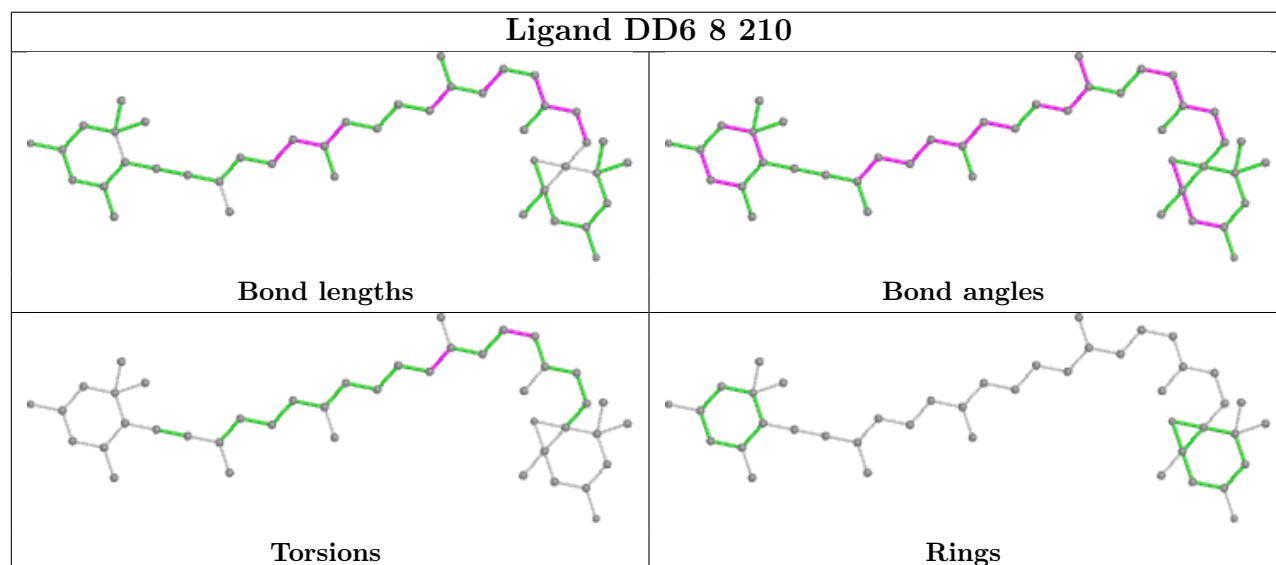
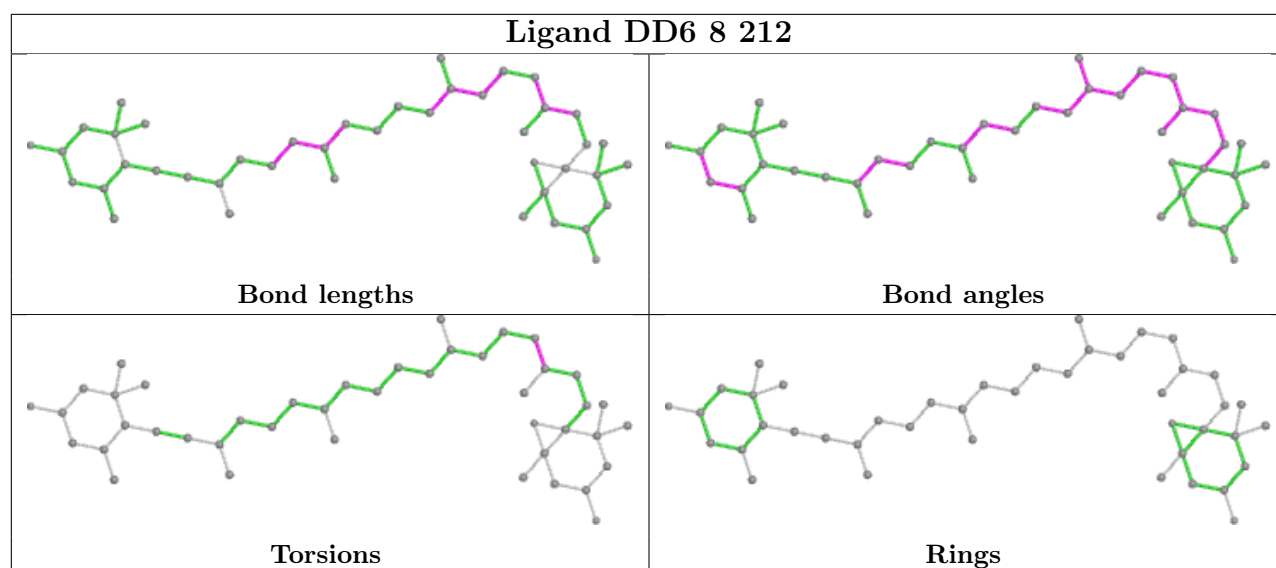
Rings

Ligand DD6 8 211

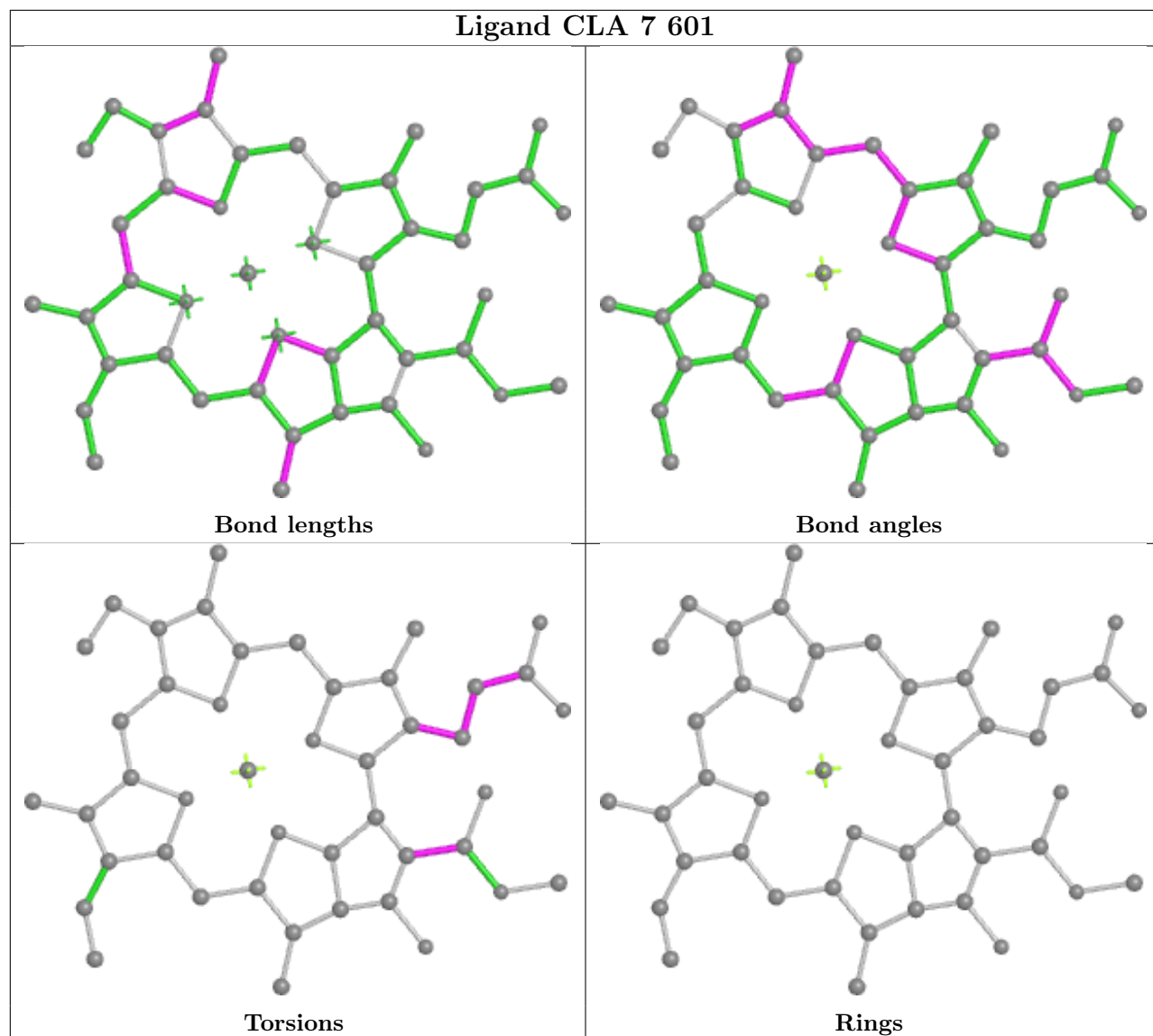


Ligand CLA A 834

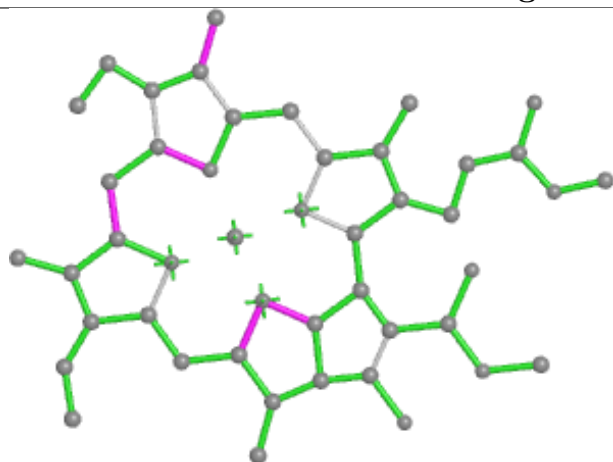




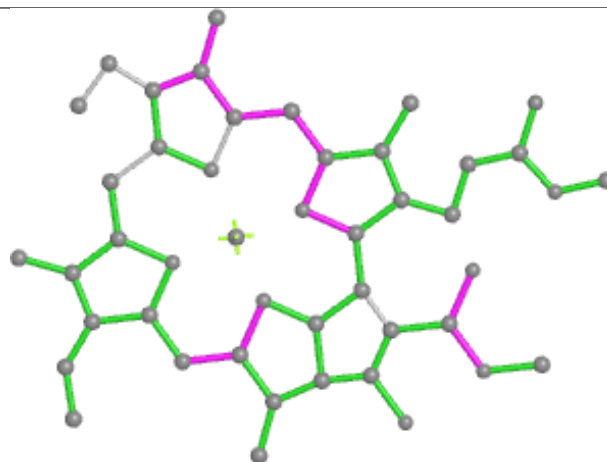
Ligand CLA 7 601



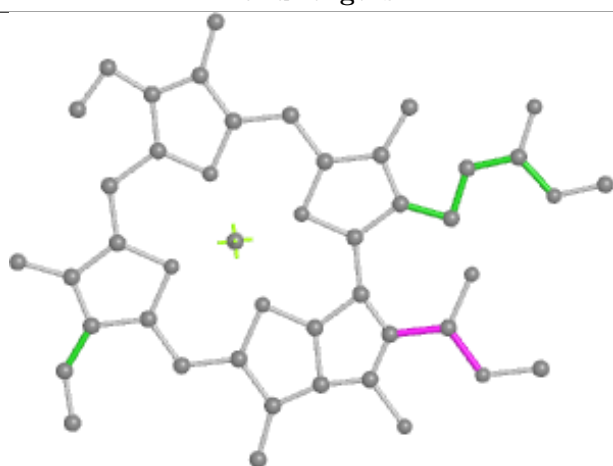
Ligand CLA 8 201



Bond lengths



Bond angles

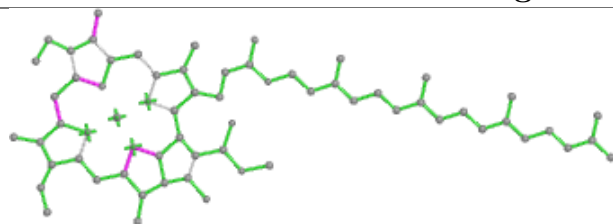


Torsions

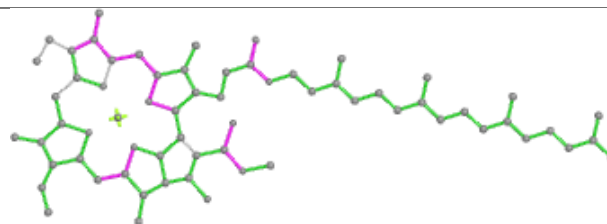


Rings

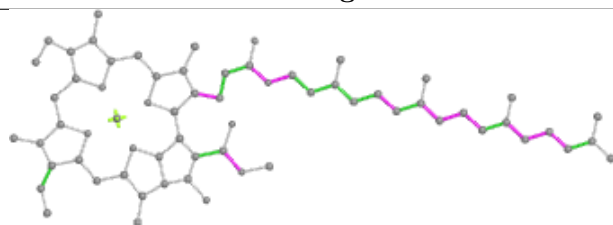
Ligand CLA B 812



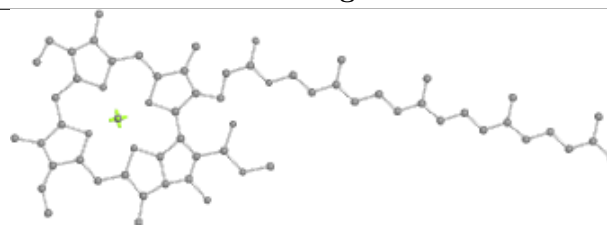
Bond lengths



Bond angles

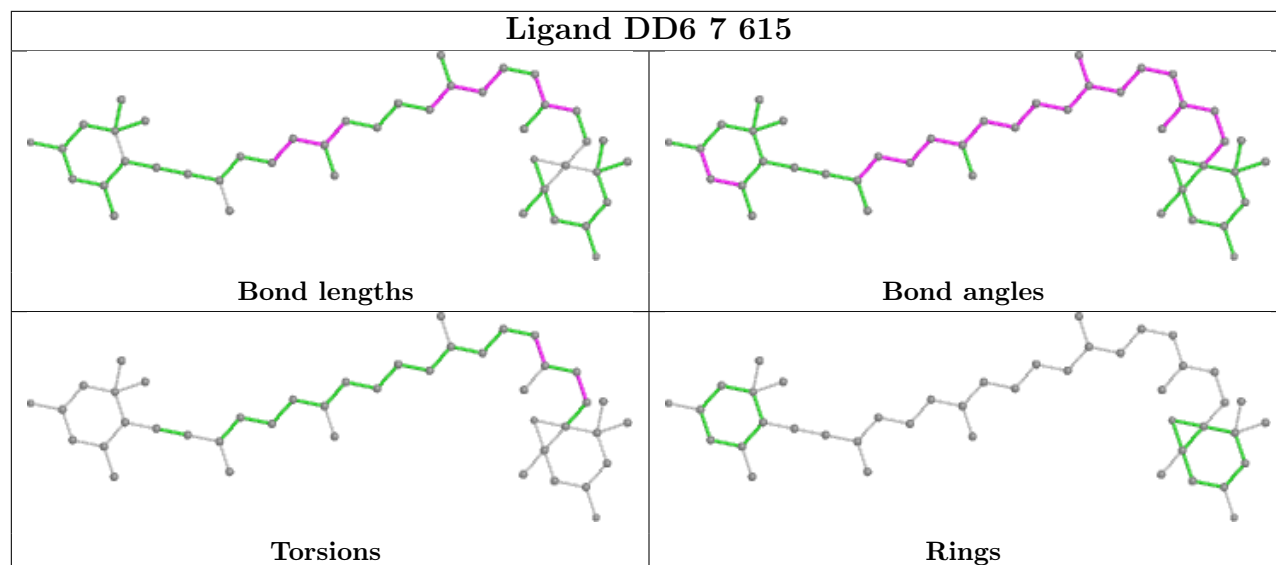


Torsions

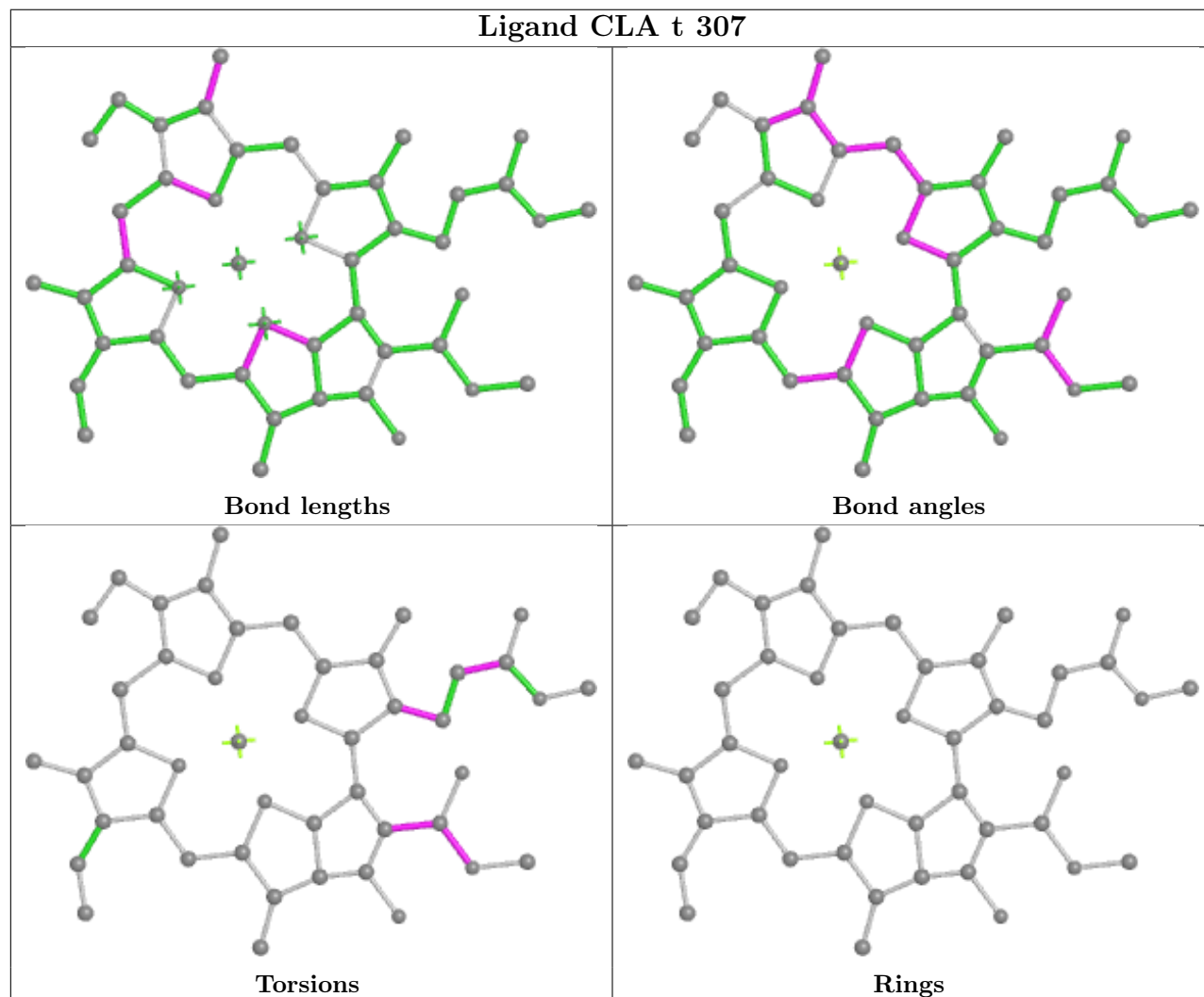


Rings

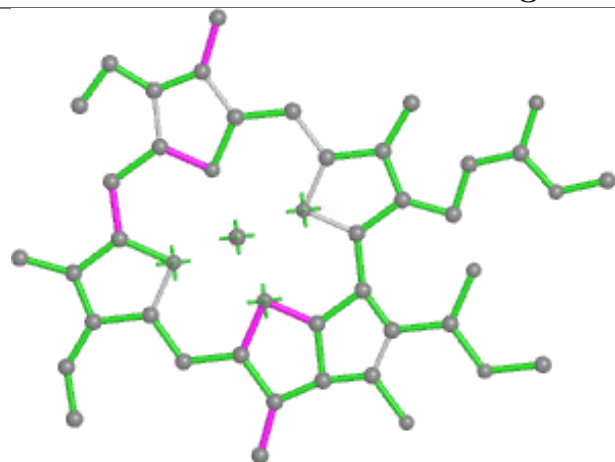
Ligand DD6 7 615



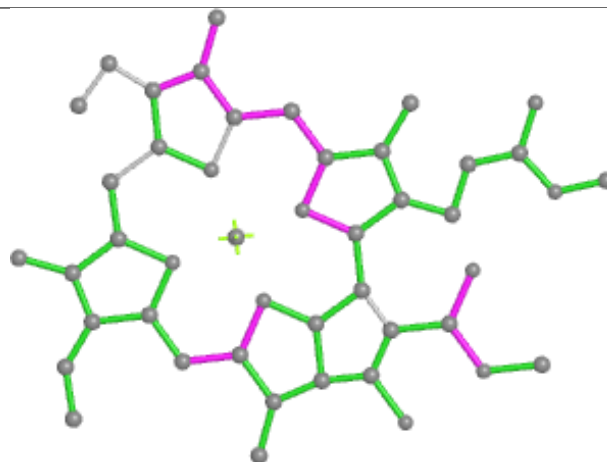
Ligand CLA t 307



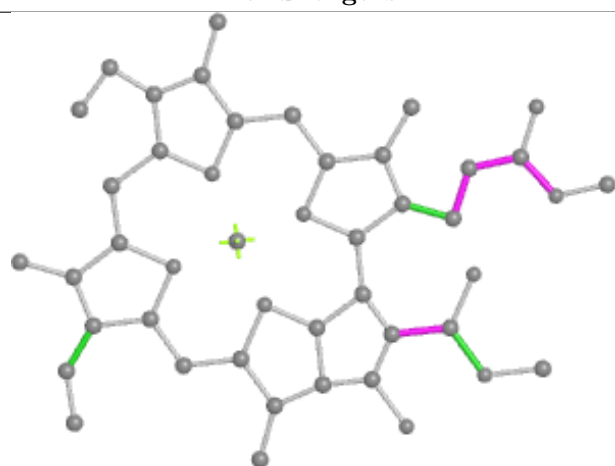
Ligand CLA k 307



Bond lengths



Bond angles

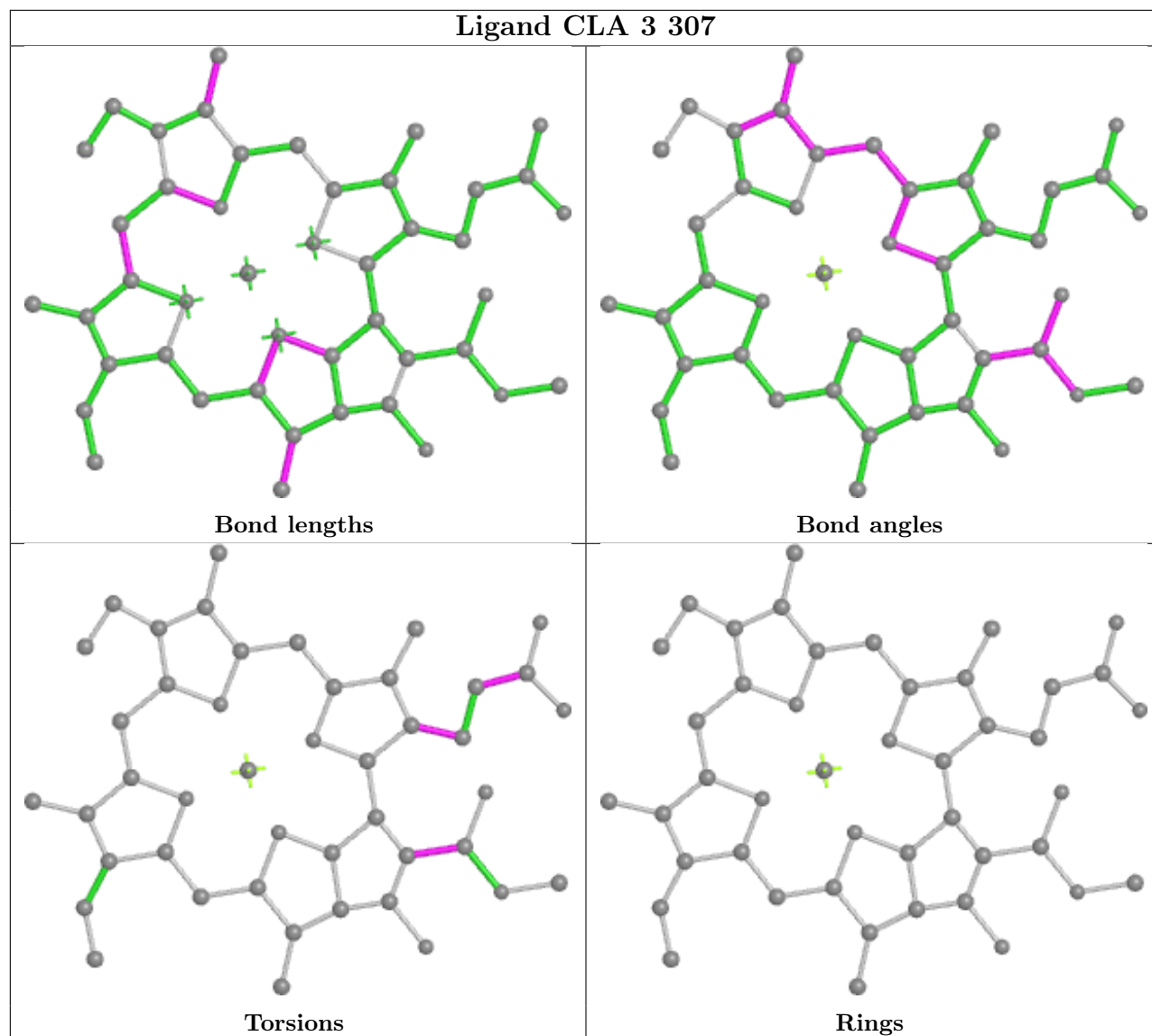


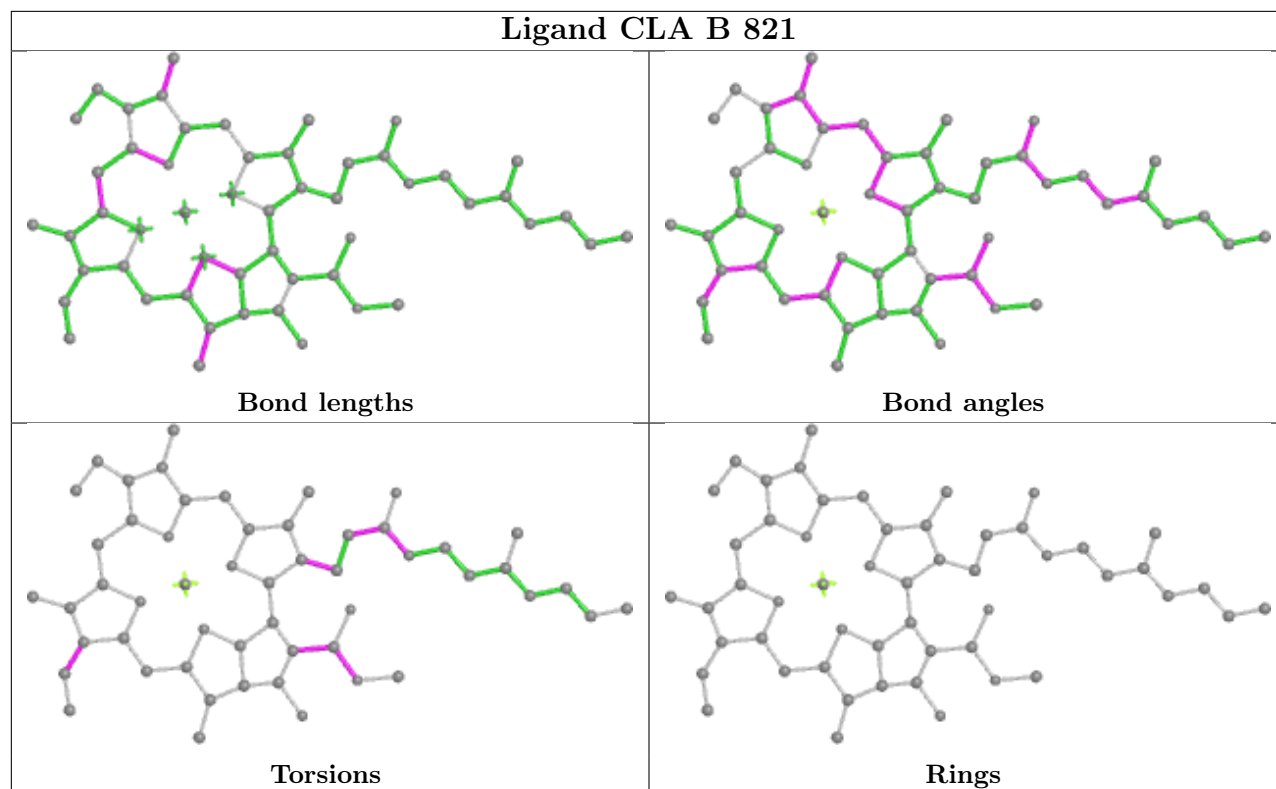
Torsions



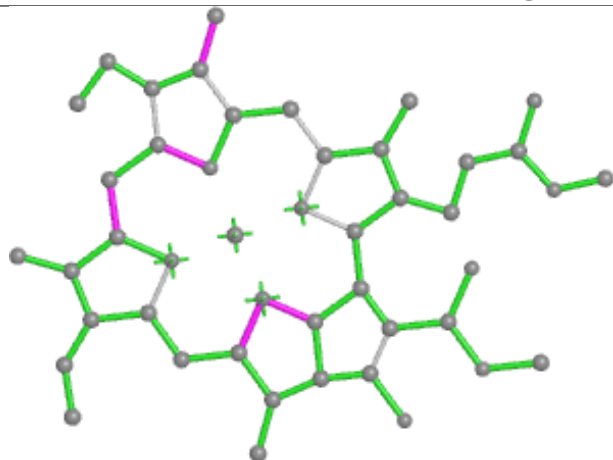
Rings

Ligand CLA 3 307

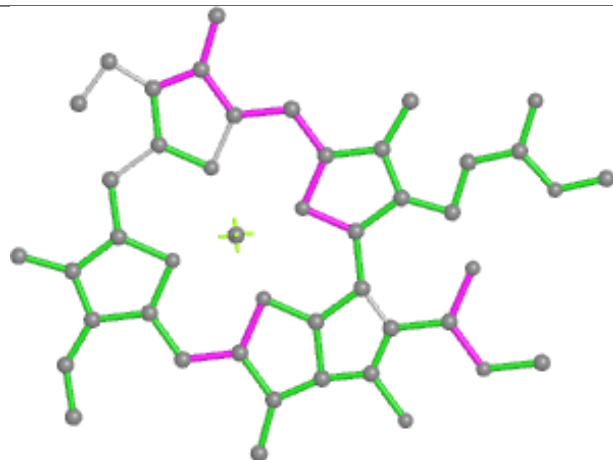




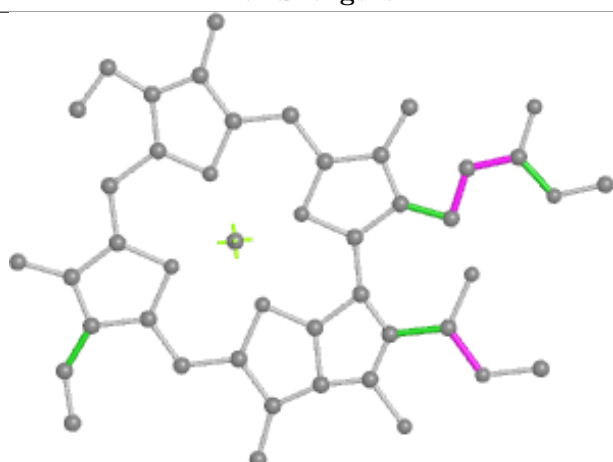
Ligand CLA t 309



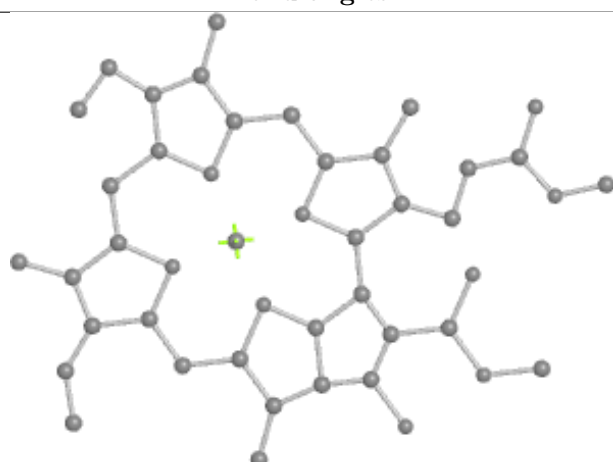
Bond lengths



Bond angles

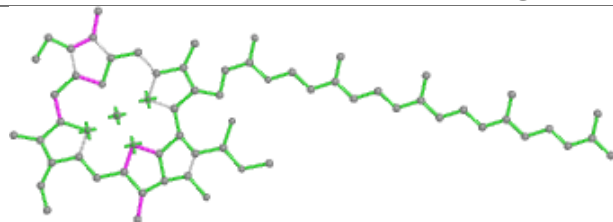


Torsions

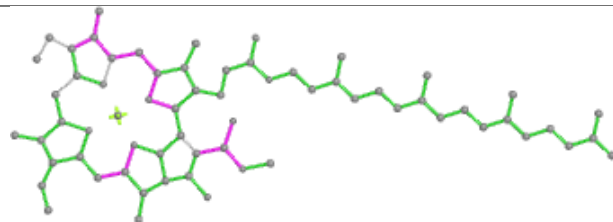


Rings

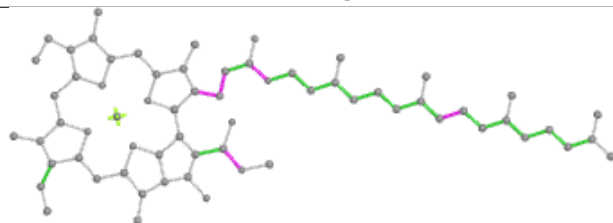
Ligand CLA B 826



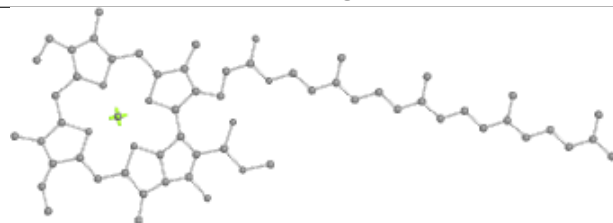
Bond lengths



Bond angles

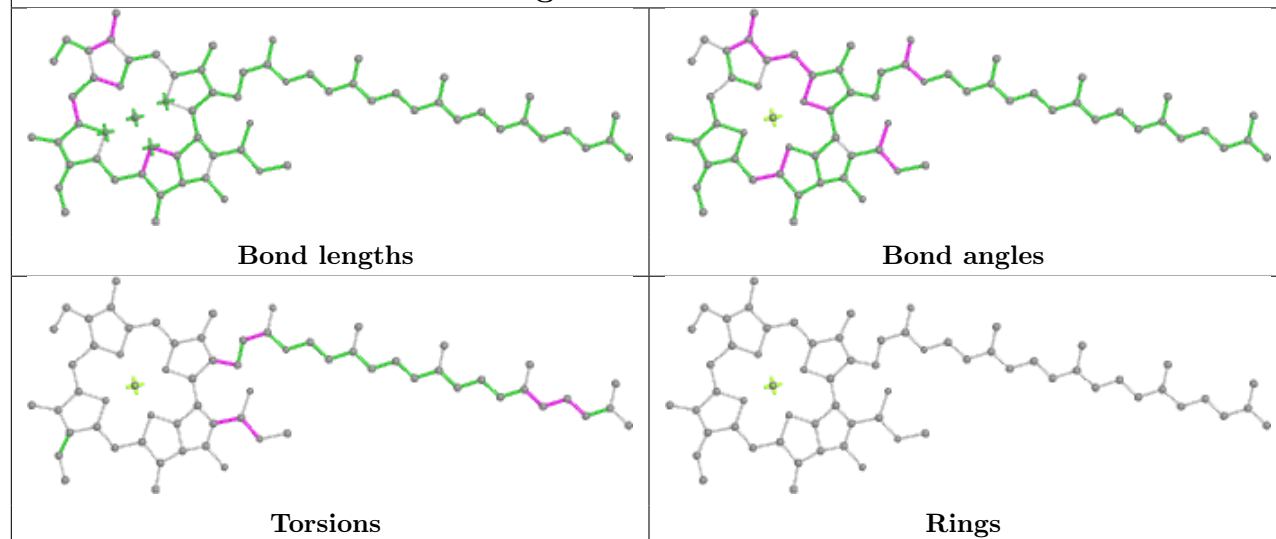


Torsions

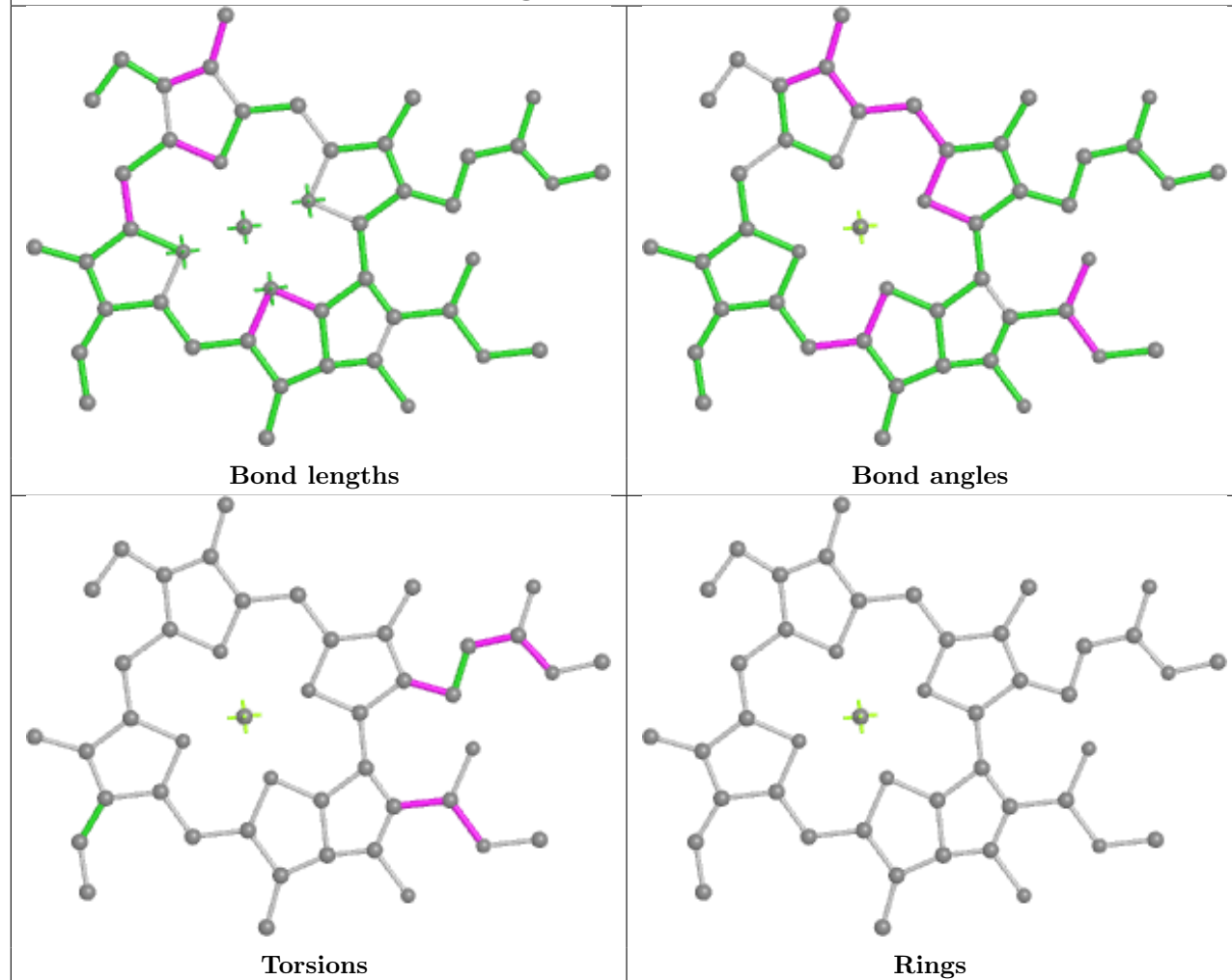


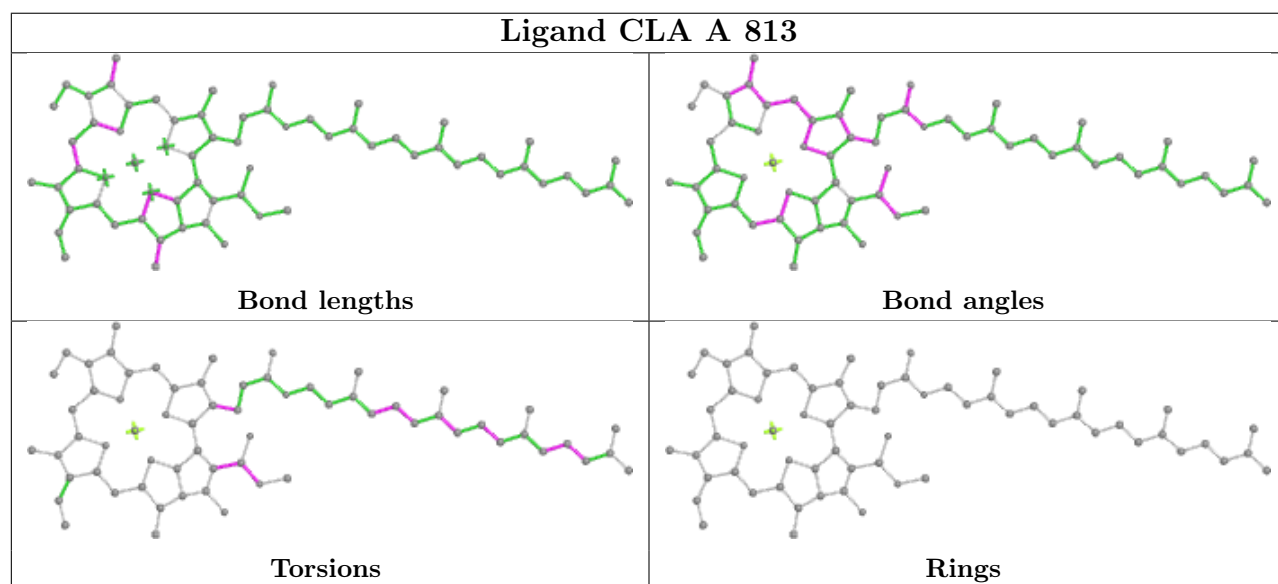
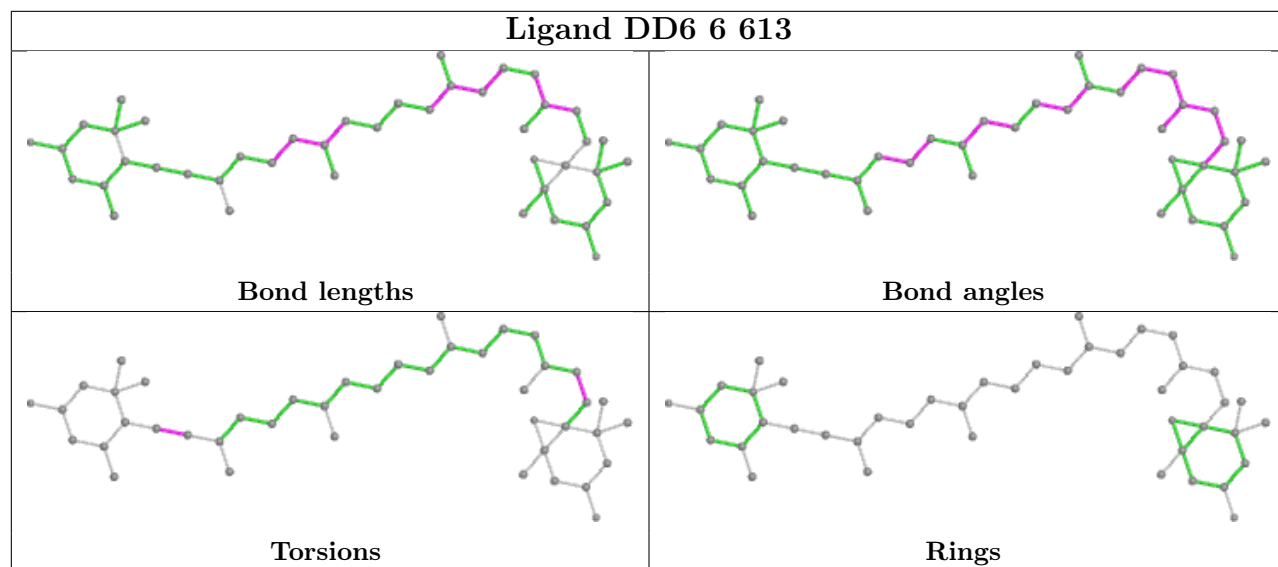
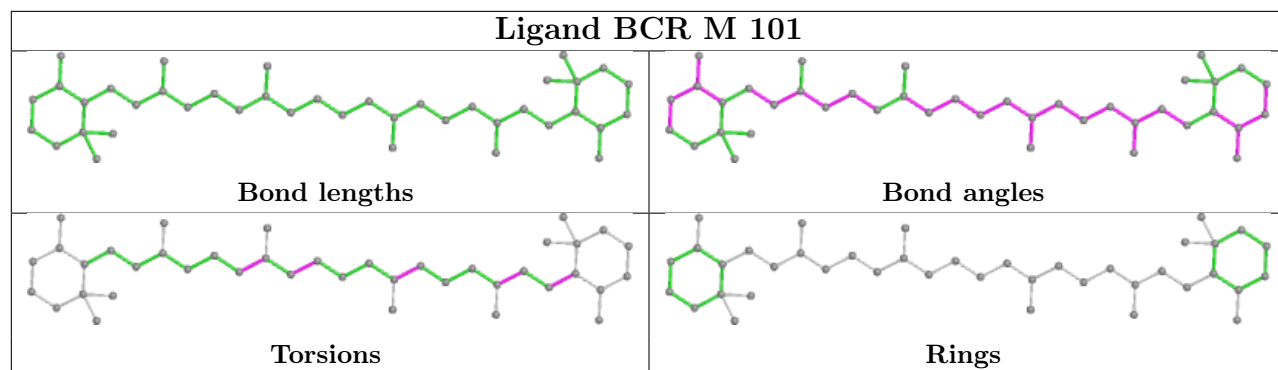
Rings

Ligand CLA 3 306

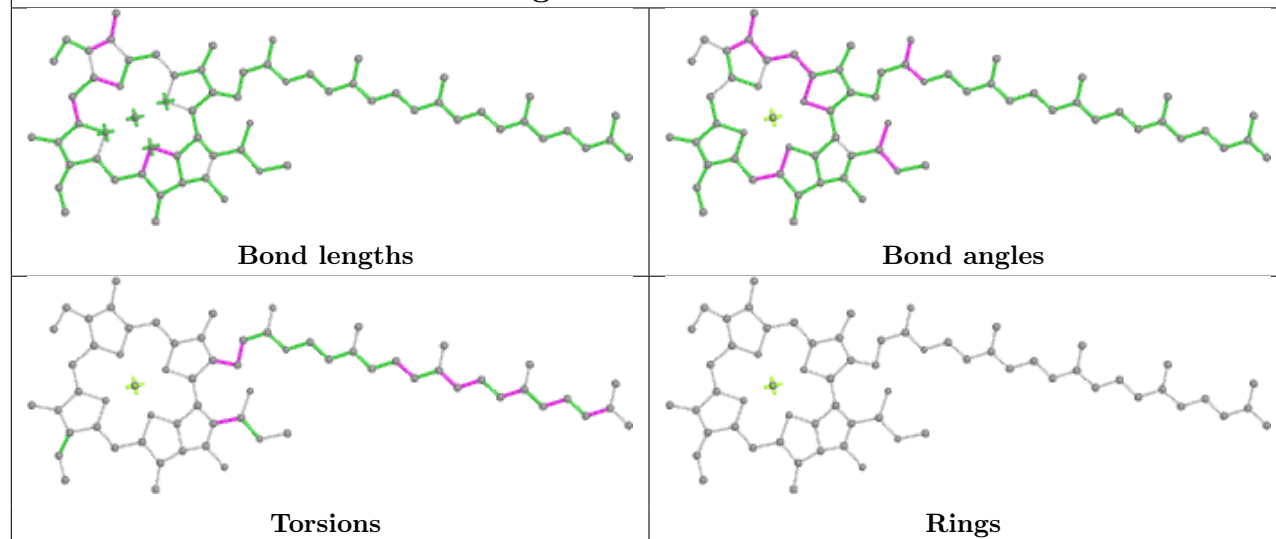


Ligand CLA 4 613

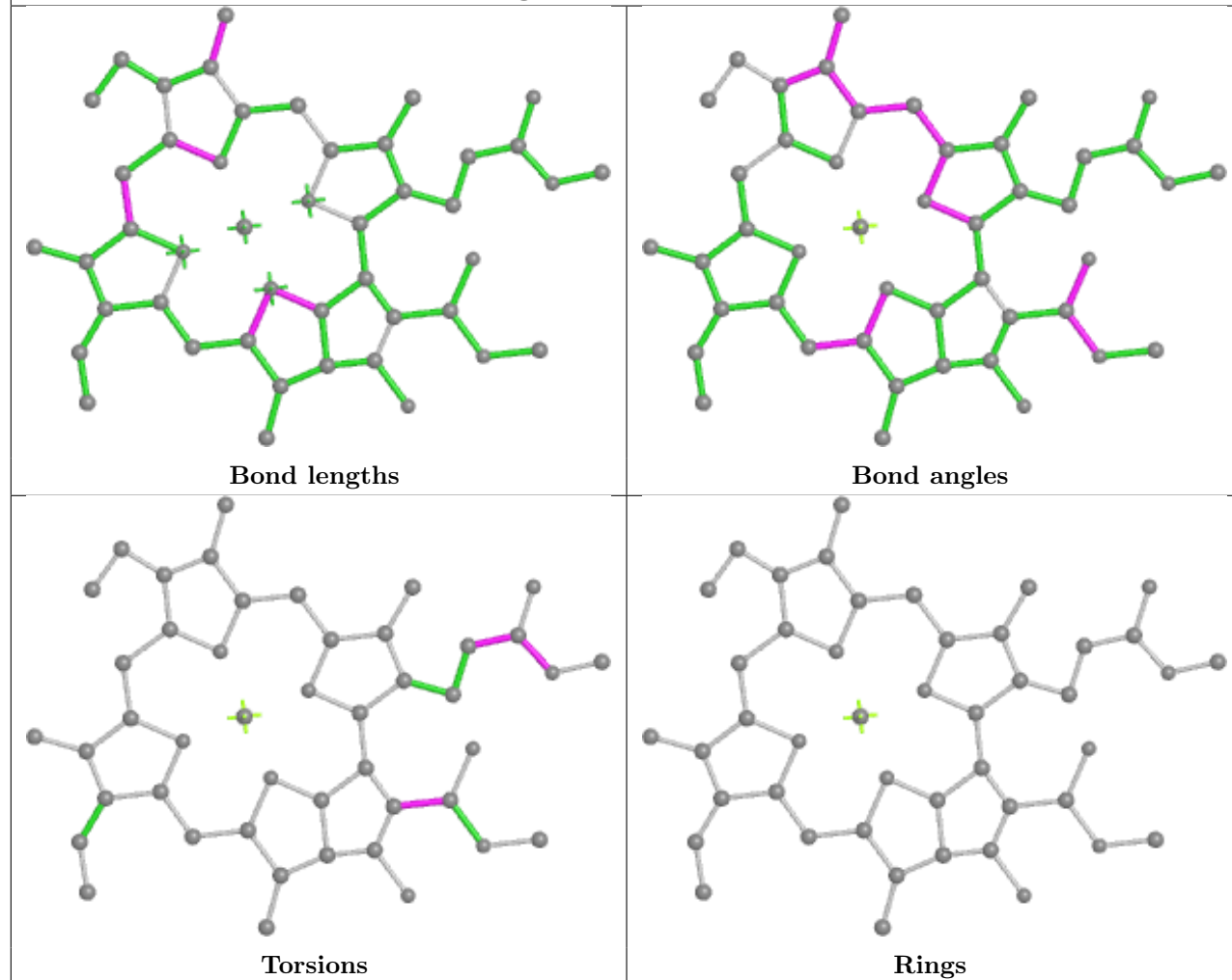




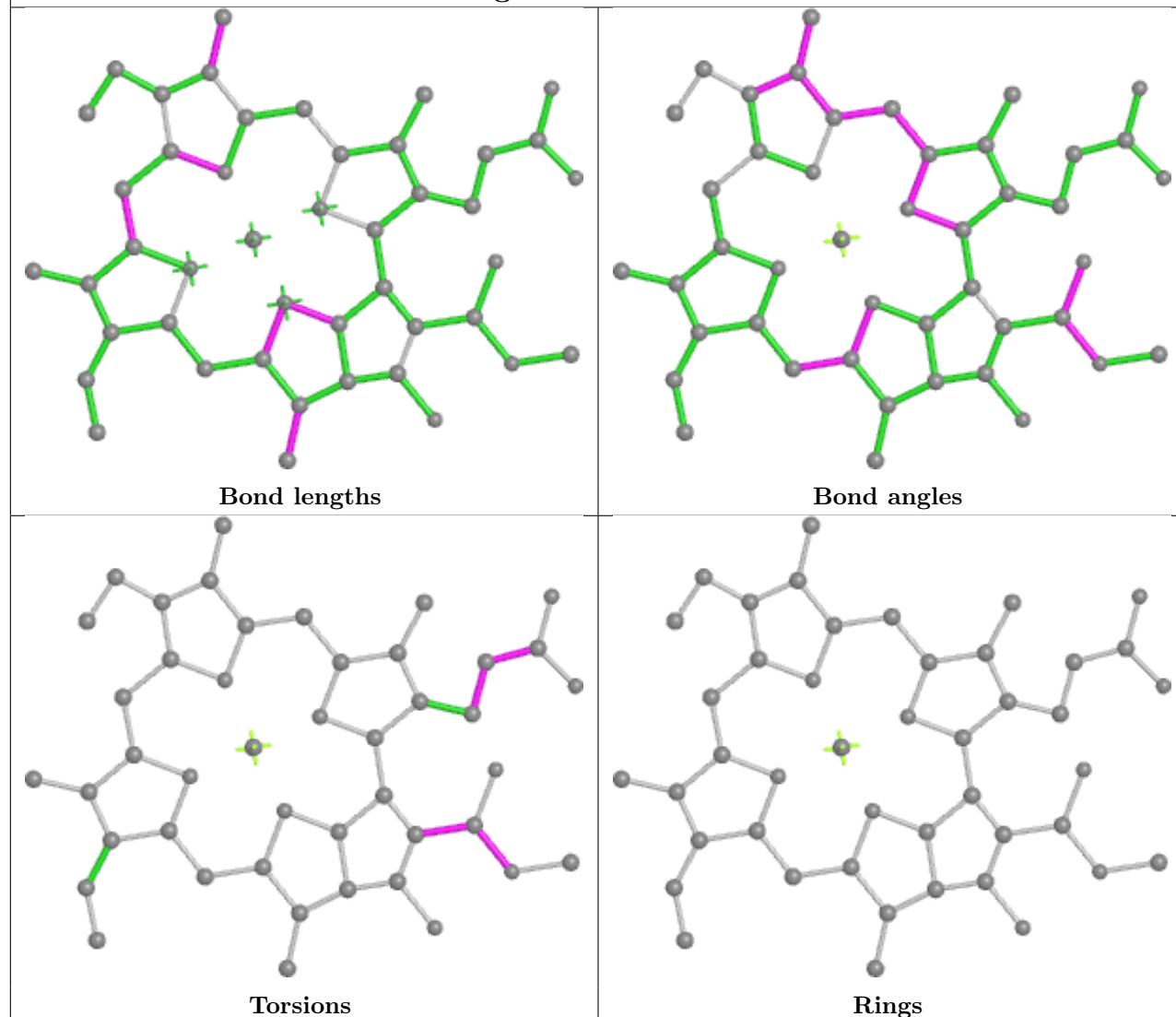
Ligand CLA B 836



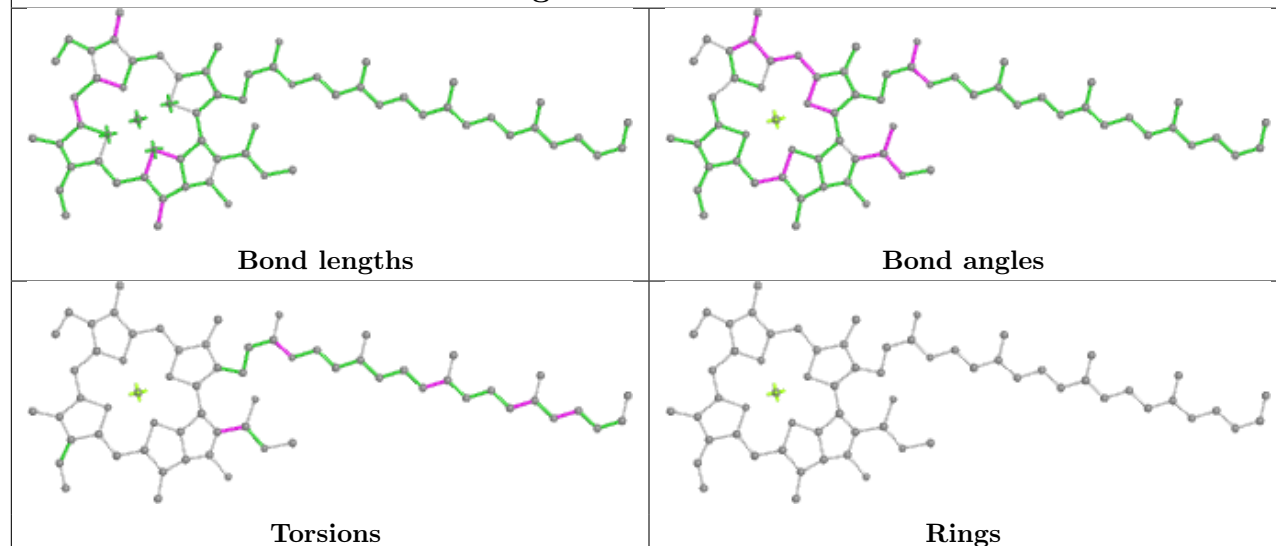
Ligand CLA F 202

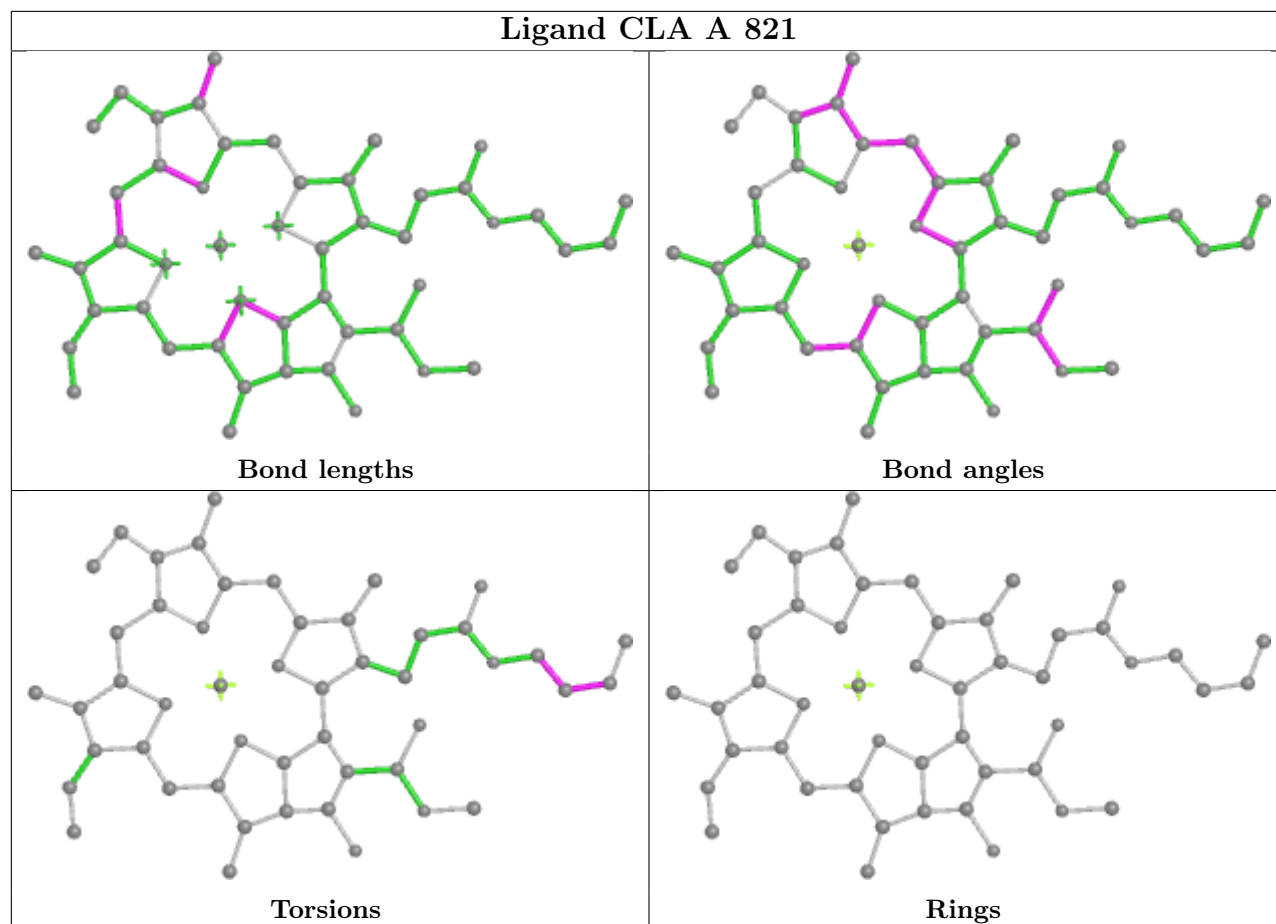
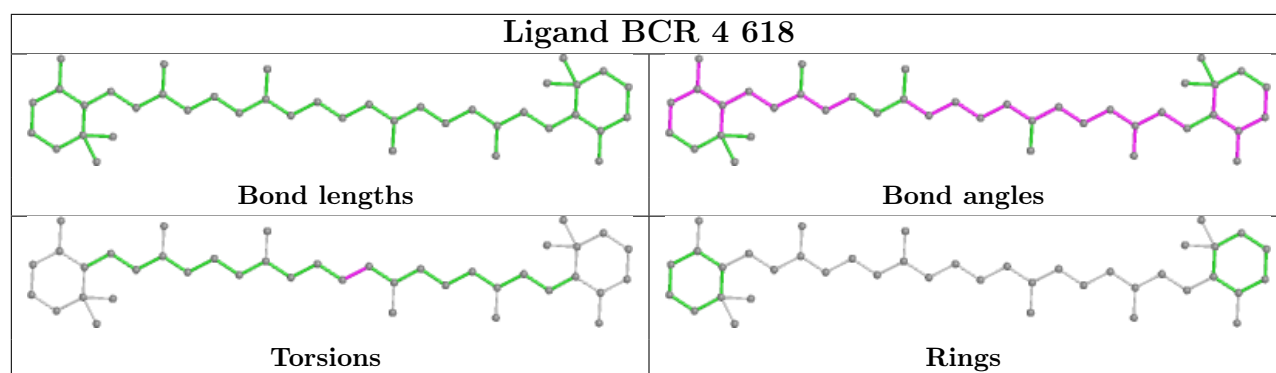


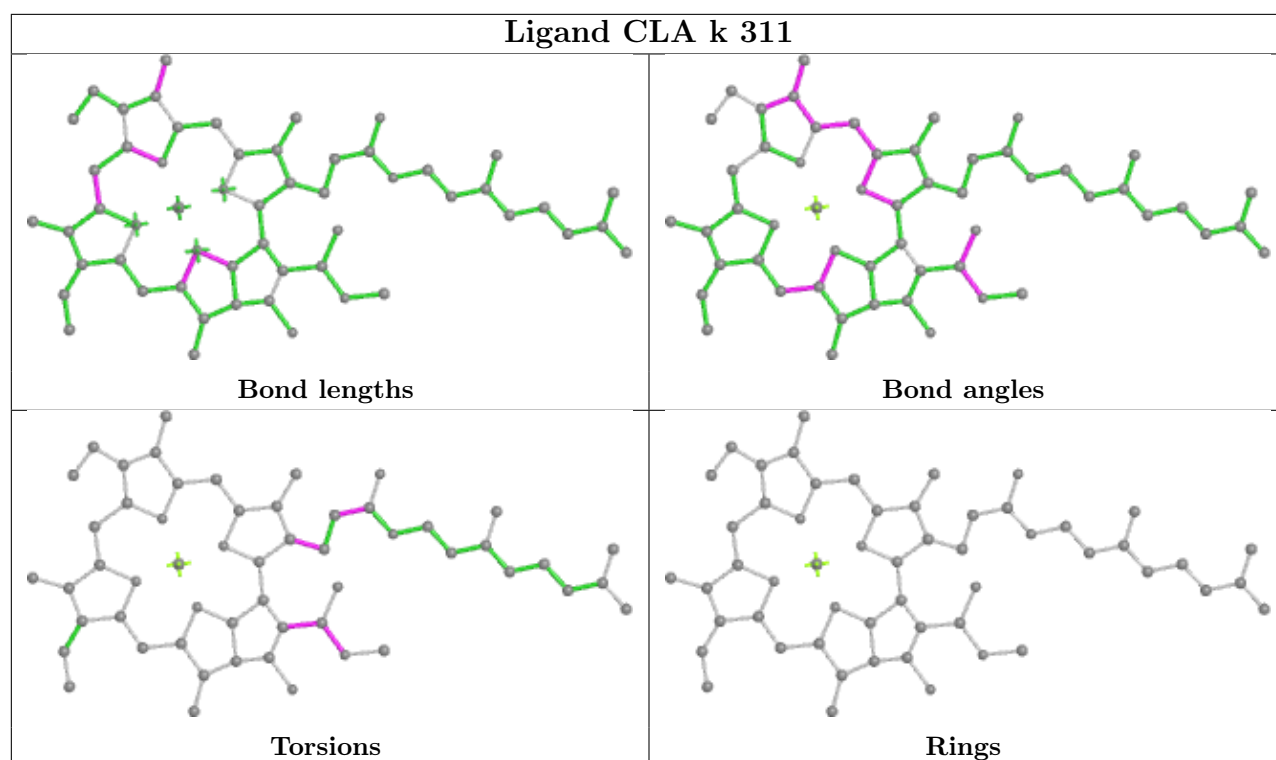
Ligand CLA 7 604



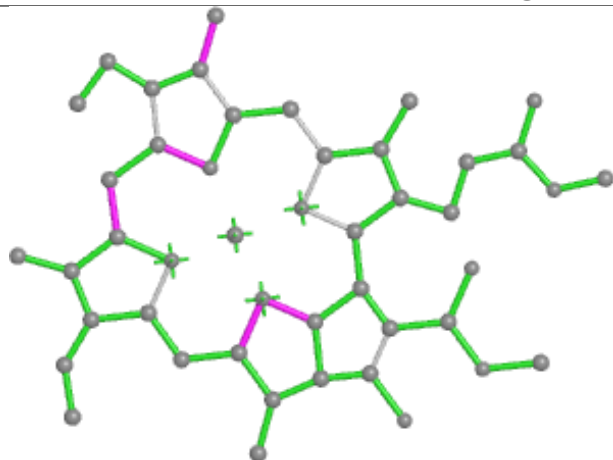
Ligand CLA B 823



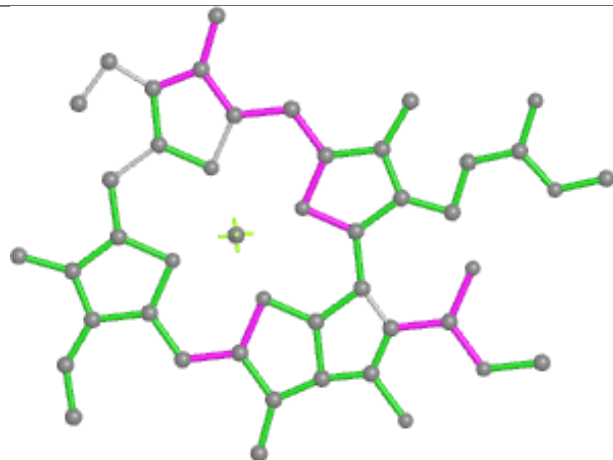




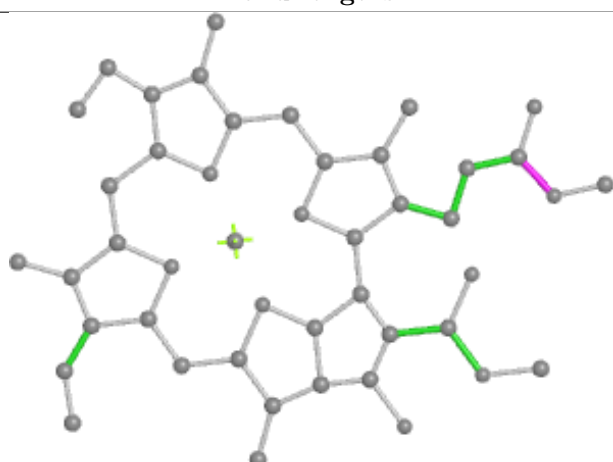
Ligand CLA 4 606



Bond lengths



Bond angles

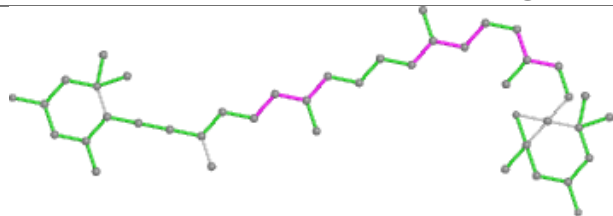


Torsions

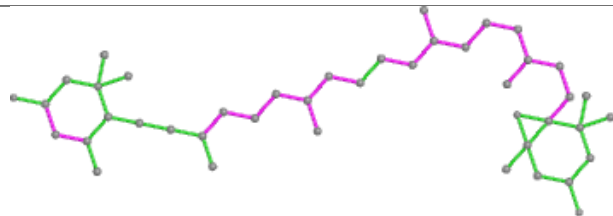


Rings

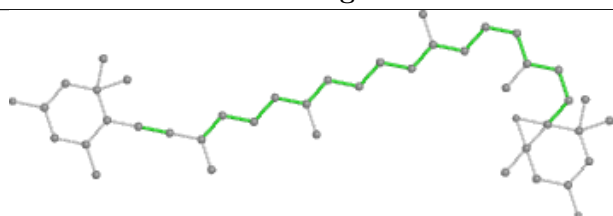
Ligand DD6 7 613



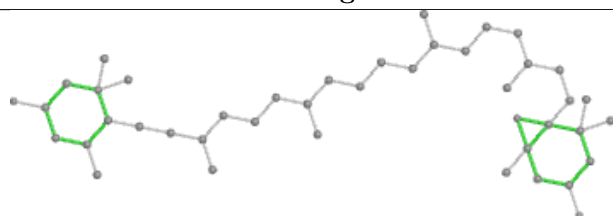
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.