



## Full wwPDB EM Validation Report ⓘ

Nov 24, 2025 – 06:09 PM JST

PDB ID : 8ZOA / pdb\_00008zoa  
EMDB ID : EMD-60286  
Title : Structure of the wild-type PSI-8VCPI supercomplex in *Nannochloropsis oceanica*  
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.  
Deposited on : 2024-05-28  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

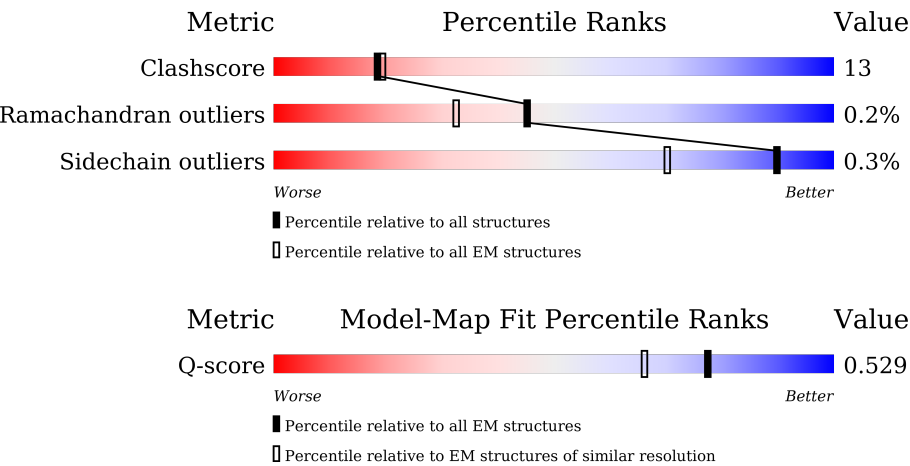
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13114 ( 2.45 - 3.45 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	5	244	<div><div>5%</div><div>52%18%31%</div></div>
2	9	232	<div><div>34%67%19%13%</div></div>
3	8	200	<div><div>62%62%18%18%</div></div>
4	4	202	<div><div>73%10%17%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	7	202	
5	3	220	
6	2	223	
7	1	208	
8	a	745	
9	b	737	
10	d	136	
11	e	67	
12	f	185	
13	h	128	
14	i	45	
15	j	41	
16	l	172	
17	m	30	
18	g	55	
19	c	81	

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
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	315	X	-	-	-
22	CLA	2	316	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	3	315	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	4	315	X	-	-	-
22	CLA	4	316	X	-	-	-
22	CLA	4	317	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	315	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	8	305	X	-	-	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	311	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	9	314	X	-	-	-
22	CLA	9	315	X	-	-	-
22	CLA	9	316	X	-	-	-
22	CLA	9	318	X	-	-	-
22	CLA	a	801	X	-	-	-
22	CLA	a	802	X	-	-	-
22	CLA	a	803	X	-	-	-
22	CLA	a	804	X	-	-	-
22	CLA	a	805	X	-	-	-
22	CLA	a	806	X	-	-	-
22	CLA	a	807	X	-	-	-
22	CLA	a	808	X	-	-	-
22	CLA	a	809	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	810	X	-	-	-
22	CLA	a	811	X	-	-	-
22	CLA	a	812	X	-	-	-
22	CLA	a	813	X	-	-	-
22	CLA	a	814	X	-	-	-
22	CLA	a	815	X	-	-	-
22	CLA	a	816	X	-	-	-
22	CLA	a	817	X	-	-	-
22	CLA	a	818	X	-	-	-
22	CLA	a	819	X	-	-	-
22	CLA	a	820	X	-	-	-
22	CLA	a	821	X	-	-	-
22	CLA	a	822	X	-	-	-
22	CLA	a	823	X	-	-	-
22	CLA	a	824	X	-	-	-
22	CLA	a	825	X	-	-	-
22	CLA	a	826	X	-	-	-
22	CLA	a	827	X	-	-	-
22	CLA	a	828	X	-	-	-
22	CLA	a	829	X	-	-	-
22	CLA	a	830	X	-	-	-
22	CLA	a	831	X	-	-	-
22	CLA	a	832	X	-	-	-
22	CLA	a	833	X	-	-	-
22	CLA	a	834	X	-	-	-
22	CLA	a	835	X	-	-	-
22	CLA	a	836	X	-	-	-
22	CLA	a	837	X	-	-	-
22	CLA	a	838	X	-	-	-
22	CLA	a	839	X	-	-	-
22	CLA	a	840	X	-	-	-
22	CLA	a	841	X	-	-	-
22	CLA	a	842	X	-	-	-
22	CLA	a	844	X	-	-	-
22	CLA	a	854	X	-	-	-
22	CLA	b	801	X	-	-	-
22	CLA	b	802	X	-	-	-
22	CLA	b	803	X	-	-	-
22	CLA	b	804	X	-	-	-
22	CLA	b	805	X	-	-	-
22	CLA	b	806	X	-	-	-
22	CLA	b	807	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	808	X	-	-	-
22	CLA	b	809	X	-	-	-
22	CLA	b	810	X	-	-	-
22	CLA	b	811	X	-	-	-
22	CLA	b	812	X	-	-	-
22	CLA	b	813	X	-	-	-
22	CLA	b	814	X	-	-	-
22	CLA	b	815	X	-	-	-
22	CLA	b	816	X	-	-	-
22	CLA	b	817	X	-	-	-
22	CLA	b	818	X	-	-	-
22	CLA	b	819	X	-	-	-
22	CLA	b	820	X	-	-	-
22	CLA	b	821	X	-	-	-
22	CLA	b	822	X	-	-	-
22	CLA	b	823	X	-	-	-
22	CLA	b	824	X	-	-	-
22	CLA	b	825	X	-	-	-
22	CLA	b	826	X	-	-	-
22	CLA	b	827	X	-	-	-
22	CLA	b	828	X	-	-	-
22	CLA	b	829	X	-	-	-
22	CLA	b	830	X	-	-	-
22	CLA	b	831	X	-	-	-
22	CLA	b	832	X	-	-	-
22	CLA	b	833	X	-	-	-
22	CLA	b	834	X	-	-	-
22	CLA	b	835	X	-	-	-
22	CLA	b	836	X	-	-	-
22	CLA	b	837	X	-	-	-
22	CLA	b	838	X	-	-	-
22	CLA	b	839	X	-	-	-
22	CLA	b	840	X	-	-	-
22	CLA	f	802	X	-	-	-
22	CLA	f	803	X	-	-	-
22	CLA	h	203	X	-	-	-
22	CLA	h	205	X	-	-	-
22	CLA	j	102	X	-	-	-
22	CLA	j	103	X	-	-	-
22	CLA	l	202	X	-	-	-
22	CLA	l	203	X	-	-	-
22	CLA	l	204	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SF4	c	102	-	-	X	-

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 41637 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 VCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1317	867	222	222	6		

- Molecule 2 is a protein called VCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	201	Total	C	N	O	S	0	0
			1466	936	256	269	5		

- Molecule 3 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	164	Total	C	N	O	S	0	0
			1258	822	203	227	6		

- Molecule 4 is a protein called VCPI-4/7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		
4	7	166	Total	C	N	O	S	0	0
			1220	791	202	222	5		

- Molecule 5 is a protein called VCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	177	Total	C	N	O	S	0	0
			1324	846	225	245	8		

- Molecule 6 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 7 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	739	Total	C	N	O	S	0	0
			5827	3828	982	1000	17		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	735	Total	C	N	O	S	0	0
			5865	3874	985	989	17		

- Molecule 10 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	130	Total	C	N	O	S	0	0
			1014	652	175	184	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	61	Total	C	N	O	0	0
			494	314	86	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	160	Total	C	N	O	S	0	0
			1266	815	213	235	3		

- Molecule 13 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	85	Total	C	N	O	S	0	0
			646	427	100	117	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	34	Total	C	N	O	S	0	0
			271	189	36	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	j	41	Total	C	N	O	S	0	0
			339	233	48	57	1		

- Molecule 16 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	171	Total	C	N	O		0	0
			1283	848	203	232			

- Molecule 17 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	m	30	Total	C	N	O	0	0
			210	137	35	38		

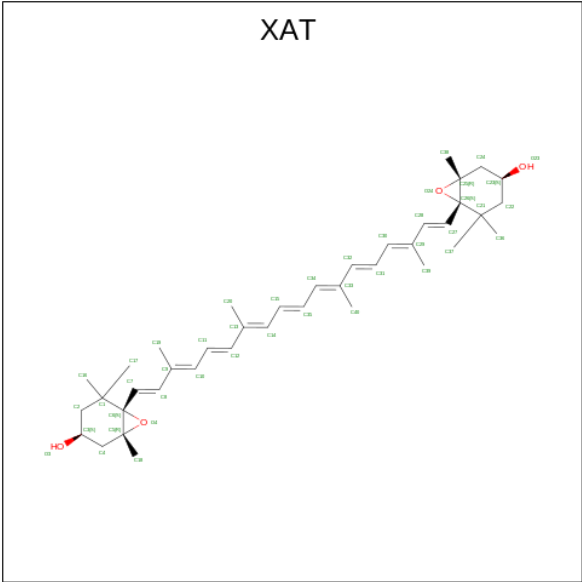
- Molecule 18 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	g	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 19 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	80	Total	C	N	O	S	0	0
			596	366	103	117	10		

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

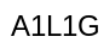
Continued on next page...



*Continued from previous page...*

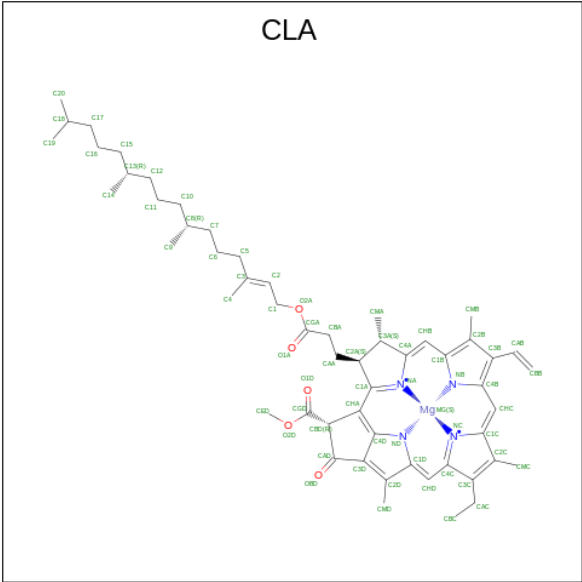
Mol	Chain	Residues	Atoms			AltConf
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	a	1	Total	C	O	0
			44	40	4	
20	j	1	Total	C	O	0
			44	40	4	

- Molecule 21 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-oxa bicyclo[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: C<sub>40</sub>H<sub>56</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltCon
21	5	1	Total 45	C 40	O 5	0
21	9	1	Total 45	C 40	O 5	0
21	9	1	Total 45	C 40	O 5	0
21	3	1	Total 45	C 40	O 5	0
21	3	1	Total 45	C 40	O 5	0
21	7	1	Total 45	C 40	O 5	0
21	1	1	Total 45	C 40	O 5	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

*Continued on next page...*

*Continued from previous page...*

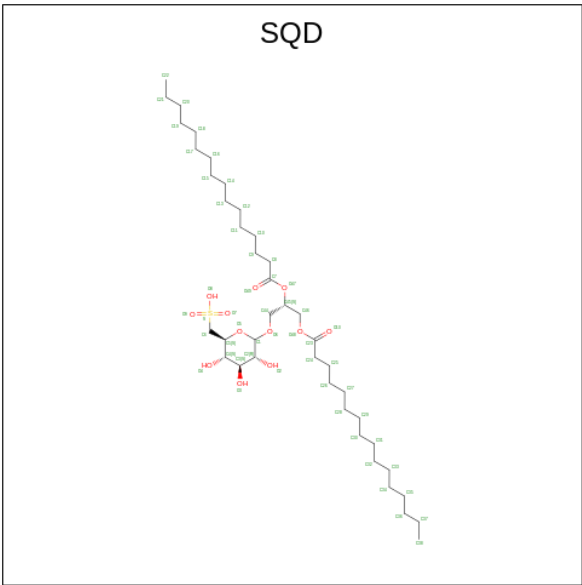
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

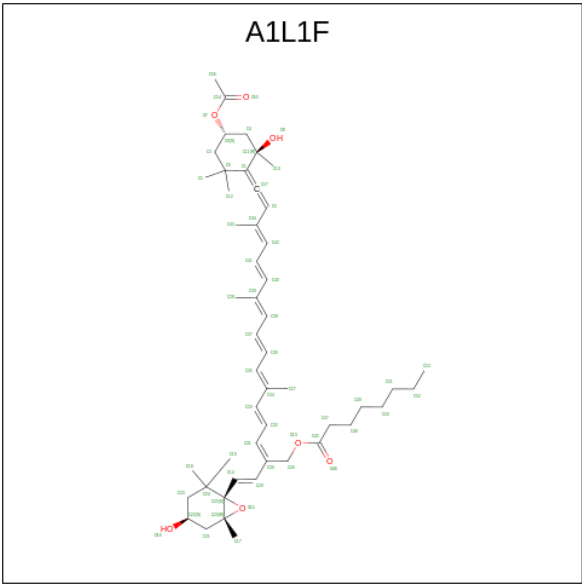
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



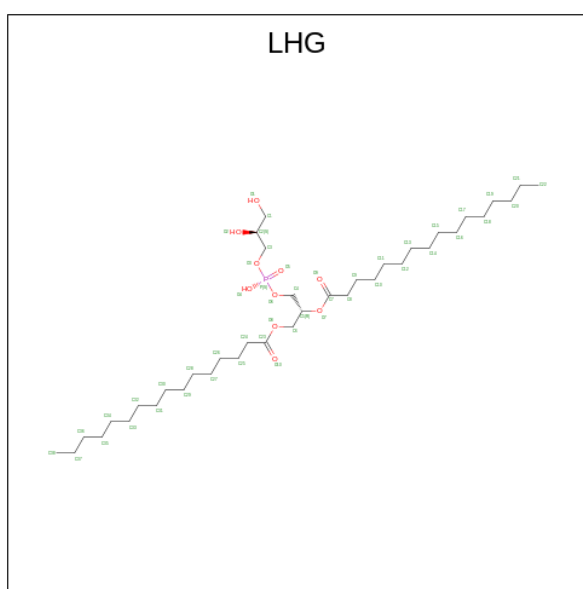
Mol	Chain	Residues	Atoms				AltConf
23	5	1	Total	C	O	S	0
			35	22	12	1	
23	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 24 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[( {E})-2-[(1 {S},4 {S}, 6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,1 0,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C<sub>50</sub>H<sub>72</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



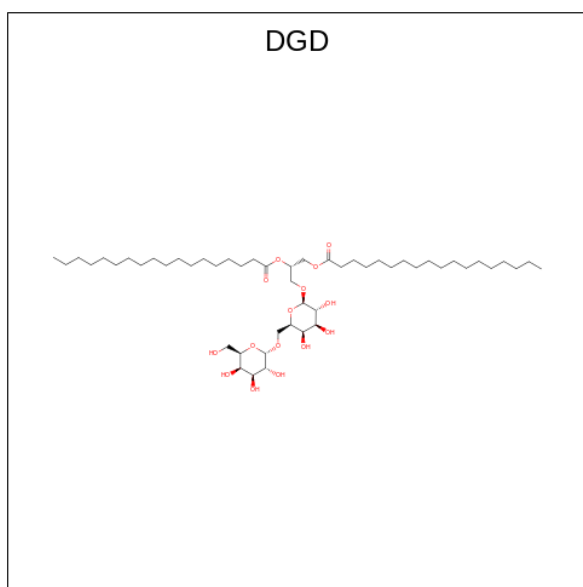
Mol	Chain	Residues	Atoms			AltConf
24	9	1	Total	C	O	0
			57	50	7	
24	8	1	Total	C	O	0
			57	50	7	
24	1	1	Total	C	O	0
			57	50	7	
24	h	1	Total	C	O	0
			57	50	7	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).



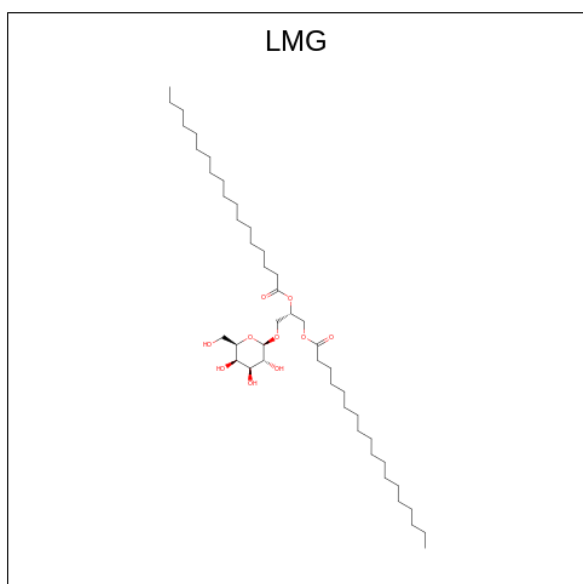
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O	P	0
			36	25	10	1	
25	9	1	Total	C	O	P	0
			46	35	10	1	
25	a	1	Total	C	O	P	0
			48	37	10	1	
25	a	1	Total	C	O	P	0
			27	16	10	1	
25	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



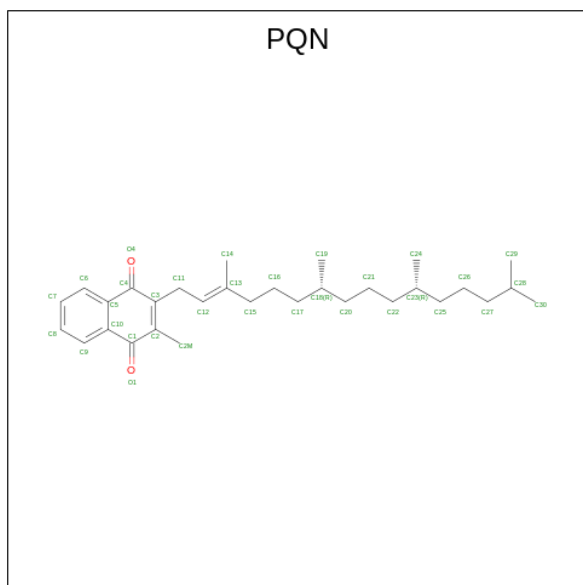
Mol	Chain	Residues	Atoms			AltConf
26	8	1	Total	C	O	0
			40	25	15	
26	4	1	Total	C	O	0
			40	25	15	
26	b	1	Total	C	O	0
			57	42	15	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



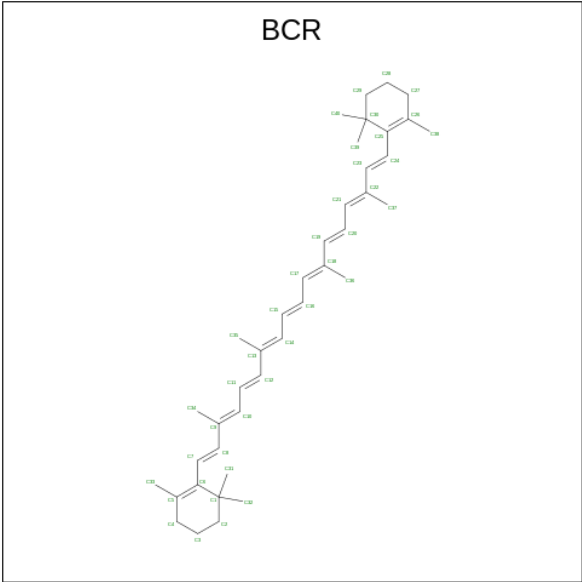
Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total	C	O	0
			35	25	10	
27	a	1	Total	C	O	0
			34	24	10	
27	j	1	Total	C	O	0
			32	22	10	

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



Mol	Chain	Residues	Atoms			AltConf
28	a	1	Total	C	O	0
			33	31	2	
28	b	1	Total	C	O	0
			33	31	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	h	1	Total C 40 40	0

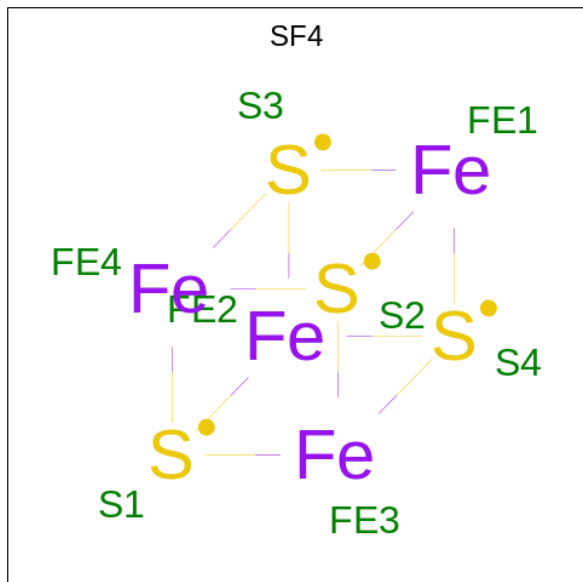
Continued on next page...



Continued from previous page...

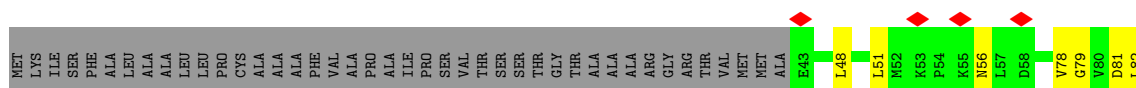
Mol	Chain	Residues	Atoms	AltConf
29	i	1	Total C 40 40	0
29	j	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	m	1	Total C 40 40	0

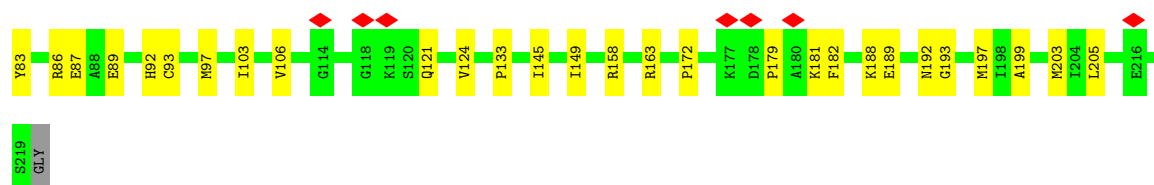
- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



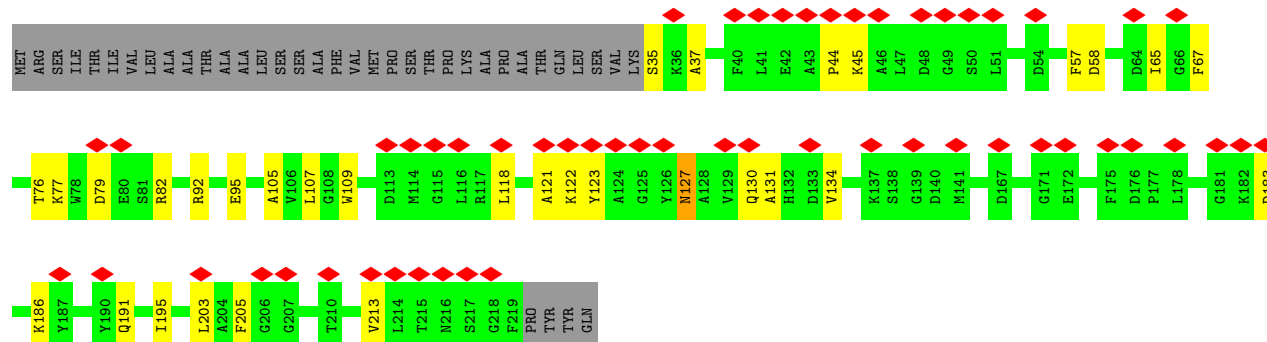
Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0



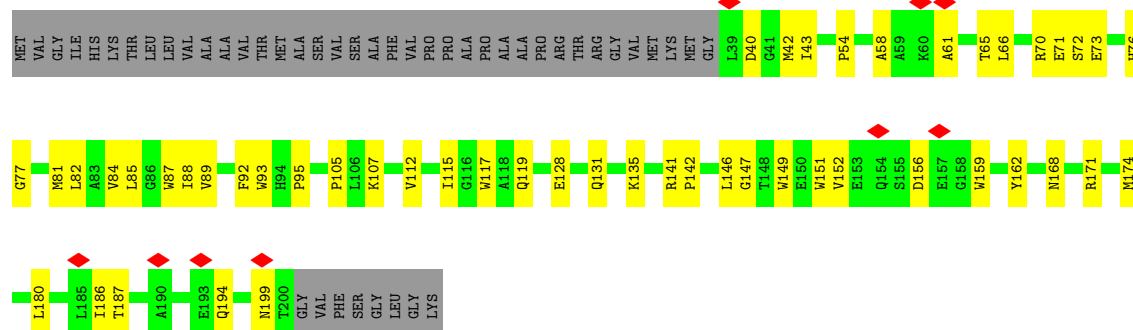




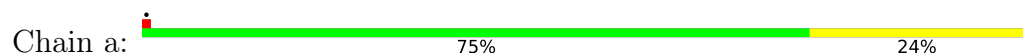
• Molecule 6: VCPI-2



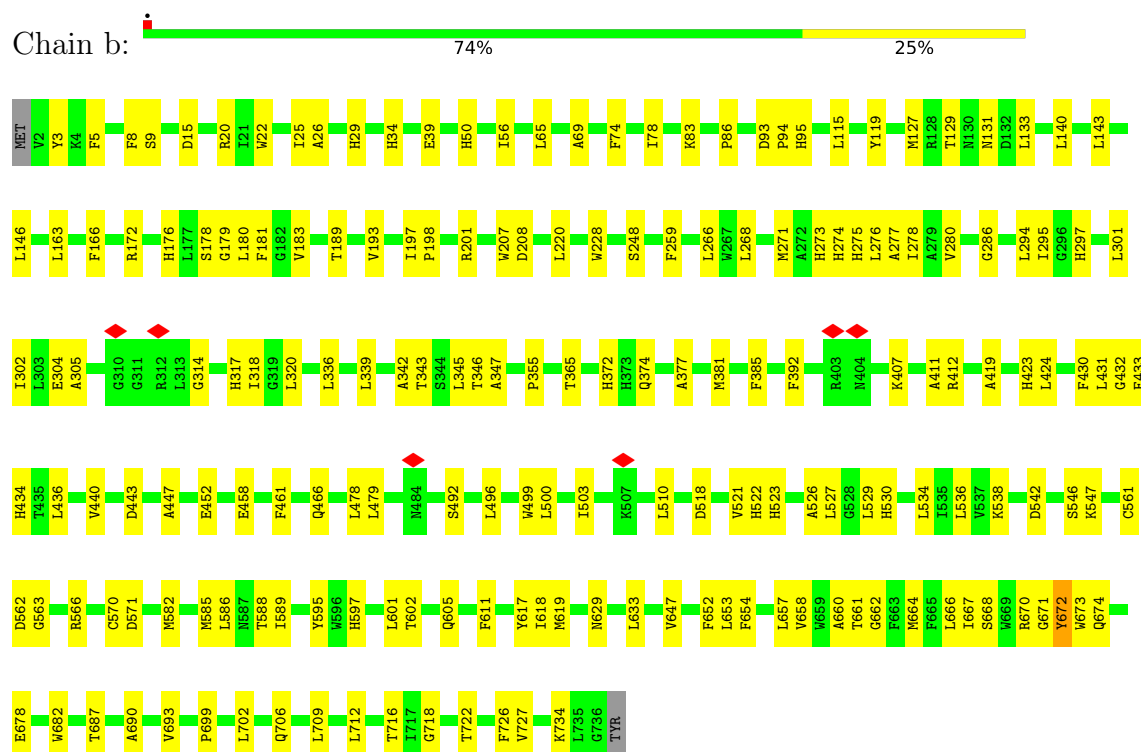
• Molecule 7: VCPI-1



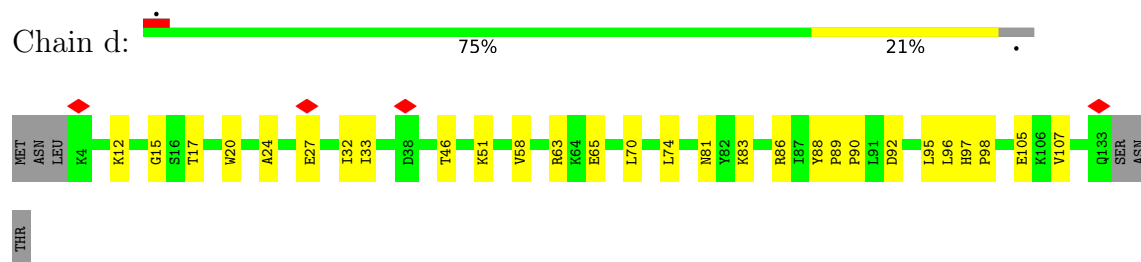
• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A1



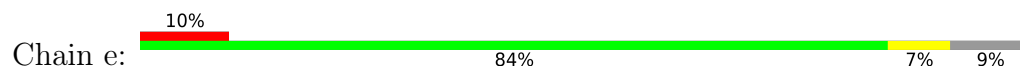
- Molecule 9: Photosystem I P700 chlorophyll a apoprotein A2

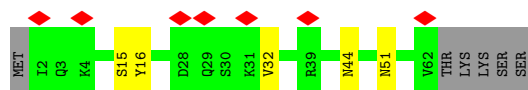


- Molecule 10: Photosystem I reaction center subunit II

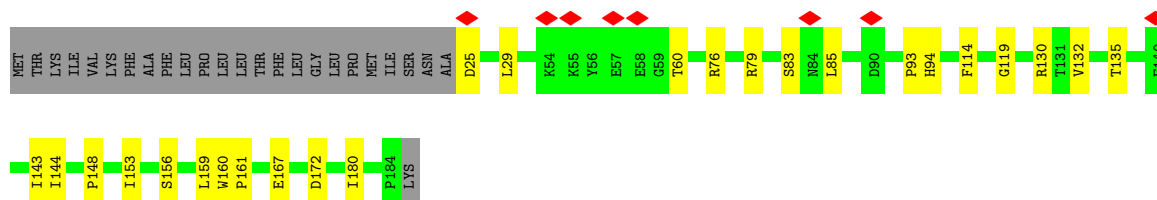


- Molecule 11: Photosystem I reaction center subunit IV

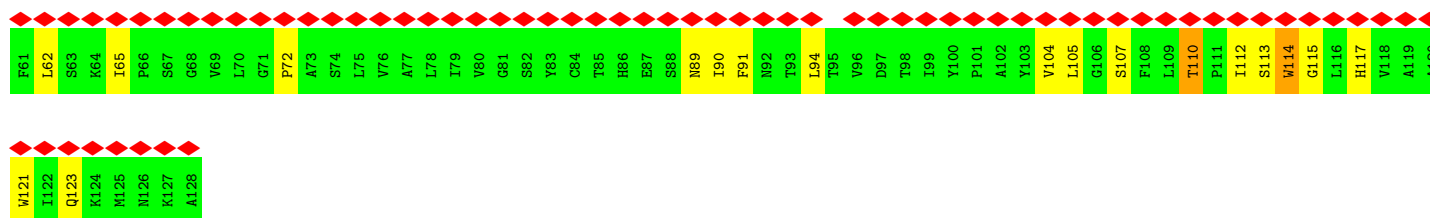
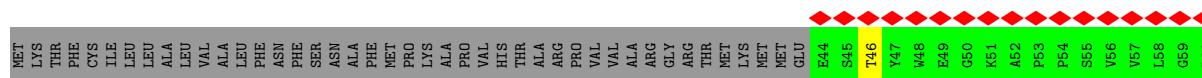




- Molecule 12: Photosystem I reaction center subunit III



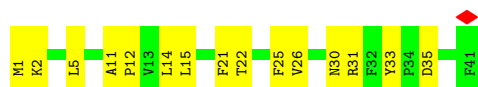
- Molecule 13: PsaR



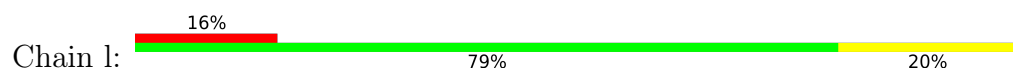
- Molecule 14: Photosystem I reaction center subunit VIII

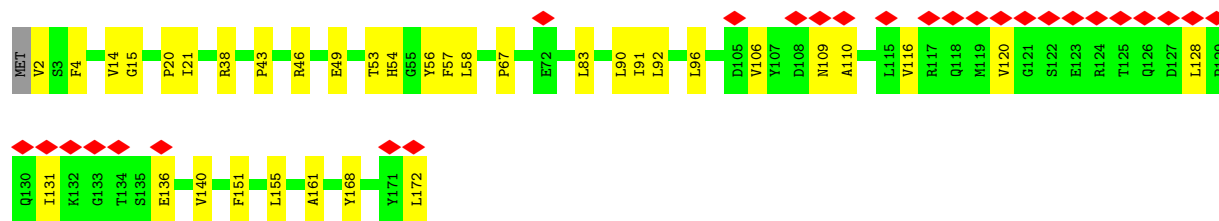


- Molecule 15: Photosystem I reaction center subunit IX



- Molecule 16: PSI subunit V





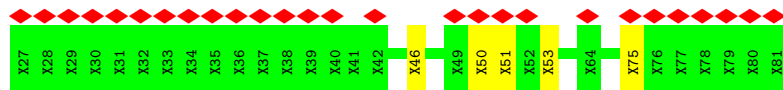
• Molecule 17: Psam

Chain m: 90% 10%



• Molecule 18: PsaS

Chain g: 49% 91% 9%



• Molecule 19: Photosystem I iron-sulfur center

Chain c: 70% 28%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.545	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.295	Depositor
Map size ( $\text{\AA}$ )	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, SF4, SQD, DGD, PQN, A1L1F, CLA, BCR, LMG, A1L1G, LHG

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	5	0.14	0/1353	0.29	0/1823
2	9	0.34	0/1496	0.34	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.31	0/1761
4	7	0.19	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	2	0.14	0/1405	0.36	0/1904
7	1	0.13	0/1293	0.33	0/1759
8	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
9	b	0.20	0/6080	0.32	1/8302 (0.0%)
10	d	0.12	0/1040	0.32	0/1402
11	e	0.09	0/502	0.20	0/681
12	f	0.14	0/1297	0.30	0/1762
13	h	0.52	1/667 (0.1%)	0.52	0/915
14	i	0.15	0/278	0.33	0/378
15	j	0.15	0/351	0.36	0/478
16	l	0.14	0/1315	0.31	0/1796
17	m	0.09	0/210	0.28	0/288
19	c	0.13	0/606	0.34	0/822
All	All	0.24	5/29099 (0.0%)	0.33	8/39586 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	580	SER	CA-C	-7.02	1.43	1.52
3	8	44	LEU	C-O	-6.16	1.15	1.23
8	a	581	ALA	CA-C	-5.42	1.45	1.52
13	h	114	TRP	C-O	-5.28	1.18	1.24
8	a	582	TRP	CA-C	-5.08	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	581	ALA	N-CA-C	-8.63	102.50	113.72
8	a	448	LEU	N-CA-C	-6.11	104.18	111.69
3	8	39	LYS	N-CA-C	-6.10	105.66	113.23
8	a	584	HIS	N-CA-C	-5.81	106.53	113.97
9	b	672	TYR	N-CA-C	-5.59	106.30	113.23
3	8	41	LEU	CA-C-N	5.09	124.80	119.82
3	8	41	LEU	C-N-CA	5.09	124.80	119.82
8	a	585	VAL	N-CA-C	-5.07	105.45	112.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	37	0
2	9	1466	0	1470	46	0
3	8	1258	0	1280	33	0
4	4	1268	0	1288	22	0
4	7	1220	0	1209	41	0
5	3	1324	0	1340	25	0
6	2	1372	0	1347	21	0
7	1	1262	0	1237	37	0
8	a	5827	0	5697	140	0
9	b	5865	0	5710	157	0
10	d	1014	0	1015	22	0
11	e	494	0	495	5	0
12	f	1266	0	1262	21	0
13	h	646	0	649	18	0
14	i	271	0	292	12	0
15	j	339	0	342	20	0
16	l	1283	0	1278	28	0
17	m	210	0	226	3	0
18	g	275	0	62	3	0
19	c	596	0	583	20	0
20	1	88	0	112	7	0
20	2	220	0	280	20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	3	176	0	224	19	0
20	4	220	0	280	31	0
20	5	132	0	168	13	0
20	7	176	0	224	25	0
20	8	132	0	168	12	0
20	9	132	0	168	17	0
20	a	44	0	56	6	0
20	j	44	0	56	7	0
21	1	45	0	0	1	0
21	3	90	0	0	0	0
21	5	45	0	0	1	0
21	7	45	0	0	2	0
21	9	90	0	0	3	0
22	1	547	0	508	15	0
22	2	544	0	452	13	0
22	3	458	0	378	9	0
22	4	613	0	522	32	0
22	5	563	0	472	22	0
22	7	576	0	444	23	0
22	8	507	0	429	20	0
22	9	519	0	452	34	0
22	a	2579	0	2562	138	0
22	b	2410	0	2464	133	0
22	f	117	0	115	2	0
22	h	120	0	121	6	0
22	j	100	0	86	9	0
22	l	148	0	123	3	0
23	1	45	0	54	2	0
23	5	35	0	34	1	0
24	1	57	0	0	2	0
24	8	57	0	0	2	0
24	9	57	0	0	2	0
24	h	57	0	0	4	0
25	9	82	0	110	5	0
25	a	75	0	93	6	0
25	b	31	0	32	0	0
26	4	40	0	38	11	0
26	8	40	0	38	2	0
26	b	57	0	72	6	0
27	2	35	0	40	3	0
27	a	34	0	38	10	0
27	j	32	0	34	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	33	0	46	4	0
28	b	33	0	46	3	0
29	a	160	0	224	12	0
29	b	240	0	336	24	0
29	f	80	0	112	14	0
29	h	80	0	112	6	0
29	i	40	0	56	3	0
29	j	40	0	56	9	0
29	l	80	0	112	14	0
29	m	40	0	56	2	0
30	a	8	0	0	0	0
30	c	16	0	0	3	0
All	All	41637	0	40703	1052	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 13.

All (1052) 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)
4:4:193:ALA:HB1	26:4:318:DGD:HE62	1.13	1.13
4:4:193:ALA:HB1	26:4:318:DGD:C6E	1.84	1.07
26:4:318:DGD:O4E	26:4:318:DGD:O5E	1.61	0.91
20:2:303:XAT:H32	22:2:308:CLA:HAB	1.52	0.90
20:5:302:XAT:H12	22:5:307:CLA:HAB	1.53	0.89
22:a:806:CLA:O1A	22:a:814:CLA:HBA1	1.81	0.80
8:a:531:ILE:HD12	22:a:801:CLA:H172	1.63	0.80
20:4:303:XAT:H12	22:4:308:CLA:HAB	1.67	0.77
22:b:825:CLA:HMA1	29:b:845:BCR:H17C	1.66	0.76
20:8:303:XAT:H12	22:8:312:CLA:HAB	1.67	0.76
22:1:312:CLA:HHC	22:1:312:CLA:HBB1	1.69	0.74
4:4:193:ALA:CB	26:4:318:DGD:HE62	2.07	0.74
20:2:303:XAT:H181	22:2:314:CLA:HBB1	1.70	0.72
22:b:833:CLA:H72	29:b:845:BCR:H391	1.72	0.71
7:1:43:ILE:O	7:1:70:ARG:NH2	2.25	0.70
22:4:317:CLA:H2A	26:4:318:DGD:HE62	1.73	0.69
22:b:807:CLA:H151	22:b:828:CLA:HBB2	1.74	0.69
15:j:22:THR:HA	15:j:25:PHE:CE1	2.28	0.69
29:a:847:BCR:H362	29:a:848:BCR:H21C	1.73	0.69
12:f:167:GLU:HG3	12:f:172:ASP:HB3	1.73	0.68
1:5:179:LEU:HD12	12:f:159:LEU:HD11	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:302:XAT:H14	22:4:310:CLA:H12	1.76	0.68
9:b:273:HIS:HD1	22:b:817:CLA:HAB	1.58	0.68
8:a:569:ASP:OD2	8:a:573:ARG:NH2	2.27	0.68
8:a:363:HIS:ND1	22:a:819:CLA:OBD	2.26	0.67
7:1:70:ARG:NH1	7:1:73:GLU:OE1	2.28	0.67
9:b:295:ILE:HG13	22:b:820:CLA:HED1	1.77	0.67
22:4:317:CLA:HAA2	26:4:318:DGD:HE5	1.77	0.66
8:a:112:TRP:HB3	20:j:101:XAT:H373	1.77	0.66
15:j:31:ARG:HD3	20:j:101:XAT:H222	1.77	0.66
7:1:194:GLN:HG3	7:1:199:ASN:HB3	1.77	0.66
9:b:304:GLU:HG2	9:b:318:ILE:HG13	1.78	0.66
22:a:804:CLA:HED1	15:j:15:LEU:HD22	1.76	0.65
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.65
22:a:808:CLA:HMB2	29:j:104:BCR:HC8	1.78	0.65
9:b:336:LEU:HD21	22:b:829:CLA:HAB	1.78	0.65
7:1:146:LEU:HD13	22:a:844:CLA:H91	1.77	0.65
8:a:197:GLY:O	8:a:201:LEU:HB2	1.97	0.65
9:b:9:SER:HB2	26:b:848:DGD:HE62	1.78	0.65
13:h:114:TRP:HA	13:h:117:HIS:NE2	2.11	0.65
2:9:191:ALA:O	2:9:195:ASN:ND2	2.30	0.64
12:f:25:ASP:N	12:f:29:LEU:O	2.30	0.64
4:7:120:ALA:HB1	22:7:311:CLA:HMD1	1.78	0.64
8:a:356:LEU:HD11	22:a:820:CLA:H71	1.78	0.64
20:4:303:XAT:H193	22:4:308:CLA:H142	1.78	0.64
9:b:115:LEU:HA	9:b:365:THR:HG22	1.80	0.64
20:3:305:XAT:H32	22:3:313:CLA:HAB	1.79	0.64
22:a:834:CLA:H142	29:b:846:BCR:H15C	1.79	0.64
14:i:29:TYR:HA	14:i:32:LYS:HE2	1.78	0.64
8:a:684:ARG:H	9:b:570:CYS:HB2	1.63	0.64
9:b:129:THR:HG22	9:b:131:ASN:H	1.63	0.63
22:b:813:CLA:H121	22:b:818:CLA:H72	1.79	0.63
4:7:50:ASP:OD1	4:7:51:GLY:N	2.32	0.63
12:f:79:ARG:NH1	15:j:35:ASP:O	2.30	0.63
22:b:823:CLA:HBB1	22:b:837:CLA:H151	1.79	0.63
4:7:136:VAL:HG22	22:7:312:CLA:HMA1	1.81	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
8:a:362:HIS:HA	8:a:365:TYR:CE1	2.33	0.63
15:j:26:VAL:HG11	29:j:104:BCR:H24C	1.81	0.62
1:5:130:PHE:CE1	20:5:302:XAT:O24	2.52	0.62
8:a:114:ILE:HB	20:j:101:XAT:H372	1.81	0.62
20:4:304:XAT:H32	22:4:313:CLA:HAB	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:7:303:XAT:H362	22:7:308:CLA:H51	1.81	0.62
8:a:298:PHE:HE1	22:a:822:CLA:HAB	1.64	0.62
2:9:182:ALA:HB3	2:9:190:GLU:HG2	1.82	0.62
9:b:424:LEU:HD13	9:b:534:LEU:HA	1.81	0.62
10:d:12:LYS:HB2	10:d:51:LYS:HB3	1.82	0.62
15:j:21:PHE:HA	22:j:103:CLA:HBB2	1.80	0.62
20:4:305:XAT:H363	20:3:301:XAT:H10	1.80	0.62
10:d:88:TYR:HB2	10:d:92:ASP:HB2	1.81	0.62
24:h:204:A1L1F:C12	24:h:204:A1L1F:C4	2.78	0.62
22:a:818:CLA:C3D	27:a:853:LMG:HC91	2.30	0.61
22:8:305:CLA:CGA	26:8:315:DGD:HE5	2.29	0.61
8:a:70:HIS:ND1	22:a:814:CLA:OBD	2.31	0.61
8:a:162:ALA:O	8:a:166:MET:HG2	2.00	0.61
8:a:298:PHE:CE1	22:a:822:CLA:HAB	2.35	0.61
9:b:660:ALA:HB3	22:b:804:CLA:HBB2	1.83	0.61
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.61
22:4:317:CLA:H2A	26:4:318:DGD:C6E	2.30	0.61
8:a:121:ASN:HB3	8:a:129:GLN:HB3	1.82	0.61
8:a:589:LEU:HD21	22:a:831:CLA:HBC1	1.81	0.61
10:d:86:ARG:HB2	10:d:96:LEU:HD11	1.82	0.61
4:7:136:VAL:HG11	22:b:820:CLA:HBA1	1.81	0.61
9:b:561:CYS:SG	9:b:563:GLY:N	2.71	0.61
22:b:830:CLA:HAB	22:b:837:CLA:HBB2	1.82	0.61
6:2:44:PRO:HG3	6:2:58:ASP:HB3	1.83	0.61
4:7:144:GLU:HB2	9:b:294:LEU:HD11	1.82	0.61
9:b:15:ASP:HB3	9:b:20:ARG:HB2	1.82	0.61
23:5:316:SQD:H2	20:4:301:XAT:H373	1.82	0.60
6:2:76:THR:O	6:2:82:ARG:NH1	2.33	0.60
22:b:823:CLA:HAB	22:b:830:CLA:HMD2	1.83	0.60
22:b:831:CLA:HBC3	29:f:804:BCR:H362	1.83	0.60
24:1:304:A1L1F:C2	22:a:844:CLA:H11	2.31	0.60
22:8:305:CLA:HAA2	26:8:315:DGD:HE5	1.82	0.60
8:a:429:ALA:O	8:a:433:HIS:ND1	2.31	0.60
22:a:833:CLA:HBC2	22:a:840:CLA:HMC2	1.83	0.60
1:5:225:ILE:HG22	22:5:314:CLA:HAB	1.82	0.60
20:2:303:XAT:H363	22:2:308:CLA:H2	1.84	0.60
8:a:53:ASP:OD2	8:a:343:HIS:NE2	2.35	0.60
9:b:412:ARG:NH2	22:b:830:CLA:O1D	2.35	0.60
5:3:92:HIS:HB3	5:3:197:MET:SD	2.42	0.60
5:3:199:ALA:O	5:3:203:MET:HG3	2.01	0.60
8:a:167:LEU:HD11	22:a:810:CLA:H193	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:302:XAT:H162	22:5:307:CLA:H2	1.82	0.59
7:1:186:ILE:HG13	7:1:187:THR:HG23	1.83	0.59
5:3:83:TYR:OH	5:3:163:ARG:NH1	2.35	0.59
21:1:301:A1L1G:C18	22:1:306:CLA:HAC2	2.32	0.59
4:4:185:PHE:CZ	20:4:303:XAT:H30	2.37	0.59
3:8:185:MET:HE2	22:8:308:CLA:HBB2	1.83	0.59
16:l:38:ARG:O	16:l:46:ARG:NH2	2.35	0.58
2:9:185:PRO:HA	22:9:313:CLA:HBA2	1.85	0.58
4:7:88:THR:HG21	20:7:304:XAT:H12	1.85	0.58
22:a:820:CLA:H92	22:a:830:CLA:H91	1.84	0.58
8:a:107:SER:HB2	8:a:124:VAL:HG11	1.85	0.58
22:a:804:CLA:ND	15:j:12:PRO:HG3	2.17	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
10:d:97:HIS:HB3	10:d:98:PRO:HD3	1.86	0.58
22:a:818:CLA:C1D	27:a:853:LMG:H291	2.34	0.58
13:h:121:TRP:CD1	22:h:203:CLA:HAA1	2.39	0.58
20:8:302:XAT:H32	22:8:307:CLA:HAB	1.85	0.58
22:b:804:CLA:CGA	22:b:804:CLA:H3A	2.34	0.58
8:a:292:LEU:HD21	22:a:818:CLA:CAB	2.34	0.57
8:a:507:VAL:HG22	8:a:517:MET:HG3	1.85	0.57
1:5:155:VAL:HG21	22:5:309:CLA:HAA2	1.86	0.57
4:4:170:MET:HE1	22:4:313:CLA:H43	1.84	0.57
22:a:802:CLA:CGA	22:a:802:CLA:H3A	2.35	0.57
20:5:301:XAT:H14	22:5:309:CLA:H12	1.86	0.57
9:b:178:SER:HB3	9:b:286:GLY:HA3	1.86	0.57
29:f:801:BCR:HC32	22:j:102:CLA:H43	1.86	0.57
5:3:86:ARG:NH1	5:3:89:GLU:OE1	2.38	0.57
8:a:7:SER:H	8:a:12:PHE:HE2	1.53	0.57
9:b:29:HIS:ND1	22:b:807:CLA:O1A	2.28	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
8:a:598:ILE:HG13	22:a:801:CLA:H192	1.86	0.57
2:9:107:LEU:HD11	2:9:140:ILE:HD11	1.87	0.57
2:9:222:ASP:HB2	2:9:230:LEU:HD13	1.86	0.57
3:8:60:PHE:HE1	22:8:305:CLA:HBC3	1.70	0.57
4:7:185:PHE:CD2	20:7:303:XAT:H12	2.39	0.57
22:b:840:CLA:HBB2	22:h:203:CLA:C2	2.34	0.57
29:b:842:BCR:H23C	29:h:202:BCR:H323	1.86	0.57
1:5:112:LEU:HD22	22:5:307:CLA:H12	1.86	0.57
22:3:312:CLA:H42	29:a:848:BCR:H272	1.85	0.57
8:a:517:MET:HE1	8:a:623:HIS:NE2	2.19	0.57
22:a:826:CLA:HBA1	22:a:830:CLA:H193	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:69:ALA:HB2	9:b:133:LEU:HB2	1.86	0.56
8:a:324:GLY:HA3	25:a:846:LHG:HC32	1.87	0.56
20:9:303:XAT:H363	3:8:135:LEU:HD12	1.86	0.56
5:3:48:LEU:HD13	5:3:51:LEU:HD12	1.87	0.56
20:2:303:XAT:C36	22:2:308:CLA:H2	2.35	0.56
27:a:853:LMG:O8	27:a:853:LMG:H112	2.05	0.56
9:b:582:MET:HG3	9:b:712:LEU:HD21	1.87	0.56
9:b:693:VAL:HG11	22:b:801:CLA:HAB	1.87	0.56
22:b:805:CLA:H18	14:i:14:VAL:HG22	1.86	0.56
4:4:140:SER:OG	15:j:1:MET:SD	2.57	0.56
9:b:39:GLU:HB3	9:b:163:LEU:HD11	1.87	0.56
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.56
8:a:441:LEU:HB3	8:a:534:PHE:HB2	1.88	0.56
22:a:818:CLA:CHD	27:a:853:LMG:H291	2.36	0.56
22:a:841:CLA:H92	29:f:801:BCR:H15C	1.88	0.56
9:b:74:PHE:O	9:b:78:ILE:HG12	2.04	0.56
14:i:26:LEU:HD13	29:l:205:BCR:HC8	1.86	0.56
4:4:136:VAL:HG22	22:4:312:CLA:HMA1	1.87	0.56
8:a:114:ILE:HG13	8:a:115:VAL:HG13	1.87	0.56
10:d:105:GLU:HG2	19:c:19:ARG:HB3	1.88	0.56
16:l:54:HIS:HA	16:l:57:PHE:CE2	2.41	0.56
27:a:853:LMG:H112	27:a:853:LMG:C9	2.35	0.56
5:3:182:PHE:HZ	22:3:313:CLA:HED3	1.70	0.56
8:a:651:VAL:HG22	8:a:739:ALA:HB3	1.87	0.56
1:5:111:TRP:NE1	22:5:308:CLA:O1A	2.32	0.55
22:a:841:CLA:H72	29:f:801:BCR:H17C	1.88	0.55
22:b:821:CLA:HHB	22:b:822:CLA:H2	1.88	0.55
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.55
7:1:88:ILE:HG22	7:1:92:PHE:HE1	1.71	0.55
22:a:825:CLA:H12	29:a:849:BCR:H14C	1.88	0.55
8:a:734:TRP:NE1	22:a:829:CLA:O1A	2.36	0.55
9:b:521:VAL:HG21	9:b:595:TYR:HB2	1.89	0.55
8:a:651:VAL:HG21	8:a:736:PHE:HA	1.87	0.55
2:9:85:GLY:O	2:9:89:MET:HG3	2.07	0.55
2:9:93:ILE:HG13	20:9:304:XAT:H8	1.89	0.55
8:a:213:ILE:HG23	8:a:233:PRO:HB3	1.87	0.55
2:9:153:PHE:HA	16:l:151:PHE:HE2	1.71	0.55
4:4:185:PHE:CE2	20:4:303:XAT:H30	2.42	0.55
8:a:686:TYR:OH	22:a:802:CLA:OBD	2.22	0.55
22:b:806:CLA:HBA1	22:b:813:CLA:HBA1	1.87	0.55
6:2:35:SER:OG	6:2:37:ALA:O	2.22	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:93:ASP:OD1	9:b:95:HIS:ND1	2.33	0.55
8:a:197:GLY:HA3	22:a:814:CLA:HBB1	1.89	0.54
8:a:667:LEU:HD11	9:b:619:MET:HB2	1.89	0.54
15:j:14:LEU:HD21	27:j:105:LMG:H141	1.89	0.54
16:l:92:LEU:HB3	29:l:205:BCR:H401	1.88	0.54
2:9:117:TRP:O	2:9:120:TRP:CD1	2.60	0.54
7:1:115:ILE:O	7:1:119:GLN:NE2	2.40	0.54
22:a:822:CLA:HBC3	22:a:828:CLA:H172	1.88	0.54
22:a:829:CLA:H101	29:j:104:BCR:H341	1.89	0.54
22:a:854:CLA:H112	15:j:14:LEU:HD22	1.88	0.54
19:c:15:THR:HG22	19:c:28:MET:HG3	1.89	0.54
8:a:210:GLN:HA	8:a:214:ALA:HB3	1.89	0.54
9:b:317:HIS:HB3	9:b:320:LEU:HD12	1.89	0.54
3:8:75:VAL:HG23	22:8:307:CLA:HMA2	1.89	0.54
24:8:304:A1L1F:C2	17:m:23:ARG:HD3	2.38	0.54
8:a:290:HIS:HB2	22:a:819:CLA:C1B	2.37	0.54
8:a:660:SER:HB2	9:b:447:ALA:HB1	1.88	0.54
8:a:573:ARG:HG3	19:c:78:GLY:HA3	1.90	0.54
10:d:63:ARG:NH2	10:d:65:GLU:OE1	2.41	0.54
2:9:149:ALA:O	2:9:153:PHE:HD1	1.89	0.54
8:a:219:LYS:HD3	8:a:246:LEU:HB3	1.90	0.54
7:1:61:ALA:HB1	7:1:65:THR:HB	1.90	0.54
9:b:355:PRO:HG3	22:b:818:CLA:HBA1	1.89	0.54
22:a:820:CLA:HAB	22:a:820:CLA:H8	1.90	0.54
11:e:32:VAL:HG11	19:c:35:LYS:HD3	1.89	0.54
21:5:303:A1L1G:C41	22:5:312:CLA:HMC1	2.37	0.54
8:a:388:VAL:HG12	8:a:596:ILE:HG23	1.89	0.54
9:b:140:LEU:HG	29:b:844:BCR:H382	1.90	0.54
9:b:443:ASP:OD1	9:b:617:TYR:HB2	2.08	0.54
2:9:162:LYS:NZ	22:9:312:CLA:O1A	2.40	0.53
2:9:179:LEU:HD23	22:9:308:CLA:HMD3	1.90	0.53
9:b:22:TRP:CG	9:b:706:GLN:HE22	2.26	0.53
22:9:312:CLA:HBA1	22:9:312:CLA:HBD	1.89	0.53
3:8:36:ALA:N	3:8:44:LEU:O	2.42	0.53
4:7:46:PRO:HG2	4:7:49:LEU:HD12	1.90	0.53
8:a:702:LYS:HB3	12:f:130:ARG:HD3	1.89	0.53
3:8:175:LYS:HB3	22:8:306:CLA:HMD2	1.90	0.53
8:a:591:TRP:HE1	22:b:804:CLA:C1D	2.21	0.53
9:b:5:PHE:HB2	14:i:30:ILE:HA	1.89	0.53
22:a:835:CLA:O2D	22:a:835:CLA:H2A	2.09	0.53
9:b:718:GLY:O	9:b:722:THR:HG22	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:823:CLA:HBB2	22:b:840:CLA:H52	1.90	0.53
22:a:825:CLA:HMA3	22:a:844:CLA:HAB	1.90	0.53
9:b:633:LEU:HD22	9:b:726:PHE:HA	1.89	0.53
22:b:816:CLA:H91	13:h:105:LEU:HG	1.91	0.53
2:9:107:LEU:HG	2:9:136:ALA:HB1	1.91	0.53
22:8:305:CLA:HBC2	4:7:134:ILE:HG13	1.91	0.53
22:a:809:CLA:CHC	22:a:810:CLA:HMD2	2.39	0.53
4:4:121:LEU:HD23	4:4:124:ILE:HD12	1.90	0.53
22:a:831:CLA:H42	25:a:845:LHG:H251	1.90	0.53
9:b:661:THR:O	9:b:664:MET:HB3	2.08	0.53
9:b:709:LEU:HD11	26:b:848:DGD:HB41	1.90	0.53
22:b:829:CLA:H42	26:b:848:DGD:HB42	1.91	0.53
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.53
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.91	0.53
4:4:83:ILE:HD11	20:4:302:XAT:H362	1.90	0.53
18:g:51:UNK:O	18:g:53:UNK:N	2.42	0.53
2:9:137:ARG:NH1	22:9:318:CLA:OBD	2.41	0.52
22:4:317:CLA:O2D	26:4:318:DGD:HE61	2.09	0.52
9:b:419:ALA:O	9:b:423:HIS:ND1	2.39	0.52
22:b:801:CLA:H101	22:b:801:CLA:HBB1	1.92	0.52
4:7:128:THR:HG23	21:7:302:A1L1G:C17	2.39	0.52
7:1:72:SER:O	7:1:76:HIS:ND1	2.28	0.52
9:b:50:HIS:ND1	22:b:813:CLA:OBD	2.38	0.52
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.52
3:8:177:GLY:O	3:8:181:MET:HG3	2.09	0.52
8:a:396:VAL:HG11	8:a:589:LEU:HG	1.91	0.52
22:b:836:CLA:HBC3	29:f:804:BCR:H401	1.91	0.52
12:f:143:ILE:HG13	12:f:144:ILE:HG13	1.92	0.52
2:9:192:GLU:HB2	22:9:312:CLA:C1B	2.40	0.52
4:7:200:PRO:O	20:7:304:XAT:O3	2.26	0.52
22:a:810:CLA:HAB	22:j:102:CLA:HMD2	1.91	0.52
22:a:827:CLA:H93	22:a:840:CLA:H52	1.92	0.52
20:5:302:XAT:C16	22:5:307:CLA:H2	2.39	0.52
3:8:70:ALA:H	22:b:811:CLA:HED1	1.75	0.52
5:3:87:GLU:OE2	5:3:163:ARG:NH2	2.31	0.52
7:1:85:LEU:HB3	22:1:308:CLA:HMC2	1.92	0.52
9:b:179:GLY:O	9:b:183:VAL:HB	2.10	0.52
10:d:95:LEU:HD22	18:g:75:UNK:HA	1.91	0.52
12:f:85:LEU:HD13	12:f:93:PRO:HB3	1.92	0.52
5:3:93:CYS:HB3	5:3:193:GLY:HA3	1.92	0.52
9:b:189:THR:HG21	9:b:276:LEU:HB2	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:662:GLY:O	9:b:666:LEU:HG	2.10	0.52
8:a:577:CYS:O	9:b:671:GLY:HA3	2.11	0.51
4:4:193:ALA:O	26:4:318:DGD:O6E	2.28	0.51
7:1:77:GLY:O	7:1:81:MET:HG3	2.09	0.51
19:c:58:CYS:SG	19:c:63:LEU:HA	2.51	0.51
19:c:11:CYS:SG	19:c:39:ILE:HG13	2.50	0.51
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
22:b:836:CLA:HBC3	29:f:804:BCR:H292	1.91	0.51
24:h:204:A1L1F:O46	22:h:205:CLA:H52	2.11	0.51
8:a:422:ARG:O	8:a:426:HIS:ND1	2.41	0.51
22:b:811:CLA:H72	22:b:812:CLA:HBC3	1.93	0.51
2:9:218:LEU:HG	22:9:314:CLA:HMA2	1.92	0.51
4:4:81:CYS:HB3	4:4:178:GLY:HA3	1.91	0.51
20:7:301:XAT:H10	22:7:315:CLA:HMD1	1.93	0.51
9:b:274:HIS:HB2	22:b:817:CLA:C1B	2.41	0.51
22:h:203:CLA:HBA1	22:h:203:CLA:HBD	1.93	0.51
6:2:121:ALA:O	6:2:122:LYS:HG2	2.10	0.51
4:7:121:LEU:HD13	22:7:316:CLA:HBC3	1.92	0.51
22:a:834:CLA:H151	28:b:841:PQN:H202	1.91	0.51
9:b:434:HIS:CD2	29:b:849:BCR:H333	2.46	0.51
22:b:807:CLA:H52	26:b:848:DGD:HB72	1.92	0.51
12:f:160:TRP:CD1	12:f:161:PRO:HD3	2.46	0.51
5:3:79:GLY:O	5:3:158:ARG:NH1	2.43	0.51
10:d:33:ILE:HG22	10:d:58:VAL:HG22	1.92	0.51
8:a:431:ILE:HG13	8:a:549:TYR:HE1	1.74	0.51
9:b:722:THR:HG23	22:b:803:CLA:O1D	2.11	0.51
24:1:304:A1L1F:C56	25:a:846:LHG:H241	2.41	0.50
22:a:818:CLA:HHC	22:a:818:CLA:HBB1	1.93	0.50
27:a:853:LMG:H131	27:a:853:LMG:H292	1.94	0.50
9:b:273:HIS:ND1	22:b:817:CLA:HAB	2.25	0.50
9:b:342:ALA:O	9:b:346:THR:HG23	2.11	0.50
20:4:303:XAT:C16	22:4:308:CLA:H2	2.41	0.50
6:2:77:LYS:O	6:2:79:ASP:N	2.43	0.50
8:a:440:PHE:HE2	22:a:839:CLA:HAB	1.76	0.50
9:b:305:ALA:HB2	13:h:46:THR:HB	1.94	0.50
9:b:602:THR:HG21	9:b:611:PHE:HB2	1.93	0.50
19:c:17:CYS:SG	19:c:18:VAL:N	2.85	0.50
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.50
20:5:301:XAT:H193	22:5:310:CLA:HBA2	1.94	0.50
22:5:312:CLA:CGA	22:5:312:CLA:H3A	2.41	0.50
27:a:853:LMG:HC92	27:a:853:LMG:C11	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:50:LEU:HD11	3:8:61:ASP:HB2	1.93	0.50
8:a:460:ARG:NH2	22:a:835:CLA:O1D	2.44	0.50
9:b:478:LEU:HG	9:b:479:LEU:HG	1.93	0.50
19:c:13:GLY:O	19:c:38:GLN:NE2	2.44	0.50
1:5:130:PHE:HE1	20:5:302:XAT:O24	1.94	0.50
4:7:45:ARG:NH1	4:7:49:LEU:O	2.42	0.50
4:7:54:VAL:HG21	4:7:74:GLN:HE21	1.77	0.50
8:a:425:ARG:NH2	10:d:15:GLY:O	2.44	0.50
22:b:832:CLA:HBB2	29:f:801:BCR:HC41	1.94	0.50
2:9:117:TRP:O	2:9:120:TRP:NE1	2.45	0.50
22:3:308:CLA:HED2	22:3:308:CLA:H2A	1.94	0.50
2:9:32:THR:H	2:9:33:PRO:HD2	1.77	0.49
21:9:301:A1L1G:C44	22:9:315:CLA:HBC3	2.41	0.49
9:b:26:ALA:HA	22:b:829:CLA:H43	1.93	0.49
9:b:492:SER:HA	9:b:496:LEU:HD12	1.94	0.49
9:b:562:ASP:OD2	9:b:566:ARG:NH2	2.38	0.49
8:a:565:ARG:HG2	8:a:715:THR:HG21	1.93	0.49
29:b:849:BCR:H23C	15:j:33:TYR:CD2	2.47	0.49
8:a:292:LEU:HD12	22:a:816:CLA:HMC3	1.95	0.49
22:a:803:CLA:H2	9:b:657:LEU:HD22	1.95	0.49
9:b:3:TYR:HB2	14:i:33:GLU:HA	1.95	0.49
9:b:25:ILE:HG12	29:l:205:BCR:H312	1.94	0.49
6:2:183:ASP:O	6:2:186:LYS:N	2.44	0.49
8:a:615:VAL:HG22	8:a:621:VAL:HG22	1.95	0.49
16:l:106:VAL:H	16:l:140:VAL:HG23	1.77	0.49
18:g:46:UNK:O	18:g:50:UNK:N	2.45	0.49
2:9:191:ALA:HB1	22:9:313:CLA:HAA1	1.93	0.49
7:1:112:VAL:HB	7:1:117:TRP:NE1	2.27	0.49
8:a:423:VAL:HA	8:a:426:HIS:CE1	2.47	0.49
4:7:42:PHE:HE2	22:7:306:CLA:HAB	1.77	0.49
22:a:818:CLA:CHD	22:a:819:CLA:HBB2	2.43	0.49
19:c:17:CYS:HB3	30:c:102:SF4:S4	2.52	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
4:7:185:PHE:O	4:7:189:VAL:HG22	2.13	0.49
9:b:443:ASP:OD1	9:b:618:ILE:N	2.46	0.49
3:8:60:PHE:CE1	22:8:305:CLA:HBC3	2.47	0.49
4:4:159:ASN:C	4:4:161:ALA:H	2.20	0.49
5:3:203:MET:HE2	20:3:305:XAT:O4	2.13	0.49
4:7:91:TRP:CE3	20:7:303:XAT:H22	2.48	0.49
4:7:97:VAL:O	4:7:97:VAL:HG13	2.13	0.49
8:a:637:ASN:HB2	9:b:653:LEU:HD11	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:802:CLA:H41	9:b:436:LEU:HD22	1.95	0.49
2:9:88:ALA:HA	20:9:303:XAT:H8	1.95	0.49
22:a:818:CLA:O1A	27:a:853:LMG:O10	2.30	0.49
9:b:65:LEU:HD11	29:b:844:BCR:H281	1.95	0.48
9:b:181:PHE:HE2	22:b:819:CLA:HAB	1.78	0.48
22:b:823:CLA:H2A	22:b:823:CLA:HED3	1.95	0.48
22:b:824:CLA:H141	22:b:824:CLA:H193	1.95	0.48
14:i:26:LEU:HD22	29:l:205:BCR:H323	1.94	0.48
16:l:43:PRO:HD3	16:l:136:GLU:CD	2.38	0.48
16:l:109:ASN:OD1	16:l:110:ALA:N	2.35	0.48
3:8:73:LYS:HD3	3:8:145:ASP:HA	1.95	0.48
24:8:304:A1L1F:C36	22:8:311:CLA:H51	2.43	0.48
22:4:309:CLA:HAC1	22:4:316:CLA:HAB	1.95	0.48
8:a:674:ALA:HB3	22:a:802:CLA:HBB2	1.94	0.48
9:b:166:PHE:O	9:b:172:ARG:NH2	2.46	0.48
9:b:271:MET:O	9:b:275:HIS:ND1	2.47	0.48
9:b:412:ARG:HH21	22:b:830:CLA:CGD	2.27	0.48
8:a:712:LEU:N	28:a:843:PQN:O4	2.45	0.48
9:b:526:ALA:O	9:b:530:HIS:ND1	2.37	0.48
3:8:172:LYS:O	3:8:176:ASN:ND2	2.39	0.48
22:a:832:CLA:HAB	22:a:840:CLA:HBB2	1.96	0.48
22:b:821:CLA:CHB	22:b:822:CLA:H2	2.44	0.48
13:h:89:ASN:O	13:h:91:PHE:N	2.46	0.48
22:9:311:CLA:H2A	22:9:311:CLA:O2D	2.14	0.48
5:3:81:ASP:N	5:3:81:ASP:OD1	2.46	0.48
4:7:81:CYS:O	4:7:85:MET:HG3	2.13	0.48
8:a:554:ARG:HB2	9:b:678:GLU:OE1	2.13	0.48
9:b:407:LYS:HB3	9:b:411:ALA:HB3	1.95	0.48
13:h:72:PRO:HG3	24:h:204:A1L1F:C56	2.43	0.48
29:b:849:BCR:H23C	15:j:33:TYR:HD2	1.79	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.48
6:2:107:LEU:HB3	22:2:310:CLA:HMC2	1.94	0.48
22:2:316:CLA:C2C	27:2:317:LMG:H111	2.44	0.48
4:7:185:PHE:HE1	20:7:303:XAT:H162	1.79	0.48
22:a:820:CLA:H203	22:a:828:CLA:H3A	1.96	0.48
22:a:839:CLA:H62	22:a:839:CLA:H41	1.54	0.48
9:b:266:LEU:HD22	22:b:817:CLA:HBA1	1.95	0.48
9:b:597:HIS:CE1	9:b:601:LEU:HD11	2.49	0.48
15:j:2:LYS:O	27:j:105:LMG:HC61	2.13	0.48
15:j:5:LEU:HB3	27:j:105:LMG:HC72	1.96	0.48
1:5:171:GLU:HG3	22:5:311:CLA:NB	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:92:ARG:NH1	6:2:95:GLU:OE1	2.47	0.48
9:b:277:ALA:HA	22:b:816:CLA:HMC2	1.96	0.48
22:b:839:CLA:H13	29:i:101:BCR:H19C	1.95	0.48
9:b:595:TYR:CZ	22:b:835:CLA:HBC3	2.49	0.48
20:2:303:XAT:H11	20:2:303:XAT:H191	1.66	0.47
7:1:42:MET:HE1	7:1:66:LEU:HD22	1.95	0.47
7:1:88:ILE:HG22	7:1:92:PHE:CE1	2.49	0.47
8:a:712:LEU:HD21	28:a:843:PQN:H151	1.95	0.47
22:a:825:CLA:H71	22:a:840:CLA:H62	1.96	0.47
9:b:8:PHE:HB2	9:b:34:HIS:CG	2.49	0.47
9:b:432:GLY:HA2	9:b:527:LEU:HD22	1.96	0.47
9:b:670:ARG:C	9:b:672:TYR:H	2.22	0.47
22:b:838:CLA:HAB	28:b:841:PQN:H172	1.96	0.47
10:d:95:LEU:HD11	10:d:98:PRO:HD2	1.95	0.47
14:i:26:LEU:HB3	29:l:205:BCR:H323	1.96	0.47
5:3:145:ILE:O	5:3:149:ILE:HG12	2.13	0.47
4:7:124:ILE:HA	22:7:311:CLA:HBC3	1.96	0.47
20:7:303:XAT:H191	20:7:303:XAT:H11	1.70	0.47
8:a:514:ILE:HD11	8:a:621:VAL:HG13	1.96	0.47
3:8:36:ALA:HB3	3:8:45:LYS:HZ2	1.78	0.47
7:1:84:VAL:O	7:1:88:ILE:HG12	2.14	0.47
8:a:38:THR:HB	8:a:710:ARG:HG3	1.97	0.47
8:a:114:ILE:HG23	8:a:115:VAL:HG22	1.95	0.47
20:5:304:XAT:C10	22:5:315:CLA:HBC3	2.43	0.47
2:9:91:GLY:HA3	20:9:303:XAT:H173	1.94	0.47
25:9:307:LHG:H341	16:l:91:ILE:HD11	1.96	0.47
20:3:304:XAT:H15	20:3:304:XAT:H201	1.78	0.47
8:a:127:ASN:HD21	12:f:60:THR:HG21	1.79	0.47
8:a:287:THR:HG23	22:a:820:CLA:HMA3	1.96	0.47
8:a:375:ILE:HG21	8:a:510:VAL:HB	1.96	0.47
22:9:316:CLA:H202	16:l:90:LEU:HD22	1.96	0.47
4:4:184:ALA:HA	22:4:315:CLA:HBB1	1.96	0.47
5:3:78:VAL:HG12	5:3:78:VAL:O	2.13	0.47
22:1:306:CLA:H93	22:1:306:CLA:H61	1.70	0.47
8:a:354:GLY:HA2	8:a:391:GLY:HA2	1.97	0.47
9:b:385:PHE:HB3	9:b:536:LEU:HB3	1.97	0.47
22:b:839:CLA:H92	22:b:839:CLA:H61	1.73	0.47
6:2:65:ILE:HG22	6:2:67:PHE:H	1.80	0.47
8:a:290:HIS:HB2	22:a:819:CLA:CHB	2.44	0.47
9:b:176:HIS:O	9:b:180:LEU:HB3	2.14	0.47
2:9:201:LEU:HD21	20:9:304:XAT:H371	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:316:CLA:H71	16:l:83:LEU:HG	1.97	0.47
22:8:311:CLA:HBB1	22:8:311:CLA:HMB3	1.97	0.47
22:3:308:CLA:H2A	22:3:308:CLA:CED	2.44	0.47
20:7:304:XAT:H191	22:7:314:CLA:HAB	1.97	0.47
8:a:476:PHE:HB3	22:a:838:CLA:H11	1.96	0.47
22:a:841:CLA:H61	22:b:832:CLA:H42	1.95	0.47
29:a:848:BCR:H15C	29:a:848:BCR:H351	1.78	0.47
9:b:127:MET:HE1	29:b:844:BCR:H282	1.97	0.47
9:b:143:LEU:HD23	9:b:146:LEU:HD12	1.97	0.47
9:b:538:LYS:O	9:b:542:ASP:HB2	2.15	0.47
9:b:586:LEU:HD21	9:b:716:THR:HG23	1.96	0.47
22:b:812:CLA:H41	22:b:812:CLA:H62	1.62	0.47
22:b:822:CLA:H43	13:h:115:GLY:C	2.40	0.47
10:d:20:TRP:CZ2	16:l:14:VAL:HG12	2.50	0.47
13:h:114:TRP:HA	13:h:117:HIS:CD2	2.49	0.47
22:a:834:CLA:CAD	29:l:201:BCR:H10C	2.45	0.47
22:b:807:CLA:H192	22:b:807:CLA:H161	1.72	0.47
22:b:812:CLA:H3A	22:b:812:CLA:HBA2	1.61	0.47
22:b:830:CLA:HAB	22:b:837:CLA:CBB	2.44	0.47
2:9:49:MET:HA	2:9:52:LYS:HD3	1.97	0.47
22:b:822:CLA:H42	13:h:62:LEU:HD11	1.97	0.47
22:b:837:CLA:H101	22:b:837:CLA:H13	1.78	0.47
11:e:51:ASN:CG	19:c:61:ASP:HB2	2.39	0.47
22:j:102:CLA:NB	29:j:104:BCR:H281	2.30	0.47
22:4:317:CLA:CGD	26:4:318:DGD:HE61	2.45	0.47
20:2:303:XAT:H15	20:2:303:XAT:H201	1.79	0.47
8:a:677:LEU:HB2	22:a:802:CLA:HMC2	1.97	0.47
2:9:187:LEU:HA	22:9:312:CLA:HMB1	1.96	0.46
6:2:191:GLN:O	6:2:195:ILE:HD12	2.15	0.46
27:2:317:LMG:H321	27:2:317:LMG:H292	1.35	0.46
22:b:838:CLA:H162	22:b:838:CLA:H192	1.73	0.46
16:l:168:TYR:O	16:l:172:LEU:HB2	2.15	0.46
4:4:185:PHE:CZ	20:4:303:XAT:H28	2.50	0.46
20:4:301:XAT:H15	20:4:301:XAT:H201	1.80	0.46
8:a:114:ILE:O	8:a:117:GLN:HG2	2.16	0.46
8:a:144:GLU:HG2	8:a:206:TRP:HH2	1.80	0.46
8:a:400:ALA:HB2	8:a:585:VAL:HG11	1.96	0.46
22:a:801:CLA:H61	22:a:803:CLA:O1D	2.15	0.46
22:a:854:CLA:H143	27:j:105:LMG:H142	1.98	0.46
9:b:297:HIS:HB3	9:b:302:ILE:HD11	1.97	0.46
9:b:452:GLU:OE2	12:f:76:ARG:NE	2.42	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:28:LEU:O	14:i:32:LYS:HG3	2.15	0.46
22:4:309:CLA:HED2	22:4:309:CLA:HBD	1.83	0.46
20:3:304:XAT:H31	20:3:304:XAT:H391	1.78	0.46
4:7:37:SER:HB2	4:7:45:ARG:HA	1.97	0.46
7:1:40:ASP:HB2	7:1:42:MET:HG3	1.98	0.46
7:1:73:GLU:HB2	22:1:306:CLA:C1B	2.45	0.46
22:1:306:CLA:H202	22:1:306:CLA:H162	1.69	0.46
8:a:68:SER:OG	8:a:174:TYR:HB2	2.14	0.46
22:b:823:CLA:HBA1	29:h:201:BCR:H16C	1.98	0.46
3:8:58:PHE:HZ	3:8:175:LYS:HZ1	1.62	0.46
6:2:118:LEU:N	22:2:310:CLA:OBD	2.47	0.46
22:h:205:CLA:HED3	22:h:205:CLA:H2A	1.97	0.46
22:j:102:CLA:H41	22:j:102:CLA:H61	1.64	0.46
4:7:120:ALA:O	4:7:124:ILE:HG13	2.16	0.46
22:a:807:CLA:H92	22:a:807:CLA:H61	1.69	0.46
22:a:829:CLA:HBB1	22:a:829:CLA:HMB1	1.97	0.46
22:b:822:CLA:HHC	22:b:840:CLA:HED1	1.98	0.46
22:9:314:CLA:CED	22:9:314:CLA:H2A	2.45	0.46
3:8:166:MET:O	3:8:170:GLU:HG3	2.16	0.46
20:7:303:XAT:H32	22:7:308:CLA:HAB	1.96	0.46
22:a:832:CLA:HBA1	22:a:832:CLA:H3A	1.80	0.46
9:b:339:LEU:O	9:b:343:THR:HG22	2.16	0.46
9:b:372:HIS:HB2	22:b:827:CLA:C1B	2.45	0.46
29:b:844:BCR:HC8	29:b:844:BCR:H311	1.97	0.46
1:5:96:VAL:HG12	22:5:307:CLA:OBD	2.15	0.46
21:9:306:A1L1G:C31	22:9:310:CLA:HBD	2.46	0.46
3:8:82:HIS:HB3	3:8:181:MET:SD	2.56	0.46
3:8:141:THR:HA	3:8:147:PRO:HB3	1.97	0.46
20:8:303:XAT:H34	22:8:313:CLA:HBB1	1.96	0.46
8:a:689:GLU:OE2	9:b:546:SER:OG	2.30	0.46
9:b:280:VAL:HG21	22:b:816:CLA:HAB	1.98	0.46
9:b:687:THR:HG23	9:b:690:ALA:HB3	1.97	0.46
22:b:817:CLA:H41	22:b:833:CLA:HAA2	1.98	0.46
3:8:171:VAL:HG13	3:8:175:LYS:HE3	1.97	0.46
4:4:37:SER:HB3	4:4:45:ARG:HA	1.98	0.46
22:a:818:CLA:NC	27:a:853:LMG:H302	2.31	0.46
9:b:392:PHE:CE2	29:b:845:BCR:HC42	2.51	0.46
12:f:143:ILE:O	15:j:11:ALA:N	2.48	0.46
2:9:80:ALA:O	2:9:84:ASN:ND2	2.49	0.46
22:9:316:CLA:HBC3	22:a:803:CLA:H151	1.97	0.46
3:8:110:ASN:HB3	3:8:113:LYS:HB2	1.96	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:806:CLA:H72	29:a:848:BCR:HC8	1.98	0.46
10:d:83:LYS:HG2	10:d:98:PRO:HG2	1.97	0.46
1:5:116:GLU:HB2	22:5:307:CLA:C1B	2.46	0.45
22:9:318:CLA:H91	22:9:318:CLA:H112	1.69	0.45
20:4:302:XAT:H30	22:4:310:CLA:H151	1.98	0.45
22:2:310:CLA:H141	22:2:310:CLA:H162	1.74	0.45
22:1:306:CLA:H91	22:1:306:CLA:H112	1.69	0.45
8:a:312:GLY:HA2	22:a:823:CLA:HMD2	1.99	0.45
8:a:665:ILE:HG23	22:a:809:CLA:H171	1.98	0.45
22:b:808:CLA:H93	22:b:808:CLA:H61	1.71	0.45
12:f:119:GLY:HA3	12:f:160:TRP:CE2	2.51	0.45
27:j:105:LMG:H292	27:j:105:LMG:H111	1.98	0.45
16:l:38:ARG:NH1	16:l:49:GLU:OE1	2.40	0.45
22:9:316:CLA:HBA2	16:l:67:PRO:HG3	1.97	0.45
6:2:127:ASN:OD1	6:2:130:GLN:N	2.46	0.45
4:7:160:PHE:HE2	20:7:304:XAT:H373	1.81	0.45
20:7:304:XAT:H32	22:7:313:CLA:HAB	1.98	0.45
22:a:801:CLA:CED	22:a:801:CLA:HAA2	2.46	0.45
22:a:827:CLA:H13	22:a:827:CLA:H172	1.77	0.45
27:a:853:LMG:H112	27:a:853:LMG:HC92	1.98	0.45
9:b:433:PHE:HZ	29:f:801:BCR:H372	1.80	0.45
20:7:305:XAT:H201	20:7:305:XAT:H15	1.69	0.45
8:a:25:PRO:HB2	8:a:41:TRP:HH2	1.81	0.45
8:a:342:TRP:CD1	22:a:826:CLA:H192	2.51	0.45
29:a:848:BCR:H11C	29:a:848:BCR:H341	1.86	0.45
9:b:228:TRP:HZ3	29:h:202:BCR:H363	1.81	0.45
9:b:268:LEU:HD23	9:b:271:MET:HE3	1.98	0.45
22:b:802:CLA:H162	22:b:802:CLA:H122	1.61	0.45
22:b:811:CLA:H51	22:b:812:CLA:H43	1.97	0.45
22:b:832:CLA:H18	29:f:804:BCR:H17C	1.98	0.45
22:b:838:CLA:H12	29:l:205:BCR:H15C	1.98	0.45
14:i:14:VAL:O	14:i:19:PRO:HD2	2.17	0.45
20:1:303:XAT:H183	22:1:308:CLA:C2B	2.47	0.45
8:a:502:ALA:HB2	8:a:516:MET:HE2	1.97	0.45
19:c:3:HIS:HB2	19:c:48:CYS:SG	2.57	0.45
3:8:93:TRP:CE2	3:8:111:PRO:HG2	2.51	0.45
4:4:193:ALA:HB1	26:4:318:DGD:O5E	2.16	0.45
20:a:852:XAT:H35	20:a:852:XAT:H401	1.85	0.45
22:b:813:CLA:H143	22:b:824:CLA:H51	1.99	0.45
22:b:825:CLA:HAA2	22:b:826:CLA:OBD	2.16	0.45
29:j:104:BCR:H15C	29:j:104:BCR:H351	1.78	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:124:MET:HE3	22:5:312:CLA:HMC2	1.98	0.45
1:5:164:PHE:HE1	22:f:802:CLA:H121	1.81	0.45
2:9:126:THR:OG1	2:9:129:GLU:OE2	2.34	0.45
29:b:849:BCR:H361	29:b:849:BCR:H20C	1.76	0.45
15:j:26:VAL:CG1	29:j:104:BCR:H403	2.47	0.45
2:9:153:PHE:CG	16:l:151:PHE:HE2	2.34	0.45
3:8:72:LEU:HD13	22:8:307:CLA:HED1	1.99	0.45
22:4:317:CLA:H62	22:4:317:CLA:H92	1.83	0.45
5:3:179:PRO:C	5:3:181:LYS:H	2.24	0.45
20:2:301:XAT:H15	20:2:301:XAT:H201	1.77	0.45
22:1:312:CLA:HMA2	23:1:315:SQD:H141	1.99	0.45
8:a:71:PHE:HD1	8:a:166:MET:HE3	1.82	0.45
22:a:835:CLA:H61	29:l:201:BCR:H363	1.99	0.45
20:4:305:XAT:H15	20:4:305:XAT:H201	1.71	0.45
20:2:303:XAT:H31	20:2:303:XAT:H391	1.70	0.45
20:7:304:XAT:H171	22:7:315:CLA:HBB1	1.99	0.45
20:1:302:XAT:H35	20:1:302:XAT:H401	1.72	0.45
22:a:834:CLA:H201	29:l:205:BCR:H343	1.98	0.45
13:h:65:ILE:O	13:h:123:GLN:NE2	2.49	0.45
13:h:112:ILE:O	13:h:115:GLY:N	2.49	0.45
4:7:170:MET:HE2	22:7:313:CLA:H12	1.99	0.45
8:a:686:TYR:CE1	9:b:538:LYS:HD2	2.52	0.45
22:a:804:CLA:H41	22:a:841:CLA:HMC1	1.98	0.45
9:b:458:GLU:OE1	12:f:94:HIS:ND1	2.46	0.45
9:b:547:LYS:NZ	11:e:15:SER:O	2.45	0.45
22:b:824:CLA:H92	22:b:824:CLA:H61	1.72	0.45
3:8:83:CYS:HB3	3:8:177:GLY:HA3	1.97	0.45
4:4:170:MET:CE	22:4:313:CLA:H12	2.47	0.45
20:7:301:XAT:H31	20:7:301:XAT:H391	1.79	0.45
22:a:826:CLA:HMB3	22:a:826:CLA:HBB1	1.99	0.45
9:b:678:GLU:HG2	19:c:81:TYR:HE1	1.82	0.45
22:b:823:CLA:HHB	22:b:840:CLA:O1D	2.16	0.45
1:5:232:HIS:HE1	20:5:304:XAT:H14	1.81	0.44
20:3:303:XAT:H35	20:3:303:XAT:H401	1.79	0.44
4:7:77:GLU:HB2	22:7:308:CLA:CHB	2.48	0.44
4:7:78:ILE:HG12	4:7:175:LEU:HD21	1.99	0.44
7:1:95:PRO:HD2	22:1:308:CLA:HMD3	1.99	0.44
8:a:407:VAL:HG11	8:a:564:PHE:N	2.32	0.44
8:a:411:ASN:ND2	8:a:414:ASN:OD1	2.37	0.44
8:a:447:GLY:HA3	22:a:835:CLA:HAB	1.98	0.44
8:a:580:SER:HB2	8:a:582:TRP:H	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:50:HIS:HE1	22:b:806:CLA:H171	1.81	0.44
9:b:654:PHE:O	9:b:658:VAL:HG23	2.17	0.44
29:l:205:BCR:H15C	29:l:205:BCR:H351	1.74	0.44
1:5:106:PHE:HB2	12:f:148:PRO:HG3	1.99	0.44
22:9:318:CLA:H111	22:9:318:CLA:H142	1.61	0.44
20:4:303:XAT:H11	20:4:303:XAT:H191	1.74	0.44
4:7:85:MET:HE3	4:7:177:ASN:HB3	1.99	0.44
7:1:156:ASP:OD2	16:l:2:VAL:N	2.51	0.44
8:a:304:MET:HG3	22:a:823:CLA:C3C	2.47	0.44
8:a:738:LEU:HD23	8:a:738:LEU:HA	1.80	0.44
22:a:822:CLA:H12	22:a:825:CLA:HBA2	1.99	0.44
9:b:172:ARG:HB2	22:b:813:CLA:HBC2	2.00	0.44
9:b:259:PHE:CZ	9:b:510:LEU:HD12	2.52	0.44
22:h:203:CLA:H141	22:h:203:CLA:H162	1.77	0.44
29:l:205:BCR:H11C	29:l:205:BCR:H341	1.84	0.44
2:9:93:ILE:CG1	20:9:304:XAT:H8	2.47	0.44
2:9:153:PHE:HA	16:l:151:PHE:CE2	2.51	0.44
22:4:310:CLA:H112	22:4:310:CLA:H142	1.78	0.44
4:7:36:LYS:HB2	4:7:45:ARG:H	1.83	0.44
7:1:89:VAL:O	7:1:93:TRP:N	2.49	0.44
8:a:194:HIS:ND1	22:a:826:CLA:OBD	2.48	0.44
22:a:831:CLA:H92	22:a:831:CLA:H61	1.70	0.44
9:b:201:ARG:HG2	9:b:248:SER:HB2	1.99	0.44
9:b:208:ASP:OD1	9:b:208:ASP:N	2.43	0.44
20:j:101:XAT:H35	20:j:101:XAT:H401	1.80	0.44
16:l:116:VAL:HG11	16:l:128:LEU:C	2.42	0.44
20:5:302:XAT:H383	22:5:309:CLA:C2B	2.48	0.44
2:9:144:HIS:CD2	22:9:314:CLA:HBC3	2.53	0.44
2:9:207:VAL:HG21	22:9:308:CLA:H191	1.99	0.44
22:9:308:CLA:H92	22:9:308:CLA:H61	1.76	0.44
20:8:302:XAT:H31	20:8:302:XAT:H391	1.88	0.44
22:4:311:CLA:H2A	22:4:311:CLA:O2D	2.16	0.44
5:3:121:GLN:HA	5:3:124:VAL:HG12	1.99	0.44
5:3:133:PRO:HB2	20:3:301:XAT:H23	2.00	0.44
6:2:131:ALA:HA	6:2:134:VAL:HG12	1.98	0.44
20:2:301:XAT:H35	20:2:301:XAT:H401	1.76	0.44
7:1:105:PRO:C	7:1:107:LYS:H	2.24	0.44
8:a:578:GLN:HA	8:a:583:ASP:OD2	2.18	0.44
22:a:807:CLA:H43	25:a:845:LHG:H252	2.00	0.44
22:b:827:CLA:H61	22:b:827:CLA:H102	1.85	0.44
12:f:153:ILE:O	12:f:156:SER:OG	2.31	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:9:301:A1L1G:O13	20:9:304:XAT:H28	2.16	0.44
22:4:308:CLA:H112	22:4:308:CLA:H143	1.66	0.44
6:2:105:ALA:HB1	20:2:303:XAT:H161	1.98	0.44
20:7:304:XAT:H401	20:7:304:XAT:H35	1.74	0.44
22:1:310:CLA:H92	22:1:310:CLA:H61	1.73	0.44
8:a:415:ASN:O	8:a:421:ASP:HB2	2.18	0.44
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.44
7:1:171:ARG:HA	7:1:174:MET:HE3	2.00	0.44
8:a:565:ARG:HD2	25:a:845:LHG:HC61	2.00	0.44
9:b:466:GLN:NE2	22:b:835:CLA:OBD	2.34	0.44
22:b:835:CLA:H12	22:b:836:CLA:O1A	2.18	0.44
10:d:20:TRP:HB2	10:d:24:ALA:HB3	1.99	0.44
29:f:804:BCR:H341	29:f:804:BCR:H11C	1.73	0.44
27:j:105:LMG:H122	27:j:105:LMG:H151	1.56	0.44
19:c:25:VAL:HG21	19:c:48:CYS:HA	2.00	0.44
20:5:301:XAT:H35	20:5:301:XAT:H401	1.77	0.44
25:9:307:LHG:H352	14:i:16:LEU:HD22	1.99	0.44
4:4:59:PHE:HE1	22:4:306:CLA:HBC3	1.83	0.44
5:3:189:GLU:HB2	22:3:313:CLA:C1B	2.47	0.44
8:a:282:LEU:HD21	8:a:367:MET:HB3	1.98	0.44
29:a:850:BCR:H11C	29:a:850:BCR:H341	1.88	0.44
9:b:26:ALA:HB1	26:b:848:DGD:O1B	2.17	0.44
9:b:172:ARG:HD2	22:b:824:CLA:OBD	2.18	0.44
9:b:605:GLN:HE21	9:b:734:LYS:HB3	1.82	0.44
12:f:79:ARG:O	12:f:83:SER:HB2	2.17	0.44
15:j:30:ASN:ND2	22:j:102:CLA:O1A	2.47	0.44
19:c:59:PRO:HD2	30:c:102:SF4:S2	2.58	0.44
22:9:314:CLA:H2A	22:9:314:CLA:O2D	2.17	0.44
22:2:307:CLA:H3A	22:2:307:CLA:HBA2	1.76	0.44
7:1:141:ARG:HD3	7:1:149:TRP:HB3	1.99	0.44
7:1:152:VAL:HG11	7:1:159:TRP:CD1	2.53	0.44
8:a:532:HIS:CE1	8:a:599:VAL:HA	2.53	0.44
8:a:673:TRP:O	8:a:676:SER:OG	2.32	0.44
22:a:820:CLA:CAD	22:a:830:CLA:H41	2.48	0.44
22:a:854:CLA:H142	22:a:854:CLA:H111	1.80	0.44
13:h:72:PRO:CG	24:h:204:A1L1F:C56	2.96	0.44
13:h:112:ILE:O	13:h:113:SER:C	2.60	0.44
22:4:310:CLA:H162	22:4:310:CLA:H141	1.70	0.44
6:2:118:LEU:HB2	6:2:123:TYR:HD2	1.83	0.44
8:a:517:MET:HE2	8:a:611:VAL:HA	2.00	0.44
22:a:829:CLA:H91	22:a:831:CLA:H192	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:844:CLA:C1C	25:a:846:LHG:HC31	2.48	0.44
9:b:302:ILE:HD13	22:b:822:CLA:HMD2	1.99	0.44
9:b:343:THR:HG23	9:b:377:ALA:HB2	1.99	0.44
9:b:529:LEU:HD23	9:b:588:THR:HG21	2.00	0.44
22:b:839:CLA:HBA1	22:b:839:CLA:H3A	1.59	0.44
10:d:81:ASN:H	10:d:81:ASN:ND2	2.16	0.44
20:8:301:XAT:H382	22:8:312:CLA:HAC2	1.99	0.43
22:2:316:CLA:C1C	27:2:317:LMG:H111	2.46	0.43
8:a:84:MET:SD	22:a:829:CLA:HED1	2.58	0.43
8:a:442:GLY:HA3	22:b:804:CLA:O1A	2.18	0.43
22:a:827:CLA:HBA2	22:a:827:CLA:H3A	1.79	0.43
22:a:833:CLA:H72	22:l:203:CLA:H12	2.00	0.43
22:b:836:CLA:H62	22:b:836:CLA:H102	1.77	0.43
20:9:305:XAT:H11	20:9:305:XAT:H191	1.60	0.43
20:8:302:XAT:H11	20:8:302:XAT:H191	1.71	0.43
22:4:310:CLA:C1A	22:4:310:CLA:CGA	2.96	0.43
8:a:367:MET:HG2	8:a:500:SER:HB2	1.99	0.43
9:b:647:VAL:HG21	22:b:809:CLA:HAC1	2.00	0.43
22:b:838:CLA:H62	22:b:838:CLA:H41	1.70	0.43
20:j:101:XAT:H15	20:j:101:XAT:H201	1.82	0.43
22:j:103:CLA:O1D	22:j:103:CLA:H2A	2.18	0.43
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.43
2:9:120:TRP:CD1	2:9:121:VAL:HG13	2.53	0.43
24:9:302:A1L1F:C42	22:9:311:CLA:O1A	2.66	0.43
4:7:112:HIS:O	4:7:116:VAL:HG13	2.18	0.43
8:a:143:ALA:HB2	8:a:371:PRO:HD2	2.00	0.43
8:a:364:MET:HE1	22:a:830:CLA:CAD	2.49	0.43
8:a:701:LEU:HD12	22:a:841:CLA:HMA2	2.00	0.43
22:a:807:CLA:H102	22:a:807:CLA:H161	2.00	0.43
22:b:818:CLA:H3A	22:b:818:CLA:HBA2	1.37	0.43
12:f:160:TRP:CG	12:f:161:PRO:HD3	2.52	0.43
22:9:318:CLA:HMC2	14:i:17:VAL:HG21	2.01	0.43
8:a:194:HIS:HE1	22:a:826:CLA:H72	1.84	0.43
22:a:822:CLA:OBD	22:a:824:CLA:HMD3	2.19	0.43
20:a:852:XAT:H201	20:a:852:XAT:H15	1.67	0.43
20:5:301:XAT:H31	20:5:301:XAT:H391	1.88	0.43
2:9:153:PHE:CE2	16:l:155:LEU:HD22	2.53	0.43
22:9:316:CLA:H112	22:9:318:CLA:HAB	1.99	0.43
8:a:683:GLY:HA3	9:b:571:ASP:HB2	1.99	0.43
22:a:806:CLA:H162	22:a:806:CLA:H141	1.59	0.43
22:a:810:CLA:HBB1	29:j:104:BCR:H23C	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:430:PHE:O	9:b:434:HIS:ND1	2.41	0.43
22:5:307:CLA:HBC1	20:4:301:XAT:H383	2.01	0.43
2:9:198:VAL:HG12	20:9:304:XAT:H34	2.01	0.43
20:9:305:XAT:H35	20:9:305:XAT:H401	1.74	0.43
3:8:47:PRO:HG2	3:8:50:LEU:HG	2.00	0.43
20:4:302:XAT:H35	20:4:302:XAT:H401	1.76	0.43
5:3:51:LEU:HD23	5:3:51:LEU:HA	1.87	0.43
4:7:142:MET:C	4:7:144:GLU:H	2.26	0.43
20:7:303:XAT:H35	20:7:303:XAT:H401	1.76	0.43
8:a:75:ALA:HB2	8:a:166:MET:HB2	2.01	0.43
8:a:651:VAL:O	8:a:654:SER:OG	2.29	0.43
28:a:843:PQN:H302	28:a:843:PQN:H261	1.75	0.43
9:b:274:HIS:HB2	22:b:817:CLA:CHB	2.48	0.43
22:b:805:CLA:H162	22:b:805:CLA:H141	1.67	0.43
22:b:838:CLA:H161	16:l:92:LEU:HD21	1.99	0.43
19:c:54:CYS:SG	19:c:55:GLU:N	2.91	0.43
3:8:172:LYS:HD3	22:8:313:CLA:HAA2	2.01	0.43
8:a:52:PHE:CD2	22:a:806:CLA:HMC2	2.53	0.43
22:a:841:CLA:HED3	22:a:841:CLA:H2A	2.01	0.43
9:b:83:LYS:HE3	9:b:83:LYS:HB3	1.85	0.43
9:b:345:LEU:CD1	22:b:826:CLA:HAA1	2.49	0.43
22:b:833:CLA:H3A	22:b:833:CLA:HBA2	1.52	0.43
22:5:309:CLA:H92	22:5:309:CLA:H61	1.77	0.43
20:8:301:XAT:H401	20:8:301:XAT:H35	1.77	0.43
4:4:183:LEU:HD11	22:4:308:CLA:HAC1	2.00	0.43
20:4:303:XAT:H15	20:4:303:XAT:H201	1.82	0.43
7:1:151:TRP:CH2	16:l:20:PRO:HA	2.54	0.43
7:1:171:ARG:HA	7:1:174:MET:CE	2.49	0.43
22:b:816:CLA:C9	13:h:105:LEU:HG	2.49	0.43
16:l:96:LEU:HG	29:l:205:BCR:H24C	2.01	0.43
20:4:304:XAT:H31	20:4:304:XAT:H391	1.92	0.43
5:3:56:ASN:HB3	5:3:82:LEU:HD22	2.01	0.43
20:2:302:XAT:H31	20:2:302:XAT:H391	1.84	0.43
9:b:526:ALA:HB2	22:b:836:CLA:HMA1	2.00	0.43
22:b:802:CLA:H41	22:b:802:CLA:H61	1.78	0.43
22:b:807:CLA:H161	22:b:807:CLA:H102	2.01	0.43
10:d:32:ILE:HG21	10:d:70:LEU:HD23	2.00	0.43
13:h:107:SER:O	13:h:110:THR:OG1	2.32	0.43
3:8:138:LEU:HB2	22:8:311:CLA:HMA1	1.99	0.43
20:3:303:XAT:H11	20:3:303:XAT:H191	1.89	0.43
20:2:303:XAT:H35	20:2:303:XAT:H401	1.71	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:87:ALA:HB1	20:7:303:XAT:H161	2.01	0.43
4:7:185:PHE:CE1	20:7:303:XAT:H162	2.53	0.43
8:a:525:ASP:HA	8:a:528:VAL:HG12	2.01	0.43
22:a:806:CLA:H202	22:a:806:CLA:H161	1.70	0.43
22:a:819:CLA:HBA2	22:a:819:CLA:H3A	1.53	0.43
29:j:104:BCR:H24C	29:j:104:BCR:H371	1.85	0.43
2:9:91:GLY:HA3	20:9:303:XAT:O4	2.19	0.42
2:9:204:VAL:HG22	22:9:308:CLA:H203	2.01	0.42
20:7:303:XAT:C36	22:7:308:CLA:H2	2.49	0.42
7:1:82:LEU:HD11	22:1:311:CLA:HBC1	2.01	0.42
7:1:128:GLU:HG3	20:1:302:XAT:H372	2.01	0.42
7:1:168:ASN:HA	7:1:171:ARG:HD2	2.01	0.42
8:a:361:ALA:HB2	8:a:387:HIS:HB2	2.01	0.42
22:a:807:CLA:H161	22:a:807:CLA:H192	1.83	0.42
22:a:823:CLA:CHD	20:a:852:XAT:H183	2.49	0.42
22:a:840:CLA:H72	29:a:850:BCR:H373	2.00	0.42
9:b:207:TRP:HE1	22:b:814:CLA:H11	1.84	0.42
9:b:699:PRO:O	19:c:81:TYR:OH	2.34	0.42
22:b:801:CLA:H51	22:b:838:CLA:H102	2.01	0.42
29:b:845:BCR:H20C	29:b:845:BCR:H361	1.86	0.42
2:9:138:ALA:O	2:9:142:ILE:HG12	2.20	0.42
3:8:38:SER:OG	3:8:41:LEU:O	2.36	0.42
20:7:303:XAT:H201	20:7:303:XAT:H15	1.78	0.42
8:a:684:ARG:NH1	8:a:711:ALA:O	2.52	0.42
29:b:842:BCR:H351	29:b:842:BCR:H15C	1.73	0.42
25:9:317:LHG:H321	25:9:317:LHG:H291	1.65	0.42
3:8:42:PRO:HB2	4:7:154:LYS:HB2	2.01	0.42
22:4:306:CLA:CHA	22:4:306:CLA:HBA1	2.48	0.42
6:2:109:TRP:CE3	20:2:303:XAT:H22	2.54	0.42
6:2:205:PHE:CD2	20:2:303:XAT:H12	2.54	0.42
4:7:174:GLU:HB2	22:7:313:CLA:C1B	2.50	0.42
8:a:692:GLU:CD	9:b:547:LYS:HB2	2.44	0.42
8:a:741:ILE:HD12	8:a:741:ILE:HA	1.93	0.42
22:a:834:CLA:H142	29:b:846:BCR:H17C	2.01	0.42
9:b:518:ASP:OD2	9:b:595:TYR:OH	2.23	0.42
9:b:682:TRP:NE1	16:l:15:GLY:O	2.43	0.42
22:b:809:CLA:H142	22:b:809:CLA:H111	1.70	0.42
12:f:114:PHE:HB2	29:f:801:BCR:C32	2.49	0.42
3:8:140:GLN:HE21	3:8:140:GLN:HB3	1.72	0.42
3:8:184:ILE:HG21	20:8:302:XAT:H12	2.01	0.42
20:4:303:XAT:H35	20:4:303:XAT:H401	1.85	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:81:CYS:SG	4:7:175:LEU:HD23	2.59	0.42
8:a:567:PRO:HB3	8:a:714:ILE:HB	2.01	0.42
1:5:98:PHE:HE1	22:5:305:CLA:HBC3	1.84	0.42
2:9:217:ILE:HG21	22:9:314:CLA:HHB	2.01	0.42
20:4:302:XAT:H11	20:4:302:XAT:H191	1.89	0.42
5:3:172:PRO:HD2	20:3:305:XAT:H242	2.00	0.42
20:3:303:XAT:H15	20:3:303:XAT:H201	1.79	0.42
20:2:302:XAT:H401	20:2:302:XAT:H35	1.71	0.42
21:7:302:A1L1G:O9	22:7:311:CLA:O1A	2.37	0.42
8:a:73:GLN:HG2	22:a:806:CLA:H3A	2.00	0.42
8:a:440:PHE:CE2	22:a:839:CLA:HAB	2.55	0.42
22:a:809:CLA:H3A	22:a:809:CLA:HBA2	1.67	0.42
9:b:220:LEU:HD21	29:b:842:BCR:H391	2.01	0.42
22:b:816:CLA:CHD	22:b:817:CLA:HBB2	2.49	0.42
29:b:842:BCR:H341	29:b:842:BCR:H11C	1.74	0.42
11:e:16:TYR:CD2	11:e:44:ASN:HA	2.54	0.42
14:i:29:TYR:HE1	17:m:30:ASN:HD21	1.67	0.42
19:c:32:ASP:OD1	19:c:32:ASP:N	2.53	0.42
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.42
2:9:222:ASP:OD1	2:9:227:GLY:HA2	2.19	0.42
3:8:153:ASP:OD1	20:8:303:XAT:O3	2.28	0.42
5:3:103:ILE:HD11	20:3:304:XAT:H363	2.01	0.42
5:3:205:LEU:HD12	5:3:205:LEU:HA	1.86	0.42
20:3:301:XAT:H35	20:3:301:XAT:H401	1.81	0.42
8:a:427:ARG:NH2	10:d:46:THR:O	2.53	0.42
22:a:831:CLA:H93	22:a:842:CLA:HED3	2.01	0.42
20:a:852:XAT:H31	20:a:852:XAT:H391	1.82	0.42
9:b:347:ALA:HB3	9:b:374:GLN:HE21	1.85	0.42
9:b:381:MET:HE1	29:b:845:BCR:H352	2.02	0.42
9:b:500:LEU:HA	9:b:503:ILE:HG22	2.02	0.42
20:9:303:XAT:H7	22:9:309:CLA:HAB	2.01	0.42
20:9:304:XAT:H35	20:9:304:XAT:H401	1.86	0.42
22:8:308:CLA:HBA1	22:8:308:CLA:H11	1.78	0.42
20:3:304:XAT:H12	22:3:309:CLA:HAB	2.01	0.42
8:a:67:PHE:HE2	8:a:173:HIS:CG	2.38	0.42
22:a:831:CLA:H62	22:a:831:CLA:H41	1.76	0.42
9:b:424:LEU:HG	22:b:837:CLA:CBB	2.49	0.42
9:b:702:LEU:HD22	9:b:706:GLN:NE2	2.35	0.42
22:b:820:CLA:HBA2	22:b:820:CLA:H3A	1.33	0.42
15:j:14:LEU:CD2	27:j:105:LMG:H141	2.49	0.42
20:9:303:XAT:H35	20:9:303:XAT:H401	1.85	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:303:XAT:C34	22:8:313:CLA:HBB1	2.49	0.42
22:4:309:CLA:H3A	22:4:309:CLA:HBA1	1.77	0.42
20:3:304:XAT:H11	20:3:304:XAT:H191	1.88	0.42
4:7:59:PHE:HE1	22:7:306:CLA:HBC3	1.85	0.42
20:7:303:XAT:H362	22:7:308:CLA:H2	2.01	0.42
9:b:56:ILE:HD11	29:m:101:BCR:HC7	2.02	0.42
9:b:597:HIS:CE1	9:b:727:VAL:HG23	2.54	0.42
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.42
2:9:120:TRP:HB3	9:b:94:PRO:HA	2.02	0.42
7:1:147:GLY:HA2	7:1:149:TRP:CZ3	2.55	0.42
8:a:272:LYS:HG2	8:a:496:LEU:HD12	2.02	0.42
8:a:356:LEU:HB2	22:a:828:CLA:H41	2.02	0.42
22:a:804:CLA:C4D	15:j:12:PRO:HG3	2.50	0.42
9:b:140:LEU:HD23	9:b:143:LEU:HD12	2.01	0.42
22:b:802:CLA:HMA1	22:b:803:CLA:H161	2.02	0.42
22:b:835:CLA:HBB1	22:b:835:CLA:HMB1	2.02	0.42
29:b:844:BCR:H351	29:b:844:BCR:H15C	1.78	0.42
20:4:304:XAT:H30	22:4:313:CLA:H71	2.02	0.42
8:a:680:LEU:HB3	9:b:667:ILE:HG12	2.02	0.42
8:a:727:LEU:HD22	22:a:842:CLA:HMA3	2.01	0.42
22:a:835:CLA:H141	22:a:835:CLA:H161	1.84	0.42
9:b:197:ILE:HB	9:b:198:PRO:HD3	2.02	0.42
29:l:201:BCR:H352	22:l:203:CLA:HAB	2.01	0.42
20:4:301:XAT:H401	20:4:301:XAT:H35	1.66	0.41
6:2:203:LEU:HD13	20:2:301:XAT:C10	2.50	0.41
4:7:71:SER:HB3	4:7:142:MET:CE	2.49	0.41
20:7:304:XAT:H30	22:7:313:CLA:H71	2.01	0.41
22:7:306:CLA:HBA2	22:7:306:CLA:H3A	1.58	0.41
22:a:816:CLA:C4B	20:a:852:XAT:H242	2.50	0.41
9:b:440:VAL:HG12	22:j:102:CLA:HAC1	2.01	0.41
22:b:814:CLA:CHA	22:b:814:CLA:HBA1	2.49	0.41
11:e:51:ASN:ND2	19:c:61:ASP:HB2	2.35	0.41
20:9:305:XAT:H31	20:9:305:XAT:H391	1.83	0.41
3:8:47:PRO:HG3	3:8:61:ASP:HB3	2.01	0.41
4:4:85:MET:HE3	4:4:177:ASN:HB3	2.00	0.41
20:3:305:XAT:H15	20:3:305:XAT:H201	1.84	0.41
22:7:308:CLA:H142	22:7:308:CLA:H111	1.77	0.41
22:1:306:CLA:H3A	22:1:306:CLA:O2A	2.20	0.41
8:a:271:PHE:HE2	8:a:495:ALA:HB2	1.84	0.41
22:a:806:CLA:H62	22:a:806:CLA:H2	1.67	0.41
22:a:818:CLA:OBD	22:a:837:CLA:HED2	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:839:CLA:H161	22:a:839:CLA:H141	1.68	0.41
29:a:849:BCR:H15C	29:a:849:BCR:H351	1.79	0.41
20:a:852:XAT:H11	20:a:852:XAT:H191	1.91	0.41
9:b:629:ASN:HA	9:b:734:LYS:HE2	2.02	0.41
28:b:841:PQN:H243	28:b:841:PQN:H262	1.84	0.41
10:d:88:TYR:HB3	10:d:89:PRO:HD2	2.01	0.41
2:9:120:TRP:CH2	22:9:318:CLA:H43	2.56	0.41
2:9:217:ILE:HB	22:9:314:CLA:H3A	2.02	0.41
25:9:317:LHG:HC81	25:9:317:LHG:HC5	1.98	0.41
22:7:307:CLA:C3D	22:7:314:CLA:HMA3	2.51	0.41
7:1:71:GLU:HG2	7:1:142:PRO:O	2.20	0.41
8:a:226:SER:HG	8:a:229:GLU:HG2	1.86	0.41
8:a:290:HIS:O	8:a:294:ILE:HG12	2.20	0.41
22:a:803:CLA:O1A	22:a:803:CLA:H3A	2.19	0.41
22:b:816:CLA:CBB	29:h:202:BCR:H14C	2.50	0.41
22:b:821:CLA:H12	22:b:822:CLA:H52	2.03	0.41
22:b:824:CLA:H141	22:b:824:CLA:H161	1.83	0.41
16:l:53:THR:HG22	22:l:202:CLA:C1B	2.49	0.41
29:m:101:BCR:H20C	29:m:101:BCR:H361	1.84	0.41
2:9:91:GLY:CA	20:9:303:XAT:H173	2.51	0.41
22:9:314:CLA:H51	22:9:314:CLA:C1C	2.50	0.41
3:8:77:ALA:HB2	3:8:147:PRO:HB2	2.02	0.41
20:3:305:XAT:H31	20:3:305:XAT:H391	1.91	0.41
6:2:57:PHE:CZ	20:2:305:XAT:H172	2.56	0.41
7:1:162:TYR:CE2	22:a:844:CLA:HBD	2.55	0.41
22:a:806:CLA:H72	29:a:848:BCR:C8	2.50	0.41
22:b:826:CLA:HED1	29:b:845:BCR:H21C	2.02	0.41
10:d:70:LEU:O	10:d:74:LEU:HG	2.19	0.41
29:j:104:BCR:H341	29:j:104:BCR:H11C	1.72	0.41
1:5:117:LEU:HD23	1:5:117:LEU:HA	1.92	0.41
20:4:301:XAT:H11	20:4:301:XAT:H191	1.86	0.41
20:4:305:XAT:H391	20:4:305:XAT:H31	1.62	0.41
7:1:54:PRO:HD2	20:1:303:XAT:H242	2.02	0.41
7:1:87:TRP:CG	7:1:180:LEU:HD13	2.56	0.41
8:a:293:ALA:HB1	22:a:818:CLA:HBC2	2.03	0.41
22:a:829:CLA:H3A	22:a:829:CLA:HBA2	1.83	0.41
22:b:809:CLA:C4A	22:b:809:CLA:HBA2	2.50	0.41
22:b:813:CLA:H192	22:b:813:CLA:H161	1.76	0.41
22:b:824:CLA:H52	22:b:824:CLA:H12	1.85	0.41
22:b:827:CLA:H143	22:b:827:CLA:H161	1.78	0.41
10:d:107:VAL:HG21	19:c:38:GLN:HB3	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:94:LEU:HD12	13:h:94:LEU:HA	1.94	0.41
29:i:101:BCR:H11C	29:i:101:BCR:H341	1.86	0.41
6:2:205:PHE:HE1	20:2:303:XAT:H162	1.85	0.41
8:a:342:TRP:HB3	22:a:806:CLA:HAC1	2.02	0.41
8:a:452:ASN:HD22	8:a:634:ILE:HB	1.85	0.41
9:b:181:PHE:CE2	22:b:819:CLA:HAB	2.56	0.41
9:b:273:HIS:HB3	22:b:817:CLA:HMB1	2.03	0.41
15:j:12:PRO:HB2	20:j:101:XAT:H21	2.01	0.41
20:9:304:XAT:H31	20:9:304:XAT:H391	1.97	0.41
20:3:301:XAT:H15	20:3:301:XAT:H201	1.79	0.41
20:3:304:XAT:H35	20:3:304:XAT:H401	1.68	0.41
20:2:302:XAT:H11	20:2:302:XAT:H191	1.93	0.41
8:a:357:SER:HB2	22:a:830:CLA:HMC2	2.01	0.41
8:a:434:LEU:HG	8:a:541:LEU:HB2	2.03	0.41
8:a:675:PHE:HZ	22:a:842:CLA:HBC2	1.86	0.41
22:a:826:CLA:H141	22:a:826:CLA:H161	1.81	0.41
9:b:547:LYS:HE2	12:f:180:ILE:HD11	2.03	0.41
29:b:846:BCR:H15C	29:b:846:BCR:H351	1.85	0.41
29:i:101:BCR:H15C	29:i:101:BCR:H351	1.85	0.41
20:4:301:XAT:H373	20:4:301:XAT:H23	1.87	0.41
22:1:311:CLA:H72	16:l:21:ILE:HG12	2.02	0.41
8:a:555:LEU:HD11	9:b:674:GLN:HB3	2.01	0.41
22:a:806:CLA:H52	29:a:848:BCR:HC8	2.03	0.41
22:a:841:CLA:HAA2	22:b:831:CLA:HMB1	2.02	0.41
29:a:849:BCR:H11C	29:a:849:BCR:H341	1.84	0.41
9:b:278:ILE:HD13	9:b:278:ILE:HA	1.93	0.41
9:b:346:THR:HG21	22:b:828:CLA:HHD	2.03	0.41
9:b:709:LEU:CD1	26:b:848:DGD:HB41	2.51	0.41
10:d:27:GLU:O	10:d:89:PRO:HD3	2.21	0.41
29:f:801:BCR:H20C	29:f:801:BCR:H361	1.85	0.41
1:5:98:PHE:CD2	22:5:305:CLA:HMD2	2.56	0.41
1:5:149:VAL:HG22	20:5:304:XAT:H182	2.02	0.41
24:9:302:A1L1F:C28	22:9:310:CLA:HMC1	2.51	0.41
20:8:302:XAT:H403	22:8:307:CLA:H202	2.02	0.41
20:4:304:XAT:H401	20:4:304:XAT:H35	1.81	0.41
22:4:307:CLA:HBD	22:4:314:CLA:OBD	2.20	0.41
7:1:58:ALA:HB1	7:1:66:LEU:HD21	2.01	0.41
8:a:318:ILE:O	8:a:322:HIS:ND1	2.54	0.41
8:a:601:PHE:CZ	22:a:801:CLA:HED3	2.55	0.41
9:b:518:ASP:O	9:b:522:HIS:ND1	2.38	0.41
9:b:585:MET:O	9:b:589:ILE:HG12	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:807:CLA:H201	22:b:827:CLA:H143	2.03	0.41
22:b:827:CLA:H13	22:b:829:CLA:H141	2.02	0.41
22:b:828:CLA:H3A	22:b:828:CLA:HBA2	1.76	0.41
22:b:828:CLA:H61	22:b:828:CLA:H41	1.75	0.41
22:b:834:CLA:H62	22:b:834:CLA:H41	1.86	0.41
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
2:9:201:LEU:HD13	22:9:308:CLA:HBC1	2.03	0.41
25:9:317:LHG:H312	17:m:22:ILE:HD12	2.02	0.41
20:4:303:XAT:H163	22:4:308:CLA:H2	2.02	0.41
4:7:39:ALA:HB2	4:7:57:VAL:HG23	2.03	0.41
20:7:301:XAT:H15	20:7:301:XAT:H201	1.81	0.41
22:7:307:CLA:CAD	22:7:314:CLA:HMA3	2.51	0.41
20:1:302:XAT:H15	20:1:302:XAT:H201	1.87	0.41
22:1:308:CLA:H192	22:1:308:CLA:H161	1.87	0.41
9:b:301:LEU:HB3	13:h:46:THR:HG21	2.02	0.41
9:b:314:GLY:HA3	9:b:412:ARG:HD2	2.02	0.41
9:b:412:ARG:NE	22:b:830:CLA:OBD	2.47	0.41
9:b:431:LEU:HD11	22:b:836:CLA:HMB1	2.03	0.41
9:b:499:TRP:CD1	22:b:833:CLA:HED2	2.57	0.41
9:b:523:HIS:CE1	29:b:849:BCR:H322	2.56	0.41
29:b:845:BCR:H24C	29:b:845:BCR:H371	1.83	0.41
2:9:218:LEU:HD23	2:9:218:LEU:HA	1.84	0.40
22:3:312:CLA:HBA1	22:3:312:CLA:H3A	1.93	0.40
22:2:309:CLA:HAC2	22:2:314:CLA:HAB	2.03	0.40
23:1:315:SQD:H132	23:1:315:SQD:H161	1.72	0.40
8:a:399:ALA:HB1	8:a:543:LEU:HB3	2.02	0.40
8:a:632:SER:O	8:a:638:GLY:HA3	2.21	0.40
22:a:828:CLA:H152	22:a:840:CLA:H191	2.03	0.40
22:a:828:CLA:H2	22:a:828:CLA:H61	1.78	0.40
22:a:834:CLA:H162	22:a:834:CLA:H202	1.79	0.40
9:b:86:PRO:HB3	9:b:119:TYR:CD2	2.56	0.40
9:b:668:SER:OG	9:b:673:TRP:NE1	2.52	0.40
22:f:802:CLA:H11	22:j:102:CLA:H122	2.03	0.40
16:l:56:TYR:CD2	16:l:161:ALA:HB2	2.56	0.40
29:l:205:BCR:H20C	29:l:205:BCR:H361	1.90	0.40
20:4:303:XAT:H383	22:4:310:CLA:C2B	2.51	0.40
20:2:305:XAT:H15	20:2:305:XAT:H201	1.78	0.40
8:a:209:HIS:HB2	22:a:815:CLA:C1C	2.52	0.40
8:a:232:LEU:HD23	8:a:232:LEU:HA	1.92	0.40
8:a:586:PHE:CE1	8:a:722:VAL:HB	2.57	0.40
8:a:685:GLY:N	9:b:570:CYS:O	2.48	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:193:VAL:O	9:b:198:PRO:HD3	2.20	0.40
9:b:461:PHE:HB2	22:b:836:CLA:CAD	2.52	0.40
22:b:805:CLA:HHC	22:b:807:CLA:OBD	2.22	0.40
10:d:89:PRO:HB2	10:d:90:PRO:HD3	2.03	0.40
13:h:104:VAL:HG22	29:h:202:BCR:H383	2.02	0.40
20:j:101:XAT:H31	20:j:101:XAT:H391	1.92	0.40
16:l:54:HIS:O	16:l:58:LEU:HB2	2.22	0.40
19:c:64:SER:HB2	30:c:102:SF4:S3	2.62	0.40
20:4:304:XAT:H11	20:4:304:XAT:H191	1.90	0.40
5:3:106:VAL:HG11	22:3:311:CLA:HED1	2.03	0.40
8:a:426:HIS:HA	10:d:17:THR:OG1	2.22	0.40
8:a:570:GLY:O	8:a:576:THR:OG1	2.32	0.40
22:a:803:CLA:HBB1	22:a:803:CLA:HMB3	2.04	0.40
22:a:826:CLA:H143	22:a:826:CLA:HMD2	2.02	0.40
22:b:804:CLA:HBC2	22:b:804:CLA:HHD	2.03	0.40
22:b:818:CLA:H91	22:b:818:CLA:H111	1.85	0.40
22:b:839:CLA:H121	22:b:839:CLA:H8	1.92	0.40
12:f:114:PHE:HB2	29:f:801:BCR:H321	2.02	0.40
29:h:201:BCR:H15C	29:h:201:BCR:H351	1.83	0.40
2:9:86:ARG:NE	2:9:192:GLU:OE2	2.36	0.40
20:4:302:XAT:H14	22:4:310:CLA:C1	2.49	0.40
20:3:305:XAT:H11	20:3:305:XAT:H191	1.99	0.40
4:7:79:LYS:HE3	4:7:79:LYS:HB2	1.79	0.40
20:7:305:XAT:H191	20:7:305:XAT:H11	1.84	0.40
7:1:131:GLN:O	7:1:135:LYS:HG3	2.21	0.40
7:1:186:ILE:HG13	7:1:187:THR:N	2.37	0.40
8:a:406:PHE:HE2	8:a:424:ILE:HD11	1.86	0.40
9:b:339:LEU:HD11	22:b:806:CLA:H51	2.04	0.40
9:b:585:MET:HE3	9:b:585:MET:HB3	1.83	0.40
9:b:633:LEU:HD21	9:b:652:PHE:CG	2.57	0.40
22:b:813:CLA:H161	22:b:813:CLA:H141	1.77	0.40
22:b:825:CLA:H3A	22:b:825:CLA:HBA2	1.72	0.40
22:b:840:CLA:H192	22:b:840:CLA:H161	1.82	0.40
16:l:4:PHE:HB3	16:l:20:PRO:HG3	2.03	0.40
22:5:305:CLA:HAB	4:4:153:PHE:O	2.21	0.40
3:8:44:LEU:HD22	4:7:137:ILE:HG22	2.03	0.40
20:8:302:XAT:H401	20:8:302:XAT:H35	1.76	0.40
5:3:97:MET:HG3	5:3:193:GLY:HA2	2.03	0.40
5:3:188:LYS:O	5:3:192:ASN:ND2	2.45	0.40
6:2:92:ARG:NH2	22:2:308:CLA:HED3	2.36	0.40
22:2:308:CLA:H51	22:2:309:CLA:H3A	2.04	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:303:XAT:H15	20:1:303:XAT:H201	1.85	0.40
20:1:303:XAT:H31	20:1:303:XAT:H391	1.93	0.40
22:a:842:CLA:H12	28:a:843:PQN:H301	2.02	0.40
9:b:433:PHE:CZ	29:f:801:BCR:H372	2.56	0.40
22:b:809:CLA:H143	22:b:809:CLA:H161	1.83	0.40
12:f:132:VAL:O	12:f:135:THR:HG22	2.22	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	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	50
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	46
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
6	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	22
7	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
8	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	72
9	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
10	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
11	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
12	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
13	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	11	29
14	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	j	39/41 (95%)	39 (100%)	0	0	100	100
16	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	29
17	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3620/4098 (88%)	3393 (94%)	218 (6%)	9 (0%)	45	67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
6	2	45	LYS
16	l	120	VAL
6	2	127	ASN
6	2	213	VAL
8	a	580	SER
16	l	131	ILE
4	4	146	SER
13	h	90	ILE

### 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	5	133/182 (73%)	133 (100%)	0	100	100
2	9	141/167 (84%)	139 (99%)	2 (1%)	62	79
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	88
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	88
5	3	136/164 (83%)	136 (100%)	0	100	100
6	2	134/172 (78%)	134 (100%)	0	100	100
7	1	128/165 (78%)	128 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	a	607/613 (99%)	603 (99%)	4 (1%)	81	90
9	b	599/602 (100%)	599 (100%)	0	100	100
10	d	107/113 (95%)	107 (100%)	0	100	100
11	e	56/62 (90%)	56 (100%)	0	100	100
12	f	138/162 (85%)	138 (100%)	0	100	100
13	h	71/107 (66%)	70 (99%)	1 (1%)	62	79
14	i	32/43 (74%)	32 (100%)	0	100	100
15	j	36/36 (100%)	36 (100%)	0	100	100
16	l	130/141 (92%)	130 (100%)	0	100	100
17	m	21/24 (88%)	21 (100%)	0	100	100
19	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2923/3299 (89%)	2914 (100%)	9 (0%)	90	96

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

Mol	Chain	Res	Type
2	9	172	LYS
2	9	174	GLU
3	8	175	LYS
4	7	95	ASP
8	a	428	ASP
8	a	448	LEU
8	a	579	VAL
8	a	580	SER
13	h	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
3	8	156	ASN
5	3	156	GLN
5	3	211	HIS
7	1	119	GLN
7	1	132	ASN
7	1	194	GLN
8	a	127	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
8	a	186	ASN
8	a	415	ASN
8	a	435	ASN
9	b	80	ASN
9	b	112	ASN
9	b	169	ASN
9	b	326	ASN
9	b	373	HIS
9	b	605	GLN
9	b	629	ASN
10	d	7	GLN
12	f	166	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

257 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	$\# Z  > 2$
22	CLA	7	310	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	819	-	54,62,73	1.63	6 (11%)	62,99,113	1.45	7 (11%)
22	CLA	a	837	8	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
22	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
27	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.13	3 (7%)
22	CLA	3	313	-	52,60,73	1.66	5 (9%)	60,97,113	1.53	9 (15%)
22	CLA	9	315	2	42,50,73	1.83	5 (11%)	48,85,113	1.61	7 (14%)
22	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	8	309	-	57,65,73	1.59	5 (8%)	66,103,113	1.46	9 (13%)
20	XAT	2	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.71	18 (33%)
22	CLA	a	824	-	46,54,73	1.78	6 (13%)	53,90,113	1.49	7 (13%)
29	BCR	f	804	-	41,41,41	0.73	0	56,56,56	2.04	16 (28%)
22	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.51	8 (13%)
22	CLA	b	831	-	49,57,73	1.70	5 (10%)	55,93,113	1.57	8 (14%)
29	BCR	b	846	-	41,41,41	0.75	0	56,56,56	1.79	15 (26%)
24	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
22	CLA	2	316	6	46,54,73	1.76	6 (13%)	53,90,113	1.54	6 (11%)
29	BCR	b	849	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
22	CLA	1	309	7	46,54,73	1.78	6 (13%)	53,90,113	1.51	7 (13%)
22	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.58	8 (13%)
22	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
25	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
29	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
22	CLA	b	825	-	64,72,73	1.48	6 (9%)	74,111,113	1.44	7 (9%)
22	CLA	7	316	-	51,59,73	1.64	6 (11%)	59,96,113	1.61	8 (13%)
22	CLA	b	809	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
30	SF4	a	851	-	0,12,12	-	-	-	-	-
22	CLA	7	313	-	54,62,73	1.66	5 (9%)	62,99,113	1.50	9 (14%)
22	CLA	b	814	-	55,63,73	1.60	6 (10%)	64,101,113	1.55	8 (12%)
22	CLA	8	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
22	CLA	1	314	-	45,53,73	1.80	5 (11%)	52,89,113	1.56	6 (11%)
22	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	9 (11%)
20	XAT	8	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.53	19 (35%)
22	CLA	9	311	-	46,54,73	1.75	5 (10%)	53,90,113	1.61	8 (15%)
22	CLA	b	820	-	50,58,73	1.71	6 (12%)	58,95,113	1.59	10 (17%)
22	CLA	7	307	-	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	BCR	b	845	-	41,41,41	0.75	0	56,56,56	2.19	22 (39%)
25	LHG	9	317	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
22	CLA	a	839	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	b	803	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
22	CLA	b	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
20	XAT	4	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.57	18 (33%)
20	XAT	7	305	-	39,47,47	0.87	1 (2%)	54,74,74	2.65	20 (37%)
21	A1L1G	1	301	-	38,47,47	1.44	6 (15%)	49,71,71	1.57	11 (22%)
22	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
22	CLA	a	815	-	45,53,73	1.78	5 (11%)	52,89,113	1.60	8 (15%)
22	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	9 (11%)
22	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.65	9 (19%)
22	CLA	9	318	-	62,70,73	1.54	6 (9%)	72,109,113	1.37	8 (11%)
22	CLA	4	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
22	CLA	9	310	-	46,54,73	1.75	5 (10%)	53,90,113	1.65	6 (11%)
22	CLA	8	314	-	41,49,73	1.86	5 (12%)	47,84,113	1.64	8 (17%)
22	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.52	6 (10%)
22	CLA	2	311	-	58,66,73	1.59	5 (8%)	67,104,113	1.41	8 (11%)
21	A1L1G	3	306	-	38,47,47	1.43	6 (15%)	49,71,71	1.50	9 (18%)
22	CLA	3	308	-	47,55,73	1.75	5 (10%)	54,91,113	1.57	8 (14%)
22	CLA	3	314	5	47,55,73	1.74	6 (12%)	54,91,113	1.56	6 (11%)
22	CLA	b	819	-	55,63,73	1.63	5 (9%)	64,101,113	1.44	8 (12%)
22	CLA	7	312	-	48,56,73	1.72	6 (12%)	55,92,113	1.55	8 (14%)
22	CLA	b	822	-	60,68,73	1.55	6 (10%)	70,107,113	1.39	8 (11%)
23	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
20	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)
22	CLA	4	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.55	8 (15%)
22	CLA	a	810	8	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
22	CLA	a	811	-	56,64,73	1.59	5 (8%)	65,102,113	1.48	8 (12%)
24	A1L1F	h	204	-	50,59,59	1.38	5 (10%)	62,85,85	2.60	22 (35%)
29	BCR	a	849	-	41,41,41	0.73	0	56,56,56	2.17	20 (35%)
20	XAT	1	302	-	39,47,47	0.90	1 (2%)	54,74,74	2.59	16 (29%)
22	CLA	4	309	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
22	CLA	a	825	-	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	XAT	9	303	-	39,47,47	0.95	1 (2%)	54,74,74	2.61	18 (33%)
22	CLA	5	309	1	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	7	314	-	45,53,73	1.79	6 (13%)	52,89,113	1.64	7 (13%)
22	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	6 (11%)
22	CLA	a	812	22	62,70,73	1.51	6 (9%)	72,109,113	1.43	8 (11%)
22	CLA	a	834	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	9 (11%)
22	CLA	a	826	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	6 (7%)
22	CLA	8	306	26	46,54,73	1.75	5 (10%)	53,90,113	1.55	7 (13%)
28	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
22	CLA	2	309	-	46,54,73	1.77	5 (10%)	53,90,113	1.55	7 (13%)
22	CLA	b	805	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	9	314	-	55,63,73	1.62	6 (10%)	64,101,113	1.50	8 (12%)
22	CLA	5	315	-	46,54,73	1.75	5 (10%)	53,90,113	1.57	7 (13%)
29	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	15 (26%)
22	CLA	8	312	3	52,60,73	1.66	5 (9%)	60,97,113	1.52	8 (13%)
29	BCR	b	843	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
22	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	10 (13%)
22	CLA	a	813	-	54,62,73	1.65	5 (9%)	62,99,113	1.44	7 (11%)
20	XAT	9	305	-	39,47,47	0.95	1 (2%)	54,74,74	2.36	17 (31%)
22	CLA	7	308	-	60,68,73	1.54	5 (8%)	70,107,113	1.44	7 (10%)
22	CLA	b	826	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	6 (7%)
20	XAT	5	302	-	39,47,47	0.92	2 (5%)	54,74,74	2.58	20 (37%)
20	XAT	1	303	-	39,47,47	0.91	1 (2%)	54,74,74	2.51	20 (37%)
21	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
22	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
22	CLA	a	829	-	62,70,73	1.52	6 (9%)	72,109,113	1.40	8 (11%)
22	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	b	833	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	b	824	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	7 (9%)
22	CLA	b	821	-	51,59,73	1.65	5 (9%)	59,96,113	1.56	9 (15%)
22	CLA	b	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	a	817	-	45,53,73	1.79	5 (11%)	52,89,113	1.59	7 (13%)
22	CLA	j	102	-	58,66,73	1.59	6 (10%)	67,104,113	1.42	8 (11%)
22	CLA	b	840	25	65,73,73	1.53	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	2	314	-	56,64,73	1.61	7 (12%)	65,102,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.55	8 (13%)
22	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.50	8 (12%)
22	CLA	2	308	6	54,62,73	1.65	5 (9%)	62,99,113	1.46	8 (12%)
22	CLA	a	836	-	50,58,73	1.70	5 (10%)	58,95,113	1.51	9 (15%)
22	CLA	b	834	-	53,61,73	1.67	6 (11%)	61,98,113	1.51	8 (13%)
27	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.30	4 (9%)
29	BCR	l	205	-	41,41,41	0.71	0	56,56,56	2.03	13 (23%)
20	XAT	2	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.43	18 (33%)
26	DGD	4	318	-	41,41,67	1.06	2 (4%)	55,55,81	1.82	6 (10%)
22	CLA	8	308	-	55,63,73	1.62	5 (9%)	64,101,113	1.51	9 (14%)
22	CLA	2	306	-	41,50,73	1.85	6 (14%)	46,85,113	1.57	6 (13%)
22	CLA	9	308	2	65,73,73	1.49	6 (9%)	76,113,113	1.42	9 (11%)
22	CLA	b	810	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	9 (11%)
20	XAT	4	302	-	39,47,47	0.90	0	54,74,74	2.57	20 (37%)
29	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
20	XAT	3	301	-	39,47,47	0.90	2 (5%)	54,74,74	2.55	18 (33%)
22	CLA	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.51	7 (11%)
22	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	8 (10%)
22	CLA	4	306	4	45,53,73	1.81	6 (13%)	52,89,113	1.58	7 (13%)
22	CLA	a	803	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	7 (9%)
22	CLA	5	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.56	7 (13%)
22	CLA	7	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.57	7 (13%)
22	CLA	a	844	25	65,73,73	1.46	5 (7%)	76,113,113	1.39	9 (11%)
22	CLA	b	829	-	65,73,73	1.51	6 (9%)	76,113,113	1.44	10 (13%)
22	CLA	b	839	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	8 (10%)
25	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
20	XAT	8	303	-	39,47,47	0.88	1 (2%)	54,74,74	2.64	18 (33%)
22	CLA	l	203	-	60,68,73	1.54	6 (10%)	70,107,113	1.48	7 (10%)
29	BCR	h	202	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
22	CLA	a	805	22	55,63,73	1.60	5 (9%)	64,101,113	1.51	8 (12%)
22	CLA	1	305	-	61,69,73	1.55	5 (8%)	71,108,113	1.40	7 (9%)
22	CLA	f	803	12	52,60,73	1.66	5 (9%)	60,97,113	1.50	8 (13%)
22	CLA	b	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	a	840	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	b	835	-	58,66,73	1.56	5 (8%)	67,104,113	1.52	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SF4	c	102	-	0,12,12	-	-	-		
22	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	7 (10%)
22	CLA	3	315	5	46,54,73	1.78	6 (13%)	53,90,113	1.52	7 (13%)
22	CLA	9	313	2	46,54,73	1.76	5 (10%)	53,90,113	1.63	6 (11%)
22	CLA	4	314	4	45,53,73	1.81	5 (11%)	52,89,113	1.57	7 (13%)
22	CLA	3	311	-	50,58,73	1.70	5 (10%)	58,95,113	1.54	9 (15%)
22	CLA	4	317	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	7 (10%)
21	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.53	8 (16%)
20	XAT	7	304	-	39,47,47	0.91	2 (5%)	54,74,74	2.68	21 (38%)
22	CLA	1	310	7	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
22	CLA	h	205	-	55,63,73	1.61	5 (9%)	64,101,113	1.47	10 (15%)
22	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
22	CLA	b	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.50	9 (13%)
22	CLA	2	312	-	47,55,73	1.74	6 (12%)	54,91,113	1.57	7 (12%)
22	CLA	b	817	-	59,67,73	1.56	5 (8%)	68,105,113	1.50	9 (13%)
22	CLA	8	313	-	46,54,73	1.79	6 (13%)	53,90,113	1.55	6 (11%)
22	CLA	9	316	-	65,73,73	1.46	5 (7%)	76,113,113	1.45	7 (9%)
22	CLA	a	814	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
29	BCR	i	101	-	41,41,41	0.74	0	56,56,56	2.13	14 (25%)
20	XAT	4	305	-	39,47,47	0.90	1 (2%)	54,74,74	2.75	19 (35%)
22	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
22	CLA	9	309	2	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)
28	PQN	b	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
21	A1L1G	3	302	-	38,47,47	1.46	6 (15%)	49,71,71	1.39	7 (14%)
22	CLA	9	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.68	8 (15%)
22	CLA	a	820	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
20	XAT	3	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.62	19 (35%)
22	CLA	1	202	-	42,50,73	1.82	5 (11%)	48,85,113	1.63	7 (14%)
22	CLA	7	315	4	41,49,73	1.86	6 (14%)	47,84,113	1.66	8 (17%)
22	CLA	5	311	-	51,59,73	1.66	5 (9%)	59,96,113	1.53	9 (15%)
29	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	15 (26%)
22	CLA	5	312	-	52,60,73	1.65	5 (9%)	60,97,113	1.55	9 (15%)
22	CLA	5	306	23	45,53,73	1.79	5 (11%)	52,89,113	1.57	7 (13%)
22	CLA	4	307	-	56,64,73	1.61	5 (8%)	65,102,113	1.44	8 (12%)
22	CLA	3	312	5	59,67,73	1.57	5 (8%)	68,105,113	1.43	7 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	1	308	7	65,73,73	1.47	5 (7%)	76,113,113	1.41	9 (11%)
22	CLA	a	808	-	51,59,73	1.70	5 (9%)	59,96,113	1.49	8 (13%)
29	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
22	CLA	1	204	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	7 (13%)
20	XAT	4	301	-	39,47,47	0.95	2 (5%)	54,74,74	2.62	19 (35%)
21	A1L1G	7	302	-	38,47,47	1.43	5 (13%)	49,71,71	1.51	9 (18%)
22	CLA	4	310	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	9 (11%)
26	DGD	8	315	22	41,41,67	1.05	2 (4%)	55,55,81	1.11	5 (9%)
20	XAT	9	304	-	39,47,47	0.94	1 (2%)	54,74,74	2.42	19 (35%)
22	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	7 (9%)
22	CLA	a	854	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
20	XAT	5	304	-	39,47,47	0.89	0	54,74,74	2.86	22 (40%)
22	CLA	3	309	5	56,64,73	1.59	6 (10%)	65,102,113	1.45	7 (10%)
21	A1L1G	5	303	-	38,47,47	1.41	6 (15%)	49,71,71	1.46	7 (14%)
20	XAT	2	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.50	18 (33%)
22	CLA	1	312	7	52,60,73	1.71	5 (9%)	60,97,113	1.48	8 (13%)
22	CLA	a	801	-	65,73,73	1.50	9 (13%)	76,113,113	1.38	7 (9%)
22	CLA	2	315	-	42,50,73	1.87	5 (11%)	48,85,113	1.56	7 (14%)
22	CLA	b	804	-	65,73,73	1.46	6 (9%)	76,113,113	1.55	12 (15%)
22	CLA	j	103	15	42,50,73	1.82	5 (11%)	48,85,113	1.64	6 (12%)
25	LHG	a	846	22	26,26,48	1.27	5 (19%)	29,32,54	1.21	2 (6%)
22	CLA	b	818	-	60,68,73	1.56	5 (8%)	70,107,113	1.41	7 (10%)
22	CLA	a	832	-	50,58,73	1.69	6 (12%)	58,95,113	1.52	9 (15%)
30	SF4	c	101	-	0,12,12	-	-	-		
20	XAT	3	303	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	20 (37%)
20	XAT	2	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.54	20 (37%)
22	CLA	5	307	1	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
22	CLA	h	203	-	65,73,73	1.51	6 (9%)	76,113,113	1.45	7 (9%)
26	DGD	b	848	-	58,58,67	1.15	7 (12%)	72,72,81	1.52	10 (13%)
22	CLA	4	313	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
20	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
22	CLA	a	806	-	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)
24	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
22	CLA	2	307	-	47,55,73	1.73	6 (12%)	54,91,113	1.63	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	XAT	8	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.66	20 (37%)
22	CLA	b	815	-	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
27	LMG	a	853	-	34,34,55	1.13	2 (5%)	42,42,63	1.15	3 (7%)
20	XAT	3	305	-	39,47,47	0.88	1 (2%)	54,74,74	2.57	17 (31%)
22	CLA	2	313	6	41,49,73	1.86	5 (12%)	47,84,113	1.70	8 (17%)
22	CLA	7	309	-	46,55,73	1.75	5 (10%)	52,91,113	1.52	7 (13%)
22	CLA	b	837	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
22	CLA	8	305	3	43,51,73	1.79	6 (13%)	49,86,113	1.66	7 (14%)
22	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
29	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
29	BCR	b	844	-	41,41,41	0.69	0	56,56,56	2.09	16 (28%)
22	CLA	3	310	-	56,64,73	1.60	5 (8%)	65,102,113	1.46	7 (10%)
22	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.43	8 (12%)
22	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
20	XAT	j	101	-	39,47,47	0.89	1 (2%)	54,74,74	2.72	18 (33%)
22	CLA	4	312	-	46,54,73	1.78	6 (13%)	53,90,113	1.52	7 (13%)
22	CLA	5	305	1	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
20	XAT	7	303	-	39,47,47	0.97	1 (2%)	54,74,74	2.59	17 (31%)
22	CLA	a	802	-	58,66,73	1.55	5 (8%)	67,104,113	1.50	7 (10%)
22	CLA	a	809	8	65,73,73	1.45	5 (7%)	76,113,113	1.44	9 (11%)
22	CLA	b	802	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
20	XAT	7	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.63	20 (37%)
22	CLA	b	816	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	9 (14%)
24	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
29	BCR	b	842	-	41,41,41	0.70	0	56,56,56	2.29	21 (37%)
29	BCR	m	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	4	315	4	41,49,73	1.87	5 (12%)	47,84,113	1.66	8 (17%)
22	CLA	b	813	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	b	823	-	53,61,73	1.64	6 (11%)	61,98,113	1.47	8 (13%)
22	CLA	a	823	-	49,57,73	1.69	5 (10%)	55,93,113	1.61	7 (12%)
22	CLA	b	808	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	9 (11%)
22	CLA	5	313	1	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
22	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	10 (15%)
20	XAT	4	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.56	17 (31%)
22	CLA	4	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
22	CLA	a	807	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
20	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
25	LHG	b	847	22	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
22	CLA	b	812	-	53,61,73	1.63	5 (9%)	61,98,113	1.49	8 (13%)
22	CLA	5	308	-	55,63,73	1.63	6 (10%)	64,101,113	1.47	7 (10%)
22	CLA	5	314	-	52,60,73	1.65	5 (9%)	60,97,113	1.55	8 (13%)
23	SQD	5	316	22	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)
22	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
29	BCR	h	201	-	41,41,41	0.71	0	56,56,56	1.97	20 (35%)
22	CLA	3	307	5	45,53,73	1.80	6 (13%)	52,89,113	1.56	6 (11%)

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
22	CLA	7	310	-	1/1/11/20	6/15/93/115	-
22	CLA	a	819	-	1/1/12/20	4/24/102/115	-
22	CLA	a	837	8	1/1/11/20	4/13/91/115	-
22	CLA	2	310	-	1/1/15/20	14/37/115/115	-
27	LMG	j	105	-	-	11/27/47/70	0/1/1/1
22	CLA	3	313	-	1/1/12/20	1/22/100/115	-
22	CLA	9	315	2	1/1/10/20	6/10/88/115	-
22	CLA	a	822	-	1/1/15/20	5/37/115/115	-
22	CLA	8	309	-	1/1/13/20	8/28/106/115	-
22	CLA	a	824	-	1/1/11/20	4/15/93/115	-
20	XAT	2	301	-	-	3/31/93/93	0/4/4/4
29	BCR	f	804	-	-	4/29/63/63	0/2/2/2
22	CLA	1	311	-	1/1/12/20	6/23/101/115	-
22	CLA	b	831	-	1/1/11/20	6/18/96/115	-
29	BCR	b	846	-	-	2/29/63/63	0/2/2/2
24	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
22	CLA	2	316	6	1/1/11/20	5/15/93/115	-
29	BCR	b	849	-	-	5/29/63/63	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	309	7	1/1/11/20	6/15/93/115	-
22	CLA	a	816	-	1/1/12/20	5/19/97/115	-
22	CLA	f	802	-	1/1/15/20	13/37/115/115	-
25	LHG	a	845	-	-	27/52/52/53	-
29	BCR	l	201	-	-	4/29/63/63	0/2/2/2
22	CLA	b	825	-	1/1/14/20	6/36/114/115	-
22	CLA	7	316	-	1/1/12/20	11/21/99/115	-
22	CLA	b	809	-	1/1/15/20	11/37/115/115	-
30	SF4	a	851	-	-	-	0/6/5/5
22	CLA	7	313	-	1/1/12/20	7/24/102/115	-
22	CLA	b	814	-	1/1/13/20	13/25/103/115	-
22	CLA	8	310	-	1/1/11/20	5/15/93/115	-
22	CLA	1	314	-	1/1/11/20	5/13/91/115	-
22	CLA	b	807	-	1/1/15/20	19/37/115/115	-
22	CLA	b	820	-	1/1/12/20	7/19/97/115	-
22	CLA	9	311	-	1/1/11/20	7/15/93/115	-
20	XAT	8	301	-	-	3/31/93/93	0/4/4/4
22	CLA	7	307	-	1/1/11/20	5/13/91/115	-
29	BCR	b	845	-	-	1/29/63/63	0/2/2/2
25	LHG	9	317	-	-	28/50/50/53	-
22	CLA	a	839	-	1/1/15/20	15/37/115/115	-
22	CLA	b	803	-	1/1/15/20	18/37/115/115	-
22	CLA	b	836	-	1/1/15/20	8/37/115/115	-
20	XAT	4	303	-	-	3/31/93/93	0/4/4/4
20	XAT	7	305	-	-	2/31/93/93	0/4/4/4
22	CLA	a	842	-	1/1/15/20	9/37/115/115	-
21	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
22	CLA	a	821	-	1/1/11/20	2/13/91/115	-
22	CLA	a	815	-	1/1/11/20	2/13/91/115	-
22	CLA	a	841	-	1/1/15/20	15/37/115/115	-
22	CLA	b	830	-	1/1/10/20	1/8/86/115	-
22	CLA	9	318	-	1/1/14/20	9/34/112/115	-
22	CLA	4	308	-	1/1/15/20	14/37/115/115	-
22	CLA	9	310	-	1/1/11/20	6/15/93/115	-
22	CLA	8	314	-	1/1/10/20	5/8/86/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	306	4	1/1/11/20	10/17/95/115	-
22	CLA	2	311	-	1/1/13/20	5/29/107/115	-
21	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
22	CLA	3	308	-	1/1/11/20	5/16/94/115	-
22	CLA	3	314	5	1/1/11/20	7/16/94/115	-
22	CLA	b	819	-	1/1/13/20	3/25/103/115	-
22	CLA	7	312	-	1/1/11/20	3/17/95/115	-
22	CLA	b	822	-	1/1/14/20	7/31/109/115	-
23	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	CLA	4	311	-	1/1/11/20	8/15/93/115	-
20	XAT	a	852	-	-	7/31/93/93	0/4/4/4
22	CLA	a	810	8	1/1/15/20	13/37/115/115	-
22	CLA	a	811	-	1/1/13/20	8/27/105/115	-
24	A1L1F	h	204	-	-	11/43/99/99	1/3/3/3
29	BCR	a	849	-	-	0/29/63/63	0/2/2/2
20	XAT	1	302	-	-	0/31/93/93	0/4/4/4
22	CLA	4	309	-	1/1/12/20	7/19/97/115	-
22	CLA	a	825	-	1/1/13/20	8/25/103/115	-
22	CLA	5	309	1	1/1/15/20	14/37/115/115	-
22	CLA	7	314	-	1/1/11/20	4/13/91/115	-
22	CLA	7	317	-	1/1/11/20	5/13/91/115	-
20	XAT	9	303	-	-	4/31/93/93	0/4/4/4
22	CLA	a	812	22	1/1/14/20	9/34/112/115	-
22	CLA	a	834	-	1/1/15/20	7/37/115/115	-
22	CLA	a	826	-	1/1/15/20	9/37/115/115	-
22	CLA	8	306	26	1/1/11/20	2/15/93/115	-
28	PQN	a	843	-	-	5/23/43/43	0/2/2/2
22	CLA	2	309	-	1/1/11/20	4/15/93/115	-
22	CLA	b	805	-	1/1/15/20	12/37/115/115	-
22	CLA	9	314	-	1/1/13/20	9/25/103/115	-
22	CLA	5	315	-	1/1/11/20	5/15/93/115	-
29	BCR	a	850	-	-	4/29/63/63	0/2/2/2
22	CLA	8	312	3	1/1/12/20	2/22/100/115	-
29	BCR	b	843	-	-	2/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	306	-	1/1/15/20	15/37/115/115	-
22	CLA	a	813	-	1/1/12/20	10/24/102/115	-
22	CLA	b	826	-	1/1/15/20	5/37/115/115	-
22	CLA	7	308	-	1/1/14/20	14/31/109/115	-
20	XAT	9	305	-	-	3/31/93/93	0/4/4/4
20	XAT	5	302	-	-	3/31/93/93	0/4/4/4
22	CLA	b	801	-	1/1/15/20	20/37/115/115	-
20	XAT	1	303	-	-	0/31/93/93	0/4/4/4
21	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
22	CLA	a	829	-	1/1/14/20	15/34/112/115	-
22	CLA	a	828	-	1/1/15/20	9/37/115/115	-
22	CLA	b	833	-	1/1/15/20	14/37/115/115	-
22	CLA	b	824	-	1/1/15/20	14/37/115/115	-
22	CLA	b	821	-	1/1/12/20	2/21/99/115	-
22	CLA	b	838	-	1/1/15/20	13/37/115/115	-
22	CLA	a	817	-	1/1/11/20	6/13/91/115	-
22	CLA	j	102	-	1/1/13/20	16/29/107/115	-
22	CLA	b	840	25	1/1/15/20	9/37/115/115	-
22	CLA	2	314	-	1/1/13/20	13/27/105/115	-
22	CLA	a	838	-	1/1/12/20	6/21/99/115	-
22	CLA	8	311	-	1/1/13/20	8/27/105/115	-
22	CLA	2	308	6	1/1/12/20	5/24/102/115	-
22	CLA	a	836	-	1/1/12/20	6/19/97/115	-
22	CLA	b	834	-	1/1/12/20	8/23/101/115	-
27	LMG	2	317	-	-	11/30/50/70	0/1/1/1
29	BCR	1	205	-	-	8/29/63/63	0/2/2/2
20	XAT	2	305	-	-	2/31/93/93	0/4/4/4
26	DGD	4	318	-	-	10/29/69/95	0/2/2/2
22	CLA	8	308	-	1/1/13/20	7/25/103/115	-
22	CLA	2	306	-	1/1/10/20	2/9/87/115	-
22	CLA	9	308	2	1/1/15/20	15/37/115/115	-
22	CLA	b	810	-	1/1/15/20	16/37/115/115	-
20	XAT	4	302	-	-	0/31/93/93	0/4/4/4
29	BCR	j	104	-	-	4/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	307	-	1/1/12/20	6/24/102/115	-
22	CLA	a	831	-	1/1/15/20	11/37/115/115	-
20	XAT	3	301	-	-	3/31/93/93	0/4/4/4
22	CLA	4	306	4	1/1/11/20	7/13/91/115	-
22	CLA	a	803	-	1/1/15/20	3/37/115/115	-
22	CLA	5	310	-	1/1/11/20	6/15/93/115	-
22	CLA	7	311	-	1/1/11/20	5/15/93/115	-
22	CLA	a	844	25	1/1/15/20	16/37/115/115	-
22	CLA	b	829	-	1/1/15/20	10/37/115/115	-
22	CLA	b	839	-	1/1/15/20	17/37/115/115	-
25	LHG	9	307	-	-	21/40/40/53	-
22	CLA	l	203	-	1/1/14/20	6/31/109/115	-
20	XAT	8	303	-	-	0/31/93/93	0/4/4/4
29	BCR	h	202	-	-	2/29/63/63	0/2/2/2
22	CLA	a	805	22	1/1/13/20	6/25/103/115	-
22	CLA	1	305	-	1/1/14/20	10/33/111/115	-
22	CLA	f	803	12	1/1/12/20	2/22/100/115	-
22	CLA	b	827	-	1/1/15/20	14/37/115/115	-
22	CLA	a	840	-	1/1/15/20	8/37/115/115	-
22	CLA	b	835	-	1/1/13/20	11/29/107/115	-
30	SF4	c	102	-	-	-	0/6/5/5
22	CLA	a	833	-	1/1/13/20	2/25/103/115	-
22	CLA	3	315	5	1/1/11/20	8/15/93/115	-
22	CLA	9	313	2	1/1/11/20	9/15/93/115	-
22	CLA	4	314	4	1/1/11/20	3/13/91/115	-
22	CLA	3	311	-	1/1/12/20	4/19/97/115	-
22	CLA	4	317	-	1/1/13/20	7/25/103/115	-
21	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
22	CLA	1	310	7	1/1/15/20	18/37/115/115	-
22	CLA	h	205	-	1/1/13/20	9/25/103/115	-
20	XAT	7	304	-	-	6/31/93/93	0/4/4/4
22	CLA	8	307	3	1/1/15/20	13/37/115/115	-
22	CLA	b	811	-	1/1/13/20	5/25/101/115	-
22	CLA	2	312	-	1/1/11/20	4/16/94/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	817	-	1/1/13/20	10/30/108/115	-
22	CLA	8	313	-	1/1/11/20	3/15/93/115	-
22	CLA	9	316	-	1/1/15/20	17/37/115/115	-
22	CLA	a	814	-	1/1/15/20	20/37/115/115	-
29	BCR	i	101	-	-	3/29/63/63	0/2/2/2
20	XAT	4	305	-	-	4/31/93/93	0/4/4/4
22	CLA	1	313	-	1/1/10/20	3/8/86/115	-
22	CLA	9	309	2	1/1/11/20	3/15/93/115	-
28	PQN	b	841	-	-	1/23/43/43	0/2/2/2
22	CLA	9	312	-	1/1/11/20	9/15/93/115	-
22	CLA	a	820	-	1/1/15/20	15/37/115/115	-
21	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
20	XAT	3	304	-	-	3/31/93/93	0/4/4/4
22	CLA	1	202	-	1/1/10/20	2/10/88/115	-
22	CLA	7	315	4	1/1/10/20	4/8/86/115	-
22	CLA	5	311	-	1/1/12/20	8/21/99/115	-
29	BCR	f	801	-	-	3/29/63/63	0/2/2/2
22	CLA	5	312	-	1/1/12/20	0/22/100/115	-
22	CLA	5	306	23	1/1/11/20	7/13/91/115	-
22	CLA	4	307	-	1/1/13/20	7/27/105/115	-
22	CLA	3	312	5	1/1/13/20	9/30/108/115	-
22	CLA	1	308	7	1/1/15/20	13/37/115/115	-
22	CLA	a	808	-	1/1/12/20	3/21/99/115	-
29	BCR	a	847	-	-	0/29/63/63	0/2/2/2
22	CLA	1	204	-	1/1/11/20	4/15/93/115	-
20	XAT	4	301	-	-	4/31/93/93	0/4/4/4
21	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
22	CLA	4	310	-	1/1/15/20	16/37/115/115	-
22	CLA	a	827	-	1/1/15/20	8/37/115/115	-
26	DGD	8	315	22	-	11/29/69/95	0/2/2/2
22	CLA	a	854	-	1/1/15/20	13/37/115/115	-
22	CLA	a	835	-	1/1/15/20	12/37/115/115	-
20	XAT	9	304	-	-	1/31/93/93	0/4/4/4
22	CLA	3	309	5	1/1/13/20	5/27/105/115	-
20	XAT	5	304	-	-	1/31/93/93	0/4/4/4

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
20	XAT	2	302	-	-	0/31/93/93	0/4/4/4
22	CLA	1	312	7	1/1/12/20	3/22/100/115	-
22	CLA	a	801	-	1/1/15/20	22/37/115/115	-
22	CLA	2	315	-	1/1/10/20	1/10/88/115	-
22	CLA	b	804	-	1/1/15/20	10/37/115/115	-
22	CLA	j	103	15	1/1/10/20	5/10/88/115	-
25	LHG	a	846	22	-	16/31/31/53	-
22	CLA	b	818	-	1/1/14/20	14/31/109/115	-
22	CLA	a	832	-	1/1/12/20	5/19/97/115	-
30	SF4	c	101	-	-	-	0/6/5/5
20	XAT	3	303	-	-	3/31/93/93	0/4/4/4
20	XAT	2	304	-	-	3/31/93/93	0/4/4/4
22	CLA	5	307	1	1/1/14/20	7/31/109/115	-
22	CLA	h	203	-	1/1/15/20	9/37/115/115	-
26	DGD	b	848	-	-	20/46/86/95	0/2/2/2
22	CLA	4	313	-	1/1/12/20	6/23/101/115	-
20	XAT	5	301	-	-	3/31/93/93	0/4/4/4
22	CLA	a	806	-	1/1/15/20	12/37/115/115	-
24	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
22	CLA	2	307	-	1/1/11/20	6/16/94/115	-
20	XAT	8	302	-	-	4/31/93/93	0/4/4/4
22	CLA	b	815	-	1/1/11/20	3/13/91/115	-
27	LMG	a	853	-	-	13/29/49/70	0/1/1/1
20	XAT	3	305	-	-	0/31/93/93	0/4/4/4
22	CLA	2	313	6	1/1/10/20	4/8/86/115	-
22	CLA	7	309	-	1/1/11/20	5/15/93/115	-
22	CLA	b	837	-	1/1/15/20	8/37/115/115	-
22	CLA	8	305	3	1/1/10/20	2/11/89/115	-
22	CLA	b	832	-	1/1/15/20	13/37/115/115	-
29	BCR	a	848	-	-	0/29/63/63	0/2/2/2
29	BCR	b	844	-	-	6/29/63/63	0/2/2/2
22	CLA	3	310	-	1/1/13/20	4/27/105/115	-
22	CLA	a	818	-	1/1/13/20	11/27/105/115	-
22	CLA	a	830	-	1/1/15/20	15/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	XAT	j	101	-	-	5/31/93/93	0/4/4/4
22	CLA	4	312	-	1/1/11/20	4/15/93/115	-
22	CLA	5	305	1	1/1/11/20	4/15/93/115	-
22	CLA	a	802	-	1/1/13/20	7/29/107/115	-
22	CLA	a	809	8	1/1/15/20	15/37/115/115	-
22	CLA	b	802	-	1/1/15/20	17/37/115/115	-
22	CLA	b	816	-	1/1/13/20	4/25/103/115	-
20	XAT	7	301	-	-	6/31/93/93	0/4/4/4
20	XAT	7	303	-	-	8/31/93/93	0/4/4/4
24	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
29	BCR	b	842	-	-	2/29/63/63	0/2/2/2
29	BCR	m	101	-	-	9/29/63/63	0/2/2/2
22	CLA	4	315	4	1/1/10/20	5/8/86/115	-
22	CLA	b	813	-	1/1/15/20	14/37/115/115	-
22	CLA	b	823	-	1/1/12/20	8/23/101/115	-
22	CLA	a	823	-	1/1/11/20	7/18/96/115	-
22	CLA	b	808	-	1/1/15/20	12/37/115/115	-
22	CLA	5	313	1	1/1/11/20	4/13/91/115	-
22	CLA	a	804	-	1/1/13/20	10/25/103/115	-
20	XAT	4	304	-	-	0/31/93/93	0/4/4/4
22	CLA	4	316	-	1/1/11/20	7/15/93/115	-
22	CLA	b	828	-	1/1/15/20	11/37/115/115	-
22	CLA	a	807	-	1/1/15/20	18/37/115/115	-
20	XAT	2	303	-	-	6/31/93/93	0/4/4/4
25	LHG	b	847	22	-	20/35/35/53	-
22	CLA	b	812	-	1/1/12/20	6/23/101/115	-
22	CLA	5	308	-	1/1/13/20	4/25/103/115	-
22	CLA	5	314	-	1/1/12/20	4/22/100/115	-
23	SQD	5	316	22	-	11/30/50/69	0/1/1/1
22	CLA	b	806	-	1/1/15/20	16/37/115/115	-
29	BCR	h	201	-	-	0/29/63/63	0/2/2/2
22	CLA	3	307	5	1/1/11/20	1/13/91/115	-

All (1145) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	312	CLA	C4B-NB	7.91	1.42	1.35
22	2	315	CLA	C4B-NB	7.81	1.42	1.35
22	a	842	CLA	C4B-NB	7.79	1.42	1.35
22	3	315	CLA	C4B-NB	7.70	1.42	1.35
22	4	315	CLA	C4B-NB	7.70	1.42	1.35
22	a	840	CLA	C4B-NB	7.69	1.42	1.35
22	a	818	CLA	C4B-NB	7.69	1.42	1.35
22	4	312	CLA	C4B-NB	7.69	1.42	1.35
22	b	837	CLA	C4B-NB	7.68	1.42	1.35
22	b	820	CLA	C4B-NB	7.68	1.42	1.35
22	5	313	CLA	C4B-NB	7.67	1.42	1.35
22	1	309	CLA	C4B-NB	7.67	1.42	1.35
22	h	203	CLA	C4B-NB	7.67	1.42	1.35
22	4	314	CLA	C4B-NB	7.65	1.42	1.35
22	a	813	CLA	C4B-NB	7.64	1.42	1.35
22	2	311	CLA	C4B-NB	7.62	1.42	1.35
22	1	305	CLA	C4B-NB	7.62	1.42	1.35
22	7	311	CLA	C4B-NB	7.61	1.42	1.35
22	4	306	CLA	C4B-NB	7.61	1.42	1.35
22	a	824	CLA	C4B-NB	7.61	1.42	1.35
22	1	314	CLA	C4B-NB	7.60	1.42	1.35
22	2	309	CLA	C4B-NB	7.60	1.42	1.35
22	9	314	CLA	C4B-NB	7.60	1.42	1.35
22	8	313	CLA	C4B-NB	7.60	1.42	1.35
22	5	305	CLA	C4B-NB	7.59	1.42	1.35
22	2	308	CLA	C4B-NB	7.59	1.42	1.35
22	b	802	CLA	C4B-NB	7.59	1.42	1.35
22	a	831	CLA	C4B-NB	7.59	1.42	1.35
22	j	102	CLA	C4B-NB	7.58	1.42	1.35
28	a	843	PQN	C3-C2	7.57	1.49	1.35
22	5	310	CLA	C4B-NB	7.57	1.42	1.35
22	a	808	CLA	C4B-NB	7.57	1.42	1.35
22	b	834	CLA	C4B-NB	7.57	1.42	1.35
22	b	840	CLA	C4B-NB	7.57	1.42	1.35
22	7	315	CLA	C4B-NB	7.56	1.42	1.35
22	7	313	CLA	C4B-NB	7.56	1.42	1.35
22	b	829	CLA	C4B-NB	7.56	1.42	1.35
22	2	313	CLA	C4B-NB	7.56	1.42	1.35
22	4	317	CLA	C4B-NB	7.56	1.41	1.35
22	7	307	CLA	C4B-NB	7.55	1.41	1.35
22	3	311	CLA	C4B-NB	7.55	1.41	1.35
22	a	825	CLA	C4B-NB	7.55	1.41	1.35
22	1	313	CLA	C4B-NB	7.55	1.41	1.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	312	CLA	C4B-NB	7.55	1.41	1.35
22	4	311	CLA	C4B-NB	7.54	1.41	1.35
22	9	318	CLA	C4B-NB	7.53	1.41	1.35
22	8	309	CLA	C4B-NB	7.53	1.41	1.35
22	4	309	CLA	C4B-NB	7.53	1.41	1.35
22	4	313	CLA	C4B-NB	7.53	1.41	1.35
22	a	817	CLA	C4B-NB	7.52	1.41	1.35
22	9	309	CLA	C4B-NB	7.52	1.41	1.35
22	7	317	CLA	C4B-NB	7.52	1.41	1.35
22	b	801	CLA	C4B-NB	7.52	1.41	1.35
22	b	828	CLA	C4B-NB	7.51	1.41	1.35
22	b	826	CLA	C4B-NB	7.51	1.41	1.35
22	2	316	CLA	C4B-NB	7.51	1.41	1.35
22	2	310	CLA	C4B-NB	7.51	1.41	1.35
22	2	314	CLA	C4B-NB	7.51	1.41	1.35
22	b	818	CLA	C4B-NB	7.50	1.41	1.35
22	a	804	CLA	C4B-NB	7.50	1.41	1.35
22	4	316	CLA	C4B-NB	7.50	1.41	1.35
22	4	307	CLA	C4B-NB	7.50	1.41	1.35
22	4	310	CLA	C4B-NB	7.49	1.41	1.35
22	2	306	CLA	C4B-NB	7.49	1.41	1.35
22	a	841	CLA	C4B-NB	7.49	1.41	1.35
22	b	839	CLA	C4B-NB	7.49	1.41	1.35
22	b	822	CLA	C4B-NB	7.48	1.41	1.35
22	3	307	CLA	C4B-NB	7.48	1.41	1.35
22	b	831	CLA	C4B-NB	7.47	1.41	1.35
22	a	810	CLA	C4B-NB	7.47	1.41	1.35
22	a	822	CLA	C4B-NB	7.47	1.41	1.35
22	a	834	CLA	C4B-NB	7.47	1.41	1.35
22	1	202	CLA	C4B-NB	7.47	1.41	1.35
22	3	312	CLA	C4B-NB	7.46	1.41	1.35
22	3	308	CLA	C4B-NB	7.46	1.41	1.35
22	8	312	CLA	C4B-NB	7.45	1.41	1.35
22	1	307	CLA	C4B-NB	7.45	1.41	1.35
22	5	306	CLA	C4B-NB	7.45	1.41	1.35
22	b	805	CLA	C4B-NB	7.45	1.41	1.35
22	3	310	CLA	C4B-NB	7.45	1.41	1.35
22	8	308	CLA	C4B-NB	7.44	1.41	1.35
22	a	837	CLA	C4B-NB	7.44	1.41	1.35
22	a	854	CLA	C4B-NB	7.44	1.41	1.35
22	b	809	CLA	C4B-NB	7.44	1.41	1.35
22	8	314	CLA	C4B-NB	7.44	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	306	CLA	C4B-NB	7.43	1.41	1.35
22	a	816	CLA	C4B-NB	7.43	1.41	1.35
22	f	803	CLA	C4B-NB	7.43	1.41	1.35
22	b	816	CLA	C4B-NB	7.43	1.41	1.35
22	9	310	CLA	C4B-NB	7.43	1.41	1.35
22	b	814	CLA	C4B-NB	7.43	1.41	1.35
22	8	310	CLA	C4B-NB	7.43	1.41	1.35
22	b	808	CLA	C4B-NB	7.42	1.41	1.35
22	a	805	CLA	C4B-NB	7.42	1.41	1.35
22	5	315	CLA	C4B-NB	7.42	1.41	1.35
22	a	820	CLA	C4B-NB	7.41	1.41	1.35
22	a	829	CLA	C4B-NB	7.41	1.41	1.35
22	7	314	CLA	C4B-NB	7.41	1.41	1.35
22	b	838	CLA	C4B-NB	7.41	1.41	1.35
22	j	103	CLA	C4B-NB	7.41	1.41	1.35
22	7	308	CLA	C4B-NB	7.40	1.41	1.35
22	1	310	CLA	C4B-NB	7.40	1.41	1.35
22	9	308	CLA	C4B-NB	7.40	1.41	1.35
22	9	313	CLA	C4B-NB	7.40	1.41	1.35
22	7	306	CLA	C4B-NB	7.40	1.41	1.35
22	b	804	CLA	C4B-NB	7.40	1.41	1.35
22	9	315	CLA	C4B-NB	7.40	1.41	1.35
22	b	827	CLA	C4B-NB	7.39	1.41	1.35
22	a	812	CLA	C4B-NB	7.39	1.41	1.35
22	a	815	CLA	C4B-NB	7.39	1.41	1.35
22	8	305	CLA	C4B-NB	7.39	1.41	1.35
22	a	823	CLA	C4B-NB	7.39	1.41	1.35
22	3	313	CLA	C4B-NB	7.39	1.41	1.35
22	b	824	CLA	C4B-NB	7.38	1.41	1.35
22	5	308	CLA	C4B-NB	7.38	1.41	1.35
22	1	308	CLA	C4B-NB	7.38	1.41	1.35
22	a	827	CLA	C4B-NB	7.38	1.41	1.35
22	7	310	CLA	C4B-NB	7.38	1.41	1.35
22	5	309	CLA	C4B-NB	7.37	1.41	1.35
22	b	811	CLA	C4B-NB	7.37	1.41	1.35
22	b	836	CLA	C4B-NB	7.37	1.41	1.35
22	a	826	CLA	C4B-NB	7.37	1.41	1.35
22	3	309	CLA	C4B-NB	7.36	1.41	1.35
28	b	841	PQN	C3-C2	7.36	1.48	1.35
22	7	312	CLA	C4B-NB	7.36	1.41	1.35
22	7	309	CLA	C4B-NB	7.36	1.41	1.35
22	a	836	CLA	C4B-NB	7.36	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	821	CLA	C4B-NB	7.35	1.41	1.35
22	a	811	CLA	C4B-NB	7.35	1.41	1.35
22	b	819	CLA	C4B-NB	7.34	1.41	1.35
22	b	832	CLA	C4B-NB	7.34	1.41	1.35
22	b	833	CLA	C4B-NB	7.34	1.41	1.35
22	l	203	CLA	C4B-NB	7.34	1.41	1.35
22	a	839	CLA	C4B-NB	7.33	1.41	1.35
22	l	204	CLA	C4B-NB	7.33	1.41	1.35
22	b	813	CLA	C4B-NB	7.33	1.41	1.35
22	l	306	CLA	C4B-NB	7.33	1.41	1.35
22	a	830	CLA	C4B-NB	7.32	1.41	1.35
22	9	311	CLA	C4B-NB	7.32	1.41	1.35
22	a	802	CLA	C4B-NB	7.31	1.41	1.35
22	a	832	CLA	C4B-NB	7.31	1.41	1.35
22	b	817	CLA	C4B-NB	7.31	1.41	1.35
22	b	803	CLA	C4B-NB	7.31	1.41	1.35
22	b	806	CLA	C4B-NB	7.31	1.41	1.35
22	a	819	CLA	C4B-NB	7.31	1.41	1.35
22	f	802	CLA	C4B-NB	7.31	1.41	1.35
22	a	833	CLA	C4B-NB	7.30	1.41	1.35
22	8	307	CLA	C4B-NB	7.30	1.41	1.35
22	5	314	CLA	C4B-NB	7.30	1.41	1.35
22	5	312	CLA	C4B-NB	7.30	1.41	1.35
22	a	835	CLA	C4B-NB	7.30	1.41	1.35
22	5	307	CLA	C4B-NB	7.29	1.41	1.35
22	a	844	CLA	C4B-NB	7.29	1.41	1.35
22	3	314	CLA	C4B-NB	7.29	1.41	1.35
22	b	823	CLA	C4B-NB	7.28	1.41	1.35
22	a	814	CLA	C4B-NB	7.28	1.41	1.35
22	b	810	CLA	C4B-NB	7.28	1.41	1.35
22	b	815	CLA	C4B-NB	7.28	1.41	1.35
22	h	205	CLA	C4B-NB	7.28	1.41	1.35
22	b	812	CLA	C4B-NB	7.27	1.41	1.35
22	8	311	CLA	C4B-NB	7.26	1.41	1.35
22	9	312	CLA	C4B-NB	7.26	1.41	1.35
22	5	311	CLA	C4B-NB	7.26	1.41	1.35
22	b	807	CLA	C4B-NB	7.26	1.41	1.35
22	a	803	CLA	C4B-NB	7.25	1.41	1.35
22	b	825	CLA	C4B-NB	7.25	1.41	1.35
22	a	838	CLA	C4B-NB	7.24	1.41	1.35
22	2	307	CLA	C4B-NB	7.23	1.41	1.35
22	b	821	CLA	C4B-NB	7.23	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	801	CLA	C4B-NB	7.23	1.41	1.35
22	b	835	CLA	C4B-NB	7.21	1.41	1.35
22	1	311	CLA	C4B-NB	7.20	1.41	1.35
22	4	308	CLA	C4B-NB	7.19	1.41	1.35
22	9	316	CLA	C4B-NB	7.18	1.41	1.35
22	b	830	CLA	C4B-NB	7.18	1.41	1.35
22	a	807	CLA	C4B-NB	7.16	1.41	1.35
22	7	316	CLA	C4B-NB	7.11	1.41	1.35
22	a	809	CLA	C4B-NB	7.09	1.41	1.35
22	a	828	CLA	C4B-NB	7.09	1.41	1.35
22	a	806	CLA	C4B-NB	6.14	1.40	1.35
28	a	843	PQN	C10-C5	4.84	1.48	1.40
28	b	841	PQN	C10-C5	4.83	1.48	1.40
23	5	316	SQD	O8-S	4.63	1.64	1.47
23	1	315	SQD	O8-S	4.60	1.63	1.47
24	h	204	A1L1F	O7-C54	4.58	1.45	1.35
24	9	302	A1L1F	O7-C54	4.57	1.45	1.35
24	8	304	A1L1F	O7-C54	4.55	1.45	1.35
24	1	304	A1L1F	O7-C54	4.46	1.45	1.35
23	1	315	SQD	O48-C23	4.29	1.45	1.33
26	8	315	DGD	O1G-C1A	4.27	1.45	1.33
24	1	304	A1L1F	O13-C45	4.23	1.45	1.33
23	5	316	SQD	O48-C23	4.23	1.45	1.33
27	a	853	LMG	O8-C28	4.22	1.45	1.33
23	1	315	SQD	O47-C7	4.20	1.46	1.34
24	h	204	A1L1F	O13-C45	4.15	1.45	1.33
27	a	853	LMG	O7-C10	4.14	1.46	1.34
27	j	105	LMG	O8-C28	4.10	1.45	1.33
23	5	316	SQD	O47-C7	4.10	1.45	1.34
24	8	304	A1L1F	O13-C45	4.09	1.45	1.33
27	2	317	LMG	O8-C28	4.05	1.45	1.33
22	a	806	CLA	C4D-ND	-4.03	1.32	1.37
26	4	318	DGD	O1G-C1A	4.02	1.45	1.33
26	b	848	DGD	O2G-C1B	4.00	1.45	1.34
22	2	313	CLA	C1D-ND	3.99	1.42	1.37
22	h	203	CLA	C1D-ND	3.98	1.42	1.37
26	b	848	DGD	O1G-C1A	3.96	1.44	1.33
22	a	804	CLA	C1D-ND	3.96	1.42	1.37
22	7	306	CLA	C1D-ND	3.96	1.42	1.37
27	2	317	LMG	O7-C10	3.95	1.45	1.34
22	8	314	CLA	C1D-ND	3.95	1.42	1.37
22	1	312	CLA	C1D-ND	3.95	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	308	CLA	C1D-ND	3.94	1.42	1.37
22	a	837	CLA	C1D-ND	3.94	1.42	1.37
22	3	314	CLA	C1D-ND	3.94	1.42	1.37
22	8	308	CLA	C1D-ND	3.94	1.42	1.37
22	8	313	CLA	C1D-ND	3.93	1.42	1.37
22	a	828	CLA	C1D-ND	3.93	1.42	1.37
24	9	302	A1L1F	O13-C45	3.92	1.44	1.33
22	5	308	CLA	C1D-ND	3.91	1.42	1.37
22	9	312	CLA	C1D-ND	3.91	1.42	1.37
22	8	310	CLA	C1D-ND	3.91	1.42	1.37
22	9	313	CLA	C1D-ND	3.90	1.42	1.37
22	9	310	CLA	C1D-ND	3.90	1.42	1.37
22	4	307	CLA	C1D-ND	3.90	1.42	1.37
21	1	301	A1L1G	C38-C39	3.89	1.40	1.35
22	9	315	CLA	C1D-ND	3.89	1.42	1.37
22	7	315	CLA	C1D-ND	3.89	1.42	1.37
22	7	307	CLA	C1D-ND	3.89	1.42	1.37
22	2	311	CLA	C1D-ND	3.88	1.42	1.37
22	b	820	CLA	C1D-ND	3.88	1.42	1.37
24	h	204	A1L1F	C57-C2	-3.88	1.25	1.32
22	2	315	CLA	C1D-ND	3.88	1.42	1.37
22	a	840	CLA	C1D-ND	3.87	1.42	1.37
22	4	306	CLA	C1D-ND	3.87	1.42	1.37
22	a	814	CLA	C1D-ND	3.87	1.42	1.37
22	l	204	CLA	C1D-ND	3.87	1.42	1.37
22	b	840	CLA	C1D-ND	3.87	1.42	1.37
22	4	316	CLA	C1D-ND	3.87	1.42	1.37
26	4	318	DGD	O2G-C1B	3.87	1.45	1.34
22	2	307	CLA	C1D-ND	3.86	1.42	1.37
22	7	308	CLA	C1D-ND	3.86	1.42	1.37
22	a	811	CLA	C1D-ND	3.86	1.42	1.37
22	b	818	CLA	C1D-ND	3.86	1.42	1.37
22	j	103	CLA	C1D-ND	3.86	1.42	1.37
22	3	315	CLA	C1D-ND	3.86	1.42	1.37
22	3	311	CLA	C1D-ND	3.86	1.42	1.37
22	2	306	CLA	C1D-ND	3.86	1.42	1.37
22	a	815	CLA	C1D-ND	3.86	1.42	1.37
27	j	105	LMG	O7-C10	3.86	1.45	1.34
22	b	814	CLA	C1D-ND	3.85	1.42	1.37
24	8	304	A1L1F	C57-C2	-3.85	1.25	1.32
22	9	314	CLA	C1D-ND	3.85	1.42	1.37
22	7	317	CLA	C1D-ND	3.85	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	305	CLA	C1D-ND	3.85	1.42	1.37
22	5	311	CLA	C1D-ND	3.84	1.42	1.37
22	5	314	CLA	C1D-ND	3.84	1.42	1.37
22	a	835	CLA	C1D-ND	3.84	1.42	1.37
22	5	313	CLA	C1D-ND	3.84	1.42	1.37
22	b	839	CLA	C1D-ND	3.84	1.42	1.37
22	7	311	CLA	C1D-ND	3.84	1.42	1.37
22	2	314	CLA	C1D-ND	3.84	1.42	1.37
22	8	309	CLA	C1D-ND	3.83	1.42	1.37
22	a	839	CLA	C1D-ND	3.83	1.42	1.37
22	b	824	CLA	C1D-ND	3.83	1.42	1.37
22	3	310	CLA	C1D-ND	3.83	1.42	1.37
22	1	310	CLA	C1D-ND	3.83	1.42	1.37
22	b	833	CLA	C1D-ND	3.83	1.42	1.37
22	4	315	CLA	C1D-ND	3.83	1.42	1.37
22	7	310	CLA	C1D-ND	3.83	1.42	1.37
22	a	817	CLA	C1D-ND	3.83	1.42	1.37
22	5	306	CLA	C1D-ND	3.82	1.42	1.37
22	4	314	CLA	C1D-ND	3.82	1.42	1.37
22	a	829	CLA	C1D-ND	3.82	1.42	1.37
22	7	316	CLA	C1D-ND	3.82	1.42	1.37
22	b	807	CLA	C1D-ND	3.82	1.42	1.37
22	j	102	CLA	C1D-ND	3.82	1.42	1.37
22	5	305	CLA	C1D-ND	3.82	1.42	1.37
22	5	309	CLA	C1D-ND	3.82	1.42	1.37
22	b	819	CLA	C1D-ND	3.82	1.42	1.37
22	a	838	CLA	C1D-ND	3.82	1.42	1.37
22	5	310	CLA	C1D-ND	3.82	1.42	1.37
22	1	311	CLA	C1D-ND	3.81	1.42	1.37
24	9	302	A1L1F	C57-C2	-3.81	1.25	1.32
22	b	817	CLA	C1D-ND	3.81	1.42	1.37
22	a	822	CLA	C1D-ND	3.81	1.42	1.37
22	b	826	CLA	C1D-ND	3.81	1.42	1.37
22	f	802	CLA	C1D-ND	3.81	1.42	1.37
22	7	313	CLA	C1D-ND	3.81	1.42	1.37
22	a	834	CLA	C1D-ND	3.81	1.42	1.37
22	a	821	CLA	C1D-ND	3.81	1.42	1.37
22	7	314	CLA	C1D-ND	3.81	1.42	1.37
22	1	314	CLA	C1D-ND	3.81	1.42	1.37
22	a	819	CLA	C1D-ND	3.81	1.42	1.37
22	a	825	CLA	C1D-ND	3.81	1.42	1.37
22	2	309	CLA	C1D-ND	3.80	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	205	CLA	C1D-ND	3.80	1.42	1.37
22	8	306	CLA	C1D-ND	3.80	1.42	1.37
22	a	809	CLA	C1D-ND	3.80	1.42	1.37
22	b	837	CLA	C1D-ND	3.80	1.42	1.37
22	1	306	CLA	C1D-ND	3.80	1.42	1.37
22	b	805	CLA	C1D-ND	3.80	1.42	1.37
22	3	313	CLA	C1D-ND	3.79	1.42	1.37
22	b	835	CLA	C1D-ND	3.79	1.42	1.37
22	b	813	CLA	C1D-ND	3.79	1.42	1.37
22	a	820	CLA	C1D-ND	3.79	1.42	1.37
22	a	826	CLA	C1D-ND	3.79	1.42	1.37
22	b	834	CLA	C1D-ND	3.79	1.42	1.37
22	2	312	CLA	C1D-ND	3.79	1.42	1.37
22	a	807	CLA	C1D-ND	3.78	1.42	1.37
22	b	838	CLA	C1D-ND	3.78	1.42	1.37
22	9	318	CLA	C1D-ND	3.78	1.42	1.37
22	b	816	CLA	C1D-ND	3.78	1.42	1.37
22	4	309	CLA	C1D-ND	3.78	1.42	1.37
22	3	309	CLA	C1D-ND	3.78	1.42	1.37
22	4	310	CLA	C1D-ND	3.78	1.42	1.37
22	7	312	CLA	C1D-ND	3.78	1.42	1.37
22	1	309	CLA	C1D-ND	3.78	1.42	1.37
22	8	307	CLA	C1D-ND	3.77	1.42	1.37
22	3	312	CLA	C1D-ND	3.77	1.42	1.37
22	a	836	CLA	C1D-ND	3.77	1.42	1.37
22	b	829	CLA	C1D-ND	3.77	1.42	1.37
22	7	309	CLA	C1D-ND	3.77	1.42	1.37
22	4	317	CLA	C1D-ND	3.77	1.42	1.37
26	8	315	DGD	O2G-C1B	3.77	1.44	1.34
22	1	308	CLA	C1D-ND	3.77	1.42	1.37
22	5	312	CLA	C1D-ND	3.76	1.42	1.37
21	7	302	A1L1G	C38-C39	3.76	1.40	1.35
22	9	316	CLA	C1D-ND	3.76	1.42	1.37
22	1	307	CLA	C1D-ND	3.76	1.42	1.37
22	a	816	CLA	C1D-ND	3.76	1.42	1.37
22	5	315	CLA	C1D-ND	3.75	1.42	1.37
22	a	841	CLA	C1D-ND	3.75	1.42	1.37
21	9	301	A1L1G	C38-C39	3.75	1.40	1.35
22	b	812	CLA	C1D-ND	3.75	1.42	1.37
22	b	831	CLA	C1D-ND	3.75	1.42	1.37
22	4	312	CLA	C1D-ND	3.74	1.42	1.37
22	a	844	CLA	C1D-ND	3.74	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	821	CLA	C1D-ND	3.74	1.42	1.37
22	a	813	CLA	C1D-ND	3.74	1.42	1.37
22	a	818	CLA	C1D-ND	3.74	1.42	1.37
22	b	808	CLA	C1D-ND	3.74	1.42	1.37
22	a	823	CLA	C1D-ND	3.74	1.42	1.37
22	a	854	CLA	C1D-ND	3.74	1.42	1.37
22	a	805	CLA	C1D-ND	3.74	1.42	1.37
22	a	808	CLA	C1D-ND	3.74	1.42	1.37
22	l	202	CLA	C1D-ND	3.73	1.42	1.37
22	2	308	CLA	C1D-ND	3.73	1.42	1.37
22	b	801	CLA	C1D-ND	3.73	1.42	1.37
21	1	301	A1L1G	C35-C34	3.73	1.40	1.35
22	1	305	CLA	C1D-ND	3.73	1.42	1.37
22	4	308	CLA	C1D-ND	3.72	1.42	1.37
22	a	803	CLA	C1D-ND	3.72	1.42	1.37
22	f	803	CLA	C1D-ND	3.72	1.42	1.37
22	b	815	CLA	C1D-ND	3.72	1.42	1.37
22	a	810	CLA	C1D-ND	3.72	1.42	1.37
22	9	308	CLA	C1D-ND	3.72	1.42	1.37
22	a	842	CLA	C1D-ND	3.72	1.42	1.37
22	b	828	CLA	C1D-ND	3.72	1.42	1.37
22	4	311	CLA	C1D-ND	3.71	1.42	1.37
22	b	825	CLA	C1D-ND	3.71	1.42	1.37
22	a	832	CLA	C1D-ND	3.71	1.42	1.37
22	b	822	CLA	C1D-ND	3.71	1.42	1.37
22	8	311	CLA	C1D-ND	3.71	1.42	1.37
22	a	824	CLA	C1D-ND	3.71	1.42	1.37
22	a	831	CLA	C1D-ND	3.70	1.42	1.37
22	a	812	CLA	C1D-ND	3.69	1.42	1.37
29	m	101	BCR	C1-C6	-3.69	1.48	1.53
22	b	809	CLA	C1D-ND	3.69	1.42	1.37
22	9	311	CLA	C1D-ND	3.68	1.42	1.37
22	l	203	CLA	C1D-ND	3.68	1.42	1.37
22	3	307	CLA	C1D-ND	3.68	1.42	1.37
22	b	810	CLA	C1D-ND	3.68	1.42	1.37
22	4	313	CLA	C1D-ND	3.68	1.42	1.37
22	b	806	CLA	C1D-ND	3.68	1.42	1.37
22	1	313	CLA	C1D-ND	3.68	1.42	1.37
22	a	830	CLA	C1D-ND	3.68	1.42	1.37
22	2	316	CLA	C1D-ND	3.67	1.42	1.37
22	b	836	CLA	C1D-ND	3.66	1.42	1.37
21	9	301	A1L1G	C35-C34	3.66	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	827	CLA	C1D-ND	3.66	1.42	1.37
22	b	823	CLA	C1D-ND	3.66	1.42	1.37
22	5	307	CLA	C1D-ND	3.65	1.42	1.37
22	8	312	CLA	C1D-ND	3.65	1.42	1.37
21	9	306	A1L1G	C35-C34	3.64	1.40	1.35
22	a	827	CLA	C1D-ND	3.63	1.42	1.37
22	2	310	CLA	C1D-ND	3.63	1.42	1.37
22	b	832	CLA	C1D-ND	3.63	1.42	1.37
21	3	302	A1L1G	C35-C34	3.62	1.40	1.35
24	1	304	A1L1F	C57-C2	-3.62	1.25	1.32
22	b	802	CLA	C1D-ND	3.62	1.42	1.37
22	b	811	CLA	C1D-ND	3.60	1.42	1.37
22	9	309	CLA	C1D-ND	3.58	1.42	1.37
21	3	306	A1L1G	C38-C39	3.57	1.40	1.35
22	b	830	CLA	C1D-ND	3.55	1.42	1.37
21	3	302	A1L1G	C38-C39	3.55	1.40	1.35
22	b	803	CLA	C1D-ND	3.54	1.42	1.37
22	a	801	CLA	C1D-ND	3.53	1.42	1.37
22	a	802	CLA	C1D-ND	3.53	1.42	1.37
22	b	811	CLA	CAB-C3B	-3.50	1.44	1.51
21	9	306	A1L1G	C38-C39	3.47	1.40	1.35
22	a	833	CLA	C1D-ND	3.46	1.42	1.37
21	5	303	A1L1G	C38-C39	3.45	1.40	1.35
21	7	302	A1L1G	C35-C34	3.44	1.40	1.35
21	3	306	A1L1G	C35-C34	3.41	1.40	1.35
21	5	303	A1L1G	C35-C34	3.40	1.40	1.35
21	3	302	A1L1G	C42-C44	3.38	1.40	1.35
22	4	313	CLA	CHC-C1C	3.32	1.43	1.35
22	b	804	CLA	C1D-ND	3.28	1.41	1.37
22	a	802	CLA	CHC-C1C	3.26	1.43	1.35
22	b	838	CLA	CHC-C1C	3.26	1.43	1.35
22	7	313	CLA	CHC-C1C	3.25	1.43	1.35
22	b	816	CLA	CHC-C1C	3.25	1.43	1.35
22	4	312	CLA	CHC-C1C	3.24	1.43	1.35
22	2	308	CLA	CHC-C1C	3.24	1.43	1.35
22	8	311	CLA	CHC-C1C	3.24	1.43	1.35
22	b	836	CLA	CHC-C1C	3.24	1.43	1.35
22	b	814	CLA	CHC-C1C	3.23	1.43	1.35
22	8	312	CLA	CHC-C1C	3.23	1.43	1.35
22	a	818	CLA	CHC-C1C	3.23	1.43	1.35
22	7	311	CLA	CHC-C1C	3.23	1.43	1.35
22	a	822	CLA	CHC-C1C	3.23	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	813	CLA	CHC-C1C	3.22	1.43	1.35
22	a	829	CLA	CHC-C1C	3.22	1.43	1.35
22	a	819	CLA	CHC-C1C	3.22	1.43	1.35
22	9	308	CLA	CHC-C1C	3.22	1.43	1.35
22	3	315	CLA	CHC-C1C	3.21	1.43	1.35
22	b	811	CLA	CHC-C1C	3.21	1.43	1.35
22	a	841	CLA	CHC-C1C	3.21	1.43	1.35
22	f	803	CLA	CHC-C1C	3.21	1.43	1.35
22	7	308	CLA	CHC-C1C	3.21	1.43	1.35
22	9	318	CLA	CHC-C1C	3.20	1.43	1.35
22	b	835	CLA	CHC-C1C	3.20	1.43	1.35
22	b	813	CLA	CHC-C1C	3.20	1.43	1.35
22	b	828	CLA	CHC-C1C	3.20	1.43	1.35
22	a	837	CLA	CHC-C1C	3.20	1.43	1.35
22	b	806	CLA	CHC-C1C	3.20	1.43	1.35
22	b	802	CLA	CHC-C1C	3.20	1.43	1.35
22	5	312	CLA	CHC-C1C	3.20	1.43	1.35
22	9	311	CLA	CHC-C1C	3.20	1.43	1.35
22	8	313	CLA	CHC-C1C	3.20	1.43	1.35
22	b	831	CLA	CHC-C1C	3.20	1.43	1.35
22	a	804	CLA	CHC-C1C	3.20	1.43	1.35
22	a	820	CLA	CHC-C1C	3.20	1.43	1.35
22	a	828	CLA	C4D-ND	-3.20	1.33	1.37
22	a	809	CLA	CHC-C1C	3.20	1.43	1.35
22	7	306	CLA	CHC-C1C	3.20	1.43	1.35
22	5	314	CLA	CHC-C1C	3.20	1.43	1.35
22	5	315	CLA	CHC-C1C	3.20	1.43	1.35
22	1	311	CLA	CHC-C1C	3.19	1.43	1.35
22	1	314	CLA	CHC-C1C	3.19	1.43	1.35
22	2	309	CLA	CHC-C1C	3.19	1.43	1.35
22	a	832	CLA	CHC-C1C	3.19	1.43	1.35
22	b	832	CLA	CHC-C1C	3.19	1.43	1.35
22	8	305	CLA	CHC-C1C	3.19	1.43	1.35
22	b	805	CLA	CHC-C1C	3.19	1.43	1.35
22	b	815	CLA	CHC-C1C	3.19	1.43	1.35
22	1	308	CLA	CHC-C1C	3.19	1.43	1.35
22	b	833	CLA	CHC-C1C	3.18	1.43	1.35
22	5	311	CLA	CHC-C1C	3.18	1.43	1.35
22	2	315	CLA	CHC-C1C	3.18	1.43	1.35
22	7	312	CLA	CHC-C1C	3.18	1.43	1.35
22	b	834	CLA	CHC-C1C	3.18	1.43	1.35
22	b	817	CLA	CHC-C1C	3.18	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	312	CLA	CHC-C1C	3.18	1.43	1.35
22	1	310	CLA	CHC-C1C	3.18	1.43	1.35
22	7	314	CLA	CHC-C1C	3.18	1.43	1.35
22	5	313	CLA	CHC-C1C	3.18	1.43	1.35
22	8	309	CLA	CHC-C1C	3.17	1.43	1.35
22	a	808	CLA	CHC-C1C	3.17	1.43	1.35
22	a	826	CLA	CHC-C1C	3.17	1.43	1.35
22	a	824	CLA	CHC-C1C	3.17	1.43	1.35
22	a	833	CLA	CHC-C1C	3.17	1.43	1.35
22	a	827	CLA	CHC-C1C	3.17	1.43	1.35
22	a	842	CLA	CHC-C1C	3.17	1.43	1.35
22	2	313	CLA	CHC-C1C	3.17	1.43	1.35
22	8	306	CLA	CHC-C1C	3.17	1.43	1.35
22	8	314	CLA	CHC-C1C	3.17	1.43	1.35
22	2	311	CLA	CHC-C1C	3.17	1.43	1.35
22	a	844	CLA	CHC-C1C	3.17	1.43	1.35
22	4	314	CLA	CHC-C1C	3.17	1.43	1.35
22	b	825	CLA	CHC-C1C	3.17	1.43	1.35
22	b	809	CLA	CHC-C1C	3.17	1.43	1.35
22	h	205	CLA	CHC-C1C	3.16	1.43	1.35
22	f	802	CLA	CHC-C1C	3.16	1.43	1.35
22	b	827	CLA	CHC-C1C	3.16	1.43	1.35
22	a	854	CLA	CHC-C1C	3.16	1.43	1.35
22	9	312	CLA	CHC-C1C	3.16	1.43	1.35
22	2	310	CLA	CHC-C1C	3.16	1.43	1.35
22	3	312	CLA	CHC-C1C	3.16	1.43	1.35
22	a	811	CLA	CHC-C1C	3.16	1.43	1.35
22	b	823	CLA	CHC-C1C	3.16	1.43	1.35
22	5	306	CLA	CHC-C1C	3.16	1.43	1.35
22	4	315	CLA	CHC-C1C	3.16	1.43	1.35
22	a	803	CLA	CHC-C1C	3.16	1.43	1.35
22	b	807	CLA	CHC-C1C	3.16	1.43	1.35
22	7	310	CLA	CHC-C1C	3.16	1.43	1.35
22	9	314	CLA	CHC-C1C	3.16	1.43	1.35
22	a	828	CLA	CHC-C1C	3.16	1.43	1.35
22	b	812	CLA	CHC-C1C	3.16	1.43	1.35
22	a	823	CLA	CHC-C1C	3.16	1.43	1.35
22	3	311	CLA	CHC-C1C	3.15	1.43	1.35
22	8	310	CLA	CHC-C1C	3.15	1.43	1.35
22	2	316	CLA	CHC-C1C	3.15	1.43	1.35
22	a	814	CLA	CHC-C1C	3.15	1.43	1.35
22	a	816	CLA	CHC-C1C	3.15	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	309	CLA	CHC-C1C	3.15	1.43	1.35
22	9	309	CLA	CHC-C1C	3.15	1.43	1.35
22	3	309	CLA	CHC-C1C	3.15	1.43	1.35
22	1	202	CLA	CHC-C1C	3.15	1.43	1.35
22	5	309	CLA	CHC-C1C	3.15	1.43	1.35
22	4	310	CLA	CHC-C1C	3.15	1.43	1.35
22	2	312	CLA	CHC-C1C	3.15	1.43	1.35
22	7	315	CLA	CHC-C1C	3.15	1.43	1.35
22	4	309	CLA	CHC-C1C	3.15	1.43	1.35
22	3	313	CLA	CHC-C1C	3.15	1.43	1.35
22	a	803	CLA	C4D-ND	-3.15	1.33	1.37
22	5	307	CLA	CHC-C1C	3.14	1.43	1.35
22	9	310	CLA	CHC-C1C	3.14	1.43	1.35
22	4	308	CLA	CHC-C1C	3.14	1.43	1.35
22	1	305	CLA	CHC-C1C	3.14	1.43	1.35
22	b	822	CLA	CHC-C1C	3.14	1.43	1.35
22	a	805	CLA	CHC-C1C	3.14	1.43	1.35
22	a	840	CLA	CHC-C1C	3.14	1.43	1.35
22	b	837	CLA	CHC-C1C	3.14	1.43	1.35
22	l	204	CLA	CHC-C1C	3.14	1.43	1.35
22	a	830	CLA	CHC-C1C	3.14	1.43	1.35
22	l	203	CLA	CHC-C1C	3.14	1.43	1.35
22	9	313	CLA	CHC-C1C	3.14	1.43	1.35
22	7	309	CLA	CHC-C1C	3.14	1.43	1.35
22	a	836	CLA	CHC-C1C	3.14	1.43	1.35
22	b	840	CLA	C4D-ND	-3.14	1.33	1.37
22	9	315	CLA	CHC-C1C	3.14	1.43	1.35
22	7	307	CLA	CHC-C1C	3.14	1.43	1.35
29	m	101	BCR	C30-C25	-3.14	1.49	1.53
22	b	830	CLA	CHC-C1C	3.14	1.43	1.35
22	5	310	CLA	CHC-C1C	3.13	1.43	1.35
22	a	834	CLA	CHC-C1C	3.13	1.43	1.35
22	b	804	CLA	CHC-C1C	3.13	1.43	1.35
22	1	307	CLA	CHC-C1C	3.13	1.43	1.35
22	j	102	CLA	CHC-C1C	3.13	1.43	1.35
22	4	317	CLA	CHC-C1C	3.13	1.43	1.35
22	4	307	CLA	CHC-C1C	3.13	1.43	1.35
22	a	815	CLA	CHC-C1C	3.13	1.43	1.35
22	b	840	CLA	CHC-C1C	3.13	1.43	1.35
22	a	817	CLA	CHC-C1C	3.13	1.43	1.35
22	b	824	CLA	CHC-C1C	3.13	1.43	1.35
22	b	821	CLA	CHC-C1C	3.13	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	839	CLA	CHC-C1C	3.13	1.43	1.35
22	4	311	CLA	CHC-C1C	3.12	1.43	1.35
22	3	307	CLA	CHC-C1C	3.12	1.43	1.35
22	a	812	CLA	CHC-C1C	3.12	1.43	1.35
22	2	314	CLA	CHC-C1C	3.12	1.43	1.35
22	1	313	CLA	CHC-C1C	3.12	1.43	1.35
22	a	838	CLA	CHC-C1C	3.12	1.43	1.35
22	5	308	CLA	CHC-C1C	3.12	1.43	1.35
22	a	835	CLA	CHC-C1C	3.11	1.42	1.35
22	3	310	CLA	CHC-C1C	3.11	1.42	1.35
22	b	820	CLA	CHC-C1C	3.11	1.42	1.35
22	b	803	CLA	CHC-C1C	3.11	1.42	1.35
22	7	317	CLA	CHC-C1C	3.11	1.42	1.35
22	2	306	CLA	CHC-C1C	3.11	1.42	1.35
22	a	810	CLA	CHC-C1C	3.11	1.42	1.35
22	5	307	CLA	C4D-ND	-3.11	1.33	1.37
22	4	308	CLA	C4D-ND	-3.11	1.33	1.37
22	h	205	CLA	C4D-ND	-3.11	1.33	1.37
22	1	306	CLA	CHC-C1C	3.11	1.42	1.35
22	h	203	CLA	CHC-C1C	3.10	1.42	1.35
22	8	308	CLA	CHC-C1C	3.10	1.42	1.35
22	8	307	CLA	CHC-C1C	3.10	1.42	1.35
22	a	821	CLA	CHC-C1C	3.10	1.42	1.35
22	5	305	CLA	CHC-C1C	3.10	1.42	1.35
22	3	314	CLA	CHC-C1C	3.09	1.42	1.35
21	7	302	A1L1G	C42-C44	3.09	1.39	1.35
22	b	801	CLA	CHC-C1C	3.09	1.42	1.35
22	b	819	CLA	C4D-ND	-3.09	1.33	1.37
22	5	312	CLA	C4D-ND	-3.09	1.33	1.37
22	b	819	CLA	CHC-C1C	3.09	1.42	1.35
22	3	308	CLA	CHC-C1C	3.09	1.42	1.35
22	a	825	CLA	CHC-C1C	3.08	1.42	1.35
22	j	103	CLA	CHC-C1C	3.08	1.42	1.35
22	b	808	CLA	CHC-C1C	3.08	1.42	1.35
22	4	306	CLA	CHC-C1C	3.08	1.42	1.35
22	4	316	CLA	CHC-C1C	3.08	1.42	1.35
22	b	826	CLA	CHC-C1C	3.08	1.42	1.35
22	a	801	CLA	CHC-C1C	3.08	1.42	1.35
22	b	826	CLA	C4D-ND	-3.07	1.33	1.37
22	a	827	CLA	C4D-ND	-3.07	1.33	1.37
22	9	316	CLA	CHC-C1C	3.07	1.42	1.35
22	a	807	CLA	CHC-C1C	3.07	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	822	CLA	C4D-ND	-3.07	1.33	1.37
22	a	829	CLA	C4D-ND	-3.07	1.33	1.37
21	9	301	A1L1G	C42-C44	3.07	1.39	1.35
22	9	308	CLA	C4D-ND	-3.07	1.33	1.37
22	b	825	CLA	C4D-ND	-3.06	1.33	1.37
22	2	307	CLA	CHC-C1C	3.06	1.42	1.35
22	b	830	CLA	C4D-ND	-3.06	1.33	1.37
22	7	316	CLA	CHC-C1C	3.06	1.42	1.35
22	1	204	CLA	C4D-ND	-3.06	1.33	1.37
22	8	307	CLA	C4D-ND	-3.05	1.33	1.37
22	7	309	CLA	C4D-ND	-3.05	1.33	1.37
22	b	817	CLA	C4D-ND	-3.05	1.33	1.37
22	a	807	CLA	C4D-ND	-3.05	1.33	1.37
22	3	309	CLA	C4D-ND	-3.05	1.33	1.37
22	a	830	CLA	C4D-ND	-3.04	1.33	1.37
22	b	829	CLA	CMB-C2B	-3.04	1.45	1.51
22	b	818	CLA	CHC-C1C	3.04	1.42	1.35
22	a	854	CLA	C4D-ND	-3.04	1.33	1.37
22	9	316	CLA	C4D-ND	-3.04	1.33	1.37
22	2	308	CLA	C4D-ND	-3.03	1.33	1.37
22	b	813	CLA	C4D-ND	-3.02	1.33	1.37
22	b	832	CLA	C4D-ND	-3.02	1.33	1.37
22	a	819	CLA	C4D-ND	-3.02	1.33	1.37
22	1	305	CLA	C4D-ND	-3.02	1.33	1.37
22	b	815	CLA	C4D-ND	-3.01	1.33	1.37
22	b	835	CLA	C4D-ND	-3.01	1.33	1.37
22	4	309	CLA	C4D-ND	-3.01	1.33	1.37
22	a	838	CLA	C4D-ND	-3.01	1.33	1.37
22	b	810	CLA	CHC-C1C	3.01	1.42	1.35
22	8	311	CLA	C4D-ND	-3.01	1.33	1.37
22	a	816	CLA	C4D-ND	-3.01	1.33	1.37
22	1	203	CLA	C4D-ND	-3.01	1.33	1.37
22	a	801	CLA	C4D-ND	-3.01	1.33	1.37
22	a	808	CLA	C4D-ND	-3.01	1.33	1.37
22	a	814	CLA	C4D-ND	-3.01	1.33	1.37
22	9	315	CLA	C4D-ND	-3.00	1.33	1.37
22	9	318	CLA	C4D-ND	-3.00	1.33	1.37
22	8	312	CLA	C4D-ND	-3.00	1.33	1.37
22	1	311	CLA	C4D-ND	-3.00	1.33	1.37
22	b	802	CLA	C4D-ND	-3.00	1.33	1.37
22	b	820	CLA	C4D-ND	-2.99	1.33	1.37
22	a	834	CLA	C4D-ND	-2.99	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	831	CLA	CMB-C2B	-2.99	1.45	1.51
22	b	836	CLA	C4D-ND	-2.99	1.33	1.37
22	b	816	CLA	C4D-ND	-2.98	1.33	1.37
22	f	802	CLA	C4D-ND	-2.98	1.33	1.37
22	b	823	CLA	C4D-ND	-2.98	1.33	1.37
22	a	831	CLA	CHC-C1C	2.98	1.42	1.35
22	b	828	CLA	C4D-ND	-2.98	1.33	1.37
22	l	202	CLA	C4D-ND	-2.97	1.33	1.37
22	7	313	CLA	C4D-ND	-2.97	1.33	1.37
22	8	313	CLA	C4D-ND	-2.97	1.33	1.37
22	3	313	CLA	C4D-ND	-2.97	1.33	1.37
22	a	806	CLA	CHC-C1C	2.96	1.42	1.35
22	5	308	CLA	C4D-ND	-2.96	1.33	1.37
22	j	102	CLA	C4D-ND	-2.96	1.33	1.37
22	b	829	CLA	CHC-C1C	2.95	1.42	1.35
22	a	832	CLA	C4D-ND	-2.95	1.33	1.37
22	b	838	CLA	C4D-ND	-2.95	1.33	1.37
22	4	316	CLA	C4D-ND	-2.95	1.33	1.37
22	9	309	CLA	C4D-ND	-2.95	1.33	1.37
22	4	312	CLA	C4D-ND	-2.95	1.33	1.37
22	9	313	CLA	C4D-ND	-2.94	1.33	1.37
22	a	824	CLA	C4D-ND	-2.94	1.33	1.37
22	a	842	CLA	C4D-ND	-2.94	1.33	1.37
24	9	302	A1L1F	C6-C1	-2.94	1.49	1.54
22	a	831	CLA	C4D-ND	-2.94	1.33	1.37
22	b	806	CLA	C4D-ND	-2.94	1.33	1.37
22	2	309	CLA	C4D-ND	-2.94	1.33	1.37
22	3	310	CLA	C4D-ND	-2.94	1.33	1.37
22	8	310	CLA	C4D-ND	-2.94	1.33	1.37
22	a	815	CLA	C4D-ND	-2.94	1.33	1.37
22	a	810	CLA	C4D-ND	-2.93	1.33	1.37
22	b	837	CLA	C4D-ND	-2.93	1.33	1.37
22	9	311	CLA	C4D-ND	-2.93	1.33	1.37
22	5	311	CLA	C4D-ND	-2.93	1.33	1.37
22	9	312	CLA	C4D-ND	-2.93	1.33	1.37
22	5	313	CLA	C4D-ND	-2.93	1.33	1.37
23	5	316	SQD	C6-S	-2.93	1.66	1.77
22	3	314	CLA	C4D-ND	-2.93	1.33	1.37
22	a	812	CLA	C4D-ND	-2.93	1.33	1.37
22	5	315	CLA	C4D-ND	-2.92	1.33	1.37
22	4	306	CLA	C4D-ND	-2.92	1.33	1.37
22	3	311	CLA	C4D-ND	-2.92	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	807	CLA	C4D-ND	-2.92	1.33	1.37
22	a	837	CLA	C4D-ND	-2.92	1.33	1.37
22	b	824	CLA	C4D-ND	-2.92	1.33	1.37
22	1	310	CLA	C4D-ND	-2.92	1.33	1.37
22	b	839	CLA	CHC-C1C	2.92	1.42	1.35
22	a	817	CLA	C4D-ND	-2.92	1.33	1.37
22	1	309	CLA	C4D-ND	-2.92	1.33	1.37
22	4	317	CLA	C4D-ND	-2.91	1.33	1.37
22	7	311	CLA	C4D-ND	-2.91	1.33	1.37
22	5	309	CLA	C4D-ND	-2.91	1.33	1.37
22	a	805	CLA	C4D-ND	-2.91	1.33	1.37
22	7	308	CLA	C4D-ND	-2.91	1.33	1.37
22	1	306	CLA	C4D-ND	-2.91	1.33	1.37
22	8	306	CLA	C4D-ND	-2.91	1.33	1.37
22	b	808	CLA	C4D-ND	-2.91	1.33	1.37
22	a	839	CLA	C4D-ND	-2.91	1.33	1.37
22	a	833	CLA	C4D-ND	-2.90	1.33	1.37
22	2	315	CLA	C4D-ND	-2.90	1.33	1.37
22	a	836	CLA	C4D-ND	-2.90	1.33	1.37
22	7	310	CLA	C4D-ND	-2.90	1.33	1.37
22	a	823	CLA	C4D-ND	-2.90	1.33	1.37
22	1	308	CLA	C4D-ND	-2.90	1.33	1.37
22	b	811	CLA	C4D-ND	-2.90	1.33	1.37
22	1	312	CLA	C4D-ND	-2.89	1.33	1.37
22	b	803	CLA	C4D-ND	-2.89	1.33	1.37
22	2	316	CLA	C4D-ND	-2.89	1.33	1.37
22	b	812	CLA	C4D-ND	-2.89	1.33	1.37
22	5	306	CLA	C4D-ND	-2.89	1.33	1.37
22	4	310	CLA	C4D-ND	-2.89	1.33	1.37
22	4	313	CLA	C4D-ND	-2.89	1.33	1.37
22	a	811	CLA	C4D-ND	-2.89	1.33	1.37
22	2	306	CLA	C4D-ND	-2.89	1.33	1.37
22	1	307	CLA	C4D-ND	-2.89	1.33	1.37
22	b	834	CLA	C4D-ND	-2.89	1.33	1.37
22	b	818	CLA	C4D-ND	-2.88	1.33	1.37
22	a	822	CLA	C4D-ND	-2.88	1.33	1.37
23	1	315	SQD	C6-S	-2.88	1.66	1.77
22	7	312	CLA	C4D-ND	-2.88	1.33	1.37
22	3	307	CLA	C4D-ND	-2.88	1.33	1.37
22	b	805	CLA	C4D-ND	-2.87	1.33	1.37
22	a	809	CLA	C4D-ND	-2.87	1.33	1.37
22	2	314	CLA	C4D-ND	-2.87	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	802	CLA	C4D-ND	-2.86	1.33	1.37
22	7	306	CLA	C4D-ND	-2.86	1.33	1.37
22	a	825	CLA	C4D-ND	-2.86	1.33	1.37
22	b	821	CLA	C4D-ND	-2.86	1.33	1.37
22	a	844	CLA	C4D-ND	-2.86	1.33	1.37
22	4	314	CLA	C4D-ND	-2.86	1.33	1.37
22	2	313	CLA	C4D-ND	-2.86	1.33	1.37
22	a	835	CLA	C4D-ND	-2.86	1.33	1.37
22	8	305	CLA	C4D-ND	-2.85	1.33	1.37
22	a	804	CLA	C4D-ND	-2.85	1.33	1.37
22	b	810	CLA	C4D-ND	-2.85	1.33	1.37
22	b	839	CLA	C4D-ND	-2.85	1.33	1.37
22	a	821	CLA	C4D-ND	-2.85	1.33	1.37
22	b	827	CLA	C4D-ND	-2.85	1.33	1.37
22	b	809	CLA	C4D-ND	-2.85	1.33	1.37
22	5	310	CLA	C4D-ND	-2.85	1.33	1.37
25	a	845	LHG	C26-C25	-2.85	1.35	1.51
22	7	317	CLA	C4D-ND	-2.84	1.33	1.37
22	a	840	CLA	C4D-ND	-2.84	1.33	1.37
21	1	301	A1L1G	C42-C44	2.84	1.39	1.35
22	a	841	CLA	C4D-ND	-2.84	1.33	1.37
22	8	314	CLA	C4D-ND	-2.84	1.33	1.37
22	8	309	CLA	C4D-ND	-2.84	1.33	1.37
22	2	310	CLA	C4D-ND	-2.84	1.33	1.37
22	a	826	CLA	C4D-ND	-2.84	1.33	1.37
22	a	818	CLA	C4D-ND	-2.83	1.33	1.37
25	9	317	LHG	C26-C25	-2.83	1.35	1.51
22	7	315	CLA	C4D-ND	-2.83	1.33	1.37
22	a	813	CLA	C4D-ND	-2.83	1.33	1.37
22	f	803	CLA	C4D-ND	-2.83	1.33	1.37
22	a	820	CLA	C4D-ND	-2.83	1.33	1.37
22	b	833	CLA	C4D-ND	-2.83	1.33	1.37
22	j	103	CLA	C4D-ND	-2.82	1.33	1.37
22	3	315	CLA	C4D-ND	-2.82	1.33	1.37
22	b	831	CLA	C4D-ND	-2.82	1.33	1.37
22	2	312	CLA	C4D-ND	-2.82	1.33	1.37
22	2	307	CLA	C4D-ND	-2.82	1.33	1.37
22	9	310	CLA	C4D-ND	-2.82	1.33	1.37
22	3	312	CLA	C4D-ND	-2.81	1.33	1.37
22	4	315	CLA	C4D-ND	-2.81	1.33	1.37
22	8	308	CLA	C4D-ND	-2.81	1.33	1.37
25	b	847	LHG	C26-C25	-2.80	1.35	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	801	CLA	C4D-ND	-2.80	1.33	1.37
22	4	307	CLA	C4D-ND	-2.80	1.33	1.37
22	2	311	CLA	C4D-ND	-2.80	1.33	1.37
25	9	307	LHG	C26-C25	-2.80	1.35	1.51
22	9	314	CLA	C4D-ND	-2.79	1.33	1.37
22	1	313	CLA	C4D-ND	-2.79	1.33	1.37
21	9	301	A1L1G	C33-C34	-2.77	1.40	1.45
22	5	314	CLA	C4D-ND	-2.77	1.33	1.37
22	5	305	CLA	C4D-ND	-2.76	1.33	1.37
22	a	801	CLA	CMB-C2B	-2.76	1.45	1.51
22	7	307	CLA	C4D-ND	-2.76	1.33	1.37
22	a	806	CLA	CMB-C2B	-2.76	1.45	1.51
22	b	829	CLA	C4D-ND	-2.75	1.33	1.37
22	3	308	CLA	C4D-ND	-2.75	1.33	1.37
22	1	314	CLA	C4D-ND	-2.74	1.33	1.37
22	4	311	CLA	C4D-ND	-2.74	1.33	1.37
22	7	314	CLA	C4D-ND	-2.73	1.33	1.37
22	b	814	CLA	C4D-ND	-2.72	1.33	1.37
22	h	203	CLA	C4D-ND	-2.70	1.34	1.37
22	7	316	CLA	C4D-ND	-2.69	1.34	1.37
24	h	204	A1L1F	O15-C20	-2.68	1.42	1.46
22	b	819	CLA	CMB-C2B	-2.66	1.46	1.51
21	5	303	A1L1G	C33-C34	-2.66	1.40	1.45
24	h	204	A1L1F	C6-C1	-2.66	1.50	1.54
22	2	307	CLA	CMB-C2B	-2.64	1.46	1.51
22	b	810	CLA	CMB-C2B	-2.64	1.46	1.51
22	b	801	CLA	CMB-C2B	-2.64	1.46	1.51
22	b	804	CLA	C4D-ND	-2.62	1.34	1.37
21	5	303	A1L1G	C42-C44	2.62	1.39	1.35
22	b	839	CLA	CMB-C2B	-2.61	1.46	1.51
21	3	306	A1L1G	C40-C39	-2.61	1.40	1.45
21	3	306	A1L1G	C33-C34	-2.61	1.40	1.45
22	a	836	CLA	CMB-C2B	-2.60	1.46	1.51
22	4	311	CLA	CMB-C2B	-2.60	1.46	1.51
22	a	832	CLA	CMB-C2B	-2.59	1.46	1.51
22	2	310	CLA	CMB-C2B	-2.58	1.46	1.51
22	b	830	CLA	CMB-C2B	-2.58	1.46	1.51
22	8	310	CLA	CMB-C2B	-2.58	1.46	1.51
22	a	820	CLA	CMB-C2B	-2.58	1.46	1.51
21	3	306	A1L1G	C42-C44	2.56	1.39	1.35
21	7	302	A1L1G	C33-C34	-2.55	1.40	1.45
22	a	806	CLA	C1D-ND	2.54	1.40	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	817	CLA	CMB-C2B	-2.53	1.46	1.51
22	a	802	CLA	CMB-C2B	-2.53	1.46	1.51
21	3	302	A1L1G	C33-C34	-2.53	1.40	1.45
21	9	306	A1L1G	C33-C34	-2.52	1.40	1.45
22	b	834	CLA	CMB-C2B	-2.52	1.46	1.51
22	3	307	CLA	CMB-C2B	-2.52	1.46	1.51
22	7	311	CLA	CMB-C2B	-2.52	1.46	1.51
22	a	824	CLA	CMB-C2B	-2.52	1.46	1.51
22	a	808	CLA	CMB-C2B	-2.51	1.46	1.51
22	b	818	CLA	CMB-C2B	-2.51	1.46	1.51
22	9	309	CLA	CMB-C2B	-2.51	1.46	1.51
22	a	822	CLA	CMB-C2B	-2.51	1.46	1.51
22	b	828	CLA	CMB-C2B	-2.51	1.46	1.51
22	a	803	CLA	CMB-C2B	-2.50	1.46	1.51
22	a	837	CLA	CMB-C2B	-2.49	1.46	1.51
22	4	317	CLA	CMB-C2B	-2.47	1.46	1.51
22	1	203	CLA	CMB-C2B	-2.47	1.46	1.51
21	5	303	A1L1G	C40-C39	-2.47	1.40	1.45
22	a	818	CLA	CMB-C2B	-2.47	1.46	1.51
21	9	306	A1L1G	C42-C44	2.47	1.39	1.35
22	4	313	CLA	CMB-C2B	-2.46	1.46	1.51
22	1	309	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	809	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	825	CLA	CMB-C2B	-2.46	1.46	1.51
22	1	307	CLA	CMB-C2B	-2.46	1.46	1.51
22	a	806	CLA	CMD-C2D	-2.46	1.45	1.50
21	9	306	A1L1G	C40-C39	-2.45	1.40	1.45
21	3	302	A1L1G	C29-C30	-2.45	1.40	1.45
22	1	202	CLA	CMB-C2B	-2.45	1.46	1.51
22	5	312	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	811	CLA	CMB-C2B	-2.44	1.46	1.51
20	9	303	XAT	O4-C5	-2.44	1.42	1.46
22	7	307	CLA	CMB-C2B	-2.44	1.46	1.51
22	a	810	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	838	CLA	CMB-C2B	-2.44	1.46	1.51
22	a	842	CLA	CMB-C2B	-2.44	1.46	1.51
22	j	103	CLA	CMB-C2B	-2.43	1.46	1.51
21	3	302	A1L1G	C40-C39	-2.43	1.40	1.45
22	1	204	CLA	CMB-C2B	-2.43	1.46	1.51
22	1	314	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	829	CLA	CMD-C2D	-2.43	1.45	1.50
22	3	311	CLA	CMB-C2B	-2.43	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	308	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	812	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	835	CLA	CMB-C2B	-2.43	1.46	1.51
22	4	314	CLA	CMB-C2B	-2.43	1.46	1.51
22	f	803	CLA	CMB-C2B	-2.42	1.46	1.51
22	a	817	CLA	CMB-C2B	-2.42	1.46	1.51
22	3	313	CLA	CMB-C2B	-2.42	1.46	1.51
22	a	834	CLA	CMB-C2B	-2.42	1.46	1.51
21	7	302	A1L1G	C40-C39	-2.42	1.40	1.45
21	1	301	A1L1G	C33-C34	-2.42	1.40	1.45
22	2	311	CLA	CMB-C2B	-2.42	1.46	1.51
22	1	310	CLA	CMB-C2B	-2.42	1.46	1.51
22	2	315	CLA	CMB-C2B	-2.42	1.46	1.51
22	7	317	CLA	CMB-C2B	-2.42	1.46	1.51
22	3	308	CLA	CMB-C2B	-2.42	1.46	1.51
22	a	854	CLA	CMB-C2B	-2.42	1.46	1.51
22	9	308	CLA	CMB-C2B	-2.42	1.46	1.51
22	8	313	CLA	CMB-C2B	-2.41	1.46	1.51
22	2	314	CLA	CMB-C2B	-2.41	1.46	1.51
22	4	315	CLA	CMB-C2B	-2.41	1.46	1.51
22	7	314	CLA	CMB-C2B	-2.41	1.46	1.51
22	3	312	CLA	CMB-C2B	-2.41	1.46	1.51
22	9	318	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	824	CLA	CMB-C2B	-2.41	1.46	1.51
22	7	315	CLA	CMB-C2B	-2.41	1.46	1.51
22	a	813	CLA	CMB-C2B	-2.41	1.46	1.51
22	8	312	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	840	CLA	CMB-C2B	-2.41	1.46	1.51
22	1	312	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	838	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	833	CLA	CMB-C2B	-2.40	1.46	1.51
22	5	310	CLA	CMB-C2B	-2.40	1.46	1.51
22	8	306	CLA	CMB-C2B	-2.40	1.46	1.51
22	1	311	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	806	CLA	CMC-C2C	-2.40	1.45	1.50
22	5	306	CLA	CMB-C2B	-2.40	1.46	1.51
22	8	314	CLA	CMB-C2B	-2.40	1.46	1.51
22	4	312	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	830	CLA	CMC-C2C	-2.39	1.45	1.50
22	a	801	CLA	CMD-C2D	-2.39	1.45	1.50
22	f	802	CLA	CMB-C2B	-2.39	1.46	1.51
22	7	312	CLA	CMB-C2B	-2.39	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	311	CLA	CMB-C2B	-2.39	1.46	1.51
22	5	315	CLA	CMB-C2B	-2.39	1.46	1.51
22	a	812	CLA	CMB-C2B	-2.38	1.46	1.51
22	5	307	CLA	CMB-C2B	-2.38	1.46	1.51
22	a	815	CLA	CMB-C2B	-2.38	1.46	1.51
22	1	305	CLA	CMB-C2B	-2.38	1.46	1.51
22	a	811	CLA	CMB-C2B	-2.38	1.46	1.51
22	a	819	CLA	CMB-C2B	-2.38	1.46	1.51
22	a	828	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	836	CLA	CMB-C2B	-2.38	1.46	1.51
24	9	302	A1L1F	O15-C20	-2.38	1.42	1.46
22	b	837	CLA	CMB-C2B	-2.38	1.46	1.51
22	a	841	CLA	CMB-C2B	-2.38	1.46	1.51
22	8	311	CLA	CMB-C2B	-2.38	1.46	1.51
22	9	314	CLA	CMB-C2B	-2.38	1.46	1.51
22	2	309	CLA	CMB-C2B	-2.38	1.46	1.51
22	1	313	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	813	CLA	CMB-C2B	-2.38	1.46	1.51
22	5	308	CLA	CMB-C2B	-2.37	1.46	1.51
22	1	306	CLA	CMB-C2B	-2.37	1.46	1.51
22	3	314	CLA	CMB-C2B	-2.37	1.46	1.51
22	a	821	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	826	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	802	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	805	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	827	CLA	CMB-C2B	-2.37	1.46	1.51
22	9	313	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	815	CLA	CMB-C2B	-2.37	1.46	1.51
22	9	315	CLA	CMB-C2B	-2.37	1.46	1.51
22	a	827	CLA	CMB-C2B	-2.37	1.46	1.51
22	1	308	CLA	CMB-C2B	-2.37	1.46	1.51
22	8	309	CLA	CMB-C2B	-2.37	1.46	1.51
22	4	306	CLA	CMB-C2B	-2.37	1.46	1.51
25	a	846	LHG	O8-C6	-2.37	1.39	1.45
22	b	822	CLA	CMB-C2B	-2.37	1.46	1.51
22	5	305	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	823	CLA	CMB-C2B	-2.36	1.46	1.51
22	8	307	CLA	CMB-C2B	-2.36	1.46	1.51
22	a	840	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	807	CLA	CMB-C2B	-2.36	1.46	1.51
22	j	102	CLA	CMB-C2B	-2.36	1.46	1.51
22	a	806	CLA	C3B-CAB	-2.36	1.43	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	307	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	808	CLA	CMB-C2B	-2.36	1.46	1.51
22	4	310	CLA	CMB-C2B	-2.36	1.46	1.51
22	5	309	CLA	CMB-C2B	-2.36	1.46	1.51
22	h	203	CLA	CMB-C2B	-2.36	1.46	1.51
22	8	305	CLA	CMB-C2B	-2.36	1.46	1.51
22	2	306	CLA	CMB-C2B	-2.36	1.46	1.51
22	5	313	CLA	CMB-C2B	-2.36	1.46	1.51
22	2	312	CLA	CMB-C2B	-2.36	1.46	1.51
22	7	313	CLA	CMB-C2B	-2.36	1.46	1.51
22	7	309	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	816	CLA	CMB-C2B	-2.36	1.46	1.51
22	2	316	CLA	CMB-C2B	-2.35	1.46	1.51
22	9	310	CLA	CMB-C2B	-2.35	1.46	1.51
22	3	310	CLA	CMB-C2B	-2.35	1.46	1.51
22	7	306	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	831	CLA	CMB-C2B	-2.35	1.46	1.51
22	5	314	CLA	CMB-C2B	-2.35	1.46	1.51
22	4	309	CLA	CMB-C2B	-2.35	1.46	1.51
22	3	315	CLA	CMB-C2B	-2.35	1.46	1.51
22	a	829	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	847	LHG	O8-C6	-2.35	1.39	1.45
25	9	317	LHG	O8-C23	2.35	1.40	1.33
22	b	835	CLA	CMB-C2B	-2.35	1.46	1.51
22	a	804	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	803	CLA	CMB-C2B	-2.35	1.46	1.51
22	4	316	CLA	CMB-C2B	-2.34	1.46	1.51
22	a	816	CLA	CMB-C2B	-2.34	1.46	1.51
22	b	806	CLA	CMB-C2B	-2.34	1.46	1.51
22	b	820	CLA	CMB-C2B	-2.34	1.46	1.51
25	a	845	LHG	O8-C6	-2.34	1.39	1.45
22	h	205	CLA	CMB-C2B	-2.34	1.46	1.51
22	a	814	CLA	CMB-C2B	-2.34	1.46	1.51
22	a	830	CLA	CMB-C2B	-2.33	1.46	1.51
22	a	825	CLA	CMB-C2B	-2.33	1.46	1.51
22	3	309	CLA	CMB-C2B	-2.33	1.46	1.51
22	2	313	CLA	CMB-C2B	-2.33	1.46	1.51
25	9	317	LHG	O8-C6	-2.33	1.39	1.45
22	a	833	CLA	CMB-C2B	-2.33	1.46	1.51
22	a	826	CLA	CMB-C2B	-2.33	1.46	1.51
25	b	847	LHG	O8-C23	2.33	1.40	1.33
22	a	807	CLA	CMB-C2B	-2.33	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	307	LHG	O8-C23	2.33	1.40	1.33
22	4	308	CLA	CMB-C2B	-2.33	1.46	1.51
22	a	839	CLA	CMB-C2B	-2.33	1.46	1.51
22	7	308	CLA	CMB-C2B	-2.32	1.46	1.51
22	5	311	CLA	CMB-C2B	-2.32	1.46	1.51
22	9	316	CLA	CMB-C2B	-2.32	1.46	1.51
22	a	844	CLA	CMB-C2B	-2.32	1.46	1.51
22	b	821	CLA	CMB-C2B	-2.31	1.46	1.51
22	7	310	CLA	CMB-C2B	-2.31	1.46	1.51
22	a	823	CLA	CMB-C2B	-2.31	1.46	1.51
22	a	805	CLA	CMB-C2B	-2.31	1.46	1.51
22	9	312	CLA	CMB-C2B	-2.31	1.46	1.51
22	b	814	CLA	CMB-C2B	-2.31	1.46	1.51
25	9	307	LHG	O7-C7	2.31	1.40	1.34
21	9	301	A1L1G	C29-C30	-2.31	1.40	1.45
25	9	307	LHG	O8-C6	-2.31	1.39	1.45
22	2	308	CLA	CMB-C2B	-2.30	1.46	1.51
22	a	806	CLA	C3B-C2B	-2.30	1.37	1.40
25	a	845	LHG	O7-C7	2.30	1.40	1.34
22	7	316	CLA	CMB-C2B	-2.30	1.46	1.51
21	1	301	A1L1G	C40-C39	-2.30	1.41	1.45
22	a	809	CLA	CMB-C2B	-2.30	1.46	1.51
22	4	311	CLA	CMD-C2D	-2.29	1.45	1.50
22	b	832	CLA	CMB-C2B	-2.28	1.46	1.51
25	a	845	LHG	O8-C23	2.28	1.40	1.33
21	3	306	A1L1G	C29-C30	-2.28	1.40	1.45
25	9	317	LHG	O7-C7	2.28	1.40	1.34
25	a	846	LHG	O7-C7	2.27	1.40	1.34
25	a	846	LHG	O8-C23	2.26	1.39	1.33
22	9	308	CLA	CMC-C2C	-2.26	1.46	1.50
21	1	301	A1L1G	C29-C30	-2.25	1.40	1.45
25	a	846	LHG	O7-C5	-2.25	1.41	1.46
24	1	304	A1L1F	C6-C1	-2.25	1.50	1.54
21	5	303	A1L1G	C29-C30	-2.24	1.40	1.45
21	9	301	A1L1G	C40-C39	-2.24	1.41	1.45
22	b	809	CLA	CMD-C2D	-2.24	1.46	1.50
22	b	822	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	847	LHG	O7-C5	-2.23	1.41	1.46
25	b	847	LHG	O7-C7	2.23	1.40	1.34
24	1	304	A1L1F	O15-C20	-2.23	1.43	1.46
21	9	306	A1L1G	C29-C30	-2.21	1.40	1.45
22	b	830	CLA	CMD-C2D	-2.21	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	823	CLA	CMD-C2D	-2.19	1.46	1.50
20	4	301	XAT	O24-C25	-2.19	1.43	1.46
22	a	830	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	804	CLA	CMB-C2B	-2.18	1.47	1.51
22	3	307	CLA	CMD-C2D	-2.18	1.46	1.50
20	3	305	XAT	O4-C5	-2.18	1.43	1.46
25	a	845	LHG	O7-C5	-2.17	1.41	1.46
22	a	801	CLA	CMC-C2C	-2.17	1.46	1.50
25	9	317	LHG	O7-C5	-2.17	1.41	1.46
22	5	305	CLA	CMD-C2D	-2.17	1.46	1.50
22	a	824	CLA	CMD-C2D	-2.17	1.46	1.50
22	a	828	CLA	CMC-C2C	-2.16	1.46	1.50
22	a	810	CLA	CMD-C2D	-2.16	1.46	1.50
22	a	801	CLA	C3B-CAB	-2.16	1.43	1.47
22	a	806	CLA	CAA-C2A	-2.16	1.50	1.54
22	7	314	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	803	CLA	CMD-C2D	-2.15	1.46	1.50
25	9	307	LHG	O7-C5	-2.15	1.41	1.46
22	7	316	CLA	CMD-C2D	-2.14	1.46	1.50
22	9	309	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	801	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	838	CLA	CMD-C2D	-2.13	1.46	1.50
20	5	302	XAT	O4-C5	-2.13	1.43	1.46
26	b	848	DGD	O3D-C3D	-2.13	1.38	1.43
22	b	811	CLA	CMD-C2D	-2.13	1.46	1.50
22	2	310	CLA	CMD-C2D	-2.13	1.46	1.50
20	4	304	XAT	O24-C25	-2.12	1.43	1.46
26	b	848	DGD	C1E-C2E	2.11	1.58	1.52
26	b	848	DGD	O4D-C4D	-2.11	1.38	1.43
20	9	305	XAT	O4-C5	-2.11	1.43	1.46
20	1	302	XAT	O4-C5	-2.11	1.43	1.46
22	b	837	CLA	CMD-C2D	-2.11	1.46	1.50
20	7	301	XAT	O24-C25	-2.10	1.43	1.46
22	b	814	CLA	CMD-C2D	-2.10	1.46	1.50
22	a	807	CLA	CMD-C2D	-2.10	1.46	1.50
22	a	804	CLA	CMC-C2C	-2.09	1.46	1.50
24	8	304	A1L1F	O15-C20	-2.09	1.43	1.46
22	a	812	CLA	CMD-C2D	-2.09	1.46	1.50
20	2	302	XAT	O4-C5	-2.08	1.43	1.46
20	2	303	XAT	O4-C5	-2.08	1.43	1.46
22	a	842	CLA	CMD-C2D	-2.08	1.46	1.50
22	a	816	CLA	CMD-C2D	-2.08	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	304	XAT	O4-C5	-2.08	1.43	1.46
22	b	828	CLA	CMD-C2D	-2.08	1.46	1.50
22	a	832	CLA	CMD-C2D	-2.07	1.46	1.50
22	9	312	CLA	CMD-C2D	-2.07	1.46	1.50
25	9	317	LHG	P-O6	2.07	1.67	1.59
20	a	852	XAT	O4-C5	-2.07	1.43	1.46
25	9	307	LHG	P-O6	2.07	1.67	1.59
22	a	821	CLA	CMD-C2D	-2.07	1.46	1.50
25	a	845	LHG	P-O6	2.07	1.67	1.59
20	5	301	XAT	O4-C5	-2.06	1.43	1.46
22	b	825	CLA	CMD-C2D	-2.06	1.46	1.50
22	a	803	CLA	C3B-CAB	-2.06	1.43	1.47
20	9	304	XAT	O4-C5	-2.06	1.43	1.46
20	8	303	XAT	O4-C5	-2.06	1.43	1.46
20	7	305	XAT	O4-C5	-2.06	1.43	1.46
25	b	847	LHG	P-O6	2.06	1.67	1.59
22	2	316	CLA	CMD-C2D	-2.06	1.46	1.50
22	4	308	CLA	CMD-C2D	-2.06	1.46	1.50
22	3	309	CLA	CMD-C2D	-2.05	1.46	1.50
22	8	313	CLA	CMD-C2D	-2.05	1.46	1.50
22	a	806	CLA	MG-ND	-2.05	2.01	2.05
22	b	809	CLA	CMC-C2C	-2.05	1.46	1.50
20	3	301	XAT	O24-C25	-2.05	1.43	1.46
22	b	827	CLA	CMD-C2D	-2.05	1.46	1.50
22	1	309	CLA	CMD-C2D	-2.05	1.46	1.50
20	4	305	XAT	O4-C5	-2.05	1.43	1.46
20	7	303	XAT	O4-C5	-2.05	1.43	1.46
22	7	311	CLA	CMD-C2D	-2.04	1.46	1.50
20	1	303	XAT	O4-C5	-2.04	1.43	1.46
22	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
20	2	305	XAT	O4-C5	-2.04	1.43	1.46
22	b	820	CLA	CMD-C2D	-2.04	1.46	1.50
22	7	312	CLA	CMD-C2D	-2.04	1.46	1.50
20	3	304	XAT	O24-C25	-2.04	1.43	1.46
20	4	301	XAT	O4-C5	-2.04	1.43	1.46
22	b	834	CLA	CMD-C2D	-2.04	1.46	1.50
22	j	102	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	815	CLA	CMC-C2C	-2.04	1.46	1.50
22	3	315	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	827	CLA	CMD-C2D	-2.04	1.46	1.50
22	2	314	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	802	CLA	CMD-C2D	-2.03	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	826	CLA	CMD-C2D	-2.03	1.46	1.50
26	b	848	DGD	O4E-C4E	-2.03	1.38	1.43
22	3	314	CLA	CMD-C2D	-2.03	1.46	1.50
26	b	848	DGD	O2D-C2D	-2.03	1.38	1.43
22	5	308	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	834	CLA	CMD-C2D	-2.03	1.46	1.50
20	a	852	XAT	O24-C25	-2.03	1.43	1.46
22	2	307	CLA	CMD-C2D	-2.03	1.46	1.50
22	1	313	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	837	CLA	CMD-C2D	-2.03	1.46	1.50
20	5	302	XAT	O24-C25	-2.03	1.43	1.46
20	j	101	XAT	O4-C5	-2.03	1.43	1.46
22	2	312	CLA	CMD-C2D	-2.02	1.46	1.50
22	1	204	CLA	CMC-C2C	-2.02	1.46	1.50
20	2	301	XAT	O4-C5	-2.02	1.43	1.46
22	2	314	CLA	CMC-C2C	-2.02	1.46	1.50
20	3	303	XAT	O4-C5	-2.02	1.43	1.46
22	9	318	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	833	CLA	CMD-C2D	-2.02	1.46	1.50
22	8	310	CLA	CMD-C2D	-2.02	1.46	1.50
22	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
22	a	807	CLA	C3B-CAB	-2.02	1.43	1.47
20	7	304	XAT	O4-C5	-2.02	1.43	1.46
22	4	306	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	803	CLA	CMC-C2C	-2.01	1.46	1.50
20	4	304	XAT	O4-C5	-2.01	1.43	1.46
22	5	310	CLA	CMD-C2D	-2.01	1.46	1.50
22	a	803	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	826	CLA	CMD-C2D	-2.01	1.46	1.50
22	h	203	CLA	CMD-C2D	-2.01	1.46	1.50
20	8	301	XAT	O4-C5	-2.01	1.43	1.46
22	4	312	CLA	CMD-C2D	-2.01	1.46	1.50
20	8	302	XAT	O4-C5	-2.01	1.43	1.46
20	4	303	XAT	O4-C5	-2.01	1.43	1.46
22	b	805	CLA	CMD-C2D	-2.01	1.46	1.50
22	9	314	CLA	CMD-C2D	-2.01	1.46	1.50
22	7	306	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	807	CLA	CMD-C2D	-2.01	1.46	1.50
22	a	814	CLA	CMD-C2D	-2.01	1.46	1.50
20	2	304	XAT	O4-C5	-2.00	1.43	1.46
22	b	832	CLA	CMD-C2D	-2.00	1.46	1.50
22	a	801	CLA	C3B-C2B	-2.00	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	305	CLA	CMD-C2D	-2.00	1.46	1.50
22	7	315	CLA	CMD-C2D	-2.00	1.46	1.50
20	3	301	XAT	O4-C5	-2.00	1.43	1.46
25	a	846	LHG	P-O6	2.00	1.67	1.59
22	b	804	CLA	CMD-C2D	-2.00	1.46	1.50
22	7	310	CLA	CMD-C2D	-2.00	1.46	1.50
22	a	829	CLA	CMD-C2D	-2.00	1.46	1.50
22	1	203	CLA	CMC-C2C	-2.00	1.46	1.50
20	7	304	XAT	O24-C25	-2.00	1.43	1.46
22	b	813	CLA	CMD-C2D	-2.00	1.46	1.50

All (2472) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	302	A1L1F	O15-C20-C21	13.24	123.33	113.38
26	4	318	DGD	C6E-C5E-C4E	-9.41	90.97	113.00
24	8	304	A1L1F	O15-C20-C21	8.54	119.79	113.38
24	9	302	A1L1F	C17-C20-C25	-8.48	108.05	122.26
24	h	204	A1L1F	O15-C20-C21	8.40	119.69	113.38
24	h	204	A1L1F	C17-C20-C25	-8.35	108.27	122.26
24	8	304	A1L1F	C17-C20-C25	-8.22	108.49	122.26
24	1	304	A1L1F	C17-C20-C25	-8.10	108.68	122.26
24	8	304	A1L1F	C37-C38-C39	-7.87	116.07	127.31
22	7	314	CLA	C4A-NA-C1A	7.40	110.03	106.71
22	9	310	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	9	313	CLA	C4A-NA-C1A	7.32	110.00	106.71
24	1	304	A1L1F	O15-C20-C21	7.27	118.84	113.38
22	1	203	CLA	C4A-NA-C1A	7.25	109.97	106.71
20	9	303	XAT	C38-C25-C24	7.23	122.41	114.28
20	3	305	XAT	C38-C25-C24	7.23	122.41	114.28
22	a	806	CLA	C4A-NA-C1A	7.23	109.95	106.71
22	b	839	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	b	803	CLA	C4A-NA-C1A	7.21	109.95	106.71
20	4	305	XAT	C38-C25-C24	7.20	122.38	114.28
20	5	304	XAT	C38-C25-C24	7.19	122.37	114.28
20	7	304	XAT	C38-C25-C24	7.17	122.34	114.28
20	1	303	XAT	C38-C25-C24	7.17	122.34	114.28
20	a	852	XAT	C15-C14-C13	-7.12	117.15	127.31
20	7	305	XAT	C38-C25-C24	7.10	122.27	114.28
22	a	833	CLA	C4A-NA-C1A	7.09	109.89	106.71
22	a	823	CLA	C4A-NA-C1A	7.07	109.89	106.71
20	j	101	XAT	C38-C25-C24	7.06	122.22	114.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	809	CLA	C4A-NA-C1A	7.05	109.88	106.71
22	a	821	CLA	C4A-NA-C1A	7.04	109.87	106.71
20	9	304	XAT	C38-C25-C24	7.03	122.19	114.28
22	b	820	CLA	C4A-NA-C1A	7.02	109.86	106.71
20	5	304	XAT	C18-C5-C4	7.02	122.18	114.28
22	4	310	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	9	308	CLA	C4A-NA-C1A	7.01	109.86	106.71
29	f	801	BCR	C24-C23-C22	-6.99	115.67	126.23
20	3	304	XAT	C38-C25-C24	6.99	122.14	114.28
20	4	304	XAT	C38-C25-C24	6.99	122.14	114.28
22	a	835	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	7	317	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	j	103	CLA	C4A-NA-C1A	6.94	109.82	106.71
22	4	317	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	a	826	CLA	C4A-NA-C1A	6.91	109.81	106.71
22	b	801	CLA	C4A-NA-C1A	6.91	109.81	106.71
22	a	810	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	a	828	CLA	C4A-NA-C1A	6.89	109.80	106.71
20	1	302	XAT	C38-C25-C24	6.88	122.02	114.28
20	5	301	XAT	C38-C25-C26	-6.88	110.73	122.26
20	2	301	XAT	C18-C5-C6	-6.88	110.74	122.26
22	4	316	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	3	308	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	f	802	CLA	C4A-NA-C1A	6.87	109.80	106.71
20	8	301	XAT	C38-C25-C24	6.87	122.01	114.28
22	5	310	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	b	827	CLA	C4A-NA-C1A	6.83	109.78	106.71
20	5	304	XAT	C6-C7-C8	-6.83	111.55	125.99
20	4	305	XAT	C38-C25-C26	-6.83	110.82	122.26
22	7	316	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	a	801	CLA	C4A-NA-C1A	6.81	109.77	106.71
20	3	304	XAT	C38-C25-C26	-6.80	110.86	122.26
20	4	303	XAT	C38-C25-C24	6.80	121.92	114.28
22	a	807	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	h	203	CLA	C4A-NA-C1A	6.79	109.76	106.71
20	9	303	XAT	C38-C25-C26	-6.79	110.89	122.26
20	8	303	XAT	C38-C25-C24	6.78	121.91	114.28
22	b	836	CLA	C4A-NA-C1A	6.78	109.75	106.71
20	2	304	XAT	C38-C25-C24	6.78	121.91	114.28
22	a	809	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	b	821	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	1	305	CLA	C4A-NA-C1A	6.76	109.75	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	308	CLA	C4A-NA-C1A	6.76	109.75	106.71
20	8	301	XAT	C38-C25-C26	-6.76	110.94	122.26
20	8	303	XAT	C18-C5-C6	-6.75	110.94	122.26
22	3	313	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	b	824	CLA	C4A-NA-C1A	6.75	109.74	106.71
20	a	852	XAT	C38-C25-C24	6.75	121.87	114.28
22	9	316	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	a	817	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	b	806	CLA	C4A-NA-C1A	6.74	109.74	106.71
22	4	315	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	1	306	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	a	805	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	2	316	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	2	312	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	7	315	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	b	814	CLA	C4A-NA-C1A	6.72	109.72	106.71
22	a	841	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	b	812	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	a	840	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	a	834	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	b	810	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	8	302	XAT	C38-C25-C24	6.70	121.82	114.28
22	a	831	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	b	805	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	4	306	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	4	311	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	3	314	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	5	314	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	4	314	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	3	312	CLA	C4A-NA-C1A	6.68	109.71	106.71
20	9	304	XAT	C38-C25-C26	-6.68	111.07	122.26
20	5	304	XAT	C18-C5-C6	-6.67	111.08	122.26
20	4	302	XAT	C38-C25-C24	6.67	121.79	114.28
20	7	304	XAT	C18-C5-C6	-6.67	111.08	122.26
20	3	303	XAT	C38-C25-C24	6.66	121.78	114.28
22	a	842	CLA	C4A-NA-C1A	6.66	109.70	106.71
20	7	301	XAT	C18-C5-C6	-6.66	111.09	122.26
20	2	301	XAT	C18-C5-C4	6.66	121.78	114.28
22	5	306	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	8	312	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	8	313	CLA	C4A-NA-C1A	6.65	109.69	106.71
20	7	301	XAT	C18-C5-C4	6.64	121.75	114.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	304	XAT	C18-C5-C4	6.64	121.75	114.28
22	l	202	CLA	C4A-NA-C1A	6.64	109.69	106.71
22	l	204	CLA	C4A-NA-C1A	6.64	109.69	106.71
20	3	304	XAT	C18-C5-C6	-6.63	111.15	122.26
22	7	310	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	b	832	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	f	803	CLA	C4A-NA-C1A	6.63	109.69	106.71
29	i	101	BCR	C24-C23-C22	-6.63	116.22	126.23
22	9	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	a	825	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	a	829	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	b	822	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	4	307	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	j	101	XAT	C38-C25-C26	-6.61	111.18	122.26
22	8	309	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	3	301	XAT	C18-C5-C4	6.61	121.71	114.28
22	a	837	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	7	307	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	8	305	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	a	839	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	a	811	CLA	C4A-NA-C1A	6.60	109.67	106.71
20	7	303	XAT	C38-C25-C26	-6.60	111.21	122.26
22	2	311	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	5	311	CLA	C4A-NA-C1A	6.59	109.67	106.71
20	7	304	XAT	C38-C25-C26	-6.59	111.22	122.26
22	5	308	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	5	313	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	2	313	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	a	838	CLA	C4A-NA-C1A	6.58	109.67	106.71
20	4	301	XAT	C31-C30-C29	-6.58	117.92	127.31
22	a	804	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	5	301	XAT	C38-C25-C24	6.58	121.68	114.28
22	a	830	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	5	302	XAT	C18-C5-C6	-6.57	111.25	122.26
22	a	812	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	b	807	CLA	C4A-NA-C1A	6.56	109.66	106.71
20	4	301	XAT	C18-C5-C4	6.56	121.66	114.28
20	8	302	XAT	C18-C5-C6	-6.56	111.27	122.26
22	8	307	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	b	818	CLA	C4A-NA-C1A	6.56	109.65	106.71
20	8	302	XAT	C38-C25-C26	-6.56	111.27	122.26
22	4	308	CLA	C4A-NA-C1A	6.55	109.65	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	831	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	2	303	XAT	C18-C5-C6	-6.55	111.28	122.26
22	b	826	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	3	305	XAT	C38-C25-C26	-6.54	111.29	122.26
22	j	102	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	3	311	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	a	818	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	b	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
20	7	303	XAT	C38-C25-C24	6.53	121.62	114.28
20	4	303	XAT	C18-C5-C6	-6.53	111.32	122.26
22	5	312	CLA	C4A-NA-C1A	6.52	109.64	106.71
20	5	304	XAT	C38-C25-C26	-6.52	111.33	122.26
22	a	844	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	a	836	CLA	C4A-NA-C1A	6.52	109.64	106.71
20	7	305	XAT	C38-C25-C26	-6.52	111.33	122.26
22	3	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	b	823	CLA	C4A-NA-C1A	6.52	109.64	106.71
20	4	302	XAT	C18-C5-C4	6.51	121.61	114.28
20	4	301	XAT	C18-C5-C6	-6.51	111.34	122.26
22	8	306	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	8	303	XAT	C18-C5-C4	6.51	121.60	114.28
22	1	307	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	2	306	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	a	815	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	7	312	CLA	C4A-NA-C1A	6.49	109.63	106.71
22	a	854	CLA	C4A-NA-C1A	6.49	109.63	106.71
20	7	303	XAT	C18-C5-C6	-6.49	111.38	122.26
22	a	822	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	8	314	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	4	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	b	833	CLA	C4A-NA-C1A	6.49	109.62	106.71
20	2	305	XAT	C18-C5-C6	-6.49	111.39	122.26
29	a	850	BCR	C24-C23-C22	-6.48	116.44	126.23
20	4	303	XAT	C38-C25-C26	-6.48	111.40	122.26
22	5	309	CLA	C4A-NA-C1A	6.47	109.62	106.71
22	a	816	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	3	310	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	2	309	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	b	838	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	1	313	CLA	C4A-NA-C1A	6.46	109.61	106.71
20	2	303	XAT	C38-C25-C26	-6.46	111.44	122.26
22	2	315	CLA	C4A-NA-C1A	6.46	109.61	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	315	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	b	815	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	b	835	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	8	308	CLA	C4A-NA-C1A	6.45	109.61	106.71
20	2	304	XAT	C38-C25-C26	-6.45	111.45	122.26
22	5	315	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	1	312	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	a	808	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	8	311	CLA	C4A-NA-C1A	6.43	109.60	106.71
20	3	303	XAT	C18-C5-C6	-6.43	111.48	122.26
22	2	307	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	2	314	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	7	308	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	9	312	CLA	C4A-NA-C1A	6.43	109.59	106.71
20	2	304	XAT	C18-C5-C6	-6.43	111.49	122.26
22	b	813	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	a	832	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	5	307	CLA	C4A-NA-C1A	6.41	109.59	106.71
20	5	302	XAT	C26-C27-C28	-6.40	112.45	125.99
20	1	302	XAT	C38-C25-C26	-6.40	111.54	122.26
22	a	827	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	3	301	XAT	C18-C5-C6	-6.39	111.55	122.26
20	7	305	XAT	C18-C5-C6	-6.39	111.55	122.26
22	b	834	CLA	C4A-NA-C1A	6.38	109.57	106.71
22	9	318	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	7	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	9	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
20	3	303	XAT	C38-C25-C26	-6.36	111.59	122.26
20	2	303	XAT	C38-C25-C24	6.36	121.44	114.28
22	1	311	CLA	C4A-NA-C1A	6.36	109.57	106.71
20	j	101	XAT	C18-C5-C6	-6.36	111.60	122.26
22	b	819	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	3	307	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	9	303	XAT	C18-C5-C6	-6.35	111.61	122.26
22	1	314	CLA	C4A-NA-C1A	6.34	109.56	106.71
20	4	302	XAT	C18-C5-C6	-6.34	111.63	122.26
22	a	819	CLA	C4A-NA-C1A	6.34	109.56	106.71
20	4	304	XAT	C18-C5-C6	-6.34	111.63	122.26
22	h	205	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	1	309	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	a	814	CLA	C4A-NA-C1A	6.33	109.55	106.71
20	1	302	XAT	C18-C5-C4	6.33	121.40	114.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	302	XAT	C38-C25-C24	6.33	121.40	114.28
22	a	802	CLA	C4A-NA-C1A	6.33	109.55	106.71
20	4	305	XAT	C31-C30-C29	-6.32	118.29	127.31
22	4	312	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	7	306	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	7	309	CLA	C4A-NA-C1A	6.31	109.55	106.71
20	1	302	XAT	C18-C5-C6	-6.31	111.68	122.26
20	4	305	XAT	C18-C5-C6	-6.31	111.68	122.26
22	b	825	CLA	C4A-NA-C1A	6.31	109.54	106.71
20	3	303	XAT	C18-C5-C4	6.31	121.37	114.28
20	7	305	XAT	C18-C5-C4	6.31	121.37	114.28
20	j	101	XAT	C18-C5-C4	6.30	121.36	114.28
20	3	305	XAT	C18-C5-C4	6.29	121.36	114.28
22	5	305	CLA	C4A-NA-C1A	6.29	109.53	106.71
20	2	302	XAT	C18-C5-C6	-6.29	111.72	122.26
22	9	315	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	2	310	CLA	C4A-NA-C1A	6.28	109.53	106.71
20	3	305	XAT	C18-C5-C6	-6.28	111.74	122.26
20	3	301	XAT	C38-C25-C26	-6.28	111.74	122.26
20	8	303	XAT	C38-C25-C26	-6.27	111.75	122.26
20	4	302	XAT	C38-C25-C26	-6.27	111.75	122.26
20	4	304	XAT	C38-C25-C26	-6.27	111.75	122.26
22	a	824	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	a	813	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	b	829	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	b	840	CLA	C4A-NA-C1A	6.26	109.52	106.71
20	8	301	XAT	C18-C5-C6	-6.25	111.78	122.26
20	8	302	XAT	C11-C10-C9	-6.25	118.39	127.31
29	i	101	BCR	C20-C21-C22	-6.25	118.39	127.31
22	7	313	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	1	310	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	3	304	XAT	C18-C5-C4	6.24	121.30	114.28
20	2	301	XAT	C38-C25-C24	6.24	121.30	114.28
20	1	303	XAT	C18-C5-C6	-6.24	111.81	122.26
20	4	303	XAT	C18-C5-C4	6.24	121.30	114.28
20	a	852	XAT	C38-C25-C26	-6.22	111.83	122.26
20	1	303	XAT	C38-C25-C26	-6.22	111.84	122.26
22	b	804	CLA	C4A-NA-C1A	6.22	109.50	106.71
20	5	301	XAT	C18-C5-C6	-6.22	111.84	122.26
20	9	305	XAT	C11-C10-C9	-6.22	118.44	127.31
22	a	820	CLA	C4A-NA-C1A	6.21	109.50	106.71
20	9	305	XAT	C18-C5-C6	-6.21	111.84	122.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	837	CLA	C4A-NA-C1A	6.21	109.50	106.71
20	2	302	XAT	C38-C25-C26	-6.20	111.87	122.26
20	4	304	XAT	C18-C5-C4	6.18	121.24	114.28
22	b	811	CLA	C4A-NA-C1A	6.17	109.48	106.71
20	3	301	XAT	C38-C25-C24	6.17	121.22	114.28
20	5	302	XAT	C38-C25-C24	6.17	121.22	114.28
22	2	308	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	b	828	CLA	C4A-NA-C1A	6.12	109.46	106.71
20	1	303	XAT	C18-C5-C4	6.11	121.15	114.28
22	b	816	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	9	309	CLA	C4A-NA-C1A	6.09	109.44	106.71
20	2	301	XAT	C38-C25-C26	-6.08	112.07	122.26
20	a	852	XAT	C26-C27-C28	-6.08	113.14	125.99
20	2	305	XAT	C18-C5-C4	6.07	121.11	114.28
20	4	305	XAT	C18-C5-C4	6.06	121.10	114.28
20	2	301	XAT	C31-C30-C29	-6.06	118.66	127.31
20	7	304	XAT	C18-C5-C4	6.02	121.06	114.28
22	b	830	CLA	C4A-NA-C1A	6.01	109.41	106.71
20	2	302	XAT	C18-C5-C4	5.99	121.01	114.28
22	b	817	CLA	C4A-NA-C1A	5.98	109.39	106.71
29	b	842	BCR	C7-C8-C9	-5.96	117.23	126.23
22	b	802	CLA	C4A-NA-C1A	5.96	109.39	106.71
20	5	304	XAT	C26-C27-C28	-5.95	113.41	125.99
22	4	313	CLA	C4A-NA-C1A	5.93	109.37	106.71
20	5	302	XAT	C18-C5-C4	5.92	120.94	114.28
22	8	310	CLA	C4A-NA-C1A	5.92	109.37	106.71
20	8	301	XAT	C18-C5-C4	5.90	120.92	114.28
20	8	302	XAT	C18-C5-C4	5.90	120.92	114.28
20	7	301	XAT	C38-C25-C24	5.90	120.91	114.28
24	h	204	A1L1F	C37-C38-C39	-5.88	118.92	127.31
20	7	303	XAT	C18-C5-C4	5.88	120.89	114.28
24	8	304	A1L1F	O15-C20-C17	5.85	122.07	115.06
20	j	101	XAT	C6-C7-C8	-5.85	113.63	125.99
20	5	301	XAT	C18-C5-C4	5.85	120.86	114.28
29	b	849	BCR	C16-C17-C18	-5.84	118.97	127.31
20	7	301	XAT	C31-C30-C29	-5.82	119.00	127.31
20	5	302	XAT	C38-C25-C26	-5.81	112.52	122.26
20	9	303	XAT	C18-C5-C4	5.79	120.80	114.28
20	7	301	XAT	C38-C25-C26	-5.79	112.55	122.26
20	2	303	XAT	C18-C5-C4	5.77	120.77	114.28
20	4	301	XAT	C35-C34-C33	-5.72	119.14	127.31
29	a	850	BCR	C20-C21-C22	-5.69	119.19	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	302	XAT	C11-C10-C9	-5.67	119.22	127.31
20	9	304	XAT	C26-C27-C28	-5.67	114.01	125.99
29	b	844	BCR	C24-C23-C22	-5.64	117.71	126.23
29	f	801	BCR	C16-C17-C18	-5.64	119.25	127.31
24	1	304	A1L1F	O15-C20-C17	5.64	121.81	115.06
20	4	301	XAT	C38-C25-C24	5.63	120.62	114.28
29	b	842	BCR	C11-C10-C9	-5.63	119.28	127.31
29	b	844	BCR	C7-C8-C9	-5.53	117.88	126.23
20	7	305	XAT	C15-C14-C13	-5.52	119.42	127.31
24	h	204	A1L1F	O15-C20-C17	5.49	121.63	115.06
20	8	303	XAT	C26-C27-C28	-5.48	114.40	125.99
29	j	104	BCR	C28-C27-C26	-5.47	104.30	114.08
29	b	845	BCR	C16-C17-C18	-5.46	119.52	127.31
22	a	803	CLA	C4A-NA-C1A	5.45	109.16	106.71
20	3	301	XAT	C6-C7-C8	-5.44	114.48	125.99
20	9	303	XAT	C15-C14-C13	-5.42	119.57	127.31
29	f	801	BCR	C20-C21-C22	-5.40	119.60	127.31
29	f	804	BCR	C15-C14-C13	-5.40	119.60	127.31
20	3	304	XAT	C35-C34-C33	-5.39	119.62	127.31
20	2	303	XAT	C35-C34-C33	-5.37	119.64	127.31
20	a	852	XAT	C18-C5-C6	-5.34	113.32	122.26
20	4	301	XAT	C38-C25-C26	-5.33	113.33	122.26
20	2	303	XAT	C31-C30-C29	-5.33	119.71	127.31
29	b	844	BCR	C33-C5-C6	-5.32	118.55	124.53
29	b	842	BCR	C3-C4-C5	-5.31	104.59	114.08
26	b	848	DGD	O2G-C1B-C2B	5.29	122.91	111.50
29	a	849	BCR	C3-C4-C5	-5.29	104.63	114.08
29	b	842	BCR	C15-C14-C13	-5.29	119.76	127.31
20	4	303	XAT	C26-C27-C28	-5.27	114.84	125.99
29	l	201	BCR	C7-C8-C9	-5.26	118.28	126.23
20	a	852	XAT	C18-C5-C4	5.26	120.19	114.28
20	4	305	XAT	C15-C14-C13	-5.25	119.81	127.31
20	4	304	XAT	C26-C27-C28	-5.24	114.91	125.99
20	a	852	XAT	C6-C7-C8	-5.24	114.92	125.99
20	2	302	XAT	C35-C34-C33	-5.24	119.83	127.31
20	7	304	XAT	C11-C10-C9	-5.24	119.83	127.31
20	2	303	XAT	C11-C10-C9	-5.23	119.84	127.31
20	2	305	XAT	C31-C30-C29	-5.23	119.84	127.31
24	8	304	A1L1F	C41-C42-C44	-5.21	119.87	127.31
20	2	304	XAT	C6-C7-C8	-5.21	114.98	125.99
20	7	301	XAT	C35-C34-C33	-5.20	119.89	127.31
20	2	301	XAT	C35-C34-C33	-5.20	119.89	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	9	303	XAT	C26-C27-C28	-5.19	115.02	125.99
20	9	305	XAT	C18-C5-C4	5.18	120.11	114.28
20	j	101	XAT	C26-C27-C28	-5.18	115.05	125.99
24	8	304	A1L1F	O7-C54-C56	5.17	120.59	111.09
20	8	303	XAT	C15-C14-C13	-5.13	119.99	127.31
29	l	205	BCR	C24-C23-C22	-5.12	118.50	126.23
29	h	201	BCR	C3-C4-C5	-5.10	104.96	114.08
20	2	305	XAT	C35-C34-C33	-5.05	120.10	127.31
20	1	302	XAT	C35-C34-C33	-5.05	120.10	127.31
20	7	305	XAT	C26-C27-C28	-5.04	115.34	125.99
20	8	303	XAT	C6-C7-C8	-5.04	115.34	125.99
20	3	305	XAT	C26-C27-C28	-5.03	115.36	125.99
29	a	847	BCR	C16-C17-C18	-5.02	120.14	127.31
20	5	301	XAT	C26-C27-C28	-5.02	115.38	125.99
29	b	849	BCR	C11-C10-C9	-4.99	120.19	127.31
20	4	304	XAT	C6-C7-C8	-4.98	115.46	125.99
20	1	302	XAT	C26-C27-C28	-4.98	115.47	125.99
29	f	804	BCR	C11-C10-C9	-4.96	120.24	127.31
29	b	849	BCR	C20-C21-C22	-4.95	120.24	127.31
20	3	305	XAT	C6-C7-C8	-4.95	115.53	125.99
29	a	850	BCR	C16-C17-C18	-4.95	120.25	127.31
20	2	301	XAT	C15-C14-C13	-4.93	120.28	127.31
29	a	849	BCR	C16-C17-C18	-4.91	120.30	127.31
20	7	304	XAT	C26-C27-C28	-4.89	115.66	125.99
20	7	303	XAT	C31-C30-C29	-4.89	120.33	127.31
20	1	303	XAT	C6-C7-C8	-4.89	115.66	125.99
20	2	305	XAT	C6-C7-C8	-4.86	115.71	125.99
20	j	101	XAT	C11-C10-C9	-4.83	120.41	127.31
20	5	302	XAT	C15-C14-C13	-4.83	120.42	127.31
20	2	301	XAT	C6-C7-C8	-4.82	115.80	125.99
29	j	104	BCR	C11-C10-C9	-4.81	120.44	127.31
20	4	303	XAT	C11-C10-C9	-4.81	120.45	127.31
20	1	302	XAT	C6-C7-C8	-4.80	115.84	125.99
29	b	849	BCR	C38-C26-C25	-4.79	119.14	124.53
20	9	305	XAT	C35-C34-C33	-4.78	120.49	127.31
22	a	831	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
20	7	301	XAT	C6-C7-C8	-4.77	115.91	125.99
20	5	304	XAT	C15-C14-C13	-4.77	120.50	127.31
29	i	101	BCR	C16-C17-C18	-4.77	120.51	127.31
29	l	205	BCR	C15-C14-C13	-4.77	120.51	127.31
29	h	202	BCR	C16-C17-C18	-4.75	120.53	127.31
20	4	302	XAT	C26-C27-C28	-4.73	115.99	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	301	XAT	C26-C27-C28	-4.72	116.00	125.99
20	7	304	XAT	C35-C34-C33	-4.72	120.57	127.31
20	7	304	XAT	C15-C14-C13	-4.71	120.59	127.31
20	9	304	XAT	C15-C14-C13	-4.70	120.60	127.31
22	b	817	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
20	4	302	XAT	C6-C7-C8	-4.69	116.07	125.99
22	b	829	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
20	7	305	XAT	C6-C7-C8	-4.68	116.10	125.99
29	b	849	BCR	C7-C8-C9	-4.68	119.17	126.23
20	3	303	XAT	C26-C27-C28	-4.66	116.14	125.99
20	9	305	XAT	C38-C25-C24	4.63	119.48	114.28
20	7	303	XAT	C11-C10-C9	-4.61	120.72	127.31
20	8	302	XAT	C15-C14-C13	-4.61	120.73	127.31
29	b	846	BCR	C16-C17-C18	-4.61	120.73	127.31
20	3	304	XAT	C6-C7-C8	-4.60	116.26	125.99
20	5	301	XAT	C35-C34-C33	-4.60	120.75	127.31
20	7	301	XAT	C27-C28-C29	-4.57	118.44	125.53
20	4	302	XAT	C35-C34-C33	-4.57	120.79	127.31
24	9	302	A1L1F	O7-C54-C56	4.56	119.49	111.09
20	4	305	XAT	C26-C27-C28	-4.56	116.35	125.99
29	b	843	BCR	C11-C10-C9	-4.56	120.80	127.31
29	b	843	BCR	C7-C8-C9	-4.54	119.37	126.23
20	2	305	XAT	C15-C14-C13	-4.54	120.83	127.31
20	8	302	XAT	C26-C27-C28	-4.52	116.44	125.99
20	3	303	XAT	C6-C7-C8	-4.51	116.45	125.99
20	8	302	XAT	C35-C34-C33	-4.51	120.87	127.31
20	2	304	XAT	C26-C27-C28	-4.49	116.50	125.99
24	h	204	A1L1F	O7-C54-C56	4.49	119.34	111.09
20	7	303	XAT	C26-C27-C28	-4.48	116.51	125.99
20	2	302	XAT	C6-C7-C8	-4.48	116.52	125.99
20	7	303	XAT	C35-C34-C33	-4.47	120.93	127.31
29	a	848	BCR	C16-C17-C18	-4.46	120.95	127.31
22	a	802	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
20	3	305	XAT	C35-C34-C33	-4.45	120.97	127.31
29	a	848	BCR	C15-C14-C13	-4.43	120.99	127.31
26	b	848	DGD	O5D-C6D-C5D	-4.41	100.88	109.05
24	9	302	A1L1F	C36-C35-C34	-4.41	121.01	127.31
29	a	850	BCR	C15-C14-C13	-4.38	121.06	127.31
29	a	849	BCR	C15-C14-C13	-4.37	121.07	127.31
29	j	104	BCR	C15-C14-C13	-4.36	121.08	127.31
24	h	204	A1L1F	C25-C14-C29	-4.36	116.78	125.99
26	4	318	DGD	O6E-C5E-C6E	4.36	117.27	106.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	317	LMG	O7-C10-C11	4.36	120.89	111.50
20	3	303	XAT	C35-C34-C33	-4.34	121.12	127.31
29	b	842	BCR	C16-C17-C18	-4.34	121.12	127.31
29	b	844	BCR	C16-C17-C18	-4.33	121.13	127.31
29	b	846	BCR	C33-C5-C6	-4.32	119.67	124.53
22	b	835	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
20	j	101	XAT	C35-C34-C33	-4.32	121.14	127.31
20	8	301	XAT	C35-C34-C33	-4.32	121.14	127.31
22	2	307	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
20	3	303	XAT	C15-C14-C13	-4.31	121.16	127.31
20	3	304	XAT	C31-C30-C29	-4.30	121.18	127.31
20	5	304	XAT	C35-C34-C33	-4.29	121.19	127.31
29	j	104	BCR	C16-C17-C18	-4.28	121.19	127.31
20	4	301	XAT	C6-C7-C8	-4.28	116.94	125.99
29	b	843	BCR	C15-C14-C13	-4.27	121.21	127.31
22	a	833	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
22	4	313	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
22	a	844	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
20	2	305	XAT	C38-C25-C24	4.24	119.05	114.28
26	4	318	DGD	O2G-C1B-C2B	4.23	120.63	111.50
22	b	825	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
20	3	301	XAT	C15-C14-C13	-4.23	121.27	127.31
21	9	301	A1L1G	C37-C36-C35	4.23	132.13	123.47
20	9	304	XAT	C18-C5-C4	4.23	119.03	114.28
22	a	826	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
20	4	304	XAT	C35-C34-C33	-4.21	121.30	127.31
22	8	305	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
20	4	305	XAT	C35-C34-C33	-4.21	121.30	127.31
22	7	308	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
22	a	809	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
29	b	844	BCR	C15-C14-C13	-4.21	121.30	127.31
20	7	303	XAT	C15-C14-C13	-4.21	121.30	127.31
29	f	804	BCR	C24-C23-C22	-4.21	119.88	126.23
24	9	302	A1L1F	C14-C29-C30	-4.20	118.06	125.47
28	b	841	PQN	C11-C12-C13	-4.20	119.80	126.79
24	h	204	A1L1F	C41-C42-C44	-4.20	121.31	127.31
22	3	310	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
29	h	202	BCR	C33-C5-C6	-4.19	119.82	124.53
25	a	845	LHG	O7-C7-C8	4.19	120.54	111.50
29	j	104	BCR	C7-C8-C9	-4.19	119.90	126.23
24	1	304	A1L1F	C37-C38-C39	-4.19	121.33	127.31
22	a	829	CLA	CMB-C2B-C1B	-4.19	122.03	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	820	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
29	l	201	BCR	C15-C14-C13	-4.18	121.34	127.31
22	a	823	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
24	1	304	A1L1F	O7-C54-C56	4.18	118.78	111.09
22	8	311	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
29	l	205	BCR	C20-C21-C22	-4.16	121.37	127.31
22	b	814	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
29	a	850	BCR	C38-C26-C25	-4.15	119.87	124.53
29	l	201	BCR	C33-C5-C6	-4.15	119.87	124.53
24	8	304	A1L1F	C41-C40-C39	-4.15	114.76	126.42
22	a	806	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
29	b	845	BCR	C24-C23-C22	-4.14	119.97	126.23
24	1	304	A1L1F	C17-C20-C21	4.14	118.94	114.28
20	7	305	XAT	C11-C10-C9	-4.14	121.41	127.31
20	3	304	XAT	C15-C14-C13	-4.13	121.42	127.31
22	a	816	CLA	CMB-C2B-C1B	-4.12	122.12	128.46
24	8	304	A1L1F	C32-C31-C30	-4.12	121.39	127.26
25	b	847	LHG	O7-C7-C8	4.12	120.38	111.50
29	h	201	BCR	C16-C17-C18	-4.11	121.44	127.31
22	8	308	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
22	b	832	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
29	b	845	BCR	C20-C21-C22	-4.10	121.45	127.31
22	7	316	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
29	f	801	BCR	C3-C4-C5	-4.09	106.77	114.08
22	9	316	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
27	a	853	LMG	O7-C10-C11	4.09	120.31	111.50
29	f	804	BCR	C7-C8-C9	-4.08	120.07	126.23
29	b	845	BCR	C7-C8-C9	-4.07	120.08	126.23
22	a	803	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
29	b	842	BCR	C28-C27-C26	-4.07	106.82	114.08
22	2	308	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
22	9	309	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
22	a	804	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
22	1	307	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
20	5	301	XAT	C11-C10-C9	-4.06	121.52	127.31
20	4	301	XAT	C15-C14-C13	-4.05	121.53	127.31
22	5	307	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
29	a	848	BCR	C11-C10-C9	-4.05	121.53	127.31
29	b	845	BCR	C16-C15-C14	-4.04	115.21	123.47
29	l	205	BCR	C38-C26-C25	-4.03	120.00	124.53
22	5	311	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
20	7	303	XAT	C6-C7-C8	-4.02	117.50	125.99

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	821	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
29	a	847	BCR	C38-C26-C25	-4.01	120.02	124.53
22	7	311	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
22	b	806	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
22	a	839	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
20	4	305	XAT	C6-C7-C8	-4.00	117.53	125.99
20	3	301	XAT	C35-C34-C33	-4.00	121.60	127.31
22	a	805	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
22	b	826	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
25	9	317	LHG	O7-C7-C8	3.99	120.10	111.50
22	b	810	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
29	b	845	BCR	C28-C27-C26	-3.98	106.96	114.08
22	b	807	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
22	4	308	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
20	a	852	XAT	C31-C30-C29	-3.97	121.65	127.31
22	8	310	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
29	l	201	BCR	C11-C10-C9	-3.96	121.65	127.31
22	9	312	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
20	9	304	XAT	C18-C5-C6	-3.96	115.62	122.26
29	f	804	BCR	C33-C5-C6	-3.96	120.08	124.53
20	4	305	XAT	C11-C10-C9	-3.96	121.66	127.31
24	8	304	A1L1F	C37-C36-C35	-3.96	115.37	123.47
25	a	846	LHG	O7-C7-C8	3.96	120.03	111.50
22	b	831	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	j	105	LMG	O7-C10-C11	3.95	120.01	111.50
22	7	313	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
20	1	303	XAT	C26-C27-C28	-3.93	117.68	125.99
29	i	101	BCR	C7-C8-C9	-3.93	120.30	126.23
22	b	813	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
22	a	838	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
29	b	845	BCR	C15-C14-C13	-3.92	121.72	127.31
22	8	307	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
22	1	308	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
20	4	303	XAT	C15-C14-C13	-3.92	121.72	127.31
22	8	312	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
22	9	314	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	3	309	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	b	802	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
20	2	302	XAT	C31-C30-C29	-3.91	121.73	127.31
22	2	310	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
22	b	816	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
22	b	804	CLA	O2D-CGD-O1D	-3.90	116.22	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	303	XAT	C15-C14-C13	-3.89	121.75	127.31
29	f	804	BCR	C38-C26-C25	-3.89	120.17	124.53
20	j	101	XAT	C15-C14-C13	-3.88	121.78	127.31
22	a	822	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
22	a	815	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
22	4	309	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
22	5	312	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
20	2	302	XAT	C15-C14-C13	-3.87	121.79	127.31
29	f	804	BCR	C20-C21-C22	-3.87	121.79	127.31
22	a	827	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
20	2	305	XAT	C27-C28-C29	-3.86	119.53	125.53
20	2	302	XAT	C26-C27-C28	-3.86	117.82	125.99
29	a	847	BCR	C20-C21-C22	-3.86	121.80	127.31
22	f	802	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
22	l	202	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
22	b	817	CLA	CMB-C2B-C3B	3.85	131.89	124.68
29	l	201	BCR	C16-C17-C18	-3.85	121.82	127.31
21	1	301	A1L1G	C37-C36-C35	3.85	131.35	123.47
26	8	315	DGD	O2G-C1B-C2B	3.84	119.78	111.50
22	2	312	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
21	3	306	A1L1G	C36-C37-C38	3.84	131.34	123.47
22	5	314	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
20	7	301	XAT	C15-C14-C13	-3.82	121.85	127.31
22	l	203	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
22	b	815	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
29	l	205	BCR	C33-C5-C6	-3.82	120.24	124.53
29	l	205	BCR	C16-C17-C18	-3.82	121.86	127.31
22	b	827	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
22	a	811	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	2	313	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	h	203	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	1	306	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
22	b	824	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
22	7	310	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
29	a	849	BCR	C28-C27-C26	-3.79	107.31	114.08
29	b	846	BCR	C15-C14-C13	-3.79	121.90	127.31
22	5	315	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	b	805	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	7	312	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
29	f	804	BCR	C16-C17-C18	-3.78	121.92	127.31
20	5	301	XAT	C15-C14-C13	-3.78	121.92	127.31
21	5	303	A1L1G	C36-C37-C38	3.77	131.20	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	104	BCR	C20-C21-C22	-3.77	121.93	127.31
22	9	315	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
22	a	814	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
23	1	315	SQD	O47-C7-C8	3.76	119.61	111.50
24	h	204	A1L1F	C36-C35-C34	-3.76	121.94	127.31
29	f	801	BCR	C16-C15-C14	-3.76	115.77	123.47
20	1	303	XAT	C35-C34-C33	-3.75	121.96	127.31
22	b	830	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
20	8	301	XAT	C15-C14-C13	-3.74	121.97	127.31
22	9	310	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
20	9	305	XAT	C15-C14-C13	-3.74	121.98	127.31
22	1	310	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
22	a	806	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
22	a	812	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
24	9	302	A1L1F	O15-C20-C17	3.72	119.52	115.06
22	2	309	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
29	h	201	BCR	C15-C14-C13	-3.72	122.00	127.31
22	7	306	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
22	9	308	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
20	2	303	XAT	C26-C27-C28	-3.71	118.14	125.99
22	b	804	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	3	313	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	a	850	BCR	C33-C5-C6	-3.71	120.37	124.53
22	1	311	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	b	843	BCR	C3-C4-C5	-3.70	107.47	114.08
20	3	301	XAT	C26-C27-C28	-3.70	118.17	125.99
22	a	803	CLA	CMB-C2B-C3B	3.70	131.59	124.68
21	9	306	A1L1G	C37-C36-C35	3.69	131.04	123.47
22	3	311	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	7	309	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	a	830	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
20	3	301	XAT	C31-C30-C29	-3.69	122.05	127.31
20	2	301	XAT	C27-C28-C29	-3.69	119.81	125.53
22	a	837	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
20	a	852	XAT	C35-C34-C33	-3.68	122.06	127.31
20	2	303	XAT	C6-C7-C8	-3.67	118.24	125.99
22	a	828	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
22	b	820	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
20	7	304	XAT	C6-C7-C8	-3.66	118.25	125.99
22	h	205	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
22	a	802	CLA	CMB-C2B-C3B	3.66	131.53	124.68
21	7	302	A1L1G	C37-C36-C35	3.66	130.97	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	309	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
29	a	849	BCR	C20-C21-C22	-3.65	122.09	127.31
22	b	834	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
22	a	821	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
22	a	826	CLA	CMB-C2B-C3B	3.65	131.51	124.68
22	b	828	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	h	202	BCR	C7-C8-C9	-3.63	120.75	126.23
24	9	302	A1L1F	C32-C31-C30	-3.63	122.09	127.26
22	b	835	CLA	CMB-C2B-C3B	3.63	131.47	124.68
20	8	301	XAT	C11-C10-C9	-3.63	122.13	127.31
22	b	836	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
20	8	301	XAT	C6-C7-C8	-3.62	118.33	125.99
22	b	838	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
29	b	845	BCR	C3-C4-C5	-3.62	107.62	114.08
20	4	302	XAT	C35-C15-C14	-3.61	116.08	123.47
22	4	310	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
20	9	305	XAT	C31-C30-C29	-3.60	122.17	127.31
22	b	812	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	a	829	CLA	CMB-C2B-C3B	3.59	131.40	124.68
22	2	307	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	b	822	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
22	b	811	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
22	8	309	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
29	a	847	BCR	C33-C5-C6	-3.58	120.51	124.53
20	1	302	XAT	C11-C10-C9	-3.58	122.20	127.31
21	9	301	A1L1G	C27-C34-C35	-3.58	117.91	122.92
29	i	101	BCR	C33-C5-C6	-3.57	120.52	124.53
22	a	808	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
29	a	849	BCR	C11-C10-C9	-3.56	122.23	127.31
22	b	811	CLA	CAB-C3B-C4B	-3.56	122.99	128.46
22	9	316	CLA	CMB-C2B-C3B	3.56	131.34	124.68
22	a	809	CLA	CMB-C2B-C3B	3.56	131.34	124.68
22	8	305	CLA	CMB-C2B-C3B	3.56	131.34	124.68
22	a	833	CLA	CMB-C2B-C3B	3.56	131.33	124.68
20	9	303	XAT	C11-C10-C9	-3.55	122.24	127.31
22	7	308	CLA	CMB-C2B-C3B	3.55	131.33	124.68
29	b	843	BCR	C33-C5-C6	-3.55	120.54	124.53
22	8	306	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	b	833	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	a	832	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	a	844	CLA	CMB-C2B-C3B	3.54	131.31	124.68
22	b	808	CLA	CMB-C2B-C1B	-3.54	123.02	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	205	BCR	C3-C4-C5	-3.54	107.75	114.08
29	l	205	BCR	C11-C10-C9	-3.54	122.26	127.31
21	9	301	A1L1G	C36-C37-C38	3.54	130.72	123.47
22	b	804	CLA	CHB-C4A-NA	3.54	129.40	124.51
22	l	204	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
20	8	303	XAT	C15-C35-C34	-3.53	116.24	123.47
20	4	303	XAT	C35-C34-C33	-3.53	122.27	127.31
29	h	202	BCR	C38-C26-C25	-3.53	120.56	124.53
22	4	313	CLA	CMB-C2B-C3B	3.53	131.28	124.68
29	a	847	BCR	C15-C14-C13	-3.53	122.28	127.31
29	a	847	BCR	C7-C8-C9	-3.52	120.91	126.23
22	8	311	CLA	CMB-C2B-C3B	3.52	131.27	124.68
22	a	842	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
21	9	306	A1L1G	C36-C37-C38	3.52	130.69	123.47
22	b	818	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
22	b	825	CLA	CMB-C2B-C3B	3.52	131.26	124.68
22	b	814	CLA	CMB-C2B-C3B	3.52	131.26	124.68
22	a	806	CLA	CAA-CBA-CGA	-3.51	102.98	113.25
22	b	832	CLA	CMB-C2B-C3B	3.51	131.25	124.68
22	3	310	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	4	314	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	1	312	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	5	305	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
20	1	303	XAT	C15-C14-C13	-3.50	122.32	127.31
21	7	302	A1L1G	C36-C37-C38	3.50	130.64	123.47
22	a	835	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	b	826	CLA	CMB-C2B-C3B	3.49	131.22	124.68
22	4	317	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
20	8	302	XAT	C31-C30-C29	-3.49	122.33	127.31
22	1	305	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
29	h	201	BCR	C24-C23-C22	-3.49	120.96	126.23
29	a	848	BCR	C24-C23-C22	-3.49	120.96	126.23
22	a	823	CLA	CMB-C2B-C3B	3.49	131.20	124.68
22	5	313	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
22	a	813	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
20	9	303	XAT	C35-C34-C33	-3.49	122.34	127.31
29	i	101	BCR	C28-C27-C26	-3.48	107.86	114.08
23	5	316	SQD	O47-C7-C8	3.48	119.01	111.50
22	3	307	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	3	314	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	8	308	CLA	CMB-C2B-C3B	3.47	131.18	124.68
22	a	807	CLA	CMB-C2B-C1B	-3.47	123.13	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	809	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	7	302	A1L1G	C27-C34-C35	-3.47	118.06	122.92
22	5	306	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
21	3	302	A1L1G	C36-C37-C38	3.46	130.57	123.47
29	a	849	BCR	C4-C5-C6	-3.46	117.71	122.73
22	4	315	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	b	819	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	a	831	CLA	CMB-C2B-C3B	3.46	131.15	124.68
20	4	302	XAT	C11-C10-C9	-3.46	122.38	127.31
22	b	802	CLA	CMB-C2B-C3B	3.46	131.15	124.68
20	2	305	XAT	C24-C23-C22	-3.46	104.10	110.77
21	3	302	A1L1G	C37-C36-C35	3.46	130.55	123.47
25	a	846	LHG	O8-C23-C24	3.45	120.44	111.38
22	3	315	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	a	817	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	b	823	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	7	316	CLA	CMB-C2B-C3B	3.45	131.13	124.68
22	j	102	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
21	9	306	A1L1G	C28-C39-C38	-3.45	118.10	122.92
22	a	819	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	a	805	CLA	CMB-C2B-C3B	3.44	131.12	124.68
22	8	313	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	9	313	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	2	308	CLA	CMB-C2B-C3B	3.44	131.11	124.68
22	2	306	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	4	306	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	a	841	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	a	825	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
21	5	303	A1L1G	C28-C39-C38	-3.43	118.11	122.92
22	a	820	CLA	CMB-C2B-C3B	3.43	131.10	124.68
22	9	318	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	a	816	CLA	CMB-C2B-C3B	3.43	131.10	124.68
22	b	837	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	1	313	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
20	2	304	XAT	C11-C10-C9	-3.43	122.42	127.31
20	3	305	XAT	C15-C14-C13	-3.43	122.42	127.31
21	3	306	A1L1G	C27-C34-C35	-3.43	118.12	122.92
21	1	301	A1L1G	C28-C39-C38	-3.43	118.12	122.92
22	4	312	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
21	7	302	A1L1G	C28-C39-C38	-3.43	118.12	122.92
22	9	314	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
22	4	316	CLA	CMB-C2B-C1B	-3.43	123.20	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	308	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	7	317	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	a	806	CLA	CMB-C2B-C3B	3.42	131.08	124.68
29	a	848	BCR	C20-C21-C22	-3.42	122.43	127.31
22	8	314	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	a	818	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
20	3	303	XAT	C11-C10-C9	-3.42	122.43	127.31
29	a	847	BCR	C24-C23-C22	-3.42	121.07	126.23
22	a	840	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
29	a	849	BCR	C7-C8-C9	-3.41	121.08	126.23
21	1	301	A1L1G	C27-C34-C35	-3.41	118.14	122.92
21	9	306	A1L1G	C27-C34-C35	-3.41	118.14	122.92
20	5	302	XAT	C6-C7-C8	-3.41	118.78	125.99
20	2	304	XAT	C31-C30-C29	-3.41	122.44	127.31
22	2	314	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	9	312	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
29	a	847	BCR	C11-C10-C9	-3.41	122.45	127.31
20	7	304	XAT	C31-C30-C29	-3.41	122.45	127.31
22	3	308	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
22	b	806	CLA	CMB-C2B-C3B	3.40	131.04	124.68
22	a	810	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
24	9	302	A1L1F	C37-C38-C39	-3.39	122.47	127.31
22	a	804	CLA	CMB-C2B-C3B	3.39	131.03	124.68
22	j	103	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	9	307	LHG	O7-C7-C8	3.39	120.26	110.80
21	9	301	A1L1G	C28-C39-C38	-3.39	118.17	122.92
22	f	803	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
21	9	301	A1L1G	C33-C34-C35	3.39	124.14	118.94
29	a	849	BCR	C24-C23-C22	-3.39	121.11	126.23
22	1	309	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	b	807	CLA	CMB-C2B-C3B	3.39	131.01	124.68
22	b	821	CLA	CMB-C2B-C3B	3.38	131.01	124.68
22	5	311	CLA	CMB-C2B-C3B	3.38	131.01	124.68
22	9	312	CLA	CMB-C2B-C3B	3.38	131.01	124.68
21	3	302	A1L1G	C28-C39-C38	-3.38	118.18	122.92
22	1	314	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	a	854	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
20	8	303	XAT	C30-C31-C32	-3.37	112.69	123.22
22	2	311	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
21	5	303	A1L1G	C37-C36-C35	3.37	130.38	123.47
22	b	804	CLA	CMB-C2B-C3B	3.37	130.99	124.68
22	2	316	CLA	CMB-C2B-C1B	-3.37	123.28	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	315	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
24	1	304	A1L1F	C8-O7-C54	-3.37	111.62	117.90
22	2	315	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
22	b	831	CLA	CMB-C2B-C3B	3.37	130.98	124.68
22	5	310	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
22	7	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	5	307	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	1	307	CLA	CMB-C2B-C3B	3.36	130.96	124.68
20	9	304	XAT	C35-C34-C33	-3.36	122.52	127.31
22	4	308	CLA	CMB-C2B-C3B	3.35	130.96	124.68
22	4	307	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
21	5	303	A1L1G	C27-C34-C35	-3.35	118.22	122.92
21	3	302	A1L1G	C27-C34-C35	-3.35	118.22	122.92
29	b	845	BCR	C10-C11-C12	-3.35	112.75	123.22
20	5	301	XAT	C7-C8-C9	-3.35	120.33	125.53
22	b	813	CLA	CMB-C2B-C3B	3.35	130.94	124.68
22	7	313	CLA	CMB-C2B-C3B	3.35	130.94	124.68
21	3	306	A1L1G	C28-C39-C38	-3.34	118.24	122.92
29	h	202	BCR	C11-C10-C9	-3.34	122.55	127.31
20	j	101	XAT	C10-C11-C12	-3.34	112.81	123.22
24	8	304	A1L1F	C31-C32-C33	-3.34	112.81	123.22
22	3	309	CLA	CMB-C2B-C3B	3.33	130.91	124.68
22	b	829	CLA	CMB-C2B-C3B	3.33	130.90	124.68
29	a	847	BCR	C3-C4-C5	-3.33	108.14	114.08
22	8	307	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	7	314	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	9	311	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	5	312	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	a	834	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
24	8	304	A1L1F	C14-C29-C30	-3.32	119.62	125.47
22	a	824	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
20	5	301	XAT	C6-C7-C8	-3.31	118.98	125.99
20	1	303	XAT	C31-C30-C29	-3.31	122.58	127.31
22	b	816	CLA	CMB-C2B-C3B	3.31	130.87	124.68
28	a	843	PQN	C14-C13-C15	3.31	120.84	115.27
22	a	838	CLA	CMB-C2B-C3B	3.31	130.87	124.68
20	4	303	XAT	C6-C7-C8	-3.31	119.00	125.99
20	1	303	XAT	C24-C23-C22	-3.31	104.39	110.77
22	a	839	CLA	CMB-C2B-C3B	3.31	130.87	124.68
22	4	311	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	a	827	CLA	CMB-C2B-C3B	3.30	130.86	124.68
29	j	104	BCR	C24-C23-C22	-3.30	121.24	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	801	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
29	i	101	BCR	C15-C14-C13	-3.30	122.60	127.31
21	1	301	A1L1G	C36-C37-C38	3.30	130.23	123.47
26	b	848	DGD	C2G-O2G-C1B	-3.30	109.68	117.79
20	9	305	XAT	C38-C25-C26	-3.29	116.74	122.26
24	9	302	A1L1F	C25-C14-C29	-3.29	119.04	125.99
22	1	308	CLA	CMB-C2B-C3B	3.29	130.83	124.68
20	5	304	XAT	C24-C23-C22	-3.29	104.43	110.77
22	9	309	CLA	CMB-C2B-C3B	3.28	130.82	124.68
22	f	802	CLA	CMB-C2B-C3B	3.28	130.82	124.68
20	4	301	XAT	C11-C10-C9	-3.28	122.63	127.31
22	8	312	CLA	CMB-C2B-C3B	3.28	130.81	124.68
22	9	311	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
29	i	101	BCR	C11-C10-C9	-3.27	122.65	127.31
20	5	301	XAT	C24-C23-C22	-3.26	104.47	110.77
22	4	309	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	7	311	CLA	CMB-C2B-C3B	3.26	130.77	124.68
20	5	304	XAT	C4-C3-C2	-3.25	104.49	110.77
22	9	314	CLA	CMB-C2B-C3B	3.25	130.76	124.68
22	b	840	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
21	9	306	A1L1G	C33-C34-C35	3.25	123.92	118.94
22	5	314	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	3	312	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
22	j	103	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	h	204	A1L1F	C31-C32-C33	-3.24	113.11	123.22
29	a	850	BCR	C7-C8-C9	-3.24	121.34	126.23
20	9	304	XAT	C11-C10-C9	-3.24	122.69	127.31
24	h	204	A1L1F	C17-C20-C21	3.23	117.92	114.28
21	1	301	A1L1G	C43-C44-C42	-3.23	118.40	122.92
22	2	312	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	b	827	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	a	815	CLA	CMB-C2B-C3B	3.22	130.70	124.68
24	1	304	A1L1F	C14-C29-C30	-3.22	119.80	125.47
22	b	805	CLA	CMB-C2B-C3B	3.22	130.69	124.68
22	h	203	CLA	CMB-C2B-C3B	3.22	130.69	124.68
22	b	809	CLA	O2A-CGA-O1A	-3.22	115.48	123.59
20	a	852	XAT	C10-C11-C12	-3.21	113.19	123.22
20	1	302	XAT	C15-C14-C13	-3.20	122.74	127.31
20	a	852	XAT	C11-C10-C9	-3.20	122.74	127.31
22	8	310	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	9	315	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	a	836	CLA	CMB-C2B-C1B	-3.20	123.55	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	304	XAT	C26-C27-C28	-3.20	119.23	125.99
22	b	820	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
29	h	201	BCR	C20-C21-C22	-3.20	122.75	127.31
29	b	849	BCR	C24-C23-C22	-3.20	121.41	126.23
21	1	301	A1L1G	C33-C34-C35	3.19	123.84	118.94
20	4	304	XAT	C15-C14-C13	-3.19	122.75	127.31
29	a	848	BCR	C33-C5-C6	-3.19	120.95	124.53
22	1	306	CLA	CMB-C2B-C3B	3.19	130.64	124.68
29	a	848	BCR	C38-C26-C25	-3.19	120.95	124.53
22	b	824	CLA	CMB-C2B-C3B	3.19	130.64	124.68
29	b	849	BCR	C33-C5-C6	-3.19	120.95	124.53
22	a	814	CLA	CMB-C2B-C3B	3.19	130.64	124.68
24	8	304	A1L1F	C26-C30-C31	-3.18	120.77	124.93
21	5	303	A1L1G	C40-C39-C38	3.18	123.83	118.94
22	a	828	CLA	CMB-C2B-C3B	3.18	130.63	124.68
29	l	201	BCR	C38-C26-C25	-3.18	120.95	124.53
22	2	313	CLA	CMB-C2B-C3B	3.18	130.63	124.68
22	b	839	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
22	a	835	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
22	b	815	CLA	CMB-C2B-C3B	3.18	130.63	124.68
20	9	305	XAT	C8-C9-C10	3.18	123.82	118.94
20	3	304	XAT	C11-C10-C9	-3.18	122.77	127.31
24	h	204	A1L1F	C37-C36-C35	-3.18	116.96	123.47
22	a	811	CLA	CMB-C2B-C3B	3.17	130.62	124.68
22	5	315	CLA	CMB-C2B-C3B	3.17	130.61	124.68
21	3	306	A1L1G	C37-C36-C35	3.17	129.97	123.47
22	a	822	CLA	CMB-C2B-C3B	3.17	130.61	124.68
22	l	202	CLA	CMB-C2B-C3B	3.16	130.59	124.68
20	9	304	XAT	C24-C23-C22	-3.16	104.67	110.77
20	9	303	XAT	C6-C7-C8	-3.16	119.32	125.99
20	7	305	XAT	C35-C34-C33	-3.16	122.81	127.31
29	a	850	BCR	C11-C10-C9	-3.16	122.81	127.31
22	7	316	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	5	312	CLA	CMB-C2B-C3B	3.15	130.58	124.68
22	a	812	CLA	CMB-C2B-C3B	3.15	130.58	124.68
29	a	848	BCR	C3-C4-C5	-3.15	108.45	114.08
29	l	201	BCR	C24-C23-C22	-3.15	121.47	126.23
20	2	301	XAT	C11-C10-C9	-3.15	122.81	127.31
20	4	304	XAT	C24-C23-C22	-3.15	104.69	110.77
22	a	804	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
20	9	305	XAT	C24-C23-C22	-3.15	104.69	110.77
29	b	843	BCR	C16-C17-C18	-3.15	122.82	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	310	CLA	CMB-C2B-C3B	3.14	130.56	124.68
29	a	849	BCR	C38-C26-C25	-3.14	121.00	124.53
20	4	303	XAT	C24-C23-C22	-3.14	104.70	110.77
22	7	312	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	1	311	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	b	810	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	1	313	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
20	9	303	XAT	C24-C23-C22	-3.14	104.71	110.77
22	1	310	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	a	818	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
22	9	308	CLA	CMB-C2B-C3B	3.14	130.55	124.68
20	3	303	XAT	C24-C23-C22	-3.13	104.72	110.77
29	b	846	BCR	C10-C11-C12	-3.13	113.45	123.22
22	a	830	CLA	CMB-C2B-C3B	3.13	130.53	124.68
20	2	301	XAT	C26-C27-C28	-3.12	119.39	125.99
22	5	309	CLA	CMB-C2B-C3B	3.12	130.51	124.68
21	1	301	A1L1G	C40-C39-C38	3.12	123.72	118.94
22	7	306	CLA	CMB-C2B-C3B	3.11	130.50	124.68
21	3	302	A1L1G	C33-C34-C35	3.11	123.71	118.94
21	3	306	A1L1G	C40-C39-C38	3.11	123.71	118.94
22	a	803	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
29	h	201	BCR	C33-C5-C4	3.11	119.58	113.62
21	7	302	A1L1G	C40-C39-C38	3.11	123.71	118.94
24	8	304	A1L1F	C36-C35-C34	-3.11	122.88	127.31
22	b	832	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	2	309	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	7	310	CLA	CMB-C2B-C3B	3.10	130.48	124.68
29	b	845	BCR	C11-C10-C9	-3.10	122.88	127.31
20	8	301	XAT	C24-C23-C22	-3.10	104.78	110.77
21	7	302	A1L1G	C33-C34-C35	3.10	123.70	118.94
22	b	809	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	h	205	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	3	313	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	4	318	DGD	O1G-C1A-C2A	3.10	121.63	111.91
22	4	316	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	b	830	CLA	CMB-C2B-C3B	3.10	130.47	124.68
22	l	203	CLA	CMB-C2B-C3B	3.10	130.47	124.68
21	9	306	A1L1G	C40-C39-C38	3.10	123.69	118.94
22	a	837	CLA	CMB-C2B-C3B	3.09	130.45	124.68
20	7	304	XAT	C24-C23-C22	-3.08	104.82	110.77
22	3	308	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
20	a	852	XAT	C35-C15-C14	-3.08	117.17	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	849	BCR	C33-C5-C4	3.08	119.53	113.62
22	b	820	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	9	306	A1L1G	C43-C44-C42	-3.07	118.62	122.92
29	h	201	BCR	C38-C26-C25	-3.07	121.08	124.53
22	b	802	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
20	4	304	XAT	C35-C15-C14	-3.07	117.19	123.47
29	b	842	BCR	C20-C21-C22	-3.07	122.93	127.31
24	8	304	A1L1F	C25-C14-C29	-3.07	119.51	125.99
20	3	304	XAT	C4-C3-C2	-3.07	104.85	110.77
22	2	310	CLA	CMB-C2B-C3B	3.06	130.41	124.68
22	4	311	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	a	821	CLA	CMB-C2B-C3B	3.06	130.41	124.68
22	b	812	CLA	CMB-C2B-C3B	3.06	130.40	124.68
22	b	836	CLA	CMB-C2B-C3B	3.05	130.39	124.68
26	8	315	DGD	O1G-C1A-C2A	3.05	121.49	111.91
22	7	309	CLA	CMB-C2B-C3B	3.05	130.39	124.68
29	1	205	BCR	C8-C7-C6	-3.05	118.63	127.20
22	3	311	CLA	CMB-C2B-C3B	3.05	130.38	124.68
20	2	303	XAT	C19-C9-C10	-3.05	118.65	122.92
20	1	302	XAT	C31-C30-C29	-3.05	122.96	127.31
22	a	809	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
20	5	301	XAT	C31-C30-C29	-3.04	122.97	127.31
24	9	302	A1L1F	C42-C41-C40	-3.04	113.72	123.22
22	4	307	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	7	302	A1L1G	C43-C44-C42	-3.04	118.67	122.92
21	9	301	A1L1G	C40-C39-C38	3.04	123.60	118.94
29	f	801	BCR	C8-C7-C6	-3.04	118.67	127.20
22	b	816	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	8	308	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	a	801	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
22	b	822	CLA	CMB-C2B-C3B	3.03	130.35	124.68
20	a	852	XAT	C31-C32-C33	-3.03	117.91	126.42
22	9	313	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
29	a	848	BCR	C8-C7-C6	-3.02	118.71	127.20
22	8	309	CLA	CMB-C2B-C3B	3.02	130.32	124.68
20	4	305	XAT	C24-C23-C22	-3.02	104.95	110.77
20	8	302	XAT	C24-C23-C22	-3.02	104.95	110.77
22	a	831	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	h	204	A1L1F	C12-C6-C1	-3.01	107.78	110.47
29	h	202	BCR	C15-C14-C13	-3.01	123.01	127.31
20	3	305	XAT	C4-C3-C2	-3.01	104.96	110.77
22	9	310	CLA	O2D-CGD-O1D	-3.01	117.95	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	303	A1L1G	C33-C34-C35	3.01	123.56	118.94
22	b	808	CLA	CMB-C2B-C3B	3.01	130.30	124.68
21	3	306	A1L1G	C33-C34-C35	3.00	123.55	118.94
29	h	202	BCR	C16-C15-C14	-3.00	117.32	123.47
21	3	302	A1L1G	C40-C39-C38	3.00	123.54	118.94
22	7	314	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	b	834	CLA	CMB-C2B-C3B	3.00	130.28	124.68
21	3	306	A1L1G	C43-C44-C42	-3.00	118.73	122.92
22	b	811	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
20	9	305	XAT	C27-C28-C29	-2.99	120.88	125.53
24	9	302	A1L1F	C26-C30-C31	-2.99	121.02	124.93
22	b	808	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	l	204	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	a	835	CLA	CMB-C2B-C3B	2.99	130.27	124.68
20	8	302	XAT	C6-C7-C8	-2.99	119.68	125.99
20	8	303	XAT	C24-C23-C22	-2.99	105.00	110.77
22	a	807	CLA	CMB-C2B-C3B	2.98	130.26	124.68
22	4	310	CLA	CMB-C2B-C3B	2.98	130.25	124.68
20	3	305	XAT	C31-C30-C29	-2.98	123.06	127.31
22	b	833	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	b	838	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	1	314	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	b	814	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
20	7	305	XAT	C4-C3-C2	-2.97	105.03	110.77
22	b	803	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
22	a	830	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
26	b	848	DGD	O3E-C3E-C2E	-2.97	103.49	110.35
22	b	814	CLA	CHB-C4A-NA	2.97	128.61	124.51
29	b	849	BCR	C16-C15-C14	-2.97	117.40	123.47
20	1	302	XAT	C35-C15-C14	-2.96	117.40	123.47
29	h	201	BCR	C8-C7-C6	-2.96	118.88	127.20
20	9	305	XAT	C19-C9-C10	-2.96	118.77	122.92
22	b	836	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	7	313	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	a	850	BCR	C28-C27-C26	-2.96	108.80	114.08
22	2	309	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	b	846	BCR	C8-C7-C6	-2.95	118.90	127.20
20	4	301	XAT	C31-C32-C33	-2.95	118.12	126.42
22	2	313	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	b	843	BCR	C38-C26-C25	-2.95	121.22	124.53
22	b	834	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	b	818	CLA	CMB-C2B-C3B	2.95	130.20	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	306	CLA	CMB-C2B-C3B	2.95	130.19	124.68
20	3	305	XAT	C24-C23-C22	-2.95	105.08	110.77
22	4	308	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	4	309	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
21	5	303	A1L1G	C43-C44-C42	-2.94	118.80	122.92
22	a	839	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
20	8	303	XAT	C4-C3-C2	-2.94	105.09	110.77
22	b	805	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	9	314	CLA	O2D-CGD-CBD	2.94	116.49	111.27
22	7	308	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	a	812	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
22	h	203	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	3	314	CLA	CMB-C2B-C3B	2.93	130.17	124.68
20	4	303	XAT	C30-C31-C32	-2.93	114.07	123.22
22	a	808	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	b	839	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	4	304	XAT	C4-C3-C2	-2.93	105.12	110.77
22	5	308	CLA	CMB-C2B-C3B	2.93	130.15	124.68
22	b	824	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	9	313	CLA	CMB-C2B-C3B	2.92	130.15	124.68
29	b	845	BCR	C33-C5-C6	-2.92	121.25	124.53
22	1	311	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	b	844	BCR	C38-C26-C25	-2.92	121.25	124.53
22	3	309	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	7	305	XAT	C24-C23-C22	-2.92	105.14	110.77
22	b	829	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	j	102	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	4	314	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	b	818	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	a	817	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	7	301	XAT	C4-C3-C2	-2.91	105.15	110.77
20	5	302	XAT	C24-C23-C22	-2.91	105.16	110.77
20	3	301	XAT	C4-C3-C2	-2.91	105.16	110.77
22	b	840	CLA	CMB-C2B-C3B	2.91	130.12	124.68
22	b	817	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	1	313	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	5	315	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
20	4	302	XAT	C24-C23-C22	-2.90	105.17	110.77
22	b	823	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	a	832	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	7	314	CLA	CMB-C2B-C3B	2.90	130.10	124.68
20	1	302	XAT	C4-C3-C2	-2.90	105.17	110.77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	826	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	2	303	XAT	C4-C3-C2	-2.90	105.18	110.77
20	2	304	XAT	C24-C23-C22	-2.90	105.18	110.77
22	a	840	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	3	307	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	b	837	CLA	CMB-C2B-C3B	2.90	130.10	124.68
23	5	316	SQD	C44-O6-C1	-2.90	108.08	113.74
20	5	302	XAT	C35-C34-C33	-2.89	123.18	127.31
22	9	312	CLA	CHB-C4A-NA	2.89	128.51	124.51
21	9	301	A1L1G	C43-C44-C42	-2.89	118.87	122.92
22	a	810	CLA	CMB-C2B-C3B	2.89	130.08	124.68
20	5	304	XAT	C5-C4-C3	-2.89	107.03	112.75
22	2	310	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	b	809	CLA	CMB-C2B-C3B	2.89	130.08	124.68
22	b	828	CLA	CMB-C2B-C3B	2.89	130.08	124.68
22	4	312	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	7	303	XAT	C19-C9-C10	-2.88	118.88	122.92
22	2	307	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	a	837	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	8	304	A1L1F	C11-C1-C6	2.88	122.55	119.70
22	l	202	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
20	1	302	XAT	C24-C23-C22	-2.88	105.22	110.77
22	8	311	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	b	806	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	a	813	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	a	819	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	a	820	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	h	202	BCR	C23-C24-C25	-2.87	119.14	127.20
22	8	306	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	4	317	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	7	315	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	b	846	BCR	C15-C16-C17	-2.87	117.60	123.47
22	5	307	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	f	801	BCR	C20-C19-C18	-2.87	118.36	126.42
22	7	312	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	2	316	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	2	314	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	3	303	XAT	C4-C3-C2	-2.86	105.24	110.77
20	8	303	XAT	C11-C10-C9	-2.86	123.22	127.31
22	1	307	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	3	307	CLA	CMB-C2B-C3B	2.86	130.03	124.68
29	f	801	BCR	C33-C5-C6	-2.86	121.31	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	310	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	2	307	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	a	852	XAT	C24-C23-C22	-2.86	105.25	110.77
22	4	315	CLA	CMB-C2B-C3B	2.86	130.02	124.68
22	a	823	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	2	305	XAT	C11-C10-C9	-2.85	123.24	127.31
22	1	309	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	a	841	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	b	804	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
22	a	811	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	9	304	XAT	C15-C35-C34	-2.85	117.64	123.47
22	5	305	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	b	838	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	8	313	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	1	305	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	3	308	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	3	311	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	a	825	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	b	837	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	1	312	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	8	305	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	h	201	BCR	C4-C5-C6	-2.84	118.61	122.73
20	4	302	XAT	C4-C3-C2	-2.84	105.29	110.77
22	j	102	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	5	309	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	a	842	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	5	310	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	a	848	BCR	C7-C8-C9	-2.84	121.95	126.23
22	7	317	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	a	817	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	a	816	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	8	304	A1L1F	C17-C20-C21	2.83	117.47	114.28
22	1	314	CLA	CMB-C2B-C3B	2.83	129.98	124.68
22	5	312	CLA	O2D-CGD-CBD	2.83	116.30	111.27
22	3	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
20	2	304	XAT	C4-C3-C2	-2.83	105.31	110.77
22	a	841	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	4	318	DGD	O5E-C6E-C5E	-2.82	101.60	111.29
22	9	315	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	a	805	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	a	813	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	8	313	CLA	O2D-CGD-O1D	-2.82	118.32	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	j	103	CLA	CMB-C2B-C3B	2.82	129.95	124.68
20	5	304	XAT	C19-C9-C8	2.82	122.52	118.08
22	a	840	CLA	CMB-C2B-C3B	2.82	129.95	124.68
21	3	302	A1L1G	C43-C44-C42	-2.82	118.98	122.92
20	j	101	XAT	C4-C3-C2	-2.82	105.33	110.77
22	a	825	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	a	826	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	f	803	CLA	CMB-C2B-C3B	2.81	129.94	124.68
20	1	303	XAT	C4-C3-C2	-2.81	105.34	110.77
22	8	312	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	9	311	CLA	CHB-C4A-NA	2.81	128.40	124.51
29	b	844	BCR	C34-C9-C10	-2.81	118.98	122.92
22	7	315	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	8	314	CLA	CMB-C2B-C3B	2.81	129.94	124.68
29	b	846	BCR	C21-C20-C19	-2.81	114.45	123.22
22	1	203	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	7	310	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
20	4	301	XAT	C4-C3-C2	-2.81	105.35	110.77
20	9	304	XAT	C4-C3-C2	-2.81	105.35	110.77
22	5	308	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	3	312	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	8	307	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
20	3	304	XAT	C24-C23-C22	-2.80	105.36	110.77
22	a	844	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	4	312	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	a	815	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	9	318	CLA	CMB-C2B-C3B	2.80	129.91	124.68
20	2	301	XAT	C4-C3-C2	-2.80	105.37	110.77
22	7	307	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	9	314	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	a	833	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	5	306	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	a	836	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	1	301	A1L1G	C20-C21-C22	-2.79	107.22	112.75
22	a	803	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	b	827	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
20	7	305	XAT	C15-C35-C34	-2.79	117.75	123.47
22	7	306	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	4	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
28	b	841	PQN	C16-C15-C13	-2.79	106.14	113.45
22	a	827	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	2	316	CLA	CMB-C2B-C3B	2.79	129.90	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	834	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	b	831	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	a	832	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	4	306	CLA	CMB-C2B-C3B	2.79	129.89	124.68
22	a	802	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
22	1	310	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
22	2	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
20	2	305	XAT	C38-C25-C26	-2.78	117.60	122.26
22	b	840	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	3	314	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	b	844	BCR	C20-C21-C22	-2.78	123.34	127.31
22	5	313	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	9	303	XAT	C15-C35-C34	-2.78	117.78	123.47
26	b	848	DGD	O1G-C1A-C2A	2.78	120.63	111.91
22	1	305	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	j	104	BCR	C38-C26-C27	2.78	118.95	113.62
24	1	304	A1L1F	C36-C35-C34	-2.78	123.35	127.31
20	9	304	XAT	C30-C31-C32	-2.77	114.56	123.22
22	b	819	CLA	CMB-C2B-C3B	2.77	129.87	124.68
22	b	821	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	2	306	CLA	CMB-C2B-C3B	2.77	129.87	124.68
22	a	821	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	8	314	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	4	304	XAT	C11-C10-C9	-2.77	123.36	127.31
22	b	801	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	2	311	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	b	823	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	9	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	b	842	BCR	C33-C5-C4	2.77	118.94	113.62
20	2	301	XAT	C24-C23-C22	-2.77	105.42	110.77
22	2	315	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	8	309	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	1	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	b	811	CLA	CMB-C2B-C3B	2.77	130.10	124.69
22	a	841	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	b	843	BCR	C21-C20-C19	-2.77	114.59	123.22
22	b	828	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
20	4	305	XAT	C4-C3-C2	-2.76	105.44	110.77
24	1	304	A1L1F	C20-C21-C22	-2.76	107.28	112.75
22	3	315	CLA	CMB-C2B-C3B	2.76	129.85	124.68
29	b	842	BCR	C38-C26-C25	-2.76	121.43	124.53
20	8	303	XAT	C39-C29-C28	2.76	122.43	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	314	CLA	CMB-C2B-C3B	2.76	129.84	124.68
20	3	301	XAT	C10-C11-C12	-2.76	114.61	123.22
22	h	205	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
20	4	301	XAT	C26-C27-C28	-2.76	120.16	125.99
27	2	317	LMG	O8-C28-C29	2.76	120.56	111.91
22	7	317	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	b	815	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	9	310	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	1	306	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
29	a	849	BCR	C2-C1-C6	2.75	114.72	110.48
22	3	315	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	7	307	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	a	819	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	9	312	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	1	304	A1L1F	C26-O13-C45	2.75	121.80	115.68
22	5	313	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	9	311	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	9	316	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	9	304	XAT	C7-C8-C9	-2.75	121.26	125.53
29	a	850	BCR	C38-C26-C27	2.75	118.90	113.62
20	4	302	XAT	C31-C30-C29	-2.75	123.39	127.31
20	7	301	XAT	C11-C10-C9	-2.75	123.39	127.31
26	b	848	DGD	C6D-O5D-C1E	2.75	119.11	113.74
22	b	830	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
29	b	844	BCR	C37-C22-C21	-2.75	119.08	122.92
20	3	303	XAT	C31-C30-C29	-2.74	123.39	127.31
22	4	316	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	h	204	A1L1F	C26-C30-C31	-2.74	121.35	124.93
22	4	306	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	2	315	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	3	312	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	l	204	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	a	807	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	4	307	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	b	835	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
27	a	853	LMG	O8-C28-C29	2.73	120.49	111.91
22	a	828	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	b	812	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
20	2	305	XAT	C4-C3-C2	-2.73	105.50	110.77
24	8	304	A1L1F	O7-C54-O55	-2.73	117.54	122.96
22	5	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	a	838	CLA	O2D-CGD-O1D	-2.73	118.50	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	824	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	5	305	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	5	310	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	a	854	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	f	802	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	7	315	CLA	CAA-C2A-C3A	-2.73	109.73	116.10
22	4	315	CLA	CHB-C4A-NA	2.73	128.28	124.51
22	f	803	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
22	7	317	CLA	CHB-C4A-NA	2.73	128.28	124.51
22	b	810	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	a	820	CLA	C1-C2-C3	-2.72	121.33	126.04
29	j	104	BCR	C23-C24-C25	-2.72	119.55	127.20
22	b	819	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	i	101	BCR	C20-C19-C18	-2.72	118.77	126.42
22	b	825	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	b	842	BCR	C4-C5-C6	-2.72	118.78	122.73
24	8	304	A1L1F	O13-C45-C47	2.72	120.44	111.91
22	2	312	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
24	9	302	A1L1F	O13-C45-C47	2.72	120.43	111.91
22	4	314	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
20	3	305	XAT	C35-C15-C14	-2.71	117.92	123.47
22	l	203	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	h	204	A1L1F	O13-C45-C47	2.71	120.42	111.91
29	h	201	BCR	C7-C8-C9	-2.71	122.14	126.23
23	1	315	SQD	O48-C23-C24	2.70	120.39	111.91
20	3	301	XAT	C19-C9-C8	2.70	122.33	118.08
20	j	101	XAT	C15-C35-C34	-2.70	117.94	123.47
20	8	301	XAT	C7-C8-C9	-2.70	121.34	125.53
20	j	101	XAT	C24-C23-C22	-2.70	105.56	110.77
29	b	849	BCR	C20-C19-C18	-2.70	118.83	126.42
20	2	301	XAT	C31-C32-C33	-2.70	118.83	126.42
22	7	311	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	9	309	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
29	b	845	BCR	C35-C13-C12	2.69	122.32	118.08
20	2	302	XAT	C35-C15-C14	-2.69	117.95	123.47
22	a	808	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	5	314	CLA	CHB-C4A-NA	2.69	128.24	124.51
22	a	805	CLA	CHB-C4A-NA	2.69	128.24	124.51
24	h	204	A1L1F	C8-O7-C54	-2.69	112.88	117.90
29	h	202	BCR	C24-C23-C22	-2.69	122.17	126.23
20	1	303	XAT	C10-C11-C12	-2.69	114.82	123.22
22	b	822	CLA	O2D-CGD-O1D	-2.69	118.58	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	315	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	2	302	XAT	C24-C23-C22	-2.69	105.58	110.77
29	b	842	BCR	C23-C24-C25	-2.69	119.66	127.20
22	h	203	CLA	C1-C2-C3	-2.68	121.40	126.04
22	3	312	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	a	829	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
29	h	201	BCR	C10-C11-C12	-2.68	114.86	123.22
22	b	811	CLA	CAB-C3B-C2B	2.68	129.93	124.69
22	b	824	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	a	814	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
29	b	842	BCR	C24-C23-C22	-2.68	122.19	126.23
20	j	101	XAT	C31-C32-C33	-2.68	118.90	126.42
22	4	313	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
20	4	302	XAT	C15-C14-C13	-2.67	123.49	127.31
20	9	305	XAT	O4-C5-C4	2.67	115.39	113.38
22	a	822	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
29	h	202	BCR	C20-C21-C22	-2.67	123.50	127.31
25	9	317	LHG	O8-C23-C24	2.67	120.28	111.91
22	b	818	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
22	a	826	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	5	302	XAT	C4-C3-C2	-2.66	105.63	110.77
29	b	842	BCR	C2-C1-C6	2.66	114.58	110.48
22	b	826	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
20	4	301	XAT	C39-C29-C30	-2.66	119.19	122.92
20	4	303	XAT	C39-C29-C28	2.66	122.27	118.08
20	j	101	XAT	C31-C30-C29	-2.66	123.51	127.31
22	a	821	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	h	203	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	5	316	SQD	O48-C23-C24	2.66	120.25	111.91
20	3	301	XAT	C27-C28-C29	-2.66	121.41	125.53
20	5	304	XAT	C10-C11-C12	-2.66	114.92	123.22
22	4	308	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
22	4	310	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
22	2	313	CLA	CAA-C2A-C3A	-2.65	109.90	116.10
26	b	848	DGD	C1E-O6E-C5E	2.65	118.90	113.69
20	2	304	XAT	C15-C14-C13	-2.65	123.53	127.31
29	a	847	BCR	C16-C15-C14	-2.65	118.05	123.47
29	b	844	BCR	C11-C10-C9	-2.65	123.53	127.31
22	5	306	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
29	i	101	BCR	C29-C30-C25	2.65	114.56	110.48
20	4	305	XAT	C31-C32-C33	-2.65	118.98	126.42
20	5	304	XAT	C31-C30-C29	-2.65	123.53	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	834	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
29	m	101	BCR	C33-C5-C6	-2.64	121.56	124.53
20	4	305	XAT	C7-C8-C9	-2.64	121.43	125.53
22	a	804	CLA	C1-C2-C3	-2.64	121.47	126.04
22	a	835	CLA	CHB-C4A-NA	2.64	128.17	124.51
22	b	819	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
28	b	841	PQN	C2M-C2-C3	-2.64	120.09	124.40
20	3	301	XAT	C24-C23-C22	-2.64	105.67	110.77
20	8	303	XAT	C35-C34-C33	-2.64	123.54	127.31
22	b	807	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	b	801	CLA	CHB-C4A-NA	2.64	128.16	124.51
20	4	303	XAT	C4-C3-C2	-2.64	105.68	110.77
20	4	301	XAT	C27-C28-C29	-2.64	121.44	125.53
29	f	801	BCR	C33-C5-C4	2.64	118.68	113.62
22	1	312	CLA	CMB-C2B-C3B	2.63	129.60	124.68
20	4	304	XAT	C31-C30-C29	-2.63	123.55	127.31
22	4	317	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	4	305	XAT	C39-C29-C30	-2.63	119.24	122.92
20	8	302	XAT	C4-C3-C2	-2.63	105.70	110.77
22	a	810	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	9	316	CLA	CHB-C4A-NA	2.62	128.14	124.51
20	5	301	XAT	C35-C15-C14	-2.62	118.10	123.47
22	b	806	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	b	802	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	9	313	CLA	CHB-C4A-NA	2.62	128.14	124.51
29	b	846	BCR	C24-C23-C22	-2.62	122.27	126.23
22	a	833	CLA	CHB-C4A-NA	2.62	128.14	124.51
29	h	202	BCR	C28-C27-C26	-2.62	109.40	114.08
29	f	801	BCR	C10-C11-C12	-2.62	115.05	123.22
29	h	202	BCR	C21-C20-C19	-2.62	115.05	123.22
22	a	829	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	b	840	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
22	4	317	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	7	316	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	a	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	9	303	XAT	C30-C31-C32	-2.61	115.07	123.22
20	7	303	XAT	C4-C3-C2	-2.61	105.73	110.77
20	7	303	XAT	C24-C23-C22	-2.61	105.73	110.77
20	7	304	XAT	C4-C3-C2	-2.61	105.73	110.77
22	j	103	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	9	311	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
22	a	824	CLA	CMB-C2B-C3B	2.61	129.56	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	311	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	1	309	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
20	2	305	XAT	C31-C32-C33	-2.60	119.10	126.42
22	b	830	CLA	CAA-C2A-C3A	-2.60	110.02	116.10
22	3	315	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	9	318	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	h	204	A1L1F	C20-C21-C22	-2.60	107.61	112.75
25	b	847	LHG	O8-C23-C24	2.60	120.06	111.91
22	a	809	CLA	CHB-C4A-NA	2.60	128.10	124.51
20	8	301	XAT	C4-C3-C2	-2.60	105.76	110.77
22	b	833	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	b	809	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	9	307	LHG	O8-C23-C24	2.59	120.05	111.91
29	a	849	BCR	C16-C15-C14	-2.59	118.16	123.47
22	a	807	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	b	813	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	1	314	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	7	309	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
22	a	818	CLA	CMB-C2B-C3B	2.59	129.52	124.68
29	h	201	BCR	C2-C1-C6	2.59	114.47	110.48
24	h	204	A1L1F	C29-C30-C31	-2.59	115.01	118.93
22	a	842	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	a	819	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	3	310	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	3	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	4	306	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	j	105	LMG	O8-C28-C29	2.59	120.02	111.91
20	2	304	XAT	C35-C15-C14	-2.58	118.18	123.47
24	1	304	A1L1F	C26-C30-C31	-2.58	121.55	124.93
22	5	311	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	m	101	BCR	C15-C16-C17	-2.58	118.18	123.47
29	l	205	BCR	C28-C27-C26	-2.58	109.47	114.08
29	m	101	BCR	C27-C26-C25	2.58	126.48	122.73
22	a	854	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	5	313	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	a	806	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	2	311	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	b	820	CLA	C1-C2-C3	-2.58	122.58	126.75
29	b	849	BCR	C15-C14-C13	-2.57	123.64	127.31
22	7	313	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
22	b	817	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
22	4	310	CLA	CHB-C4A-NA	2.57	128.07	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	304	A1L1F	O13-C45-C47	2.57	119.98	111.91
22	1	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	b	809	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
22	b	816	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
29	b	845	BCR	C38-C26-C25	-2.57	121.64	124.53
20	5	304	XAT	C8-C9-C10	-2.57	115.00	118.94
22	b	801	CLA	CMB-C2B-C3B	2.57	129.49	124.68
22	a	832	CLA	C1-C2-C3	-2.57	122.60	126.75
22	8	311	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
29	a	849	BCR	C23-C24-C25	-2.57	119.99	127.20
22	8	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	b	825	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
25	a	845	LHG	O8-C23-C24	2.56	119.96	111.91
22	4	315	CLA	CAA-C2A-C3A	-2.56	110.11	116.10
29	b	845	BCR	C8-C7-C6	-2.56	120.00	127.20
22	2	307	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	2	308	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	a	802	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	9	309	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	2	311	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	b	835	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	l	201	BCR	C20-C21-C22	-2.56	123.66	127.31
22	a	804	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	2	306	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
22	5	311	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	8	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	a	852	XAT	O4-C5-C4	2.55	115.30	113.38
22	b	803	CLA	CMB-C2B-C3B	2.55	129.46	124.68
20	8	302	XAT	C11-C12-C13	-2.55	119.24	126.42
22	9	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	3	312	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	5	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	2	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	a	832	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	j	104	BCR	C33-C5-C6	-2.55	121.66	124.53
22	a	836	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	812	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	3	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	a	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	813	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	3	309	CLA	C1B-CHB-C4A	-2.55	125.07	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	302	XAT	C19-C9-C10	-2.55	119.35	122.92
22	4	314	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	5	306	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	2	312	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	9	303	XAT	C4-C3-C2	-2.54	105.86	110.77
22	8	307	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	a	840	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	5	308	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	a	838	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	f	802	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	8	301	XAT	C31-C30-C29	-2.54	123.69	127.31
29	l	201	BCR	C34-C9-C10	-2.54	119.37	122.92
22	1	308	CLA	C1-C2-C3	-2.54	121.65	126.04
20	2	302	XAT	C4-C3-C2	-2.54	105.87	110.77
22	a	827	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
20	2	302	XAT	C11-C10-C9	-2.54	123.69	127.31
22	b	834	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
20	5	304	XAT	C15-C35-C34	-2.54	118.28	123.47
22	a	816	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	5	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	8	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	l	204	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	1	312	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	829	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
29	b	846	BCR	C34-C9-C8	2.53	122.06	118.08
22	a	801	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
22	b	831	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	829	CLA	C2D-C1D-ND	-2.53	108.24	110.10
22	a	814	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	8	314	CLA	CAA-C2A-C3A	-2.53	110.20	116.10
22	5	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
29	b	845	BCR	C33-C5-C4	2.53	118.47	113.62
22	7	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	f	803	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	1	315	SQD	O8-S-C6	2.53	109.77	105.74
27	a	853	LMG	C8-O7-C10	-2.53	111.57	117.79
22	b	833	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	a	825	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	b	843	BCR	C24-C23-C22	-2.52	122.42	126.23
22	1	307	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	a	823	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	5	316	SQD	O7-S-C6	2.52	109.93	106.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	311	CLA	CMB-C2B-C3B	2.52	129.39	124.68
22	4	307	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	a	827	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	1	309	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	b	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	b	804	CLA	CHD-C1D-ND	-2.52	122.14	124.45
22	l	203	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	7	315	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	a	831	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
29	b	846	BCR	C20-C21-C22	-2.51	123.72	127.31
22	8	309	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	836	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	9	303	XAT	C7-C8-C9	-2.51	121.63	125.53
20	1	303	XAT	C35-C15-C14	-2.51	118.33	123.47
22	b	803	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	8	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	1	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	a	817	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	l	201	BCR	C28-C27-C26	-2.51	109.60	114.08
22	a	822	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	b	837	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	3	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	f	804	BCR	C15-C16-C17	-2.51	118.34	123.47
22	a	815	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	a	837	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	4	316	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	b	822	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
22	3	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	7	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	5	305	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	8	305	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	a	822	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	a	811	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	b	833	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	2	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	8	301	XAT	C35-C15-C14	-2.50	118.36	123.47
22	b	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	a	836	CLA	CMB-C2B-C3B	2.50	129.35	124.68
22	a	802	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	l	205	BCR	C15-C16-C17	-2.50	118.36	123.47
29	l	205	BCR	C38-C26-C27	2.49	118.41	113.62
29	l	205	BCR	C33-C5-C4	2.49	118.41	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	h	204	A1L1F	C27-C34-C33	2.49	122.00	118.08
20	5	302	XAT	C19-C9-C10	-2.49	119.44	122.92
22	h	203	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	b	839	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	a	820	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	b	808	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	a	810	CLA	CHB-C4A-NA	2.48	127.95	124.51
21	9	301	A1L1G	C20-C21-C22	-2.48	107.84	112.75
29	j	104	BCR	C27-C26-C25	-2.48	119.13	122.73
22	7	310	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	a	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	f	801	BCR	C2-C1-C6	2.48	114.30	110.48
22	9	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	a	841	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
20	5	304	XAT	C39-C29-C28	2.48	121.98	118.08
22	b	819	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	l	202	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	8	303	XAT	C28-C29-C30	-2.48	115.14	118.94
26	b	848	DGD	O2G-C1B-O1B	-2.47	117.73	123.70
22	2	316	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	b	846	BCR	C38-C26-C25	-2.47	121.75	124.53
22	8	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	2	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	4	301	XAT	C35-C15-C14	-2.47	118.42	123.47
20	7	304	XAT	C19-C9-C10	-2.47	119.47	122.92
22	a	802	CLA	C1-C2-C3	-2.47	121.78	126.04
20	5	304	XAT	C30-C31-C32	-2.47	115.52	123.22
22	b	805	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	b	838	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	7	306	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	b	834	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	a	818	CLA	CHB-C4A-NA	2.46	127.92	124.51
28	b	841	PQN	C14-C13-C15	2.46	119.41	115.27
24	8	304	A1L1F	C12-C6-C1	-2.46	108.27	110.47
20	7	301	XAT	C35-C15-C14	-2.46	118.44	123.47
22	a	835	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	l	203	CLA	CHD-C1D-ND	-2.46	122.19	124.45
22	2	309	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	1	310	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	a	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	a	837	CLA	C1B-CHB-C4A	-2.46	125.25	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	302	A1L1F	C36-C37-C38	-2.46	118.44	123.47
29	b	843	BCR	C15-C16-C17	-2.46	118.44	123.47
22	9	316	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
22	a	812	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	b	815	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	b	820	CLA	O2D-CGD-CBD	2.45	115.63	111.27
29	b	845	BCR	C39-C30-C25	-2.45	106.32	110.30
21	3	306	A1L1G	C17-C20-C21	2.45	117.04	114.28
22	5	308	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	1	310	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	a	841	CLA	C1-C2-C3	-2.45	121.81	126.04
22	a	809	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
20	7	304	XAT	C11-C12-C13	-2.45	119.53	126.42
29	b	842	BCR	C15-C16-C17	-2.45	118.45	123.47
29	j	104	BCR	C15-C16-C17	-2.45	118.45	123.47
22	4	309	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	a	812	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	a	839	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	7	311	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	h	205	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	l	204	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	9	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	3	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	a	820	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	a	830	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
20	5	301	XAT	C4-C3-C2	-2.44	106.06	110.77
20	7	305	XAT	C31-C30-C29	-2.44	123.83	127.31
22	b	803	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	b	827	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	2	315	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
20	5	302	XAT	C31-C30-C29	-2.44	123.83	127.31
22	8	308	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	a	805	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	b	821	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	9	309	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	b	828	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
22	a	836	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
29	h	201	BCR	C21-C20-C19	-2.43	115.63	123.22
22	4	308	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	l	201	BCR	C21-C20-C19	-2.43	115.63	123.22
29	h	201	BCR	C33-C5-C6	-2.43	121.80	124.53
24	h	204	A1L1F	C41-C40-C39	-2.43	119.59	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	808	CLA	CHB-C4A-NA	2.43	127.87	124.51
20	9	305	XAT	C35-C15-C14	-2.43	118.50	123.47
22	b	831	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	7	308	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	b	827	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	3	311	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	a	814	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
29	a	848	BCR	C33-C5-C4	2.42	118.27	113.62
22	5	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	a	806	CLA	O1D-CGD-CBD	2.42	129.44	124.48
22	b	813	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	4	309	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	b	833	CLA	CHD-C1D-ND	-2.42	122.23	124.45
22	b	822	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	a	842	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	2	311	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	a	832	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
20	2	303	XAT	C8-C9-C10	2.42	122.65	118.94
22	1	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	3	310	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	a	834	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	4	312	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
29	h	202	BCR	C33-C5-C4	2.41	118.25	113.62
22	a	840	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	9	314	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	5	307	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
24	1	304	A1L1F	C27-C34-C33	2.41	121.88	118.08
22	h	205	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	5	314	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
22	a	854	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
22	b	806	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	f	804	BCR	C28-C27-C26	-2.41	109.78	114.08
20	9	304	XAT	C39-C29-C28	2.41	121.87	118.08
29	a	850	BCR	C8-C7-C6	-2.41	120.44	127.20
22	a	804	CLA	O2D-CGD-CBD	2.41	115.54	111.27
24	h	204	A1L1F	C23-C22-C21	-2.41	106.13	110.77
22	9	318	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	b	842	BCR	C29-C30-C25	2.41	114.19	110.48
22	8	310	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	b	811	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	7	312	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	9	312	CLA	C1B-CHB-C4A	-2.40	125.36	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	818	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	a	807	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	b	830	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	a	835	CLA	O2D-CGD-CBD	2.40	115.53	111.27
20	3	304	XAT	C31-C32-C33	-2.40	119.67	126.42
22	5	315	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	8	307	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
29	b	844	BCR	C28-C27-C26	-2.40	109.79	114.08
20	2	303	XAT	C24-C23-C22	-2.40	106.14	110.77
29	b	842	BCR	C21-C20-C19	-2.40	115.73	123.22
22	8	306	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	3	311	CLA	C1-C2-C3	-2.40	122.87	126.75
20	3	305	XAT	C10-C11-C12	-2.40	115.74	123.22
22	a	813	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	4	312	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	a	825	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	b	816	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	8	312	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	7	304	XAT	O4-C5-C4	2.39	115.18	113.38
22	9	311	CLA	O2D-CGD-CBD	2.39	115.51	111.27
22	1	311	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	4	302	XAT	C10-C11-C12	-2.39	115.77	123.22
29	a	850	BCR	C10-C11-C12	-2.39	115.77	123.22
22	7	312	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	a	810	CLA	C1-C2-C3	-2.39	121.91	126.04
22	9	318	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	b	825	CLA	CHB-C4A-NA	2.39	127.81	124.51
29	h	202	BCR	C8-C7-C6	-2.39	120.50	127.20
22	9	313	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	a	808	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
22	a	818	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
20	8	302	XAT	C7-C8-C9	-2.38	121.83	125.53
22	b	811	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	1	313	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	5	311	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	a	854	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	7	314	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
29	a	850	BCR	C16-C15-C14	-2.38	118.59	123.47
20	7	303	XAT	C8-C9-C10	2.38	122.59	118.94
22	a	812	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	b	816	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	a	806	CLA	C5-C3-C2	-2.38	116.30	121.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	307	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	1	313	CLA	CAA-C2A-C3A	-2.38	110.55	116.10
22	a	803	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	j	102	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	7	303	XAT	O4-C5-C4	2.38	115.17	113.38
24	8	304	A1L1F	C28-C39-C38	-2.38	119.59	122.92
22	a	833	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
22	b	815	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	9	304	XAT	O4-C5-C4	2.37	115.17	113.38
22	8	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	b	832	CLA	CHD-C1D-ND	-2.37	122.27	124.45
22	a	834	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	4	313	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	b	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	a	839	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	9	315	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	4	315	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	8	304	A1L1F	C23-C22-C21	-2.37	106.20	110.77
20	3	303	XAT	C30-C31-C32	-2.37	115.82	123.22
22	a	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	1	305	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	a	804	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	2	315	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	4	311	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	a	801	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	b	824	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	3	310	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	b	810	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	j	102	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	7	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	1	313	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
29	j	104	BCR	C38-C26-C25	-2.36	121.87	124.53
20	8	303	XAT	C40-C33-C32	2.36	121.80	118.08
22	a	816	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	b	849	BCR	C36-C18-C17	-2.36	119.61	122.92
27	j	105	LMG	C8-O7-C10	-2.36	111.98	117.79
22	b	836	CLA	CHD-C1D-ND	-2.36	122.29	124.45
29	b	843	BCR	C28-C27-C26	-2.36	109.86	114.08
22	b	812	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	7	302	A1L1G	C17-C20-C21	2.36	116.93	114.28
29	a	848	BCR	C15-C16-C17	-2.36	118.64	123.47
22	f	802	CLA	C1B-CHB-C4A	-2.36	125.45	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	309	CLA	CHD-C1D-ND	-2.36	122.29	124.45
22	a	801	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	h	201	BCR	C16-C15-C14	-2.36	118.65	123.47
22	b	832	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	b	836	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
22	3	308	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
22	3	315	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
22	b	820	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
26	8	315	DGD	C2G-O2G-C1B	-2.35	112.00	117.79
22	9	310	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	1	308	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	h	202	BCR	C10-C11-C12	-2.35	115.88	123.22
22	7	314	CLA	C2A-C1A-CHA	2.35	127.97	123.86
22	a	827	CLA	CHD-C1D-ND	-2.35	122.29	124.45
22	b	838	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	2	314	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	b	830	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	4	313	CLA	CHD-C1D-ND	-2.35	122.30	124.45
20	4	302	XAT	C30-C31-C32	-2.35	115.89	123.22
22	3	313	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
20	5	304	XAT	C25-C24-C23	-2.35	108.11	112.75
22	a	826	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	7	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	i	101	BCR	C37-C22-C21	-2.34	119.64	122.92
22	a	844	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
29	a	847	BCR	C23-C24-C25	-2.34	120.62	127.20
22	7	309	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	a	828	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	a	819	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	b	840	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	l	202	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
29	l	201	BCR	C15-C16-C17	-2.34	118.68	123.47
22	1	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	a	815	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	7	310	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	7	311	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	4	312	CLA	CHD-C1D-ND	-2.34	122.31	124.45
22	a	830	CLA	C1-C2-C3	-2.34	122.00	126.04
22	9	311	CLA	CHD-C1D-ND	-2.34	122.31	124.45
22	8	309	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	8	313	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	a	811	CLA	C1B-CHB-C4A	-2.33	125.50	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	304	A1L1F	C31-C32-C33	-2.33	115.94	123.22
29	b	842	BCR	C38-C26-C27	2.33	118.10	113.62
22	5	310	CLA	CHD-C1D-ND	-2.33	122.31	124.45
29	b	843	BCR	C33-C5-C4	2.33	118.09	113.62
22	b	835	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	f	803	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
24	h	204	A1L1F	O7-C54-O55	-2.33	118.34	122.96
22	a	806	CLA	C6-C5-C3	-2.33	107.35	113.45
20	9	303	XAT	C39-C29-C28	2.33	121.74	118.08
24	9	302	A1L1F	O7-C54-O55	-2.33	118.34	122.96
29	b	843	BCR	C23-C24-C25	-2.33	120.67	127.20
29	a	848	BCR	C10-C11-C12	-2.32	115.97	123.22
22	5	309	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	b	825	CLA	CHD-C1D-ND	-2.32	122.32	124.45
28	a	843	PQN	C11-C12-C13	-2.32	122.92	126.79
22	b	807	CLA	C1-C2-C3	-2.32	122.03	126.04
22	4	317	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	7	314	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	b	807	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	b	804	CLA	C3C-C4C-NC	-2.32	107.97	110.57
29	a	847	BCR	C33-C5-C4	2.32	118.07	113.62
22	j	103	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
29	f	804	BCR	C3-C4-C5	-2.32	109.94	114.08
22	b	839	CLA	CMB-C2B-C3B	2.32	129.01	124.68
22	3	314	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
29	f	804	BCR	C11-C12-C13	-2.32	119.91	126.42
22	8	306	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
22	a	841	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
20	4	301	XAT	C40-C33-C34	-2.31	119.68	122.92
22	2	312	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	b	823	CLA	CHB-C4A-NA	2.31	127.71	124.51
29	b	842	BCR	C11-C12-C13	-2.31	119.92	126.42
22	a	824	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	b	805	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	7	316	CLA	O2D-CGD-CBD	2.31	115.37	111.27
22	a	828	CLA	C1-C2-C3	-2.31	122.05	126.04
22	5	310	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
20	7	301	XAT	C31-C32-C33	-2.31	119.93	126.42
22	1	307	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
20	2	301	XAT	C10-C11-C12	-2.31	116.02	123.22
22	7	313	CLA	CHD-C1D-ND	-2.31	122.33	124.45
22	b	803	CLA	CHB-C4A-NA	2.31	127.70	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	842	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
20	5	302	XAT	C15-C35-C34	-2.30	118.76	123.47
20	j	101	XAT	C39-C29-C28	2.30	121.70	118.08
22	b	801	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
29	m	101	BCR	C8-C7-C6	-2.30	120.74	127.20
22	a	836	CLA	C1-C2-C3	-2.30	123.03	126.75
22	3	311	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
29	j	104	BCR	C34-C9-C10	-2.30	119.70	122.92
22	b	814	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	8	314	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	5	312	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	5	306	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	a	816	CLA	C1-C2-C3	-2.29	123.04	126.75
22	a	810	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
22	a	844	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	a	825	CLA	CHD-C1D-ND	-2.29	122.35	124.45
20	2	304	XAT	C35-C34-C33	-2.29	124.04	127.31
22	4	314	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	i	101	BCR	C16-C15-C14	-2.29	118.78	123.47
22	4	310	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	1	304	A1L1F	C37-C36-C35	-2.29	118.78	123.47
22	1	312	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	a	838	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	b	837	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	7	306	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
20	2	302	XAT	C10-C11-C12	-2.29	116.08	123.22
20	a	852	XAT	C19-C9-C8	2.29	121.68	118.08
20	3	301	XAT	C15-C35-C34	-2.29	118.79	123.47
22	8	305	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
22	3	307	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
29	b	849	BCR	C23-C24-C25	-2.28	120.79	127.20
22	2	306	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
20	9	303	XAT	O4-C5-C4	2.28	115.10	113.38
20	2	303	XAT	O4-C5-C4	2.28	115.10	113.38
22	2	310	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	1	314	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
20	1	303	XAT	C27-C28-C29	-2.28	121.99	125.53
22	2	313	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	b	806	CLA	CHD-C1D-ND	-2.28	122.36	124.45
22	5	313	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	a	817	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	5	314	CLA	O2A-CGA-O1A	-2.28	117.84	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	301	XAT	O4-C5-C4	2.28	115.09	113.38
20	2	302	XAT	O4-C5-C4	2.28	115.09	113.38
22	1	305	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	7	313	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
29	a	848	BCR	C16-C15-C14	-2.27	118.82	123.47
22	7	316	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	a	821	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	a	823	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	7	317	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	7	301	XAT	C26-C27-C28	-2.27	121.19	125.99
21	1	301	A1L1G	C17-C20-C21	2.27	116.83	114.28
22	8	309	CLA	C1-C2-C3	-2.27	122.12	126.04
22	1	311	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	b	826	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	4	306	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
20	3	304	XAT	C40-C33-C34	-2.27	119.75	122.92
22	a	805	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	a	836	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	a	810	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
22	a	813	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
22	a	820	CLA	CHD-C1D-ND	-2.26	122.38	124.45
20	4	303	XAT	O4-C5-C4	2.26	115.08	113.38
22	2	310	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	l	201	BCR	C23-C24-C25	-2.26	120.85	127.20
22	b	821	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
29	b	849	BCR	C38-C26-C27	2.26	117.95	113.62
22	8	308	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	1	306	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	3	304	XAT	C27-C28-C29	-2.26	122.03	125.53
22	a	805	CLA	CHD-C1D-ND	-2.26	122.38	124.45
29	b	845	BCR	C21-C20-C19	-2.26	116.18	123.22
29	a	849	BCR	C38-C26-C27	2.26	117.95	113.62
29	b	845	BCR	C34-C9-C8	2.26	121.63	118.08
22	4	309	CLA	CHD-C1D-ND	-2.25	122.38	124.45
22	2	309	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	b	832	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	b	831	CLA	CHD-C1D-ND	-2.25	122.38	124.45
22	2	316	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	a	824	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	4	308	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	b	804	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
29	b	845	BCR	C38-C26-C27	2.25	117.94	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	827	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
22	4	307	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
20	4	305	XAT	C15-C35-C34	-2.25	118.87	123.47
29	f	801	BCR	C28-C27-C26	-2.25	110.06	114.08
24	1	304	A1L1F	O7-C54-O55	-2.25	118.50	122.96
22	b	809	CLA	O2D-CGD-CBD	2.25	115.26	111.27
22	a	829	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	b	829	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	m	101	BCR	C24-C23-C22	-2.25	122.84	126.23
22	1	309	CLA	CHD-C1D-ND	-2.24	122.39	124.45
24	9	302	A1L1F	C26-O13-C45	2.24	120.67	115.68
29	f	801	BCR	C34-C9-C8	2.24	121.61	118.08
22	5	305	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	a	806	CLA	CHD-C1D-ND	-2.24	122.39	124.45
24	9	302	A1L1F	C20-C21-C22	-2.24	108.31	112.75
20	8	301	XAT	C30-C31-C32	-2.24	116.22	123.22
29	a	848	BCR	C21-C20-C19	-2.24	116.22	123.22
22	b	821	CLA	C1-C2-C3	-2.24	122.17	126.04
22	a	808	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	a	841	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	5	316	SQD	C45-O47-C7	-2.24	112.28	117.79
29	h	201	BCR	C11-C10-C9	-2.24	124.12	127.31
21	9	301	A1L1G	C29-C30-C31	2.24	122.32	118.93
23	1	315	SQD	O9-S-C6	2.23	109.59	106.94
22	7	307	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	1	305	CLA	CHD-C1D-ND	-2.23	122.40	124.45
20	2	305	XAT	C19-C9-C8	2.23	121.59	118.08
22	8	308	CLA	C1-C2-C3	-2.23	122.19	126.04
22	4	310	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
21	1	301	A1L1G	C14-C29-C30	-2.23	121.54	125.47
20	2	303	XAT	C39-C29-C30	-2.23	119.80	122.92
22	b	818	CLA	CHD-C1D-ND	-2.23	122.41	124.45
20	5	302	XAT	C11-C12-C13	-2.23	120.16	126.42
22	7	315	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
22	b	823	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
22	h	205	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	4	316	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
20	7	301	XAT	C39-C29-C30	-2.22	119.81	122.92
20	9	303	XAT	O24-C25-C38	2.22	117.72	115.06
22	7	311	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	a	822	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	b	836	CLA	O2A-CGA-O1A	-2.22	117.98	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	302	XAT	C8-C9-C10	2.22	122.35	118.94
20	2	304	XAT	C20-C13-C12	2.22	121.58	118.08
29	f	801	BCR	C15-C14-C13	-2.22	124.14	127.31
20	7	301	XAT	C24-C23-C22	-2.22	106.48	110.77
22	a	818	CLA	O2D-CGD-CBD	2.22	115.21	111.27
22	a	806	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
20	8	302	XAT	O4-C5-C4	2.22	115.05	113.38
22	b	834	CLA	CHD-C1D-ND	-2.22	122.42	124.45
21	7	302	A1L1G	C20-C21-C22	-2.22	108.37	112.75
22	2	311	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
29	h	202	BCR	C37-C22-C23	2.21	121.56	118.08
22	a	815	CLA	CHD-C1D-ND	-2.21	122.42	124.45
29	a	850	BCR	C20-C19-C18	-2.21	120.21	126.42
22	2	308	CLA	CHB-C4A-NA	2.21	127.56	124.51
20	5	302	XAT	O4-C5-C4	2.21	115.04	113.38
22	a	830	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	b	810	CLA	C1-C2-C3	-2.21	122.23	126.04
29	b	844	BCR	C33-C5-C4	2.20	117.85	113.62
20	2	301	XAT	O4-C5-C4	2.20	115.04	113.38
21	9	301	A1L1G	C14-C29-C30	-2.20	121.59	125.47
22	3	313	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	a	820	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	f	803	CLA	CHD-C1D-ND	-2.20	122.43	124.45
24	9	302	A1L1F	C31-C32-C33	-2.20	116.36	123.22
22	j	102	CLA	CHD-C1D-ND	-2.20	122.43	124.45
20	8	302	XAT	C20-C13-C14	-2.20	119.84	122.92
29	a	849	BCR	C21-C20-C19	-2.20	116.36	123.22
20	3	303	XAT	C15-C35-C34	-2.20	118.97	123.47
22	a	833	CLA	C1-C2-C3	-2.20	122.25	126.04
20	4	305	XAT	O4-C5-C4	2.20	115.03	113.38
23	5	316	SQD	O9-S-C6	2.19	109.55	106.94
29	i	101	BCR	C23-C22-C21	2.19	122.31	118.94
22	1	312	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	5	307	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	7	305	XAT	C39-C29-C28	2.19	121.53	118.08
22	8	310	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	b	813	CLA	C1-C2-C3	-2.19	122.25	126.04
20	5	301	XAT	C30-C31-C32	-2.19	116.38	123.22
22	7	308	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	b	845	BCR	C23-C24-C25	-2.19	121.05	127.20
20	8	301	XAT	O24-C25-C38	2.19	117.68	115.06
20	3	303	XAT	O24-C25-C38	2.19	117.68	115.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	839	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	4	303	XAT	O24-C25-C38	2.19	117.68	115.06
20	7	305	XAT	C30-C31-C32	-2.19	116.39	123.22
22	b	835	CLA	CAC-C3C-C4C	2.19	127.65	124.81
29	b	846	BCR	C35-C13-C12	2.19	121.52	118.08
20	j	101	XAT	O4-C5-C4	2.18	115.02	113.38
22	5	309	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	f	801	BCR	C35-C13-C12	2.18	121.52	118.08
20	2	303	XAT	C40-C33-C34	-2.18	119.87	122.92
20	5	301	XAT	O24-C25-C38	2.18	117.67	115.06
22	b	839	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
29	b	844	BCR	C7-C6-C5	-2.18	116.18	121.46
22	8	311	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	a	854	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	1	303	XAT	C19-C9-C8	2.18	121.51	118.08
22	4	310	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	a	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	1	303	XAT	O4-C5-C4	2.18	115.02	113.38
22	b	805	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	a	819	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	9	302	A1L1F	C23-C22-C21	-2.18	106.57	110.77
20	2	305	XAT	C15-C35-C34	-2.18	119.02	123.47
22	8	312	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
22	a	801	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	b	804	CLA	O1D-CGD-CBD	2.17	128.93	124.48
22	8	309	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	3	305	XAT	C19-C9-C8	2.17	121.50	118.08
20	4	305	XAT	O24-C25-C38	2.17	117.66	115.06
20	7	304	XAT	O24-C25-C38	2.17	117.66	115.06
29	b	843	BCR	C37-C22-C23	2.17	121.50	118.08
21	3	306	A1L1G	C20-C21-C22	-2.17	108.45	112.75
22	3	311	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	2	309	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	a	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	7	312	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	b	840	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	2	303	XAT	C31-C32-C33	-2.17	120.33	126.42
20	4	303	XAT	C7-C8-C9	-2.17	122.17	125.53
22	b	838	CLA	CHD-C1D-ND	-2.16	122.47	124.45
20	3	304	XAT	O4-C5-C18	2.16	117.65	115.06
20	3	301	XAT	C8-C9-C10	-2.16	115.62	118.94
29	1	201	BCR	C29-C30-C25	2.16	113.81	110.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	848	BCR	C23-C24-C25	-2.16	121.13	127.20
22	b	821	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
29	h	201	BCR	C34-C9-C8	2.16	121.48	118.08
29	h	202	BCR	C35-C13-C12	2.16	121.48	118.08
22	a	834	CLA	C1-C2-C3	-2.16	122.31	126.04
20	8	301	XAT	O4-C5-C4	2.16	115.00	113.38
29	b	843	BCR	C11-C12-C13	-2.16	120.35	126.42
22	b	828	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	1	301	A1L1G	C29-C30-C31	2.16	122.20	118.93
20	3	303	XAT	C35-C15-C14	-2.16	119.06	123.47
22	a	804	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
29	b	846	BCR	C37-C22-C23	2.15	121.47	118.08
29	b	843	BCR	C36-C18-C19	2.15	121.47	118.08
20	5	302	XAT	C20-C13-C14	-2.15	119.91	122.92
22	a	809	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	1	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	5	311	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	b	848	DGD	O3D-C3D-C4D	-2.15	105.38	110.35
20	8	303	XAT	O4-C5-C18	2.15	117.63	115.06
22	3	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	a	849	BCR	C8-C7-C6	-2.15	121.17	127.20
20	4	302	XAT	C39-C29-C28	2.15	121.46	118.08
22	a	831	CLA	O2D-CGD-CBD	2.15	115.08	111.27
20	8	302	XAT	O24-C25-C38	2.15	117.63	115.06
22	8	308	CLA	O2D-CGD-CBD	2.15	115.08	111.27
20	5	304	XAT	O24-C25-C38	2.14	117.63	115.06
29	l	201	BCR	C39-C30-C25	-2.14	106.82	110.30
20	a	852	XAT	C40-C33-C32	2.14	121.45	118.08
20	j	101	XAT	O24-C25-C38	2.14	117.62	115.06
22	a	831	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
22	1	308	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	5	312	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	9	316	CLA	CHD-C1D-ND	-2.14	122.49	124.45
22	8	305	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	3	303	XAT	C39-C29-C28	2.14	121.45	118.08
20	2	304	XAT	O24-C25-C38	2.14	117.62	115.06
22	7	316	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	9	304	XAT	O24-C25-C38	2.14	117.62	115.06
20	7	305	XAT	O4-C5-C18	2.14	117.62	115.06
24	h	204	A1L1F	C26-O13-C45	2.14	120.44	115.68
28	a	843	PQN	C2M-C2-C3	-2.14	120.91	124.40
20	4	301	XAT	O4-C5-C4	2.14	114.99	113.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	306	CLA	CHD-C1D-ND	-2.13	122.49	124.45
22	a	811	CLA	CHD-C1D-ND	-2.13	122.49	124.45
22	b	837	CLA	C1-C2-C3	-2.13	122.35	126.04
29	h	201	BCR	C23-C24-C25	-2.13	121.21	127.20
20	9	304	XAT	C10-C11-C12	-2.13	116.56	123.22
20	3	303	XAT	O4-C5-C4	2.13	114.98	113.38
29	a	847	BCR	C38-C26-C27	2.13	117.71	113.62
29	l	201	BCR	C3-C4-C5	-2.13	110.27	114.08
29	m	101	BCR	C15-C14-C13	-2.13	124.27	127.31
22	1	310	CLA	CHD-C1D-ND	-2.13	122.50	124.45
20	7	304	XAT	C25-C24-C23	-2.13	108.53	112.75
20	5	302	XAT	O4-C5-C18	2.13	117.61	115.06
20	a	852	XAT	O24-C25-C38	2.13	117.61	115.06
22	a	834	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	b	808	CLA	CHD-C1D-ND	-2.13	122.50	124.45
29	b	845	BCR	C29-C30-C25	2.13	113.76	110.48
29	a	849	BCR	C10-C11-C12	-2.13	116.58	123.22
20	2	303	XAT	O4-C5-C18	2.13	117.61	115.06
29	a	847	BCR	C8-C7-C6	-2.13	121.23	127.20
22	3	313	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	a	839	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
20	7	305	XAT	O24-C25-C38	2.13	117.60	115.06
27	2	317	LMG	C8-O7-C10	-2.12	112.56	117.79
22	b	812	CLA	CHD-C1D-ND	-2.12	122.50	124.45
29	i	101	BCR	C10-C11-C12	-2.12	116.59	123.22
22	5	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
22	l	202	CLA	CHD-C1D-ND	-2.12	122.50	124.45
22	f	802	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	a	812	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	a	838	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	4	308	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	b	835	CLA	C1-C2-C3	-2.12	122.38	126.04
22	7	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
20	9	305	XAT	C5-C4-C3	2.12	116.94	112.75
22	a	806	CLA	C6-C7-C8	-2.12	109.08	115.92
22	9	318	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
22	b	802	CLA	CHD-C1D-ND	-2.11	122.51	124.45
20	4	304	XAT	O4-C5-C4	2.11	114.97	113.38
20	4	302	XAT	C20-C13-C12	2.11	121.40	118.08
22	b	816	CLA	C1-C2-C3	-2.11	122.39	126.04
22	9	314	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	f	804	BCR	C35-C13-C14	-2.11	119.97	122.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	303	XAT	C10-C11-C12	-2.11	116.63	123.22
22	b	839	CLA	C1-C2-C3	-2.11	122.39	126.04
29	a	849	BCR	C15-C16-C17	-2.11	119.15	123.47
22	4	307	CLA	O2D-CGD-CBD	2.11	115.02	111.27
22	9	318	CLA	CHD-C1D-ND	-2.11	122.52	124.45
20	7	301	XAT	C10-C11-C12	-2.11	116.63	123.22
29	j	104	BCR	C3-C4-C5	-2.11	110.31	114.08
20	2	304	XAT	C10-C11-C12	-2.11	116.63	123.22
22	5	311	CLA	CHD-C1D-ND	-2.11	122.52	124.45
20	2	305	XAT	O4-C5-C4	2.11	114.97	113.38
20	9	305	XAT	C31-C32-C33	-2.11	120.49	126.42
22	b	829	CLA	C1-C2-C3	-2.11	122.40	126.04
22	b	822	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	8	307	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	4	313	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
29	j	104	BCR	C16-C15-C14	-2.11	119.16	123.47
22	b	807	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	8	309	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	b	823	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	4	301	XAT	C28-C29-C30	2.10	122.17	118.94
29	h	201	BCR	C15-C16-C17	-2.10	119.17	123.47
20	2	301	XAT	C39-C29-C30	-2.10	119.98	122.92
20	3	301	XAT	O4-C5-C18	2.10	117.57	115.06
29	b	846	BCR	C23-C24-C25	-2.10	121.30	127.20
22	b	817	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	1	306	CLA	C1-C2-C3	-2.10	122.41	126.04
22	a	829	CLA	CHD-C1D-ND	-2.10	122.53	124.45
20	2	305	XAT	O4-C5-C18	2.10	117.57	115.06
22	b	820	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	9	303	XAT	C11-C12-C13	-2.10	120.52	126.42
20	2	301	XAT	O24-C25-C38	2.10	117.57	115.06
29	b	849	BCR	C32-C1-C6	-2.10	106.90	110.30
20	4	304	XAT	O4-C5-C18	2.10	117.57	115.06
22	b	811	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	4	308	CLA	O2D-CGD-CBD	2.10	114.99	111.27
20	8	301	XAT	O4-C5-C18	2.10	117.57	115.06
20	7	301	XAT	O4-C5-C4	2.10	114.96	113.38
22	b	802	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	7	303	XAT	O24-C25-C38	2.09	117.56	115.06
22	b	829	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	a	847	BCR	C28-C27-C26	-2.09	110.34	114.08
22	9	308	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	829	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	a	844	CLA	C1-C2-C3	-2.09	122.42	126.04
20	5	304	XAT	C35-C15-C14	-2.09	119.19	123.47
27	2	317	LMG	C4-C3-C2	-2.09	107.17	110.82
20	2	302	XAT	O24-C25-C38	2.09	117.56	115.06
20	4	303	XAT	C35-C15-C14	-2.09	119.19	123.47
20	1	302	XAT	O24-C25-C38	2.09	117.56	115.06
22	1	306	CLA	CAC-C3C-C4C	2.09	127.52	124.81
22	a	837	CLA	CHD-C1D-ND	-2.09	122.54	124.45
22	a	807	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	a	836	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	b	801	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
20	5	304	XAT	O4-C5-C18	2.09	117.56	115.06
22	4	309	CLA	C1-C2-C3	-2.09	123.38	126.75
22	3	309	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	b	812	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	8	315	DGD	O2G-C1B-O1B	-2.08	118.67	123.70
22	a	827	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	4	311	CLA	O2D-CGD-CBD	2.08	114.97	111.27
20	3	303	XAT	O4-C5-C18	2.08	117.55	115.06
20	9	304	XAT	C40-C33-C32	2.08	121.36	118.08
22	2	308	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	9	308	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	4	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	5	306	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	3	311	CLA	CHD-C1D-ND	-2.08	122.54	124.45
20	5	302	XAT	C30-C31-C32	-2.08	116.73	123.22
22	2	308	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	b	821	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	b	823	CLA	C1-C2-C3	-2.08	122.45	126.04
20	3	304	XAT	C35-C15-C14	-2.08	119.22	123.47
22	b	838	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	9	312	CLA	CHD-C1D-ND	-2.08	122.55	124.45
29	1	201	BCR	C37-C22-C23	2.08	121.35	118.08
22	b	805	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	b	808	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
22	b	834	CLA	C1-C2-C3	-2.07	122.45	126.04
20	7	303	XAT	C15-C35-C34	-2.07	119.22	123.47
22	7	307	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	4	316	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	a	844	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	b	831	CLA	O2A-CGA-O1A	-2.07	118.37	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	303	XAT	O24-C25-C38	2.07	117.53	115.06
20	7	305	XAT	O4-C5-C4	2.07	114.94	113.38
24	8	304	A1L1F	C27-C34-C33	2.07	121.33	118.08
22	b	819	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	a	848	BCR	C34-C9-C8	2.07	121.33	118.08
22	b	827	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	7	313	CLA	C1-C2-C3	-2.07	122.47	126.04
20	9	305	XAT	C11-C12-C13	-2.07	120.61	126.42
22	b	828	CLA	CHD-C1D-ND	-2.07	122.56	124.45
22	l	204	CLA	CHD-C1D-ND	-2.07	122.56	124.45
22	b	830	CLA	CMA-C3A-C2A	-2.06	111.28	116.10
22	9	308	CLA	C1-C2-C3	-2.06	122.47	126.04
20	5	302	XAT	O24-C25-C26	-2.06	57.25	58.96
22	a	825	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	9	309	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	2	304	XAT	O4-C5-C18	2.06	117.53	115.06
20	4	303	XAT	O4-C5-C18	2.06	117.53	115.06
20	3	304	XAT	O24-C25-C38	2.06	117.53	115.06
22	1	310	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	3	310	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	1	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	2	302	XAT	C27-C28-C29	-2.06	122.33	125.53
22	5	315	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	5	314	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	b	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	b	815	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	j	102	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	b	844	BCR	C8-C9-C10	2.06	122.10	118.94
29	a	849	BCR	C37-C22-C23	2.06	121.32	118.08
29	b	846	BCR	C33-C5-C4	2.06	117.56	113.62
22	a	834	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	a	854	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
22	f	803	CLA	C1-C2-C3	-2.05	122.49	126.04
22	a	844	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	8	312	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	b	849	BCR	C34-C9-C10	-2.05	120.05	122.92
22	h	205	CLA	O2D-CGD-CBD	2.05	114.92	111.27
22	b	820	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	f	802	CLA	C1-C2-C3	-2.05	122.49	126.04
20	a	852	XAT	C20-C13-C14	-2.05	120.05	122.92
22	b	839	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	5	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	304	XAT	C20-C13-C14	-2.05	120.05	122.92
29	b	844	BCR	C16-C15-C14	-2.05	119.27	123.47
29	b	842	BCR	C37-C22-C23	2.05	121.31	118.08
24	9	302	A1L1F	C17-C20-C21	2.05	116.59	114.28
22	a	840	CLA	C1-C2-C3	-2.05	122.50	126.04
22	a	824	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	b	816	CLA	O2D-CGD-CBD	2.05	114.91	111.27
22	8	311	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
20	5	301	XAT	C39-C29-C28	2.05	121.31	118.08
22	5	308	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	a	801	CLA	O1D-CGD-CBD	2.05	128.68	124.48
29	j	104	BCR	C29-C30-C25	2.05	113.63	110.48
22	4	317	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	b	840	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	b	803	CLA	O2D-CGD-CBD	2.05	114.91	111.27
20	3	305	XAT	O24-C25-C38	2.05	117.51	115.06
22	2	314	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	b	810	CLA	CHD-C1D-ND	-2.05	122.57	124.45
20	2	303	XAT	O24-C25-C38	2.05	117.51	115.06
22	7	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	a	822	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	8	304	A1L1F	C20-C21-C22	-2.05	108.70	112.75
20	3	301	XAT	O24-C25-C38	2.05	117.51	115.06
22	a	809	CLA	O2D-CGD-CBD	2.05	114.90	111.27
20	2	302	XAT	C19-C9-C8	2.04	121.30	118.08
20	7	301	XAT	C19-C9-C8	2.04	121.30	118.08
20	8	303	XAT	O24-C25-C38	2.04	117.50	115.06
20	a	852	XAT	C39-C29-C28	2.04	121.30	118.08
20	7	304	XAT	C8-C9-C10	2.04	122.08	118.94
22	a	818	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	3	304	XAT	O4-C5-C4	2.04	114.92	113.38
20	7	305	XAT	C7-C8-C9	-2.04	122.36	125.53
22	b	837	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	8	302	XAT	O4-C5-C18	2.04	117.50	115.06
22	2	312	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	h	205	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	2	311	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	9	306	A1L1G	C20-C21-C22	2.04	116.78	112.75
26	b	848	DGD	O5E-C6E-C5E	-2.04	104.30	111.29
22	b	813	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	3	305	XAT	O4-C5-C4	2.04	114.91	113.38
22	2	307	CLA	C2A-C1A-CHA	2.04	127.42	123.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	301	XAT	O4-C5-C18	2.04	117.50	115.06
22	2	310	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	3	308	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
22	a	808	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
22	b	819	CLA	CHD-C1D-ND	-2.03	122.58	124.45
20	2	304	XAT	C15-C35-C34	-2.03	119.31	123.47
22	2	315	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	a	817	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	3	313	CLA	C1-C2-C3	-2.03	122.53	126.04
20	2	304	XAT	C40-C33-C32	2.03	121.28	118.08
22	1	311	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	a	814	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	b	822	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	4	307	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	3	315	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	b	817	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	b	814	CLA	C1-C2-C3	-2.03	122.53	126.04
20	9	304	XAT	C31-C30-C29	-2.03	124.41	127.31
20	1	303	XAT	C11-C10-C9	-2.03	124.41	127.31
20	4	302	XAT	O24-C25-C38	2.03	117.49	115.06
20	7	304	XAT	C31-C32-C33	-2.03	120.71	126.42
20	7	305	XAT	C11-C12-C13	-2.03	120.71	126.42
22	b	808	CLA	O2D-CGD-CBD	2.03	114.88	111.27
22	4	311	CLA	C2D-C1D-ND	-2.03	108.61	110.10
20	7	304	XAT	O4-C5-C18	2.03	117.49	115.06
20	1	302	XAT	O4-C5-C18	2.03	117.49	115.06
29	f	804	BCR	C8-C7-C6	-2.03	121.50	127.20
29	l	201	BCR	C33-C5-C4	2.03	117.51	113.62
29	f	804	BCR	C33-C5-C4	2.03	117.51	113.62
22	1	306	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	4	315	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	a	811	CLA	C1-C2-C3	-2.03	122.54	126.04
22	a	832	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	4	305	XAT	O4-C5-C18	2.03	117.48	115.06
22	3	308	CLA	O2D-CGD-CBD	2.03	114.87	111.27
22	8	307	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	2	304	XAT	C30-C31-C32	-2.02	116.90	123.22
22	8	306	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	a	804	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	a	840	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	5	311	CLA	C1-C2-C3	-2.02	122.54	126.04
29	h	201	BCR	C28-C27-C26	-2.02	110.46	114.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	315	DGD	C4D-C3D-C2D	-2.02	107.29	110.82
20	4	302	XAT	O4-C5-C18	2.02	117.48	115.06
20	2	305	XAT	C10-C11-C12	-2.02	116.91	123.22
29	b	842	BCR	C33-C5-C6	-2.02	122.26	124.53
29	f	804	BCR	C21-C20-C19	-2.02	116.91	123.22
22	b	807	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	a	823	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	a	832	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	a	821	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
29	a	847	BCR	C20-C19-C18	-2.02	120.75	126.42
20	4	304	XAT	C19-C9-C8	2.02	121.25	118.08
20	4	302	XAT	O4-C5-C4	2.02	114.90	113.38
22	1	307	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
20	7	301	XAT	O4-C5-C18	2.02	117.47	115.06
22	b	804	CLA	O2D-CGD-CBD	2.02	114.85	111.27
20	4	304	XAT	O24-C25-C38	2.01	117.47	115.06
22	a	830	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
29	a	848	BCR	C28-C27-C26	-2.01	110.48	114.08
29	b	842	BCR	C16-C15-C14	-2.01	119.35	123.47
22	a	838	CLA	C1-C2-C3	-2.01	122.56	126.04
22	b	817	CLA	C1-C2-C3	-2.01	122.56	126.04
29	b	845	BCR	C2-C1-C6	2.01	113.58	110.48
22	9	315	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	1	306	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	b	801	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	a	850	BCR	C37-C22-C21	-2.01	120.11	122.92
24	1	304	A1L1F	C25-C14-C29	-2.01	121.74	125.99
20	1	303	XAT	O4-C5-C18	2.01	117.47	115.06
20	1	303	XAT	C20-C13-C12	2.01	121.25	118.08
23	1	315	SQD	O7-S-C6	2.01	109.33	106.94
26	4	318	DGD	C4D-C3D-C2D	-2.01	107.31	110.82
20	3	305	XAT	O4-C5-C18	2.01	117.46	115.06
22	b	824	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	b	804	CLA	CAC-C3C-C4C	2.01	127.42	124.81
22	b	829	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	a	815	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
22	a	842	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	a	809	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	b	810	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	a	803	CLA	CHB-C4A-NA	2.01	127.29	124.51
29	j	104	BCR	C21-C20-C19	-2.01	116.96	123.22
22	h	205	CLA	C1-C2-C3	-2.01	122.58	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	316	SQD	O8-S-C6	2.00	108.94	105.74
22	8	314	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	2	313	CLA	CHD-C1D-ND	-2.00	122.61	124.45
20	4	301	XAT	O4-C5-C18	2.00	117.45	115.06
29	b	844	BCR	C1-C6-C7	2.00	121.44	115.78
20	8	301	XAT	C39-C29-C28	2.00	121.23	118.08
20	1	302	XAT	O4-C5-C4	2.00	114.89	113.38
22	b	814	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	5	305	CLA	ND
22	5	306	CLA	ND
22	5	307	CLA	ND
22	5	308	CLA	ND
22	5	309	CLA	ND
22	5	310	CLA	ND
22	5	311	CLA	ND
22	5	312	CLA	ND
22	5	313	CLA	ND
22	5	314	CLA	ND
22	5	315	CLA	ND
22	9	308	CLA	ND
22	9	309	CLA	ND
22	9	310	CLA	ND
22	9	311	CLA	ND
22	9	312	CLA	ND
22	9	313	CLA	ND
22	9	314	CLA	ND
22	9	315	CLA	ND
22	9	316	CLA	ND
22	9	318	CLA	ND
22	8	305	CLA	ND
22	8	306	CLA	ND
22	8	307	CLA	ND
22	8	308	CLA	ND
22	8	309	CLA	ND
22	8	310	CLA	ND
22	8	311	CLA	ND
22	8	312	CLA	ND
22	8	313	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
22	8	314	CLA	ND
22	4	306	CLA	ND
22	4	307	CLA	ND
22	4	308	CLA	ND
22	4	309	CLA	ND
22	4	310	CLA	ND
22	4	311	CLA	ND
22	4	312	CLA	ND
22	4	313	CLA	ND
22	4	314	CLA	ND
22	4	315	CLA	ND
22	4	316	CLA	ND
22	4	317	CLA	ND
22	3	307	CLA	ND
22	3	308	CLA	ND
22	3	309	CLA	ND
22	3	310	CLA	ND
22	3	311	CLA	ND
22	3	312	CLA	ND
22	3	313	CLA	ND
22	3	314	CLA	ND
22	3	315	CLA	ND
22	2	306	CLA	ND
22	2	307	CLA	ND
22	2	308	CLA	ND
22	2	309	CLA	ND
22	2	310	CLA	ND
22	2	311	CLA	ND
22	2	312	CLA	ND
22	2	313	CLA	ND
22	2	314	CLA	ND
22	2	315	CLA	ND
22	2	316	CLA	ND
22	7	306	CLA	ND
22	7	307	CLA	ND
22	7	308	CLA	ND
22	7	309	CLA	ND
22	7	310	CLA	ND
22	7	311	CLA	ND
22	7	312	CLA	ND
22	7	313	CLA	ND
22	7	314	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
22	7	315	CLA	ND
22	7	316	CLA	ND
22	7	317	CLA	ND
22	1	305	CLA	ND
22	1	306	CLA	ND
22	1	307	CLA	ND
22	1	308	CLA	ND
22	1	309	CLA	ND
22	1	310	CLA	ND
22	1	311	CLA	ND
22	1	312	CLA	ND
22	1	313	CLA	ND
22	1	314	CLA	ND
22	a	801	CLA	ND
22	a	802	CLA	ND
22	a	803	CLA	ND
22	a	804	CLA	ND
22	a	805	CLA	ND
22	a	806	CLA	ND
22	a	807	CLA	ND
22	a	808	CLA	ND
22	a	809	CLA	ND
22	a	810	CLA	ND
22	a	811	CLA	ND
22	a	812	CLA	ND
22	a	813	CLA	ND
22	a	814	CLA	ND
22	a	815	CLA	ND
22	a	816	CLA	ND
22	a	817	CLA	ND
22	a	818	CLA	ND
22	a	819	CLA	ND
22	a	820	CLA	ND
22	a	821	CLA	ND
22	a	822	CLA	ND
22	a	823	CLA	ND
22	a	824	CLA	ND
22	a	825	CLA	ND
22	a	826	CLA	ND
22	a	827	CLA	ND
22	a	828	CLA	ND
22	a	829	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
22	a	830	CLA	ND
22	a	831	CLA	ND
22	a	832	CLA	ND
22	a	833	CLA	ND
22	a	834	CLA	ND
22	a	835	CLA	ND
22	a	836	CLA	ND
22	a	837	CLA	ND
22	a	838	CLA	ND
22	a	839	CLA	ND
22	a	840	CLA	ND
22	a	841	CLA	ND
22	a	842	CLA	ND
22	a	844	CLA	ND
22	a	854	CLA	ND
22	b	801	CLA	ND
22	b	802	CLA	ND
22	b	803	CLA	ND
22	b	804	CLA	ND
22	b	805	CLA	ND
22	b	806	CLA	ND
22	b	807	CLA	ND
22	b	808	CLA	ND
22	b	809	CLA	ND
22	b	810	CLA	ND
22	b	811	CLA	ND
22	b	812	CLA	ND
22	b	813	CLA	ND
22	b	814	CLA	ND
22	b	815	CLA	ND
22	b	816	CLA	ND
22	b	817	CLA	ND
22	b	818	CLA	ND
22	b	819	CLA	ND
22	b	820	CLA	ND
22	b	821	CLA	ND
22	b	822	CLA	ND
22	b	823	CLA	ND
22	b	824	CLA	ND
22	b	825	CLA	ND
22	b	826	CLA	ND
22	b	827	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
22	b	828	CLA	ND
22	b	829	CLA	ND
22	b	830	CLA	ND
22	b	831	CLA	ND
22	b	832	CLA	ND
22	b	833	CLA	ND
22	b	834	CLA	ND
22	b	835	CLA	ND
22	b	836	CLA	ND
22	b	837	CLA	ND
22	b	838	CLA	ND
22	b	839	CLA	ND
22	b	840	CLA	ND
22	f	802	CLA	ND
22	f	803	CLA	ND
22	h	203	CLA	ND
22	h	205	CLA	ND
22	j	102	CLA	ND
22	j	103	CLA	ND
22	l	202	CLA	ND
22	l	203	CLA	ND
22	l	204	CLA	ND

All (1985) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	5	302	XAT	O4-C6-C7-C8
20	5	302	XAT	C7-C8-C9-C10
20	5	302	XAT	C7-C8-C9-C19
20	9	303	XAT	O4-C6-C7-C8
20	9	304	XAT	O24-C26-C27-C28
20	9	305	XAT	O4-C6-C7-C8
20	9	305	XAT	C7-C8-C9-C10
20	9	305	XAT	C7-C8-C9-C19
20	8	301	XAT	C7-C8-C9-C19
20	8	302	XAT	O4-C6-C7-C8
20	8	302	XAT	C7-C8-C9-C10
20	8	302	XAT	C7-C8-C9-C19
20	4	301	XAT	C27-C28-C29-C30
20	4	301	XAT	C27-C28-C29-C39
20	4	303	XAT	O4-C6-C7-C8
20	4	303	XAT	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	4	303	XAT	C7-C8-C9-C19
20	4	305	XAT	O24-C26-C27-C28
20	3	301	XAT	O4-C6-C7-C8
20	3	301	XAT	C27-C28-C29-C30
20	3	301	XAT	C27-C28-C29-C39
20	3	303	XAT	C27-C28-C29-C30
20	3	303	XAT	C27-C28-C29-C39
20	3	304	XAT	O24-C26-C27-C28
20	3	304	XAT	C27-C28-C29-C30
20	3	304	XAT	C27-C28-C29-C39
20	2	303	XAT	O4-C6-C7-C8
20	2	303	XAT	O24-C26-C27-C28
20	2	303	XAT	C27-C28-C29-C30
20	2	303	XAT	C27-C28-C29-C39
20	2	305	XAT	C25-C26-C27-C28
20	7	301	XAT	O4-C6-C7-C8
20	7	301	XAT	C27-C28-C29-C30
20	7	301	XAT	C27-C28-C29-C39
20	7	303	XAT	O4-C6-C7-C8
20	7	303	XAT	O24-C26-C27-C28
20	7	303	XAT	C27-C28-C29-C30
20	7	303	XAT	C27-C28-C29-C39
20	7	304	XAT	O4-C6-C7-C8
20	7	304	XAT	C11-C12-C13-C14
20	7	304	XAT	C11-C12-C13-C20
20	a	852	XAT	C7-C8-C9-C10
20	a	852	XAT	C7-C8-C9-C19
20	a	852	XAT	C11-C12-C13-C14
20	a	852	XAT	C11-C12-C13-C20
20	a	852	XAT	C27-C28-C29-C30
20	a	852	XAT	C27-C28-C29-C39
20	j	101	XAT	O4-C6-C7-C8
20	j	101	XAT	C7-C8-C9-C10
20	j	101	XAT	C7-C8-C9-C19
20	j	101	XAT	O24-C26-C27-C28
21	5	303	A1L1G	C26-C30-C31-C32
21	5	303	A1L1G	C31-C32-C33-C34
21	5	303	A1L1G	C32-C33-C34-C27
21	5	303	A1L1G	C32-C33-C34-C35
21	5	303	A1L1G	C41-C42-C44-C2
21	5	303	A1L1G	C41-C42-C44-C43
21	9	301	A1L1G	O13-C26-C30-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	9	301	A1L1G	C26-C30-C31-C32
21	9	301	A1L1G	C31-C32-C33-C34
21	9	301	A1L1G	C28-C39-C40-C41
21	9	301	A1L1G	C38-C39-C40-C41
21	9	301	A1L1G	C39-C40-C41-C42
21	9	306	A1L1G	C45-C2-C44-C42
21	9	306	A1L1G	C45-C2-C44-C43
21	9	306	A1L1G	C29-C14-C25-C24
21	9	306	A1L1G	C25-C14-C29-C30
21	9	306	A1L1G	C35-C36-C37-C38
21	9	306	A1L1G	C37-C38-C39-C28
21	9	306	A1L1G	C37-C38-C39-C40
21	3	302	A1L1G	C25-C14-C29-C30
21	3	302	A1L1G	C14-C29-C30-C26
21	3	302	A1L1G	C26-C30-C31-C32
21	3	302	A1L1G	C29-C30-C31-C32
21	3	302	A1L1G	C41-C42-C44-C2
21	3	302	A1L1G	C41-C42-C44-C43
21	3	306	A1L1G	C45-C2-C44-C42
21	3	306	A1L1G	C45-C2-C44-C43
21	3	306	A1L1G	O13-C26-C30-C29
21	3	306	A1L1G	C37-C38-C39-C28
21	3	306	A1L1G	C37-C38-C39-C40
21	3	306	A1L1G	C39-C40-C41-C42
21	3	306	A1L1G	C41-C42-C44-C2
21	3	306	A1L1G	C41-C42-C44-C43
21	7	302	A1L1G	C45-C2-C44-C42
21	7	302	A1L1G	C29-C14-C25-C24
21	7	302	A1L1G	C35-C36-C37-C38
21	7	302	A1L1G	C37-C38-C39-C28
21	7	302	A1L1G	C37-C38-C39-C40
21	7	302	A1L1G	C39-C40-C41-C42
21	7	302	A1L1G	C41-C42-C44-C2
21	7	302	A1L1G	C41-C42-C44-C43
21	1	301	A1L1G	C45-C2-C44-C42
21	1	301	A1L1G	C45-C2-C44-C43
21	1	301	A1L1G	O13-C26-C30-C29
21	1	301	A1L1G	C27-C34-C35-C36
21	1	301	A1L1G	C33-C34-C35-C36
21	1	301	A1L1G	C35-C36-C37-C38
21	1	301	A1L1G	C28-C39-C40-C41
21	1	301	A1L1G	C38-C39-C40-C41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	1	301	A1L1G	C39-C40-C41-C42
22	5	307	CLA	CHA-CBD-CGD-O1D
22	5	307	CLA	CHA-CBD-CGD-O2D
22	5	308	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CHA-CBD-CGD-O1D
22	5	309	CLA	CHA-CBD-CGD-O2D
22	5	309	CLA	CAD-CBD-CGD-O1D
22	5	309	CLA	CAD-CBD-CGD-O2D
22	5	310	CLA	CBD-CGD-O2D-CED
22	5	314	CLA	C1A-C2A-CAA-CBA
22	5	314	CLA	C3A-C2A-CAA-CBA
22	5	315	CLA	CBD-CGD-O2D-CED
22	5	315	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	CHA-CBD-CGD-O1D
22	9	310	CLA	CHA-CBD-CGD-O2D
22	9	311	CLA	CHA-CBD-CGD-O1D
22	9	311	CLA	CHA-CBD-CGD-O2D
22	9	311	CLA	CBD-CGD-O2D-CED
22	9	311	CLA	O1D-CGD-O2D-CED
22	9	313	CLA	C2A-CAA-CBA-CGA
22	9	314	CLA	CHA-CBD-CGD-O1D
22	9	314	CLA	CHA-CBD-CGD-O2D
22	9	315	CLA	CHA-CBD-CGD-O1D
22	9	315	CLA	CHA-CBD-CGD-O2D
22	9	315	CLA	CBD-CGD-O2D-CED
22	9	316	CLA	C1A-C2A-CAA-CBA
22	9	316	CLA	CHA-CBD-CGD-O1D
22	9	316	CLA	CHA-CBD-CGD-O2D
22	9	316	CLA	CAD-CBD-CGD-O1D
22	8	307	CLA	CHA-CBD-CGD-O1D
22	8	307	CLA	CHA-CBD-CGD-O2D
22	8	311	CLA	C2-C3-C5-C6
22	8	311	CLA	C4-C3-C5-C6
22	4	306	CLA	C1A-C2A-CAA-CBA
22	4	307	CLA	CHA-CBD-CGD-O2D
22	4	309	CLA	CHA-CBD-CGD-O1D
22	4	309	CLA	CHA-CBD-CGD-O2D
22	4	309	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	C1A-C2A-CAA-CBA
22	4	311	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	4	312	CLA	C1A-C2A-CAA-CBA
22	4	312	CLA	C3A-C2A-CAA-CBA
22	4	313	CLA	CHA-CBD-CGD-O1D
22	4	313	CLA	CHA-CBD-CGD-O2D
22	4	315	CLA	CHA-CBD-CGD-O1D
22	4	315	CLA	CHA-CBD-CGD-O2D
22	4	316	CLA	C2A-CAA-CBA-CGA
22	4	316	CLA	CBD-CGD-O2D-CED
22	4	317	CLA	CBD-CGD-O2D-CED
22	3	309	CLA	CHA-CBD-CGD-O1D
22	3	309	CLA	CHA-CBD-CGD-O2D
22	3	310	CLA	C2-C3-C5-C6
22	3	310	CLA	C4-C3-C5-C6
22	3	312	CLA	C1A-C2A-CAA-CBA
22	3	315	CLA	C1A-C2A-CAA-CBA
22	2	307	CLA	CBD-CGD-O2D-CED
22	2	308	CLA	CHA-CBD-CGD-O1D
22	2	308	CLA	CHA-CBD-CGD-O2D
22	2	309	CLA	CBD-CGD-O2D-CED
22	2	312	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C3A-C2A-CAA-CBA
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	307	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBA-CGA-O2A-C1
22	7	311	CLA	CBA-CGA-O2A-C1
22	7	313	CLA	CHA-CBD-CGD-O1D
22	7	313	CLA	CHA-CBD-CGD-O2D
22	7	314	CLA	CBD-CGD-O2D-CED
22	7	315	CLA	CHA-CBD-CGD-O1D
22	7	315	CLA	CBD-CGD-O2D-CED
22	7	316	CLA	C1A-C2A-CAA-CBA
22	7	316	CLA	C3A-C2A-CAA-CBA
22	1	305	CLA	CHA-CBD-CGD-O1D
22	1	305	CLA	CHA-CBD-CGD-O2D
22	1	305	CLA	C11-C10-C8-C9
22	1	310	CLA	CBD-CGD-O2D-CED
22	1	311	CLA	CHA-CBD-CGD-O1D
22	1	311	CLA	CHA-CBD-CGD-O2D
22	1	313	CLA	CBD-CGD-O2D-CED
22	1	314	CLA	C1A-C2A-CAA-CBA
22	1	314	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	a	801	CLA	CHA-CBD-CGD-O1D
22	a	801	CLA	CHA-CBD-CGD-O2D
22	a	801	CLA	CBD-CGD-O2D-CED
22	a	805	CLA	C1A-C2A-CAA-CBA
22	a	805	CLA	C3A-C2A-CAA-CBA
22	a	806	CLA	CHA-CBD-CGD-O1D
22	a	806	CLA	CHA-CBD-CGD-O2D
22	a	806	CLA	O2A-C1-C2-C3
22	a	809	CLA	C1A-C2A-CAA-CBA
22	a	809	CLA	C3A-C2A-CAA-CBA
22	a	811	CLA	CHA-CBD-CGD-O1D
22	a	811	CLA	CHA-CBD-CGD-O2D
22	a	811	CLA	CBD-CGD-O2D-CED
22	a	818	CLA	C1A-C2A-CAA-CBA
22	a	818	CLA	C3A-C2A-CAA-CBA
22	a	818	CLA	CHA-CBD-CGD-O1D
22	a	818	CLA	CHA-CBD-CGD-O2D
22	a	819	CLA	C3A-C2A-CAA-CBA
22	a	820	CLA	C1A-C2A-CAA-CBA
22	a	820	CLA	C3A-C2A-CAA-CBA
22	a	823	CLA	C1A-C2A-CAA-CBA
22	a	823	CLA	C3A-C2A-CAA-CBA
22	a	825	CLA	CHA-CBD-CGD-O1D
22	a	825	CLA	CHA-CBD-CGD-O2D
22	a	829	CLA	C1A-C2A-CAA-CBA
22	a	829	CLA	CBD-CGD-O2D-CED
22	a	831	CLA	C2-C3-C5-C6
22	a	831	CLA	C4-C3-C5-C6
22	a	832	CLA	C1A-C2A-CAA-CBA
22	a	832	CLA	C3A-C2A-CAA-CBA
22	a	838	CLA	C1A-C2A-CAA-CBA
22	a	838	CLA	C2-C3-C5-C6
22	a	838	CLA	C4-C3-C5-C6
22	a	839	CLA	C2-C3-C5-C6
22	a	839	CLA	C4-C3-C5-C6
22	a	840	CLA	CHA-CBD-CGD-O1D
22	a	840	CLA	CHA-CBD-CGD-O2D
22	a	841	CLA	CHA-CBD-CGD-O1D
22	a	841	CLA	CHA-CBD-CGD-O2D
22	a	844	CLA	CHA-CBD-CGD-O1D
22	a	844	CLA	CHA-CBD-CGD-O2D
22	a	854	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	803	CLA	CHA-CBD-CGD-O1D
22	b	803	CLA	CHA-CBD-CGD-O2D
22	b	803	CLA	CBD-CGD-O2D-CED
22	b	804	CLA	CBD-CGD-O2D-CED
22	b	805	CLA	C2A-CAA-CBA-CGA
22	b	806	CLA	C1A-C2A-CAA-CBA
22	b	806	CLA	C3A-C2A-CAA-CBA
22	b	806	CLA	CHA-CBD-CGD-O1D
22	b	806	CLA	CHA-CBD-CGD-O2D
22	b	806	CLA	CAD-CBD-CGD-O1D
22	b	810	CLA	C1A-C2A-CAA-CBA
22	b	810	CLA	C2A-CAA-CBA-CGA
22	b	812	CLA	C1A-C2A-CAA-CBA
22	b	812	CLA	C2-C3-C5-C6
22	b	812	CLA	C4-C3-C5-C6
22	b	814	CLA	C1A-C2A-CAA-CBA
22	b	814	CLA	CBD-CGD-O2D-CED
22	b	817	CLA	C3A-C2A-CAA-CBA
22	b	818	CLA	C1A-C2A-CAA-CBA
22	b	818	CLA	C3A-C2A-CAA-CBA
22	b	820	CLA	C1A-C2A-CAA-CBA
22	b	820	CLA	C3A-C2A-CAA-CBA
22	b	820	CLA	CHA-CBD-CGD-O1D
22	b	820	CLA	CHA-CBD-CGD-O2D
22	b	823	CLA	CHA-CBD-CGD-O1D
22	b	823	CLA	CHA-CBD-CGD-O2D
22	b	826	CLA	CHA-CBD-CGD-O1D
22	b	826	CLA	CHA-CBD-CGD-O2D
22	b	828	CLA	C1A-C2A-CAA-CBA
22	b	828	CLA	C3A-C2A-CAA-CBA
22	b	832	CLA	C1A-C2A-CAA-CBA
22	b	832	CLA	C3A-C2A-CAA-CBA
22	b	833	CLA	C1A-C2A-CAA-CBA
22	b	833	CLA	C3A-C2A-CAA-CBA
22	b	833	CLA	C11-C12-C13-C14
22	b	834	CLA	CBD-CGD-O2D-CED
22	b	836	CLA	CHA-CBD-CGD-O1D
22	b	836	CLA	CHA-CBD-CGD-O2D
22	b	839	CLA	C1A-C2A-CAA-CBA
22	b	839	CLA	C3A-C2A-CAA-CBA
22	b	839	CLA	CHA-CBD-CGD-O1D
22	b	839	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	839	CLA	CAD-CBD-CGD-O1D
22	b	839	CLA	CBD-CGD-O2D-CED
22	h	203	CLA	C1A-C2A-CAA-CBA
22	j	102	CLA	C1A-C2A-CAA-CBA
22	j	102	CLA	C2-C3-C5-C6
22	j	102	CLA	C4-C3-C5-C6
22	j	103	CLA	CAD-CBD-CGD-O1D
22	j	103	CLA	CAD-CBD-CGD-O2D
22	j	103	CLA	CBD-CGD-O2D-CED
22	l	202	CLA	CHA-CBD-CGD-O1D
22	l	202	CLA	CHA-CBD-CGD-O2D
22	l	203	CLA	CHA-CBD-CGD-O1D
22	l	203	CLA	CHA-CBD-CGD-O2D
22	l	203	CLA	C6-C7-C8-C9
23	5	316	SQD	O49-C7-O47-C45
23	5	316	SQD	C8-C7-O47-C45
23	5	316	SQD	C5-C6-S-O7
23	5	316	SQD	C5-C6-S-O8
23	5	316	SQD	C5-C6-S-O9
23	1	315	SQD	O5-C5-C6-S
23	1	315	SQD	C5-C6-S-O7
23	1	315	SQD	C5-C6-S-O8
23	1	315	SQD	C5-C6-S-O9
24	9	302	A1L1F	C4-C8-O7-C54
24	9	302	A1L1F	O13-C26-C30-C31
24	8	304	A1L1F	C32-C33-C34-C27
24	8	304	A1L1F	C32-C33-C34-C35
24	8	304	A1L1F	C56-C54-O7-C8
24	8	304	A1L1F	O55-C54-O7-C8
24	1	304	A1L1F	C32-C33-C34-C27
24	1	304	A1L1F	C32-C33-C34-C35
24	1	304	A1L1F	C28-C39-C40-C41
24	1	304	A1L1F	C38-C39-C40-C41
24	h	204	A1L1F	C56-C54-O7-C8
24	h	204	A1L1F	O55-C54-O7-C8
25	9	307	LHG	C3-O3-P-O4
25	9	307	LHG	C3-O3-P-O5
25	9	307	LHG	C3-O3-P-O6
25	9	307	LHG	O9-C7-O7-C5
25	9	307	LHG	C8-C7-O7-C5
25	9	317	LHG	C1-C2-C3-O3
25	9	317	LHG	C3-O3-P-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	9	317	LHG	O9-C7-O7-C5
25	9	317	LHG	C8-C7-O7-C5
25	a	845	LHG	O1-C1-C2-C3
25	a	845	LHG	C3-O3-P-O4
25	a	845	LHG	C4-O6-P-O3
25	a	845	LHG	C4-O6-P-O5
25	a	845	LHG	O6-C4-C5-O7
25	a	845	LHG	O7-C5-C6-O8
25	a	846	LHG	O1-C1-C2-C3
25	a	846	LHG	O6-C4-C5-O7
25	b	847	LHG	O1-C1-C2-C3
25	b	847	LHG	C1-C2-C3-O3
25	b	847	LHG	O2-C2-C3-O3
25	b	847	LHG	C3-O3-P-O5
25	b	847	LHG	C4-O6-P-O3
25	b	847	LHG	C4-O6-P-O4
25	b	847	LHG	C4-O6-P-O5
26	8	315	DGD	C2B-C1B-O2G-C2G
26	8	315	DGD	C2E-C1E-O5D-C6D
26	8	315	DGD	O6E-C1E-O5D-C6D
26	4	318	DGD	C2B-C1B-O2G-C2G
26	4	318	DGD	O1B-C1B-O2G-C2G
26	4	318	DGD	C2E-C1E-O5D-C6D
26	4	318	DGD	O6E-C1E-O5D-C6D
27	2	317	LMG	O1-C7-C8-O7
27	a	853	LMG	C11-C10-O7-C8
27	j	105	LMG	O9-C10-O7-C8
27	j	105	LMG	C11-C10-O7-C8
29	a	850	BCR	C23-C24-C25-C26
29	b	842	BCR	C7-C8-C9-C10
29	b	842	BCR	C7-C8-C9-C34
29	b	844	BCR	C1-C6-C7-C8
29	b	844	BCR	C5-C6-C7-C8
29	i	101	BCR	C21-C22-C23-C24
29	i	101	BCR	C37-C22-C23-C24
29	j	104	BCR	C7-C8-C9-C10
29	j	104	BCR	C7-C8-C9-C34
29	m	101	BCR	C1-C6-C7-C8
29	m	101	BCR	C7-C8-C9-C34
29	m	101	BCR	C21-C22-C23-C24
29	m	101	BCR	C37-C22-C23-C24
24	9	302	A1L1F	C56-C54-O7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	9	302	A1L1F	O55-C54-O7-C8
22	5	310	CLA	O1D-CGD-O2D-CED
22	9	315	CLA	O1D-CGD-O2D-CED
22	4	309	CLA	O1D-CGD-O2D-CED
22	2	314	CLA	O1D-CGD-O2D-CED
22	7	314	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	O1D-CGD-O2D-CED
22	2	309	CLA	O1D-CGD-O2D-CED
22	2	313	CLA	O1D-CGD-O2D-CED
22	7	307	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	a	812	CLA	O1D-CGD-O2D-CED
22	b	803	CLA	O1D-CGD-O2D-CED
22	b	834	CLA	O1D-CGD-O2D-CED
22	5	313	CLA	CBD-CGD-O2D-CED
22	9	318	CLA	CBD-CGD-O2D-CED
22	8	306	CLA	CBD-CGD-O2D-CED
22	4	306	CLA	CBD-CGD-O2D-CED
22	2	314	CLA	CBD-CGD-O2D-CED
22	1	309	CLA	CBD-CGD-O2D-CED
22	a	812	CLA	CBD-CGD-O2D-CED
22	8	308	CLA	O1A-CGA-O2A-C1
22	1	307	CLA	O1A-CGA-O2A-C1
22	a	806	CLA	O1A-CGA-O2A-C1
22	b	814	CLA	O1A-CGA-O2A-C1
25	9	317	LHG	O10-C23-O8-C6
27	2	317	LMG	O10-C28-O8-C9
22	7	310	CLA	O1A-CGA-O2A-C1
22	4	316	CLA	O1D-CGD-O2D-CED
22	7	315	CLA	O1D-CGD-O2D-CED
22	b	804	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	4	317	CLA	O1D-CGD-O2D-CED
22	2	312	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	a	801	CLA	O1D-CGD-O2D-CED
22	a	811	CLA	O1D-CGD-O2D-CED
22	a	829	CLA	O1D-CGD-O2D-CED
22	b	814	CLA	O1D-CGD-O2D-CED
22	b	839	CLA	O1D-CGD-O2D-CED
22	j	103	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	8	308	CLA	CBA-CGA-O2A-C1
22	1	307	CLA	CBA-CGA-O2A-C1
22	a	806	CLA	CBA-CGA-O2A-C1
22	b	814	CLA	CBA-CGA-O2A-C1
25	9	317	LHG	C24-C23-O8-C6
22	5	305	CLA	CBD-CGD-O2D-CED
22	5	306	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	CBD-CGD-O2D-CED
22	9	314	CLA	CBD-CGD-O2D-CED
22	8	309	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	2	316	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	a	804	CLA	CBD-CGD-O2D-CED
22	a	814	CLA	CBD-CGD-O2D-CED
22	b	806	CLA	CBD-CGD-O2D-CED
22	b	819	CLA	CBD-CGD-O2D-CED
22	b	835	CLA	CBD-CGD-O2D-CED
22	h	205	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	O1A-CGA-O2A-C1
22	2	310	CLA	O1A-CGA-O2A-C1
22	2	311	CLA	O1A-CGA-O2A-C1
22	7	312	CLA	O1A-CGA-O2A-C1
22	a	805	CLA	O1A-CGA-O2A-C1
22	a	818	CLA	O1A-CGA-O2A-C1
22	b	821	CLA	O1A-CGA-O2A-C1
22	f	802	CLA	O1A-CGA-O2A-C1
25	b	847	LHG	O10-C23-O8-C6
26	8	315	DGD	O1A-C1A-O1G-C1G
27	a	853	LMG	O10-C28-O8-C9
22	4	311	CLA	O1A-CGA-O2A-C1
22	7	311	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	O1D-CGD-O2D-CED
22	4	311	CLA	O1D-CGD-O2D-CED
22	4	307	CLA	CBD-CGD-O2D-CED
22	7	308	CLA	CBD-CGD-O2D-CED
22	a	818	CLA	CBD-CGD-O2D-CED
22	a	837	CLA	CBD-CGD-O2D-CED
26	8	315	DGD	O1B-C1B-O2G-C2G
27	a	853	LMG	O9-C10-O7-C8
22	1	309	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	1	304	A1L1F	C56-C54-O7-C8
22	1	309	CLA	O1A-CGA-O2A-C1
22	1	204	CLA	O1A-CGA-O2A-C1
22	1	309	CLA	O1D-CGD-O2D-CED
22	3	312	CLA	C3-C5-C6-C7
22	2	310	CLA	C3-C5-C6-C7
22	2	311	CLA	C3-C5-C6-C7
22	2	314	CLA	C3-C5-C6-C7
22	7	308	CLA	C3-C5-C6-C7
22	a	810	CLA	C3-C5-C6-C7
22	b	802	CLA	C3-C5-C6-C7
22	b	805	CLA	C3-C5-C6-C7
22	b	807	CLA	C3-C5-C6-C7
22	b	809	CLA	C3-C5-C6-C7
22	2	310	CLA	CBA-CGA-O2A-C1
22	2	311	CLA	CBA-CGA-O2A-C1
22	7	312	CLA	CBA-CGA-O2A-C1
22	a	805	CLA	CBA-CGA-O2A-C1
22	a	818	CLA	CBA-CGA-O2A-C1
22	a	836	CLA	CBA-CGA-O2A-C1
22	b	821	CLA	CBA-CGA-O2A-C1
22	b	823	CLA	CBA-CGA-O2A-C1
22	f	802	CLA	CBA-CGA-O2A-C1
27	2	317	LMG	C29-C28-O8-C9
27	a	853	LMG	C29-C28-O8-C9
24	1	304	A1L1F	O55-C54-O7-C8
22	9	316	CLA	CBD-CGD-O2D-CED
22	3	309	CLA	CBD-CGD-O2D-CED
22	3	315	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	O1A-CGA-O2A-C1
22	9	309	CLA	CBA-CGA-O2A-C1
22	1	204	CLA	CBA-CGA-O2A-C1
22	a	813	CLA	C4-C3-C5-C6
22	a	825	CLA	C4-C3-C5-C6
22	b	828	CLA	C4-C3-C5-C6
22	b	823	CLA	CBD-CGD-O2D-CED
22	b	827	CLA	CBD-CGD-O2D-CED
22	9	311	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	C2A-CAA-CBA-CGA
22	7	317	CLA	C2A-CAA-CBA-CGA
22	a	817	CLA	C2A-CAA-CBA-CGA
22	a	825	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	a	842	CLA	C2A-CAA-CBA-CGA
22	b	820	CLA	C2A-CAA-CBA-CGA
22	b	833	CLA	C2A-CAA-CBA-CGA
22	b	838	CLA	C2A-CAA-CBA-CGA
22	9	308	CLA	C3-C5-C6-C7
22	8	308	CLA	C3-C5-C6-C7
22	1	307	CLA	C3-C5-C6-C7
22	1	310	CLA	C3-C5-C6-C7
22	b	818	CLA	C3-C5-C6-C7
22	9	316	CLA	CBA-CGA-O2A-C1
22	4	310	CLA	CBA-CGA-O2A-C1
22	1	305	CLA	CBA-CGA-O2A-C1
22	a	807	CLA	CBA-CGA-O2A-C1
22	a	811	CLA	CBA-CGA-O2A-C1
22	b	806	CLA	CBA-CGA-O2A-C1
22	b	818	CLA	CBA-CGA-O2A-C1
25	9	307	LHG	C24-C23-O8-C6
25	b	847	LHG	C24-C23-O8-C6
26	8	315	DGD	C2A-C1A-O1G-C1G
27	j	105	LMG	C29-C28-O8-C9
27	j	105	LMG	C12-C13-C14-C15
22	7	317	CLA	CBD-CGD-O2D-CED
22	a	835	CLA	CBD-CGD-O2D-CED
22	a	841	CLA	CBD-CGD-O2D-CED
27	j	105	LMG	C4-C5-C6-O5
22	5	311	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	O1A-CGA-O2A-C1
22	a	811	CLA	O1A-CGA-O2A-C1
22	a	812	CLA	O1A-CGA-O2A-C1
22	a	820	CLA	O1A-CGA-O2A-C1
22	b	806	CLA	O1A-CGA-O2A-C1
22	b	818	CLA	O1A-CGA-O2A-C1
27	j	105	LMG	O10-C28-O8-C9
21	9	301	A1L1G	C30-C31-C32-C33
21	9	301	A1L1G	C40-C41-C42-C44
21	3	302	A1L1G	C30-C31-C32-C33
21	7	302	A1L1G	C30-C31-C32-C33
24	8	304	A1L1F	C30-C31-C32-C33
22	4	308	CLA	CBD-CGD-O2D-CED
22	a	807	CLA	CBD-CGD-O2D-CED
22	a	810	CLA	CBD-CGD-O2D-CED
22	a	834	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	840	CLA	CBD-CGD-O2D-CED
22	9	318	CLA	O1D-CGD-O2D-CED
22	8	306	CLA	O1D-CGD-O2D-CED
25	9	307	LHG	O2-C2-C3-O3
25	9	317	LHG	O2-C2-C3-O3
25	a	845	LHG	O2-C2-C3-O3
22	7	306	CLA	CBA-CGA-O2A-C1
22	a	812	CLA	CBA-CGA-O2A-C1
22	b	839	CLA	CBA-CGA-O2A-C1
22	a	836	CLA	O1A-CGA-O2A-C1
22	b	823	CLA	O1A-CGA-O2A-C1
25	9	307	LHG	O10-C23-O8-C6
22	4	306	CLA	O1D-CGD-O2D-CED
22	9	312	CLA	CBA-CGA-O2A-C1
22	5	311	CLA	CBD-CGD-O2D-CED
22	b	839	CLA	O1A-CGA-O2A-C1
24	9	302	A1L1F	C47-C48-C49-C50
25	a	845	LHG	C12-C13-C14-C15
27	2	317	LMG	C29-C30-C31-C32
26	b	848	DGD	O6E-C5E-C6E-O5E
22	b	822	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	C3-C5-C6-C7
22	a	807	CLA	C3-C5-C6-C7
22	a	835	CLA	C3-C5-C6-C7
22	5	311	CLA	CBA-CGA-O2A-C1
22	a	820	CLA	CBA-CGA-O2A-C1
25	a	845	LHG	C28-C29-C30-C31
22	9	316	CLA	O1A-CGA-O2A-C1
22	a	807	CLA	O1A-CGA-O2A-C1
22	8	313	CLA	CBA-CGA-O2A-C1
22	1	312	CLA	C3-C5-C6-C7
22	9	312	CLA	O1A-CGA-O2A-C1
22	a	825	CLA	C2-C3-C5-C6
22	5	310	CLA	C2A-CAA-CBA-CGA
22	4	311	CLA	C2A-CAA-CBA-CGA
22	b	801	CLA	C2A-CAA-CBA-CGA
22	b	826	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	O1D-CGD-O2D-CED
27	a	853	LMG	O6-C5-C6-O5
27	j	105	LMG	O6-C5-C6-O5
22	9	309	CLA	O1A-CGA-O2A-C1
22	7	316	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	a	845	LHG	C23-C24-C25-C26
22	a	804	CLA	O1D-CGD-O2D-CED
22	b	806	CLA	O1D-CGD-O2D-CED
22	9	312	CLA	O1D-CGD-O2D-CED
22	9	314	CLA	O1D-CGD-O2D-CED
22	8	309	CLA	O1D-CGD-O2D-CED
22	7	310	CLA	O1D-CGD-O2D-CED
22	b	835	CLA	O1D-CGD-O2D-CED
25	9	307	LHG	C1-C2-C3-O3
25	a	845	LHG	C1-C2-C3-O3
22	h	205	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	CBA-CGA-O2A-C1
22	8	311	CLA	CBA-CGA-O2A-C1
22	3	311	CLA	CBA-CGA-O2A-C1
22	a	809	CLA	CBA-CGA-O2A-C1
22	a	839	CLA	CBA-CGA-O2A-C1
22	a	854	CLA	CBA-CGA-O2A-C1
22	b	820	CLA	CBA-CGA-O2A-C1
22	b	826	CLA	CBA-CGA-O2A-C1
22	b	833	CLA	CBA-CGA-O2A-C1
22	h	203	CLA	CBA-CGA-O2A-C1
22	4	315	CLA	CBD-CGD-O2D-CED
22	b	807	CLA	CBD-CGD-O2D-CED
22	h	203	CLA	CBD-CGD-O2D-CED
27	a	853	LMG	C4-C5-C6-O5
22	5	305	CLA	O1D-CGD-O2D-CED
21	5	303	A1L1G	C40-C41-C42-C44
24	8	304	A1L1F	C40-C41-C42-C44
22	a	810	CLA	C13-C15-C16-C17
22	a	854	CLA	O1A-CGA-O2A-C1
22	9	318	CLA	C8-C10-C11-C12
22	8	307	CLA	C5-C6-C7-C8
22	a	807	CLA	C5-C6-C7-C8
22	b	809	CLA	C5-C6-C7-C8
25	a	846	LHG	O2-C2-C3-O3
27	a	853	LMG	C28-C29-C30-C31
22	7	306	CLA	O2A-C1-C2-C3
22	8	311	CLA	O1A-CGA-O2A-C1
22	a	809	CLA	O1A-CGA-O2A-C1
22	a	813	CLA	C2-C3-C5-C6
22	9	318	CLA	C11-C10-C8-C9
22	9	318	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	8	307	CLA	C11-C10-C8-C9
22	8	311	CLA	C6-C7-C8-C9
22	2	310	CLA	C11-C12-C13-C14
22	1	306	CLA	C6-C7-C8-C9
22	1	306	CLA	C11-C12-C13-C14
22	1	310	CLA	C14-C13-C15-C16
22	a	829	CLA	C11-C10-C8-C9
22	b	801	CLA	C11-C10-C8-C9
22	b	801	CLA	C14-C13-C15-C16
22	b	805	CLA	C11-C10-C8-C9
22	b	818	CLA	C11-C10-C8-C9
22	b	824	CLA	C6-C7-C8-C9
22	b	829	CLA	C14-C13-C15-C16
22	b	838	CLA	C6-C7-C8-C9
22	f	802	CLA	C11-C12-C13-C14
22	2	316	CLA	O1D-CGD-O2D-CED
22	b	807	CLA	C15-C16-C17-C18
22	2	310	CLA	C2A-CAA-CBA-CGA
22	7	310	CLA	C2A-CAA-CBA-CGA
22	h	205	CLA	C2A-CAA-CBA-CGA
20	2	301	XAT	C27-C28-C29-C39
20	2	304	XAT	C7-C8-C9-C19
21	3	306	A1L1G	C28-C39-C40-C41
21	7	302	A1L1G	C32-C33-C34-C27
24	8	304	A1L1F	C28-C39-C40-C41
29	b	849	BCR	C7-C8-C9-C34
29	l	205	BCR	C7-C8-C9-C34
29	l	205	BCR	C37-C22-C23-C24
20	2	301	XAT	C27-C28-C29-C30
21	3	306	A1L1G	C38-C39-C40-C41
29	b	849	BCR	C7-C8-C9-C10
29	l	205	BCR	C7-C8-C9-C10
29	l	205	BCR	C21-C22-C23-C24
22	a	814	CLA	O1D-CGD-O2D-CED
24	1	304	A1L1F	C49-C50-C51-C52
26	b	848	DGD	C1A-C2A-C3A-C4A
22	3	311	CLA	O1A-CGA-O2A-C1
22	b	820	CLA	O1A-CGA-O2A-C1
22	h	203	CLA	O1A-CGA-O2A-C1
22	a	809	CLA	C5-C6-C7-C8
22	b	801	CLA	C15-C16-C17-C18
22	9	313	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	4	316	CLA	CBA-CGA-O2A-C1
22	2	312	CLA	CBA-CGA-O2A-C1
22	b	838	CLA	CBA-CGA-O2A-C1
22	2	310	CLA	C15-C16-C17-C18
22	a	834	CLA	C15-C16-C17-C18
22	b	832	CLA	C13-C15-C16-C17
22	b	833	CLA	C13-C15-C16-C17
22	5	309	CLA	O1D-CGD-O2D-CED
22	b	826	CLA	O1A-CGA-O2A-C1
22	8	310	CLA	CBD-CGD-O2D-CED
21	3	302	A1L1G	C35-C36-C37-C38
22	5	309	CLA	C13-C15-C16-C17
22	9	308	CLA	C5-C6-C7-C8
22	9	318	CLA	C10-C11-C12-C13
22	4	308	CLA	C10-C11-C12-C13
22	1	306	CLA	C8-C10-C11-C12
22	a	802	CLA	C5-C6-C7-C8
22	a	809	CLA	C8-C10-C11-C12
22	a	814	CLA	C13-C15-C16-C17
22	a	830	CLA	C13-C15-C16-C17
22	a	831	CLA	C5-C6-C7-C8
22	b	809	CLA	C8-C10-C11-C12
22	b	840	CLA	C13-C15-C16-C17
22	l	203	CLA	C10-C11-C12-C13
22	5	308	CLA	O1A-CGA-O2A-C1
25	a	846	LHG	C7-C8-C9-C10
25	b	847	LHG	C7-C8-C9-C10
27	a	853	LMG	C10-C11-C12-C13
22	f	802	CLA	CBD-CGD-O2D-CED
22	1	306	CLA	C5-C6-C7-C8
22	b	813	CLA	C15-C16-C17-C18
22	b	829	CLA	C8-C10-C11-C12
22	b	823	CLA	C3-C5-C6-C7
22	3	308	CLA	O1D-CGD-O2D-CED
22	b	819	CLA	O1D-CGD-O2D-CED
22	a	807	CLA	C15-C16-C17-C18
22	a	841	CLA	C5-C6-C7-C8
22	b	814	CLA	C5-C6-C7-C8
22	b	836	CLA	C5-C6-C7-C8
24	1	304	A1L1F	C45-C47-C48-C49
22	b	802	CLA	CBD-CGD-O2D-CED
22	7	309	CLA	O2A-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	7	308	CLA	C4-C3-C5-C6
22	a	837	CLA	O1D-CGD-O2D-CED
22	1	310	CLA	C11-C10-C8-C7
22	a	801	CLA	C12-C13-C15-C16
22	a	809	CLA	C12-C13-C15-C16
22	a	828	CLA	C12-C13-C15-C16
22	a	831	CLA	C11-C10-C8-C7
22	a	844	CLA	C12-C13-C15-C16
22	b	808	CLA	C12-C13-C15-C16
22	a	801	CLA	C3-C5-C6-C7
22	a	839	CLA	O1A-CGA-O2A-C1
22	b	833	CLA	O1A-CGA-O2A-C1
22	b	827	CLA	CBA-CGA-O2A-C1
22	a	830	CLA	C2A-CAA-CBA-CGA
22	5	306	CLA	O1D-CGD-O2D-CED
22	7	308	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	C8-C10-C11-C12
22	1	306	CLA	C15-C16-C17-C18
22	5	305	CLA	CBA-CGA-O2A-C1
22	a	826	CLA	CBD-CGD-O2D-CED
22	a	841	CLA	C15-C16-C17-C18
22	b	840	CLA	C10-C11-C12-C13
22	a	818	CLA	O1D-CGD-O2D-CED
21	5	303	A1L1G	C39-C40-C41-C42
21	9	306	A1L1G	C39-C40-C41-C42
21	3	302	A1L1G	C39-C40-C41-C42
21	7	302	A1L1G	C31-C32-C33-C34
22	a	801	CLA	C8-C10-C11-C12
22	a	828	CLA	C13-C15-C16-C17
22	a	828	CLA	C15-C16-C17-C18
22	a	831	CLA	C15-C16-C17-C18
22	f	802	CLA	C13-C15-C16-C17
22	h	205	CLA	C5-C6-C7-C8
22	4	307	CLA	O1D-CGD-O2D-CED
22	2	312	CLA	O1A-CGA-O2A-C1
22	7	316	CLA	O1A-CGA-O2A-C1
22	7	308	CLA	C10-C11-C12-C13
22	b	836	CLA	C8-C10-C11-C12
28	b	841	PQN	C23-C25-C26-C27
22	3	315	CLA	O1D-CGD-O2D-CED
22	a	839	CLA	C13-C15-C16-C17
22	b	801	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	802	CLA	C8-C10-C11-C12
22	b	827	CLA	C13-C15-C16-C17
22	f	802	CLA	C5-C6-C7-C8
22	l	203	CLA	C8-C10-C11-C12
25	a	845	LHG	C3-O3-P-O6
25	b	847	LHG	C3-O3-P-O6
22	7	313	CLA	C3-C5-C6-C7
26	b	848	DGD	C4E-C5E-C6E-O5E
22	4	317	CLA	CBA-CGA-O2A-C1
22	a	816	CLA	CBA-CGA-O2A-C1
22	b	802	CLA	CBA-CGA-O2A-C1
22	b	831	CLA	CBA-CGA-O2A-C1
22	b	801	CLA	C8-C10-C11-C12
22	9	316	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	C4-C3-C5-C6
22	8	313	CLA	O1A-CGA-O2A-C1
22	7	316	CLA	C2C-C3C-CAC-CBC
22	5	306	CLA	C2A-CAA-CBA-CGA
22	1	314	CLA	C2A-CAA-CBA-CGA
22	b	828	CLA	C2A-CAA-CBA-CGA
22	9	316	CLA	C16-C17-C18-C20
22	a	801	CLA	C16-C17-C18-C20
22	b	833	CLA	C16-C17-C18-C19
22	4	313	CLA	C3-C5-C6-C7
22	a	814	CLA	CBA-CGA-O2A-C1
22	a	838	CLA	CBA-CGA-O2A-C1
21	9	306	A1L1G	C40-C41-C42-C44
22	3	309	CLA	O1D-CGD-O2D-CED
23	1	315	SQD	C8-C7-O47-C45
22	9	310	CLA	CBA-CGA-O2A-C1
22	a	824	CLA	CBA-CGA-O2A-C1
22	b	824	CLA	C5-C6-C7-C8
22	b	829	CLA	C10-C11-C12-C13
22	b	839	CLA	C5-C6-C7-C8
21	9	301	A1L1G	C41-C42-C44-C43
21	9	306	A1L1G	C41-C42-C44-C43
21	3	302	A1L1G	C37-C38-C39-C28
21	3	306	A1L1G	C27-C34-C35-C36
25	9	307	LHG	C31-C32-C33-C34
25	9	307	LHG	C34-C35-C36-C37
25	a	845	LHG	C11-C10-C9-C8
26	4	318	DGD	C3B-C4B-C5B-C6B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	b	848	DGD	C9B-CAB-CBB-CCB
22	a	841	CLA	O1D-CGD-O2D-CED
22	b	823	CLA	O1D-CGD-O2D-CED
22	b	840	CLA	C16-C17-C18-C20
22	a	833	CLA	CBA-CGA-O2A-C1
22	a	844	CLA	CBA-CGA-O2A-C1
23	1	315	SQD	C24-C23-O48-C46
23	1	315	SQD	O49-C7-O47-C45
22	a	854	CLA	C5-C6-C7-C8
22	a	836	CLA	CBD-CGD-O2D-CED
25	9	307	LHG	C27-C28-C29-C30
25	9	307	LHG	C28-C29-C30-C31
25	a	845	LHG	C27-C28-C29-C30
22	a	835	CLA	O1D-CGD-O2D-CED
22	b	838	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C13-C14-C15-C16
22	7	317	CLA	O1D-CGD-O2D-CED
22	a	834	CLA	O1D-CGD-O2D-CED
22	b	827	CLA	O1D-CGD-O2D-CED
21	5	303	A1L1G	C29-C30-C31-C32
21	9	301	A1L1G	C29-C30-C31-C32
21	9	306	A1L1G	C29-C30-C31-C32
24	9	302	A1L1F	C45-C47-C48-C49
21	9	301	A1L1G	C41-C42-C44-C2
21	9	306	A1L1G	C41-C42-C44-C2
21	3	302	A1L1G	C37-C38-C39-C40
21	3	306	A1L1G	C33-C34-C35-C36
25	9	317	LHG	C9-C10-C11-C12
22	4	317	CLA	O1A-CGA-O2A-C1
22	a	816	CLA	O1A-CGA-O2A-C1
22	b	802	CLA	O1A-CGA-O2A-C1
22	4	310	CLA	C4-C3-C5-C6
22	b	839	CLA	C4-C3-C5-C6
22	1	308	CLA	C2-C3-C5-C6
22	b	807	CLA	C2-C3-C5-C6
22	b	828	CLA	C2-C3-C5-C6
21	9	306	A1L1G	C14-C29-C30-C31
21	3	302	A1L1G	C14-C29-C30-C31
22	a	828	CLA	C14-C13-C15-C16
22	a	839	CLA	C6-C7-C8-C9
22	a	840	CLA	C14-C13-C15-C16
22	b	825	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
27	2	317	LMG	C28-C29-C30-C31
25	9	317	LHG	C11-C12-C13-C14
26	4	318	DGD	C2B-C3B-C4B-C5B
26	b	848	DGD	C4A-C5A-C6A-C7A
22	a	814	CLA	C10-C11-C12-C13
22	a	814	CLA	C2A-CAA-CBA-CGA
22	b	831	CLA	C2A-CAA-CBA-CGA
22	a	814	CLA	O1A-CGA-O2A-C1
22	b	827	CLA	O1A-CGA-O2A-C1
20	9	303	XAT	C7-C8-C9-C19
20	2	303	XAT	C7-C8-C9-C19
21	9	301	A1L1G	C32-C33-C34-C27
21	3	302	A1L1G	C32-C33-C34-C27
29	a	850	BCR	C37-C22-C23-C24
29	f	801	BCR	C37-C22-C23-C24
22	5	315	CLA	C2C-C3C-CAC-CBC
26	b	848	DGD	C3B-C4B-C5B-C6B
20	9	303	XAT	C7-C8-C9-C10
20	8	301	XAT	C7-C8-C9-C10
20	2	303	XAT	C7-C8-C9-C10
20	7	304	XAT	C7-C8-C9-C10
21	9	301	A1L1G	C32-C33-C34-C35
21	3	302	A1L1G	C32-C33-C34-C35
24	8	304	A1L1F	C38-C39-C40-C41
29	a	850	BCR	C21-C22-C23-C24
29	f	801	BCR	C21-C22-C23-C24
22	b	840	CLA	O1D-CGD-O2D-CED
22	b	827	CLA	C8-C10-C11-C12
28	a	843	PQN	C25-C26-C27-C28
25	9	317	LHG	C28-C29-C30-C31
24	8	304	A1L1F	C45-C47-C48-C49
22	9	316	CLA	C16-C17-C18-C19
22	4	308	CLA	C16-C17-C18-C20
22	b	811	CLA	C6-C7-C8-C9
22	f	802	CLA	C16-C17-C18-C19
22	f	802	CLA	C16-C17-C18-C20
22	a	827	CLA	C8-C10-C11-C12
22	a	841	CLA	C8-C10-C11-C12
22	b	806	CLA	C15-C16-C17-C18
22	b	835	CLA	C5-C6-C7-C8
22	h	203	CLA	C10-C11-C12-C13
23	1	315	SQD	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	1	304	A1L1F	C47-C48-C49-C50
25	9	317	LHG	C14-C15-C16-C17
22	a	814	CLA	C5-C6-C7-C8
22	b	809	CLA	C10-C11-C12-C13
24	9	302	A1L1F	C48-C49-C50-C51
24	h	204	A1L1F	C47-C48-C49-C50
22	9	310	CLA	C3A-C2A-CAA-CBA
22	9	313	CLA	C3A-C2A-CAA-CBA
22	4	310	CLA	C3A-C2A-CAA-CBA
22	3	312	CLA	C3A-C2A-CAA-CBA
22	3	314	CLA	C3A-C2A-CAA-CBA
22	2	306	CLA	C3A-C2A-CAA-CBA
22	7	311	CLA	C3A-C2A-CAA-CBA
22	a	807	CLA	C3A-C2A-CAA-CBA
22	a	838	CLA	C3A-C2A-CAA-CBA
22	a	854	CLA	C3A-C2A-CAA-CBA
22	b	810	CLA	C3A-C2A-CAA-CBA
22	b	812	CLA	C3A-C2A-CAA-CBA
22	b	814	CLA	C3A-C2A-CAA-CBA
22	f	803	CLA	C3A-C2A-CAA-CBA
22	h	203	CLA	C3A-C2A-CAA-CBA
22	4	308	CLA	O1D-CGD-O2D-CED
22	a	807	CLA	O1D-CGD-O2D-CED
22	a	810	CLA	O1D-CGD-O2D-CED
22	b	831	CLA	O1A-CGA-O2A-C1
22	b	801	CLA	C16-C17-C18-C20
22	b	811	CLA	C6-C7-C8-C10
26	b	848	DGD	C4B-C5B-C6B-C7B
22	3	314	CLA	CBD-CGD-O2D-CED
26	b	848	DGD	C2B-C3B-C4B-C5B
21	9	301	A1L1G	C35-C36-C37-C38
21	3	306	A1L1G	C35-C36-C37-C38
29	m	101	BCR	C14-C15-C16-C17
22	b	816	CLA	CBA-CGA-O2A-C1
22	4	310	CLA	C2-C3-C5-C6
22	a	828	CLA	C2-C3-C5-C6
22	b	839	CLA	C2-C3-C5-C6
22	j	102	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	O1-C1-C2-O2
25	a	846	LHG	O1-C1-C2-O2
25	b	847	LHG	O1-C1-C2-O2
22	b	833	CLA	C16-C17-C18-C20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	808	CLA	C5-C6-C7-C8
22	9	308	CLA	CBA-CGA-O2A-C1
22	a	833	CLA	O1A-CGA-O2A-C1
22	a	838	CLA	O1A-CGA-O2A-C1
22	a	844	CLA	O1A-CGA-O2A-C1
23	1	315	SQD	O10-C23-O48-C46
22	a	818	CLA	C2-C1-O2A-CGA
22	9	313	CLA	O1A-CGA-O2A-C1
22	4	316	CLA	O1A-CGA-O2A-C1
22	b	808	CLA	C3-C5-C6-C7
29	a	850	BCR	C23-C24-C25-C30
29	b	843	BCR	C1-C6-C7-C8
29	b	843	BCR	C5-C6-C7-C8
29	l	201	BCR	C1-C6-C7-C8
29	l	205	BCR	C23-C24-C25-C26
29	l	205	BCR	C23-C24-C25-C30
29	m	101	BCR	C5-C6-C7-C8
25	9	307	LHG	C30-C31-C32-C33
22	a	823	CLA	CBA-CGA-O2A-C1
22	b	807	CLA	CBA-CGA-O2A-C1
22	b	835	CLA	CBA-CGA-O2A-C1
22	a	809	CLA	C13-C15-C16-C17
22	b	829	CLA	C15-C16-C17-C18
22	b	838	CLA	C15-C16-C17-C18
22	j	102	CLA	C8-C10-C11-C12
25	a	845	LHG	C26-C27-C28-C29
22	2	314	CLA	C11-C10-C8-C9
22	a	840	CLA	C13-C15-C16-C17
22	b	805	CLA	C13-C15-C16-C17
22	1	310	CLA	C4-C3-C5-C6
22	a	807	CLA	C4-C3-C5-C6
22	a	828	CLA	C4-C3-C5-C6
22	9	316	CLA	C2-C3-C5-C6
22	3	312	CLA	C6-C7-C8-C10
22	1	305	CLA	C11-C10-C8-C7
22	1	308	CLA	C11-C10-C8-C7
22	a	801	CLA	C11-C12-C13-C15
22	a	826	CLA	C11-C10-C8-C7
22	a	829	CLA	C11-C10-C8-C7
22	a	839	CLA	C6-C7-C8-C10
22	a	840	CLA	C12-C13-C15-C16
22	b	802	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	807	CLA	C11-C12-C13-C15
22	b	810	CLA	C11-C10-C8-C7
22	b	837	CLA	C11-C12-C13-C15
22	9	308	CLA	O1A-CGA-O2A-C1
22	b	804	CLA	C2C-C3C-CAC-CBC
22	b	810	CLA	C5-C6-C7-C8
27	2	317	LMG	C10-C11-C12-C13
22	a	825	CLA	CBA-CGA-O2A-C1
22	b	824	CLA	CBA-CGA-O2A-C1
22	4	308	CLA	C15-C16-C17-C18
22	a	806	CLA	C13-C15-C16-C17
22	b	832	CLA	C15-C16-C17-C18
26	b	848	DGD	CAB-CBB-CCB-CDB
22	a	811	CLA	C11-C10-C8-C7
23	1	315	SQD	C7-C8-C9-C10
26	b	848	DGD	C6A-C7A-C8A-C9A
22	4	307	CLA	C3-C5-C6-C7
26	8	315	DGD	C2B-C3B-C4B-C5B
22	b	816	CLA	O1A-CGA-O2A-C1
26	4	318	DGD	O6D-C1D-O3G-C3G
22	8	307	CLA	C15-C16-C17-C18
22	5	311	CLA	O1D-CGD-O2D-CED
25	a	846	LHG	C8-C7-O7-C5
26	b	848	DGD	C2B-C1B-O2G-C2G
25	b	847	LHG	O6-C4-C5-O7
21	9	306	A1L1G	C31-C32-C33-C34
22	9	313	CLA	CBD-CGD-O2D-CED
22	a	808	CLA	CBD-CGD-O2D-CED
25	a	846	LHG	O9-C7-O7-C5
22	2	308	CLA	C3-C5-C6-C7
26	4	318	DGD	O1G-C1G-C2G-O2G
22	b	840	CLA	C16-C17-C18-C19
22	b	809	CLA	C15-C16-C17-C18
22	9	316	CLA	C4-C3-C5-C6
22	b	807	CLA	C4-C3-C5-C6
22	b	834	CLA	C4-C3-C5-C6
22	8	310	CLA	CBA-CGA-O2A-C1
22	3	315	CLA	CBA-CGA-O2A-C1
22	7	308	CLA	C2-C3-C5-C6
22	a	804	CLA	C2-C3-C5-C6
22	b	803	CLA	C2-C3-C5-C6
22	4	308	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	3	312	CLA	C6-C7-C8-C9
22	2	310	CLA	C14-C13-C15-C16
22	1	308	CLA	C11-C10-C8-C9
22	1	310	CLA	C11-C10-C8-C9
22	a	807	CLA	C14-C13-C15-C16
22	a	814	CLA	C11-C10-C8-C9
22	a	826	CLA	C11-C10-C8-C9
22	a	831	CLA	C11-C10-C8-C9
22	b	802	CLA	C11-C12-C13-C14
22	b	807	CLA	C11-C12-C13-C14
22	b	807	CLA	C14-C13-C15-C16
22	b	810	CLA	C11-C10-C8-C9
22	b	818	CLA	C6-C7-C8-C9
22	b	822	CLA	C6-C7-C8-C9
22	b	824	CLA	C11-C10-C8-C9
22	b	825	CLA	C6-C7-C8-C9
22	b	837	CLA	C11-C12-C13-C14
22	8	308	CLA	C2A-CAA-CBA-CGA
22	a	806	CLA	C2A-CAA-CBA-CGA
22	a	810	CLA	C2A-CAA-CBA-CGA
22	b	832	CLA	C2A-CAA-CBA-CGA
20	5	301	XAT	C7-C8-C9-C19
20	7	304	XAT	C7-C8-C9-C19
21	9	306	A1L1G	C32-C33-C34-C27
22	4	308	CLA	C13-C15-C16-C17
22	a	823	CLA	O1A-CGA-O2A-C1
22	b	807	CLA	O1A-CGA-O2A-C1
22	b	835	CLA	O1A-CGA-O2A-C1
22	5	306	CLA	C1A-C2A-CAA-CBA
22	9	310	CLA	C1A-C2A-CAA-CBA
22	9	313	CLA	C1A-C2A-CAA-CBA
22	4	313	CLA	C1A-C2A-CAA-CBA
22	3	314	CLA	C1A-C2A-CAA-CBA
22	2	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	311	CLA	C1A-C2A-CAA-CBA
22	7	313	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	a	807	CLA	C1A-C2A-CAA-CBA
22	a	817	CLA	C1A-C2A-CAA-CBA
22	a	819	CLA	C1A-C2A-CAA-CBA
22	a	825	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	816	CLA	C1A-C2A-CAA-CBA
22	b	817	CLA	C1A-C2A-CAA-CBA
22	b	837	CLA	C1A-C2A-CAA-CBA
22	f	803	CLA	C1A-C2A-CAA-CBA
22	a	801	CLA	C16-C17-C18-C19
22	b	801	CLA	C16-C17-C18-C19
22	7	316	CLA	C4C-C3C-CAC-CBC
24	9	302	A1L1F	C49-C50-C51-C52
24	h	204	A1L1F	C40-C41-C42-C44
22	b	807	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	C8-C10-C11-C12
22	a	844	CLA	C10-C11-C12-C13
22	b	810	CLA	C10-C11-C12-C13
25	9	317	LHG	C3-O3-P-O6
22	7	313	CLA	C5-C6-C7-C8
25	9	317	LHG	C29-C30-C31-C32
22	b	822	CLA	O1D-CGD-O2D-CED
26	b	848	DGD	CBB-CCB-CDB-CEB
22	b	829	CLA	C13-C15-C16-C17
25	a	845	LHG	O6-C4-C5-C6
22	5	315	CLA	C4C-C3C-CAC-CBC
22	4	315	CLA	O1D-CGD-O2D-CED
22	a	812	CLA	C10-C11-C12-C13
22	b	824	CLA	O1A-CGA-O2A-C1
22	a	806	CLA	C16-C17-C18-C19
25	9	317	LHG	C12-C13-C14-C15
22	b	813	CLA	C3-C5-C6-C7
22	b	835	CLA	C2C-C3C-CAC-CBC
22	h	203	CLA	O1D-CGD-O2D-CED
22	a	822	CLA	C2A-CAA-CBA-CGA
22	a	820	CLA	C16-C17-C18-C20
22	b	814	CLA	C6-C7-C8-C10
22	a	839	CLA	C3-C5-C6-C7
22	b	801	CLA	C3-C5-C6-C7
25	a	845	LHG	C4-C5-C6-O8
25	b	847	LHG	C4-C5-C6-O8
26	4	318	DGD	O1G-C1G-C2G-C3G
22	a	829	CLA	C10-C11-C12-C13
24	1	304	A1L1F	C50-C51-C52-C53
27	j	105	LMG	C13-C14-C15-C16
24	h	204	A1L1F	C4-C8-O7-C54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	8	310	CLA	O1D-CGD-O2D-CED
22	a	820	CLA	C8-C10-C11-C12
26	b	848	DGD	C3A-C4A-C5A-C6A
22	5	310	CLA	CAA-CBA-CGA-O2A
25	9	317	LHG	C11-C10-C9-C8
25	b	847	LHG	C8-C7-O7-C5
22	a	854	CLA	C10-C11-C12-C13
28	a	843	PQN	C23-C25-C26-C27
22	a	804	CLA	C4-C3-C5-C6
22	a	820	CLA	C4-C3-C5-C6
22	b	803	CLA	C4-C3-C5-C6
22	b	813	CLA	C4-C3-C5-C6
22	a	844	CLA	C16-C17-C18-C19
22	8	307	CLA	CBA-CGA-O2A-C1
24	h	204	A1L1F	C48-C49-C50-C51
22	1	311	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	C13-C15-C16-C17
22	b	839	CLA	C13-C15-C16-C17
27	a	853	LMG	C14-C15-C16-C17
22	8	314	CLA	CBD-CGD-O2D-CED
22	9	314	CLA	C3-C5-C6-C7
22	b	802	CLA	O1D-CGD-O2D-CED
22	f	802	CLA	O1D-CGD-O2D-CED
22	a	829	CLA	C8-C10-C11-C12
26	b	848	DGD	CCB-CDB-CEB-CFB
22	a	835	CLA	CBA-CGA-O2A-C1
22	a	825	CLA	O1A-CGA-O2A-C1
22	3	315	CLA	CAA-CBA-CGA-O2A
22	b	818	CLA	C11-C12-C13-C14
25	a	845	LHG	C7-C8-C9-C10
22	1	310	CLA	C5-C6-C7-C8
22	b	836	CLA	C2C-C3C-CAC-CBC
22	1	308	CLA	C15-C16-C17-C18
22	a	810	CLA	C5-C6-C7-C8
22	a	826	CLA	C15-C16-C17-C18
26	4	318	DGD	C2D-C1D-O3G-C3G
22	b	804	CLA	C15-C16-C17-C18
22	b	814	CLA	C6-C7-C8-C9
22	a	801	CLA	C4-C3-C5-C6
22	b	838	CLA	C4-C3-C5-C6
22	9	316	CLA	C11-C12-C13-C15
22	4	308	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	1	306	CLA	C6-C7-C8-C10
22	a	807	CLA	C12-C13-C15-C16
22	a	809	CLA	C6-C7-C8-C10
22	a	810	CLA	C12-C13-C15-C16
22	a	812	CLA	C6-C7-C8-C10
22	a	820	CLA	C2-C3-C5-C6
22	a	822	CLA	C6-C7-C8-C10
22	a	830	CLA	C12-C13-C15-C16
22	a	841	CLA	C11-C10-C8-C7
22	a	844	CLA	C11-C12-C13-C15
22	b	803	CLA	C12-C13-C15-C16
22	b	807	CLA	C11-C10-C8-C7
22	b	807	CLA	C12-C13-C15-C16
22	b	813	CLA	C2-C3-C5-C6
22	b	818	CLA	C6-C7-C8-C10
22	b	822	CLA	C6-C7-C8-C10
22	b	824	CLA	C11-C10-C8-C7
22	b	825	CLA	C6-C7-C8-C10
22	b	827	CLA	C6-C7-C8-C10
22	b	828	CLA	C12-C13-C15-C16
22	b	833	CLA	C11-C12-C13-C15
22	b	838	CLA	C6-C7-C8-C10
22	f	802	CLA	C11-C12-C13-C15
22	4	317	CLA	C3-C5-C6-C7
22	b	833	CLA	C3-C5-C6-C7
22	9	316	CLA	C11-C12-C13-C14
22	7	308	CLA	C11-C10-C8-C9
22	a	801	CLA	C11-C12-C13-C14
22	a	807	CLA	C11-C12-C13-C14
22	a	809	CLA	C14-C13-C15-C16
22	a	810	CLA	C14-C13-C15-C16
22	a	822	CLA	C6-C7-C8-C9
22	a	827	CLA	C11-C10-C8-C9
22	a	830	CLA	C14-C13-C15-C16
22	a	835	CLA	C6-C7-C8-C9
22	a	841	CLA	C11-C10-C8-C9
22	a	842	CLA	C11-C12-C13-C14
22	a	844	CLA	C11-C10-C8-C9
22	a	844	CLA	C11-C12-C13-C14
22	a	844	CLA	C14-C13-C15-C16
22	b	801	CLA	C11-C12-C13-C14
22	b	803	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	803	CLA	C11-C10-C8-C9
22	b	808	CLA	C11-C10-C8-C9
22	b	828	CLA	C11-C12-C13-C14
22	b	836	CLA	C14-C13-C15-C16
22	j	102	CLA	C6-C7-C8-C9
24	h	204	A1L1F	C3-C8-O7-C54
25	9	307	LHG	C25-C26-C27-C28
22	4	307	CLA	CBA-CGA-O2A-C1
22	a	841	CLA	CBA-CGA-O2A-C1
22	a	812	CLA	C8-C10-C11-C12
22	a	819	CLA	C2A-CAA-CBA-CGA
20	7	303	XAT	C7-C8-C9-C19
21	3	306	A1L1G	C32-C33-C34-C27
24	h	204	A1L1F	C28-C39-C40-C41
22	a	844	CLA	C16-C17-C18-C20
20	4	305	XAT	C27-C28-C29-C30
25	b	847	LHG	C9-C10-C11-C12
22	a	826	CLA	O1D-CGD-O2D-CED
22	b	827	CLA	C15-C16-C17-C18
22	9	310	CLA	O1A-CGA-O2A-C1
22	a	824	CLA	O1A-CGA-O2A-C1
22	8	307	CLA	O1A-CGA-O2A-C1
26	b	848	DGD	C2A-C1A-O1G-C1G
22	b	805	CLA	C16-C17-C18-C20
25	b	847	LHG	O6-C4-C5-C6
22	h	205	CLA	C3-C5-C6-C7
22	a	844	CLA	C15-C16-C17-C18
22	a	836	CLA	O1D-CGD-O2D-CED
22	b	802	CLA	C4-C3-C5-C6
22	a	801	CLA	C2-C3-C5-C6
22	a	807	CLA	C2-C3-C5-C6
22	b	807	CLA	C10-C11-C12-C13
22	j	102	CLA	C5-C6-C7-C8
26	b	848	DGD	O1B-C1B-O2G-C2G
22	a	811	CLA	C11-C10-C8-C9
22	b	832	CLA	C3-C5-C6-C7
22	a	805	CLA	C6-C7-C8-C9
22	3	314	CLA	CBA-CGA-O2A-C1
22	1	306	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	b	828	CLA	CBA-CGA-O2A-C1
25	9	317	LHG	C2-C3-O3-P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	4	311	CLA	C3A-C2A-CAA-CBA
22	3	315	CLA	C3A-C2A-CAA-CBA
22	2	314	CLA	C3A-C2A-CAA-CBA
22	a	829	CLA	C3A-C2A-CAA-CBA
22	j	102	CLA	C3A-C2A-CAA-CBA
22	b	812	CLA	C5-C6-C7-C8
22	b	801	CLA	C5-C6-C7-C8
25	a	845	LHG	C34-C35-C36-C37
22	a	805	CLA	C6-C7-C8-C10
22	a	831	CLA	CBA-CGA-O2A-C1
22	b	811	CLA	CBA-CGA-O2A-C1
22	a	830	CLA	C5-C6-C7-C8
23	1	315	SQD	O6-C44-C45-C46
25	a	846	LHG	C4-C5-C6-O8
27	2	317	LMG	O1-C7-C8-C9
22	a	806	CLA	CBD-CGD-O2D-CED
22	b	835	CLA	C3-C5-C6-C7
25	9	307	LHG	C33-C34-C35-C36
26	b	848	DGD	C7A-C8A-C9A-CAA
22	a	840	CLA	C4-C3-C5-C6
22	b	818	CLA	C11-C12-C13-C15
22	3	314	CLA	O1D-CGD-O2D-CED
22	a	827	CLA	C3-C5-C6-C7
22	7	314	CLA	C2A-CAA-CBA-CGA
22	a	809	CLA	C2A-CAA-CBA-CGA
22	4	317	CLA	C5-C6-C7-C8
22	a	803	CLA	C15-C16-C17-C18
27	j	105	LMG	C28-C29-C30-C31
22	9	314	CLA	CBA-CGA-O2A-C1
22	a	835	CLA	O1A-CGA-O2A-C1
22	a	806	CLA	C16-C17-C18-C20
22	a	820	CLA	C16-C17-C18-C19
22	4	307	CLA	O1A-CGA-O2A-C1
22	b	806	CLA	C10-C11-C12-C13
22	4	308	CLA	C16-C17-C18-C19
22	b	827	CLA	C16-C17-C18-C20
22	b	822	CLA	C10-C11-C12-C13
21	9	301	A1L1G	O13-C26-C30-C31
25	b	847	LHG	O9-C7-O7-C5
22	7	308	CLA	C2-C1-O2A-CGA
24	1	304	A1L1F	C14-C29-C30-C31
22	b	803	CLA	C13-C15-C16-C17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	9	308	CLA	C11-C10-C8-C9
22	4	310	CLA	C11-C10-C8-C9
22	1	306	CLA	C11-C10-C8-C9
22	1	310	CLA	C6-C7-C8-C9
22	a	814	CLA	C11-C12-C13-C14
22	a	840	CLA	C11-C10-C8-C9
22	b	802	CLA	C6-C7-C8-C9
22	b	802	CLA	C11-C10-C8-C9
22	b	804	CLA	C6-C7-C8-C9
22	b	806	CLA	C6-C7-C8-C9
22	b	810	CLA	C6-C7-C8-C9
22	b	824	CLA	C11-C12-C13-C14
22	b	832	CLA	C14-C13-C15-C16
22	b	837	CLA	C14-C13-C15-C16
22	b	838	CLA	C11-C12-C13-C14
22	5	309	CLA	C5-C6-C7-C8
22	1	310	CLA	C16-C17-C18-C20
29	b	846	BCR	C5-C6-C7-C8
29	b	849	BCR	C23-C24-C25-C26
29	b	849	BCR	C23-C24-C25-C30
29	f	804	BCR	C23-C24-C25-C26
29	l	201	BCR	C5-C6-C7-C8
29	l	205	BCR	C1-C6-C7-C8
29	l	205	BCR	C5-C6-C7-C8
22	a	854	CLA	C8-C10-C11-C12
22	b	810	CLA	CAA-CBA-CGA-O2A
20	4	305	XAT	C27-C28-C29-C39
20	7	303	XAT	C7-C8-C9-C10
21	9	306	A1L1G	C26-C30-C31-C32
21	7	302	A1L1G	C32-C33-C34-C35
22	2	315	CLA	C1A-C2A-CAA-CBA
22	j	103	CLA	C1A-C2A-CAA-CBA
22	4	310	CLA	C15-C16-C17-C18
22	9	313	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	C16-C17-C18-C20
22	1	306	CLA	C16-C17-C18-C20
22	b	807	CLA	C5-C6-C7-C8
22	b	828	CLA	C5-C6-C7-C8
27	a	853	LMG	C12-C13-C14-C15
25	9	317	LHG	O6-C4-C5-C6
25	a	846	LHG	O6-C4-C5-C6
25	9	307	LHG	C32-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	9	308	CLA	C11-C12-C13-C15
22	9	318	CLA	C11-C10-C8-C7
22	8	307	CLA	C11-C10-C8-C7
22	8	309	CLA	C11-C10-C8-C7
22	4	310	CLA	C11-C10-C8-C7
22	1	308	CLA	C11-C12-C13-C15
22	a	801	CLA	C6-C7-C8-C10
22	a	802	CLA	C6-C7-C8-C10
22	a	807	CLA	C11-C12-C13-C15
22	a	814	CLA	C6-C7-C8-C10
22	a	814	CLA	C11-C12-C13-C15
22	a	820	CLA	C11-C12-C13-C15
22	a	827	CLA	C11-C10-C8-C7
22	a	829	CLA	C6-C7-C8-C10
22	a	835	CLA	C6-C7-C8-C10
22	a	840	CLA	C2-C3-C5-C6
22	a	842	CLA	C11-C12-C13-C15
22	a	844	CLA	C11-C10-C8-C7
22	b	801	CLA	C11-C12-C13-C15
22	b	803	CLA	C6-C7-C8-C10
22	b	803	CLA	C11-C10-C8-C7
22	b	808	CLA	C11-C10-C8-C7
22	b	810	CLA	C6-C7-C8-C10
22	b	813	CLA	C11-C10-C8-C7
22	b	824	CLA	C6-C7-C8-C10
22	b	829	CLA	C12-C13-C15-C16
22	b	836	CLA	C12-C13-C15-C16
22	b	837	CLA	C12-C13-C15-C16
22	b	838	CLA	C12-C13-C15-C16
22	j	102	CLA	C6-C7-C8-C10
23	1	315	SQD	C9-C10-C11-C12
21	9	306	A1L1G	C30-C31-C32-C33
21	3	306	A1L1G	C40-C41-C42-C44
21	7	302	A1L1G	C34-C35-C36-C37
22	b	805	CLA	C16-C17-C18-C19
22	a	827	CLA	C5-C6-C7-C8
22	a	842	CLA	C8-C10-C11-C12
22	a	841	CLA	O1A-CGA-O2A-C1
27	2	317	LMG	C31-C32-C33-C34
22	4	313	CLA	CBA-CGA-O2A-C1
22	a	808	CLA	O1D-CGD-O2D-CED
21	7	302	A1L1G	C45-C2-C44-C43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	5	314	CLA	CAD-CBD-CGD-O2D
22	9	309	CLA	CAD-CBD-CGD-O2D
22	8	313	CLA	CAD-CBD-CGD-O2D
22	3	310	CLA	CAD-CBD-CGD-O2D
22	7	306	CLA	CAD-CBD-CGD-O2D
22	a	808	CLA	CAD-CBD-CGD-O2D
22	a	810	CLA	CAD-CBD-CGD-O2D
22	a	815	CLA	CAD-CBD-CGD-O2D
22	a	821	CLA	CAD-CBD-CGD-O2D
22	a	824	CLA	CAD-CBD-CGD-O2D
22	a	832	CLA	CAD-CBD-CGD-O2D
22	a	842	CLA	CAD-CBD-CGD-O2D
22	a	854	CLA	CAD-CBD-CGD-O2D
22	b	802	CLA	CAD-CBD-CGD-O2D
22	b	806	CLA	CAD-CBD-CGD-O2D
22	b	811	CLA	CAD-CBD-CGD-O2D
22	b	825	CLA	CAD-CBD-CGD-O2D
22	b	830	CLA	CAD-CBD-CGD-O2D
22	b	833	CLA	CAD-CBD-CGD-O2D
22	b	838	CLA	CAD-CBD-CGD-O2D
22	b	839	CLA	CAD-CBD-CGD-O2D
24	8	304	A1L1F	C57-C2-C44-C43
27	a	853	LMG	C9-C8-O7-C10
22	a	841	CLA	C13-C15-C16-C17
22	b	838	CLA	C13-C15-C16-C17
22	9	308	CLA	C16-C17-C18-C19
27	2	317	LMG	C33-C34-C35-C36
26	8	315	DGD	C1G-C2G-C3G-O3G
22	7	313	CLA	CBD-CGD-O2D-CED
22	b	811	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C9-C10-C11-C12
22	2	307	CLA	C2A-CAA-CBA-CGA
22	2	314	CLA	C2A-CAA-CBA-CGA
22	2	310	CLA	C16-C17-C18-C19
22	b	810	CLA	C16-C17-C18-C19
22	8	308	CLA	CHA-CBD-CGD-O1D
22	8	308	CLA	CHA-CBD-CGD-O2D
22	8	309	CLA	CHA-CBD-CGD-O1D
22	8	309	CLA	CHA-CBD-CGD-O2D
22	8	314	CLA	CHA-CBD-CGD-O1D
22	8	314	CLA	CHA-CBD-CGD-O2D
22	4	307	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	3	308	CLA	CHA-CBD-CGD-O1D
22	3	308	CLA	CHA-CBD-CGD-O2D
22	2	313	CLA	CHA-CBD-CGD-O1D
22	7	308	CLA	CHA-CBD-CGD-O1D
22	7	308	CLA	CHA-CBD-CGD-O2D
22	7	315	CLA	CHA-CBD-CGD-O2D
22	7	316	CLA	CHA-CBD-CGD-O1D
22	7	316	CLA	CHA-CBD-CGD-O2D
22	a	809	CLA	CHA-CBD-CGD-O1D
22	a	809	CLA	CHA-CBD-CGD-O2D
22	a	814	CLA	CHA-CBD-CGD-O1D
22	a	814	CLA	CHA-CBD-CGD-O2D
22	a	823	CLA	CHA-CBD-CGD-O1D
22	a	828	CLA	CHA-CBD-CGD-O1D
22	a	831	CLA	CHA-CBD-CGD-O1D
22	a	831	CLA	CHA-CBD-CGD-O2D
22	a	837	CLA	CHA-CBD-CGD-O1D
22	a	839	CLA	CHA-CBD-CGD-O1D
22	a	839	CLA	CHA-CBD-CGD-O2D
22	b	804	CLA	CHA-CBD-CGD-O1D
22	b	804	CLA	CHA-CBD-CGD-O2D
22	b	809	CLA	CHA-CBD-CGD-O1D
22	b	809	CLA	CHA-CBD-CGD-O2D
22	b	814	CLA	CHA-CBD-CGD-O1D
22	b	829	CLA	CHA-CBD-CGD-O1D
22	b	829	CLA	CHA-CBD-CGD-O2D
22	b	834	CLA	CHA-CBD-CGD-O1D
22	b	834	CLA	CHA-CBD-CGD-O2D
22	b	835	CLA	CHA-CBD-CGD-O1D
22	3	314	CLA	O1A-CGA-O2A-C1
26	b	848	DGD	O1A-C1A-O1G-C1G
22	7	312	CLA	O2A-C1-C2-C3
26	8	315	DGD	O2G-C2G-C3G-O3G
22	9	318	CLA	CBA-CGA-O2A-C1
22	a	831	CLA	O1A-CGA-O2A-C1
22	b	828	CLA	O1A-CGA-O2A-C1
22	j	102	CLA	O1D-CGD-O2D-CED
22	b	817	CLA	C10-C11-C12-C13
22	9	314	CLA	O1A-CGA-O2A-C1
22	4	313	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	1	310	CLA	C2-C3-C5-C6
27	a	853	LMG	C31-C32-C33-C34
22	1	308	CLA	C11-C12-C13-C14
22	a	807	CLA	C11-C10-C8-C9
22	a	829	CLA	C6-C7-C8-C9
22	b	802	CLA	C2A-CAA-CBA-CGA
22	b	808	CLA	C2A-CAA-CBA-CGA
20	5	301	XAT	C7-C8-C9-C10
24	h	204	A1L1F	C38-C39-C40-C41
22	1	306	CLA	C3-C5-C6-C7
22	3	311	CLA	C1A-C2A-CAA-CBA
22	2	314	CLA	C1A-C2A-CAA-CBA
22	a	824	CLA	C1A-C2A-CAA-CBA
22	b	813	CLA	C1A-C2A-CAA-CBA
22	b	823	CLA	C1A-C2A-CAA-CBA
20	2	304	XAT	C33-C34-C35-C15
22	8	314	CLA	O1D-CGD-O2D-CED
22	a	806	CLA	O1D-CGD-O2D-CED
25	9	317	LHG	C4-O6-P-O3
22	1	308	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	C5-C6-C7-C8
22	2	314	CLA	C4-C3-C5-C6
22	8	311	CLA	C3-C5-C6-C7
25	9	307	LHG	C2-C3-O3-P
22	b	834	CLA	C2-C3-C5-C6
25	9	317	LHG	C3-O3-P-O5
25	9	317	LHG	C4-O6-P-O5
25	a	845	LHG	C3-O3-P-O5
25	a	846	LHG	C4-O6-P-O5
22	2	310	CLA	C16-C17-C18-C20
22	1	310	CLA	C16-C17-C18-C19
22	a	830	CLA	C8-C10-C11-C12
23	1	315	SQD	C13-C14-C15-C16
22	3	311	CLA	C2A-CAA-CBA-CGA
22	b	808	CLA	C16-C17-C18-C20
24	8	304	A1L1F	C47-C48-C49-C50
25	a	846	LHG	C10-C11-C12-C13
22	5	311	CLA	C2-C3-C5-C6
22	9	313	CLA	CAD-CBD-CGD-O1D
22	9	315	CLA	CAD-CBD-CGD-O1D
22	8	309	CLA	CAD-CBD-CGD-O1D
22	8	314	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	4	315	CLA	CAD-CBD-CGD-O1D
22	1	313	CLA	CAD-CBD-CGD-O1D
22	a	806	CLA	CAD-CBD-CGD-O1D
22	a	814	CLA	CAD-CBD-CGD-O1D
22	a	828	CLA	CAD-CBD-CGD-O1D
22	a	839	CLA	CAD-CBD-CGD-O1D
22	a	844	CLA	CAD-CBD-CGD-O1D
22	b	832	CLA	CAD-CBD-CGD-O1D
22	b	835	CLA	CAD-CBD-CGD-O1D
22	b	836	CLA	CAD-CBD-CGD-O1D
22	f	802	CLA	CAD-CBD-CGD-O1D
22	4	312	CLA	CBA-CGA-O2A-C1
22	9	308	CLA	C10-C11-C12-C13
22	b	840	CLA	C15-C16-C17-C18
22	5	307	CLA	C11-C10-C8-C7
22	9	316	CLA	C3A-C2A-CAA-CBA
22	8	307	CLA	C6-C7-C8-C10
22	2	310	CLA	C11-C12-C13-C15
22	a	842	CLA	C12-C13-C15-C16
22	b	801	CLA	C11-C10-C8-C7
22	b	801	CLA	C12-C13-C15-C16
22	b	806	CLA	C11-C12-C13-C15
22	b	827	CLA	C11-C10-C8-C7
22	b	829	CLA	C11-C12-C13-C15
22	b	832	CLA	C12-C13-C15-C16
25	9	317	LHG	O6-C4-C5-O7
28	a	843	PQN	C22-C23-C25-C26
22	b	818	CLA	C8-C10-C11-C12
22	a	834	CLA	C5-C6-C7-C8
22	b	824	CLA	C8-C10-C11-C12
22	8	309	CLA	C2A-CAA-CBA-CGA
22	1	308	CLA	C16-C17-C18-C19
23	5	316	SQD	C44-C45-C46-O48
23	5	316	SQD	O47-C45-C46-O48
23	1	315	SQD	O6-C44-C45-O47
25	a	846	LHG	O7-C5-C6-O8
25	b	847	LHG	O7-C5-C6-O8
22	3	315	CLA	O1A-CGA-O2A-C1
22	b	814	CLA	C3-C5-C6-C7
22	9	318	CLA	O1A-CGA-O2A-C1
22	1	311	CLA	CBA-CGA-O2A-C1
22	b	805	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	8	310	CLA	O1A-CGA-O2A-C1
25	9	317	LHG	C10-C11-C12-C13
22	5	309	CLA	C6-C7-C8-C9
22	9	308	CLA	C11-C12-C13-C14
22	8	309	CLA	C11-C10-C8-C9
22	4	308	CLA	C14-C13-C15-C16
22	2	311	CLA	C11-C10-C8-C9
22	a	801	CLA	C6-C7-C8-C9
22	a	802	CLA	C6-C7-C8-C9
22	a	807	CLA	C6-C7-C8-C9
22	a	809	CLA	C6-C7-C8-C9
22	a	814	CLA	C6-C7-C8-C9
22	a	820	CLA	C11-C12-C13-C14
22	a	842	CLA	C14-C13-C15-C16
22	b	804	CLA	C11-C12-C13-C14
22	b	813	CLA	C11-C10-C8-C9
22	b	838	CLA	C14-C13-C15-C16
22	a	854	CLA	CBD-CGD-O2D-CED
22	b	839	CLA	C2C-C3C-CAC-CBC
22	2	308	CLA	C6-C7-C8-C9
22	3	308	CLA	CAA-CBA-CGA-O2A
22	a	809	CLA	C10-C11-C12-C13
21	9	306	A1L1G	C32-C33-C34-C35
22	7	308	CLA	C8-C10-C11-C12
22	b	827	CLA	C10-C11-C12-C13
21	1	301	A1L1G	C37-C38-C39-C28
25	9	317	LHG	C13-C14-C15-C16
22	8	307	CLA	C16-C17-C18-C20
22	a	823	CLA	C1-C2-C3-C4
22	b	831	CLA	C1-C2-C3-C4
22	b	803	CLA	C3-C5-C6-C7
22	a	801	CLA	CAA-CBA-CGA-O2A
23	1	315	SQD	C46-C45-O47-C7
22	1	311	CLA	O1D-CGD-O2D-CED
22	4	317	CLA	C2A-CAA-CBA-CGA
22	1	305	CLA	C2A-CAA-CBA-CGA
22	1	308	CLA	C2A-CAA-CBA-CGA
22	a	813	CLA	C2A-CAA-CBA-CGA
22	a	821	CLA	C2A-CAA-CBA-CGA
22	b	824	CLA	C2A-CAA-CBA-CGA
22	b	827	CLA	C2A-CAA-CBA-CGA
22	5	311	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	7	306	CLA	C2-C1-O2A-CGA
22	a	816	CLA	C2-C1-O2A-CGA
22	a	822	CLA	C2-C1-O2A-CGA
22	b	810	CLA	C2-C1-O2A-CGA
23	5	316	SQD	C7-C8-C9-C10
22	b	832	CLA	C2C-C3C-CAC-CBC
22	b	805	CLA	O1A-CGA-O2A-C1
22	b	822	CLA	C3-C5-C6-C7
22	1	311	CLA	O1A-CGA-O2A-C1
25	b	847	LHG	C25-C26-C27-C28
22	h	205	CLA	C4-C3-C5-C6
22	1	308	CLA	O1D-CGD-O2D-CED
29	b	846	BCR	C1-C6-C7-C8
29	f	804	BCR	C23-C24-C25-C30
22	b	838	CLA	C2-C3-C5-C6
22	b	817	CLA	O1A-CGA-O2A-C1
22	b	817	CLA	CBA-CGA-O2A-C1
22	a	830	CLA	C16-C17-C18-C19
22	b	808	CLA	C16-C17-C18-C19
22	a	839	CLA	C15-C16-C17-C18
25	9	307	LHG	C4-O6-P-O3
25	a	846	LHG	C3-O3-P-O6
25	a	846	LHG	C4-O6-P-O3
22	b	803	CLA	C16-C17-C18-C20
22	a	841	CLA	C4-C3-C5-C6
22	4	308	CLA	C11-C12-C13-C15
22	2	311	CLA	C11-C10-C8-C7
22	b	825	CLA	C11-C10-C8-C7
22	f	802	CLA	C6-C7-C8-C10
22	b	801	CLA	O1A-CGA-O2A-C1
22	a	801	CLA	C14-C13-C15-C16
22	a	812	CLA	C6-C7-C8-C9
22	b	803	CLA	C14-C13-C15-C16
22	b	827	CLA	C11-C10-C8-C9
22	b	828	CLA	C14-C13-C15-C16
28	a	843	PQN	C24-C23-C25-C26
22	5	307	CLA	C8-C10-C11-C12
22	a	830	CLA	C15-C16-C17-C18
22	h	203	CLA	C13-C15-C16-C17
20	4	301	XAT	C29-C30-C31-C32
21	3	302	A1L1G	C36-C37-C38-C39
29	m	101	BCR	C13-C14-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	a	854	CLA	C15-C16-C17-C18
20	7	303	XAT	C11-C12-C13-C20
22	b	801	CLA	CBA-CGA-O2A-C1
22	5	315	CLA	CAA-CBA-CGA-O2A
21	3	306	A1L1G	C32-C33-C34-C35
22	2	314	CLA	C11-C10-C8-C7
25	a	846	LHG	C1-C2-C3-O3
22	a	813	CLA	O1A-CGA-O2A-C1
22	8	312	CLA	CBD-CGD-O2D-CED
22	b	827	CLA	C16-C17-C18-C19
22	a	813	CLA	CBA-CGA-O2A-C1
22	a	832	CLA	CBD-CGD-O2D-CED
22	a	854	CLA	O1D-CGD-O2D-CED
22	8	305	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	CBD-CGD-O2D-CED
22	3	312	CLA	CBA-CGA-O2A-C1
22	9	314	CLA	C2A-CAA-CBA-CGA
22	5	310	CLA	CAA-CBA-CGA-O1A
20	7	301	XAT	C29-C30-C31-C32
20	j	101	XAT	C9-C10-C11-C12
21	3	302	A1L1G	C40-C41-C42-C44
22	a	820	CLA	C13-C15-C16-C17
22	b	839	CLA	C16-C17-C18-C20
22	7	313	CLA	O1D-CGD-O2D-CED
22	a	812	CLA	C3-C5-C6-C7
25	a	845	LHG	C25-C26-C27-C28
22	2	314	CLA	C2-C3-C5-C6
22	b	802	CLA	C2-C3-C5-C6
22	b	813	CLA	C10-C11-C12-C13
22	a	810	CLA	C2-C1-O2A-CGA
22	a	814	CLA	C2-C1-O2A-CGA
22	5	309	CLA	C2A-CAA-CBA-CGA
22	9	316	CLA	C2A-CAA-CBA-CGA
22	8	307	CLA	C2A-CAA-CBA-CGA
22	2	309	CLA	C2A-CAA-CBA-CGA
22	7	306	CLA	C2A-CAA-CBA-CGA
22	a	803	CLA	C2A-CAA-CBA-CGA
22	b	809	CLA	C2A-CAA-CBA-CGA
26	b	848	DGD	O2G-C2G-C3G-O3G
22	2	310	CLA	C3A-C2A-CAA-CBA
22	b	813	CLA	C3A-C2A-CAA-CBA
22	b	831	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
27	2	317	LMG	O9-C10-O7-C8
21	3	306	A1L1G	C30-C31-C32-C33
22	a	832	CLA	O1D-CGD-O2D-CED
24	9	302	A1L1F	C3-C8-O7-C54
22	a	802	CLA	C4-C3-C5-C6
22	5	307	CLA	C11-C10-C8-C9
22	1	310	CLA	C11-C12-C13-C14
22	a	822	CLA	C11-C10-C8-C9
22	a	829	CLA	C11-C12-C13-C14
22	a	831	CLA	C6-C7-C8-C9
22	a	844	CLA	C6-C7-C8-C9
22	a	854	CLA	C11-C10-C8-C9
22	b	808	CLA	C6-C7-C8-C9
22	a	830	CLA	C16-C17-C18-C20
22	a	839	CLA	C16-C17-C18-C20
22	5	306	CLA	CAA-CBA-CGA-O1A
29	b	844	BCR	C11-C10-C9-C34
29	b	844	BCR	C20-C21-C22-C37
29	f	804	BCR	C35-C13-C14-C15
29	l	201	BCR	C11-C10-C9-C34
22	8	312	CLA	O1D-CGD-O2D-CED
22	3	315	CLA	CAA-CBA-CGA-O1A
22	8	305	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C14-C15-C16-C17
22	8	307	CLA	C16-C17-C18-C19
22	1	308	CLA	C16-C17-C18-C20
22	a	801	CLA	CBA-CGA-O2A-C1
22	b	840	CLA	CBA-CGA-O2A-C1
26	8	315	DGD	O6D-C1D-O3G-C3G
20	7	301	XAT	C7-C8-C9-C19
22	b	817	CLA	CBD-CGD-O2D-CED
22	4	311	CLA	C1A-C2A-CAA-CBA
22	4	316	CLA	C1A-C2A-CAA-CBA
22	2	310	CLA	C1A-C2A-CAA-CBA
22	2	316	CLA	C1A-C2A-CAA-CBA
22	b	815	CLA	C1A-C2A-CAA-CBA
22	b	822	CLA	C1A-C2A-CAA-CBA
22	b	834	CLA	C1A-C2A-CAA-CBA
25	9	317	LHG	C15-C16-C17-C18
22	a	807	CLA	C11-C10-C8-C7
22	a	814	CLA	C11-C10-C8-C7
22	b	802	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	3	312	CLA	O1A-CGA-O2A-C1
22	a	801	CLA	O1A-CGA-O2A-C1
22	b	840	CLA	O1A-CGA-O2A-C1
22	4	314	CLA	CAA-CBA-CGA-O2A
22	a	817	CLA	CAA-CBA-CGA-O1A
22	h	203	CLA	C8-C10-C11-C12
27	a	853	LMG	C11-C12-C13-C14
22	1	305	CLA	C3-C5-C6-C7
22	4	306	CLA	C2A-CAA-CBA-CGA
22	a	817	CLA	CAA-CBA-CGA-O2A
22	4	310	CLA	O1D-CGD-O2D-CED
22	b	839	CLA	C4C-C3C-CAC-CBC
22	4	314	CLA	CAA-CBA-CGA-O1A
22	4	310	CLA	C13-C15-C16-C17
22	a	841	CLA	C2-C3-C5-C6
22	1	307	CLA	C6-C7-C8-C9
29	b	844	BCR	C11-C10-C9-C8
29	b	844	BCR	C20-C21-C22-C23
29	f	804	BCR	C12-C13-C14-C15
29	l	201	BCR	C11-C10-C9-C8
21	9	301	A1L1G	C34-C35-C36-C37
21	7	302	A1L1G	C36-C37-C38-C39
21	1	301	A1L1G	C40-C41-C42-C44
27	2	317	LMG	C11-C10-O7-C8
22	5	313	CLA	CAA-CBA-CGA-O1A
22	a	830	CLA	C4-C3-C5-C6
22	a	839	CLA	C2-C1-O2A-CGA
22	b	817	CLA	O1D-CGD-O2D-CED
22	a	802	CLA	C2-C3-C5-C6
22	b	808	CLA	C14-C13-C15-C16
22	5	310	CLA	CBA-CGA-O2A-C1
22	5	306	CLA	CAA-CBA-CGA-O2A
23	1	315	SQD	C15-C16-C17-C18
22	5	311	CLA	C4-C3-C5-C6
22	a	819	CLA	CAA-CBA-CGA-O2A
22	5	307	CLA	C2A-CAA-CBA-CGA
22	a	839	CLA	C2A-CAA-CBA-CGA
26	b	848	DGD	C1B-C2B-C3B-C4B
22	a	842	CLA	O1A-CGA-O2A-C1
29	h	202	BCR	C23-C24-C25-C30
29	j	104	BCR	C1-C6-C7-C8
29	m	101	BCR	C23-C24-C25-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	9	312	CLA	CAA-CBA-CGA-O2A
25	9	317	LHG	O1-C1-C2-C3
22	a	804	CLA	O1A-CGA-O2A-C1
24	h	204	A1L1F	C36-C37-C38-C39
20	2	304	XAT	C7-C8-C9-C10
20	a	852	XAT	C31-C32-C33-C34
22	a	830	CLA	O1A-CGA-O2A-C1
22	b	835	CLA	C4C-C3C-CAC-CBC
22	b	802	CLA	C10-C11-C12-C13
22	a	813	CLA	C6-C7-C8-C9
22	5	313	CLA	CAA-CBA-CGA-O2A
22	7	307	CLA	CAA-CBA-CGA-O2A
22	5	307	CLA	C11-C12-C13-C14
22	b	813	CLA	C16-C17-C18-C19
22	7	307	CLA	CAA-CBA-CGA-O1A
22	1	314	CLA	CAA-CBA-CGA-O2A
22	9	308	CLA	C2A-CAA-CBA-CGA
22	a	830	CLA	CBA-CGA-O2A-C1
22	a	842	CLA	CBA-CGA-O2A-C1
22	a	826	CLA	C13-C15-C16-C17
22	8	311	CLA	C6-C7-C8-C10
22	b	802	CLA	C11-C10-C8-C7
22	7	317	CLA	CAA-CBA-CGA-O2A
20	8	302	XAT	C9-C10-C11-C12
26	8	315	DGD	C2D-C1D-O3G-C3G
22	b	813	CLA	C5-C6-C7-C8
22	2	314	CLA	O1A-CGA-O2A-C1
22	4	308	CLA	C3-C5-C6-C7
22	1	314	CLA	CAA-CBA-CGA-O1A
22	4	309	CLA	CAA-CBA-CGA-O2A
22	1	306	CLA	C16-C17-C18-C19
22	a	804	CLA	CBA-CGA-O2A-C1
25	9	317	LHG	C35-C36-C37-C38
27	j	105	LMG	C11-C12-C13-C14
22	5	314	CLA	C4-C3-C5-C6
22	b	808	CLA	C4-C3-C5-C6
22	9	316	CLA	C8-C10-C11-C12
22	a	830	CLA	C2-C3-C5-C6
24	h	204	A1L1F	C14-C29-C30-C31
22	8	307	CLA	C6-C7-C8-C9
22	4	308	CLA	C6-C7-C8-C9
22	a	801	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	806	CLA	C11-C12-C13-C14
22	b	829	CLA	C11-C12-C13-C14
22	9	311	CLA	C3A-C2A-CAA-CBA
22	4	306	CLA	C3A-C2A-CAA-CBA
22	2	316	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	b	809	CLA	C3A-C2A-CAA-CBA
22	b	837	CLA	CAA-CBA-CGA-O2A
22	5	306	CLA	CAD-CBD-CGD-O2D
22	5	311	CLA	CAD-CBD-CGD-O2D
22	9	312	CLA	CAD-CBD-CGD-O2D
22	8	310	CLA	CAD-CBD-CGD-O2D
22	8	311	CLA	CAD-CBD-CGD-O2D
22	4	311	CLA	CAD-CBD-CGD-O2D
22	3	314	CLA	CAD-CBD-CGD-O2D
22	2	316	CLA	CAD-CBD-CGD-O2D
22	7	307	CLA	CAD-CBD-CGD-O2D
22	7	311	CLA	CAD-CBD-CGD-O2D
22	1	307	CLA	CAD-CBD-CGD-O2D
22	1	309	CLA	CAD-CBD-CGD-O2D
22	a	827	CLA	CAD-CBD-CGD-O2D
22	a	829	CLA	CAD-CBD-CGD-O2D
22	b	812	CLA	CAD-CBD-CGD-O2D
22	b	813	CLA	CAD-CBD-CGD-O2D
22	b	816	CLA	CAD-CBD-CGD-O2D
22	b	837	CLA	CAD-CBD-CGD-O2D
22	l	204	CLA	CAD-CBD-CGD-O2D
22	a	804	CLA	C6-C7-C8-C9
22	b	818	CLA	C2A-CAA-CBA-CGA
22	b	803	CLA	C10-C11-C12-C13
22	b	813	CLA	C13-C15-C16-C17
22	a	835	CLA	C4-C3-C5-C6
22	b	833	CLA	C4-C3-C5-C6
22	7	317	CLA	CAA-CBA-CGA-O1A
22	b	808	CLA	C2-C3-C5-C6
22	a	818	CLA	CAA-CBA-CGA-O2A
22	b	801	CLA	CAA-CBA-CGA-O2A
22	l	204	CLA	CAA-CBA-CGA-O2A
29	f	801	BCR	C17-C18-C19-C20
20	5	301	XAT	O4-C6-C7-C8
20	5	304	XAT	O24-C26-C27-C28
20	9	303	XAT	O24-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	8	301	XAT	O24-C26-C27-C28
20	4	301	XAT	O4-C6-C7-C8
20	4	305	XAT	O4-C6-C7-C8
20	3	303	XAT	O4-C6-C7-C8
20	2	301	XAT	O4-C6-C7-C8
20	2	305	XAT	O24-C26-C27-C28
20	7	305	XAT	O4-C6-C7-C8
20	7	305	XAT	O24-C26-C27-C28
21	3	302	A1L1G	C29-C14-C25-O15
23	1	315	SQD	O47-C7-C8-C9
28	a	843	PQN	C18-C20-C21-C22
22	4	309	CLA	O2A-C1-C2-C3
22	3	310	CLA	O2A-C1-C2-C3
22	2	314	CLA	O2A-C1-C2-C3
22	1	305	CLA	O2A-C1-C2-C3
22	a	826	CLA	O2A-C1-C2-C3
22	b	817	CLA	O2A-C1-C2-C3
22	b	832	CLA	O2A-C1-C2-C3
22	4	308	CLA	C2A-CAA-CBA-CGA
22	2	308	CLA	C2A-CAA-CBA-CGA
22	b	833	CLA	C15-C16-C17-C18
22	a	836	CLA	CAA-CBA-CGA-O2A
22	4	306	CLA	CAA-CBA-CGA-O2A
20	7	304	XAT	C9-C10-C11-C12
22	4	310	CLA	CHA-CBD-CGD-O1D
22	4	314	CLA	CHA-CBD-CGD-O2D
22	2	307	CLA	CHA-CBD-CGD-O1D
22	2	307	CLA	CHA-CBD-CGD-O2D
22	2	310	CLA	CHA-CBD-CGD-O1D
22	2	310	CLA	CHA-CBD-CGD-O2D
22	2	313	CLA	CHA-CBD-CGD-O2D
22	a	802	CLA	CHA-CBD-CGD-O1D
22	a	802	CLA	CHA-CBD-CGD-O2D
22	a	804	CLA	CHA-CBD-CGD-O1D
22	a	804	CLA	CHA-CBD-CGD-O2D
22	a	816	CLA	CHA-CBD-CGD-O1D
22	a	817	CLA	CHA-CBD-CGD-O1D
22	a	817	CLA	CHA-CBD-CGD-O2D
22	a	820	CLA	CHA-CBD-CGD-O1D
22	a	820	CLA	CHA-CBD-CGD-O2D
22	a	823	CLA	CHA-CBD-CGD-O2D
22	a	828	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	a	830	CLA	CHA-CBD-CGD-O1D
22	a	830	CLA	CHA-CBD-CGD-O2D
22	a	837	CLA	CHA-CBD-CGD-O2D
22	b	801	CLA	CHA-CBD-CGD-O1D
22	b	801	CLA	CHA-CBD-CGD-O2D
22	b	805	CLA	CHA-CBD-CGD-O1D
22	b	805	CLA	CHA-CBD-CGD-O2D
22	b	814	CLA	CHA-CBD-CGD-O2D
22	b	815	CLA	CHA-CBD-CGD-O1D
22	b	815	CLA	CHA-CBD-CGD-O2D
22	b	824	CLA	CHA-CBD-CGD-O1D
22	b	824	CLA	CHA-CBD-CGD-O2D
22	b	835	CLA	CHA-CBD-CGD-O2D
22	j	102	CLA	CHA-CBD-CGD-O2D
22	9	313	CLA	CAA-CBA-CGA-O2A
22	b	807	CLA	CAA-CBA-CGA-O2A
22	2	314	CLA	CBA-CGA-O2A-C1
22	a	835	CLA	C2-C3-C5-C6
24	9	302	A1L1F	C50-C51-C52-C53
22	a	827	CLA	C10-C11-C12-C13
22	4	312	CLA	O1A-CGA-O2A-C1
22	a	810	CLA	CAA-CBA-CGA-O2A
22	h	205	CLA	CAA-CBA-CGA-O2A
25	9	307	LHG	O7-C5-C6-O8
22	b	803	CLA	CAA-CBA-CGA-O2A
22	a	829	CLA	CAA-CBA-CGA-O2A
22	9	308	CLA	C11-C10-C8-C7
22	1	310	CLA	C12-C13-C15-C16
22	a	801	CLA	C11-C10-C8-C7
22	a	835	CLA	C11-C12-C13-C15
22	b	810	CLA	C2-C3-C5-C6
21	3	306	A1L1G	C14-C29-C30-C31
22	1	306	CLA	CAA-CBA-CGA-O2A
22	1	309	CLA	CAA-CBA-CGA-O2A
22	b	809	CLA	CAA-CBA-CGA-O2A
22	b	817	CLA	CAA-CBA-CGA-O2A
22	a	834	CLA	C11-C12-C13-C14
22	f	802	CLA	C6-C7-C8-C9
22	b	824	CLA	C10-C11-C12-C13
22	1	312	CLA	CAA-CBA-CGA-O2A
22	b	832	CLA	CAA-CBA-CGA-O2A
25	a	845	LHG	O8-C23-C24-C25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	837	CLA	CAA-CBA-CGA-O1A
23	5	316	SQD	C4-C5-C6-S
24	9	302	A1L1F	O13-C26-C30-C29
22	b	807	CLA	C16-C17-C18-C19
22	a	829	CLA	C2A-CAA-CBA-CGA
22	a	841	CLA	C2A-CAA-CBA-CGA
22	4	309	CLA	CAA-CBA-CGA-O1A
22	j	102	CLA	CAA-CBA-CGA-O2A
22	b	810	CLA	CAA-CBA-CGA-O1A
22	j	102	CLA	C10-C11-C12-C13
22	4	306	CLA	CAA-CBA-CGA-O1A
22	a	818	CLA	CAA-CBA-CGA-O1A
22	b	801	CLA	CAA-CBA-CGA-O1A
22	b	817	CLA	CAA-CBA-CGA-O1A
23	1	315	SQD	O49-C7-C8-C9
20	7	301	XAT	C7-C8-C9-C10
29	i	101	BCR	C17-C18-C19-C20
22	9	311	CLA	C1A-C2A-CAA-CBA
22	9	312	CLA	C1A-C2A-CAA-CBA
22	1	310	CLA	C1A-C2A-CAA-CBA
22	a	803	CLA	C1A-C2A-CAA-CBA
22	a	804	CLA	C1A-C2A-CAA-CBA
22	a	814	CLA	C1A-C2A-CAA-CBA
22	a	815	CLA	C1A-C2A-CAA-CBA
22	b	825	CLA	C1A-C2A-CAA-CBA
22	b	831	CLA	C1A-C2A-CAA-CBA
22	b	819	CLA	C6-C7-C8-C9
22	a	827	CLA	C2-C1-O2A-CGA
22	a	829	CLA	C2-C1-O2A-CGA
22	b	807	CLA	C2-C1-O2A-CGA
22	b	834	CLA	C2-C1-O2A-CGA
27	j	105	LMG	C7-C8-C9-O8
24	8	304	A1L1F	C3-C8-O7-C54
22	b	804	CLA	C4C-C3C-CAC-CBC
25	9	317	LHG	C27-C28-C29-C30
22	b	803	CLA	C5-C6-C7-C8
22	b	813	CLA	CBD-CGD-O2D-CED
25	9	317	LHG	C30-C31-C32-C33
22	h	205	CLA	C2-C3-C5-C6
22	a	826	CLA	C10-C11-C12-C13
25	a	846	LHG	C3-O3-P-O5
22	b	807	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	809	CLA	CAA-CBA-CGA-O1A
22	b	832	CLA	CAA-CBA-CGA-O1A
22	h	205	CLA	CAA-CBA-CGA-O1A
22	3	312	CLA	CAA-CBA-CGA-O2A
29	b	849	BCR	C1-C6-C7-C8
29	h	202	BCR	C23-C24-C25-C26
29	j	104	BCR	C5-C6-C7-C8
29	m	101	BCR	C23-C24-C25-C26
22	1	312	CLA	CAA-CBA-CGA-O1A
22	a	836	CLA	CAA-CBA-CGA-O1A
22	b	804	CLA	CAA-CBA-CGA-O2A
22	a	814	CLA	C16-C17-C18-C19
22	b	810	CLA	C16-C17-C18-C20
22	7	309	CLA	CBA-CGA-O2A-C1
22	9	315	CLA	C2C-C3C-CAC-CBC
22	a	834	CLA	C10-C11-C12-C13
22	4	310	CLA	CAD-CBD-CGD-O1D
22	4	316	CLA	CAD-CBD-CGD-O1D
22	3	307	CLA	CAD-CBD-CGD-O1D
22	2	309	CLA	CAD-CBD-CGD-O1D
22	7	316	CLA	C2-C3-C5-C6
22	a	816	CLA	CAD-CBD-CGD-O1D
22	b	814	CLA	CAD-CBD-CGD-O1D
22	b	818	CLA	CAD-CBD-CGD-O1D
23	5	316	SQD	O5-C5-C6-S
25	9	307	LHG	C6-C5-O7-C7
22	7	309	CLA	O1A-CGA-O2A-C1
24	9	302	A1L1F	O46-C45-O13-C26
22	7	308	CLA	CAA-CBA-CGA-O2A
22	a	813	CLA	CAA-CBA-CGA-O2A
22	b	805	CLA	C11-C12-C13-C14
22	b	806	CLA	C11-C10-C8-C9
22	j	102	CLA	C11-C10-C8-C9
22	a	820	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	C8-C10-C11-C12
24	9	302	A1L1F	C47-C45-O13-C26
22	a	810	CLA	C16-C17-C18-C20
22	9	314	CLA	CAA-CBA-CGA-O2A
22	a	813	CLA	CBD-CGD-O2D-CED
23	5	316	SQD	C10-C11-C12-C13
22	5	309	CLA	C15-C16-C17-C18
22	a	801	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	3	309	CLA	C2A-CAA-CBA-CGA
22	7	308	CLA	C2A-CAA-CBA-CGA
22	5	309	CLA	CAA-CBA-CGA-O2A
22	7	309	CLA	CAA-CBA-CGA-O2A
22	7	316	CLA	CAA-CBA-CGA-O2A
22	a	826	CLA	CAA-CBA-CGA-O2A
22	j	102	CLA	C3-C5-C6-C7
22	a	810	CLA	CAA-CBA-CGA-O1A
22	8	308	CLA	C4-C3-C5-C6
22	3	313	CLA	C4-C3-C5-C6
22	b	810	CLA	C4-C3-C5-C6
22	b	824	CLA	C15-C16-C17-C18
22	9	312	CLA	C3A-C2A-CAA-CBA
22	7	309	CLA	CHA-CBD-CGD-O1D
22	1	306	CLA	C3A-C2A-CAA-CBA
22	a	834	CLA	C11-C12-C13-C15
22	b	805	CLA	C11-C12-C13-C15
22	b	818	CLA	C11-C10-C8-C7
22	l	203	CLA	C6-C7-C8-C10
22	j	102	CLA	CAA-CBA-CGA-O1A
22	4	310	CLA	CAA-CBA-CGA-O2A
22	7	310	CLA	CAA-CBA-CGA-O2A
22	a	835	CLA	CAA-CBA-CGA-O2A
20	7	303	XAT	C11-C12-C13-C14
29	b	845	BCR	C7-C8-C9-C10
22	5	309	CLA	CAA-CBA-CGA-O1A
22	3	312	CLA	CAA-CBA-CGA-O1A
22	7	308	CLA	CAA-CBA-CGA-O1A
22	a	813	CLA	CAA-CBA-CGA-O1A
23	1	315	SQD	C12-C13-C14-C15
22	2	307	CLA	CAA-CBA-CGA-O2A
22	a	854	CLA	CAA-CBA-CGA-O2A
22	a	813	CLA	O1D-CGD-O2D-CED
22	7	316	CLA	CAA-CBA-CGA-O1A
22	a	835	CLA	CAA-CBA-CGA-O1A
25	a	845	LHG	O10-C23-C24-C25
22	7	314	CLA	CAA-CBA-CGA-O2A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	h	204	A1L1F	C1-C11-C3-C4-C6-C8

217 monomers are involved in 660 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	819	CLA	5	0
22	a	837	CLA	1	0
22	2	310	CLA	3	0
27	j	105	LMG	7	0
22	3	313	CLA	3	0
22	9	315	CLA	1	0
22	a	822	CLA	5	0
20	2	301	XAT	3	0
22	a	824	CLA	1	0
29	f	804	BCR	5	0
22	1	311	CLA	2	0
22	b	831	CLA	2	0
29	b	846	BCR	3	0
24	9	302	A1L1F	2	0
22	2	316	CLA	2	0
29	b	849	BCR	5	0
22	a	816	CLA	2	0
22	f	802	CLA	2	0
25	a	845	LHG	3	0
29	l	201	BCR	3	0
22	b	825	CLA	3	0
22	7	316	CLA	1	0
22	b	809	CLA	4	0
22	7	313	CLA	4	0
22	b	814	CLA	2	0
22	b	807	CLA	7	0
20	8	301	XAT	2	0
22	9	311	CLA	2	0
22	b	820	CLA	3	0
22	7	307	CLA	2	0
29	b	845	BCR	7	0
25	9	317	LHG	3	0
22	a	839	CLA	4	0
22	b	803	CLA	2	0
22	b	836	CLA	7	0
20	4	303	XAT	11	0
20	7	305	XAT	2	0
21	1	301	A1L1G	1	0
22	a	842	CLA	4	0
22	a	815	CLA	1	0
22	a	841	CLA	7	0
22	b	830	CLA	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	9	318	CLA	6	0
22	4	308	CLA	6	0
22	9	310	CLA	2	0
22	7	306	CLA	3	0
22	3	308	CLA	2	0
22	b	819	CLA	2	0
22	7	312	CLA	1	0
22	b	822	CLA	7	0
23	1	315	SQD	2	0
20	a	852	XAT	6	0
22	4	311	CLA	1	0
22	a	810	CLA	4	0
24	h	204	A1L1F	4	0
29	a	849	BCR	3	0
20	1	302	XAT	3	0
22	4	309	CLA	3	0
22	a	825	CLA	4	0
20	9	303	XAT	7	0
22	5	309	CLA	4	0
22	7	314	CLA	3	0
22	a	834	CLA	6	0
22	a	826	CLA	7	0
22	8	306	CLA	1	0
28	a	843	PQN	4	0
22	2	309	CLA	2	0
22	b	805	CLA	3	0
22	9	314	CLA	7	0
22	5	315	CLA	1	0
29	a	850	BCR	2	0
22	8	312	CLA	2	0
22	1	306	CLA	6	0
20	9	305	XAT	3	0
22	7	308	CLA	6	0
22	b	826	CLA	3	0
20	5	302	XAT	6	0
20	1	303	XAT	4	0
21	9	301	A1L1G	2	0
22	b	801	CLA	3	0
22	a	829	CLA	6	0
22	a	828	CLA	5	0
22	b	833	CLA	4	0
22	b	824	CLA	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	821	CLA	3	0
22	b	838	CLA	6	0
22	j	102	CLA	7	0
22	b	840	CLA	5	0
22	2	314	CLA	2	0
22	a	838	CLA	1	0
22	8	311	CLA	3	0
22	2	308	CLA	5	0
22	b	834	CLA	1	0
27	2	317	LMG	3	0
29	1	205	BCR	11	0
20	2	305	XAT	2	0
26	4	318	DGD	11	0
22	8	308	CLA	2	0
22	9	308	CLA	5	0
20	4	302	XAT	6	0
29	j	104	BCR	9	0
20	3	301	XAT	4	0
22	a	831	CLA	6	0
22	4	306	CLA	2	0
22	a	803	CLA	5	0
22	5	310	CLA	1	0
22	7	311	CLA	3	0
22	a	844	CLA	5	0
22	b	829	CLA	4	0
22	b	839	CLA	4	0
25	9	307	LHG	2	0
20	8	303	XAT	4	0
22	l	203	CLA	2	0
29	h	202	BCR	4	0
22	b	827	CLA	5	0
22	a	840	CLA	6	0
22	b	835	CLA	4	0
30	c	102	SF4	3	0
22	a	833	CLA	2	0
22	9	313	CLA	2	0
22	4	314	CLA	1	0
22	3	311	CLA	1	0
22	4	317	CLA	6	0
21	9	306	A1L1G	1	0
20	7	304	XAT	8	0
22	1	310	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	h	205	CLA	2	0
22	8	307	CLA	4	0
22	b	811	CLA	3	0
22	b	817	CLA	8	0
22	8	313	CLA	3	0
22	9	316	CLA	5	0
22	a	814	CLA	3	0
29	i	101	BCR	3	0
20	4	305	XAT	3	0
22	9	309	CLA	1	0
28	b	841	PQN	3	0
22	9	312	CLA	4	0
22	a	820	CLA	6	0
20	3	304	XAT	6	0
22	l	202	CLA	1	0
22	7	315	CLA	2	0
22	5	311	CLA	1	0
29	f	801	BCR	9	0
22	5	312	CLA	3	0
22	4	307	CLA	1	0
22	3	312	CLA	2	0
22	1	308	CLA	4	0
22	a	808	CLA	1	0
29	a	847	BCR	1	0
20	4	301	XAT	6	0
21	7	302	A1L1G	2	0
22	4	310	CLA	7	0
22	a	827	CLA	3	0
26	8	315	DGD	2	0
20	9	304	XAT	7	0
22	a	835	CLA	5	0
22	a	854	CLA	3	0
20	5	304	XAT	3	0
22	3	309	CLA	1	0
21	5	303	A1L1G	1	0
20	2	302	XAT	3	0
22	1	312	CLA	2	0
22	a	801	CLA	5	0
22	b	804	CLA	5	0
22	j	103	CLA	2	0
25	a	846	LHG	3	0
22	b	818	CLA	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	832	CLA	2	0
20	3	303	XAT	3	0
22	5	307	CLA	7	0
22	h	203	CLA	4	0
26	b	848	DGD	6	0
22	4	313	CLA	4	0
20	5	301	XAT	4	0
22	a	806	CLA	10	0
24	1	304	A1L1F	2	0
22	2	307	CLA	1	0
20	8	302	XAT	6	0
27	a	853	LMG	10	0
20	3	305	XAT	6	0
22	b	837	CLA	5	0
22	8	305	CLA	5	0
22	b	832	CLA	3	0
29	a	848	BCR	7	0
29	b	844	BCR	5	0
22	a	818	CLA	10	0
22	a	830	CLA	5	0
20	j	101	XAT	7	0
22	4	312	CLA	1	0
22	5	305	CLA	3	0
20	7	303	XAT	12	0
22	a	802	CLA	5	0
22	a	809	CLA	3	0
22	b	802	CLA	3	0
20	7	301	XAT	3	0
22	b	816	CLA	6	0
24	8	304	A1L1F	2	0
29	b	842	BCR	4	0
29	m	101	BCR	2	0
22	4	315	CLA	1	0
22	b	813	CLA	7	0
22	b	823	CLA	6	0
22	a	823	CLA	3	0
22	b	808	CLA	1	0
22	a	804	CLA	4	0
20	4	304	XAT	5	0
22	4	316	CLA	1	0
22	b	828	CLA	4	0
22	a	807	CLA	4	0

*Continued on next page...*

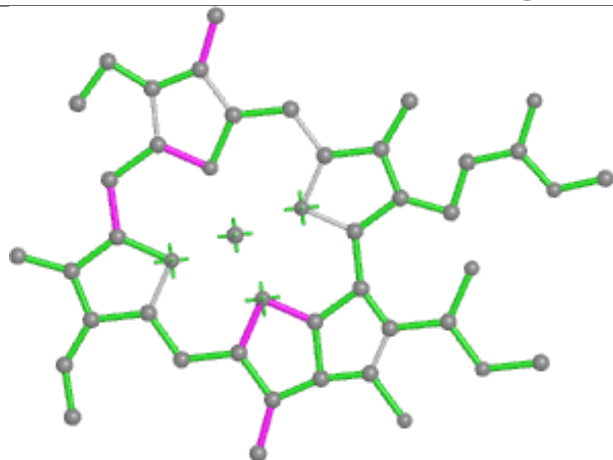
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	303	XAT	12	0
22	b	812	CLA	4	0
22	5	308	CLA	1	0
22	5	314	CLA	1	0
23	5	316	SQD	1	0
22	b	806	CLA	3	0
29	h	201	BCR	2	0

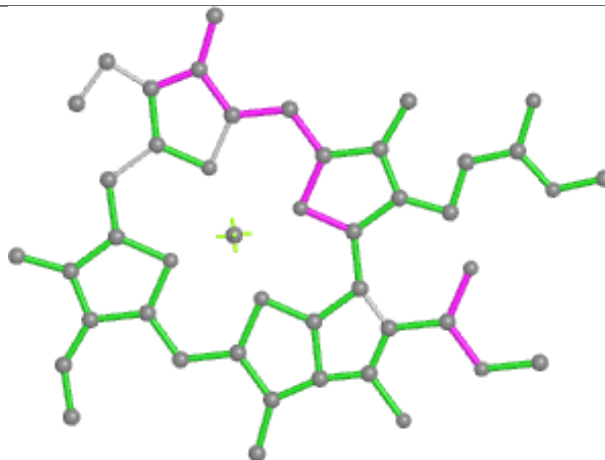
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



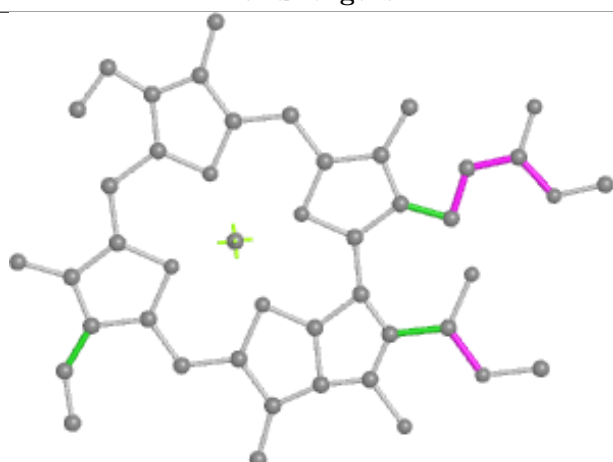
## Ligand CLA 7 310



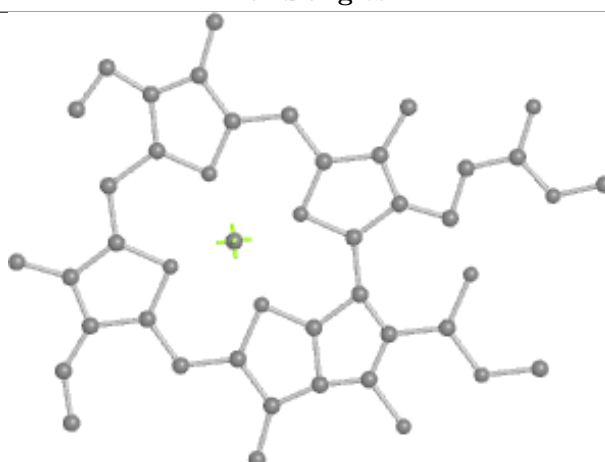
Bond lengths



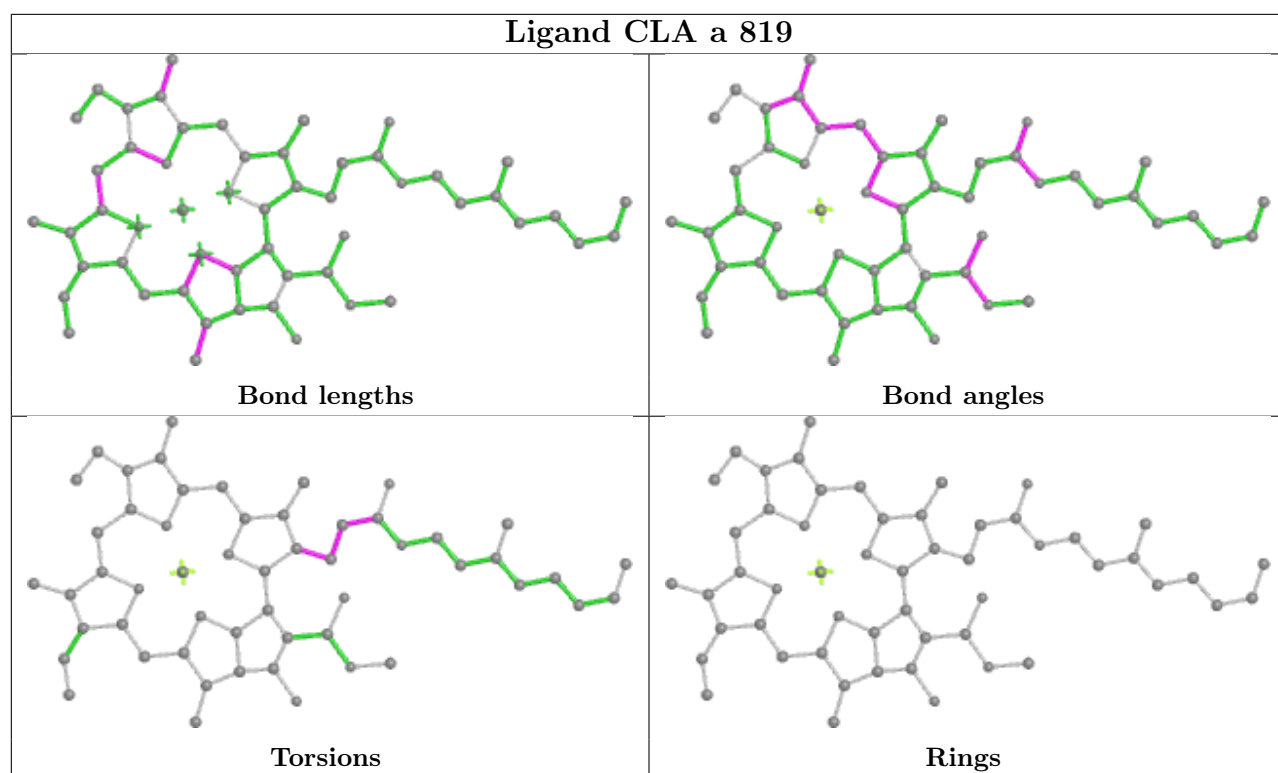
Bond angles



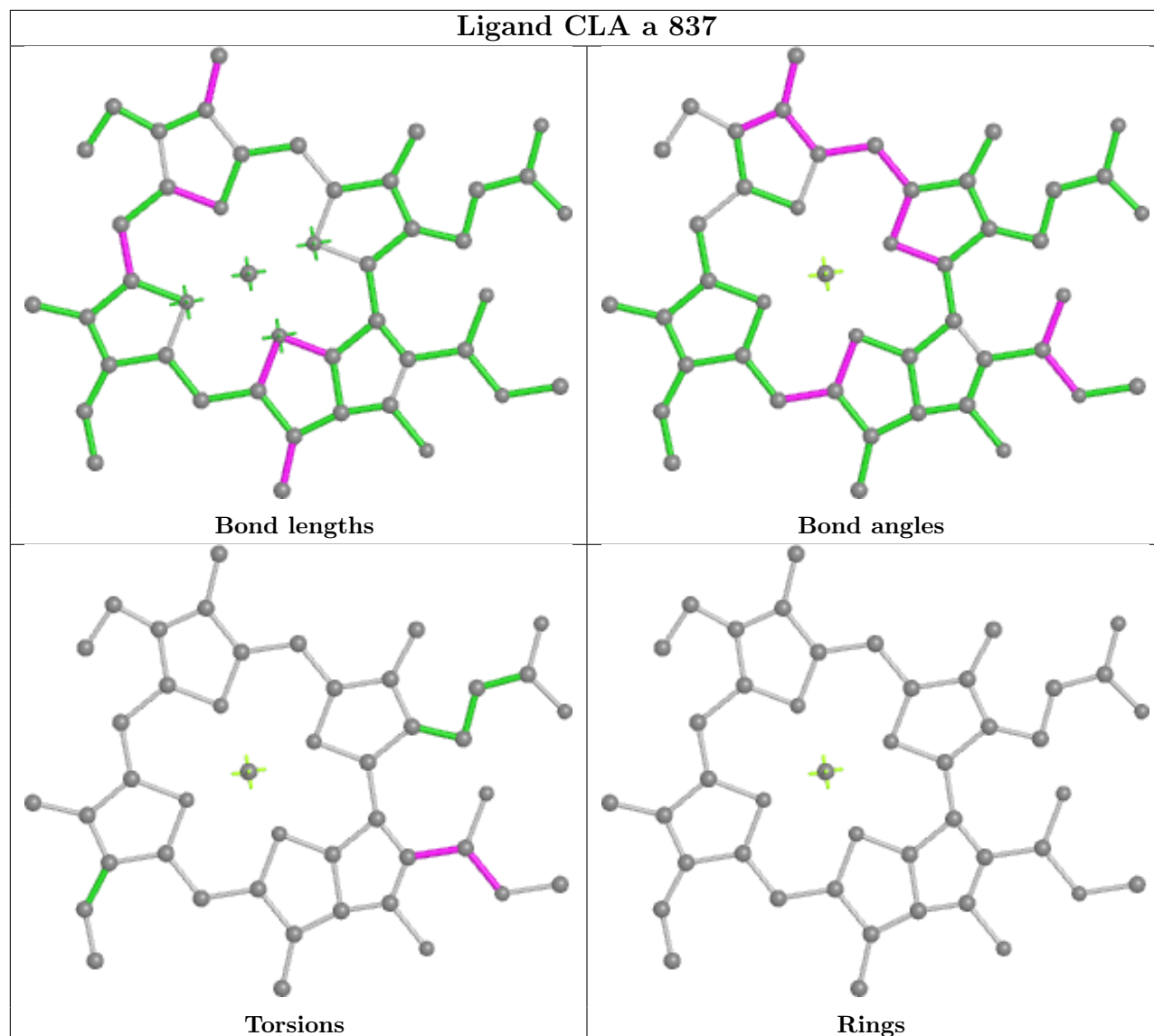
Torsions



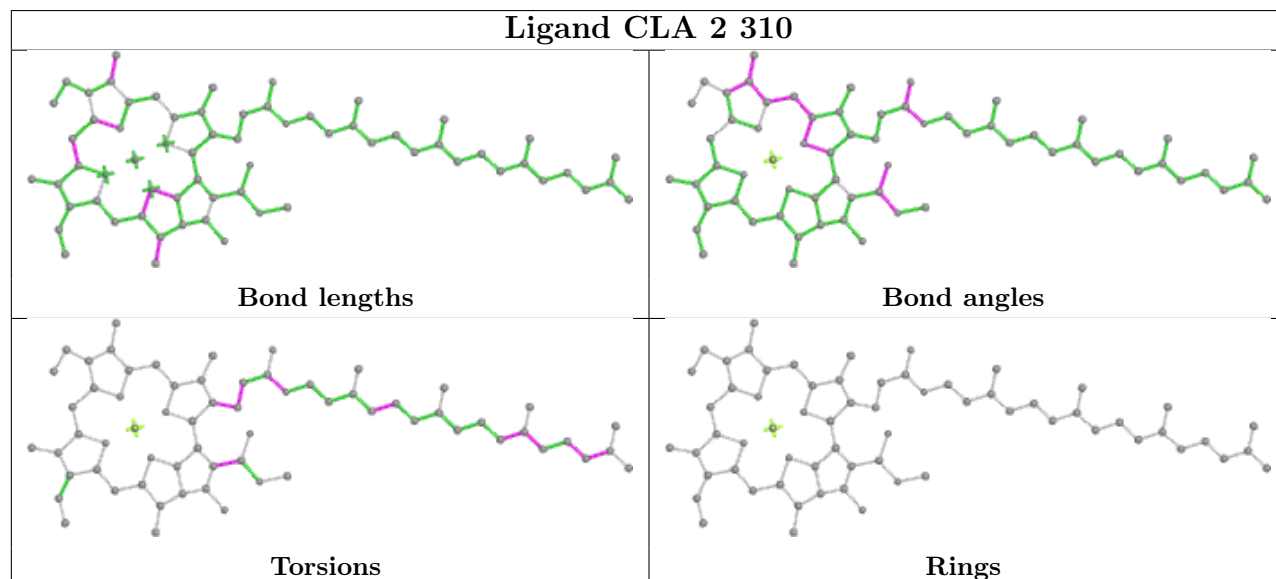
Rings



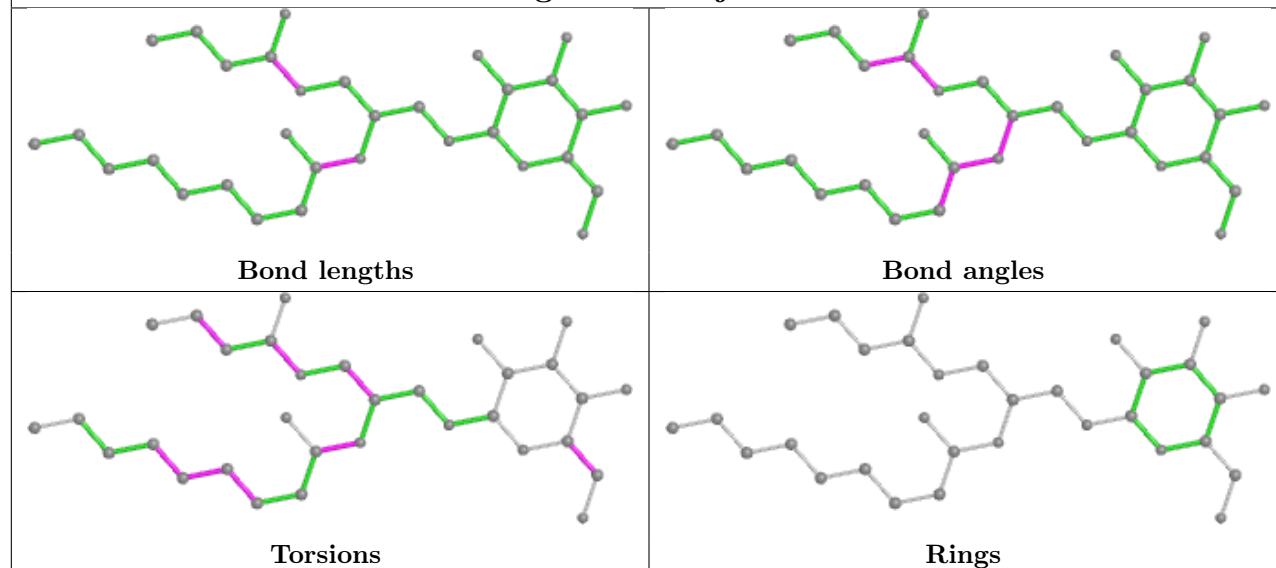
## Ligand CLA a 837



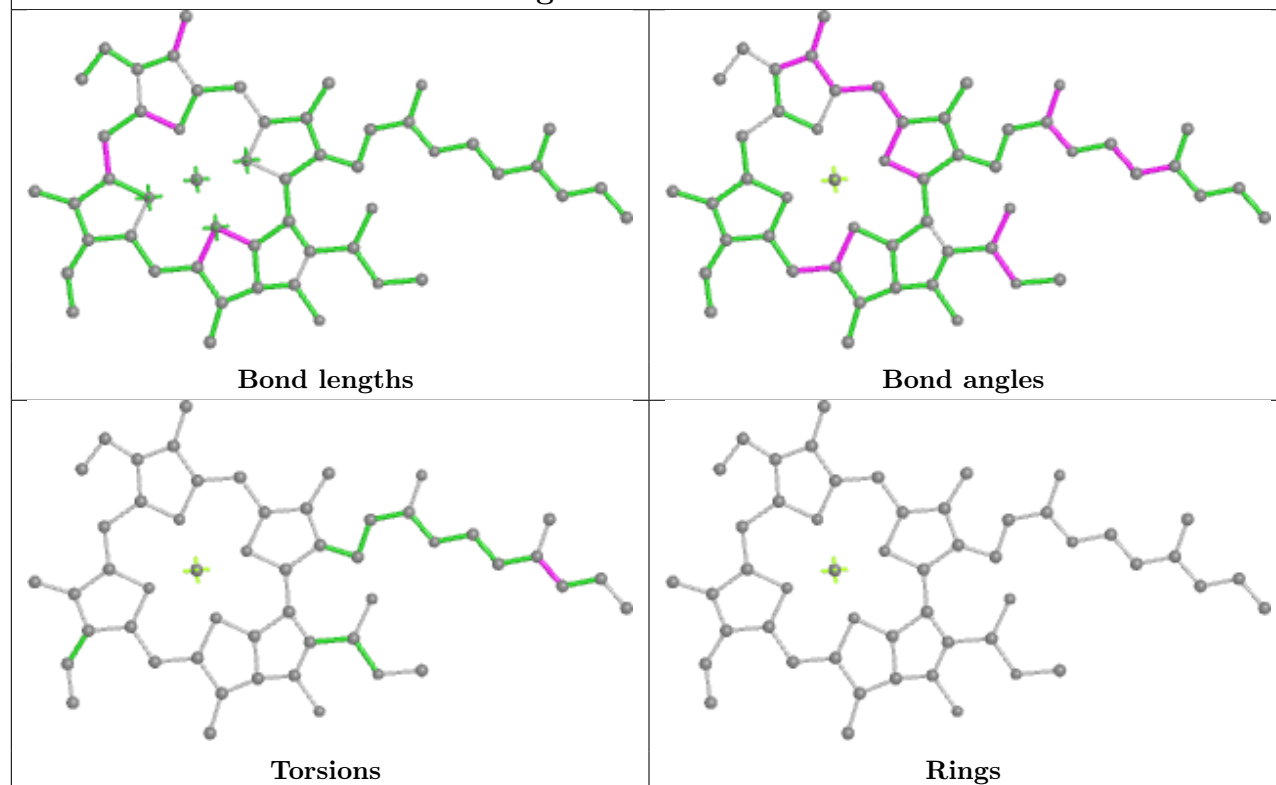
## Ligand CLA 2 310



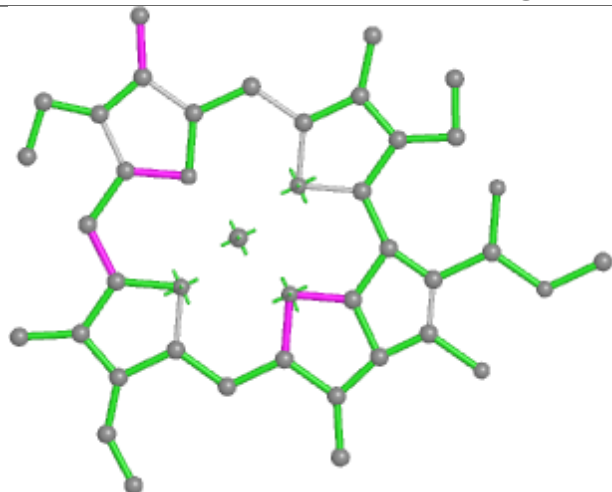
## Ligand LMG j 105



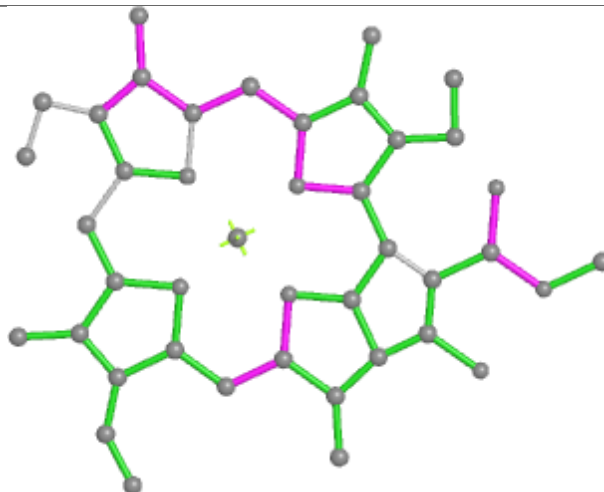
## Ligand CLA 3 313



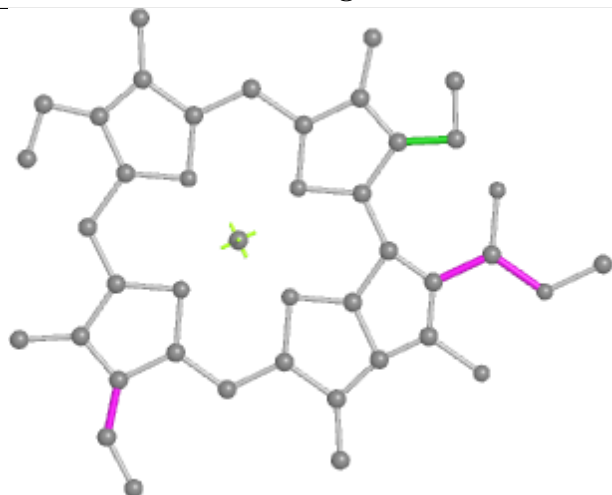
## Ligand CLA 9 315



Bond lengths



Bond angles

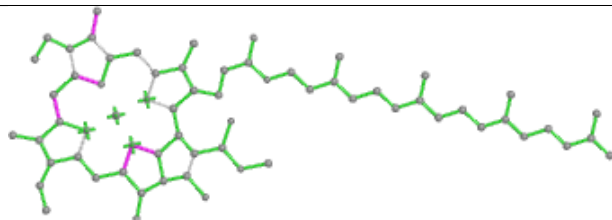


Torsions

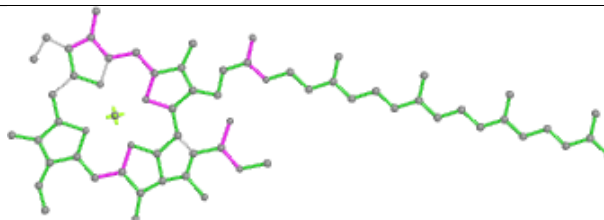


Rings

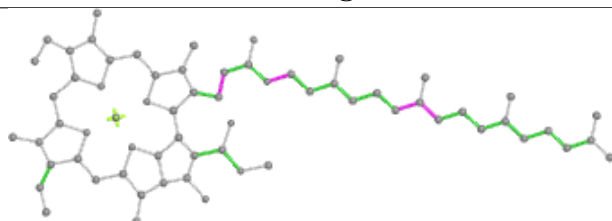
## Ligand CLA a 822



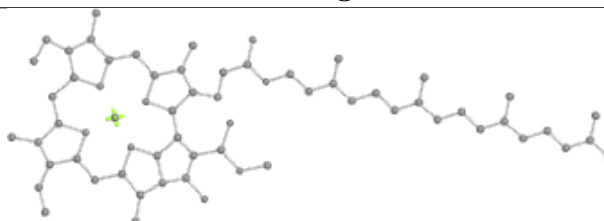
Bond lengths



Bond angles

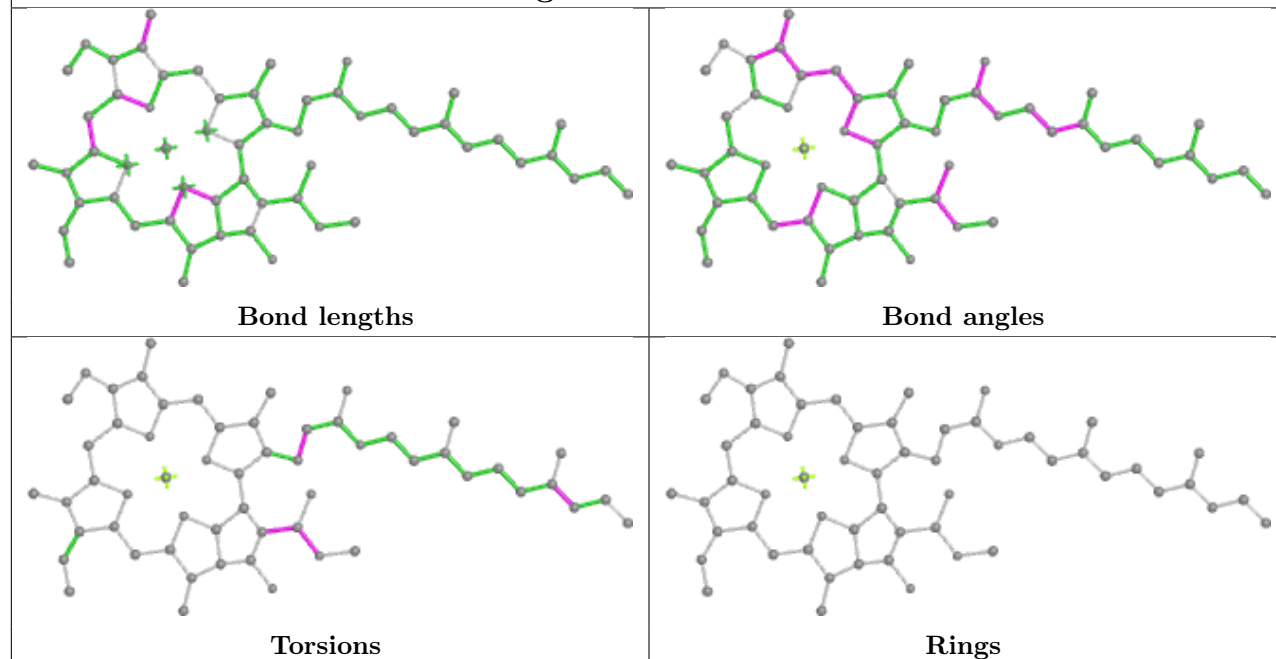


Torsions

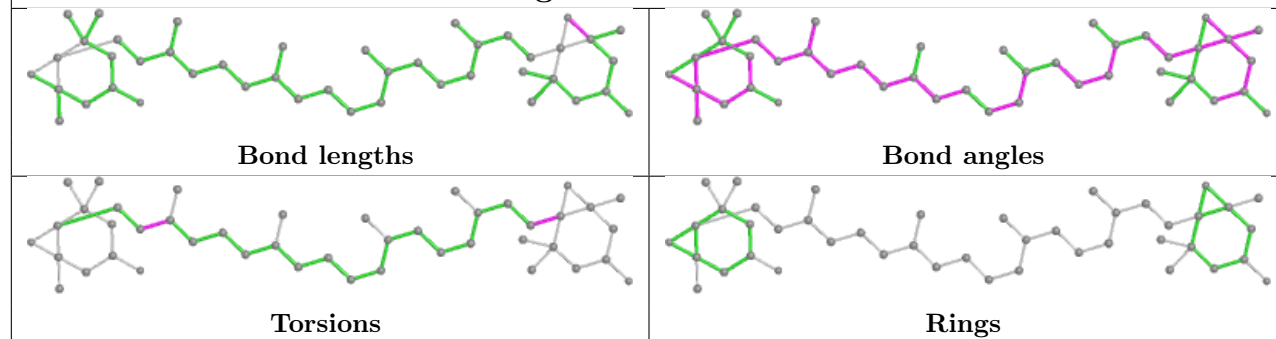


Rings

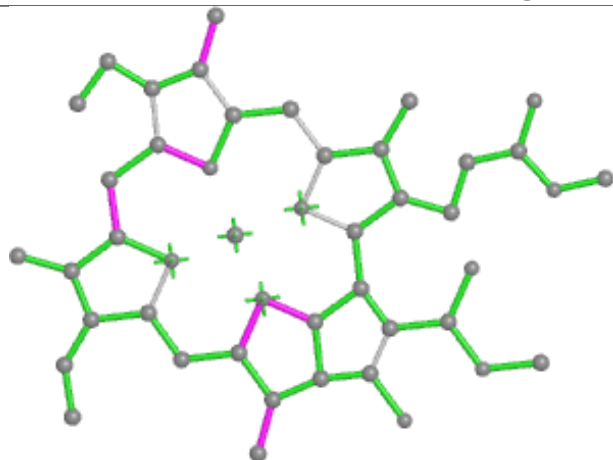
## Ligand CLA 8 309



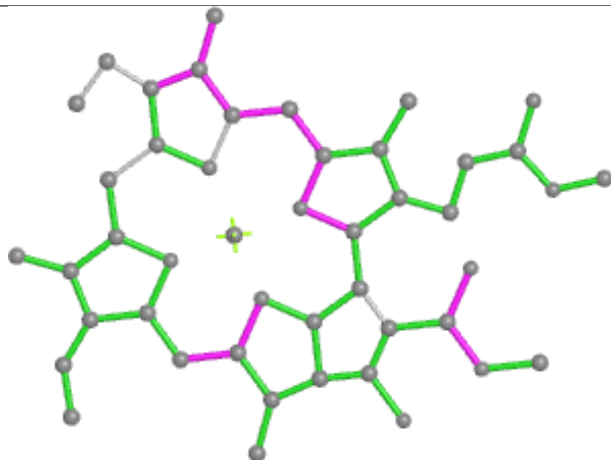
## Ligand XAT 2 301



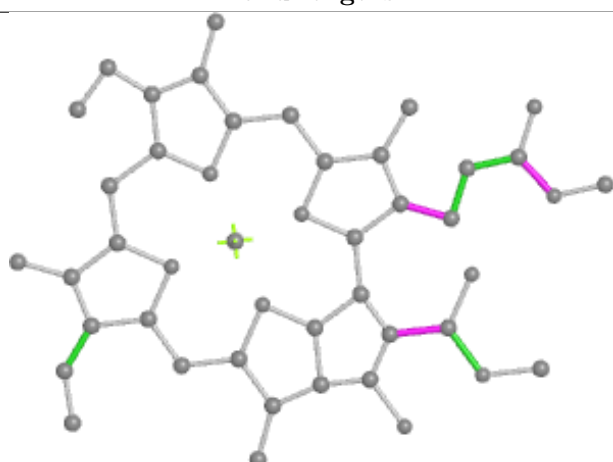
## Ligand CLA a 824



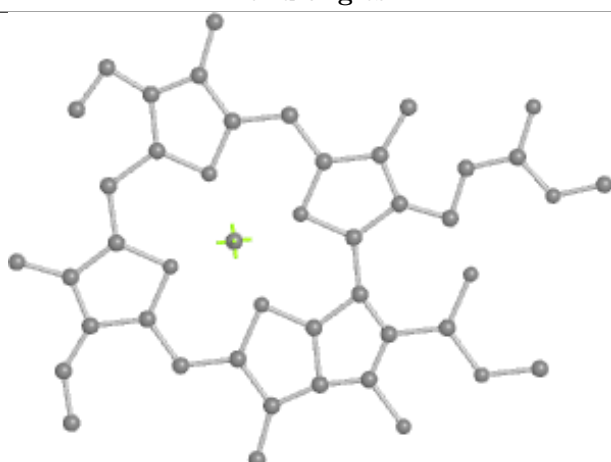
Bond lengths



Bond angles

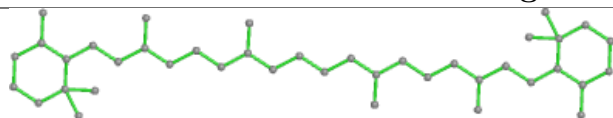


Torsions

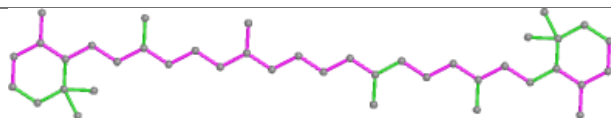


Rings

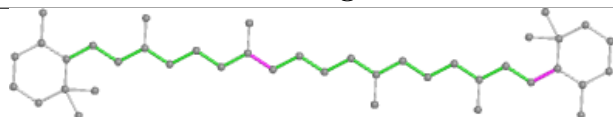
## Ligand BCR f 804



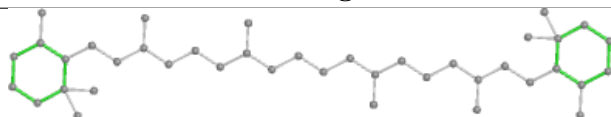
Bond lengths



Bond angles

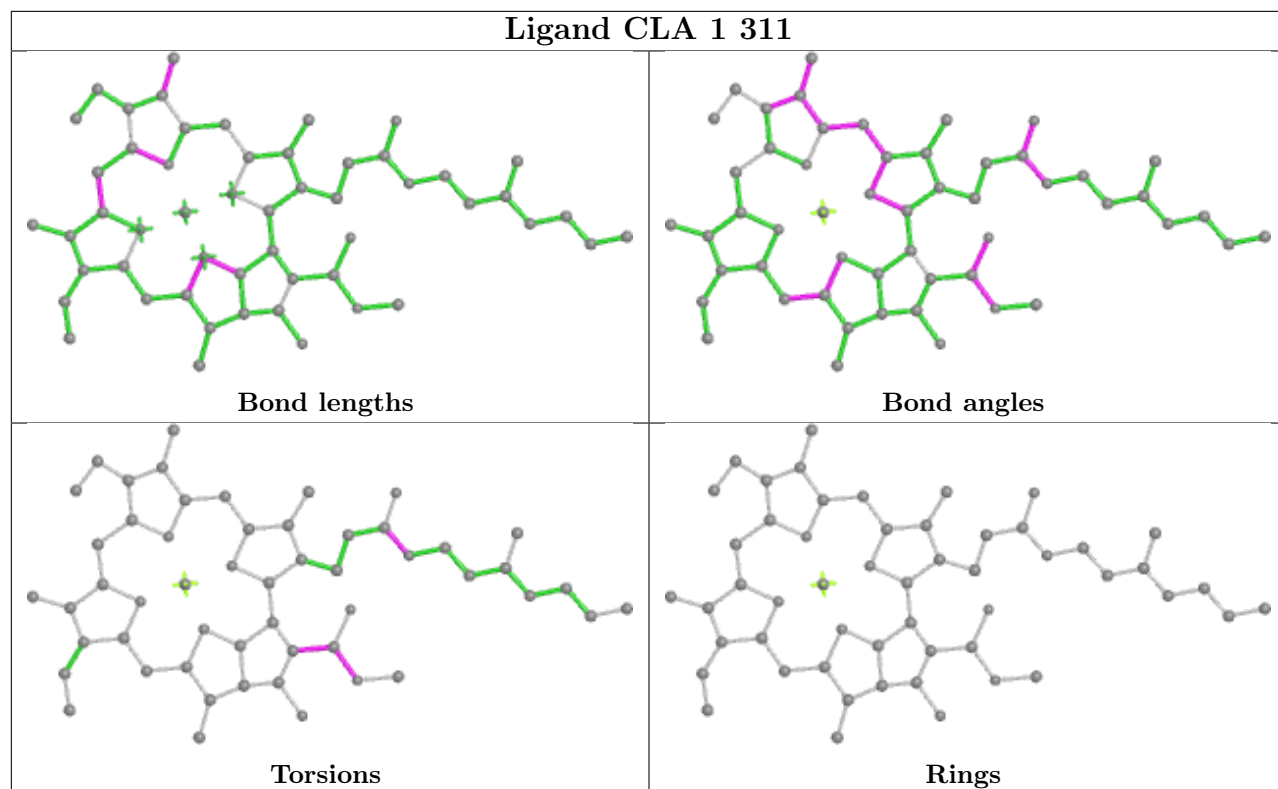


Torsions

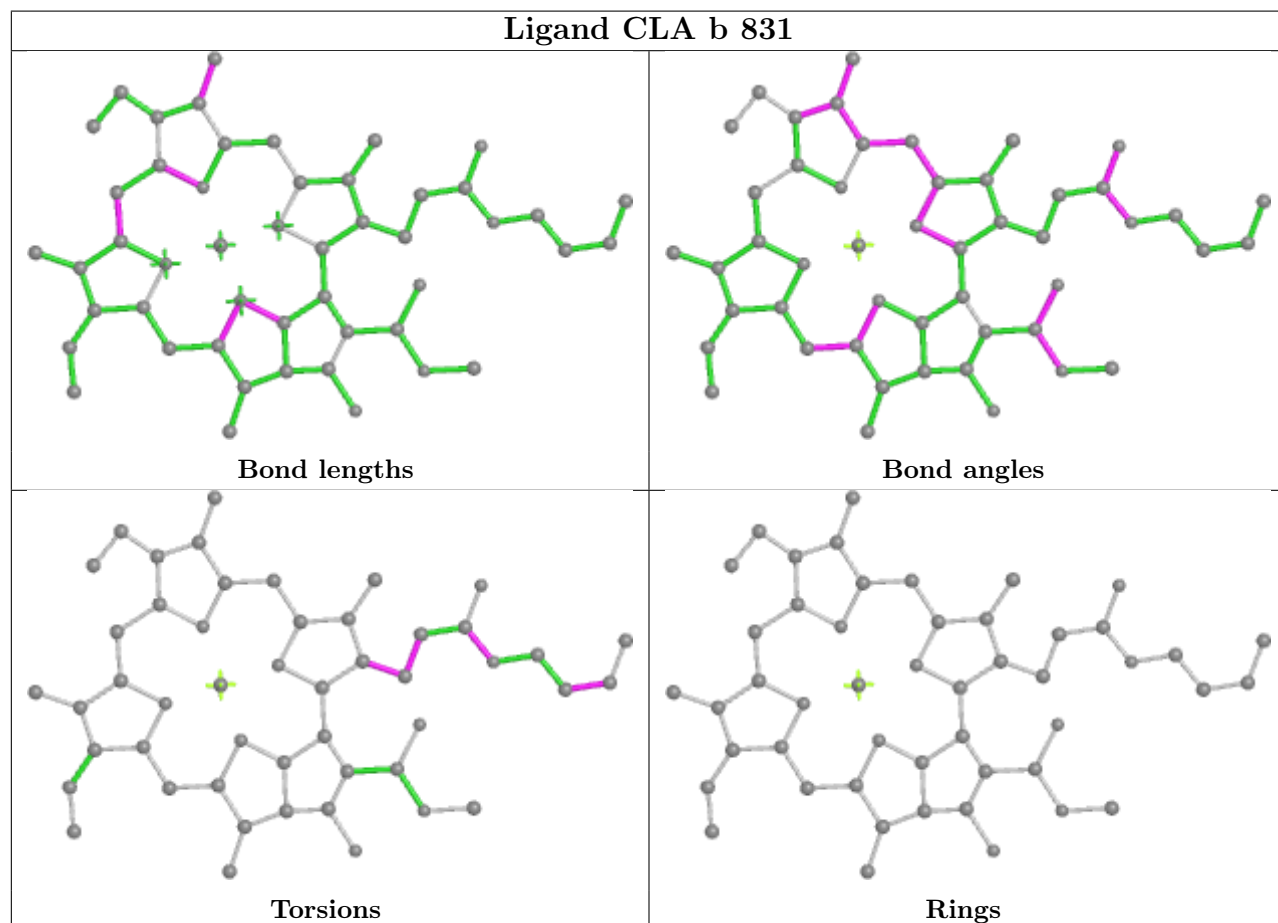


Rings

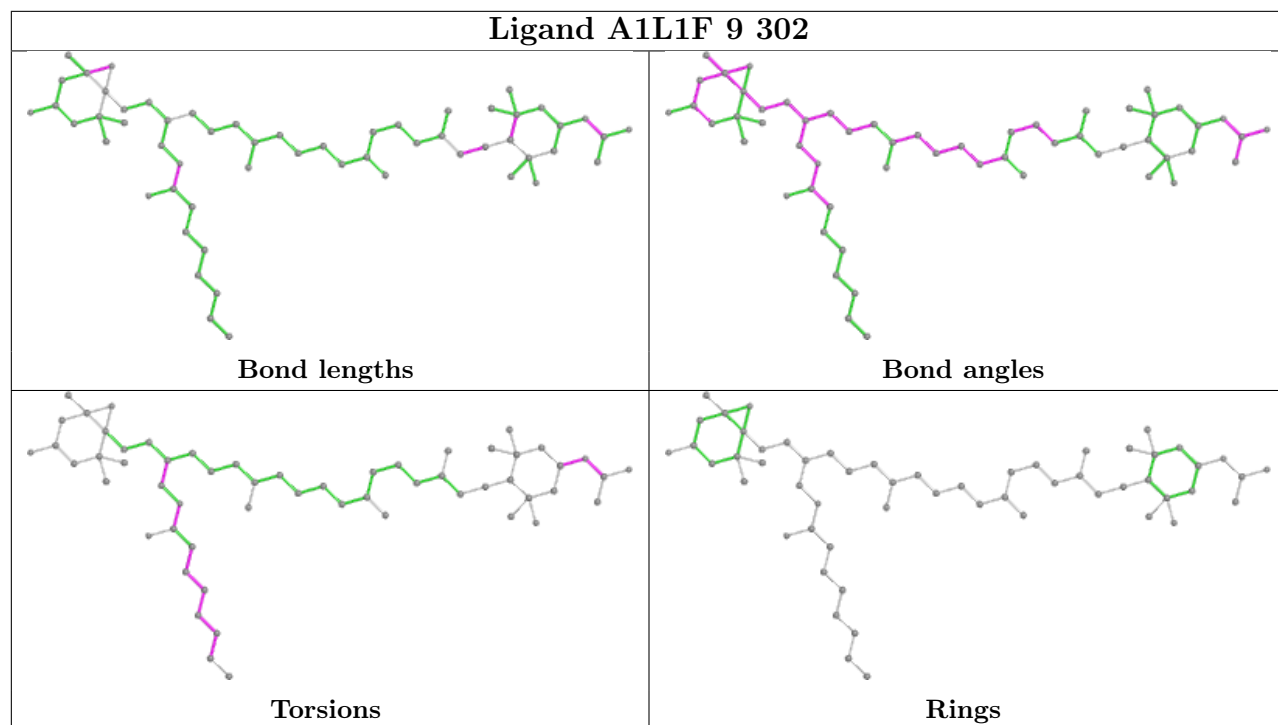
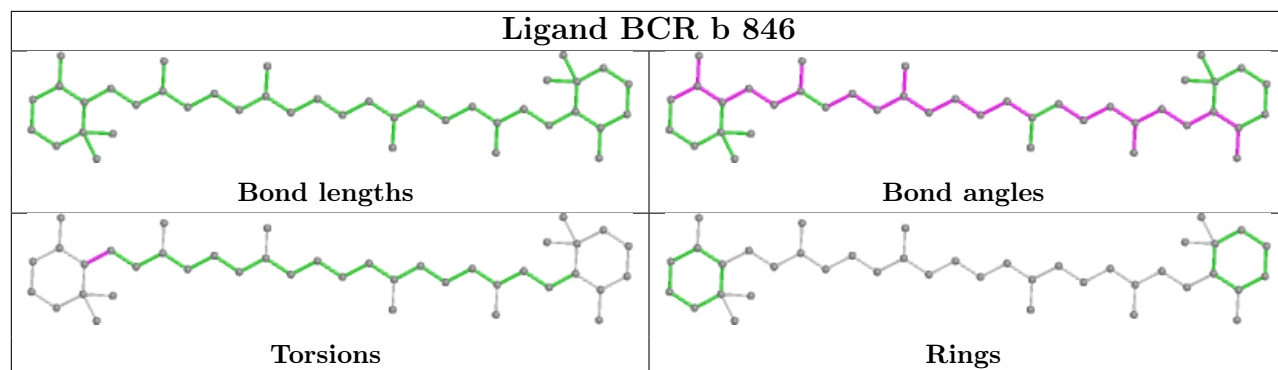
## Ligand CLA 1 311



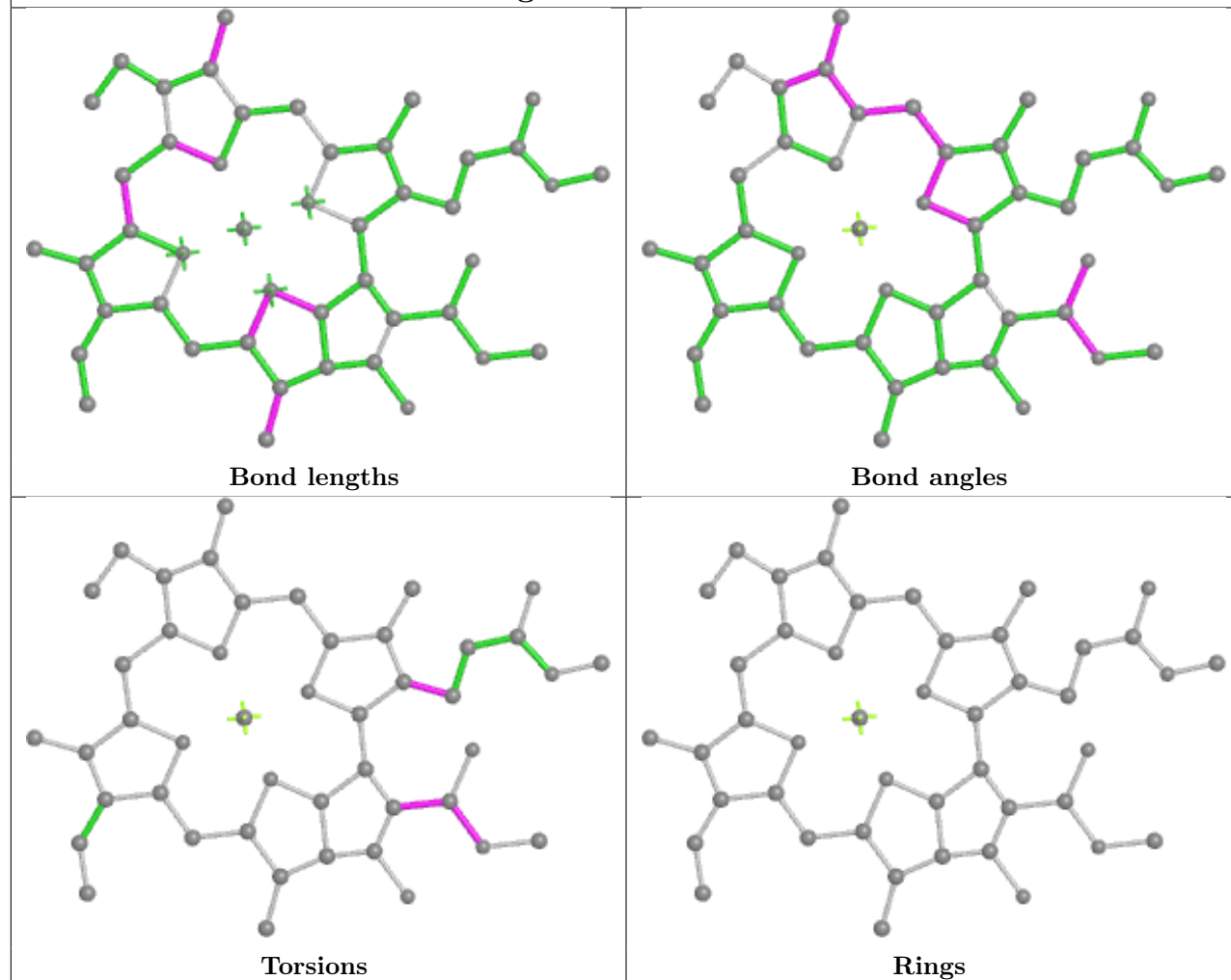
## Ligand CLA b 831



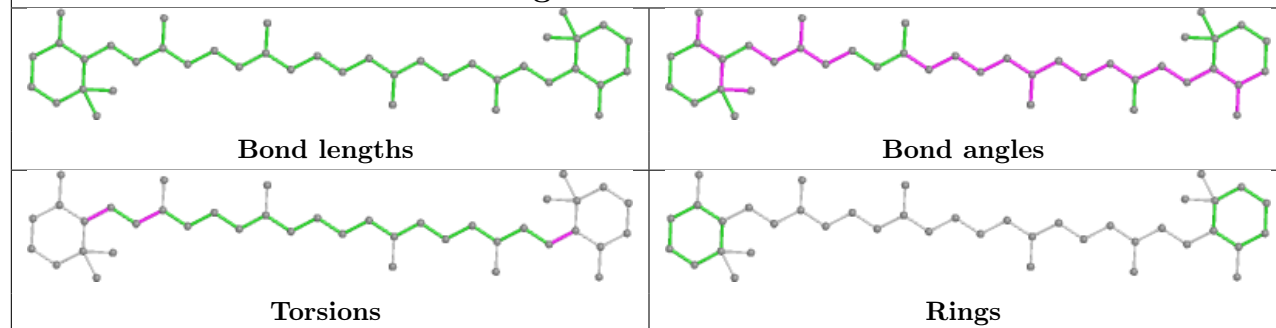




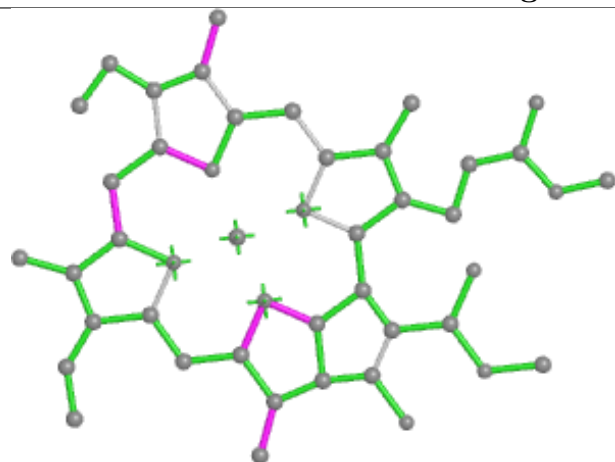
## Ligand CLA 2 316



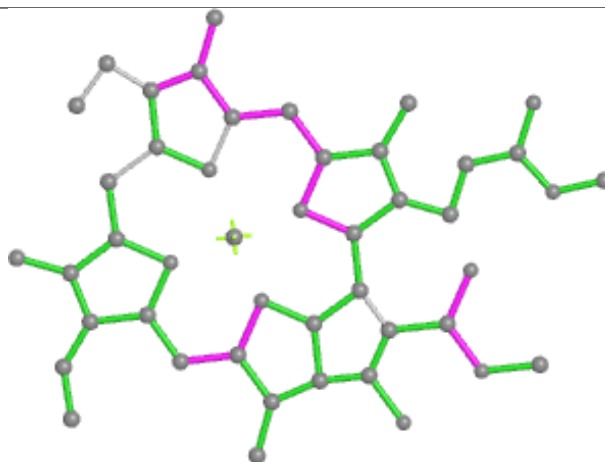
## Ligand BCR b 849



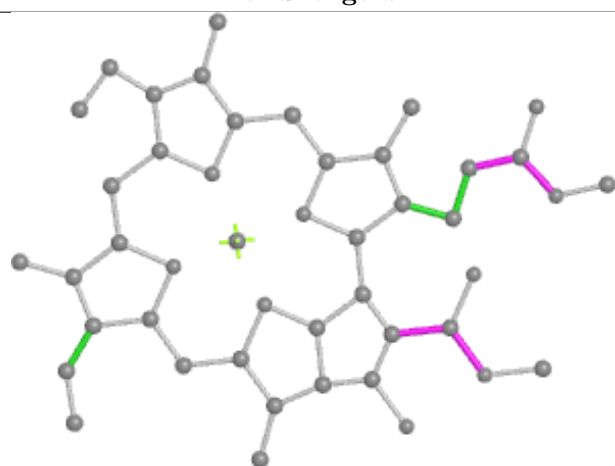
## Ligand CLA 1 309



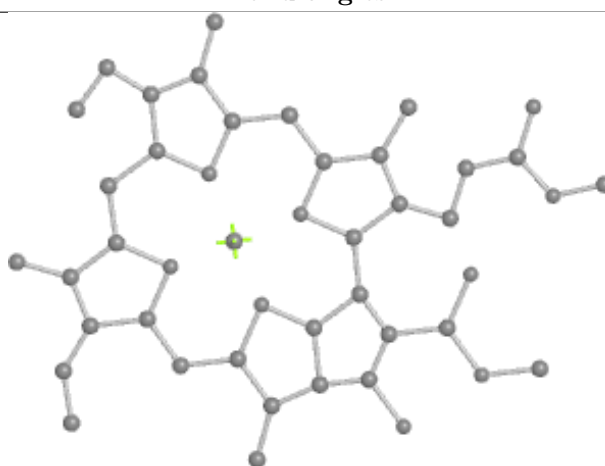
Bond lengths



Bond angles

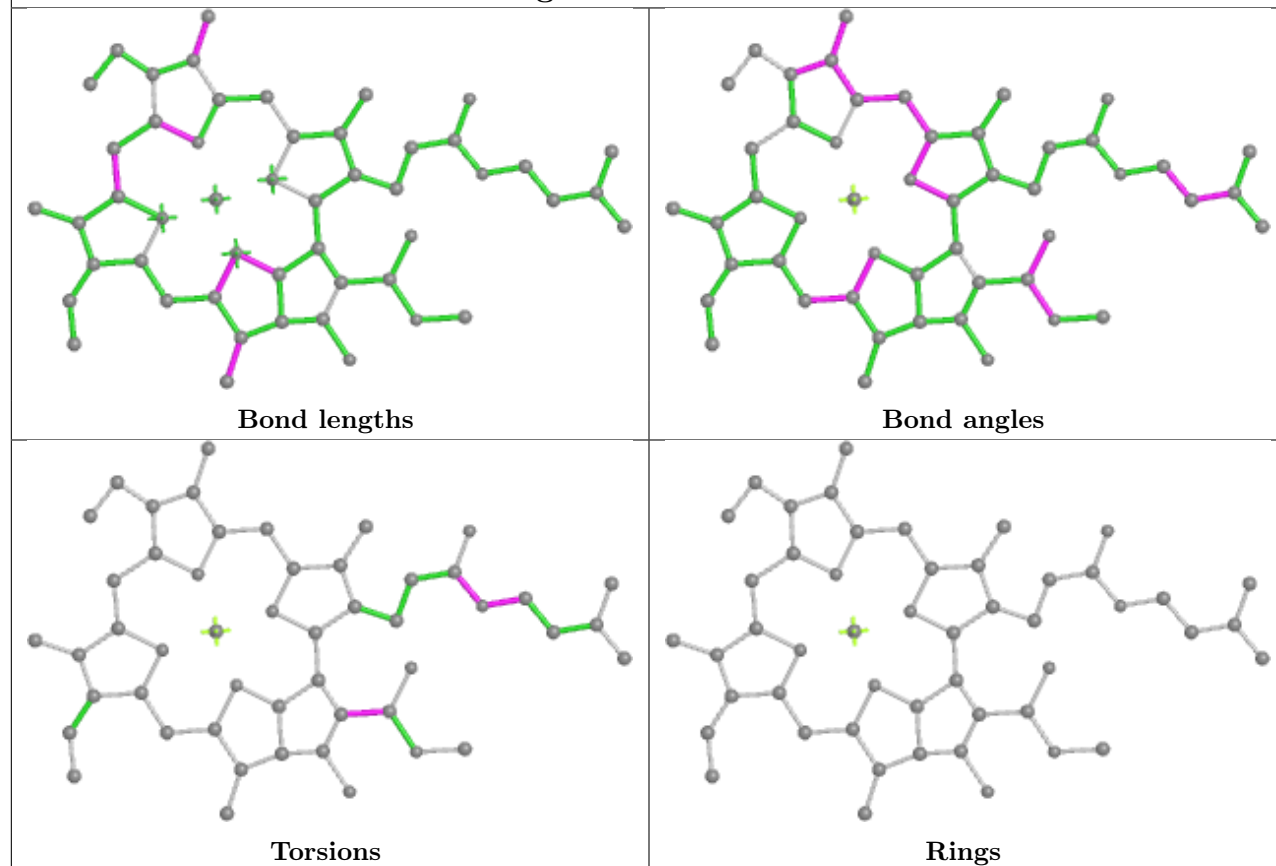


Torsions

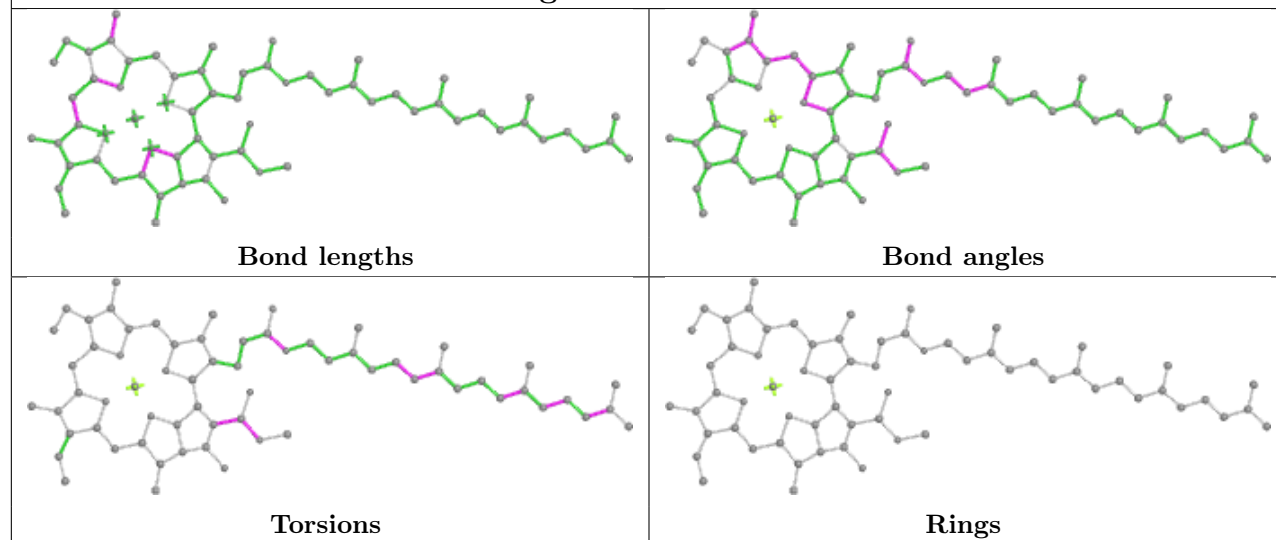


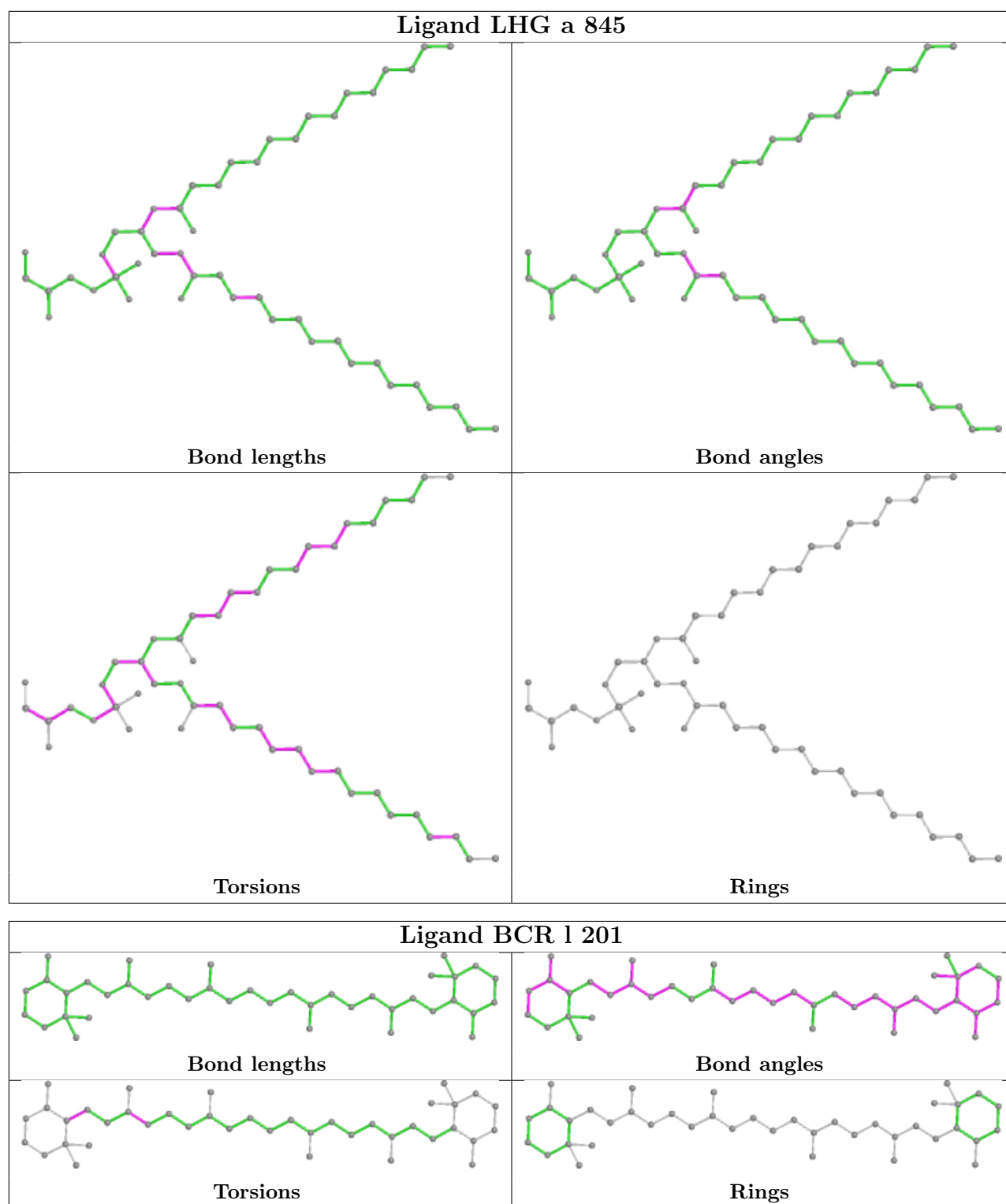
Rings

## Ligand CLA a 816

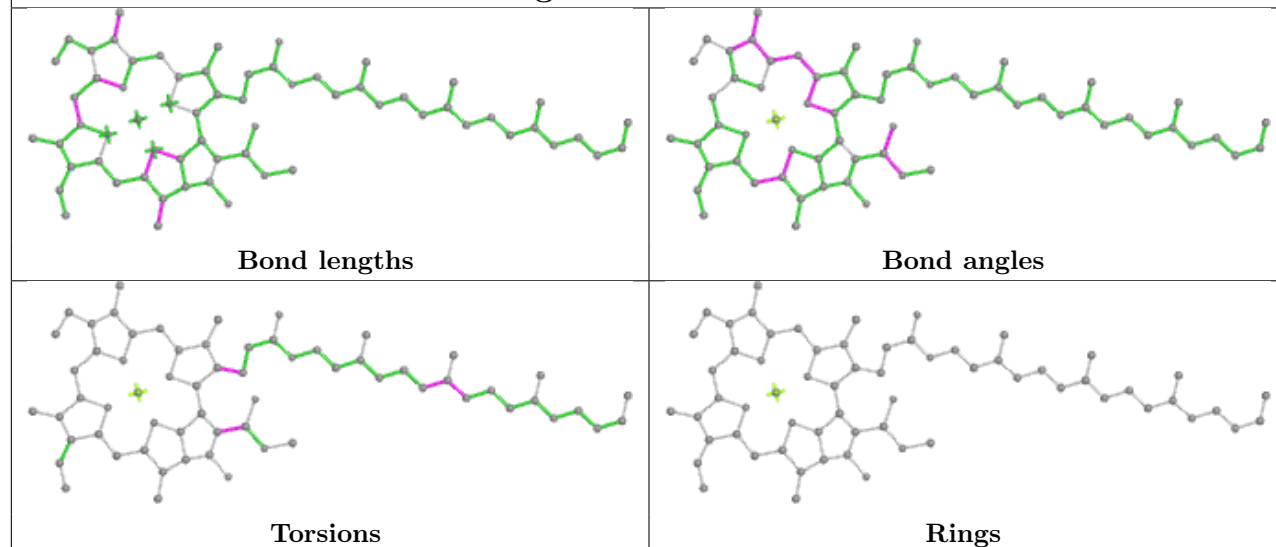


## Ligand CLA f 802

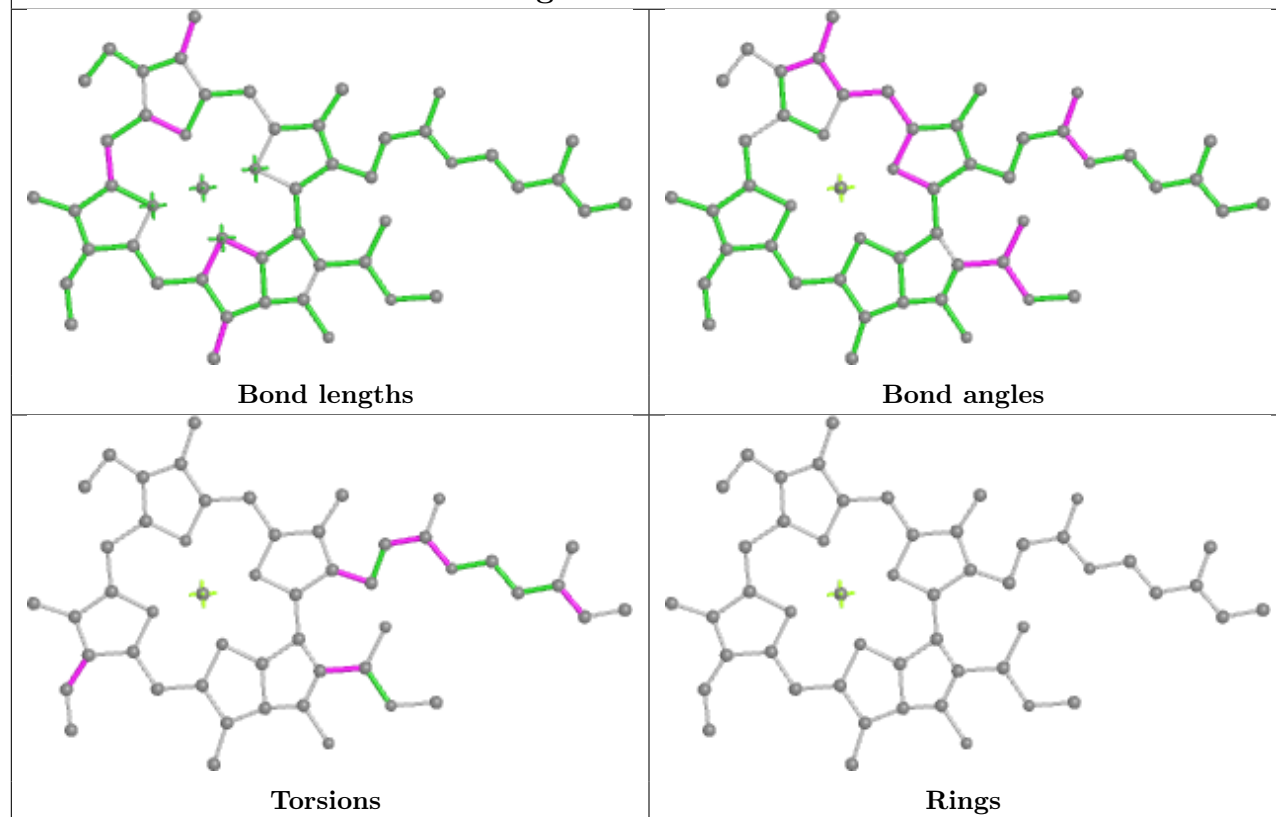




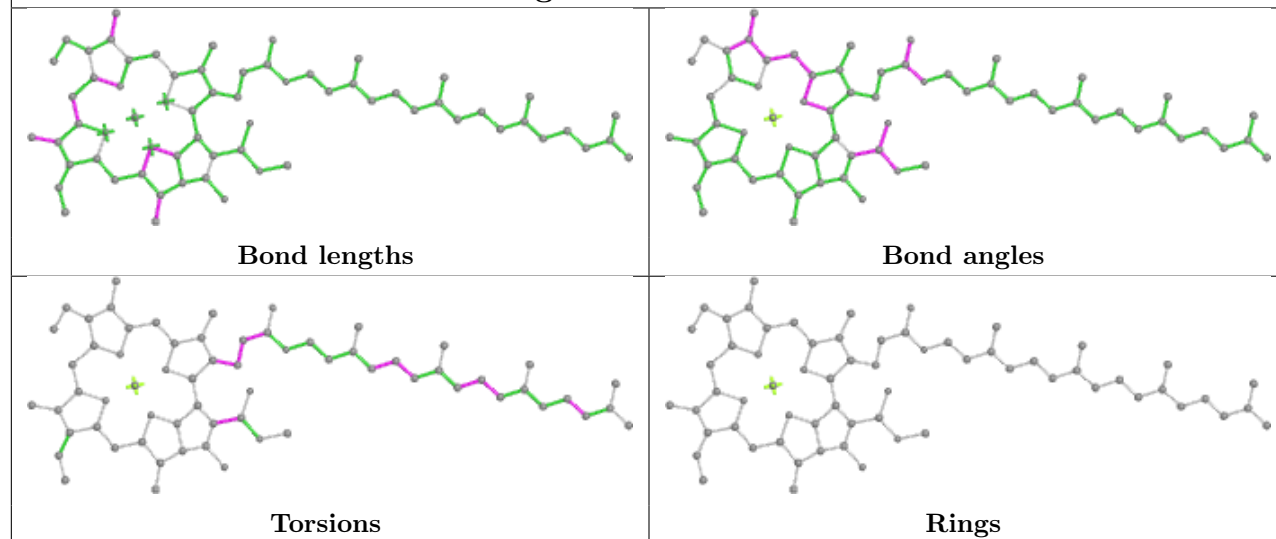
## Ligand CLA b 825



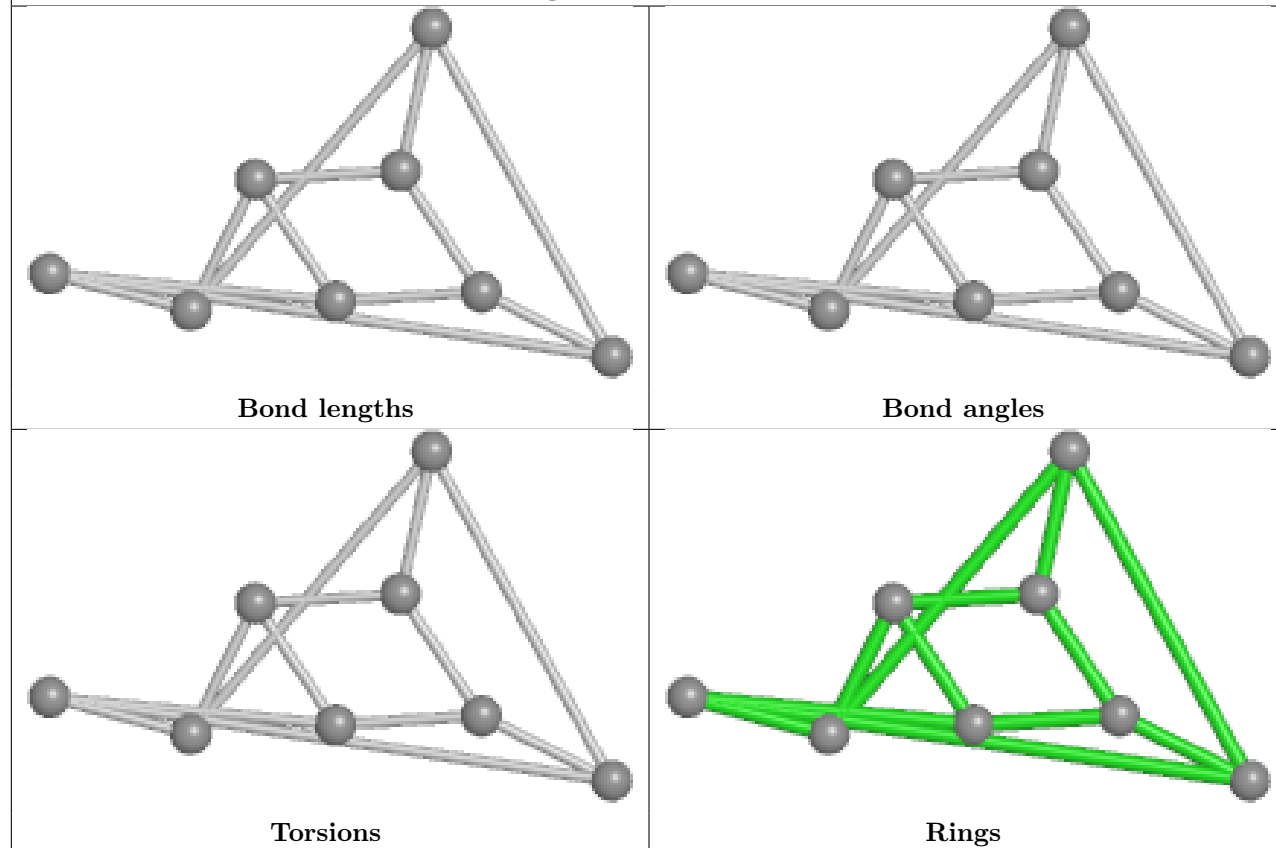
## Ligand CLA 7 316



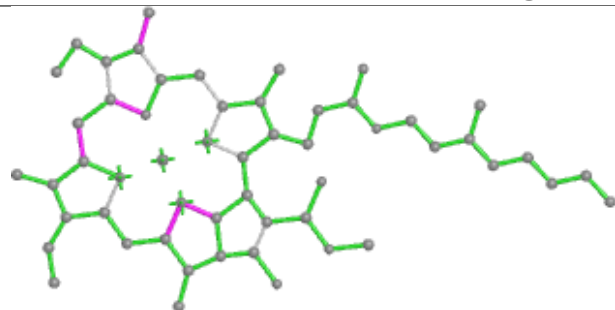
## Ligand CLA b 809



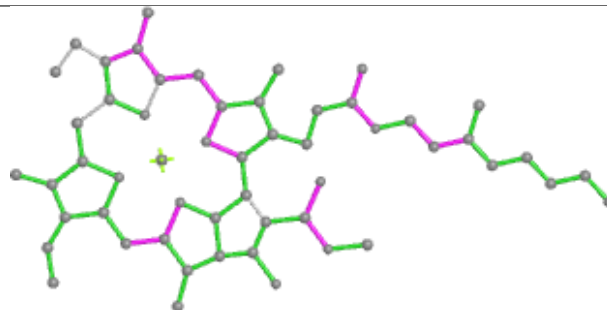
## Ligand SF4 a 851



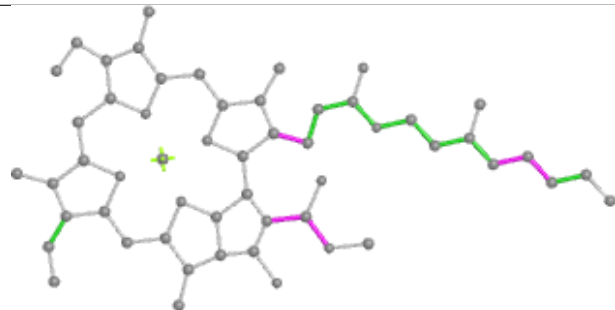
## Ligand CLA 7 313



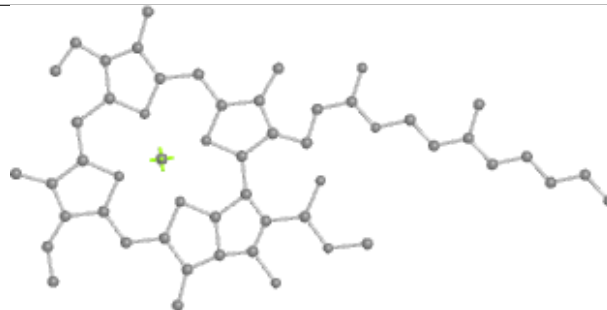
Bond lengths



Bond angles

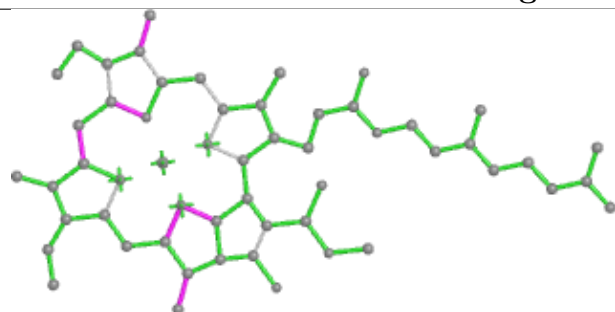


Torsions

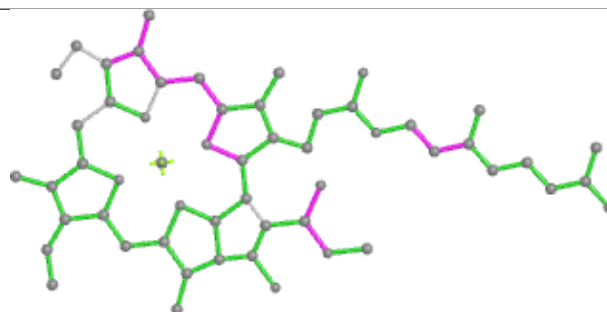


Rings

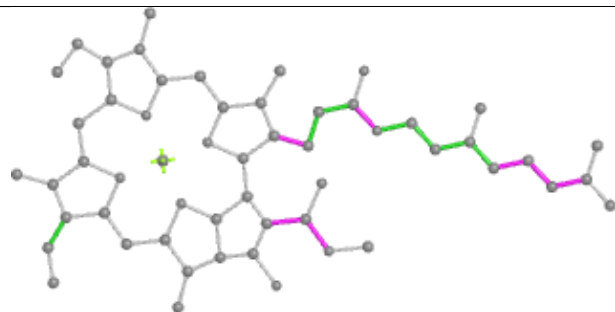
## Ligand CLA b 814



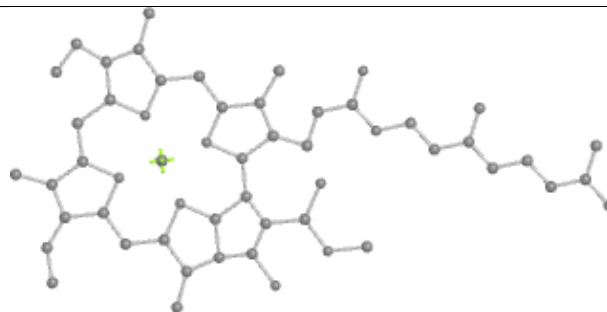
Bond lengths



Bond angles



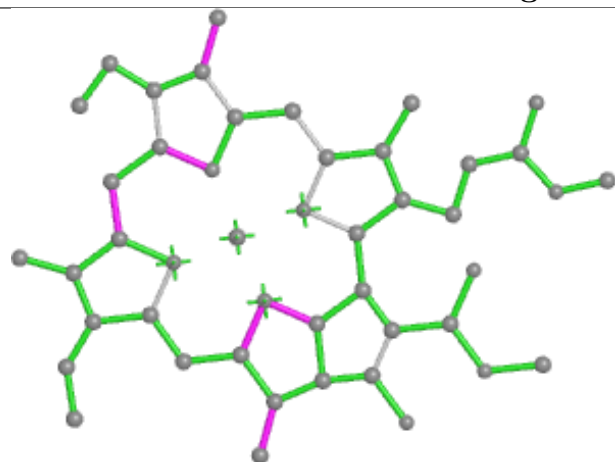
Torsions



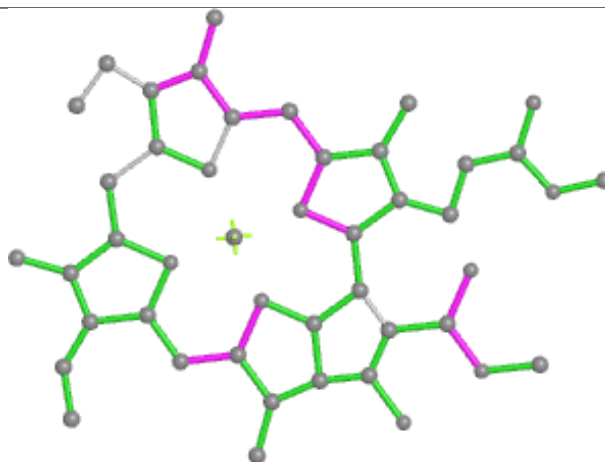
Rings



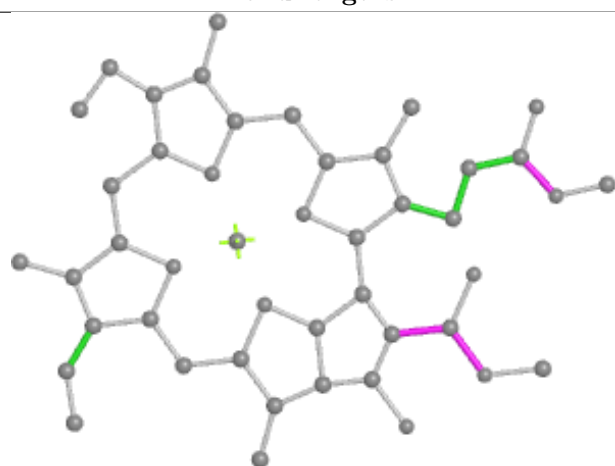
## Ligand CLA 8 310



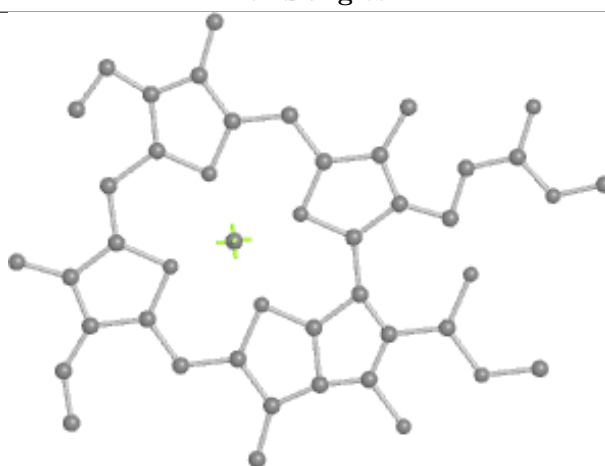
Bond lengths



Bond angles

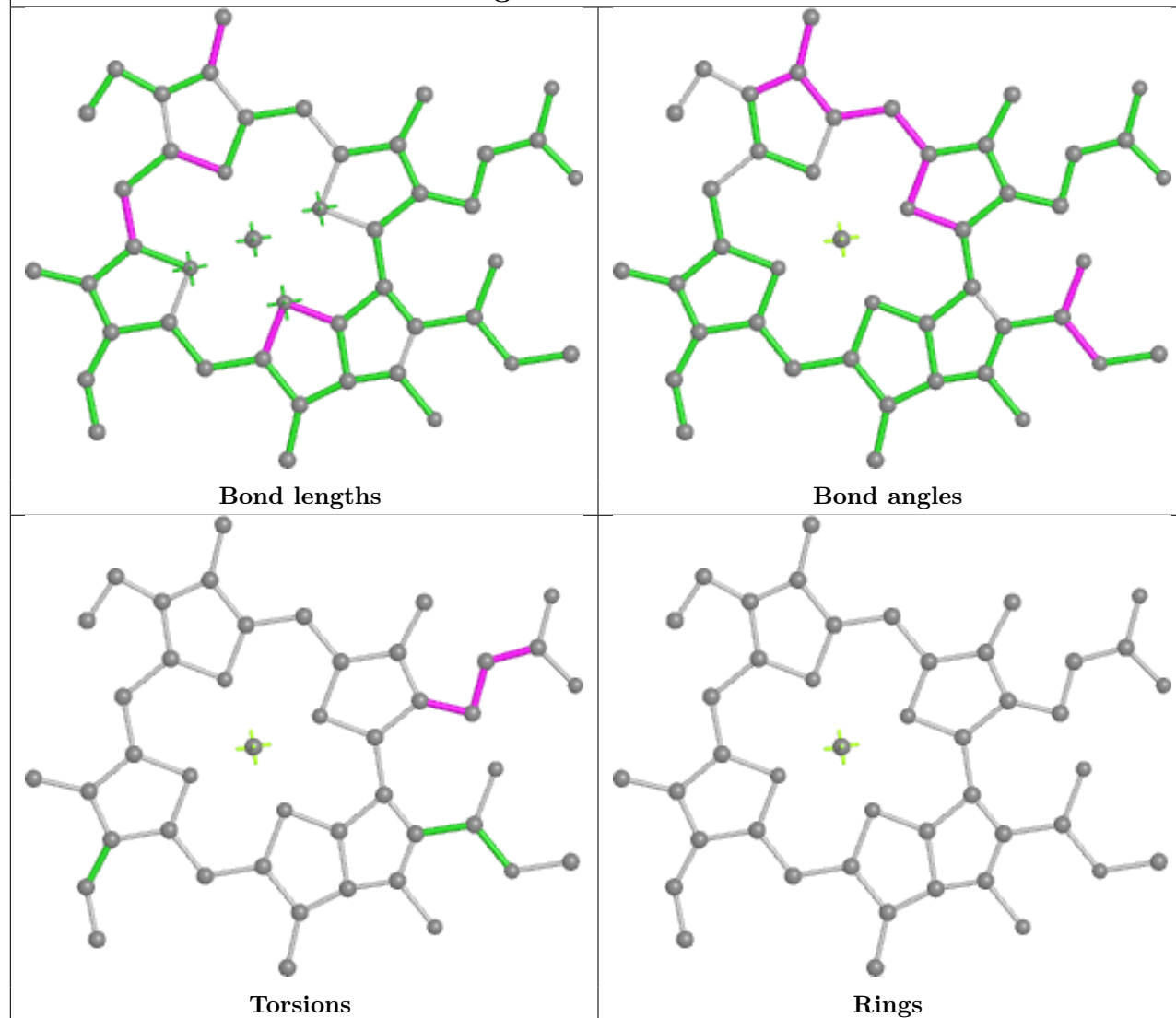


Torsions

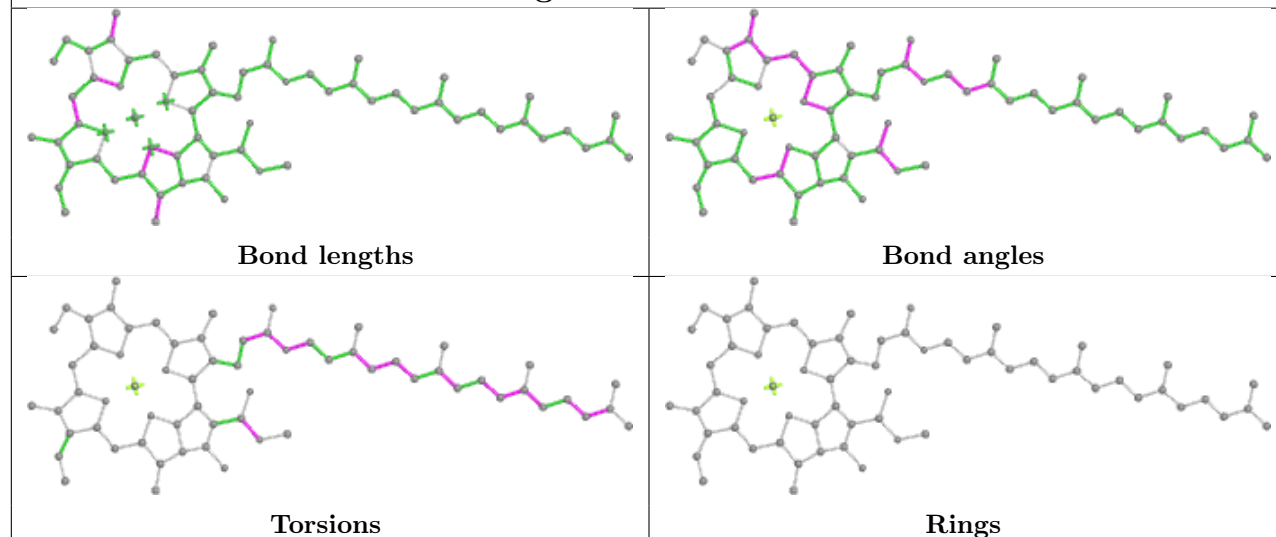


Rings

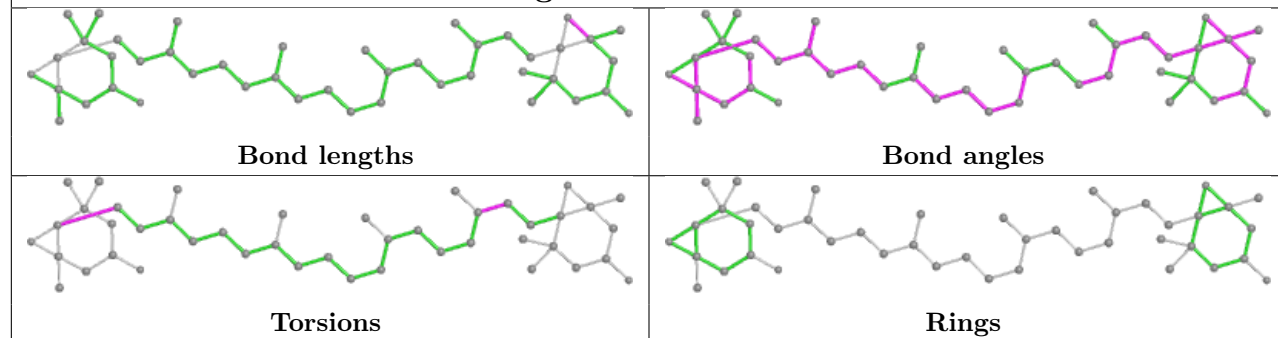
## Ligand CLA 1 314



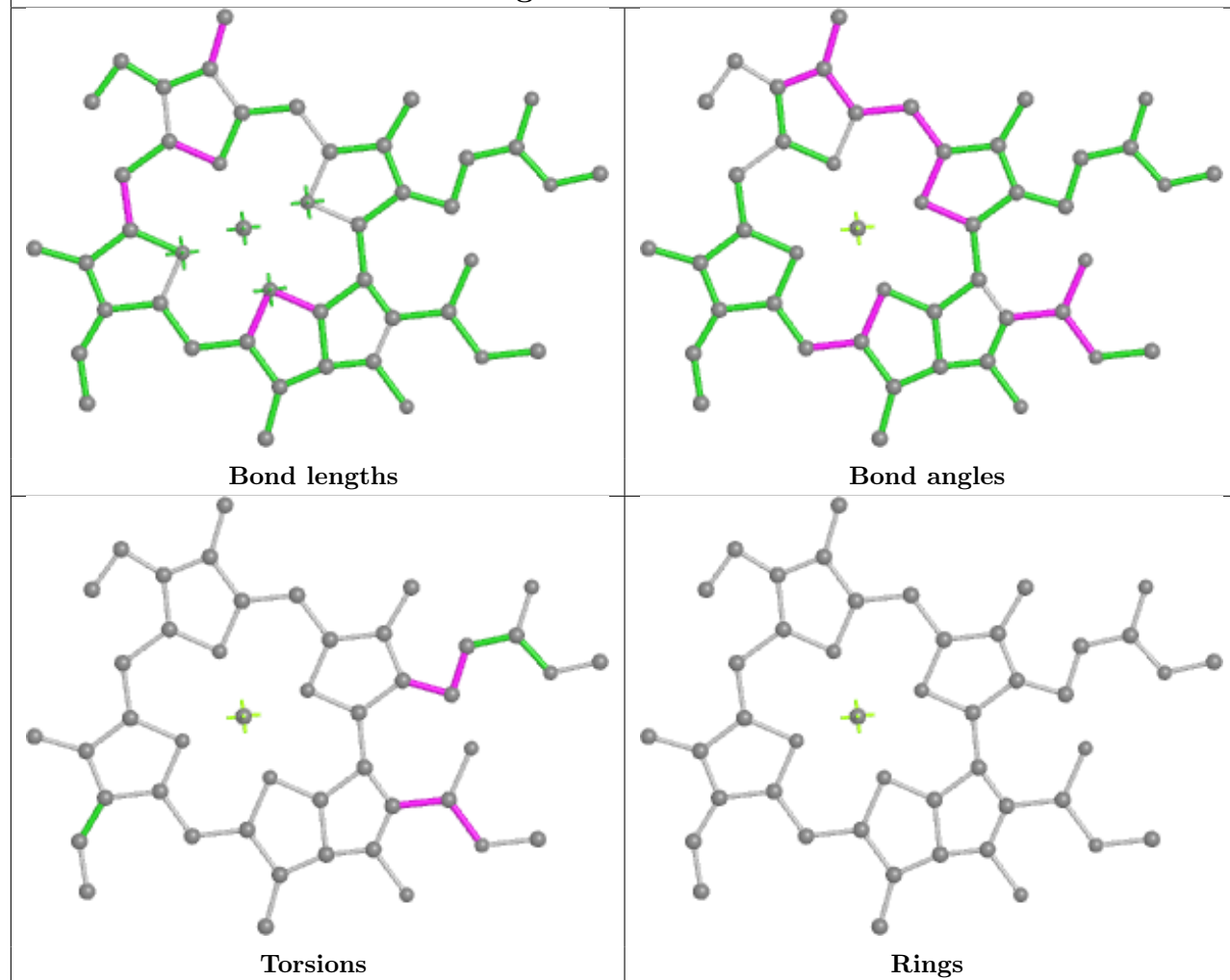
## Ligand CLA b 807

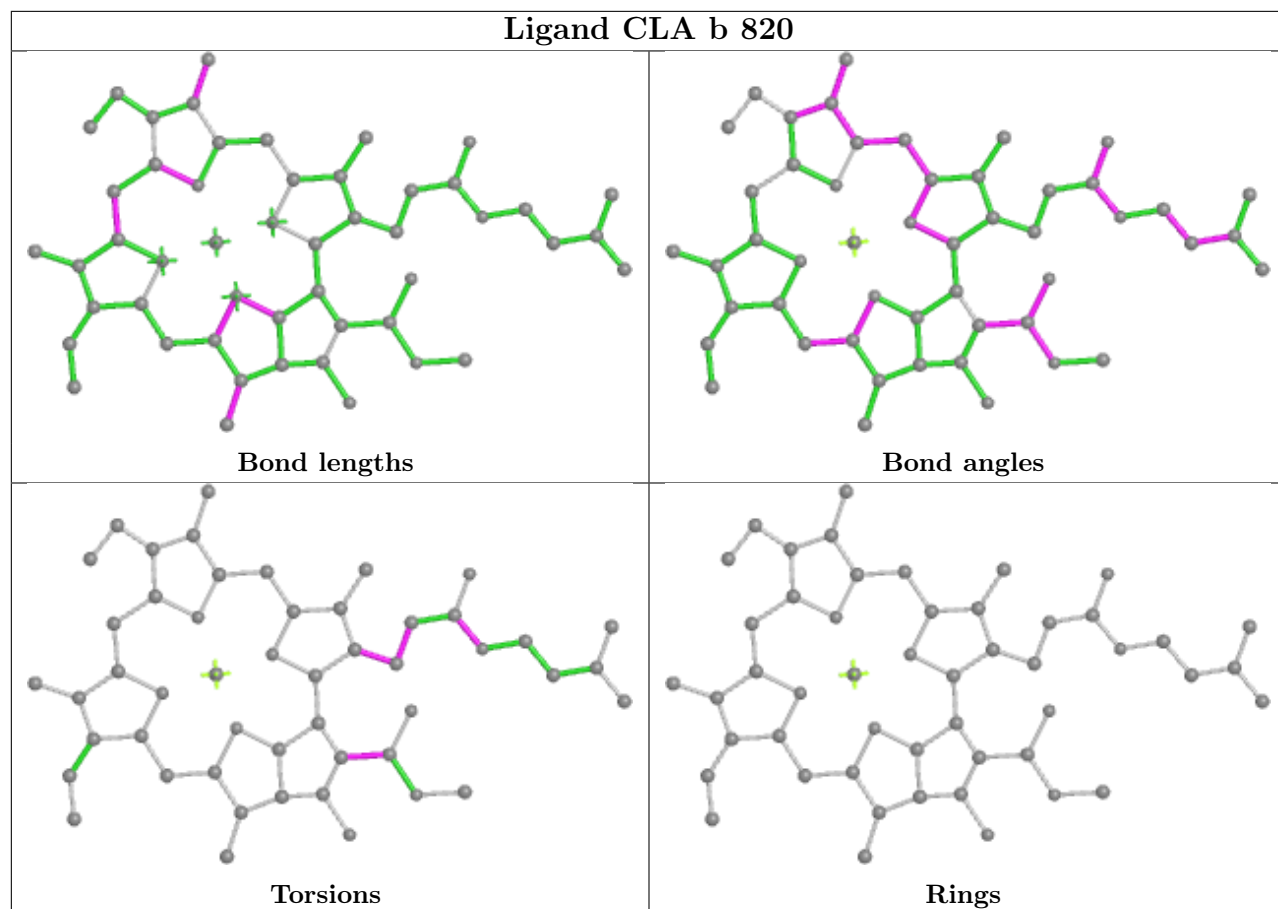


## Ligand XAT 8 301

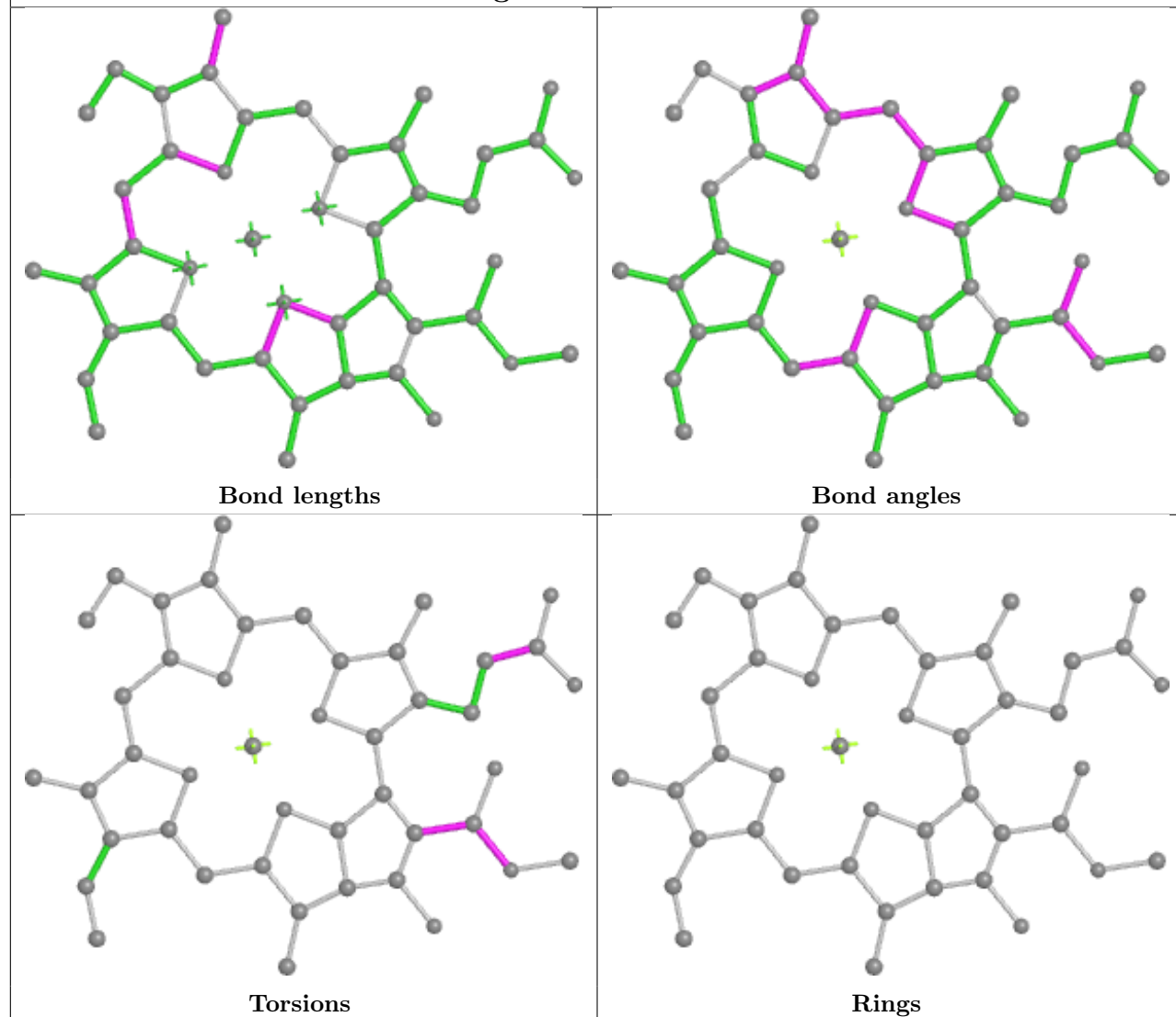


## Ligand CLA 9 311

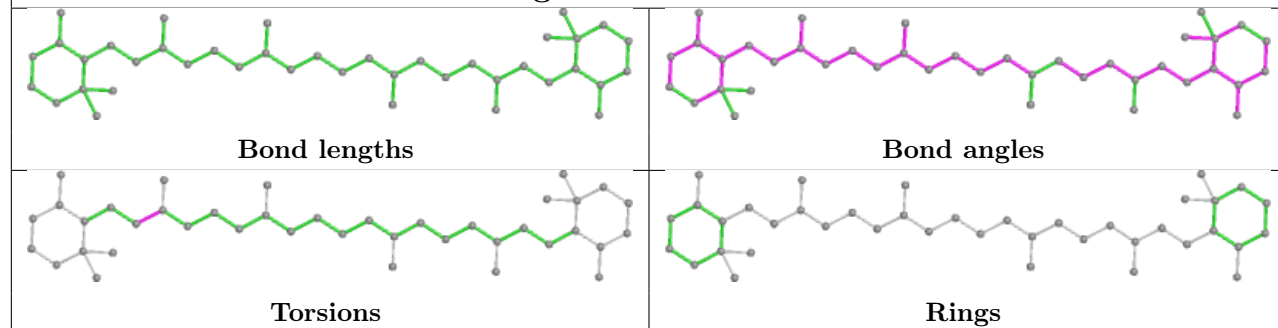




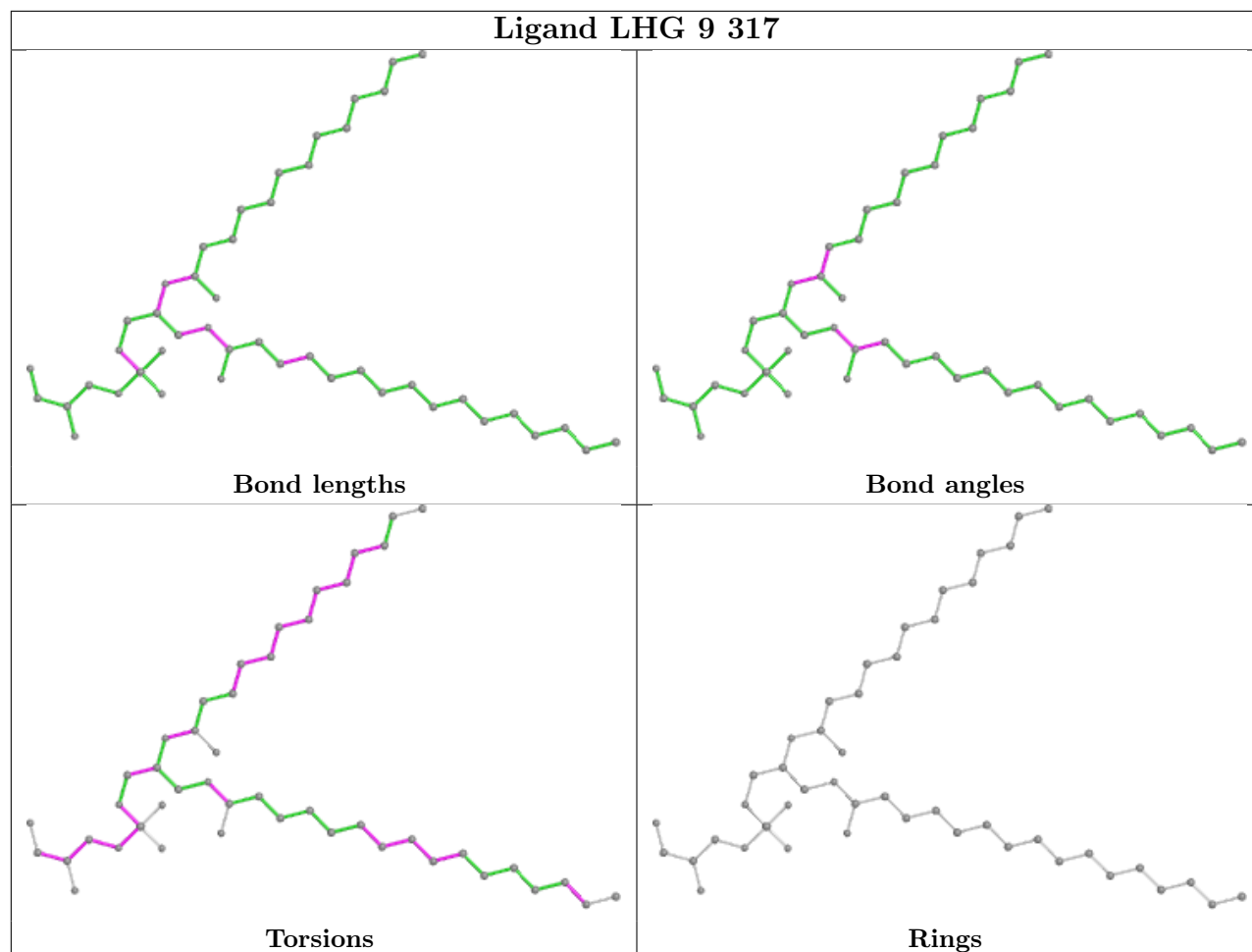
## Ligand CLA 7 307



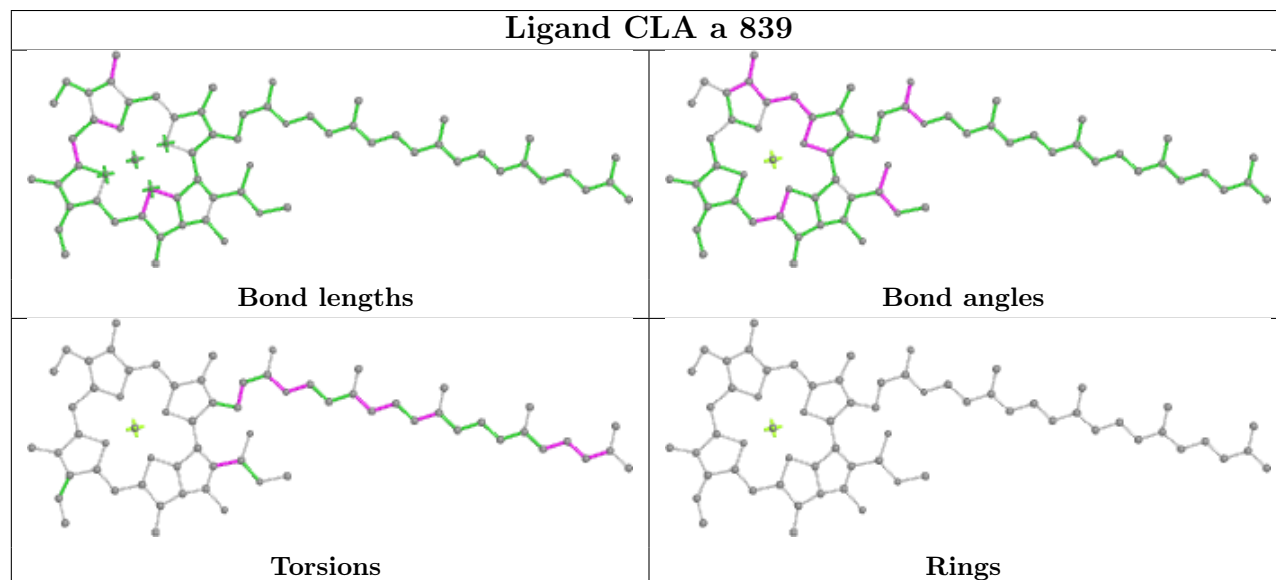
## Ligand BCR b 845



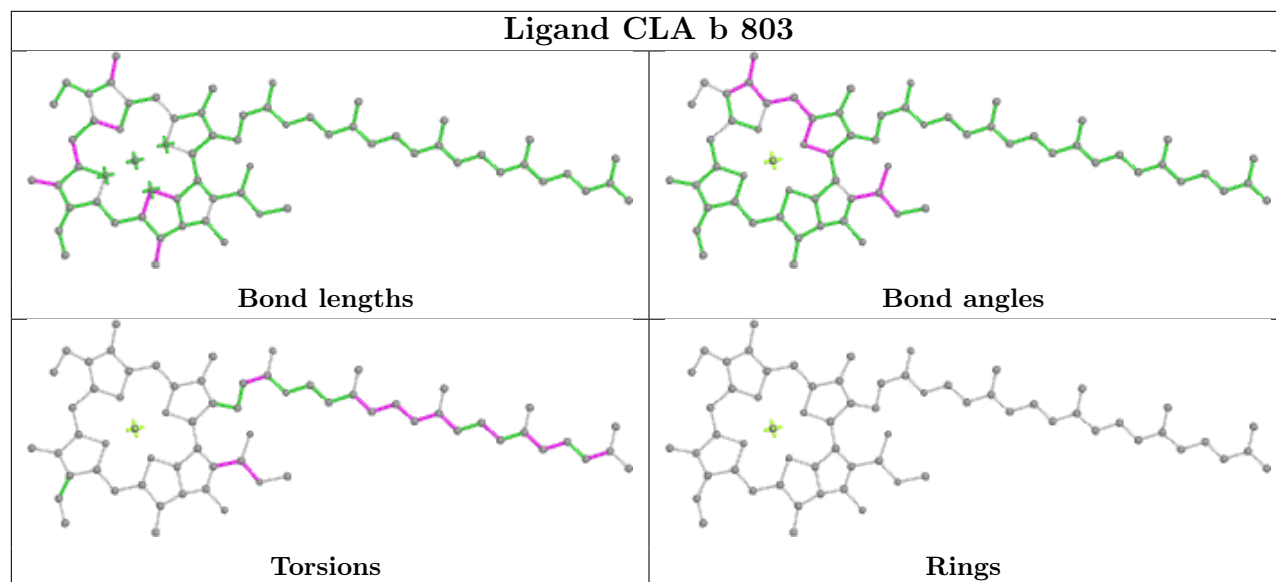
## Ligand LHG 9 317



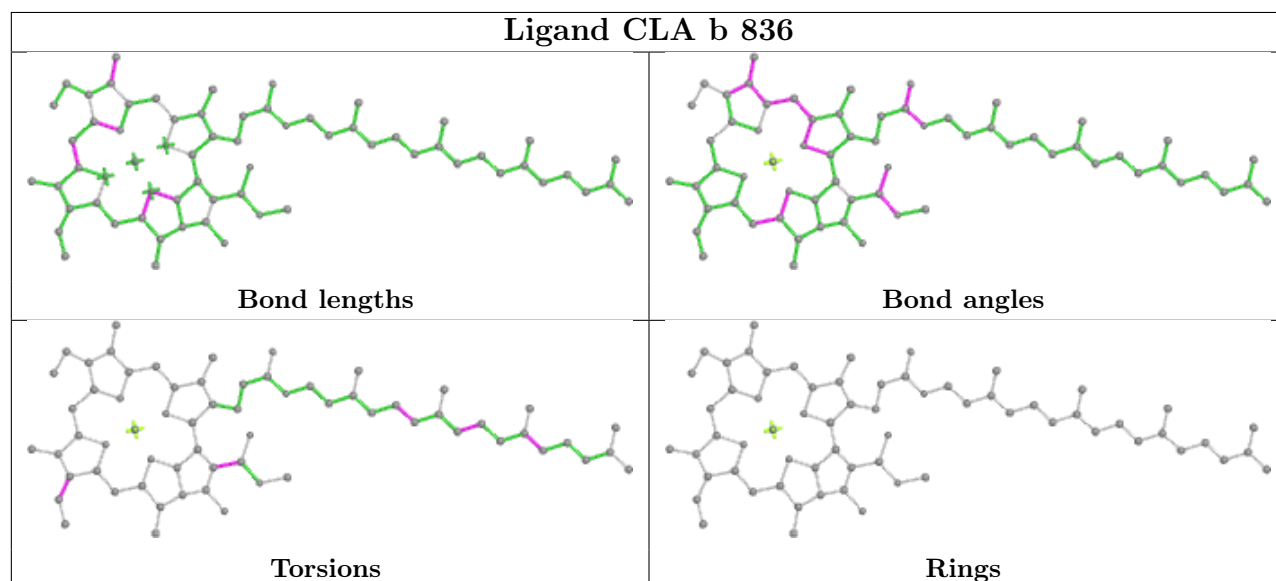
## Ligand CLA a 839



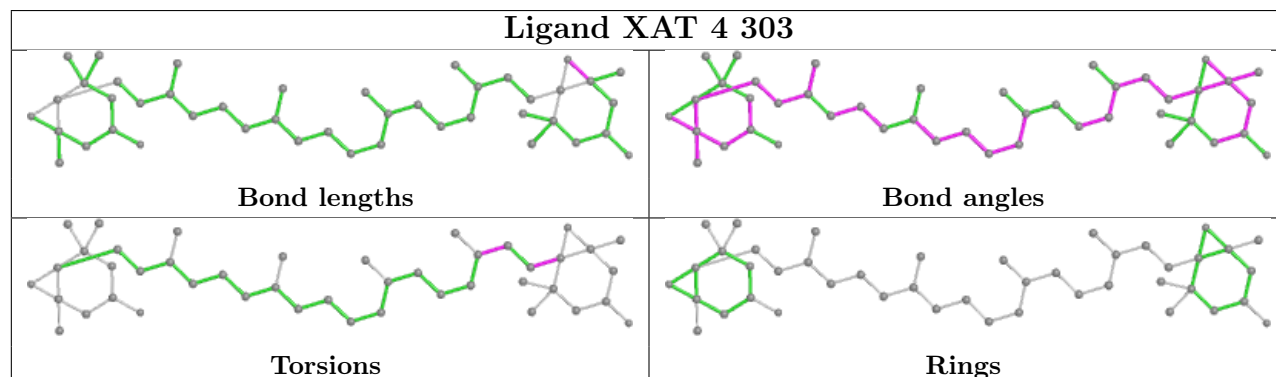
## Ligand CLA b 803

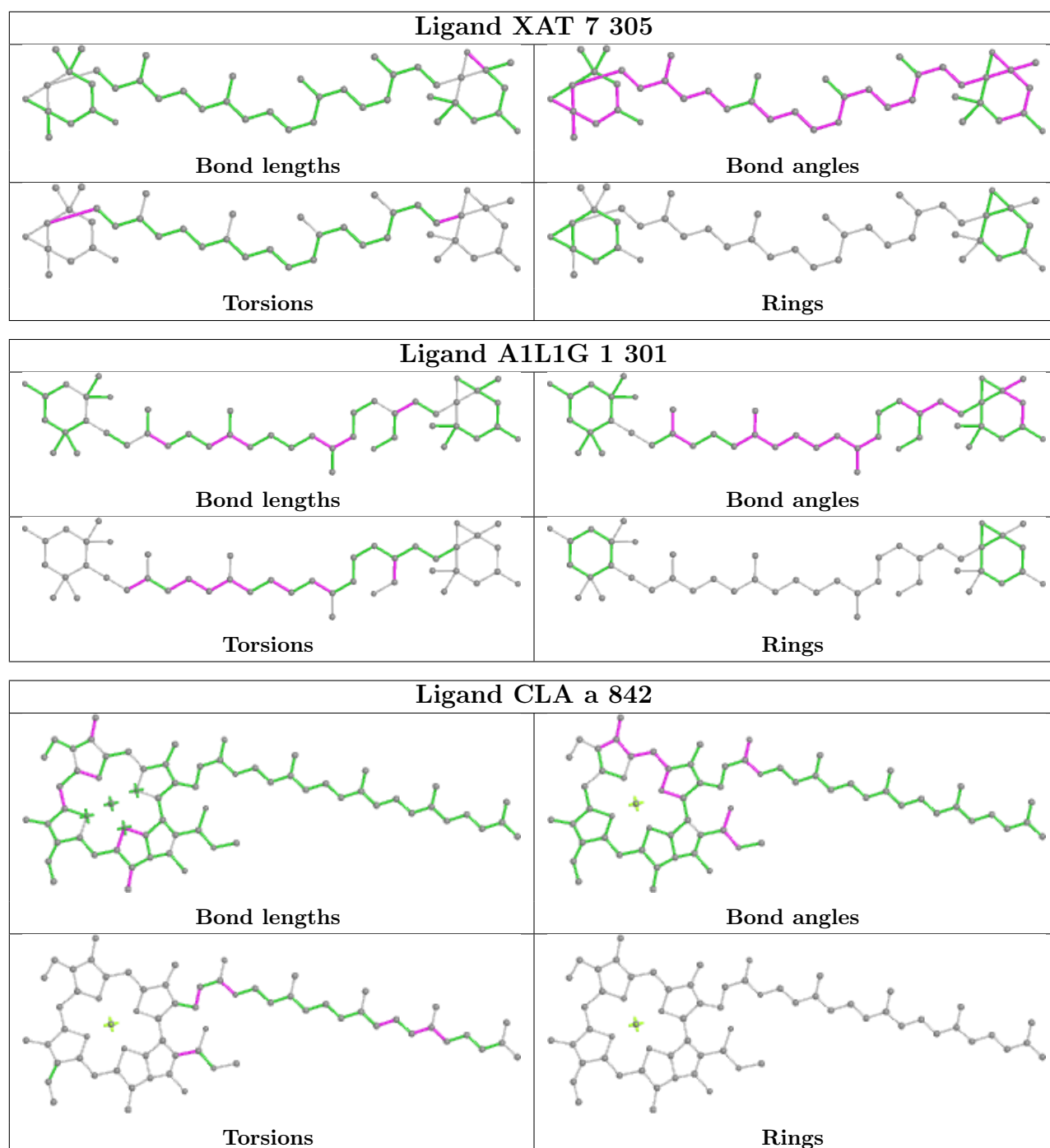


## Ligand CLA b 836



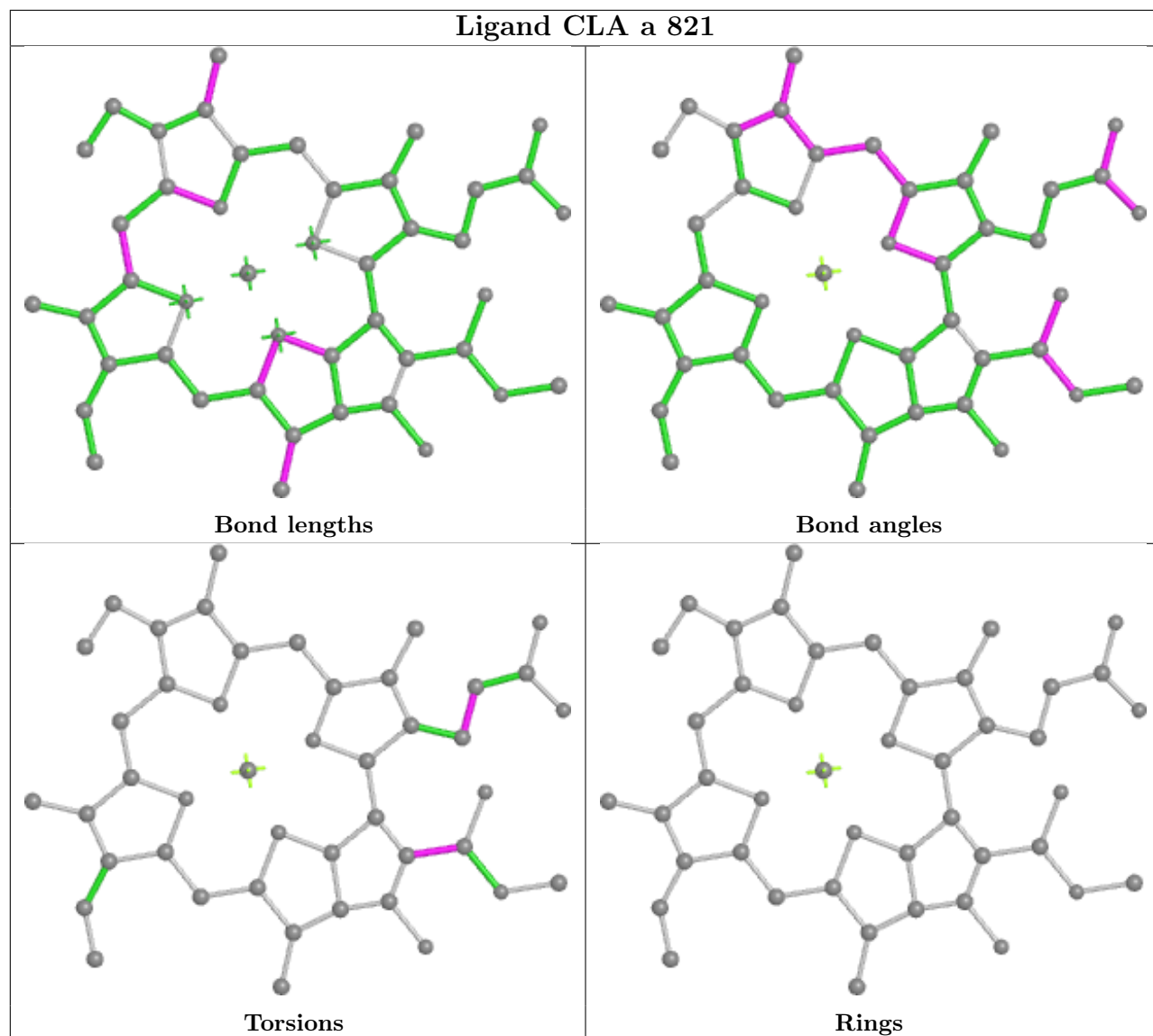
## Ligand XAT 4 303



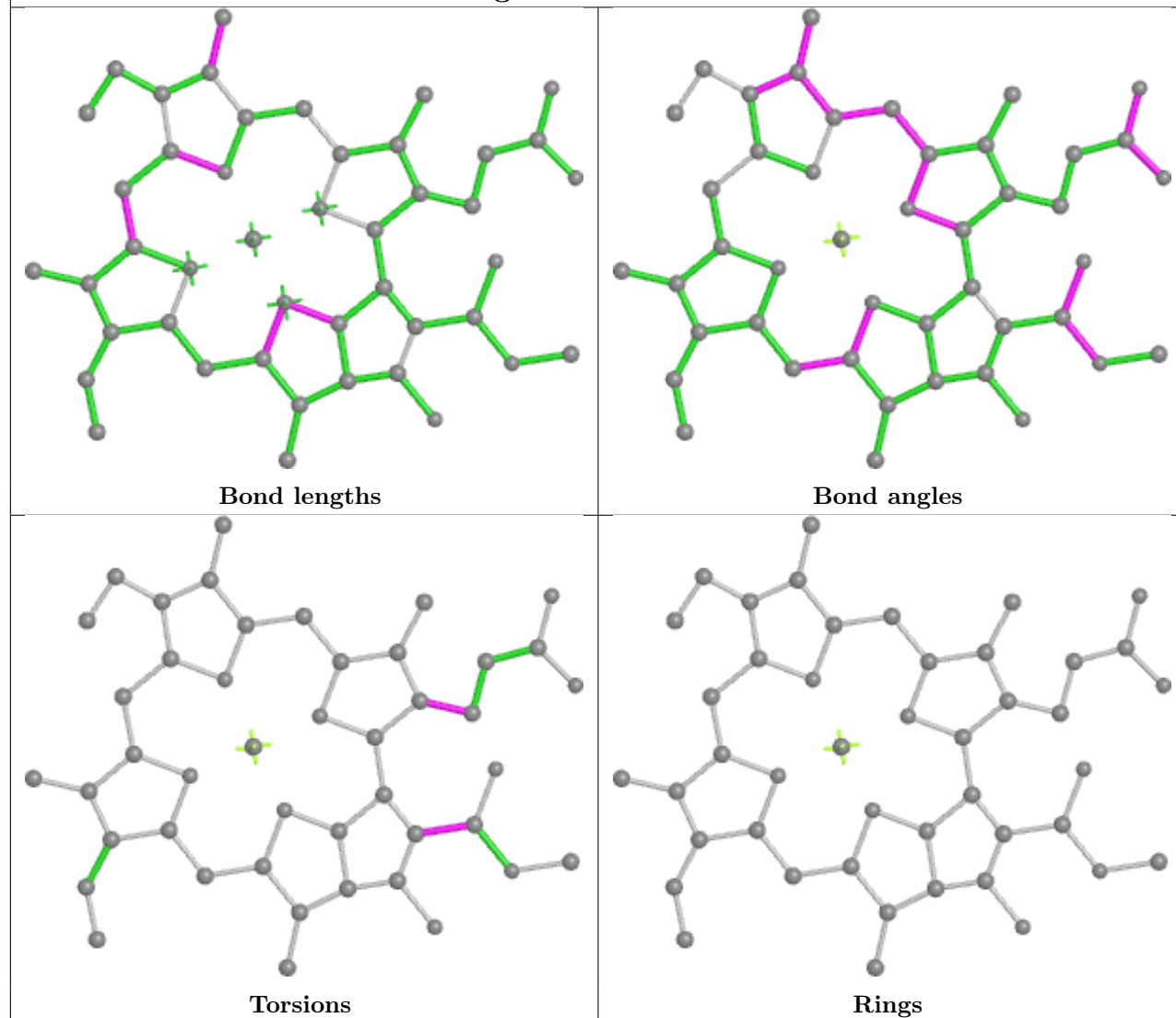




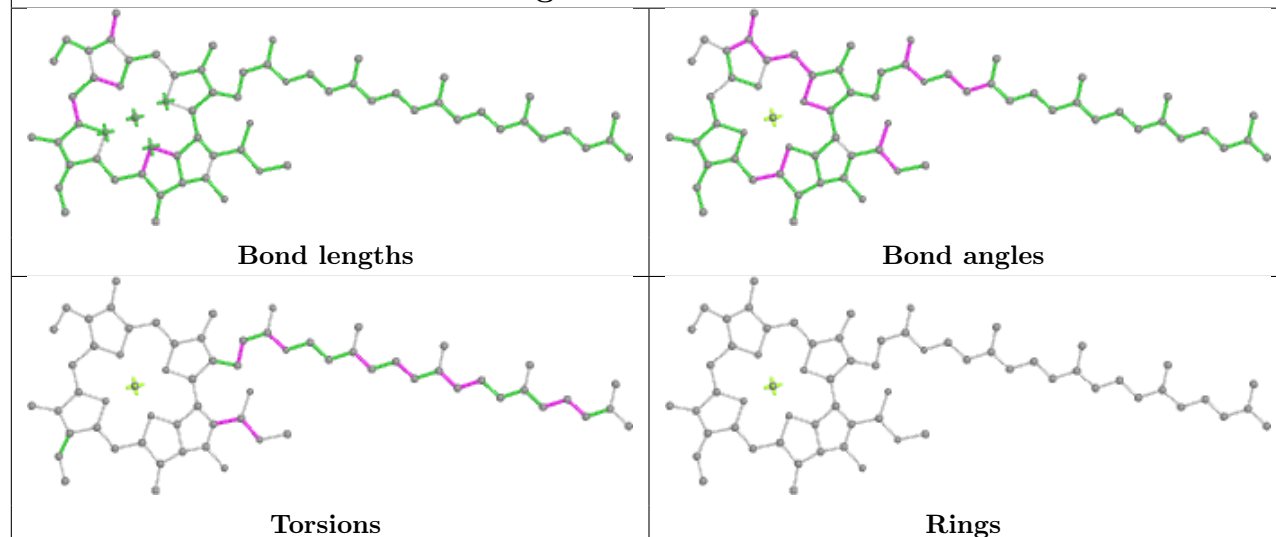
## Ligand CLA a 821



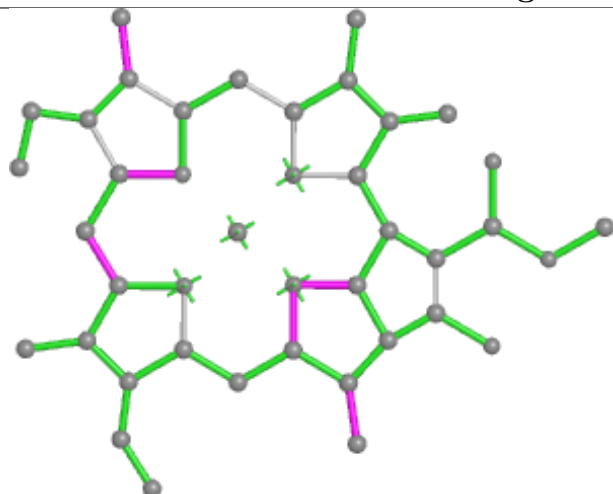
## Ligand CLA a 815



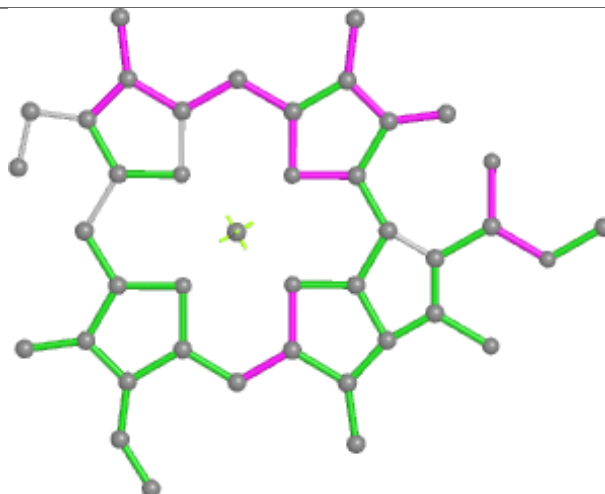
## Ligand CLA a 841



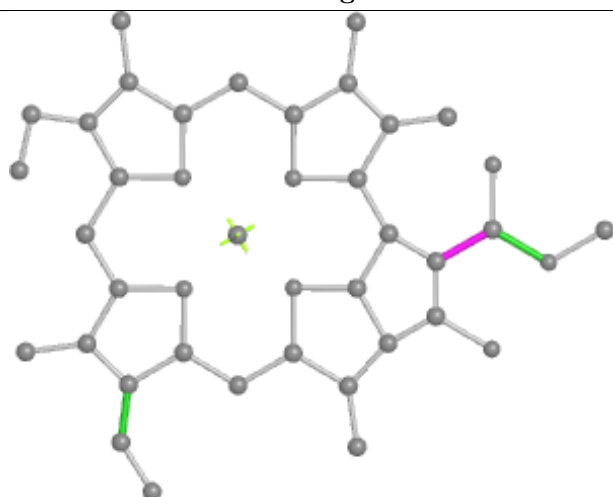
## Ligand CLA b 830



Bond lengths



Bond angles

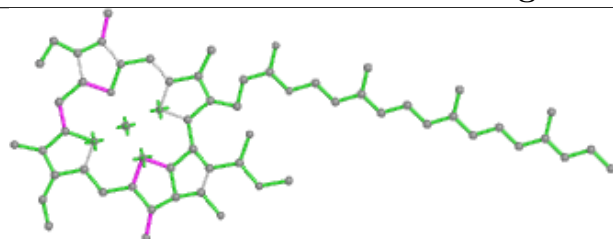


Torsions

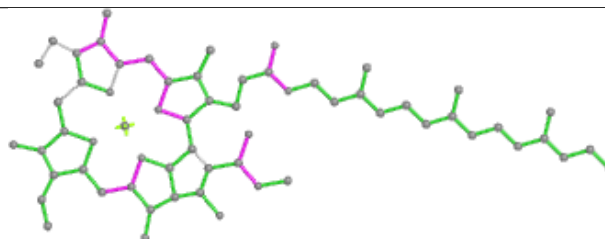


Rings

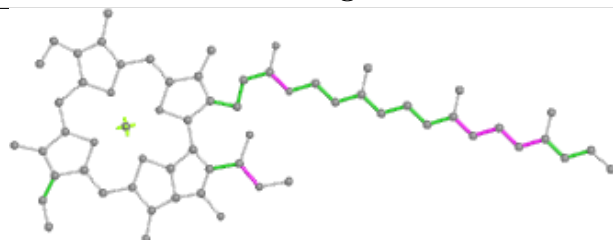
## Ligand CLA 9 318



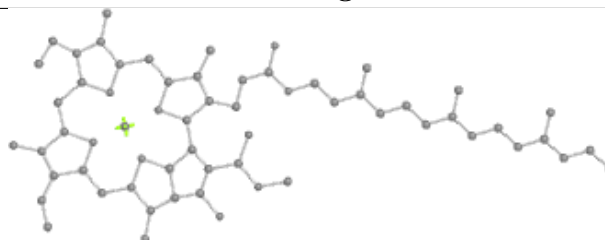
Bond lengths



Bond angles

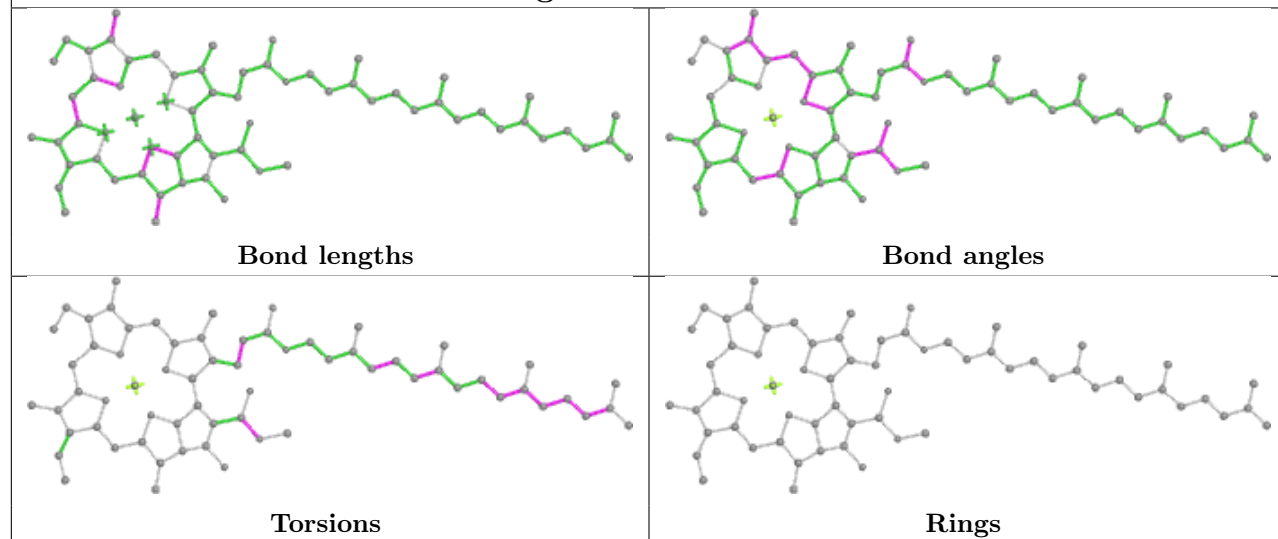


Torsions

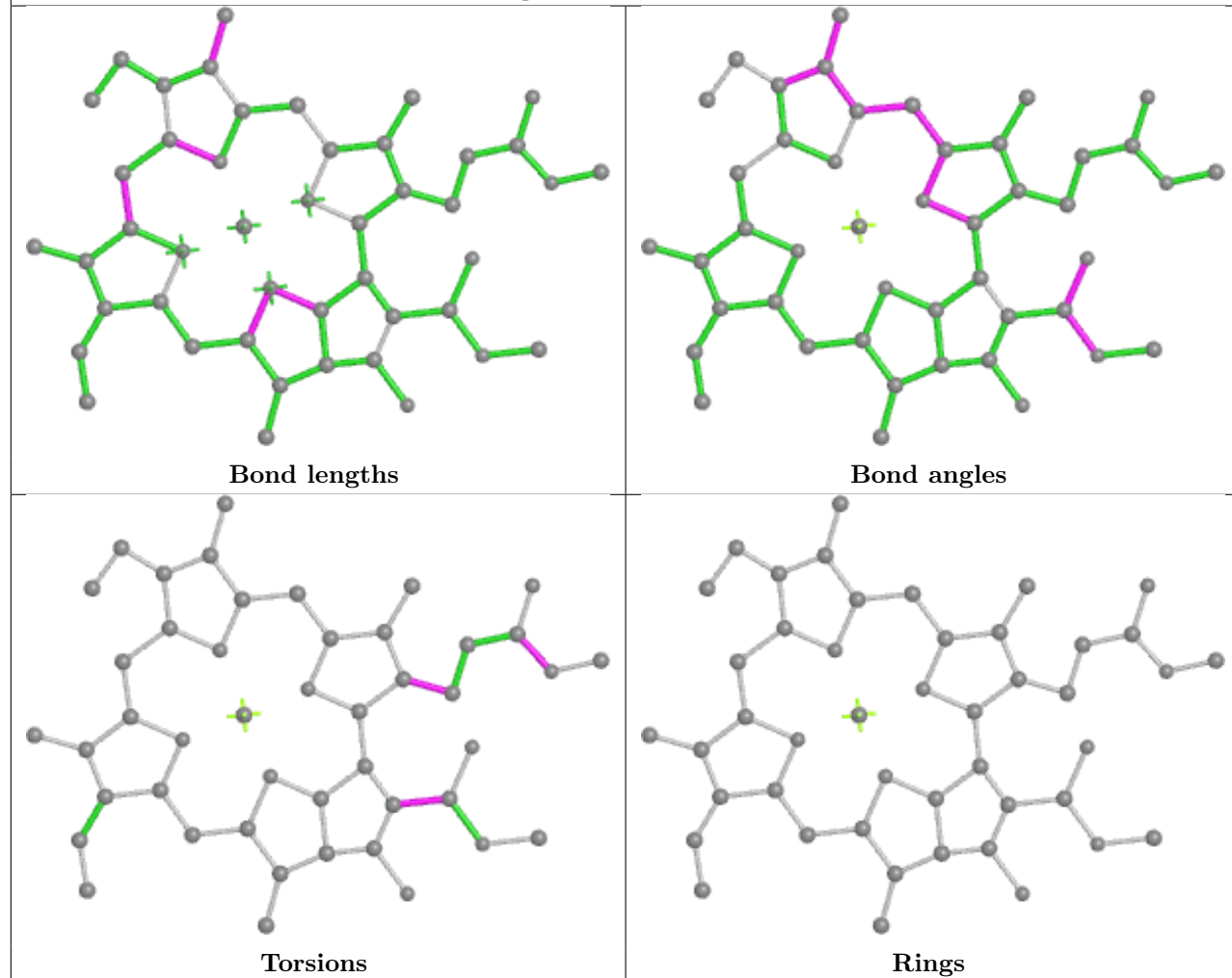


Rings

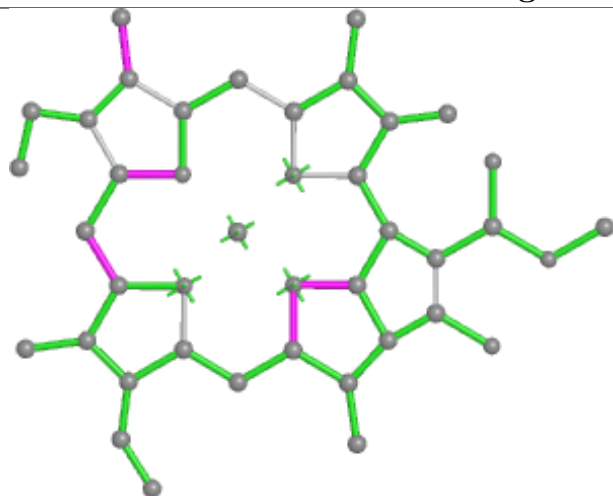
## Ligand CLA 4 308



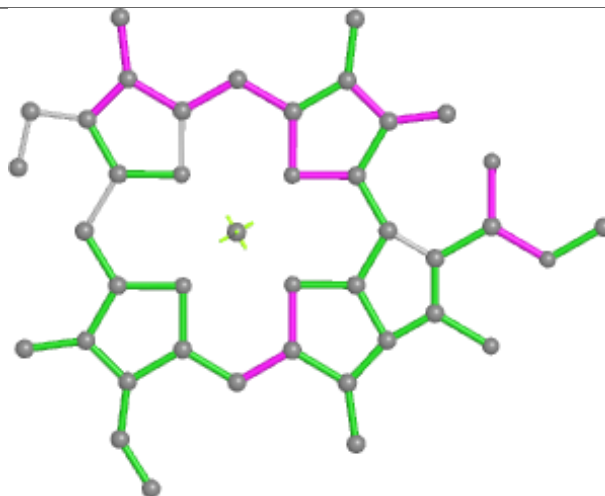
## Ligand CLA 9 310



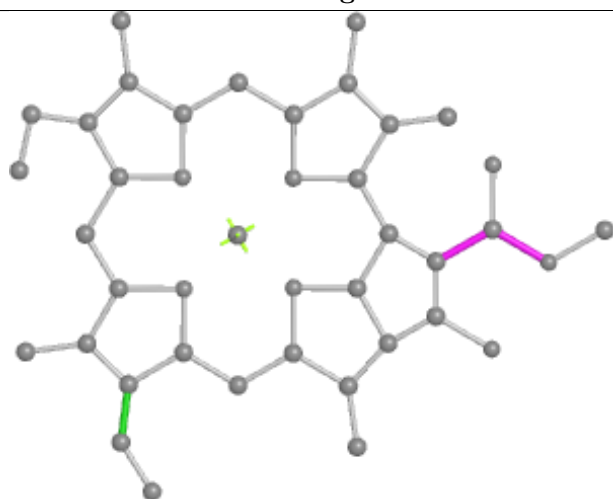
## Ligand CLA 8 314



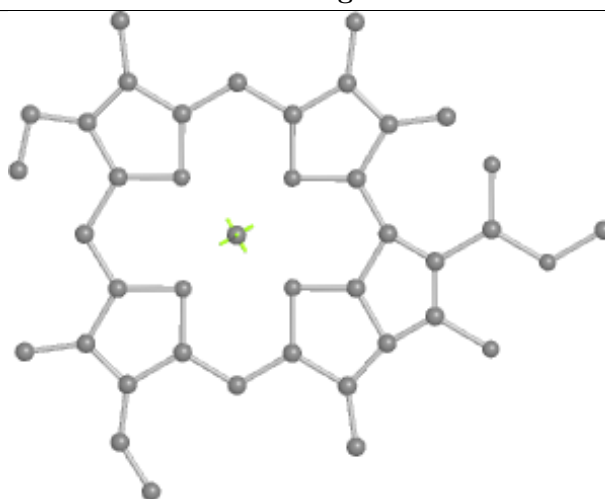
Bond lengths



Bond angles

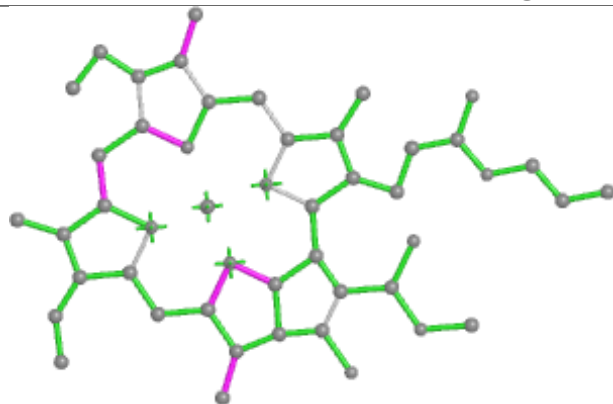


Torsions

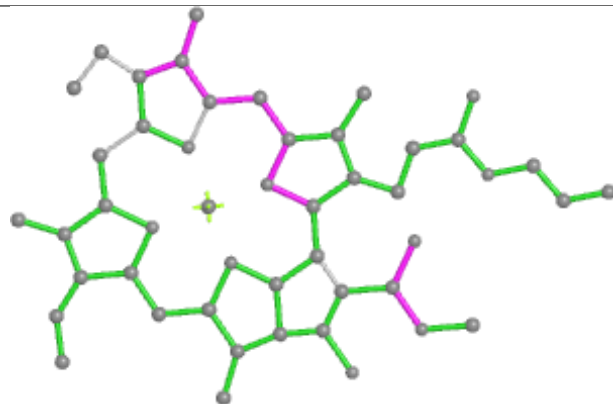


Rings

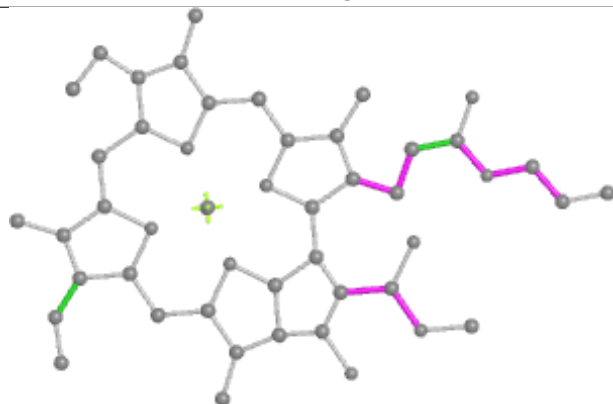
## Ligand CLA 7 306



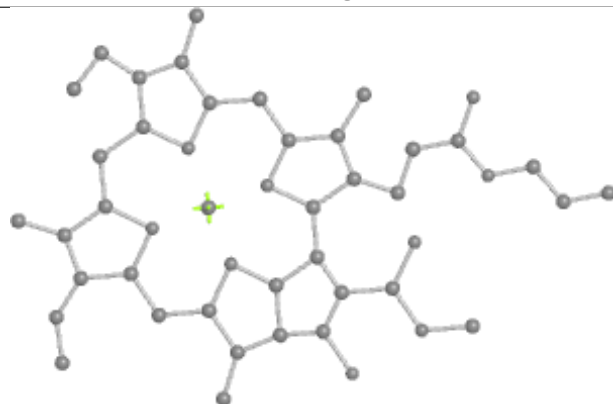
Bond lengths



Bond angles

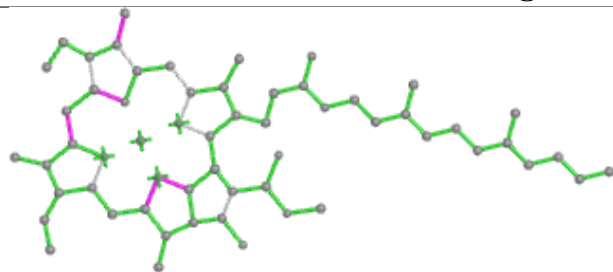


Torsions

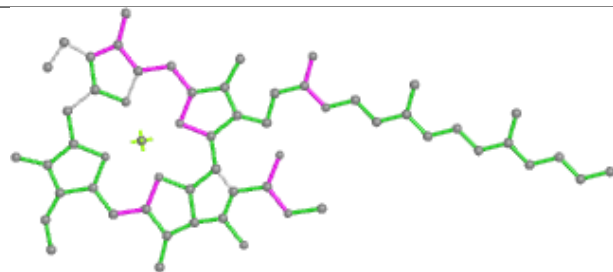


Rings

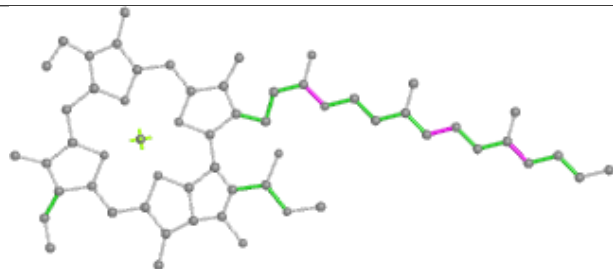
## Ligand CLA 2 311



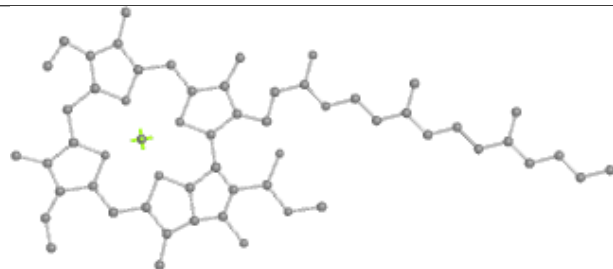
Bond lengths



Bond angles

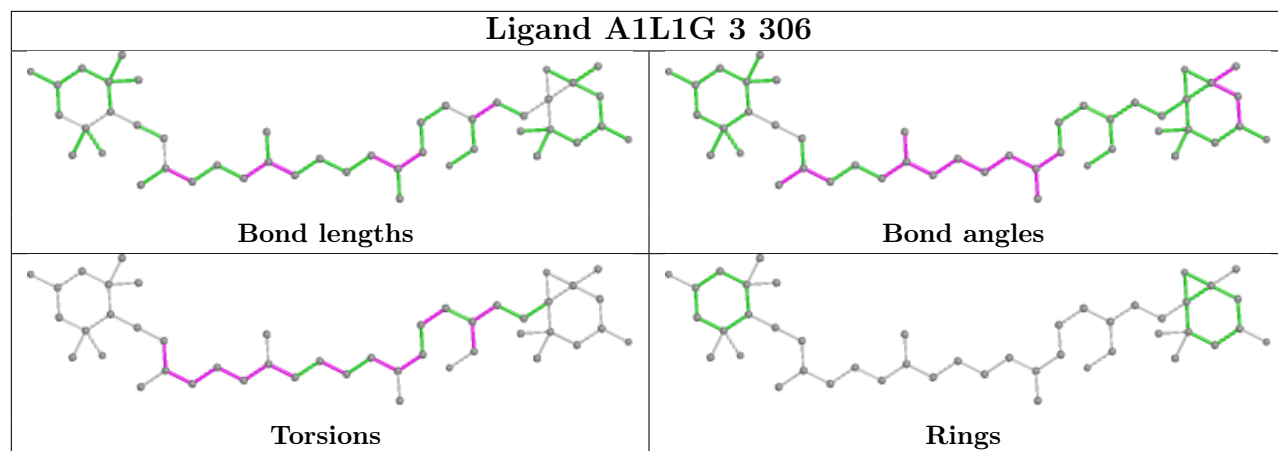


Torsions

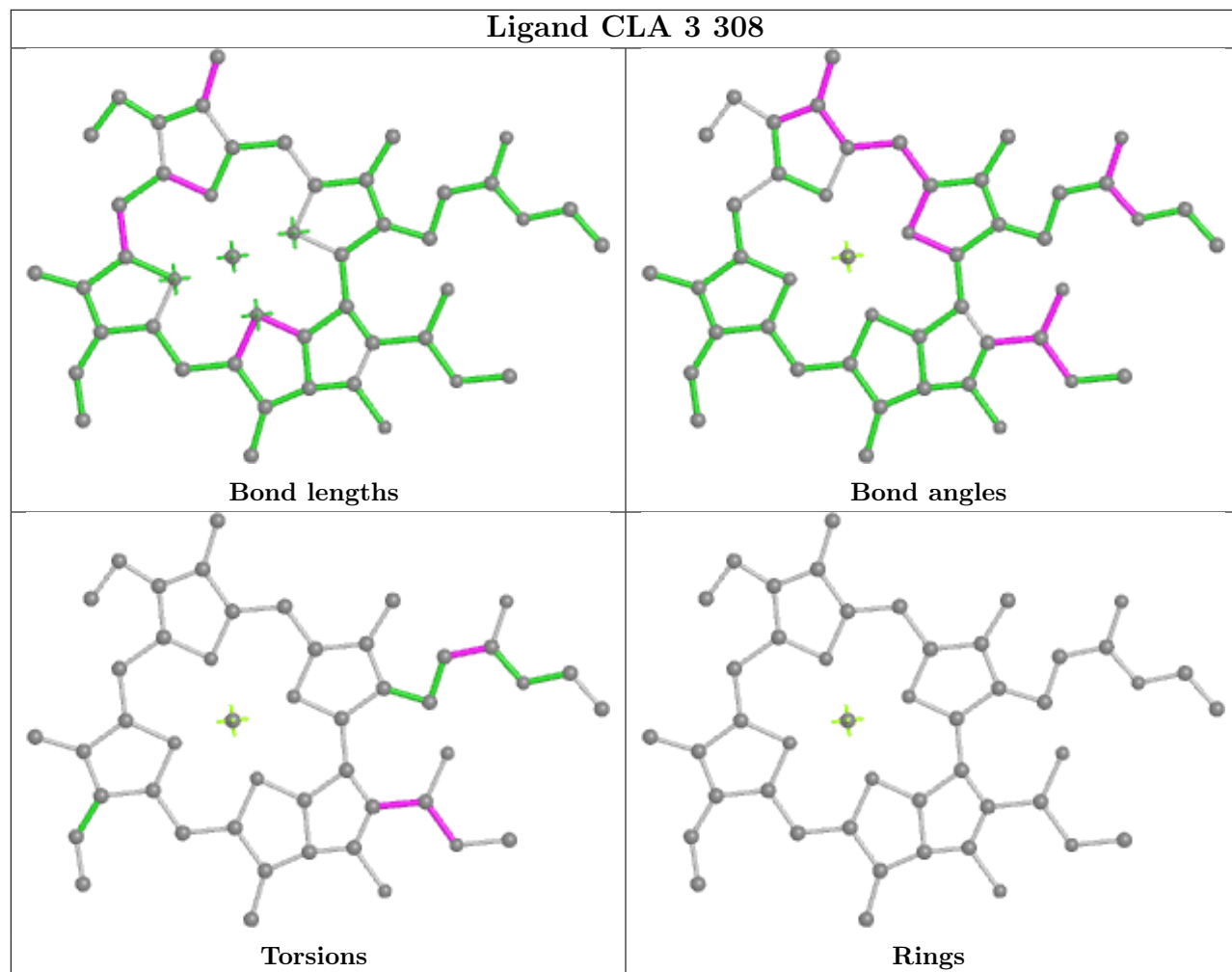


Rings

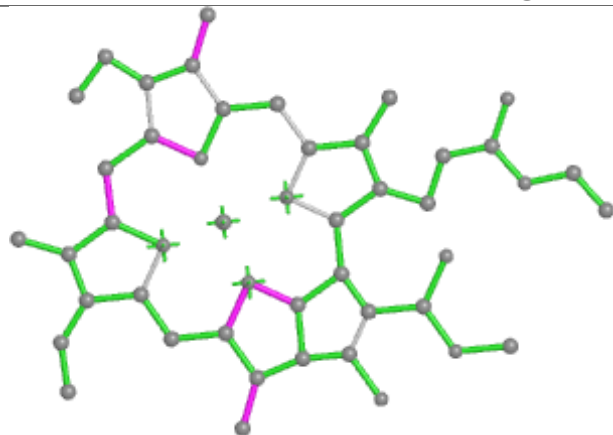
## Ligand A1L1G 3 306



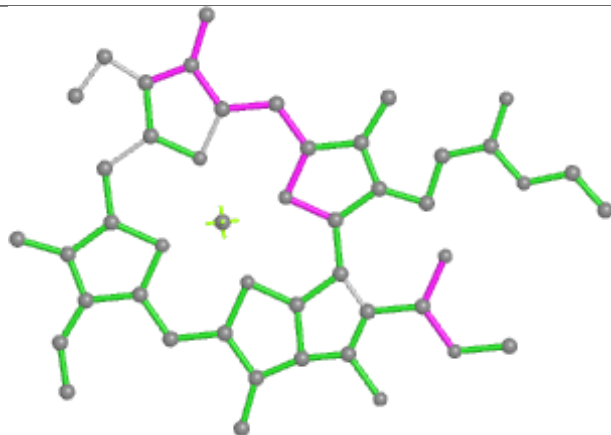
## Ligand CLA 3 308



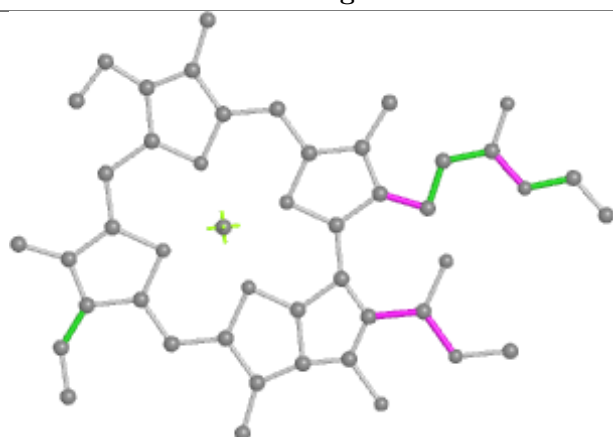
## Ligand CLA 3 314



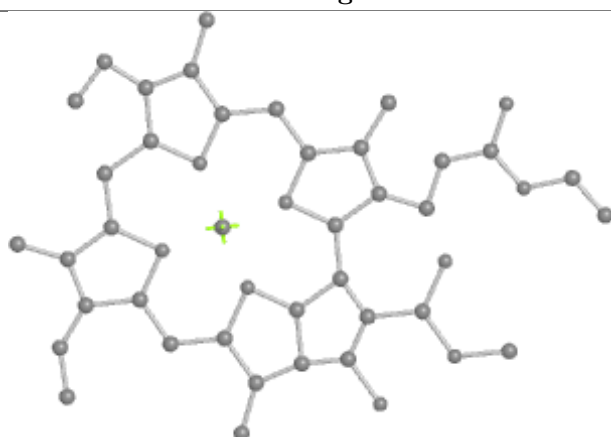
Bond lengths



Bond angles

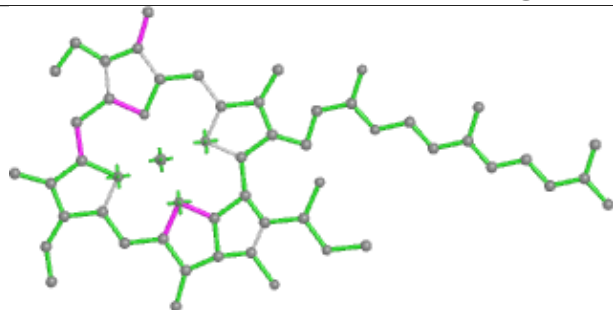


Torsions

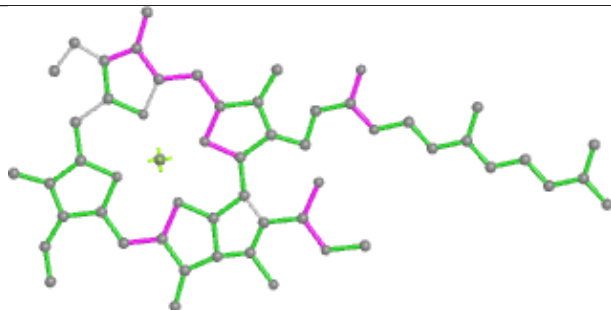


Rings

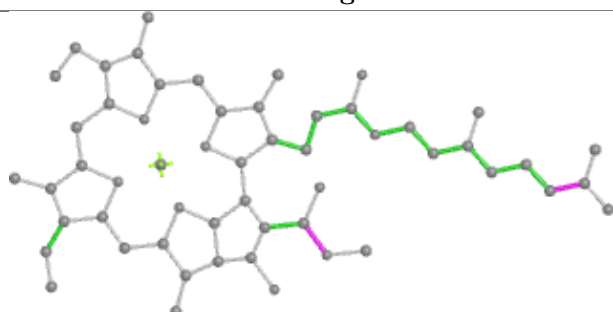
## Ligand CLA b 819



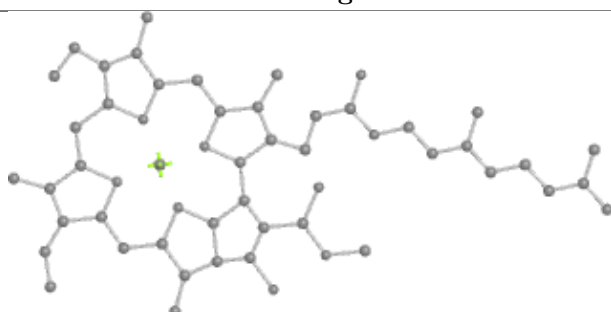
Bond lengths



Bond angles



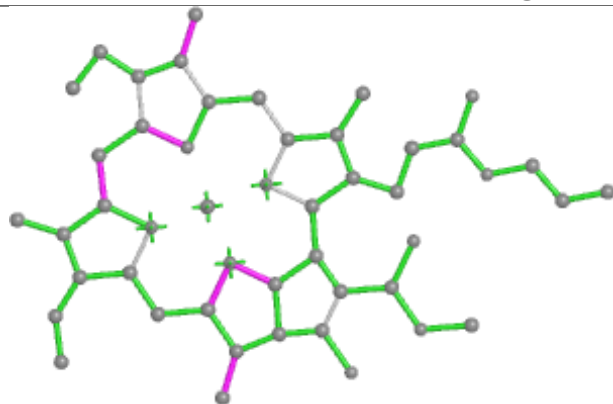
Torsions



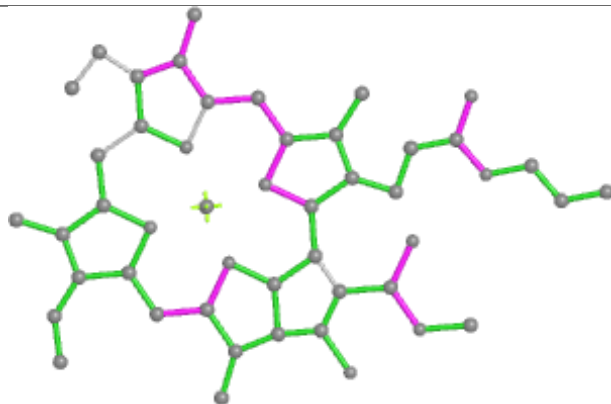
Rings



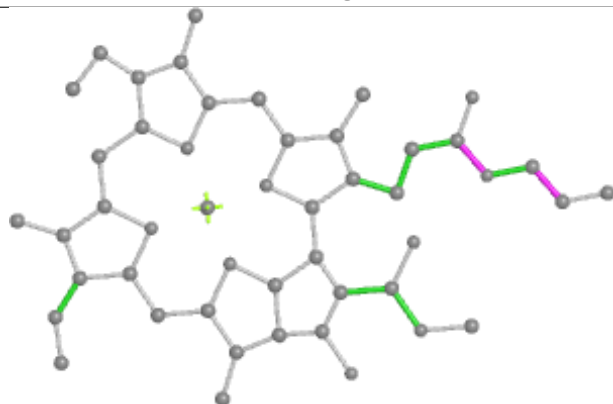
## Ligand CLA 7 312



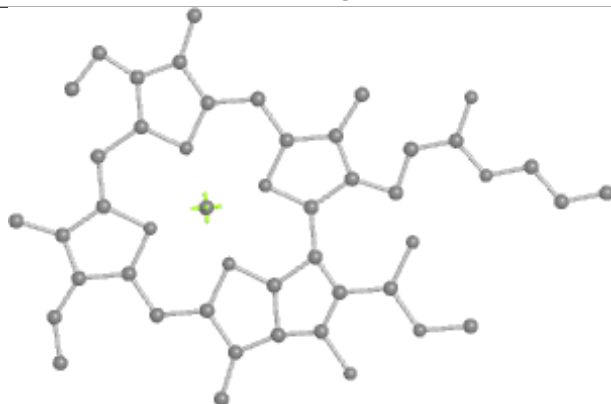
Bond lengths



Bond angles

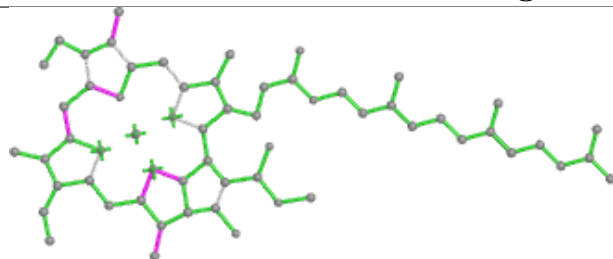


Torsions

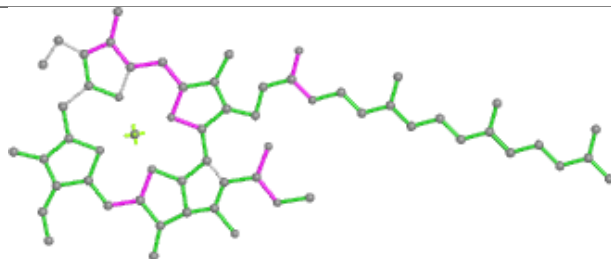


Rings

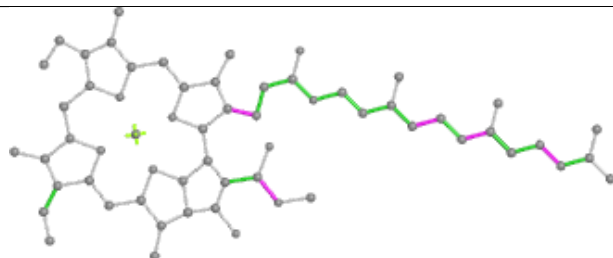
## Ligand CLA b 822



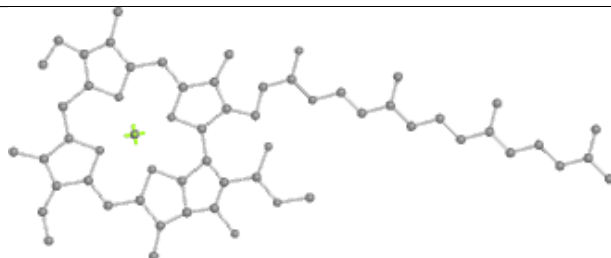
Bond lengths



Bond angles

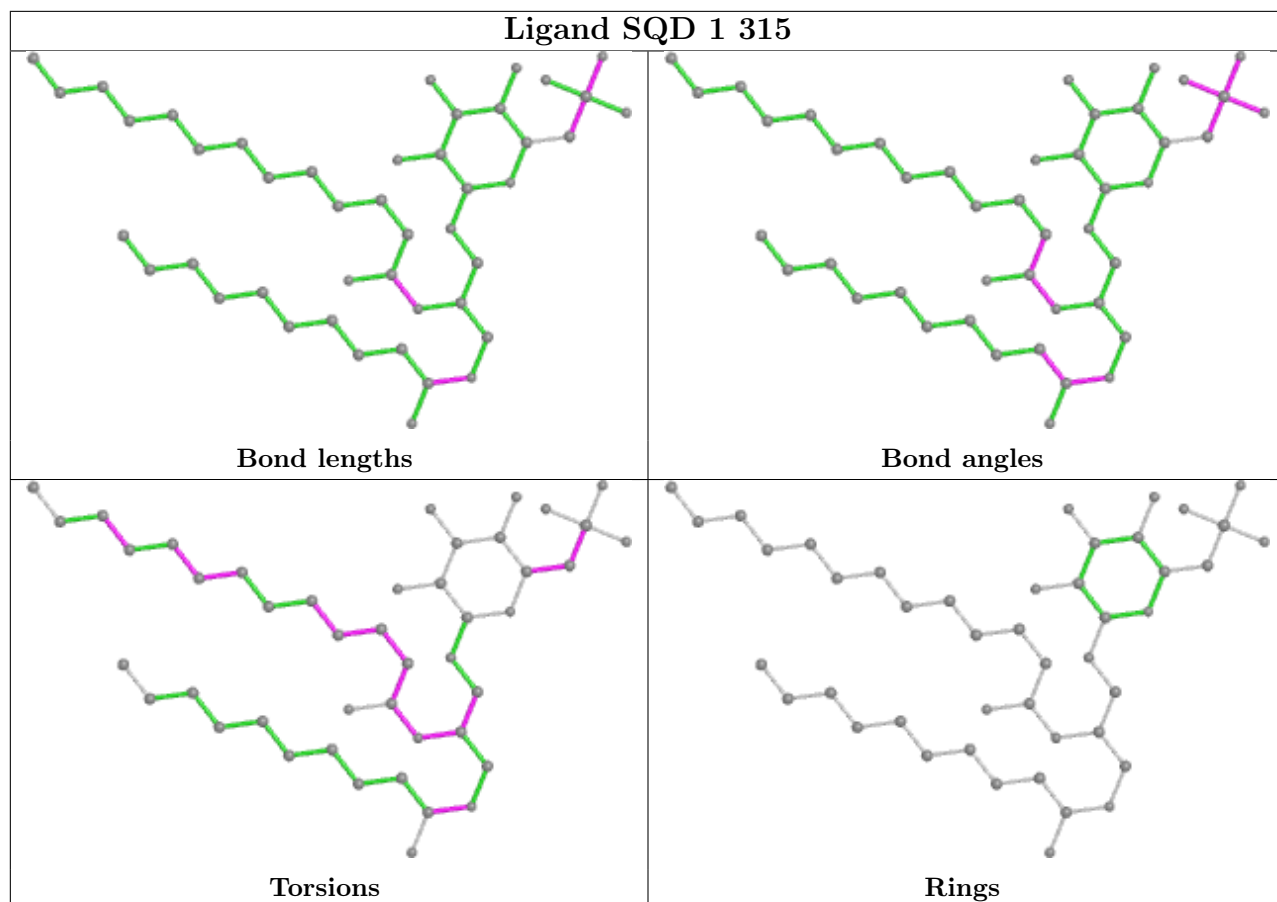


Torsions

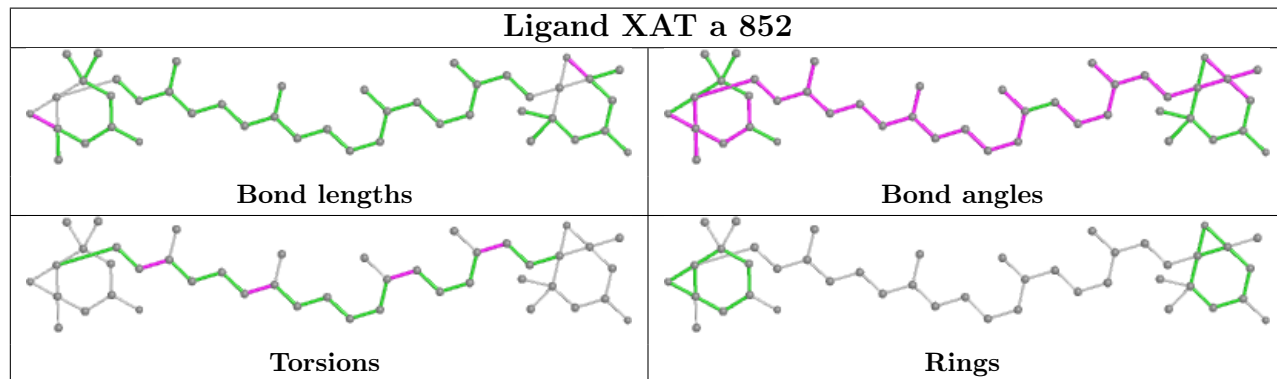


Rings

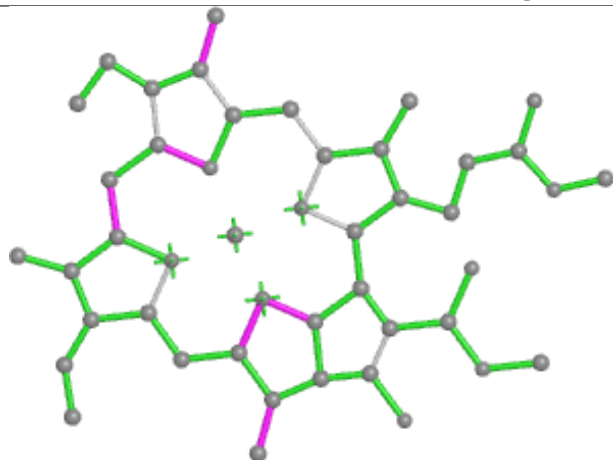
## Ligand SQD 1 315



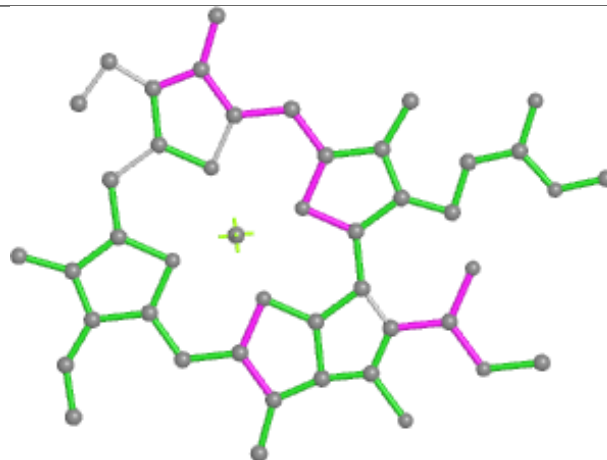
## Ligand XAT a 852



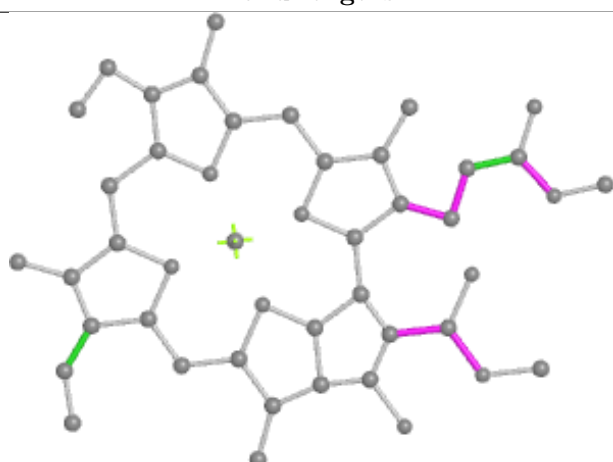
## Ligand CLA 4 311



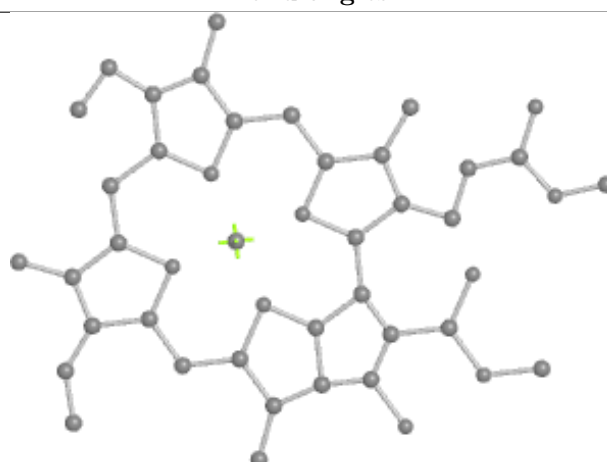
Bond lengths



Bond angles

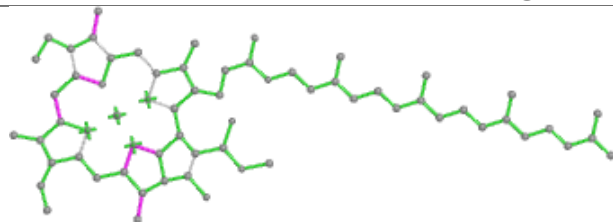


Torsions

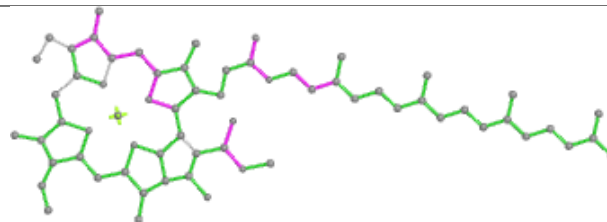


Rings

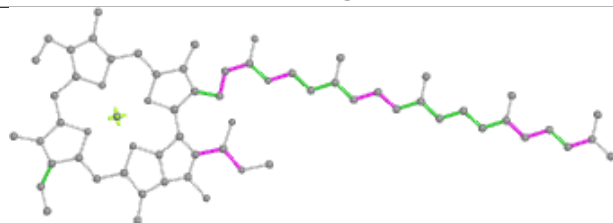
## Ligand CLA a 810



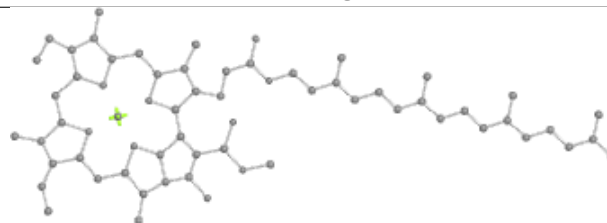
Bond lengths



Bond angles

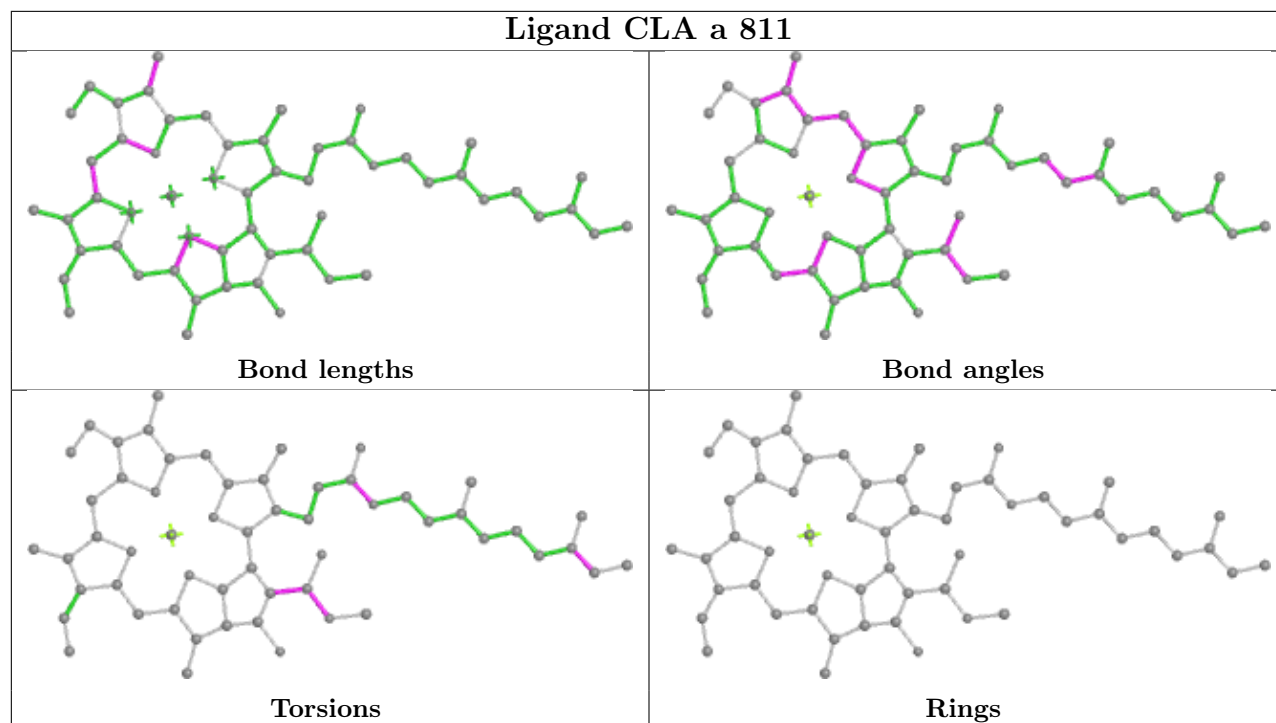


Torsions

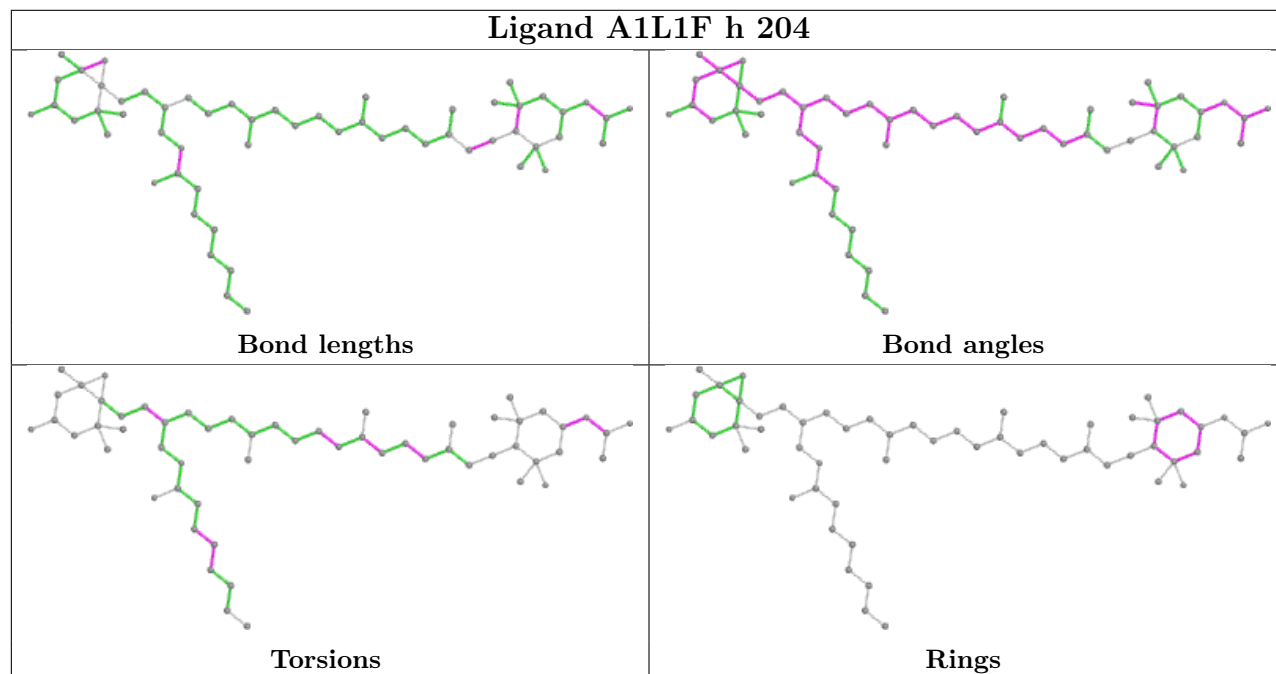


Rings

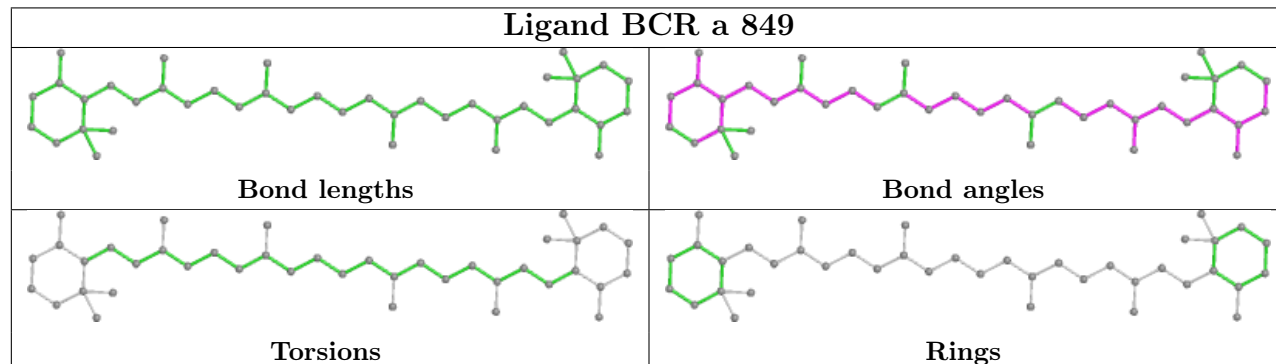
## Ligand CLA a 811

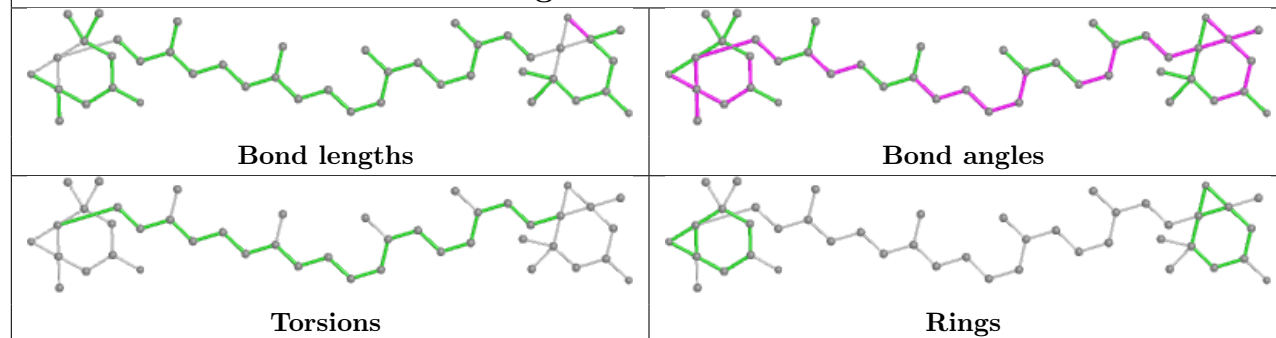
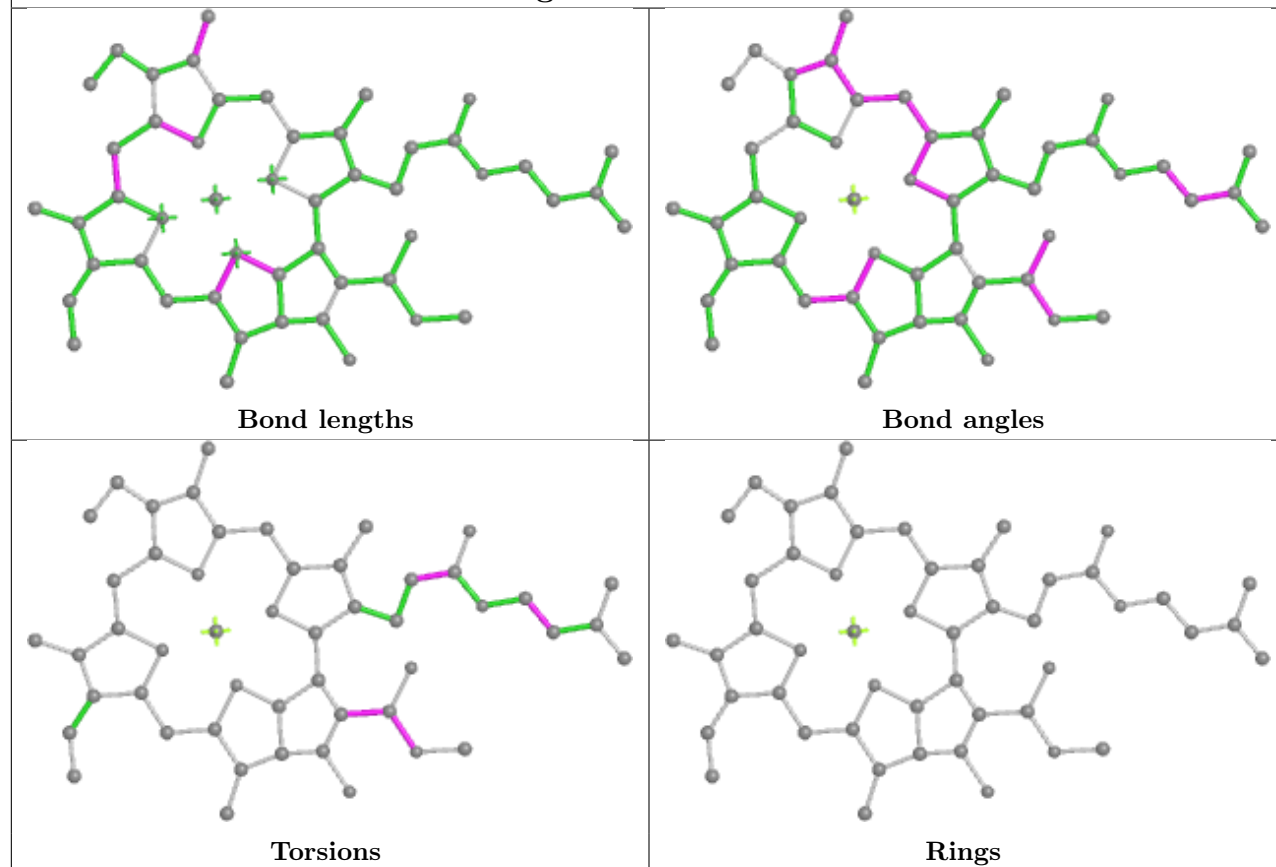


## Ligand A1L1F h 204

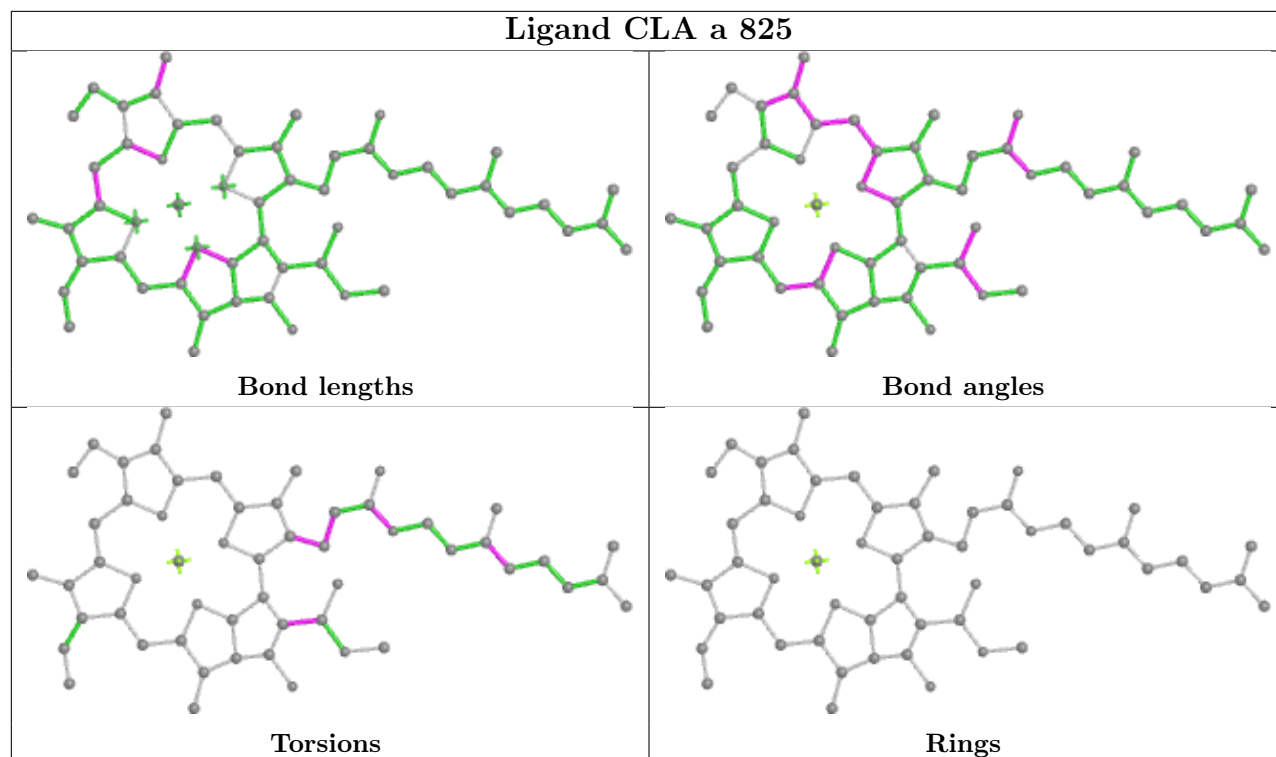


## Ligand BCR a 849

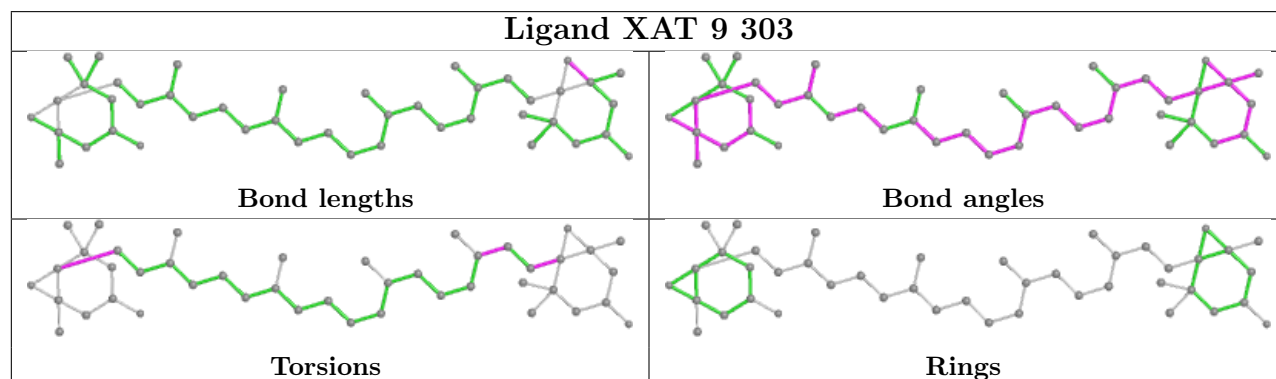


**Ligand XAT 1 302****Ligand CLA 4 309**

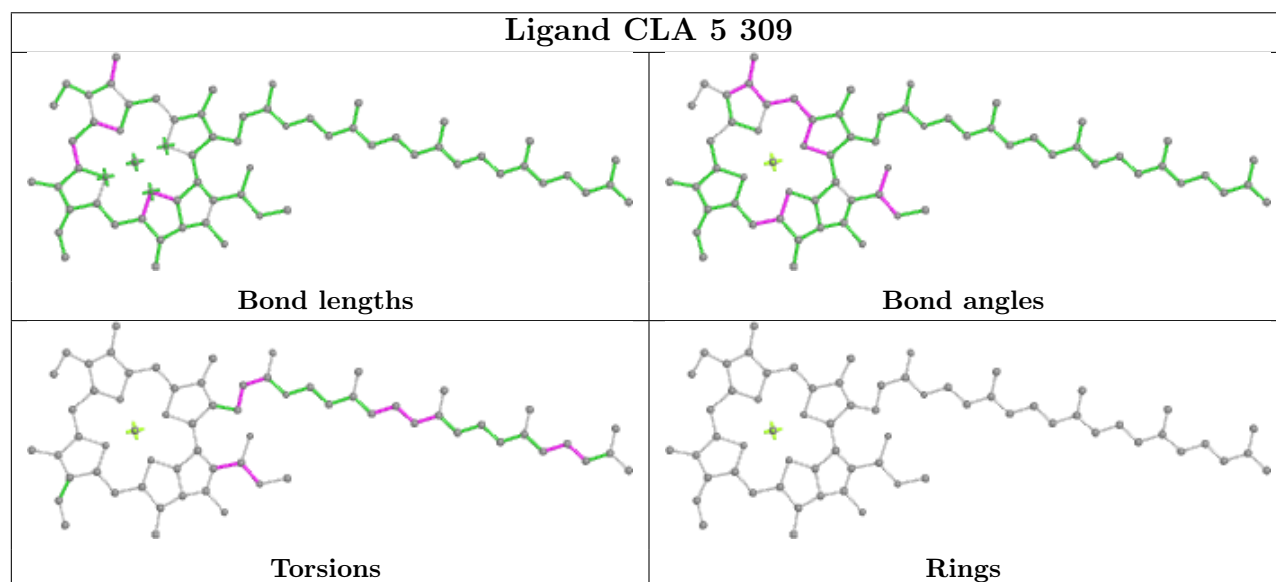
## Ligand CLA a 825



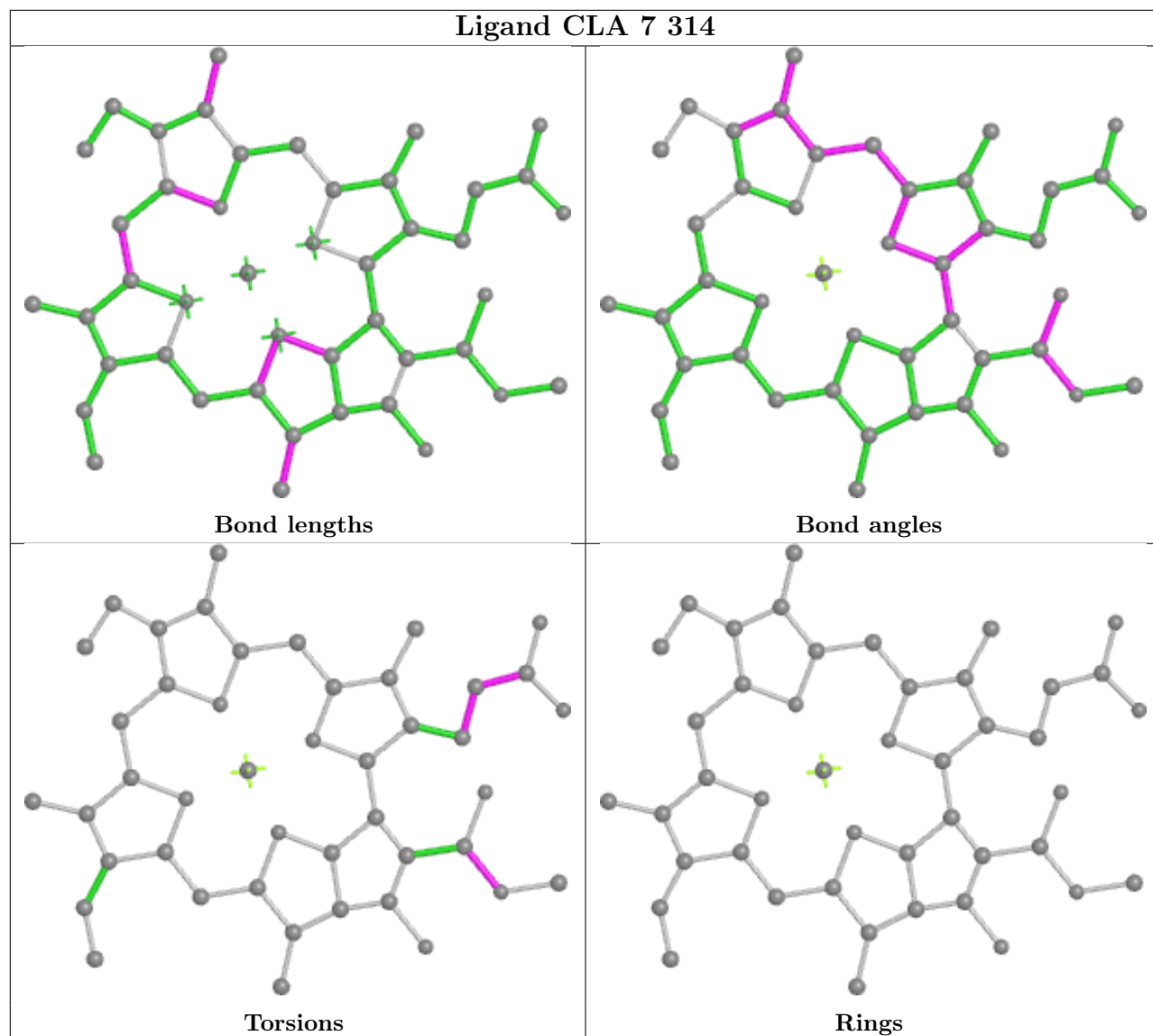
## Ligand XAT 9 303



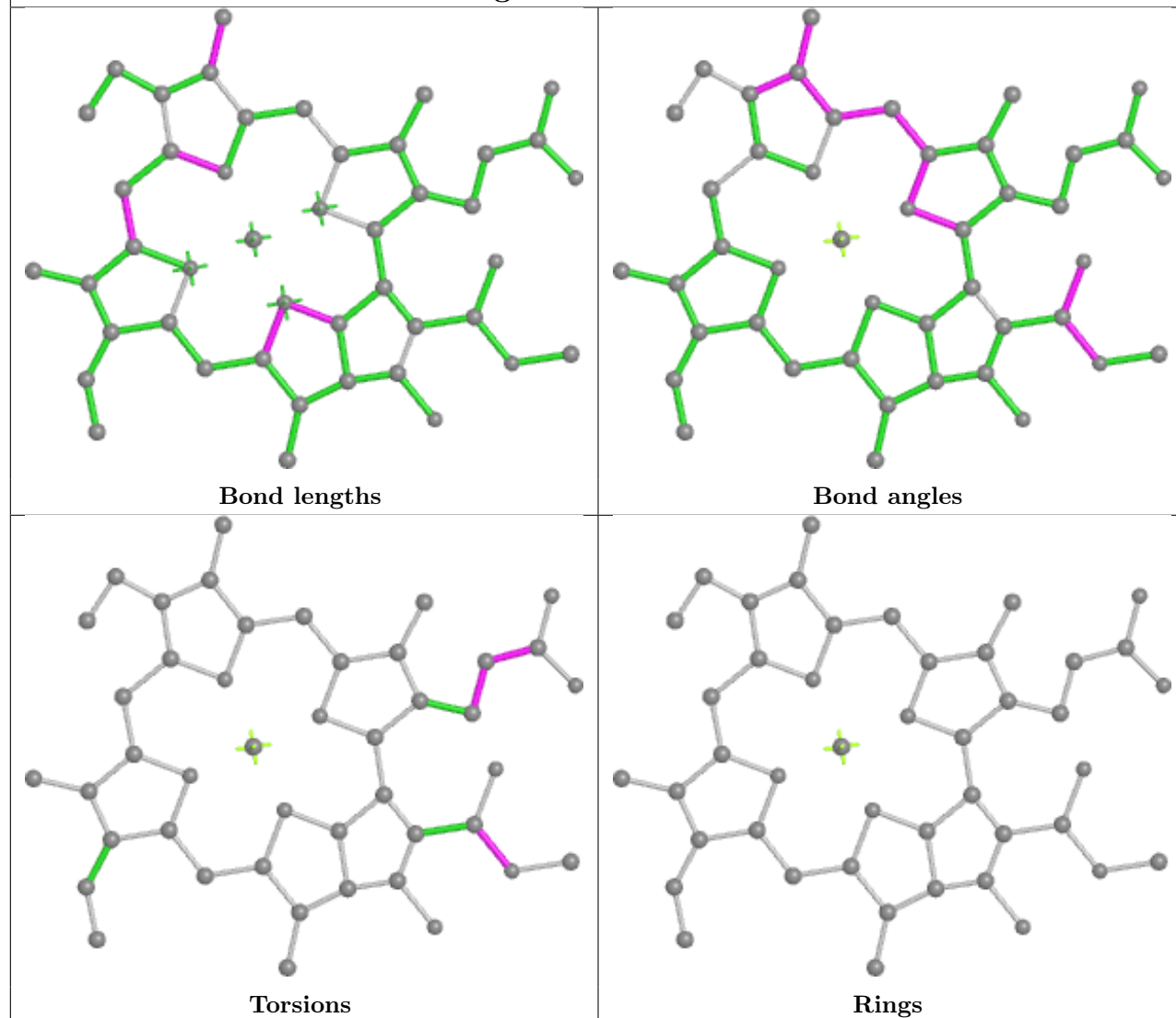
## Ligand CLA 5 309



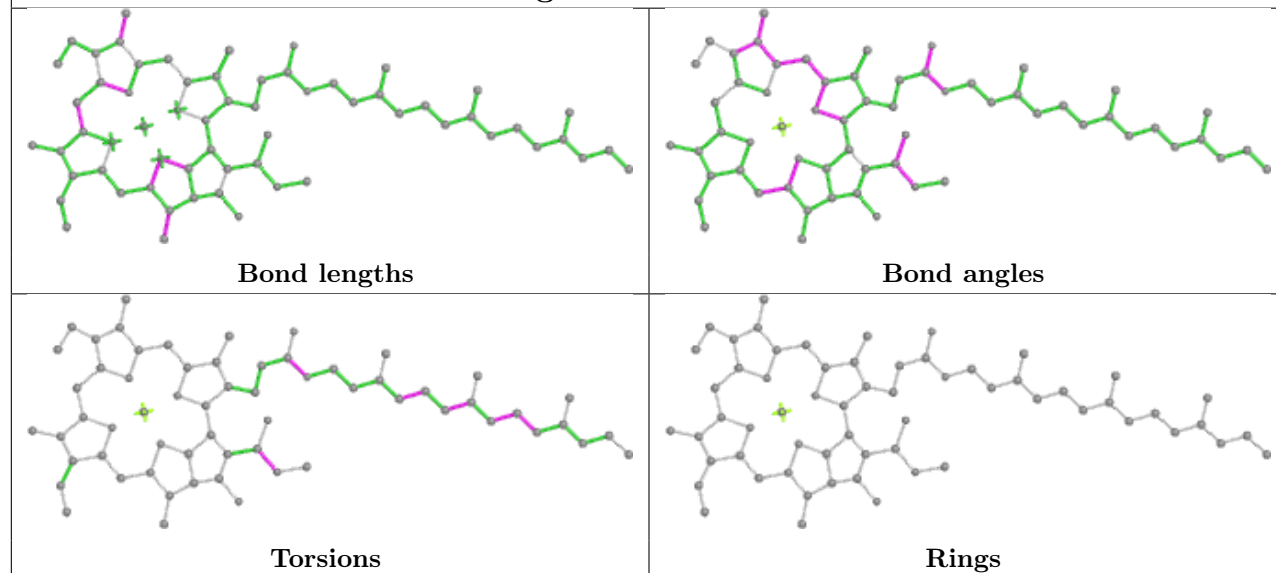
## Ligand CLA 7 314



## Ligand CLA 7 317

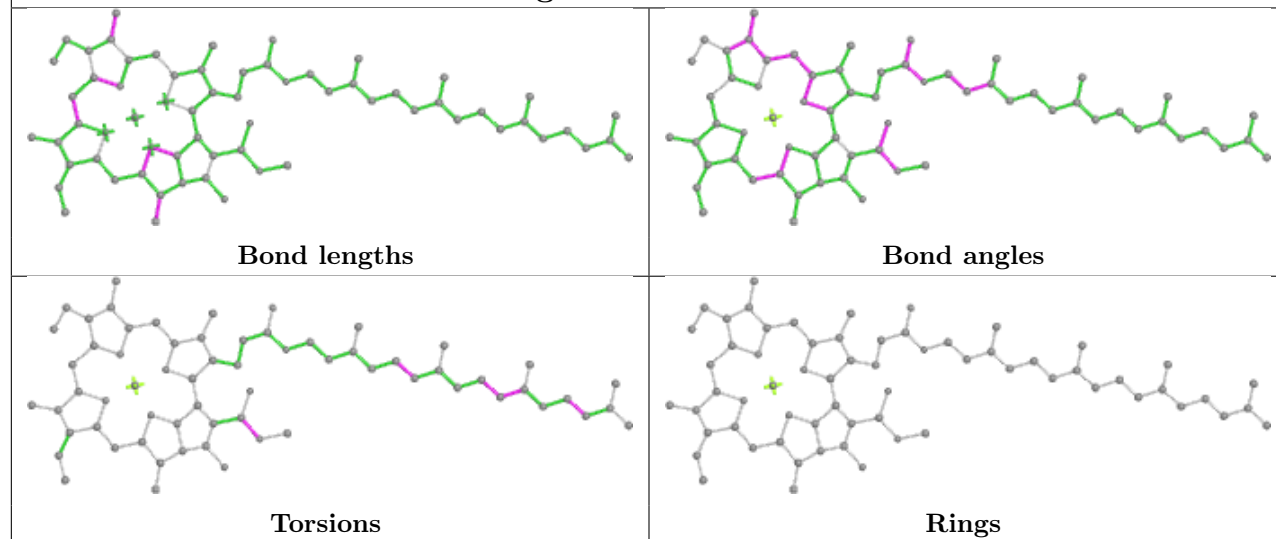


## Ligand CLA a 812

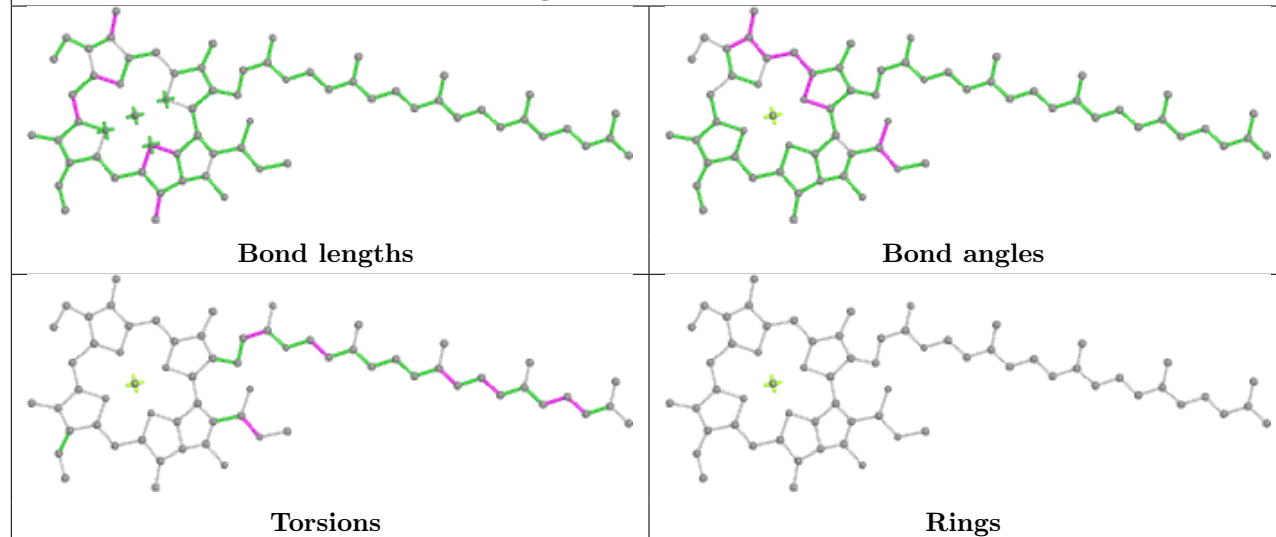




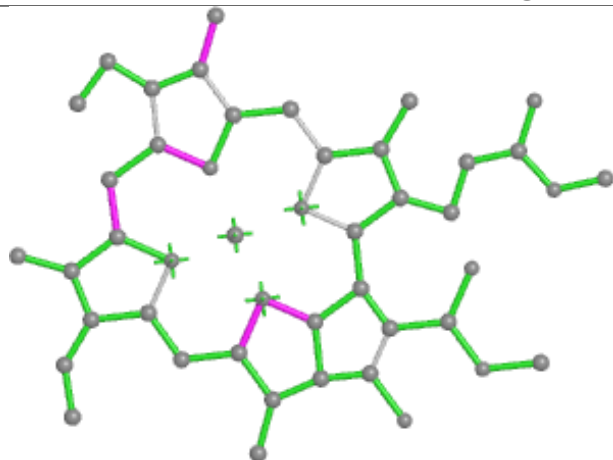
## Ligand CLA a 834



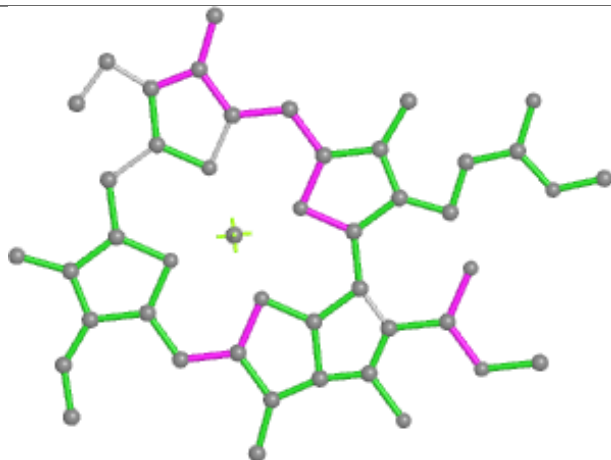
## Ligand CLA a 826



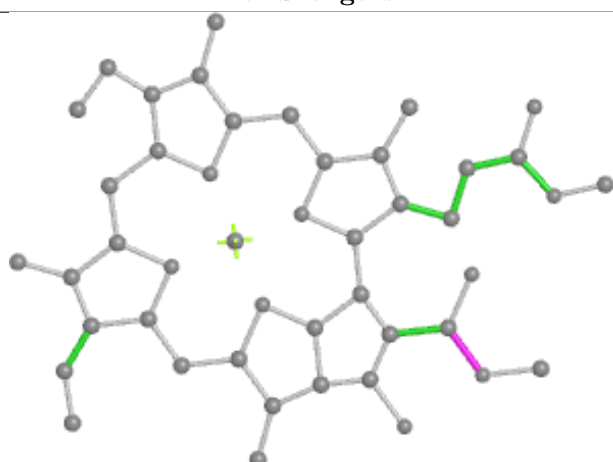
## Ligand CLA 8 306



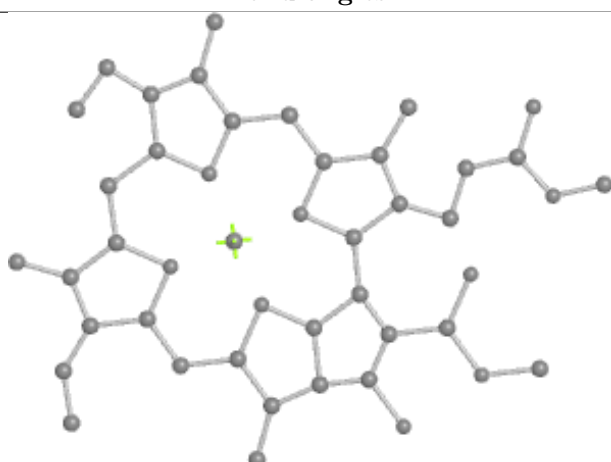
Bond lengths



Bond angles

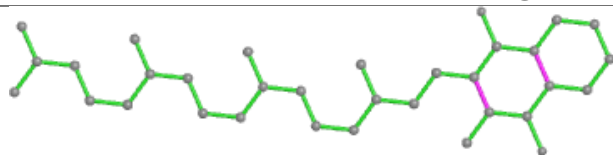


Torsions

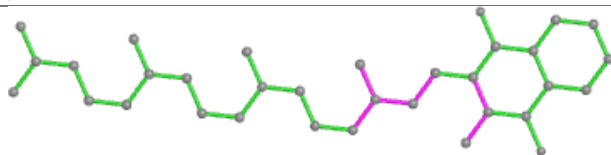


Rings

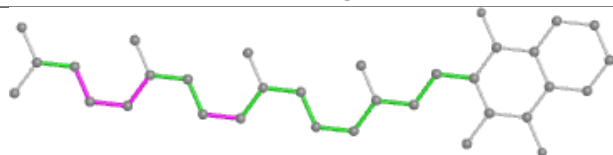
## Ligand PQN a 843



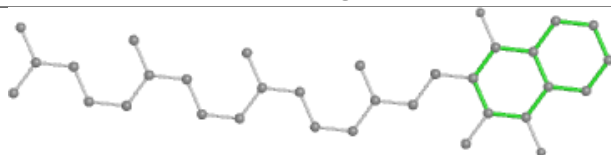
Bond lengths



Bond angles

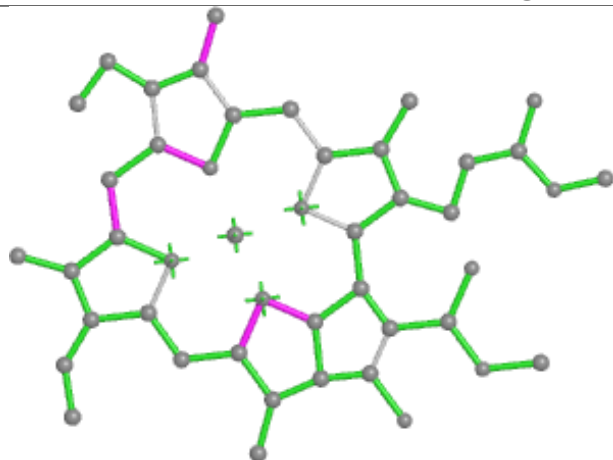


Torsions

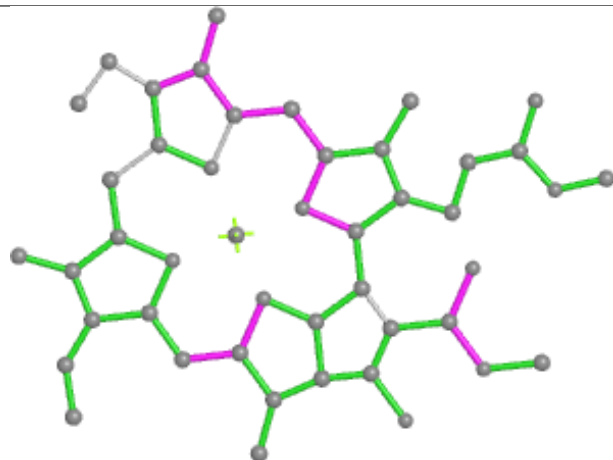


Rings

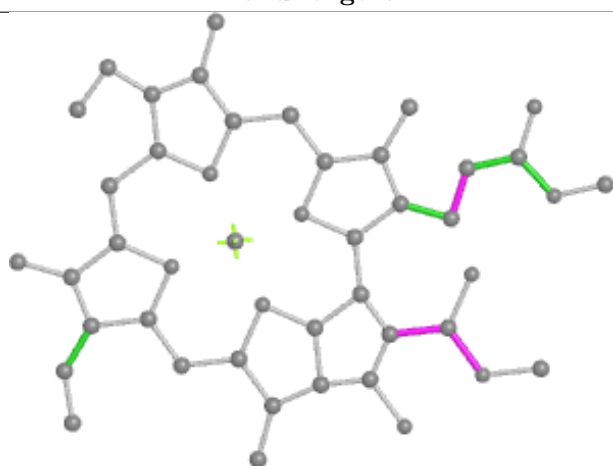
## Ligand CLA 2 309



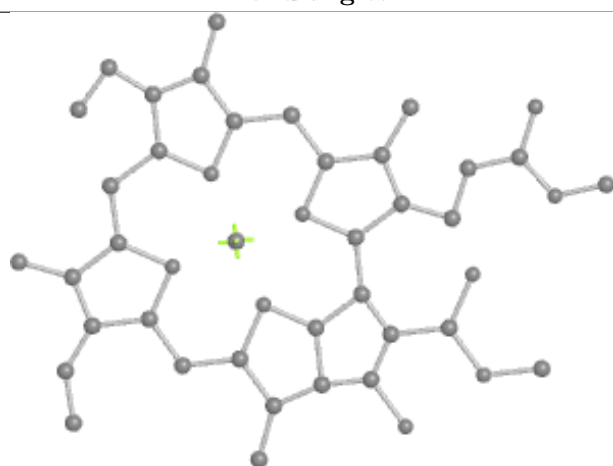
Bond lengths



Bond angles

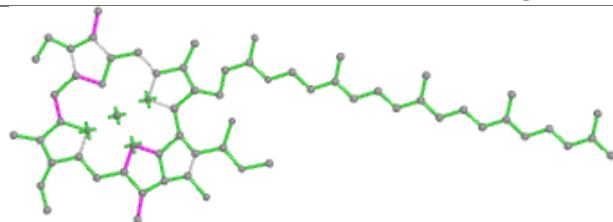


Torsions

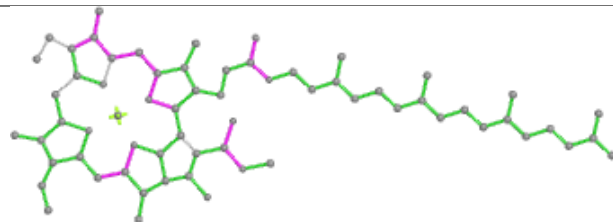


Rings

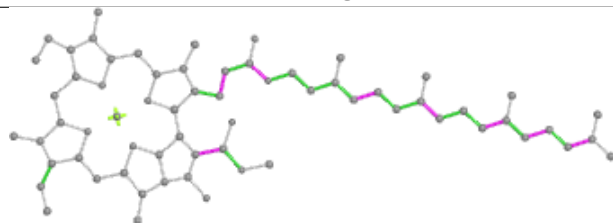
## Ligand CLA b 805



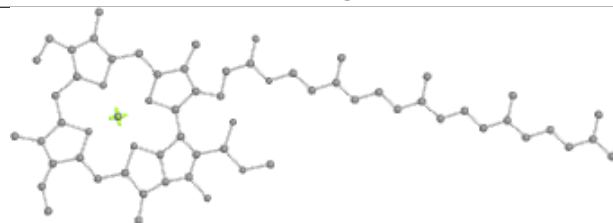
Bond lengths



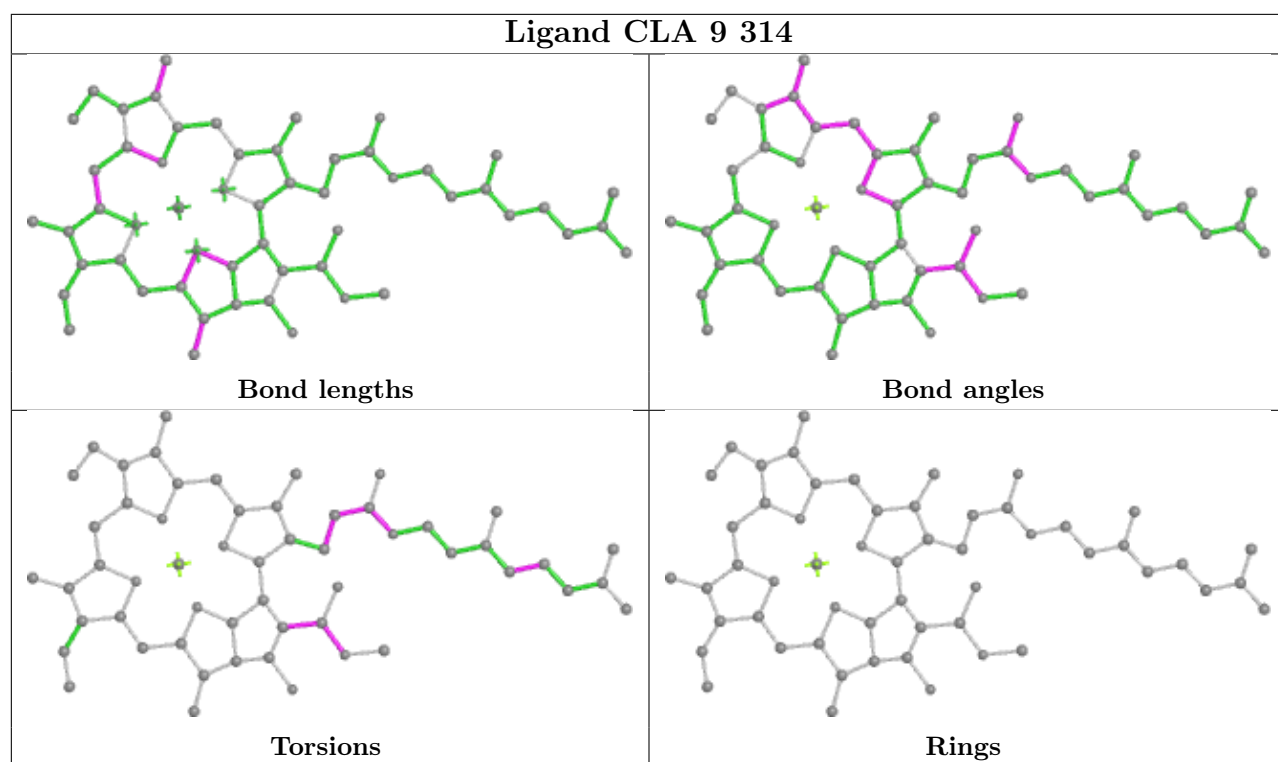
Bond angles



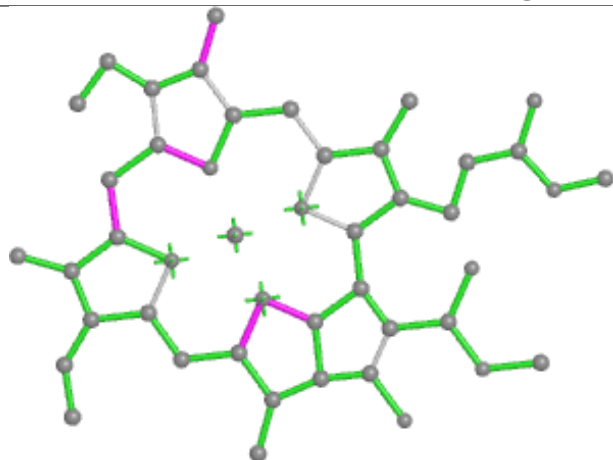
Torsions



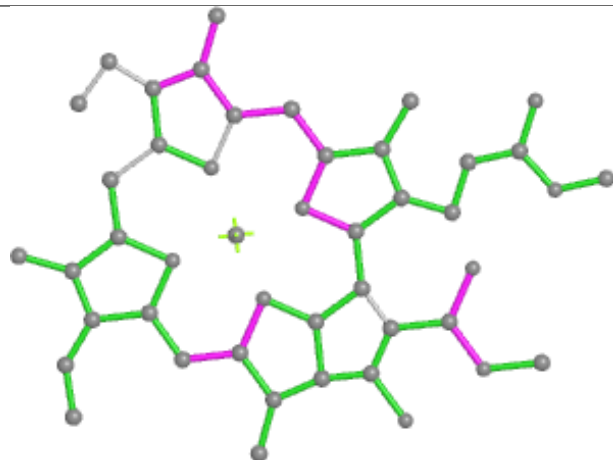
Rings



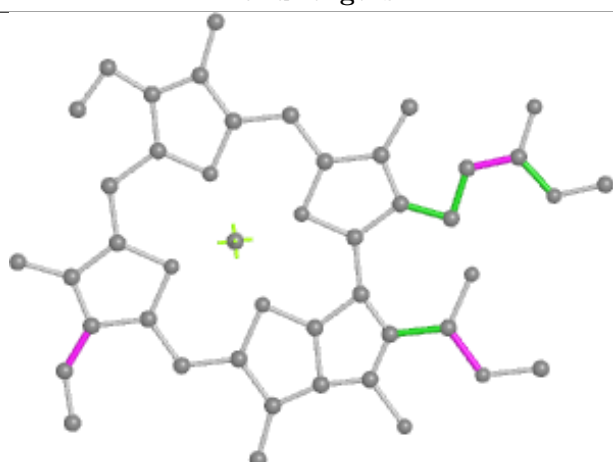
## Ligand CLA 5 315



Bond lengths



Bond angles

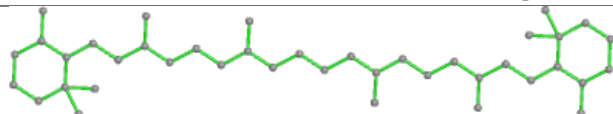


Torsions

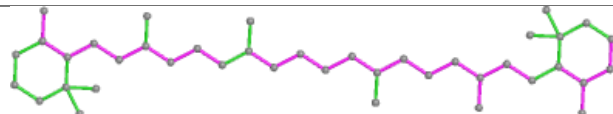


Rings

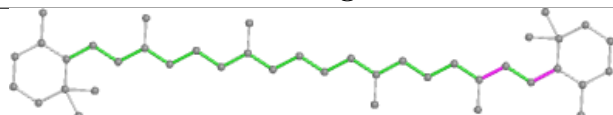
## Ligand BCR a 850



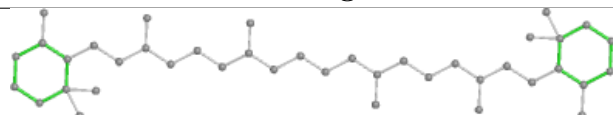
Bond lengths



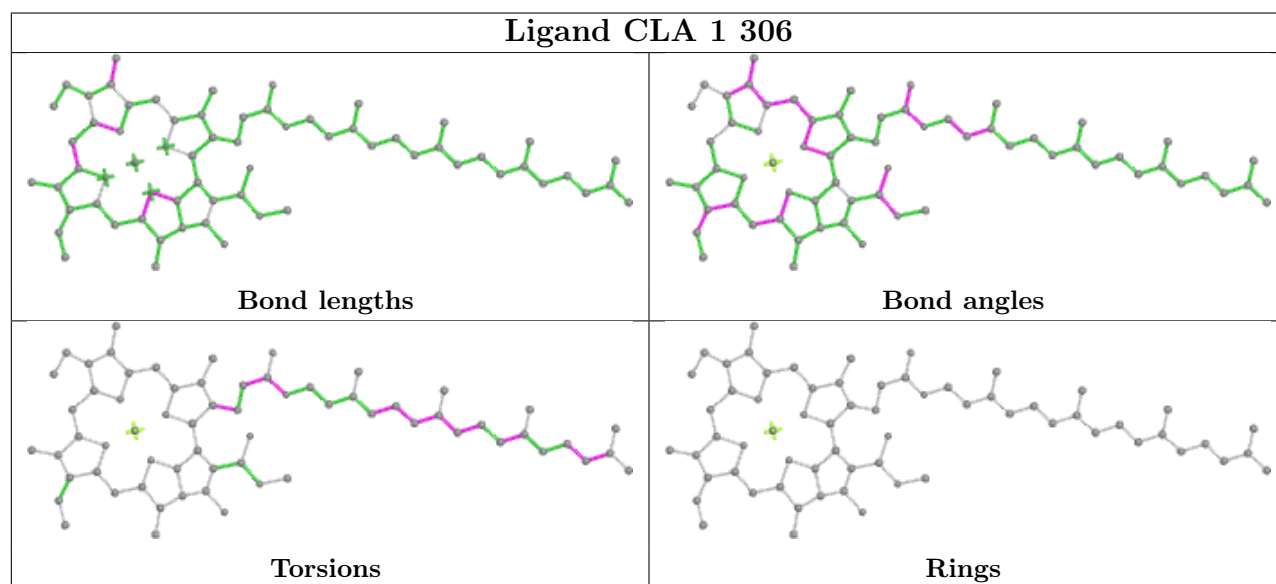
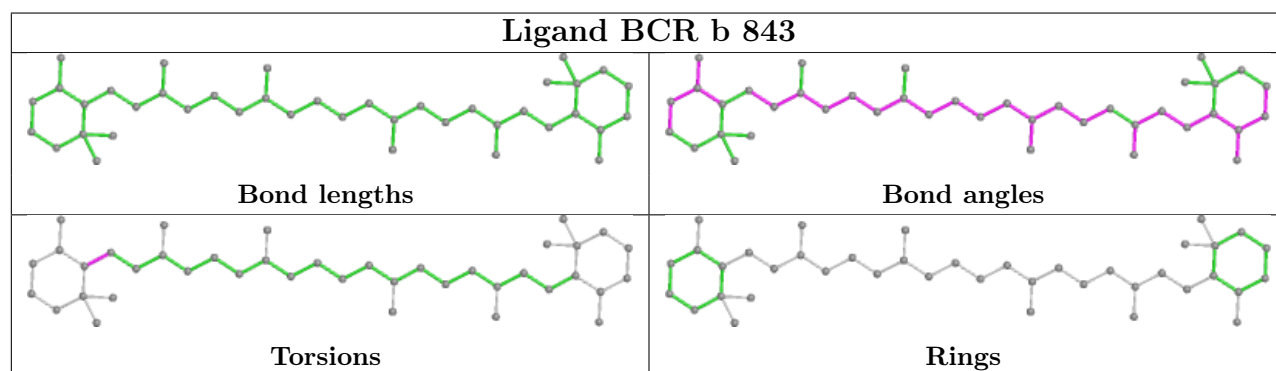
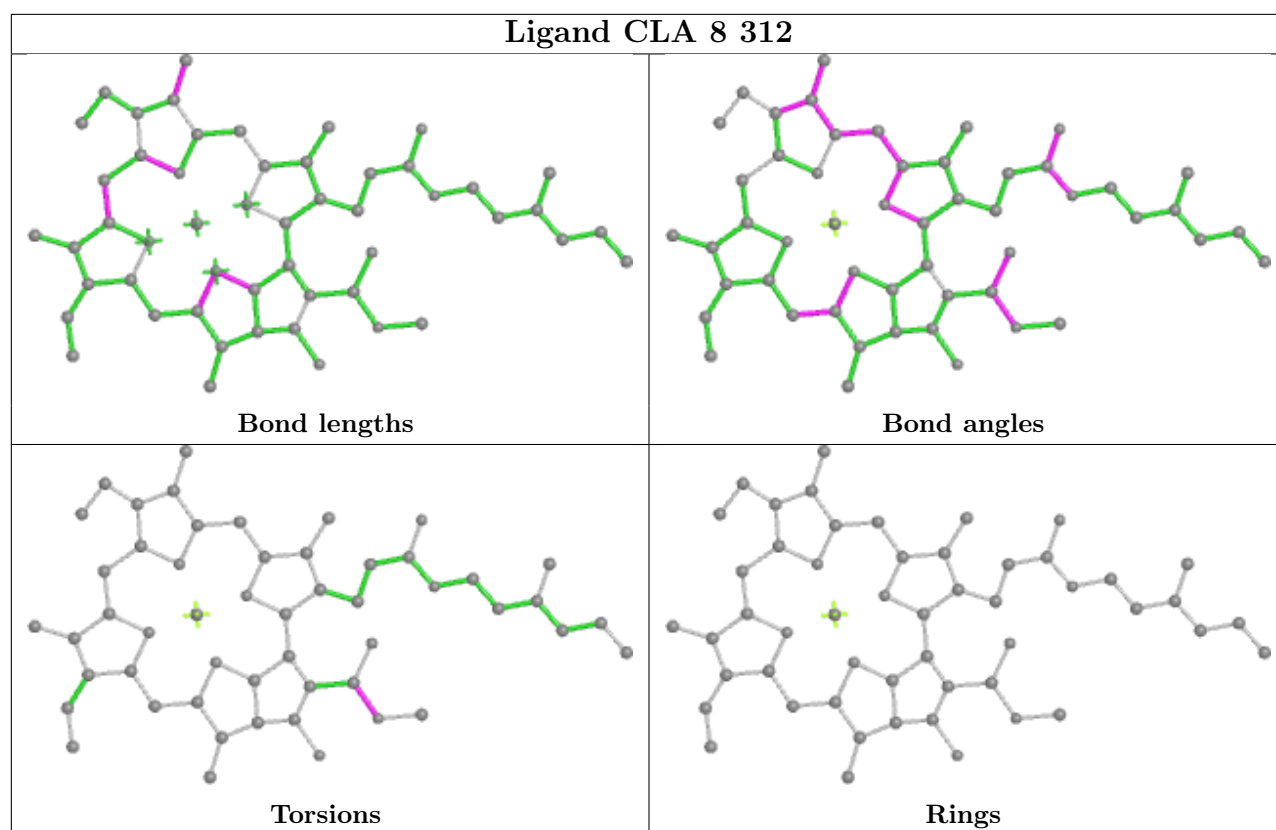
Bond angles

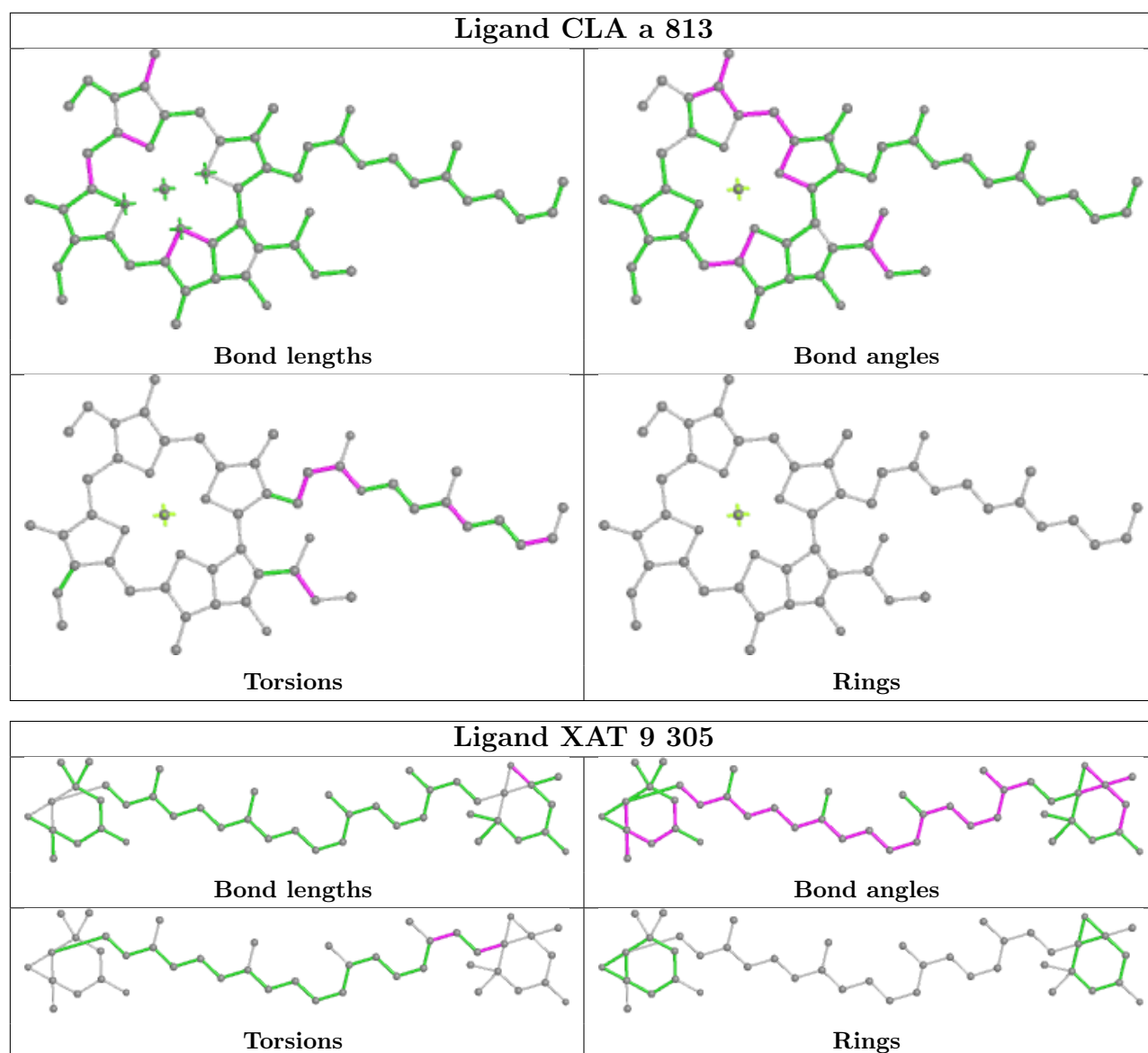


Torsions

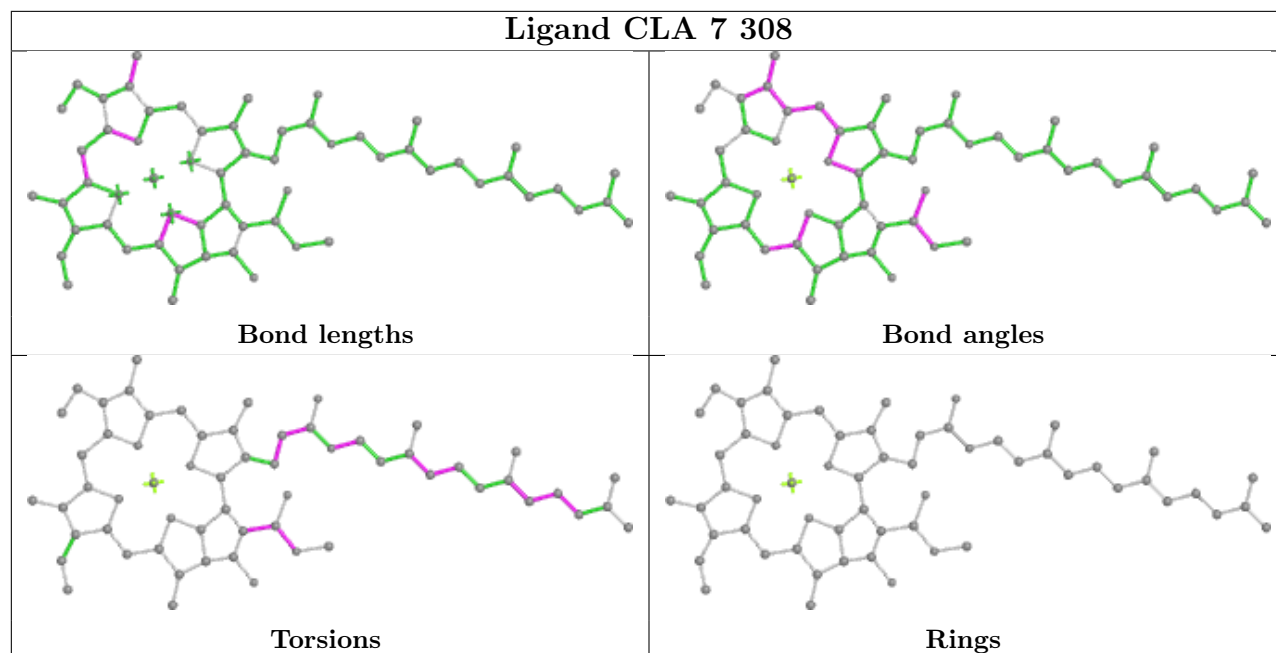


Rings

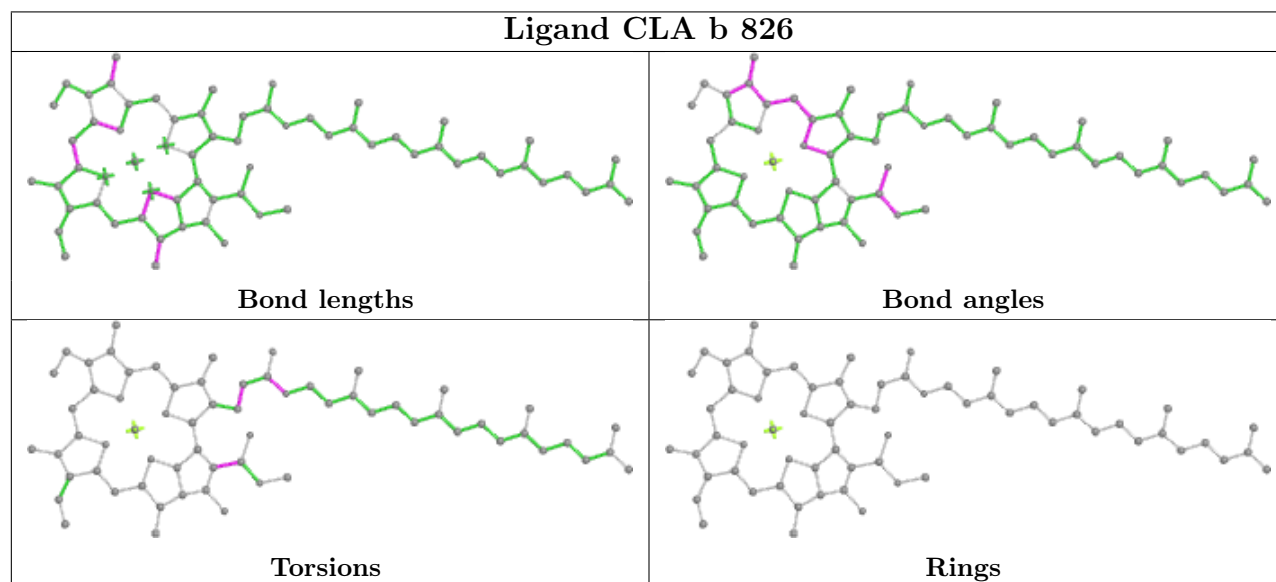




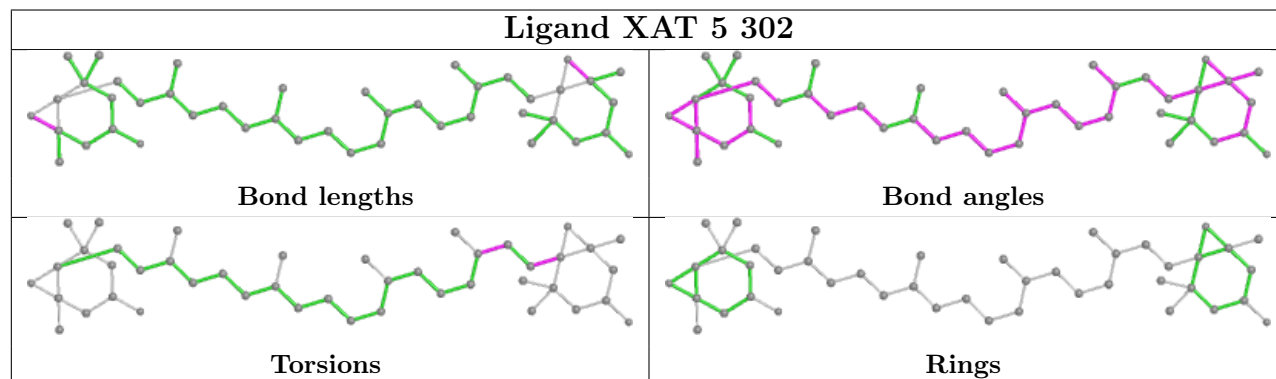
## Ligand CLA 7 308



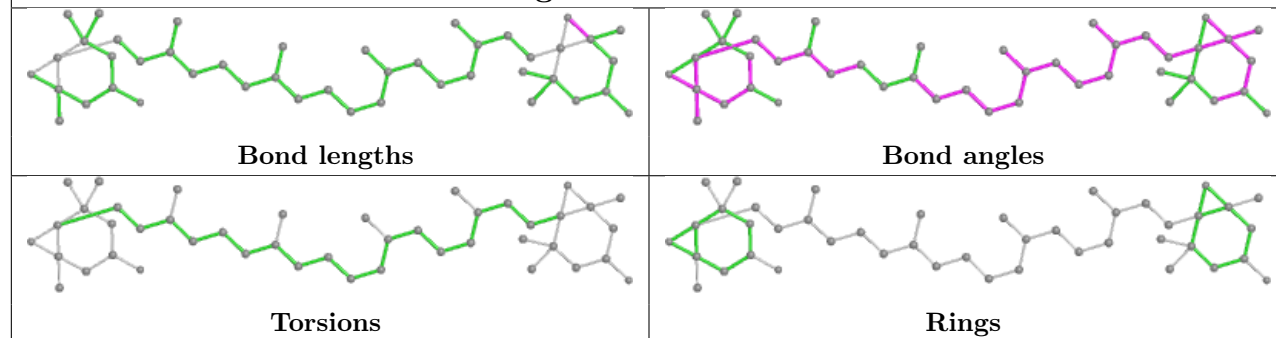
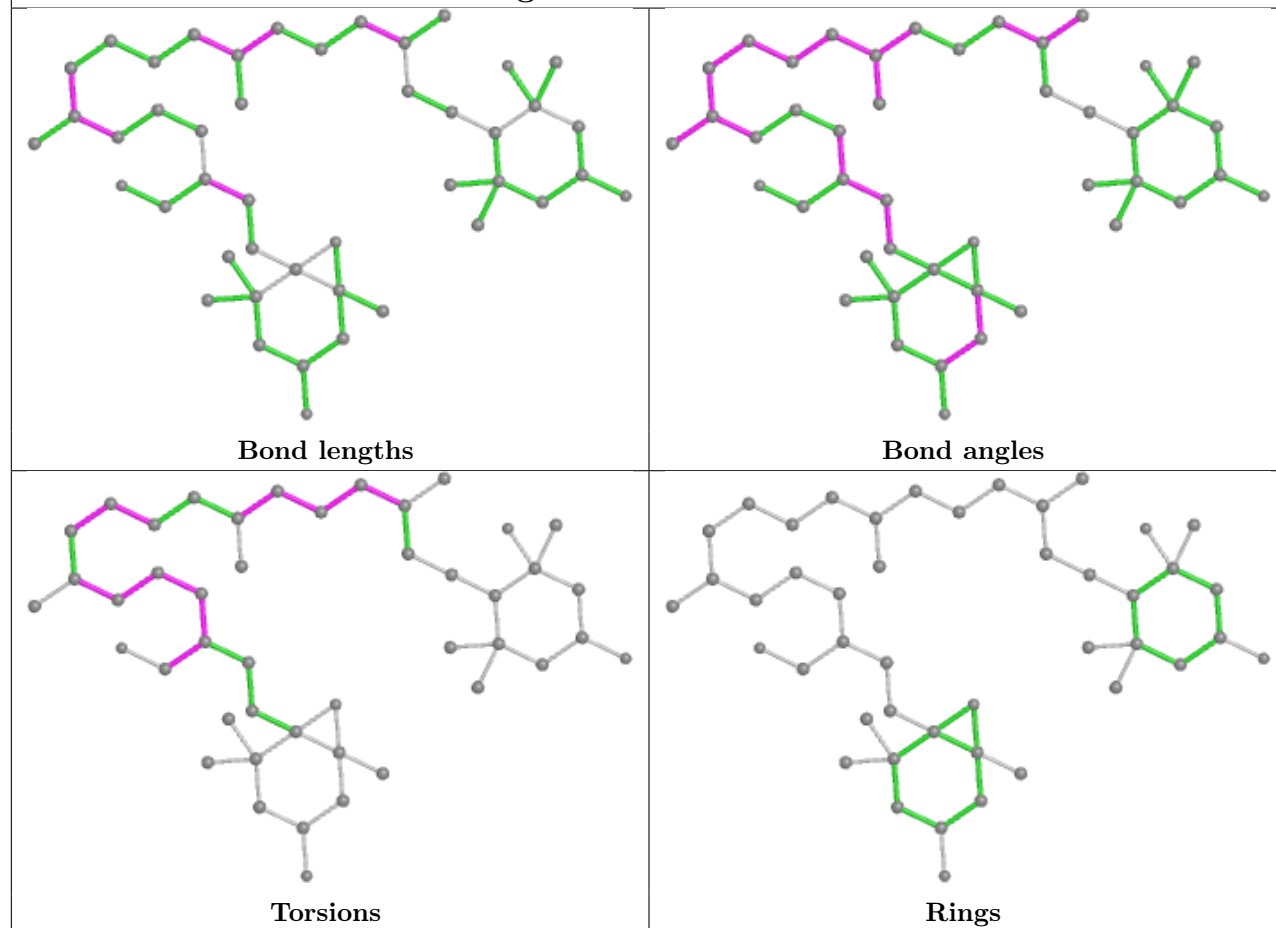
## Ligand CLA b 826



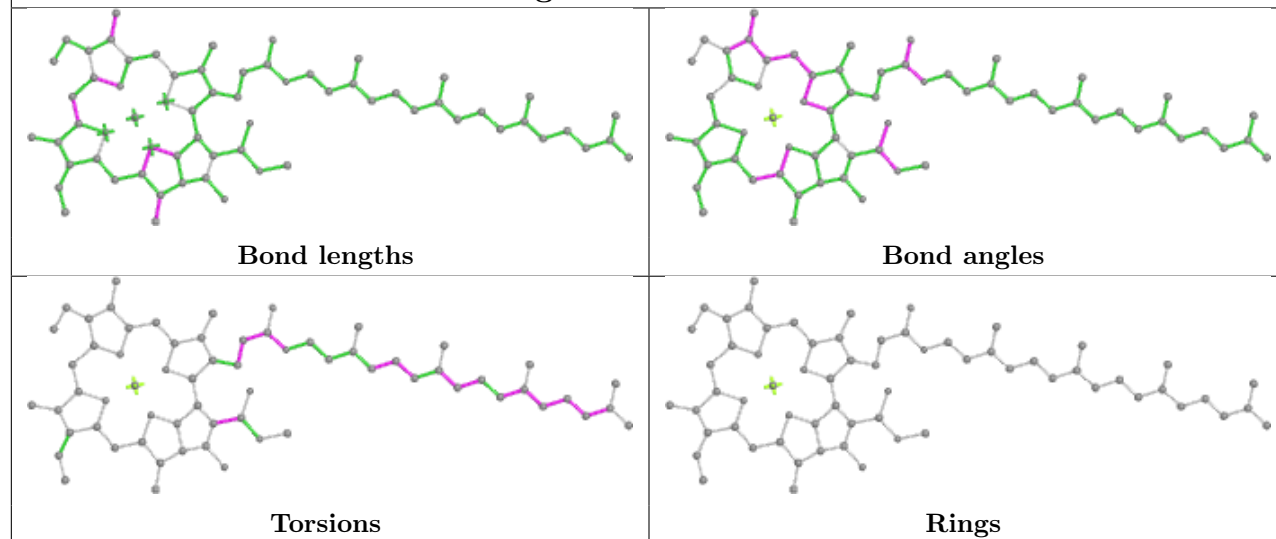
## Ligand XAT 5 302



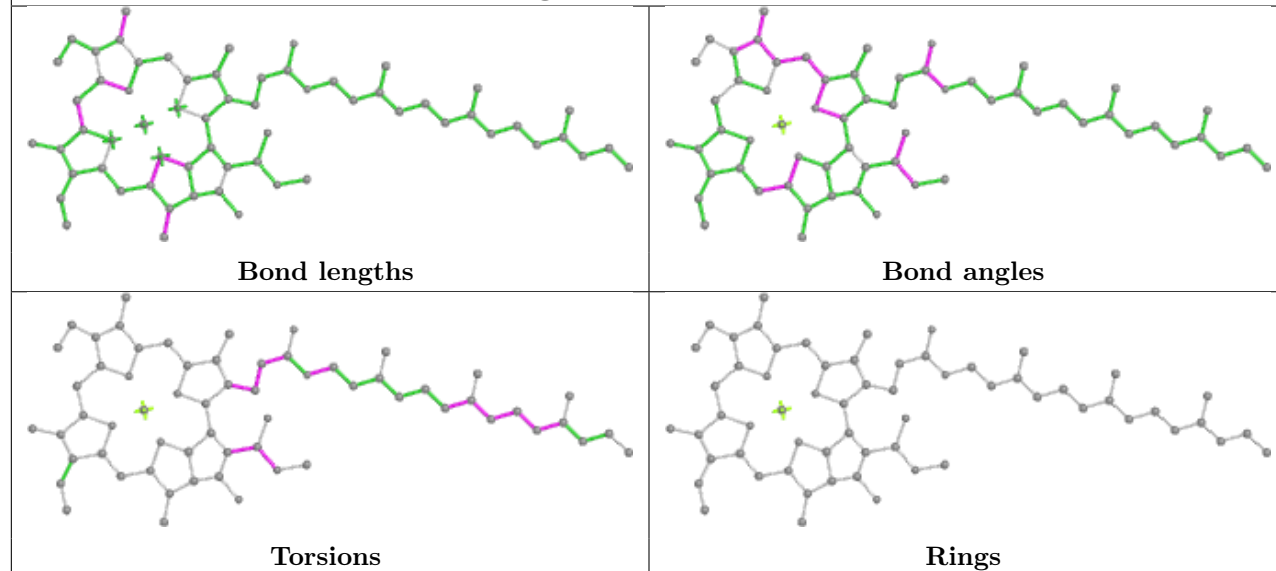


**Ligand XAT 1 303****Ligand A1L1G 9 301**

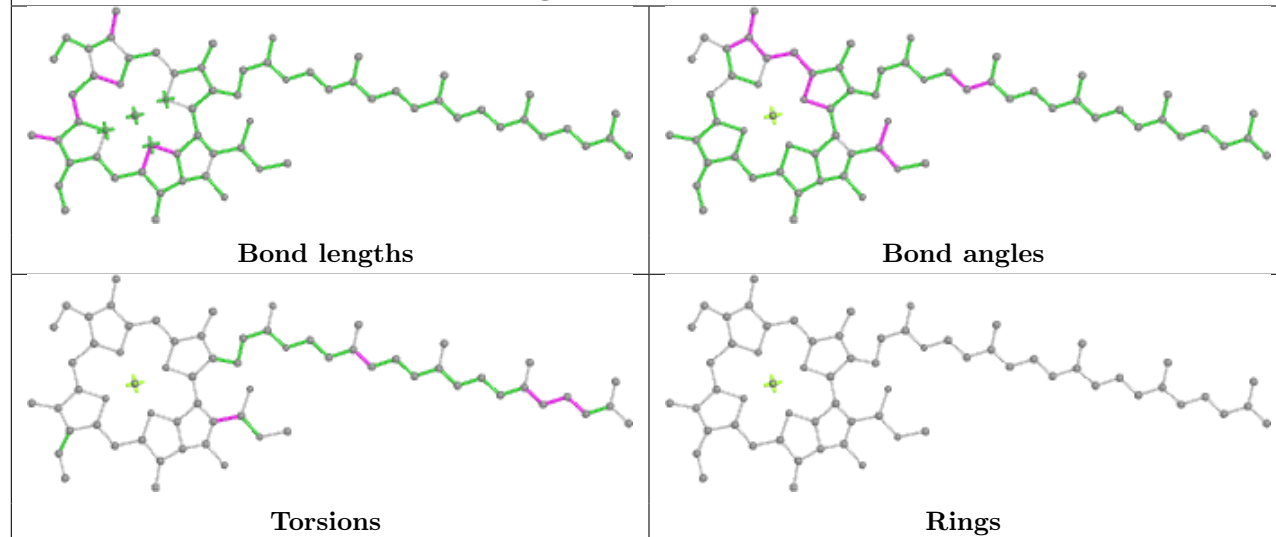
## Ligand CLA b 801

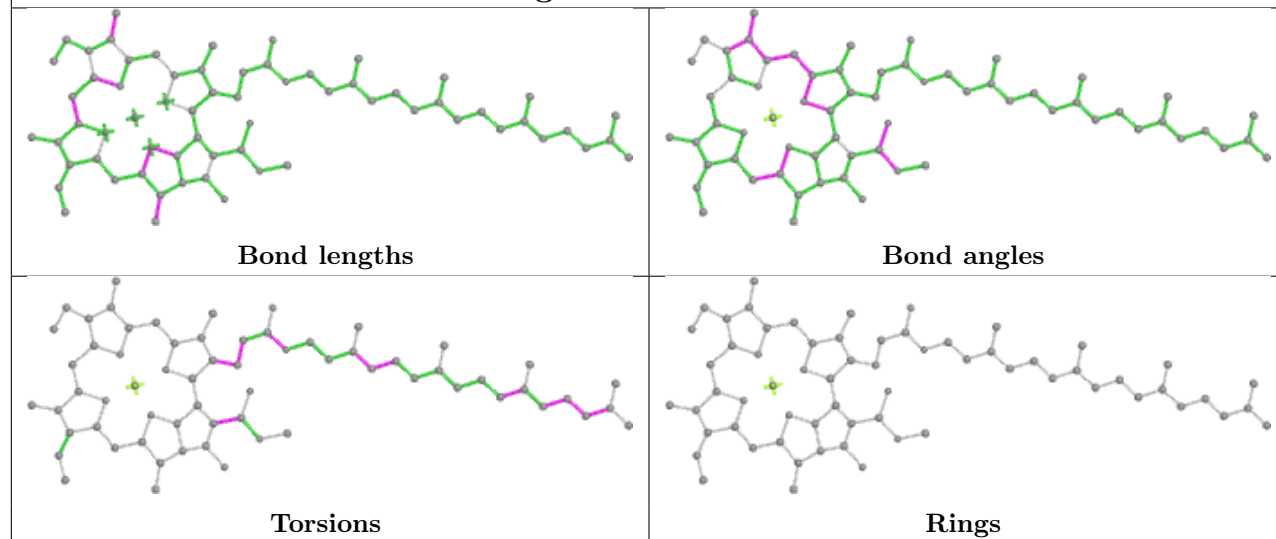
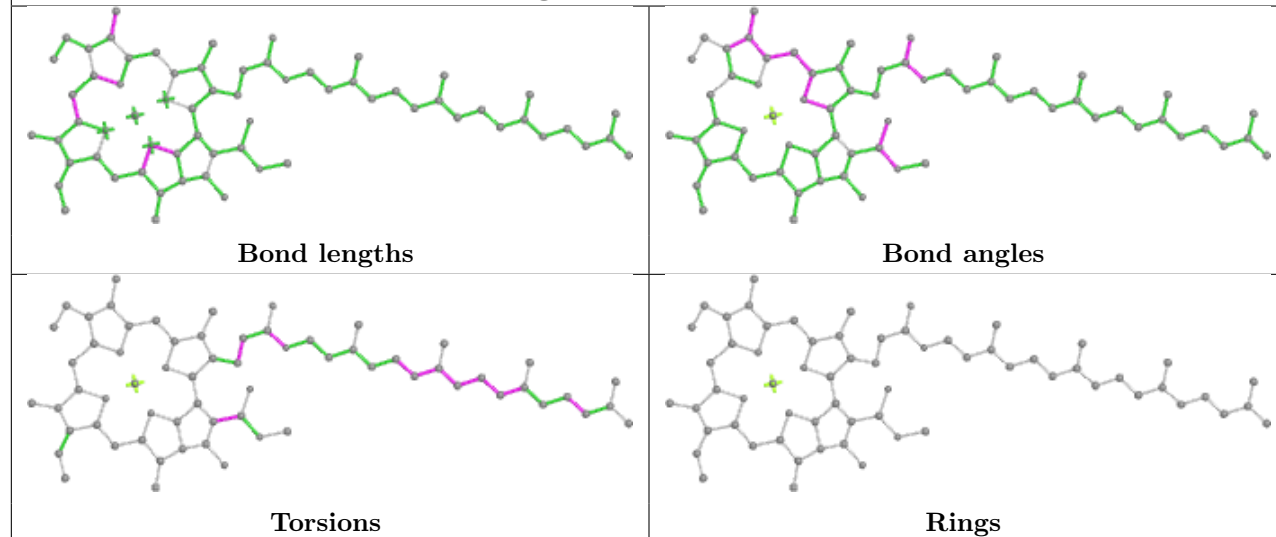


## Ligand CLA a 829

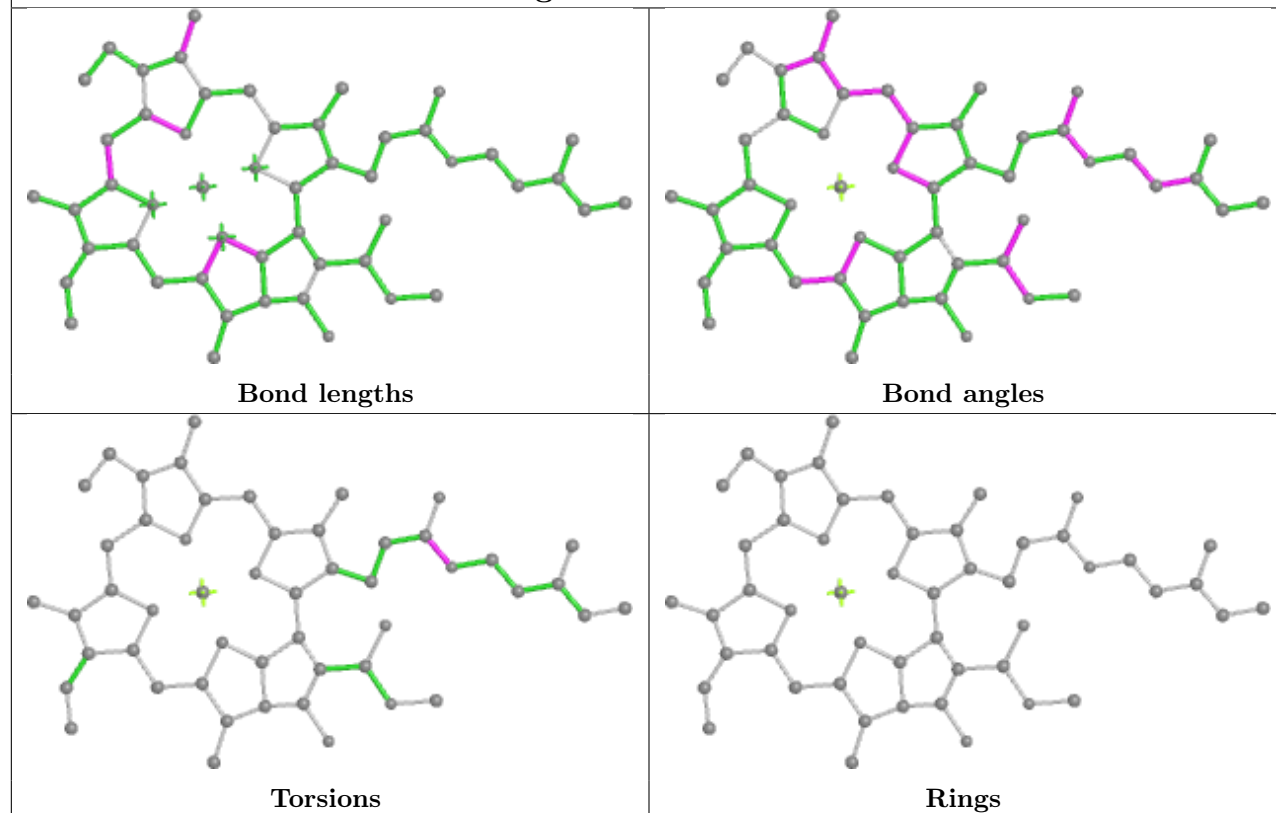


## Ligand CLA a 828

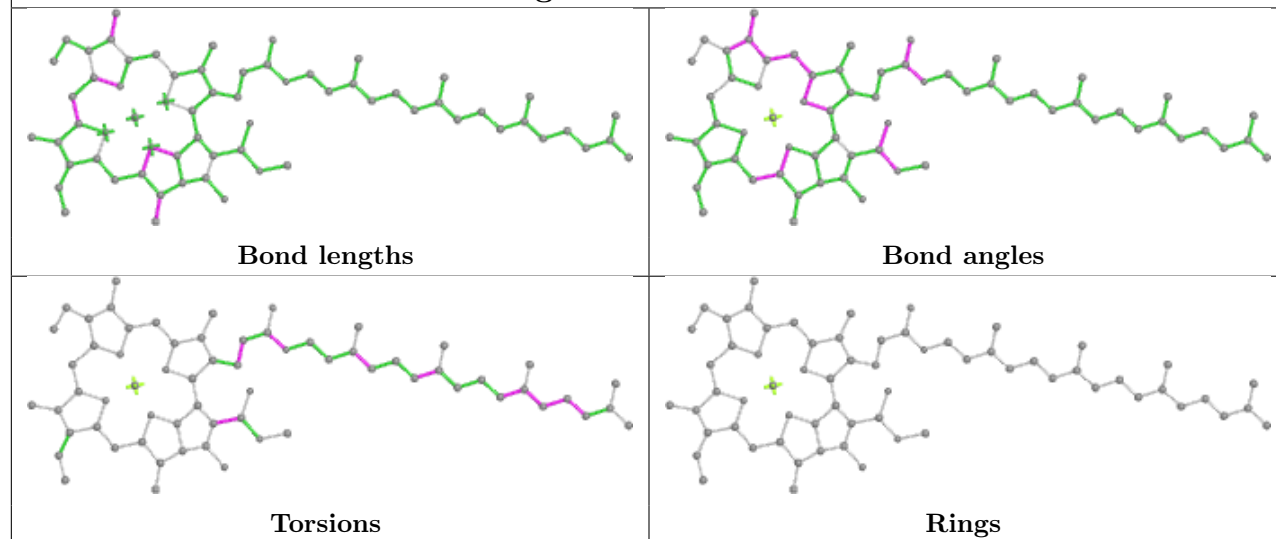


**Ligand CLA b 833****Ligand CLA b 824**

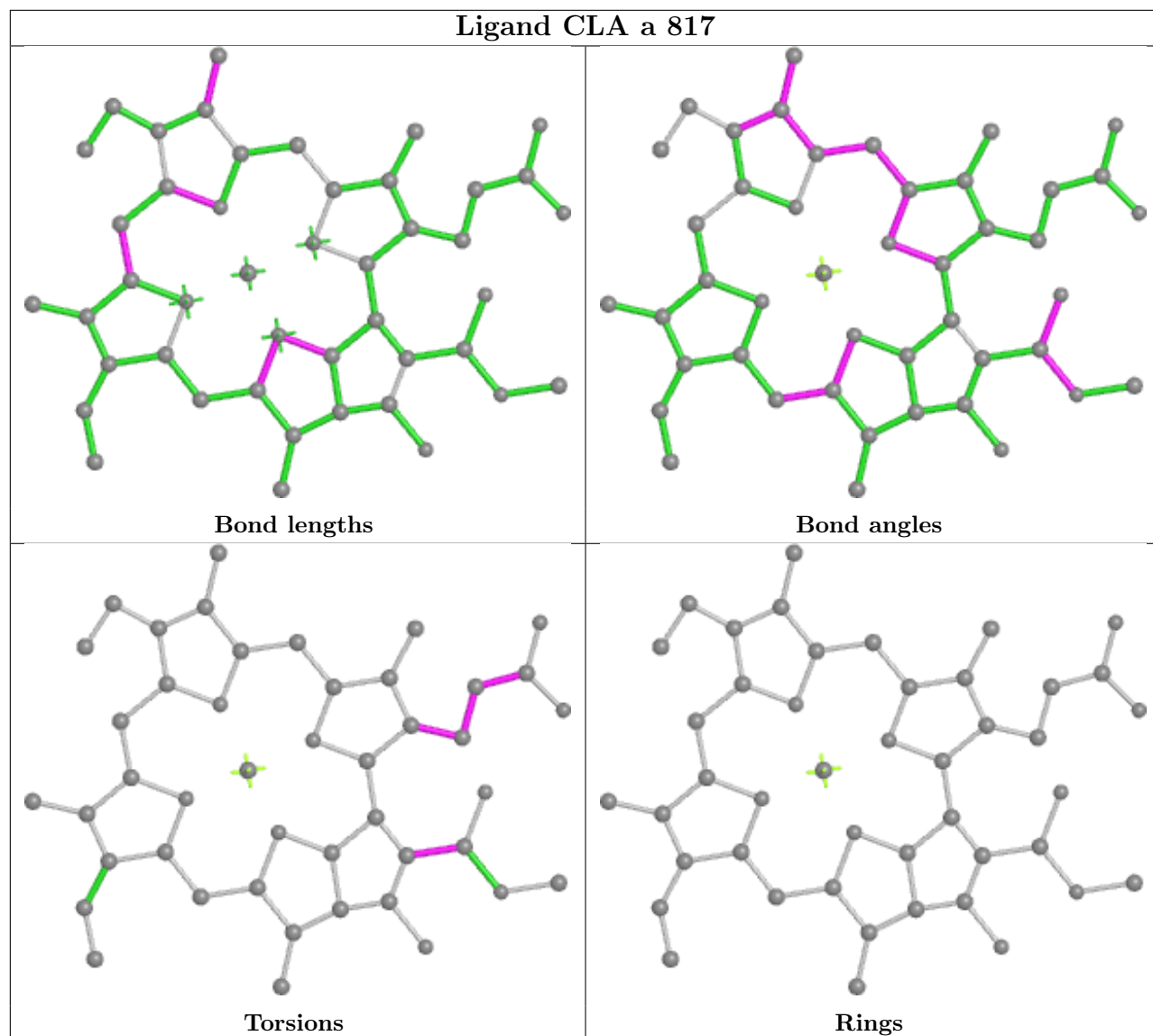
## Ligand CLA b 821



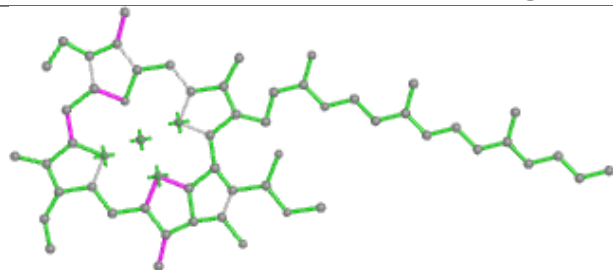
## Ligand CLA b 838



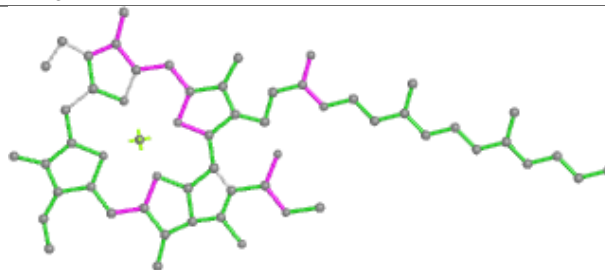
## Ligand CLA a 817



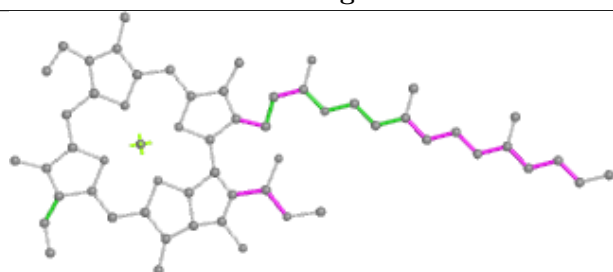
## Ligand CLA j 102



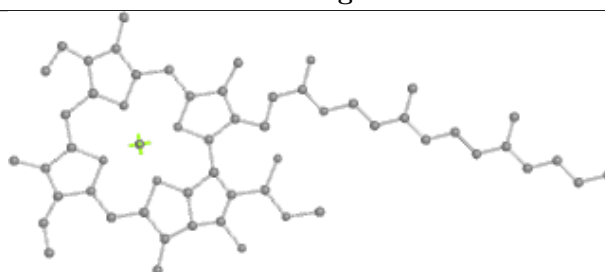
Bond lengths



Bond angles

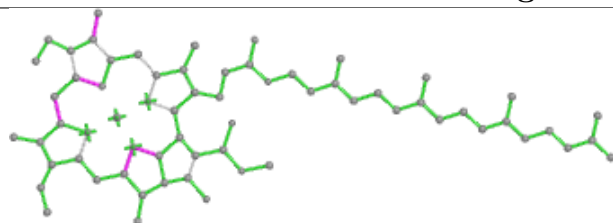


Torsions

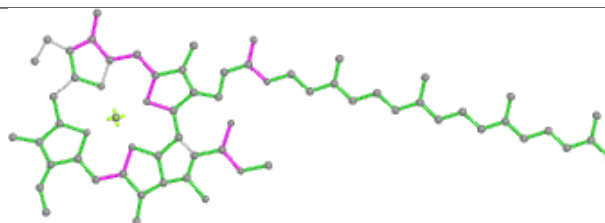


Rings

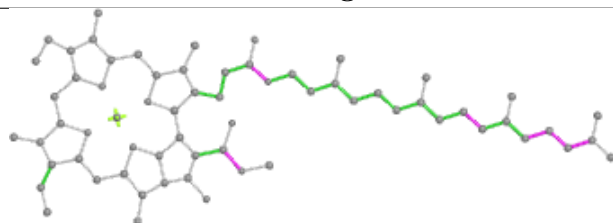
## Ligand CLA b 840



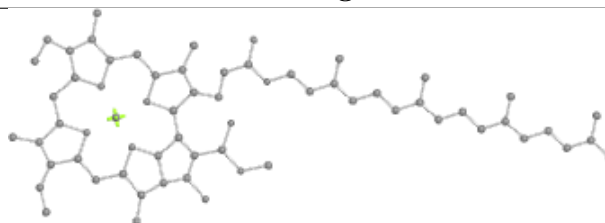
Bond lengths



Bond angles

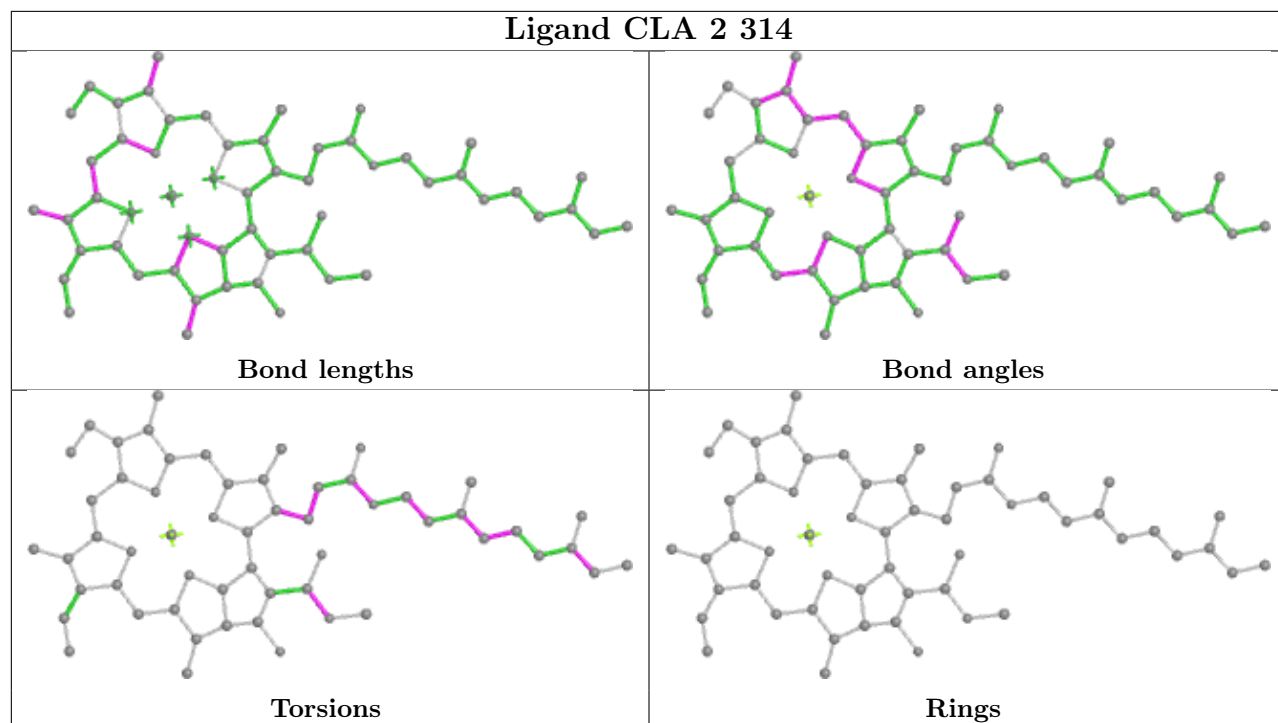


Torsions

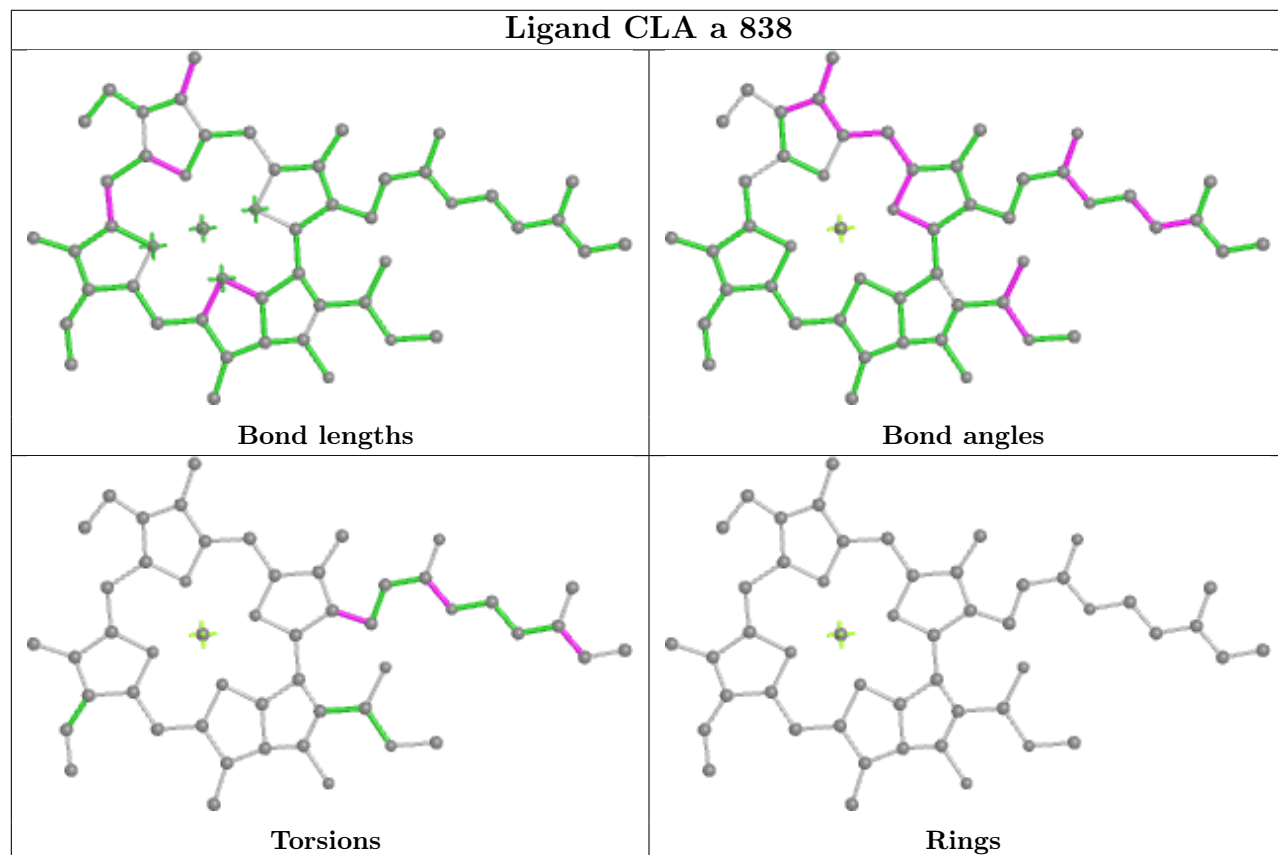


Rings

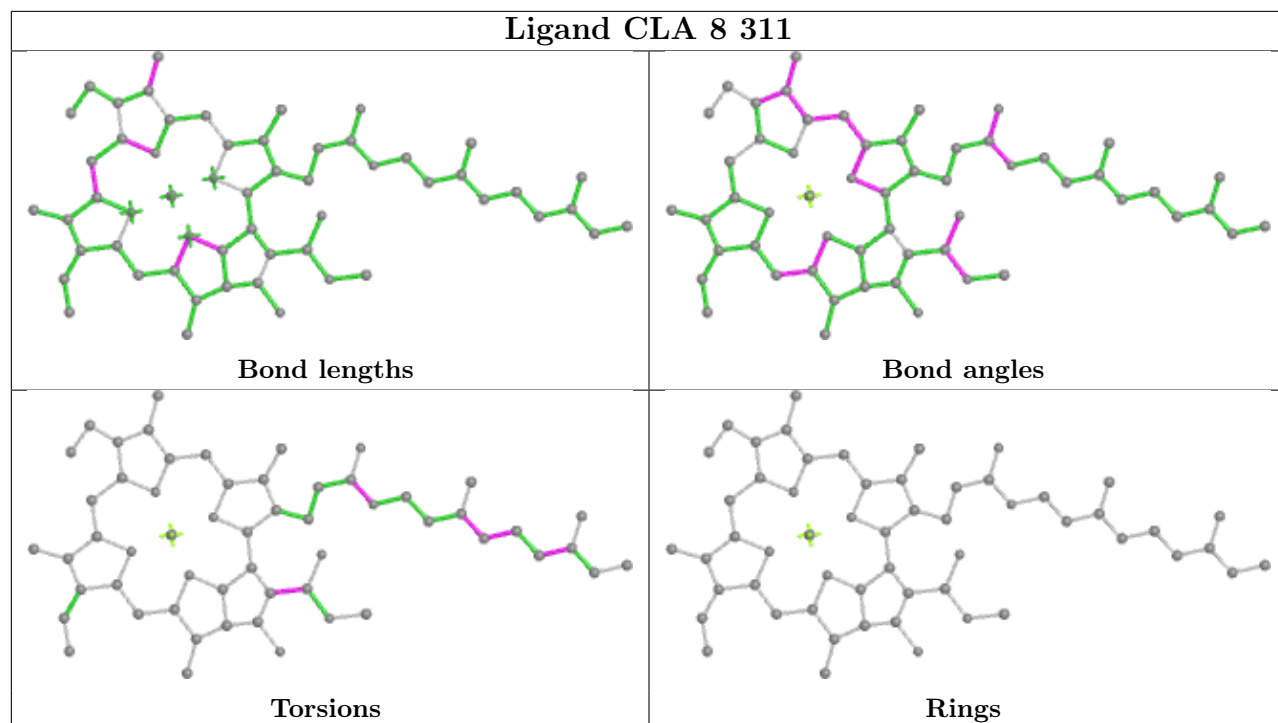
## Ligand CLA 2 314



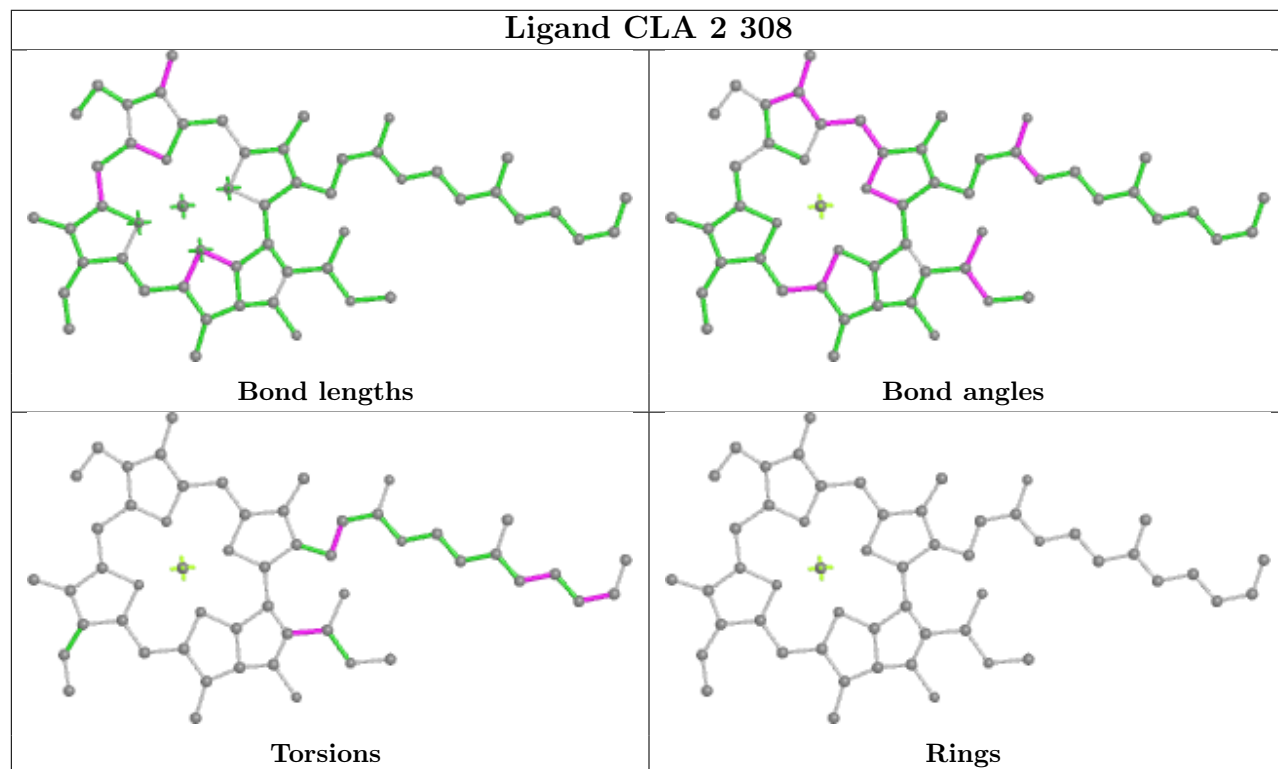
## Ligand CLA a 838



## Ligand CLA 8 311

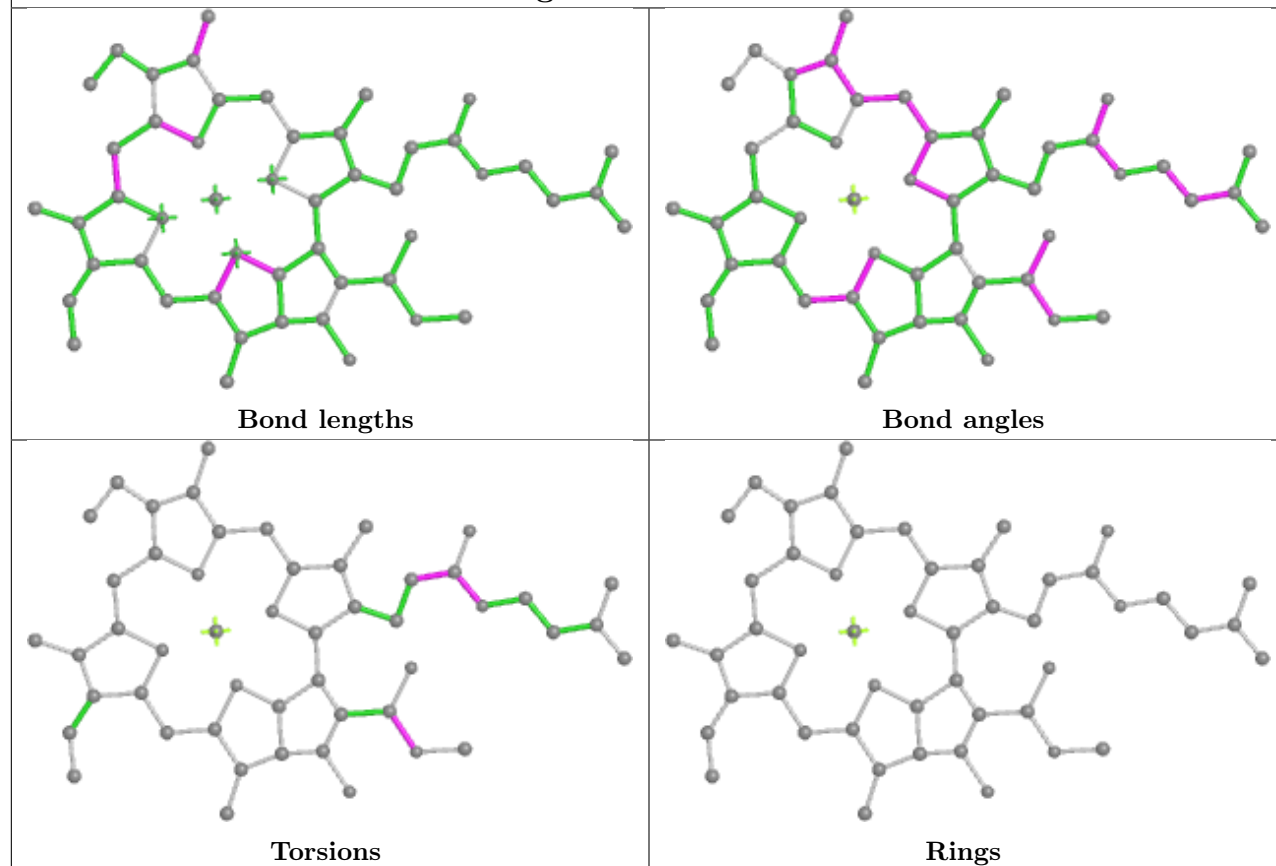


## Ligand CLA 2 308

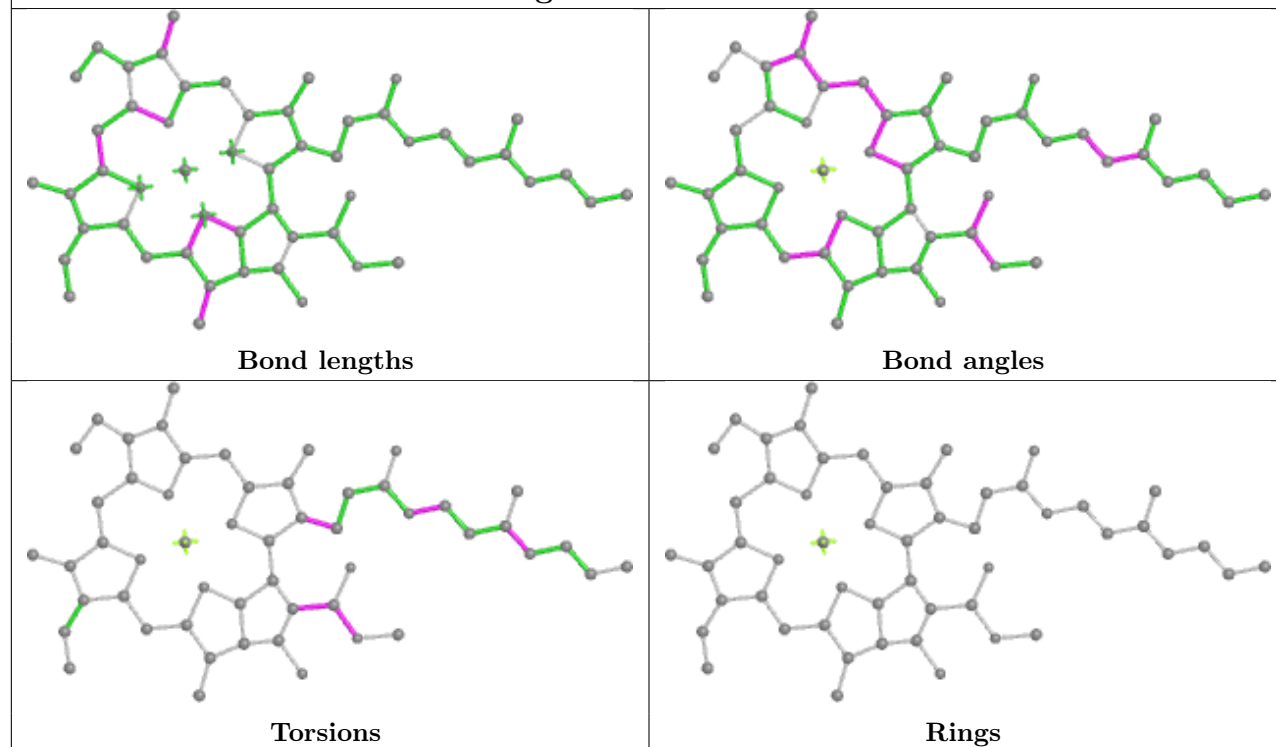


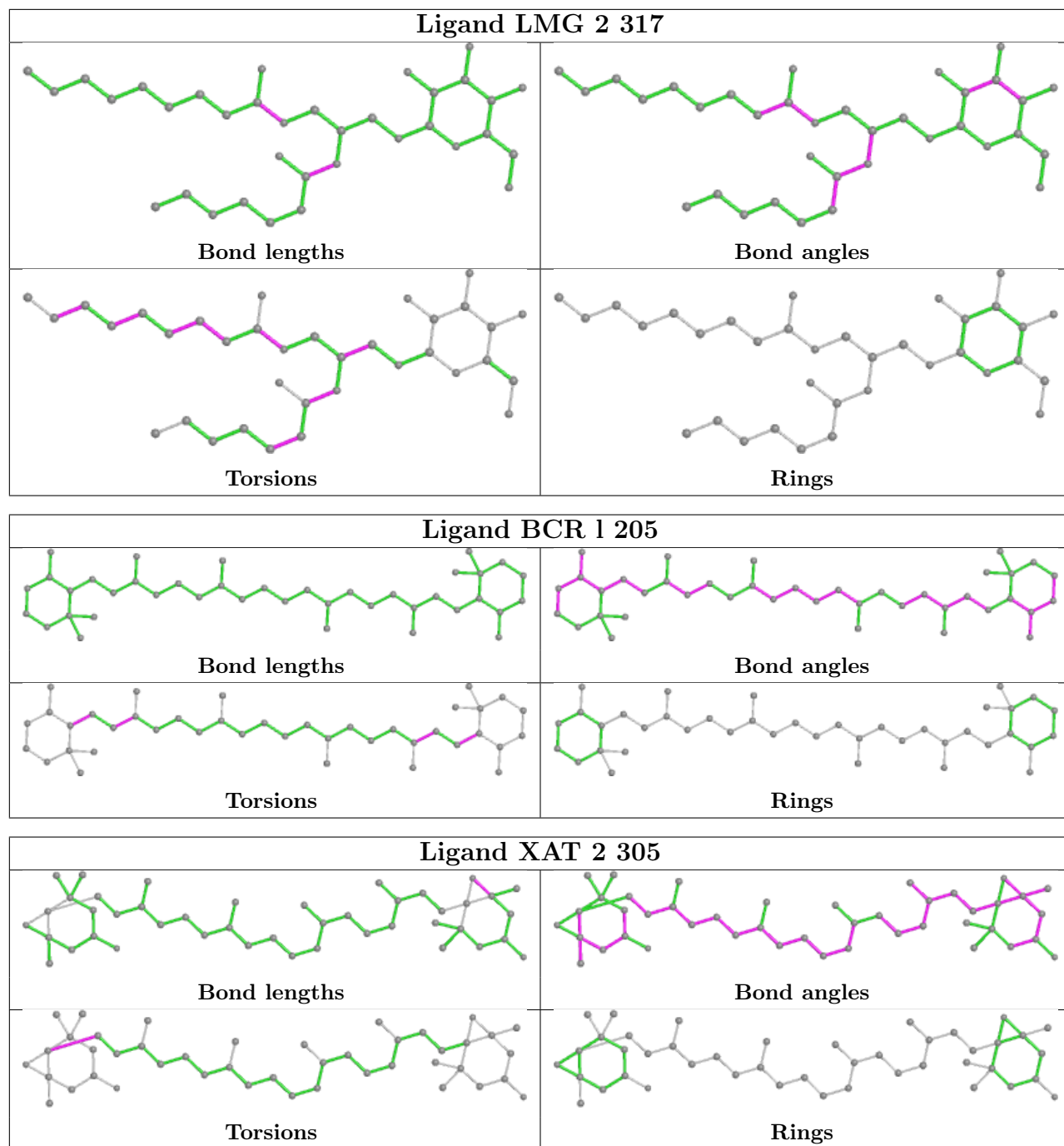


## Ligand CLA a 836

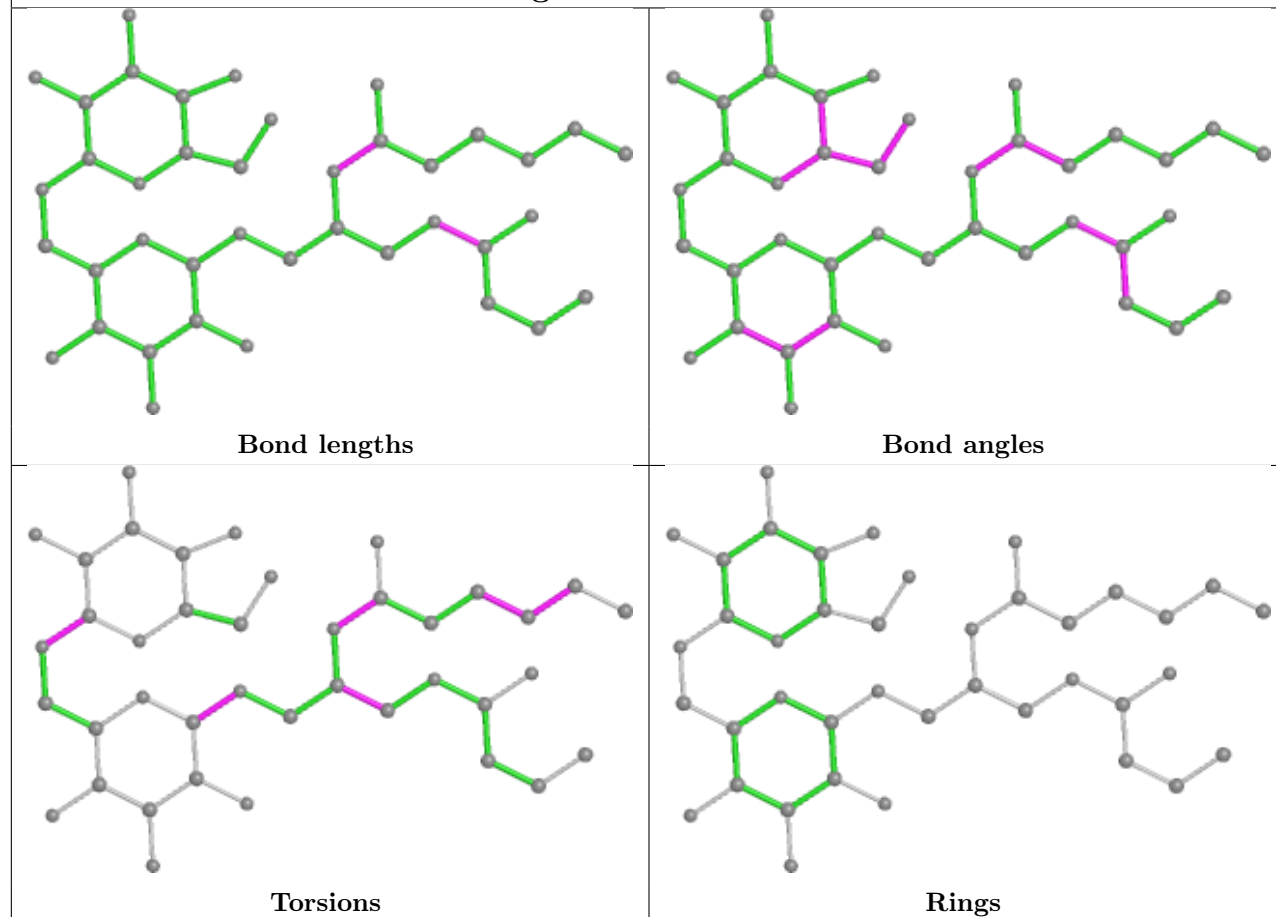


## Ligand CLA b 834

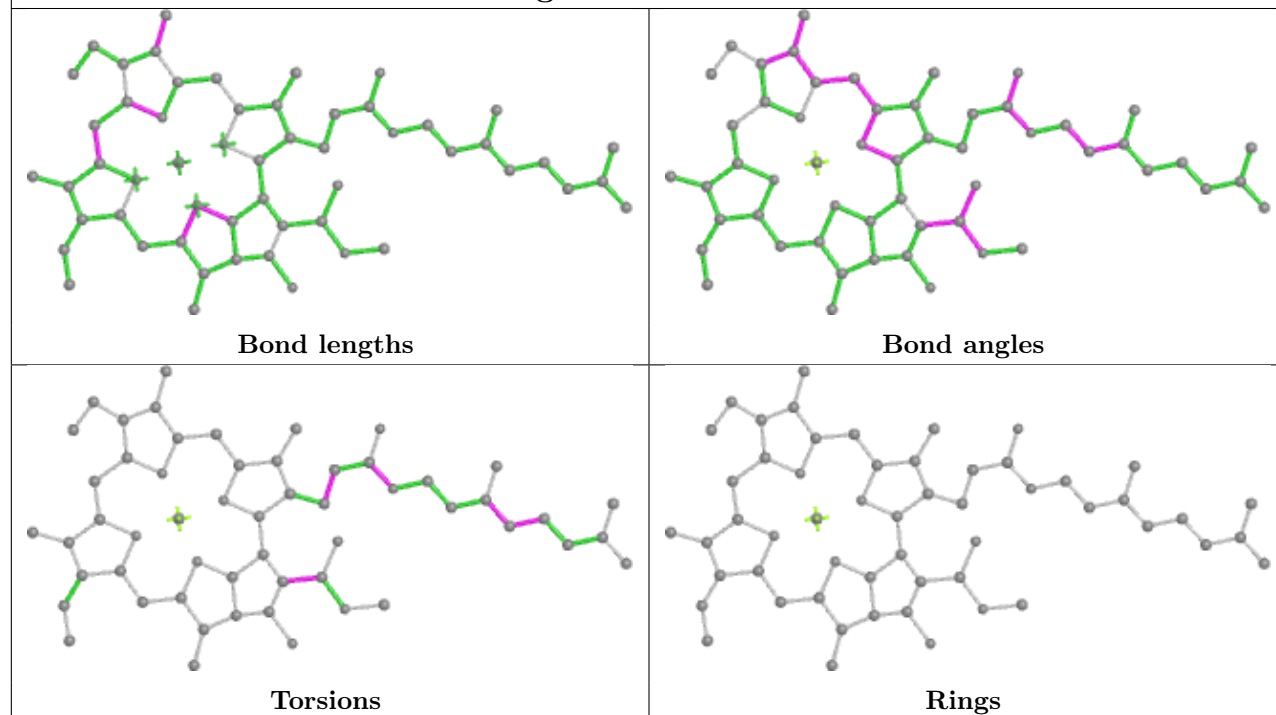




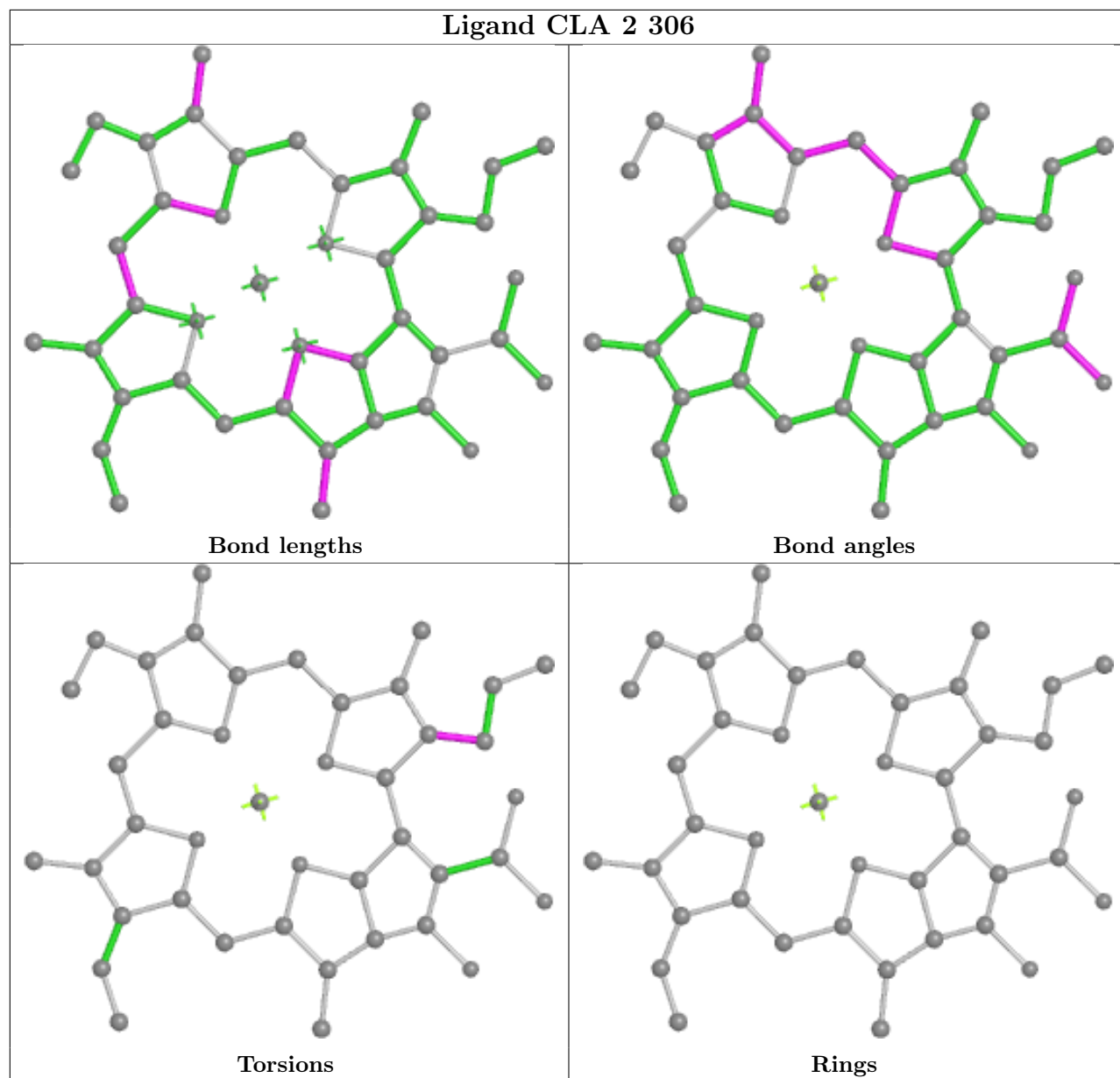
## Ligand DGD 4 318



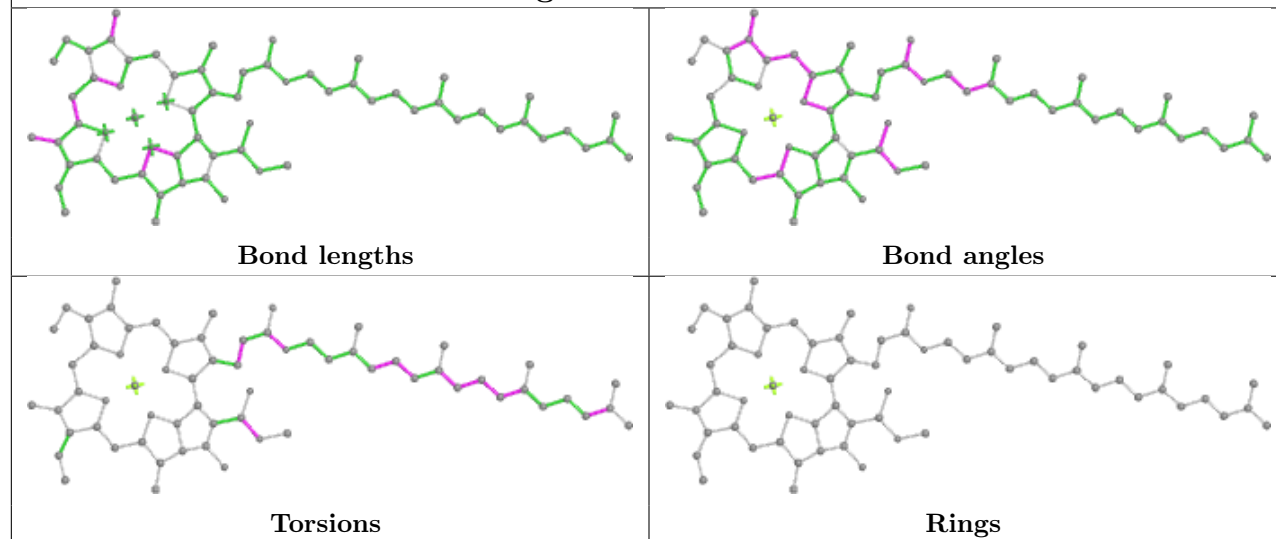
## Ligand CLA 8 308



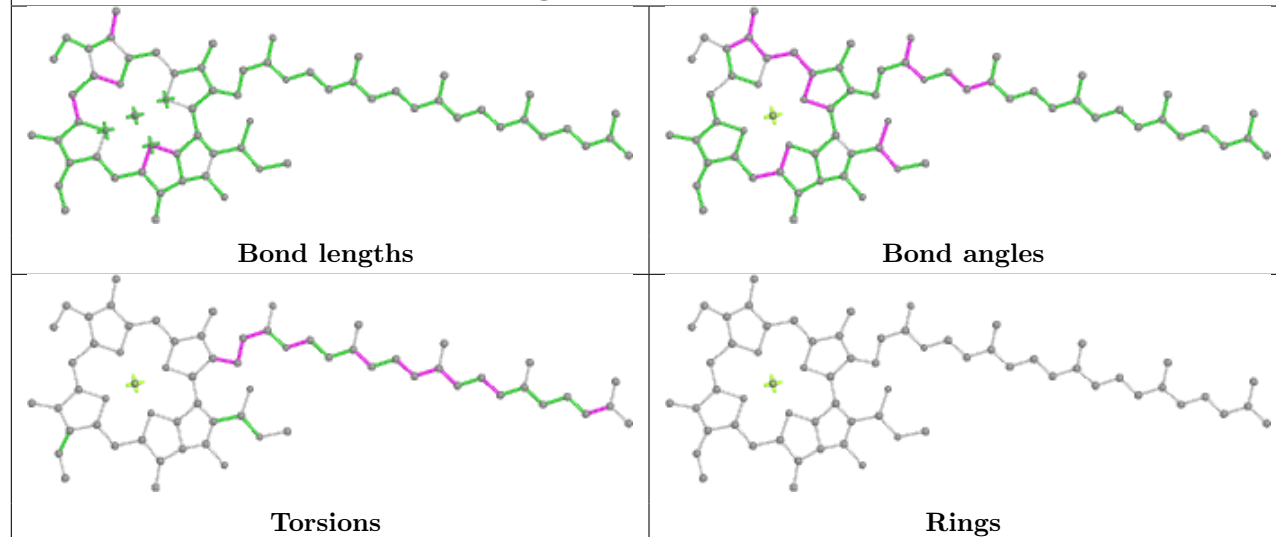
## Ligand CLA 2 306



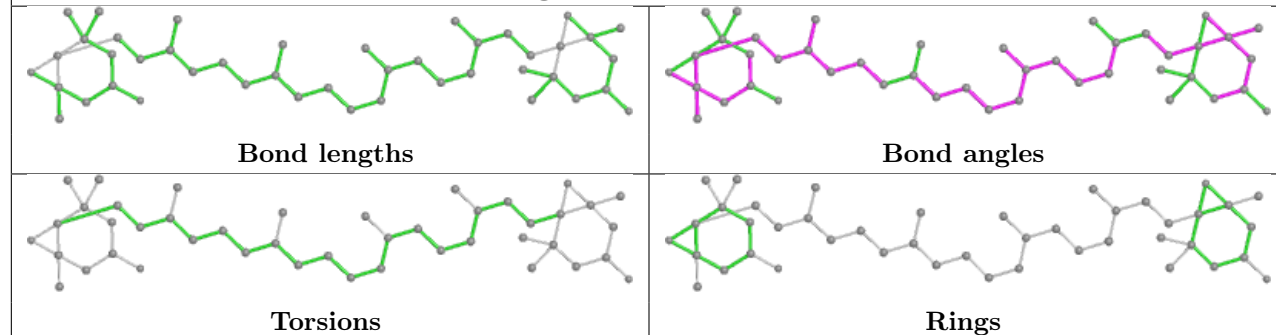
## Ligand CLA 9 308

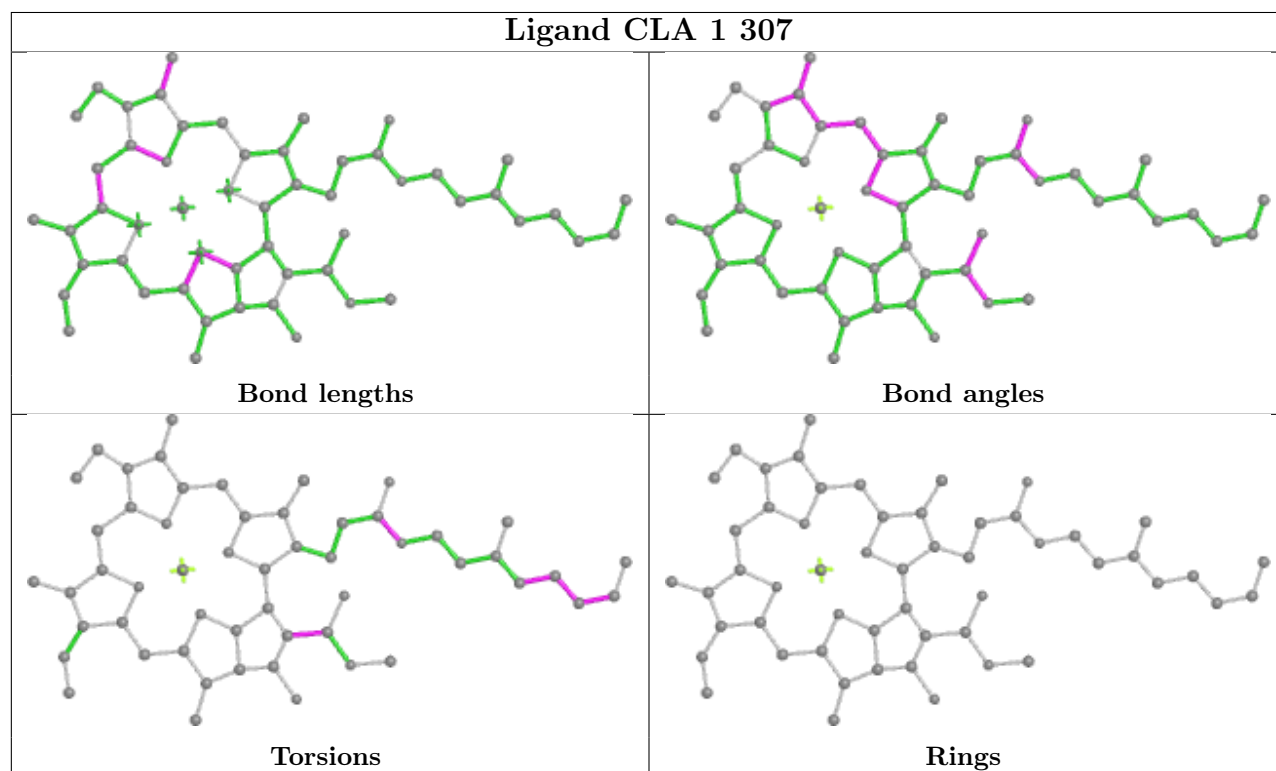
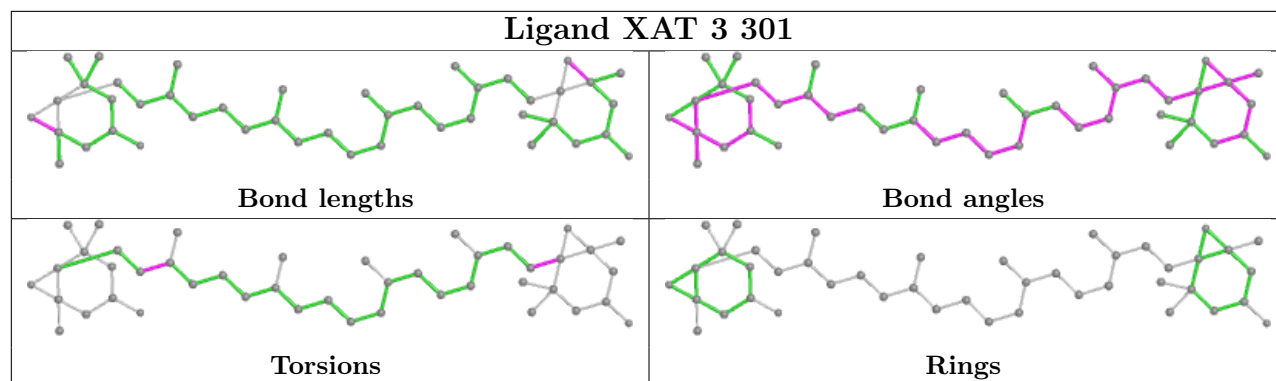
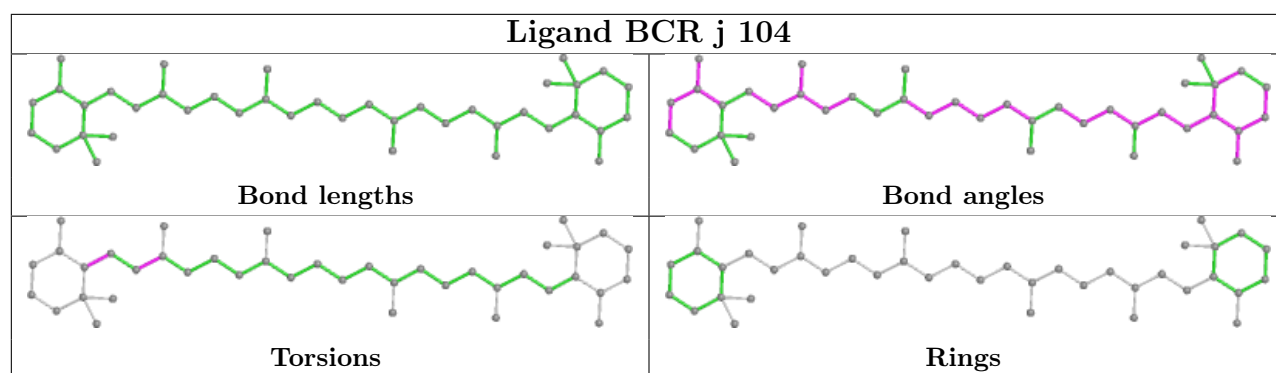


## Ligand CLA b 810

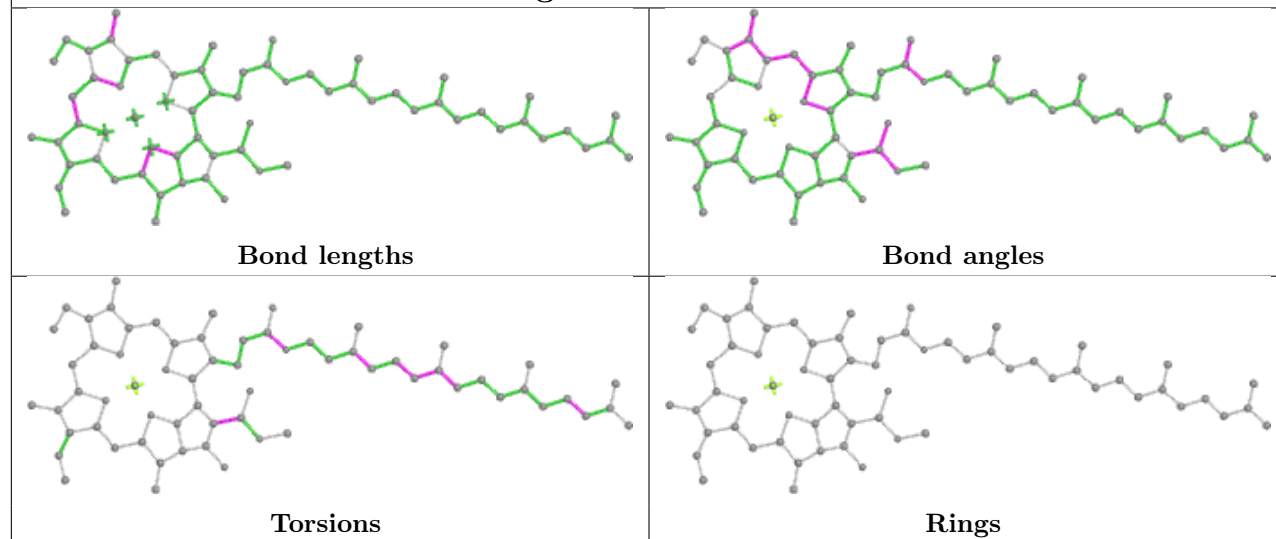


## Ligand XAT 4 302

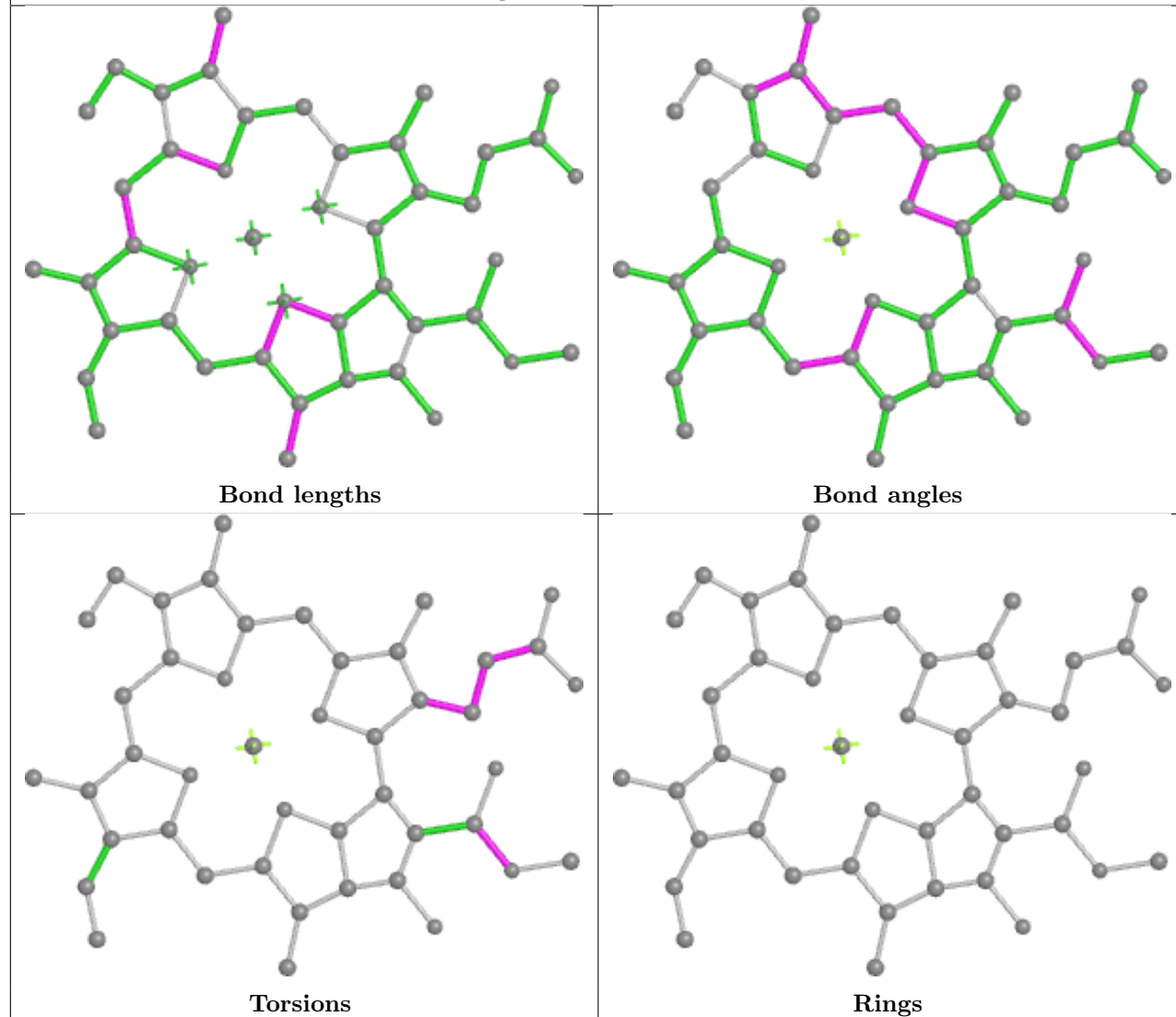




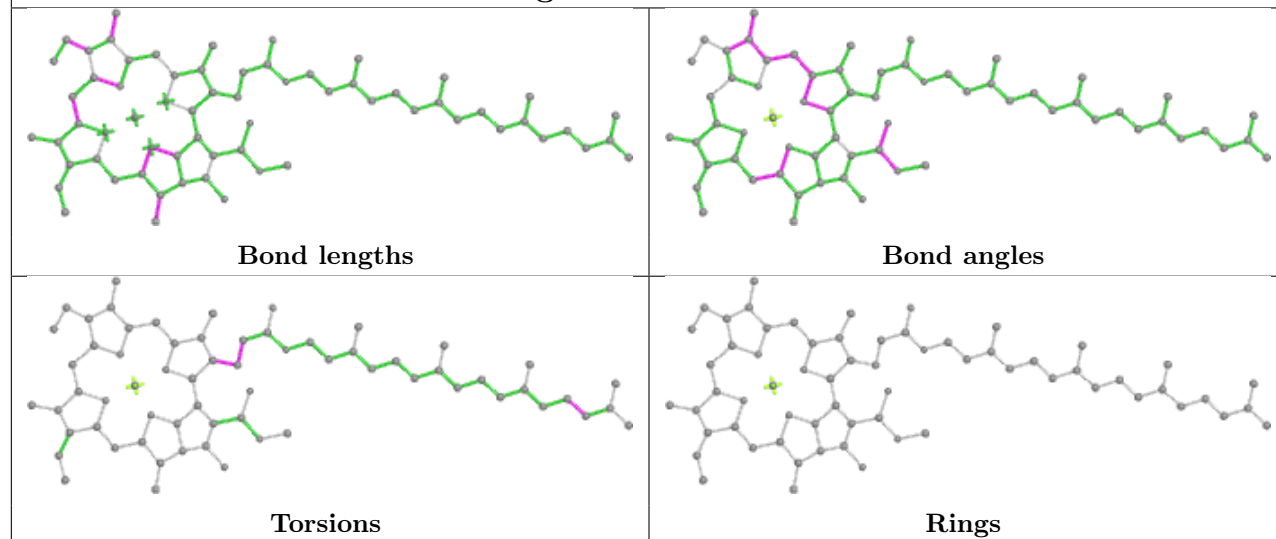
## Ligand CLA a 831



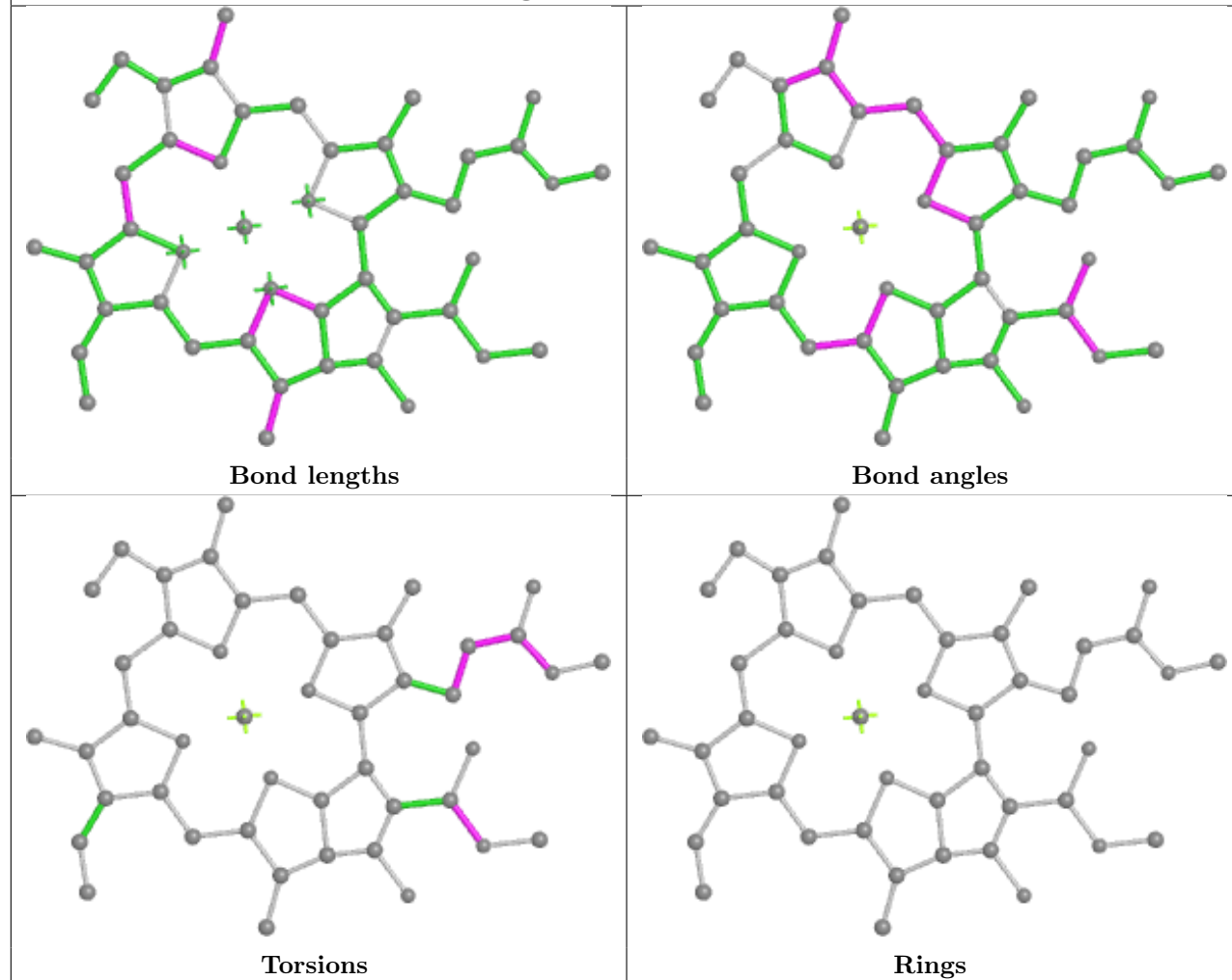
## Ligand CLA 4 306



## Ligand CLA a 803

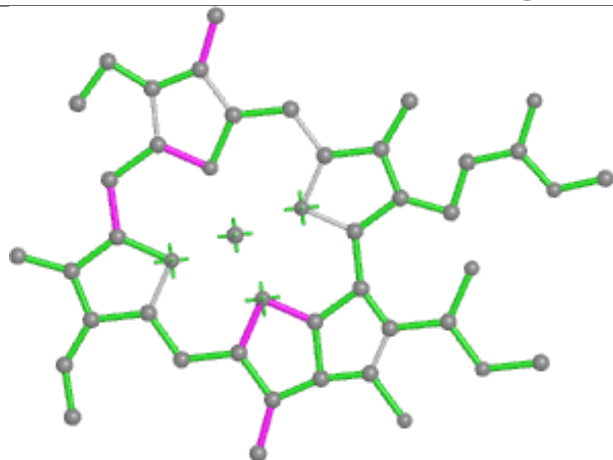


## Ligand CLA 5 310

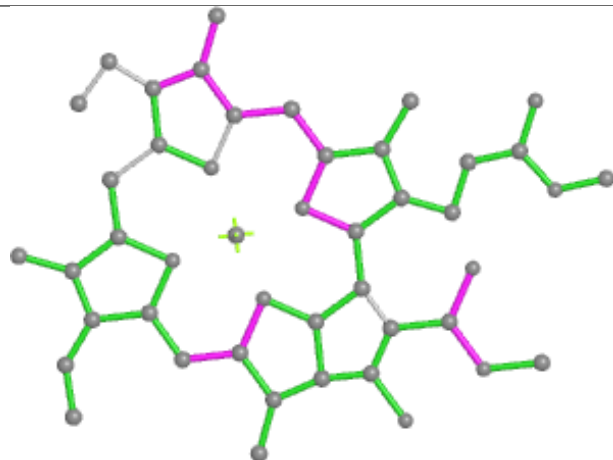




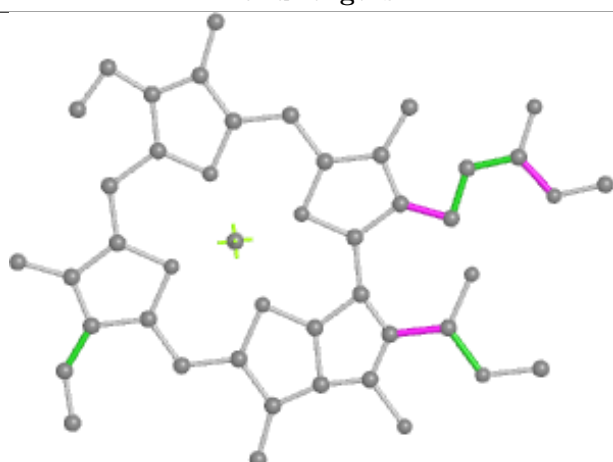
## Ligand CLA 7 311



Bond lengths



Bond angles

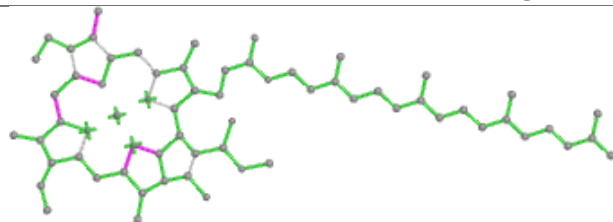


Torsions

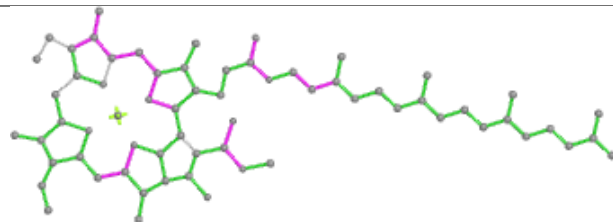


Rings

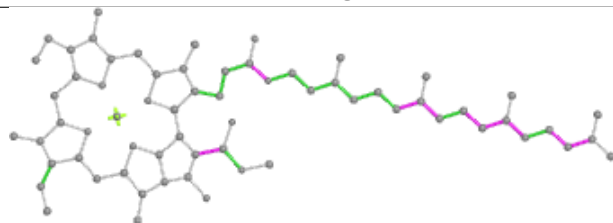
## Ligand CLA a 844



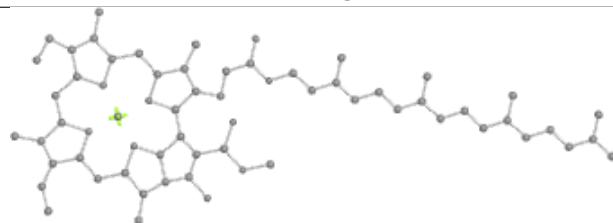
Bond lengths



Bond angles

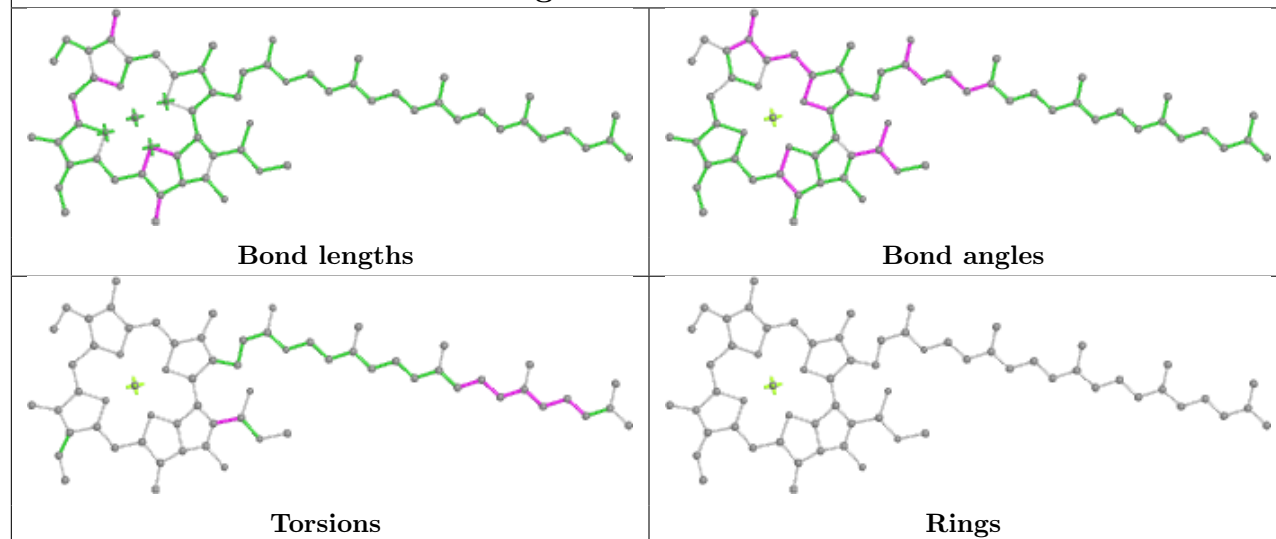


Torsions

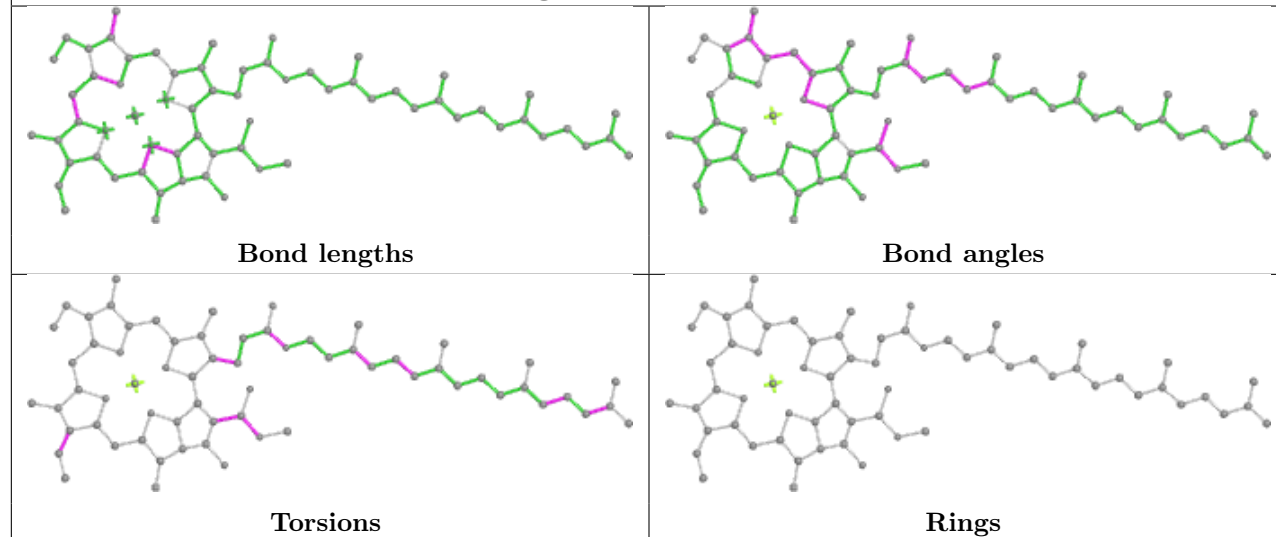


Rings

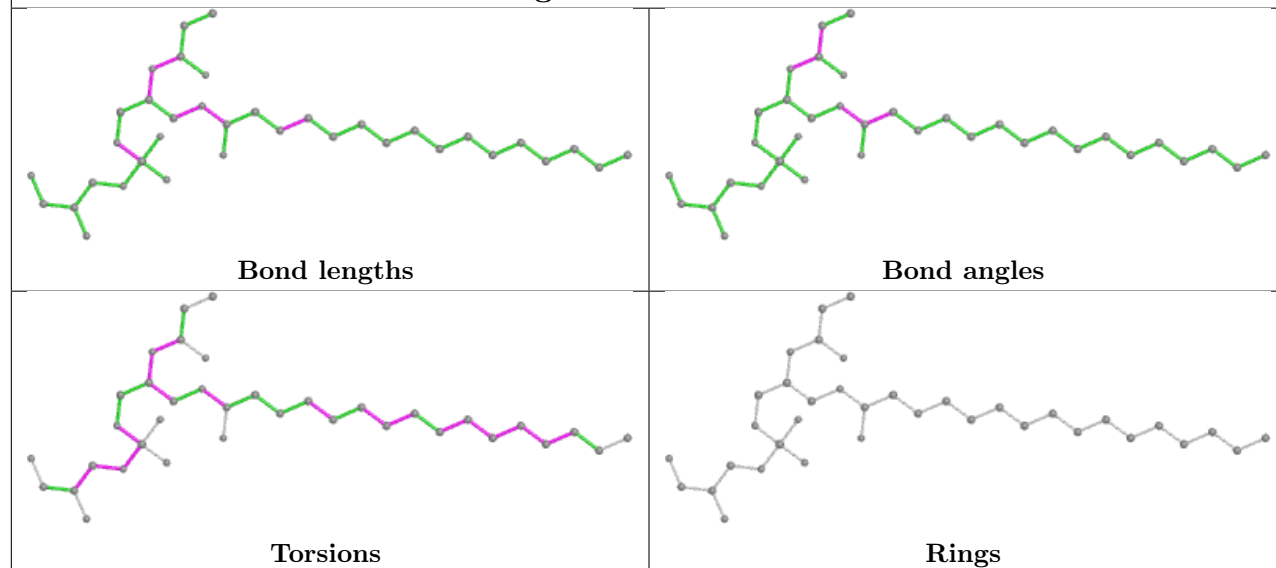
## Ligand CLA b 829

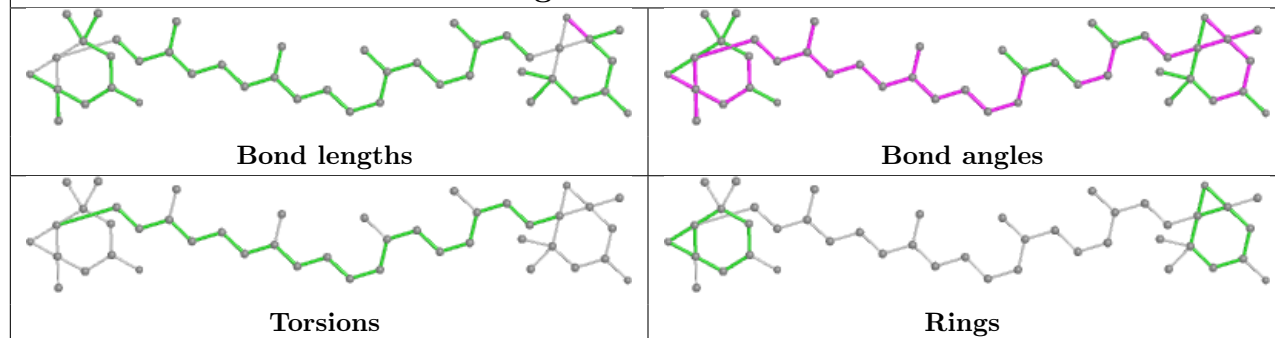
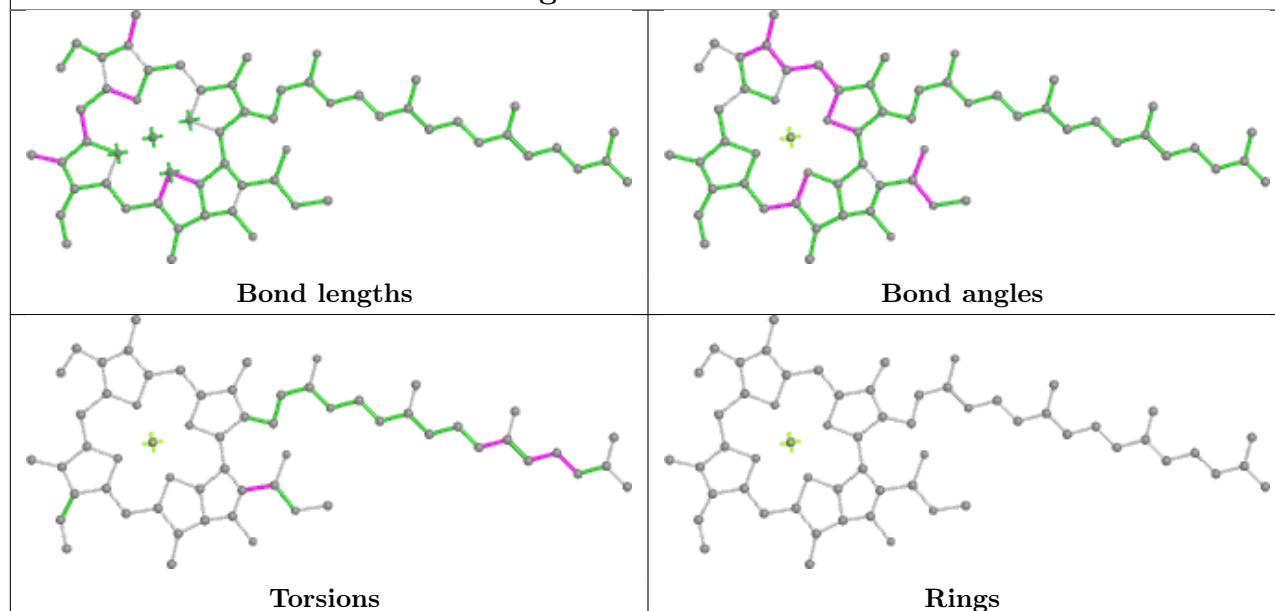
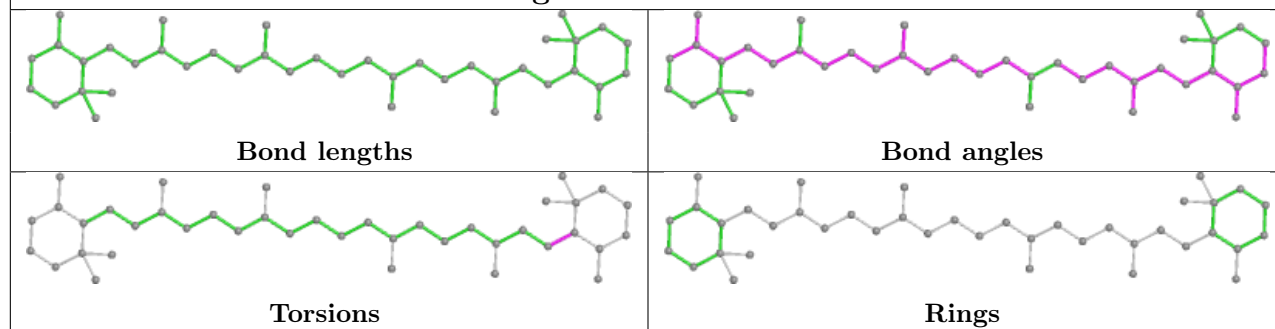


## Ligand CLA b 839

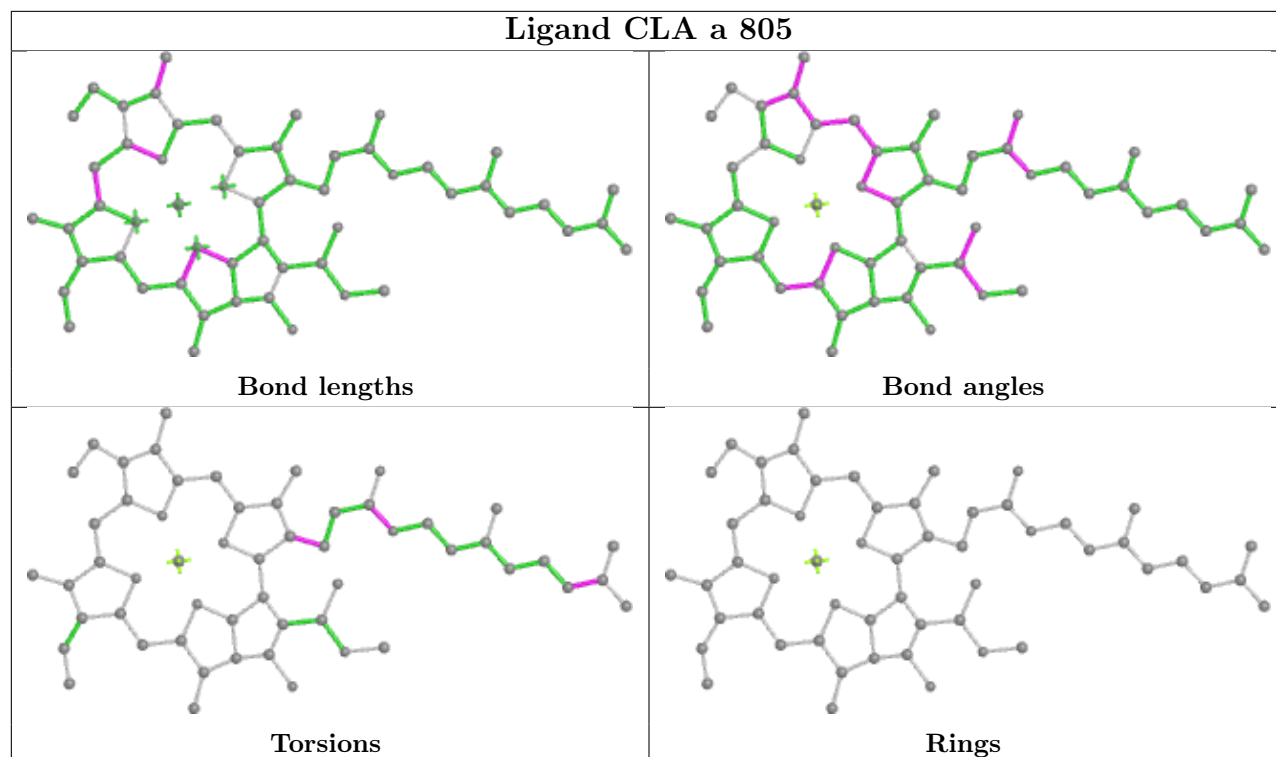


## Ligand LHG 9 307

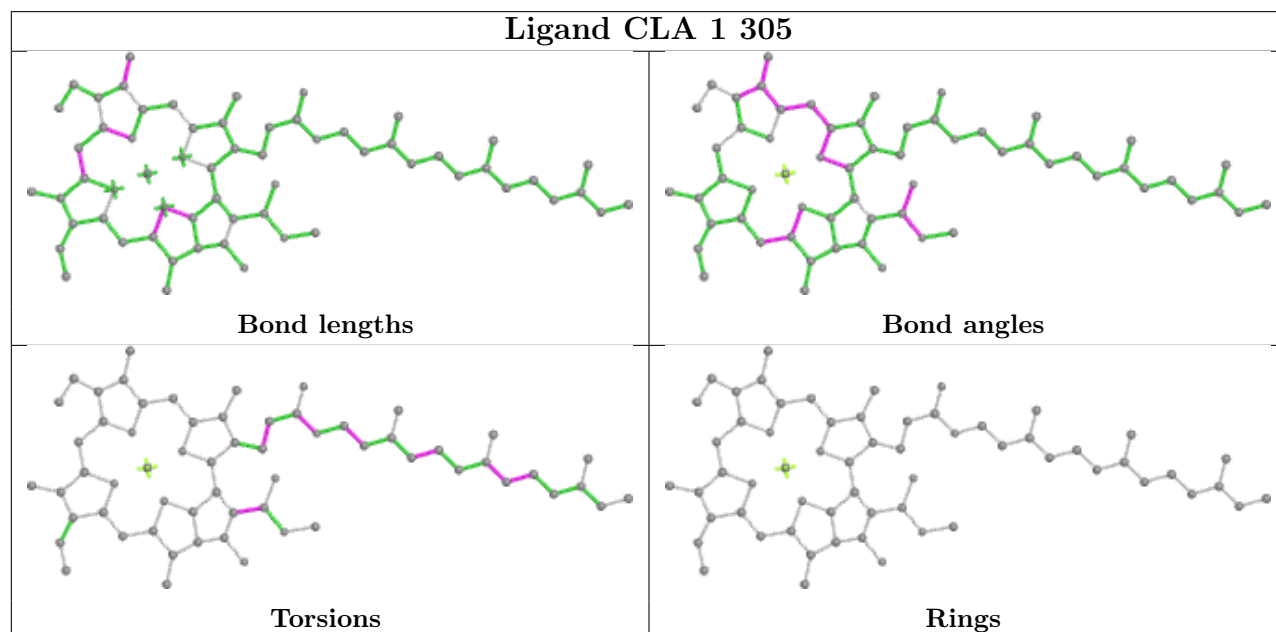


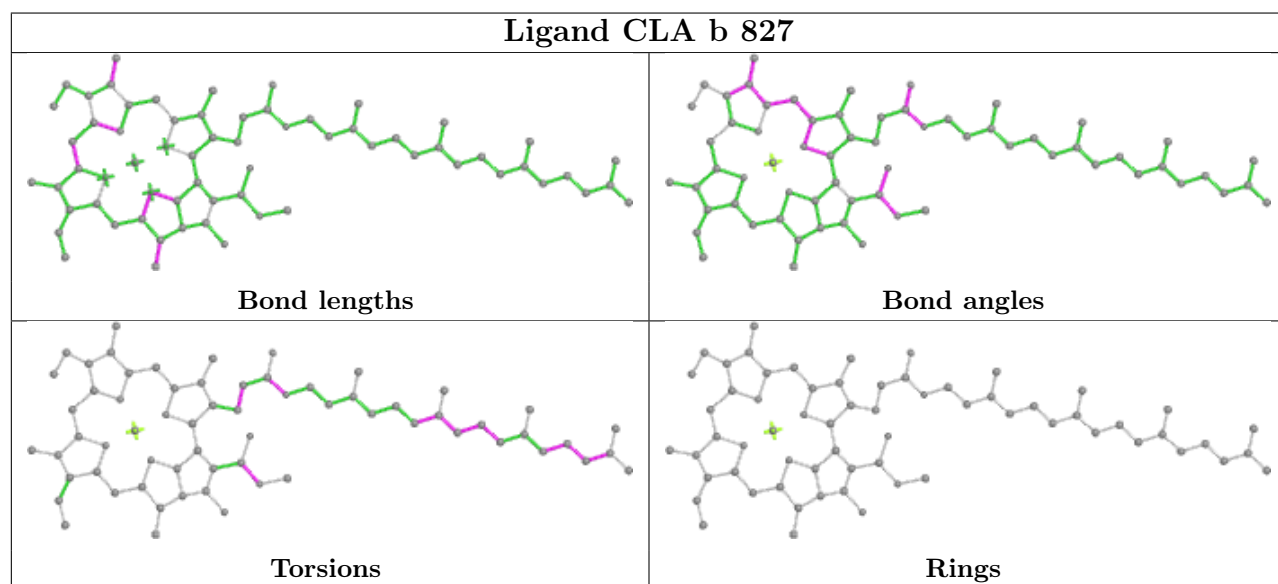
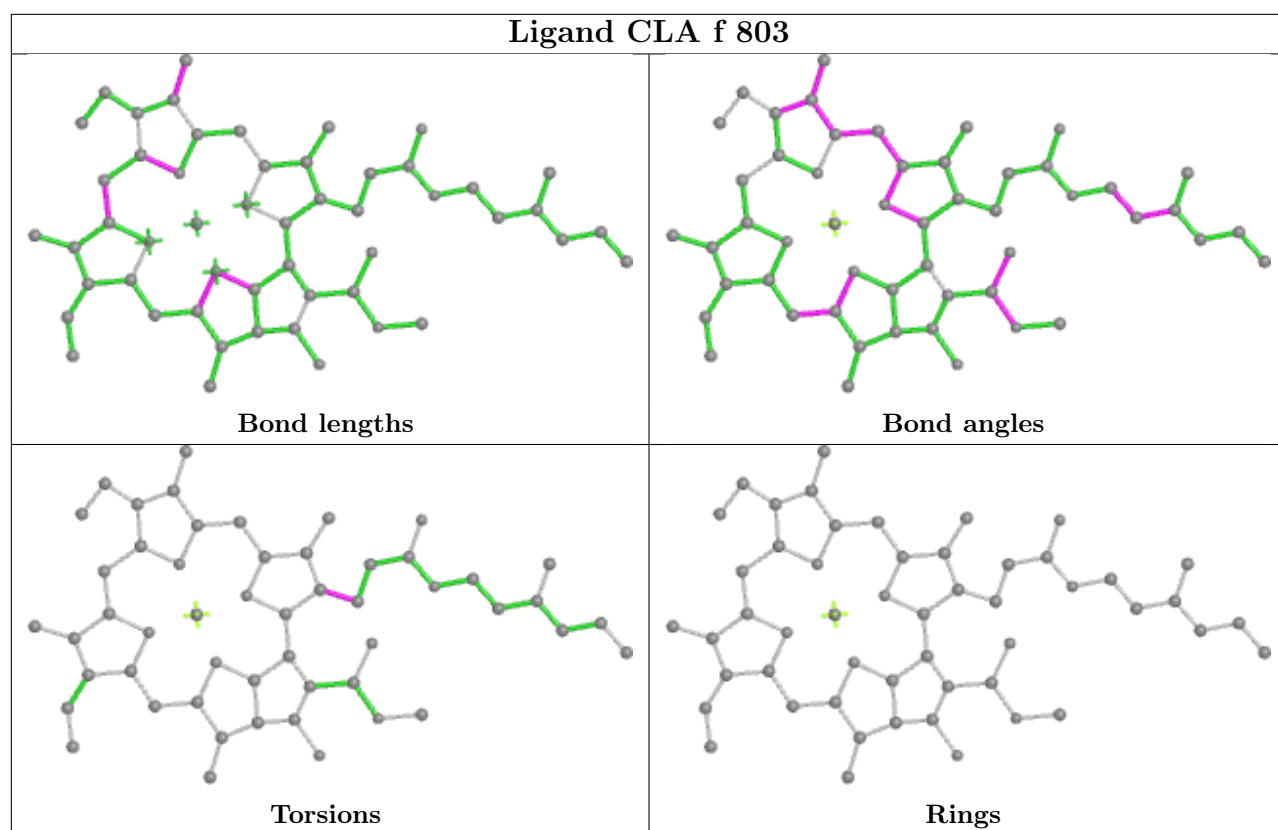
**Ligand XAT 8 303****Ligand CLA 1 203****Ligand BCR h 202**

## Ligand CLA a 805

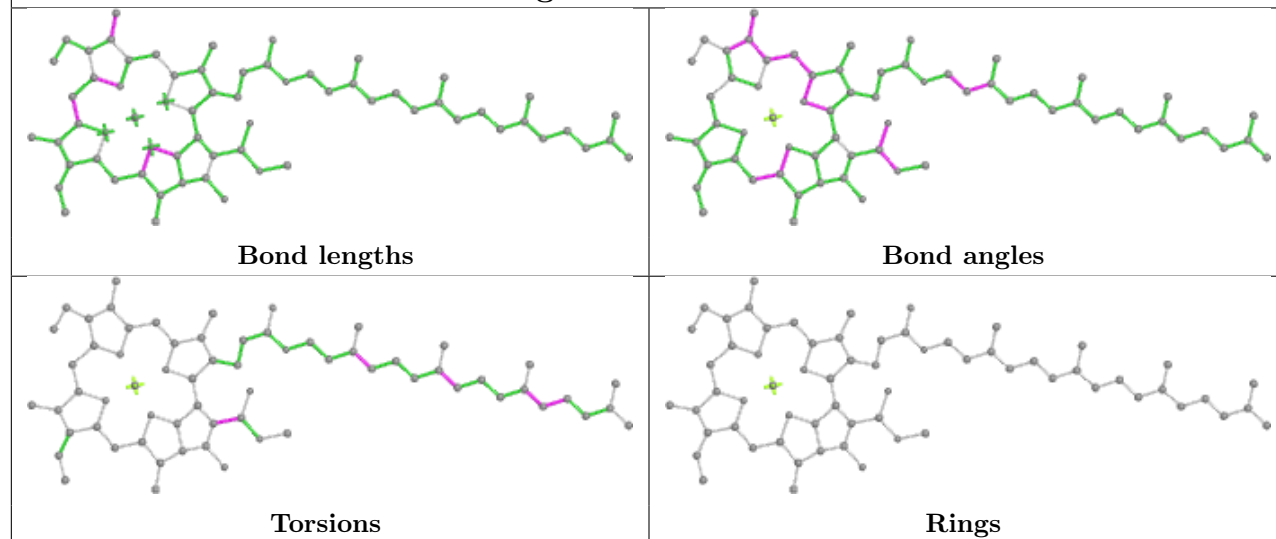


## Ligand CLA 1 305

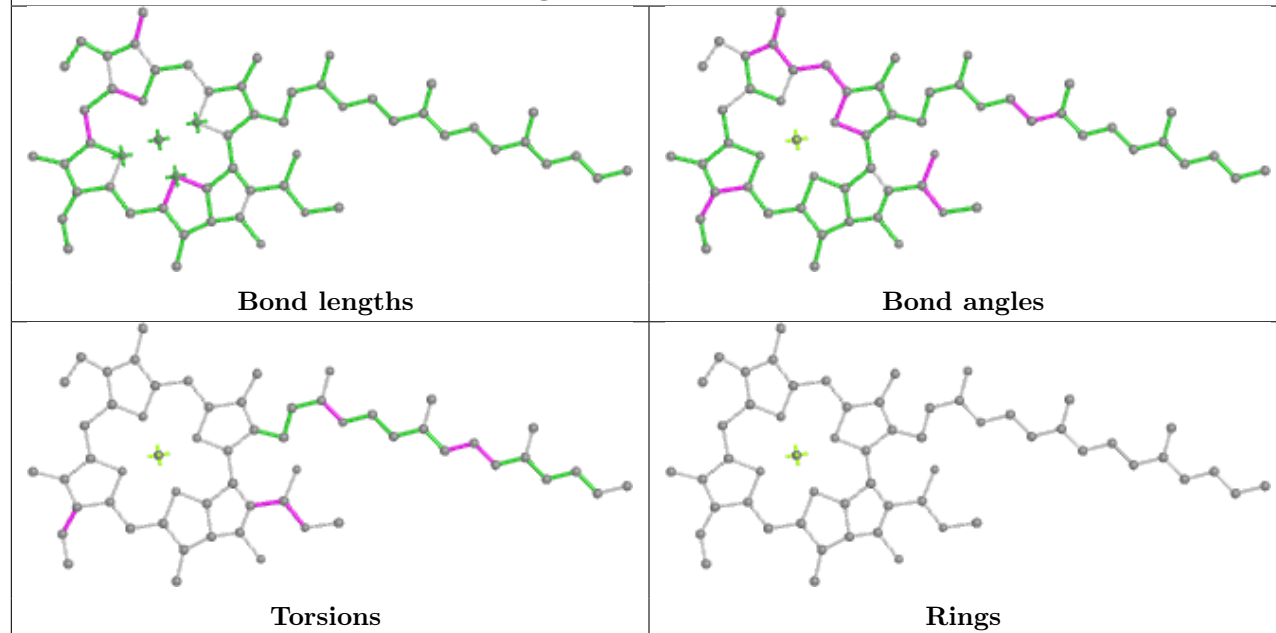




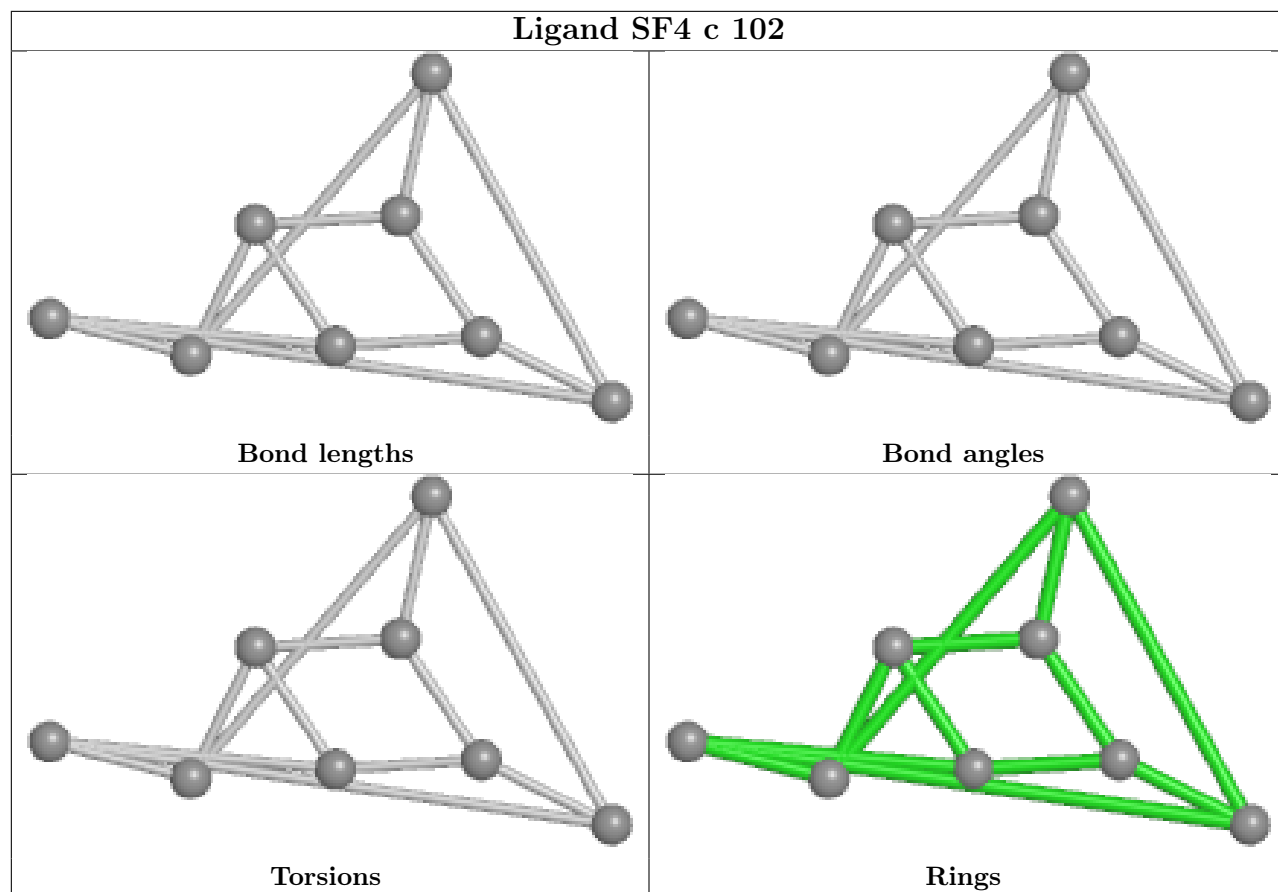
## Ligand CLA a 840



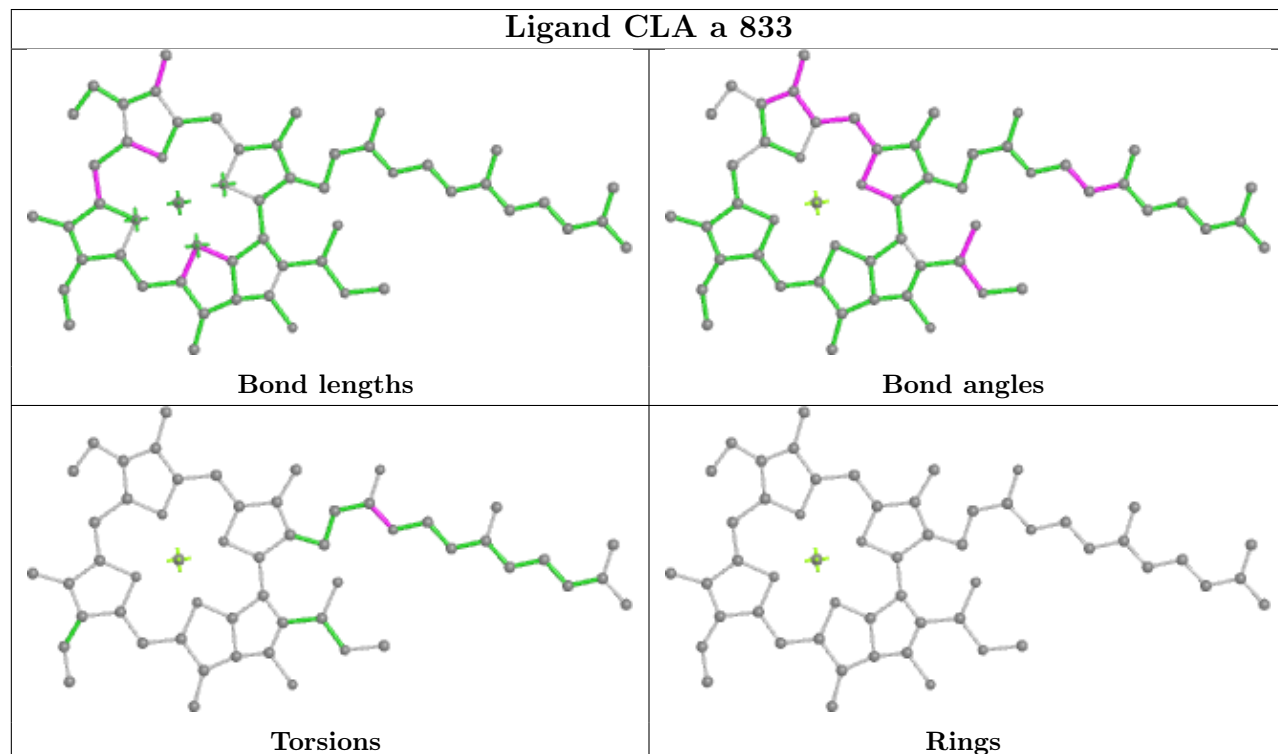
## Ligand CLA b 835



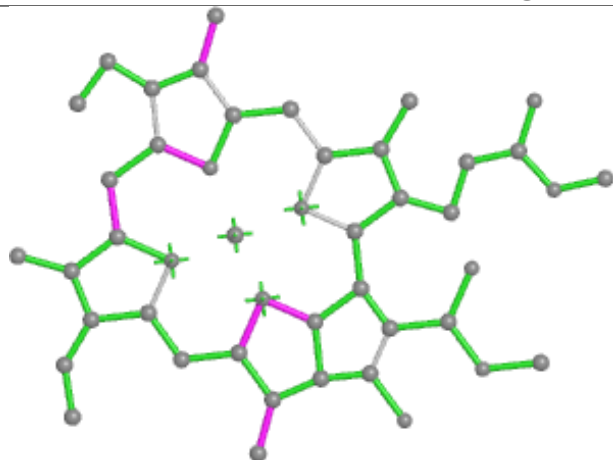
## Ligand SF4 c 102



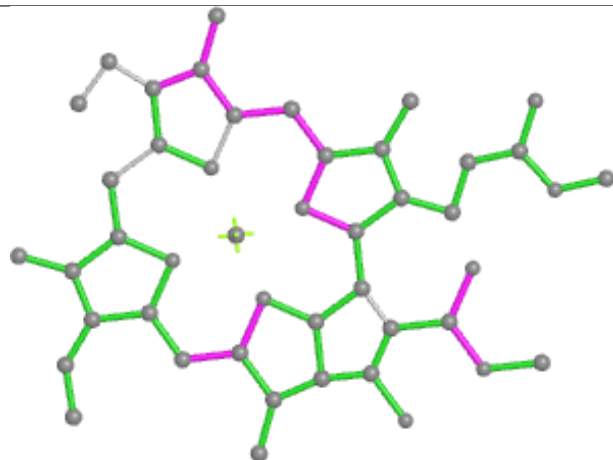
## Ligand CLA a 833



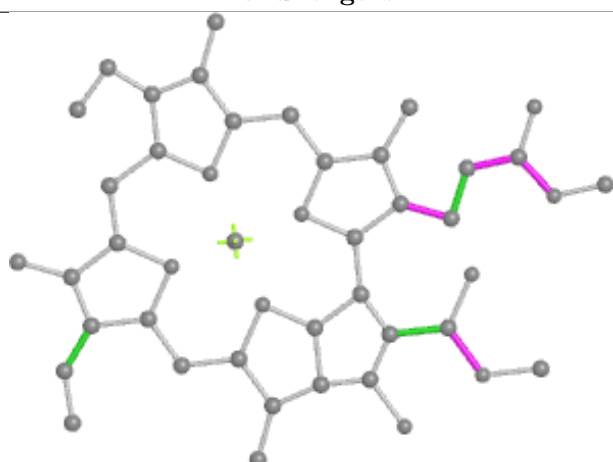
## Ligand CLA 3 315



Bond lengths



Bond angles



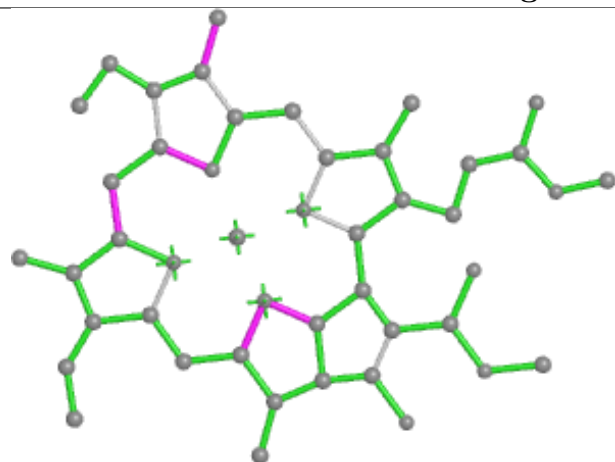
Torsions



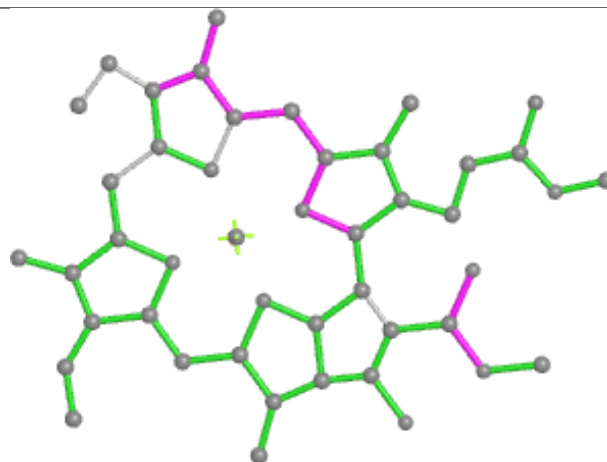
Rings



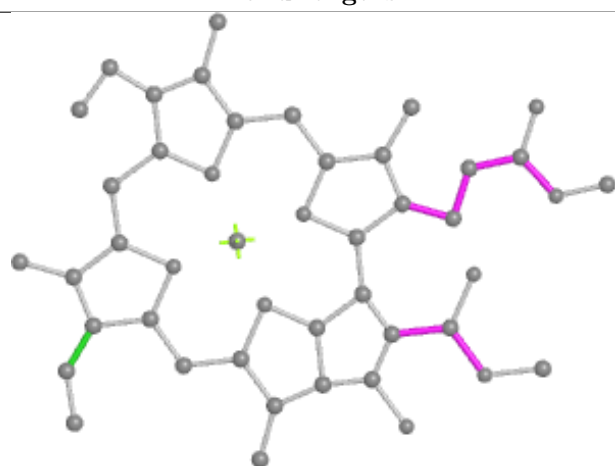
## Ligand CLA 9 313



Bond lengths



Bond angles

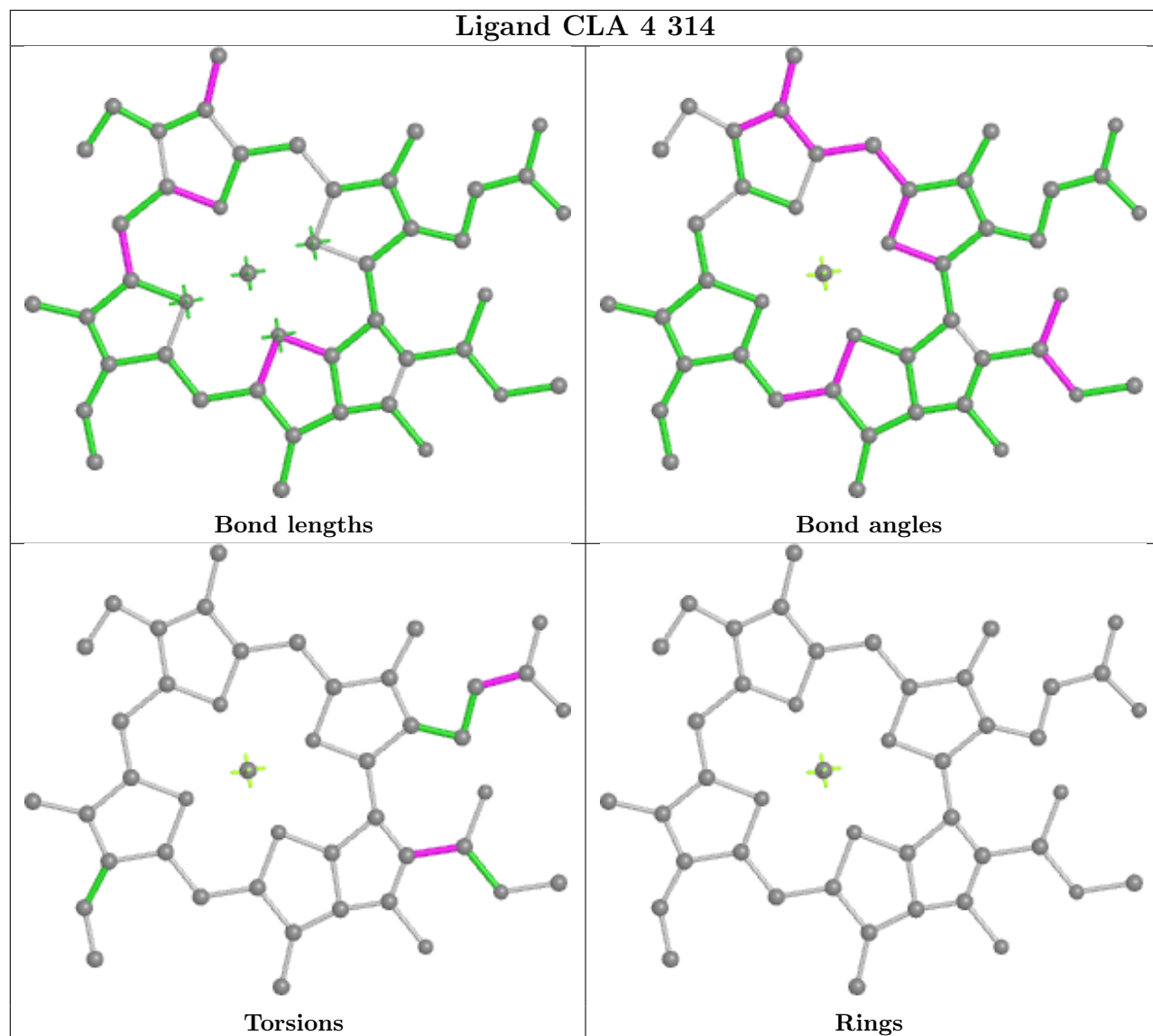


Torsions

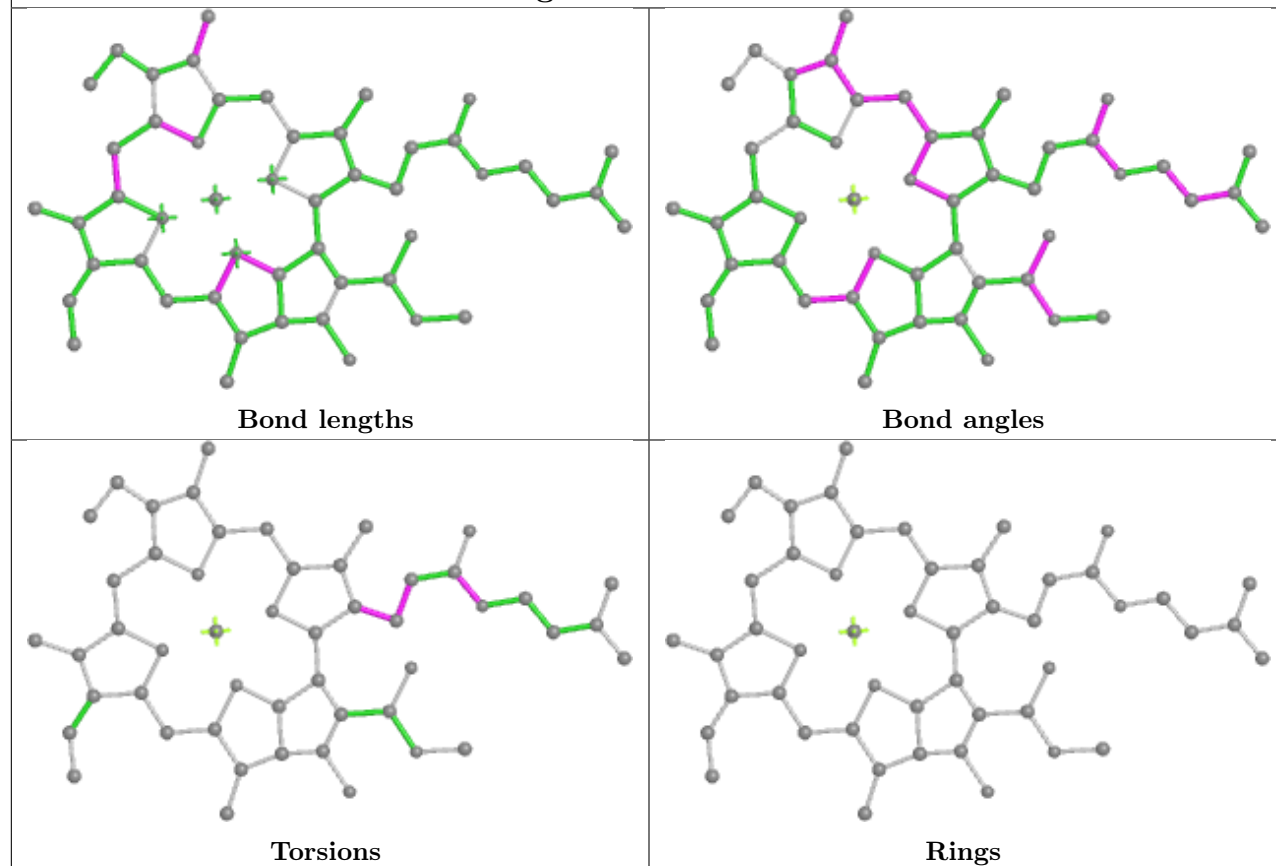


Rings

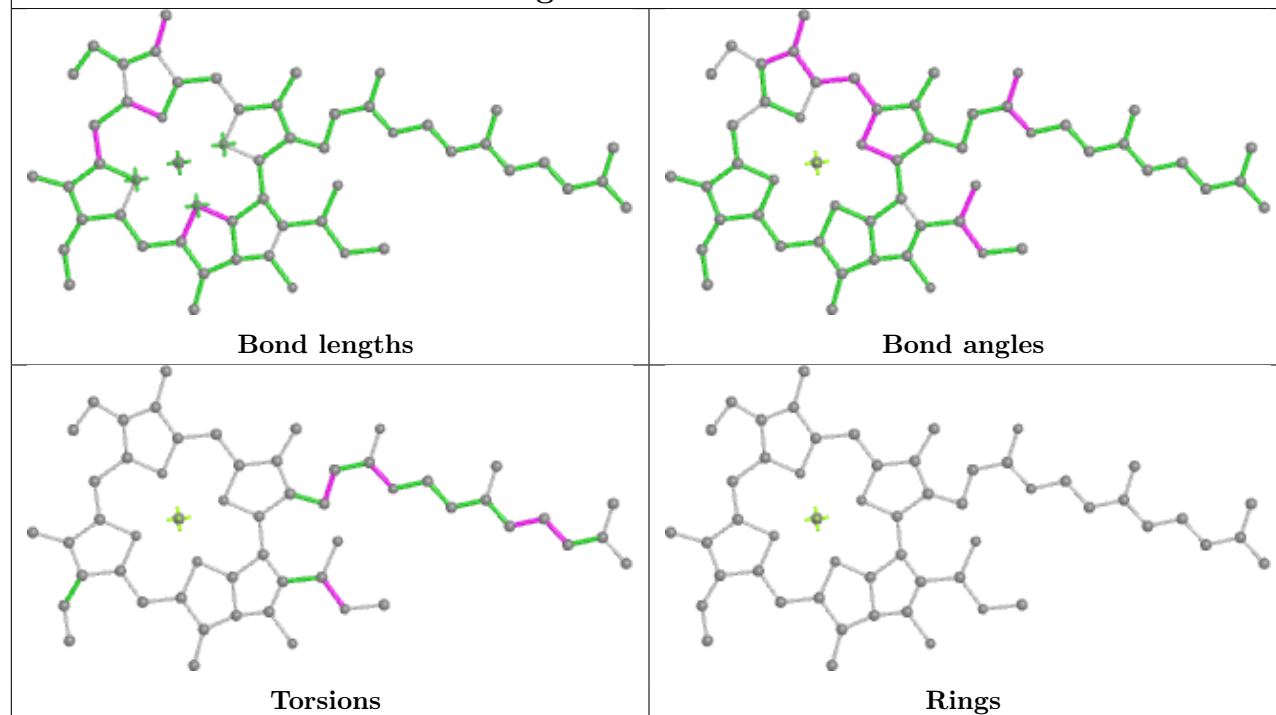
## Ligand CLA 4 314

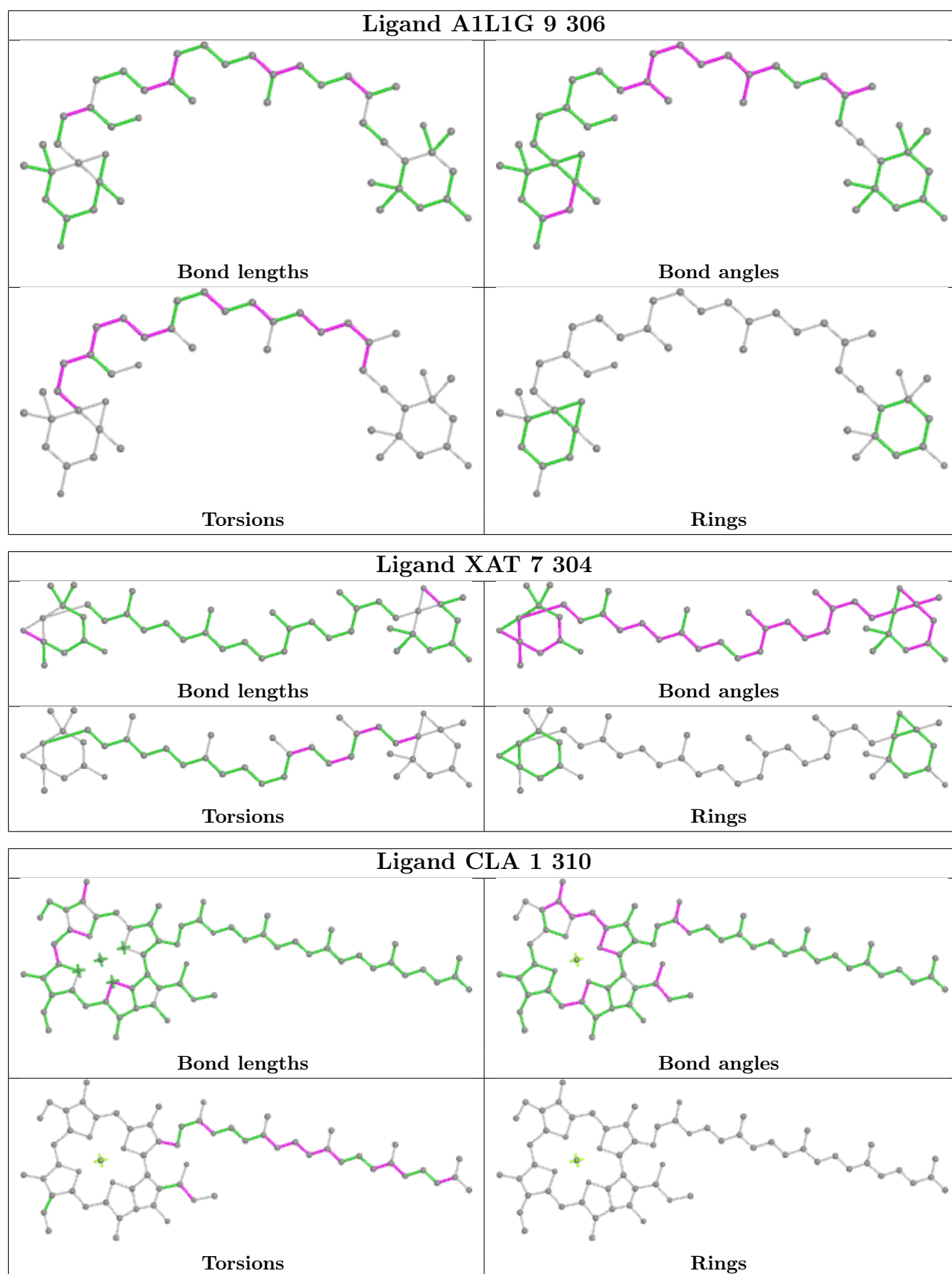


## Ligand CLA 3 311

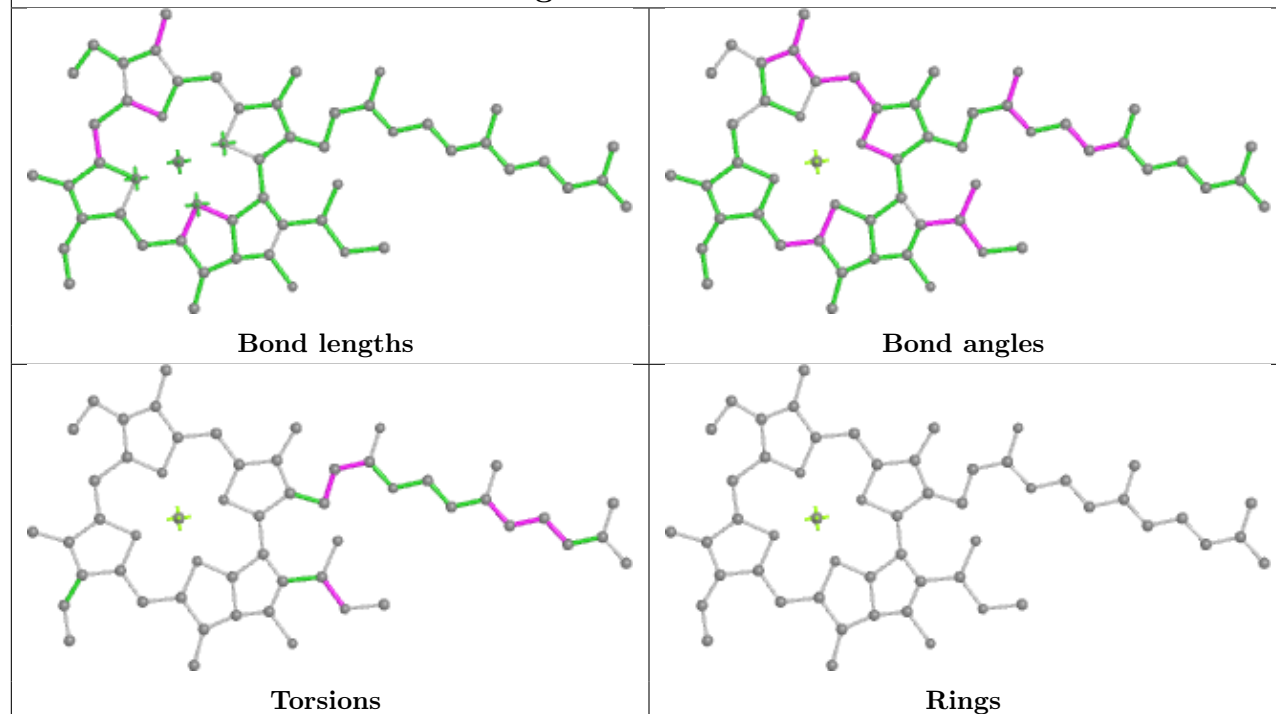


## Ligand CLA 4 317

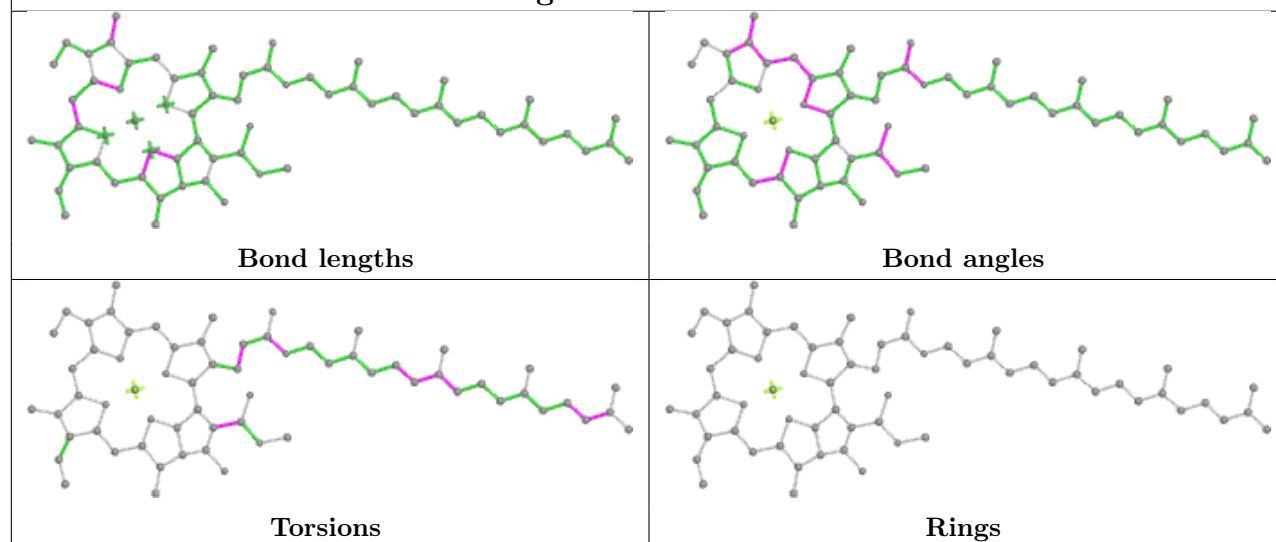




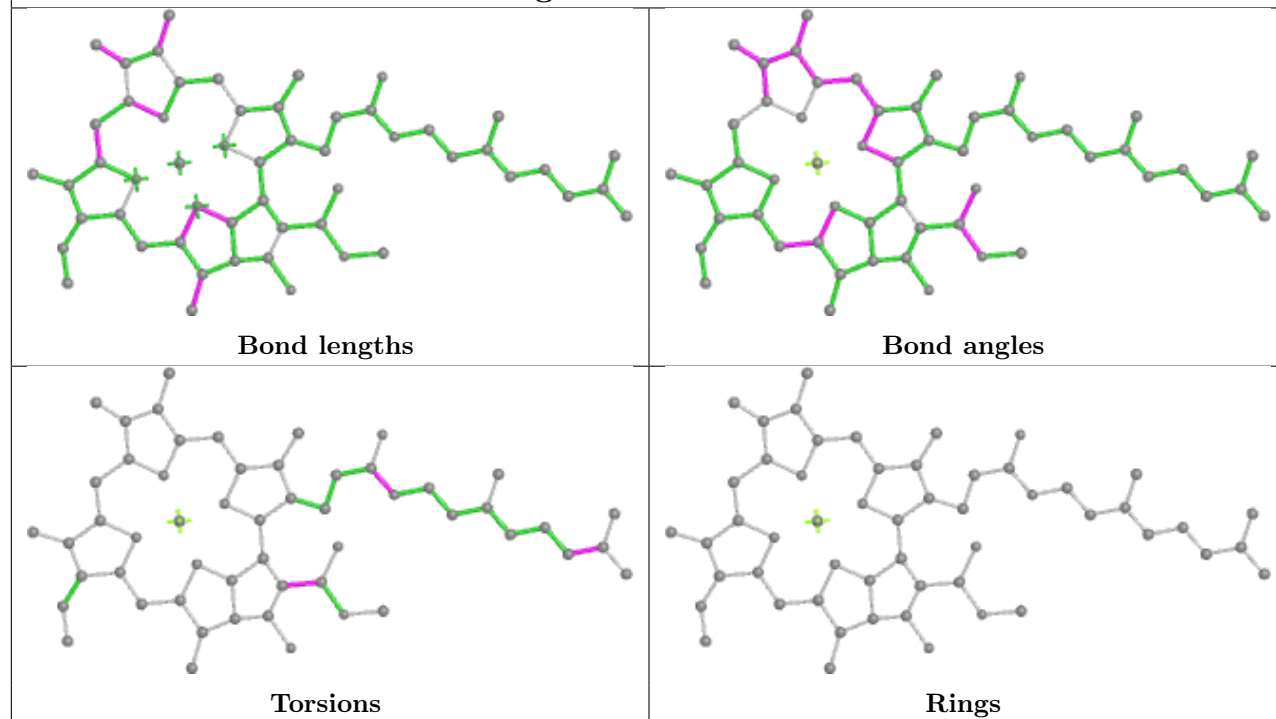
## Ligand CLA h 205



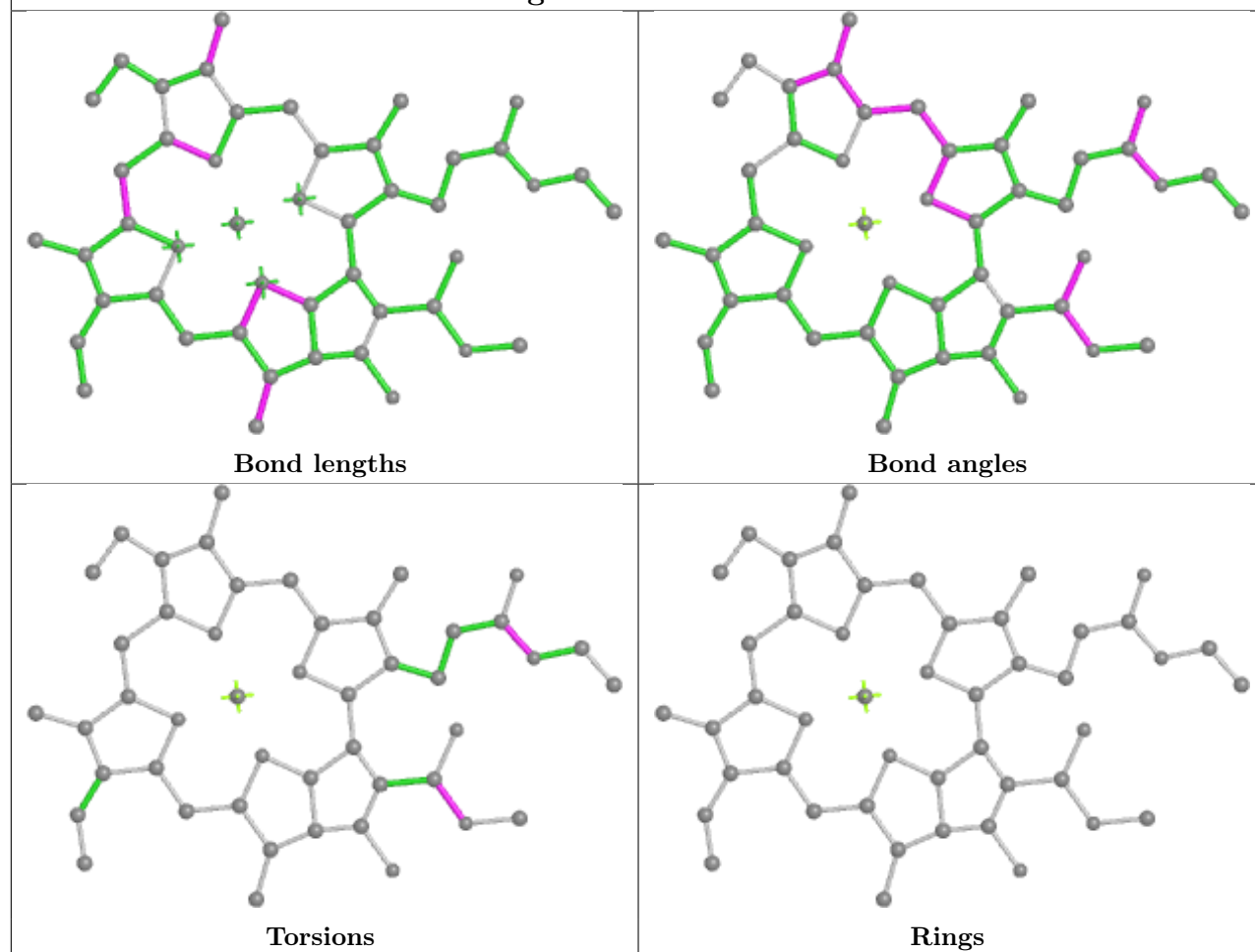
## Ligand CLA 8 307



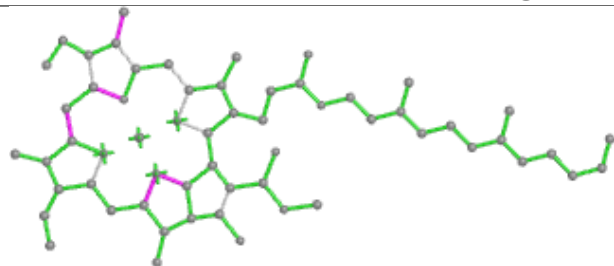
## Ligand CLA b 811



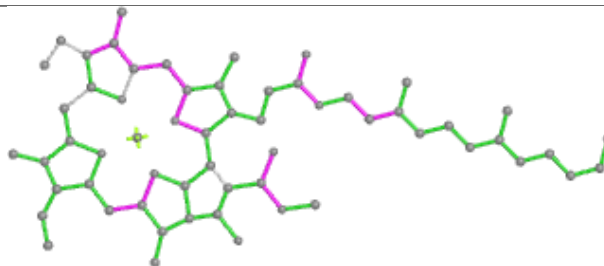
## Ligand CLA 2 312



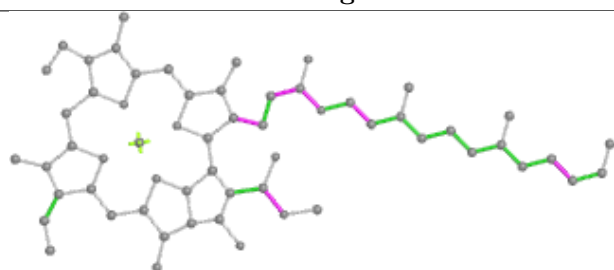
## Ligand CLA b 817



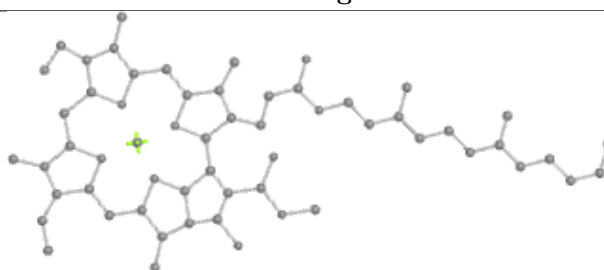
Bond lengths



Bond angles

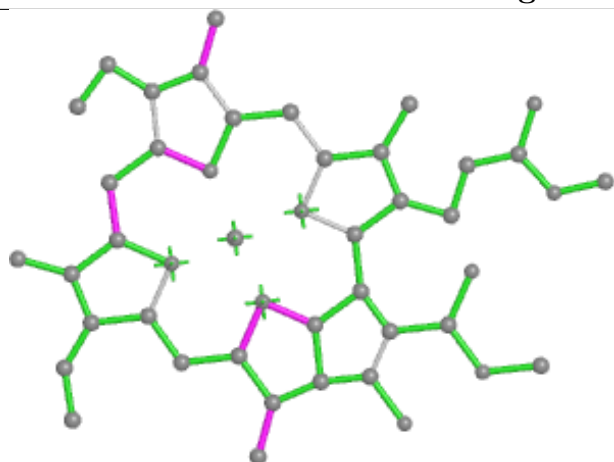


Torsions

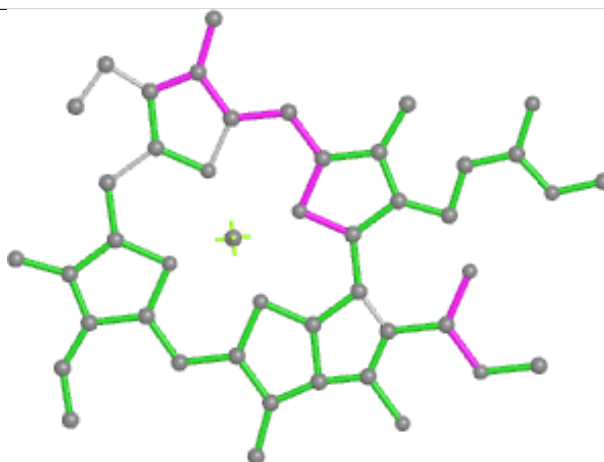


Rings

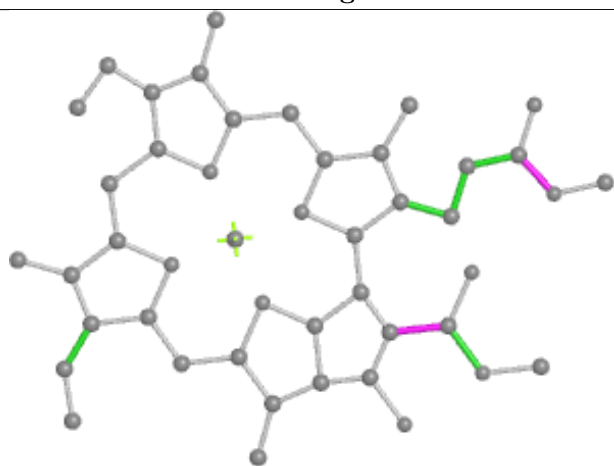
## Ligand CLA 8 313



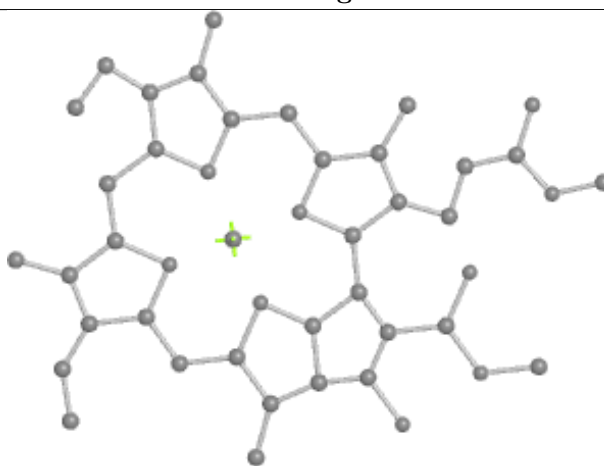
Bond lengths



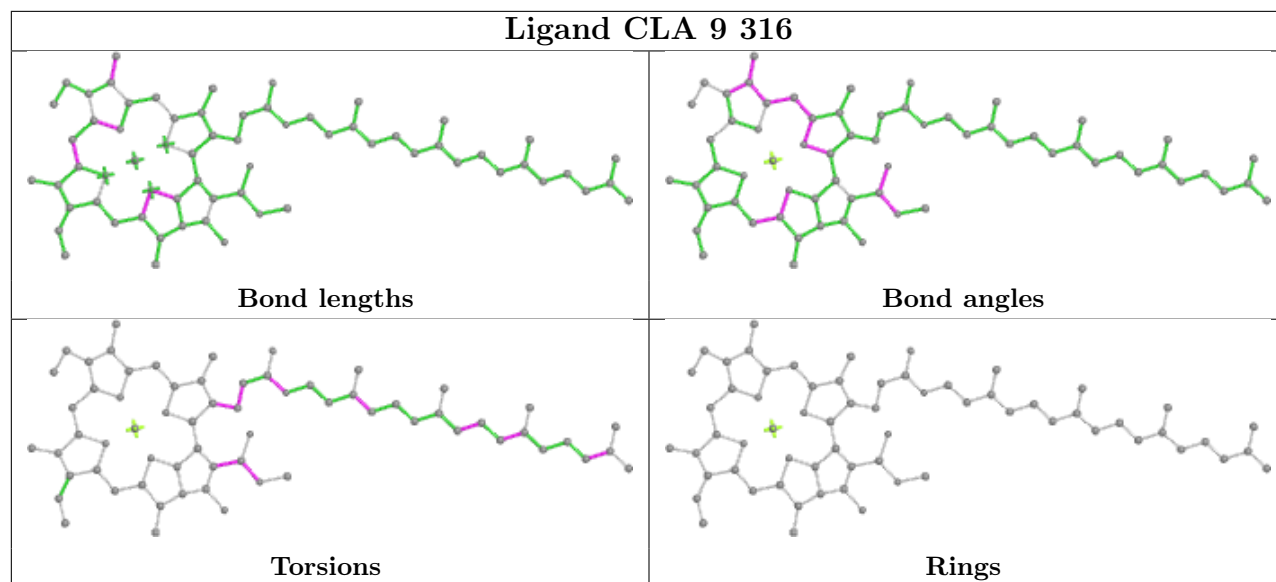
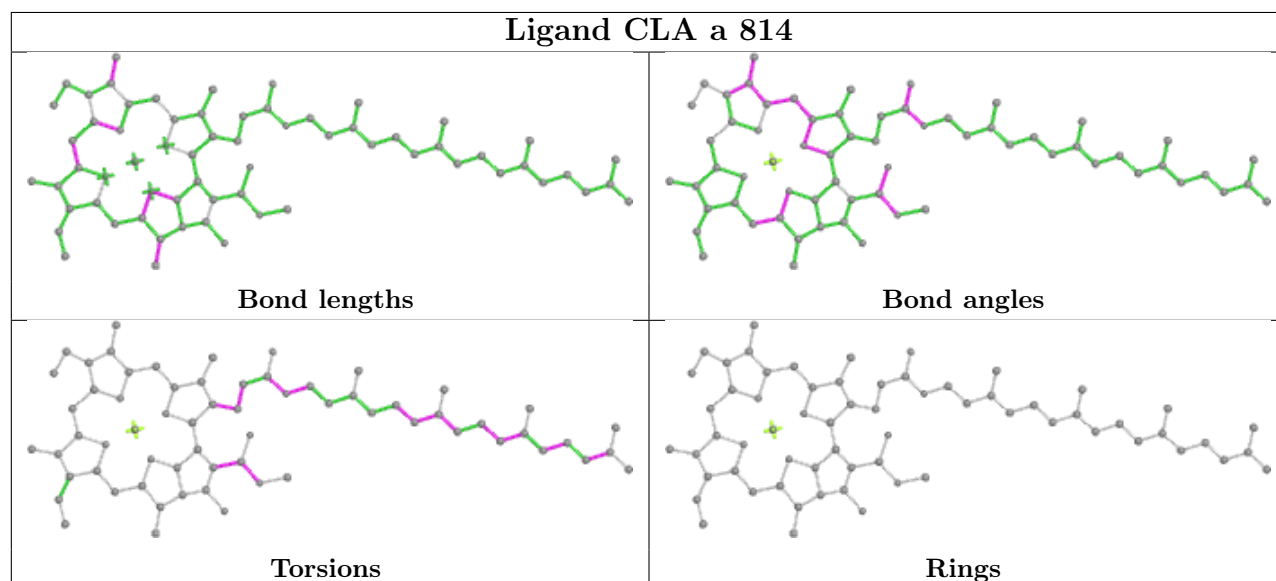
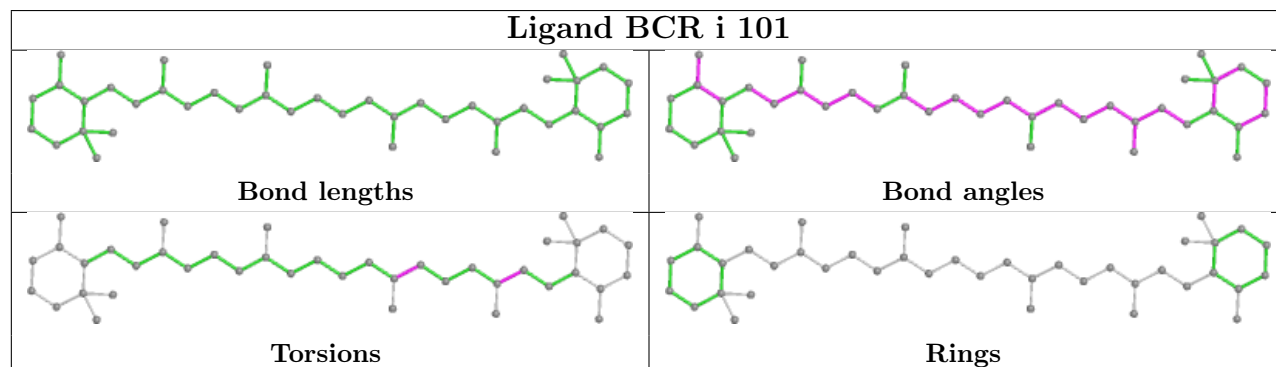
Bond angles



Torsions

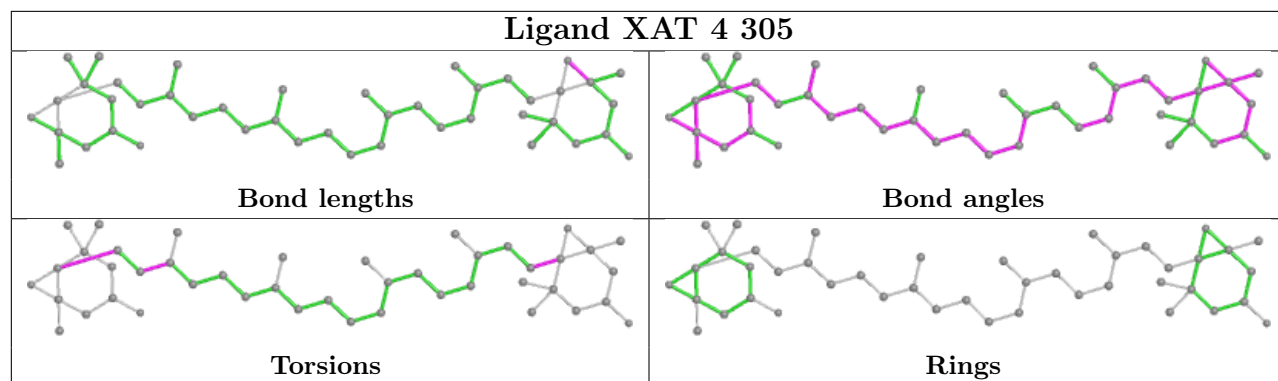


Rings

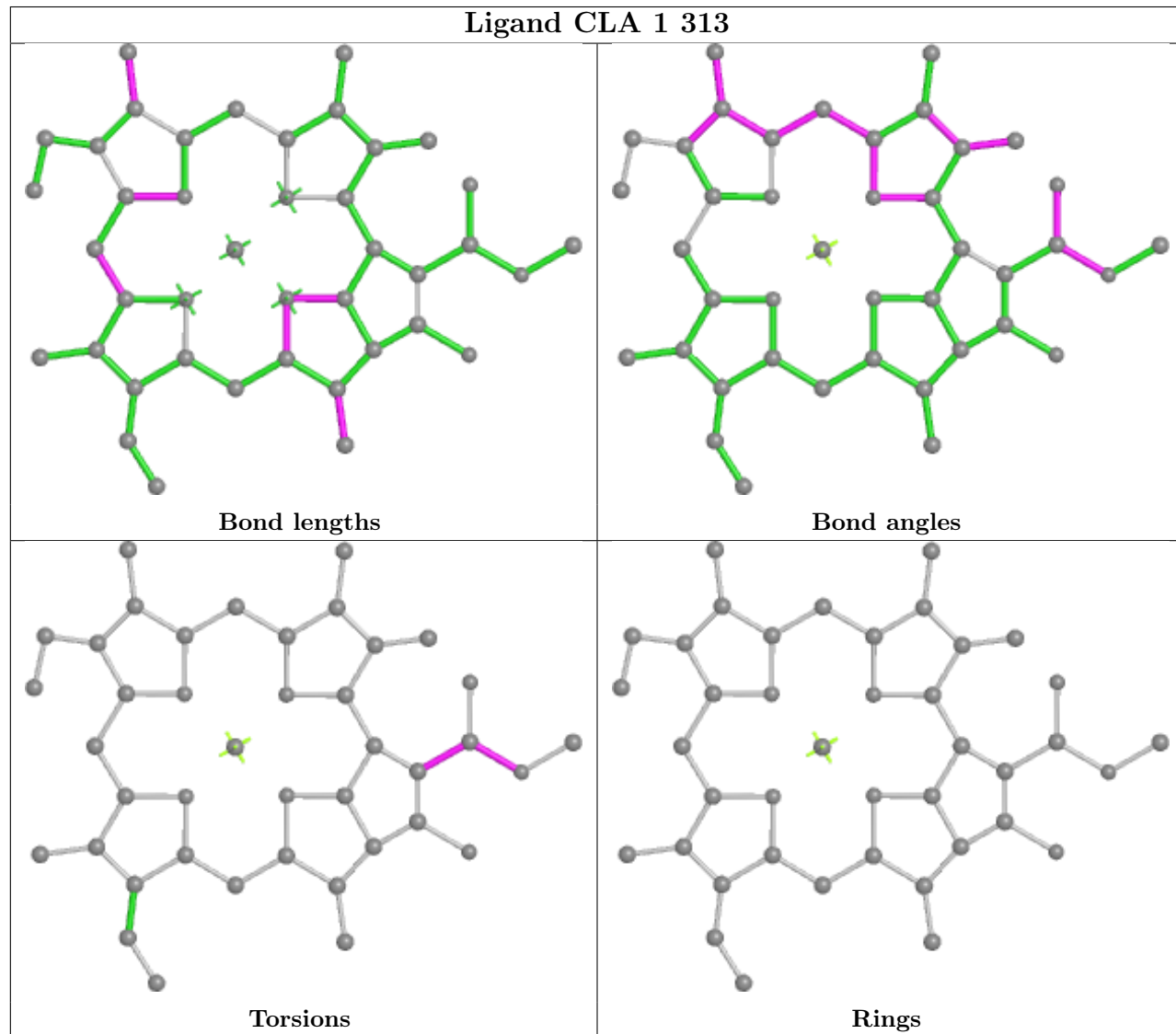
**Ligand CLA 9 316****Ligand CLA a 814****Ligand BCR i 101**



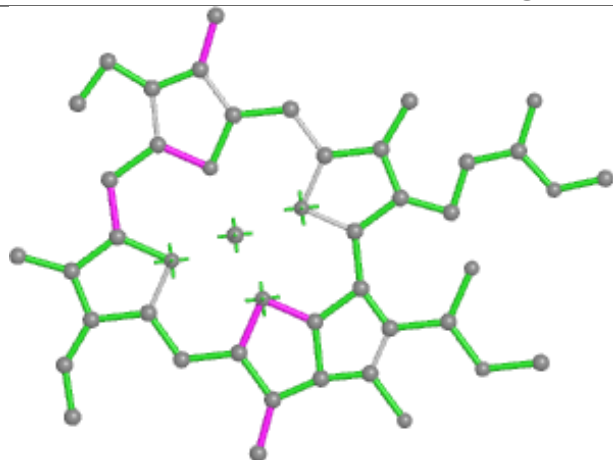
## Ligand XAT 4 305



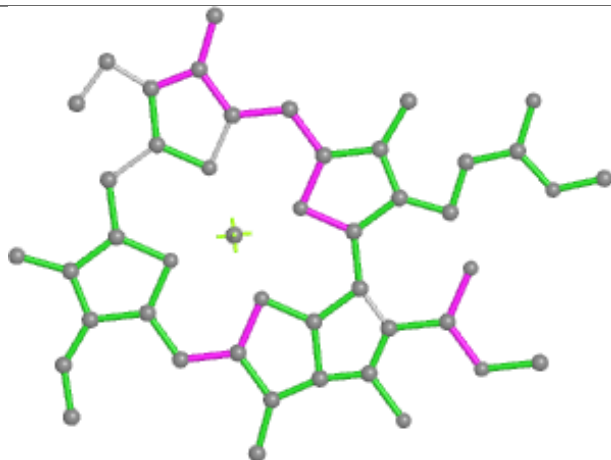
## Ligand CLA 1 313



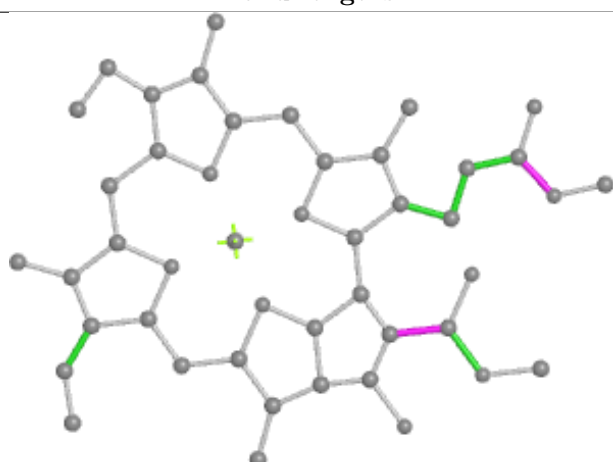
## Ligand CLA 9 309



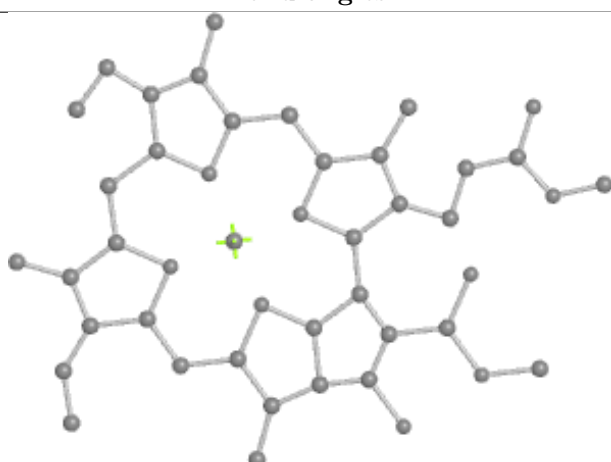
Bond lengths



Bond angles

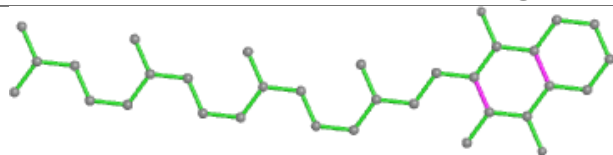


Torsions

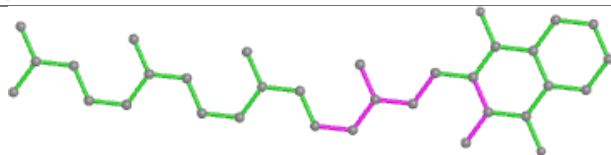


Rings

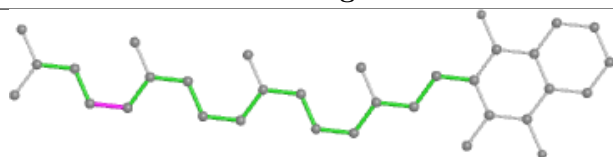
## Ligand PQN b 841



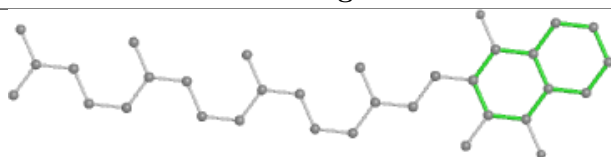
Bond lengths



Bond angles

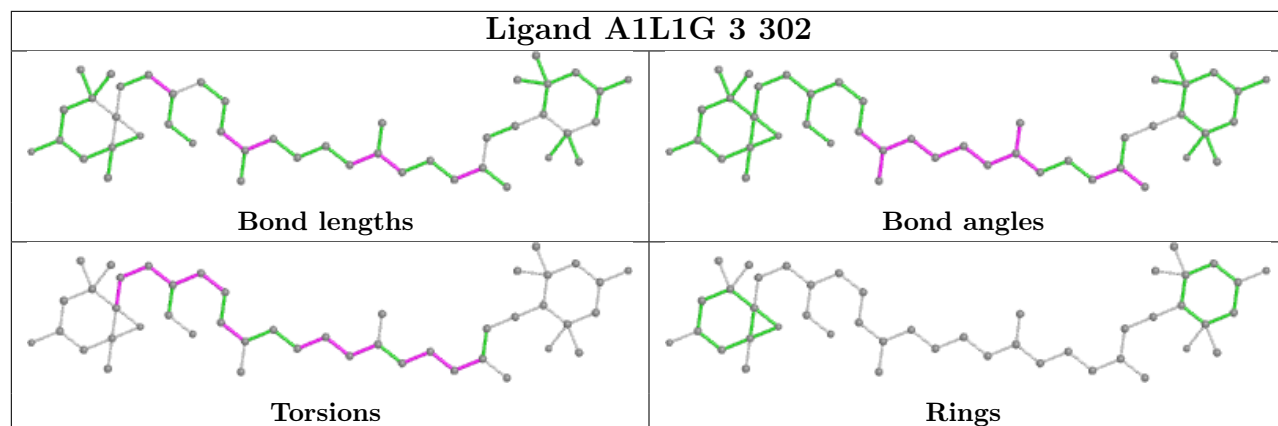


Torsions

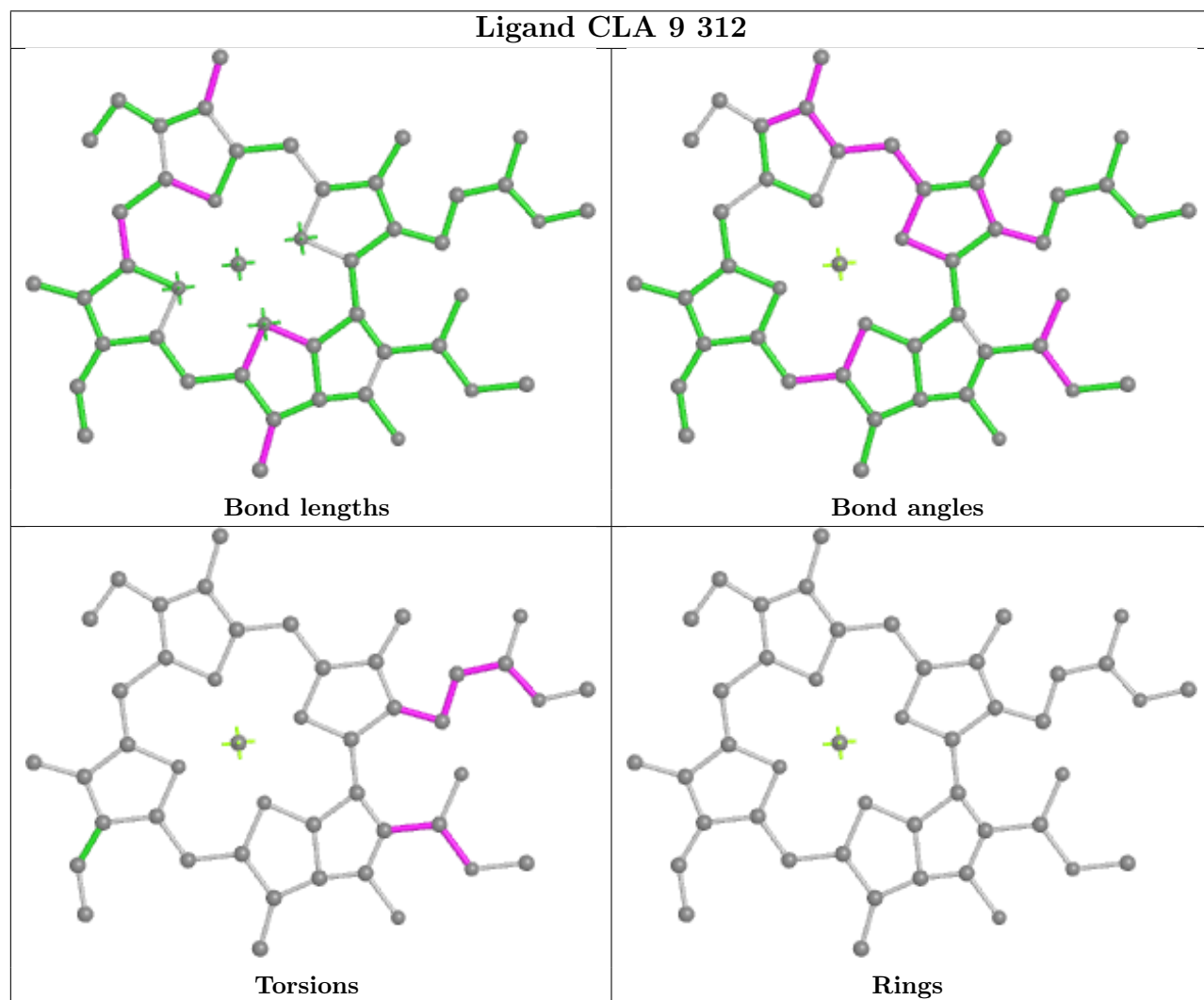


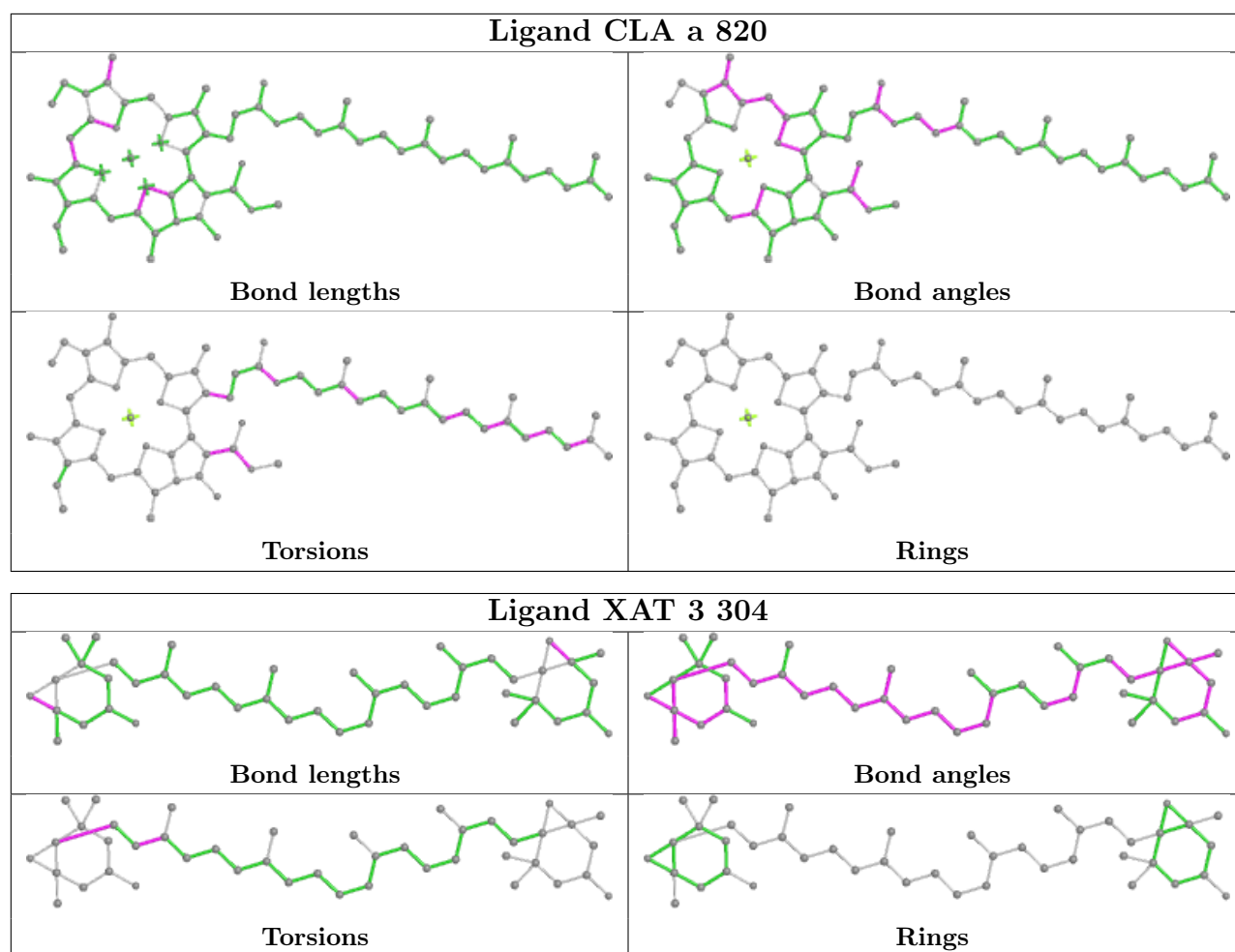
Rings

## Ligand A1L1G 3 302

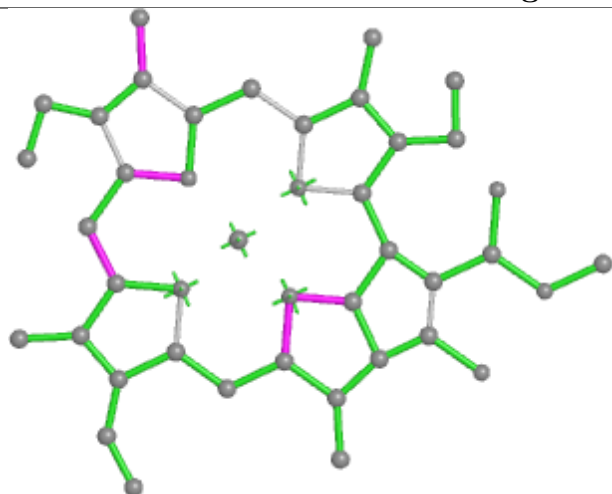


## Ligand CLA 9 312

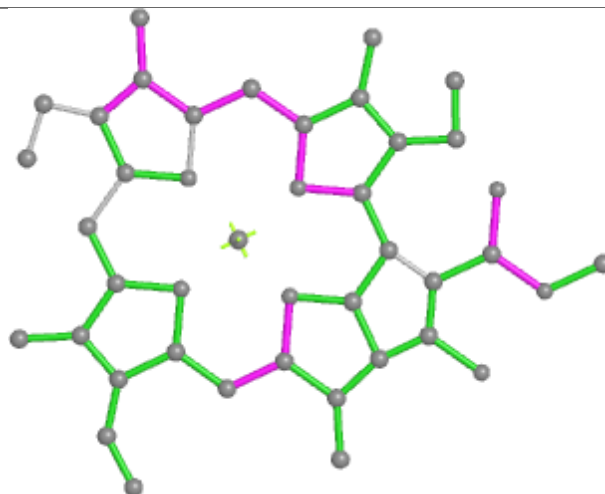




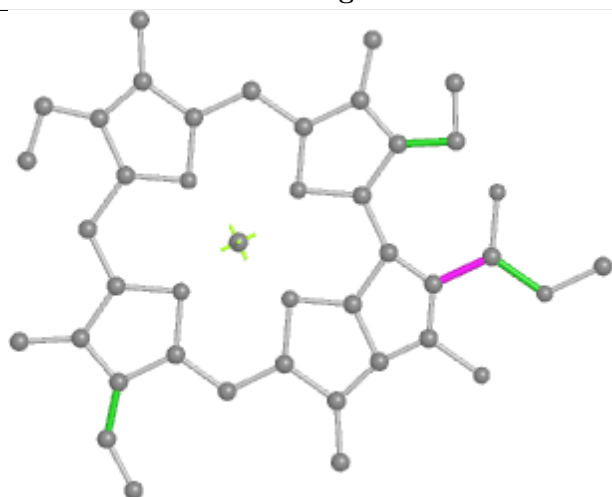
## Ligand CLA 1 202



Bond lengths



Bond angles

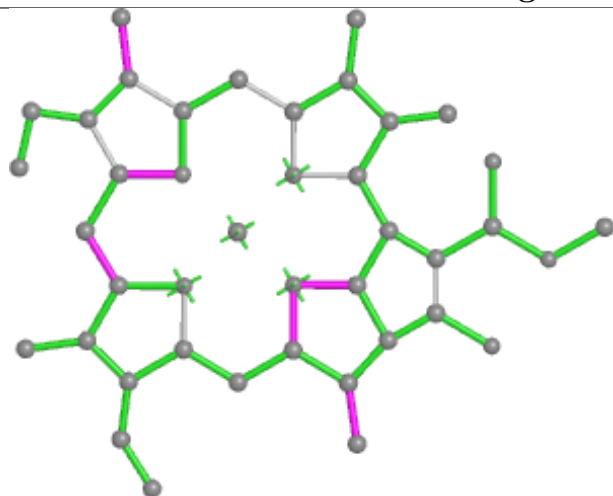


Torsions

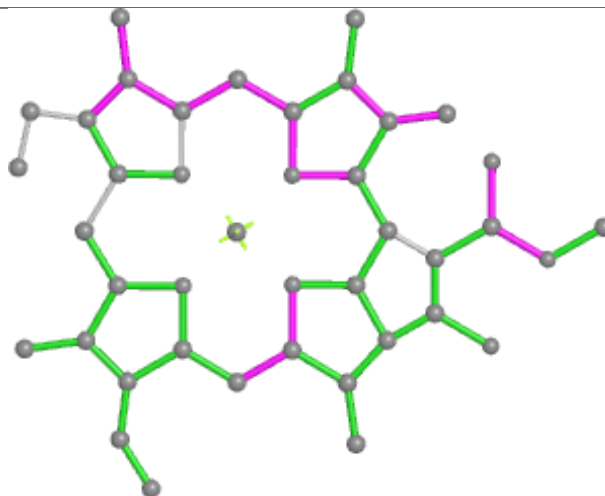


Rings

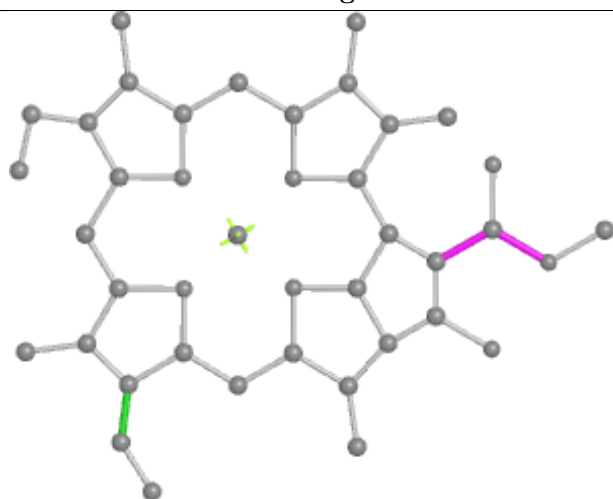
## Ligand CLA 7 315



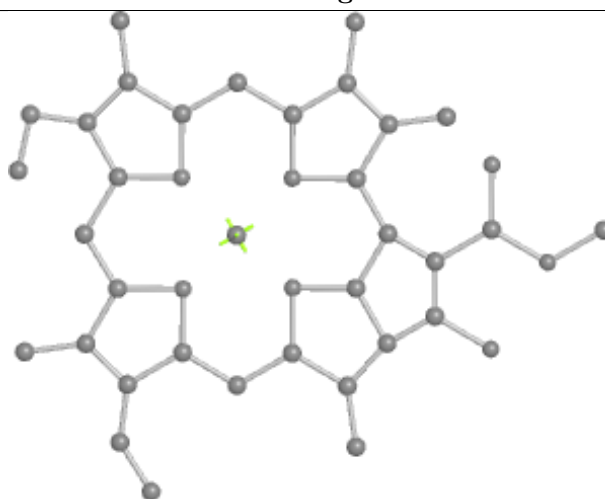
Bond lengths



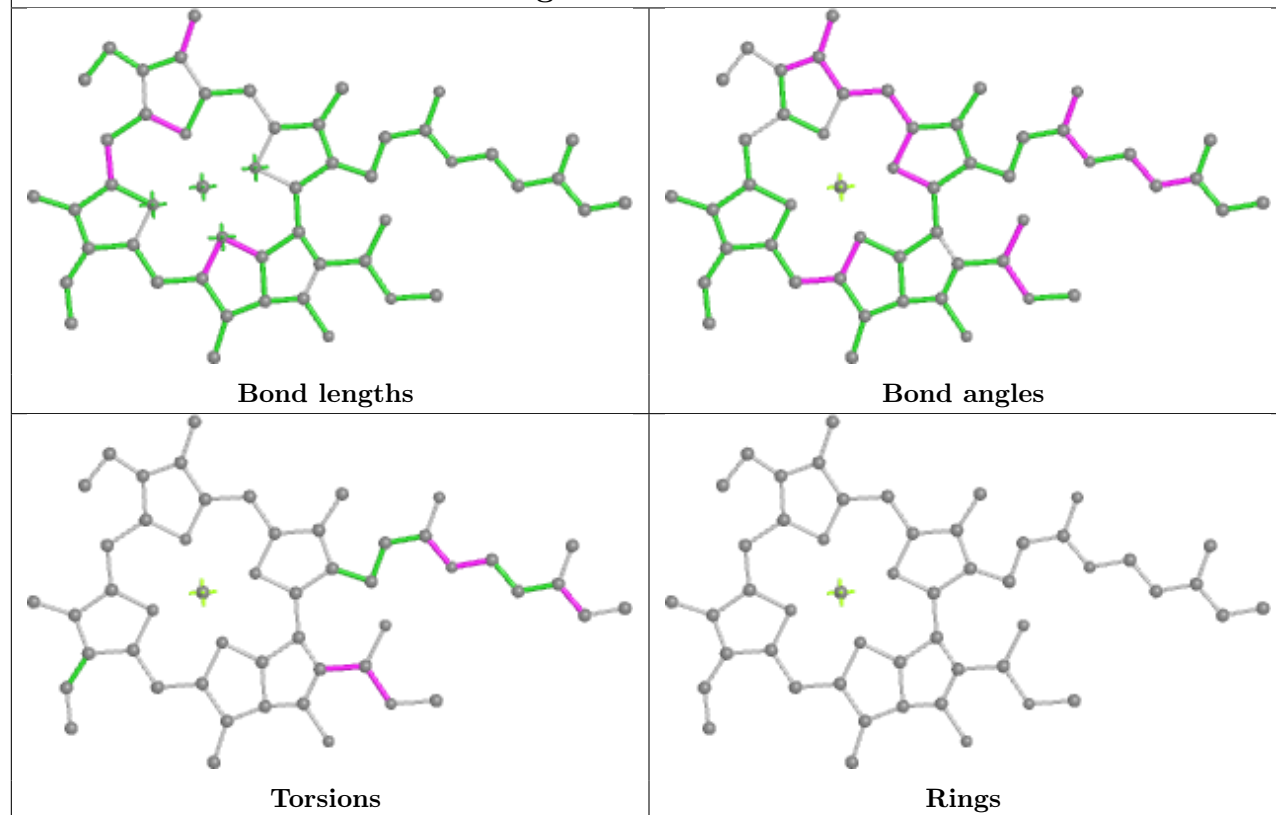
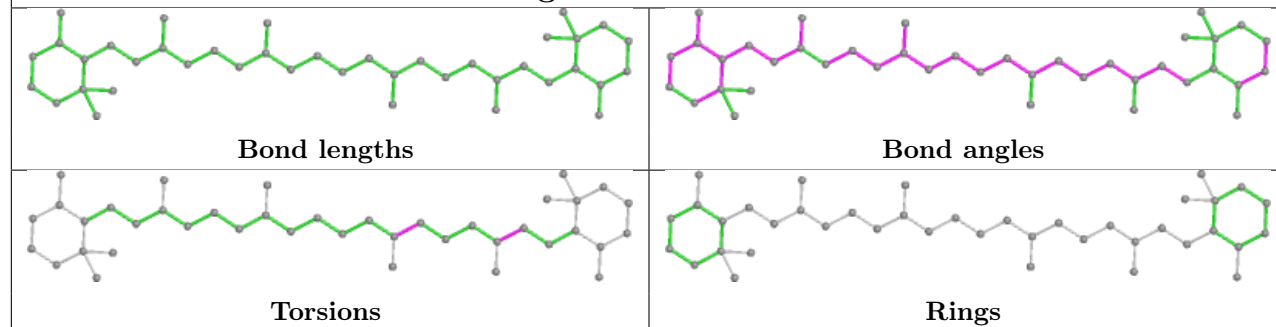
Bond angles

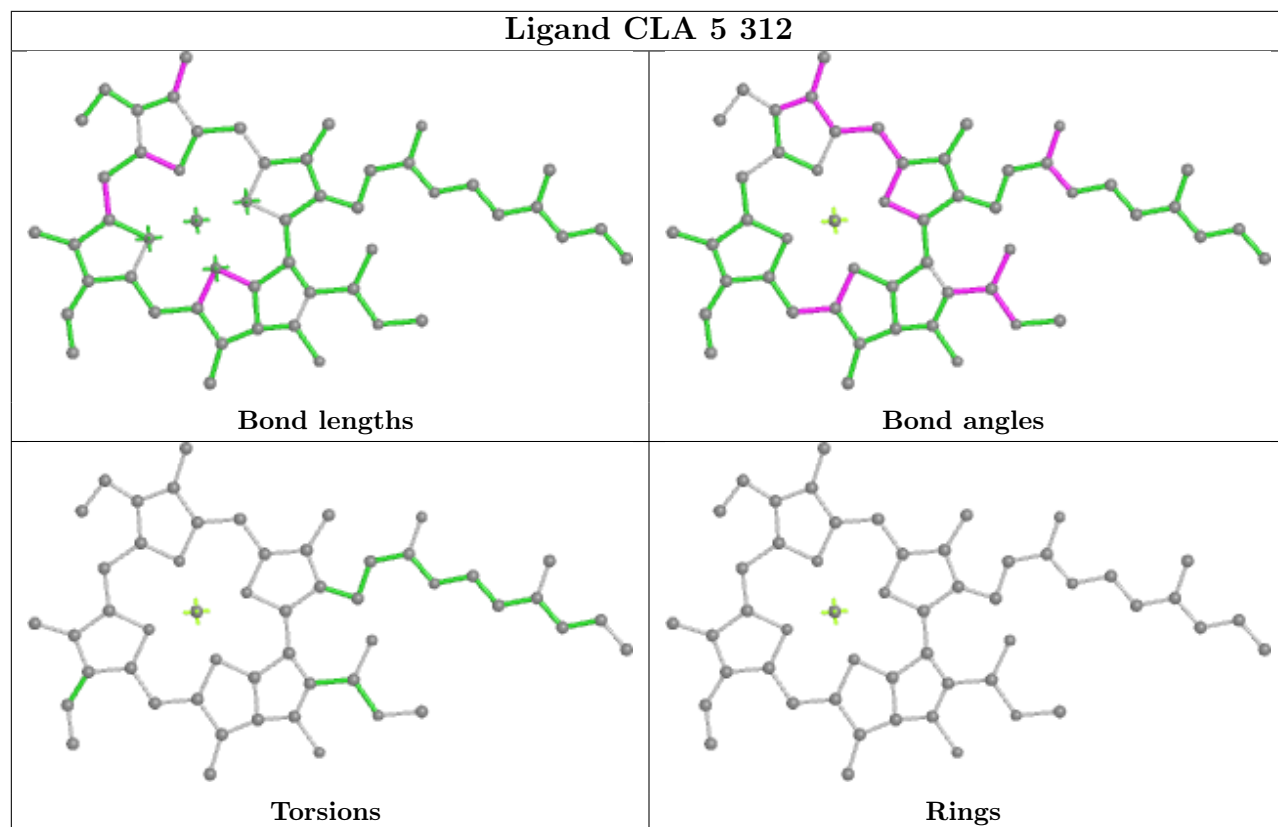


Torsions



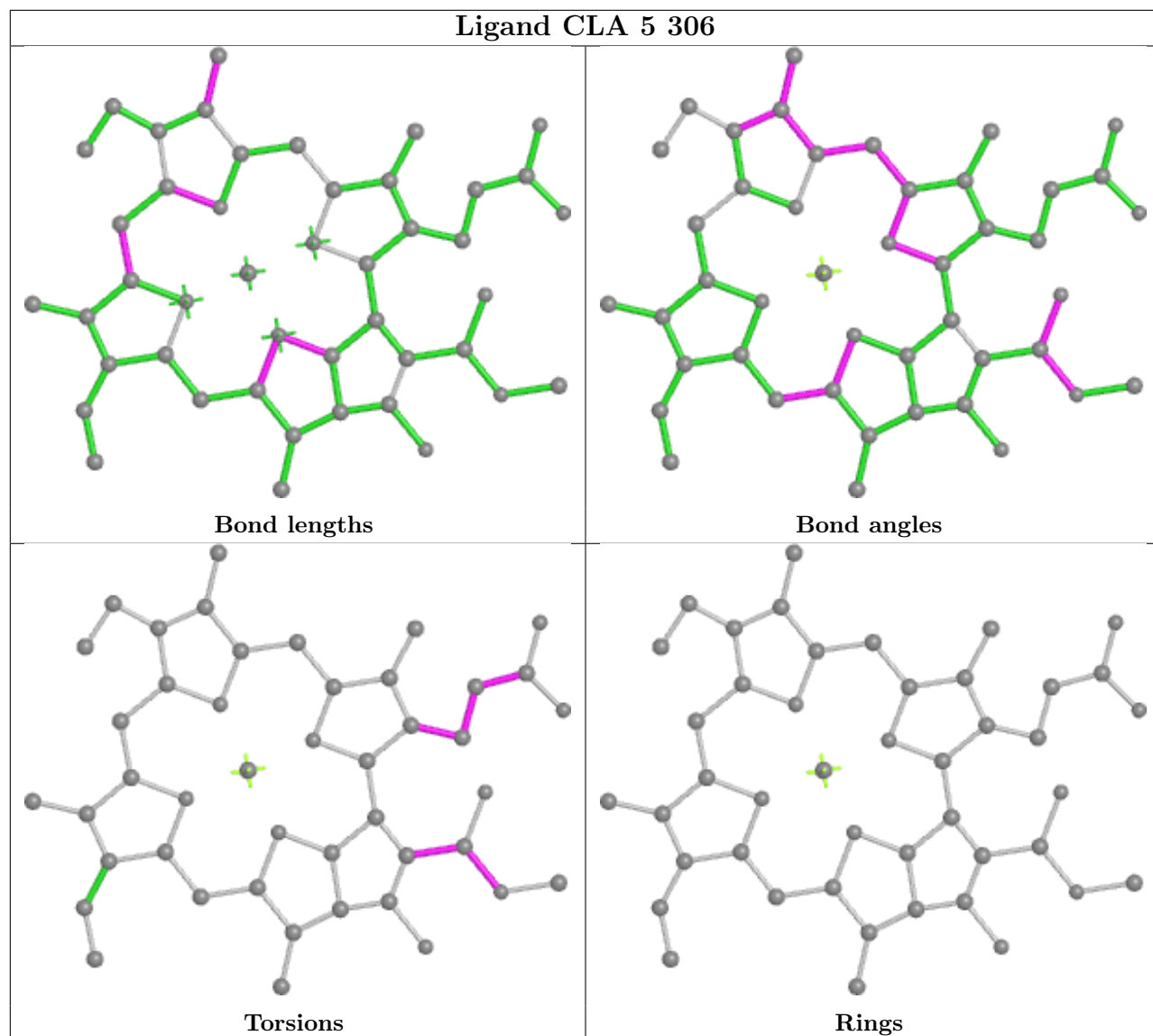
Rings

**Ligand CLA 5 311****Ligand BCR f 801**

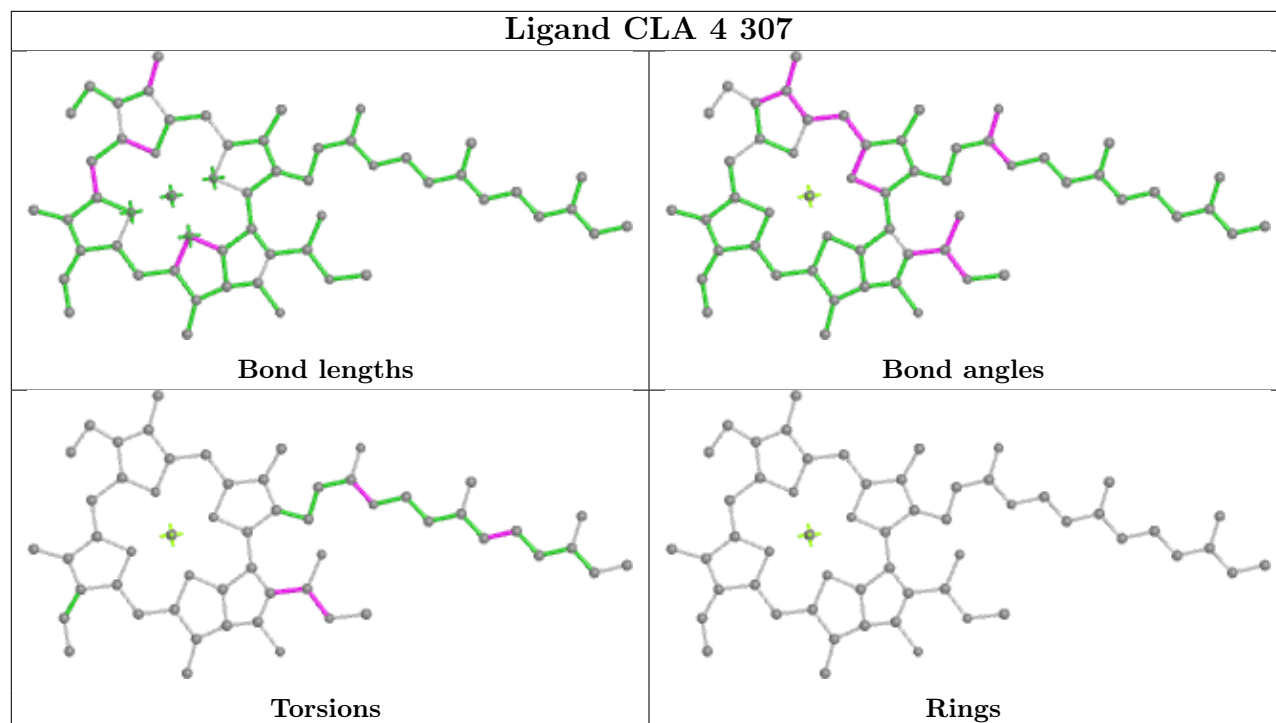




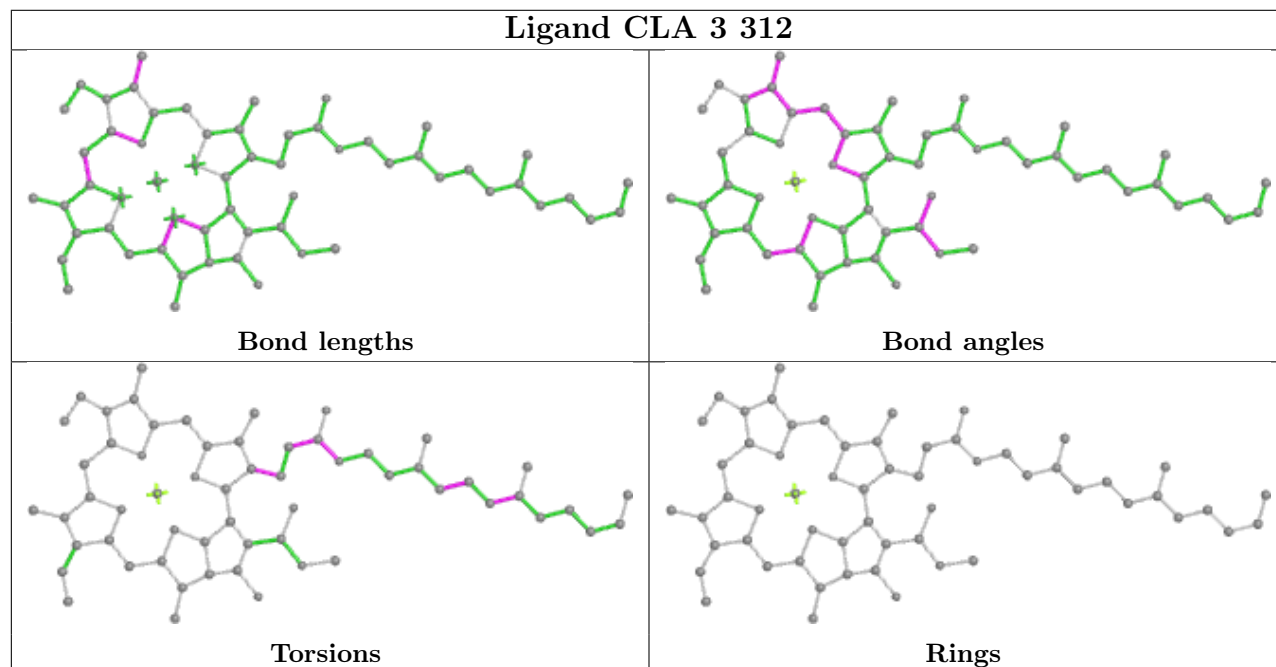
## Ligand CLA 5 306



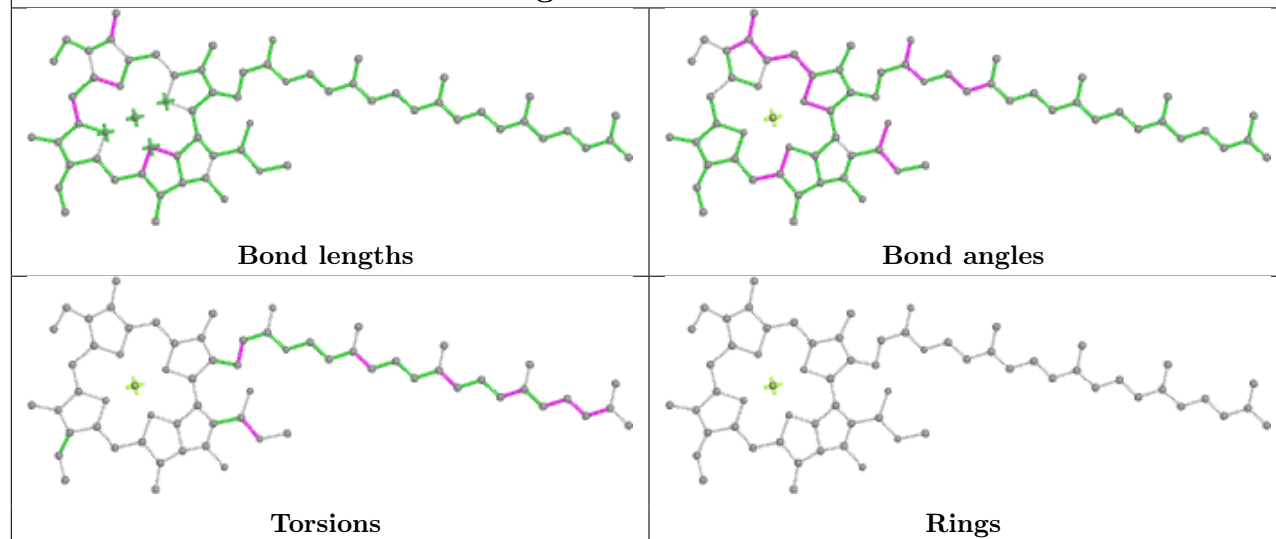
## Ligand CLA 4 307



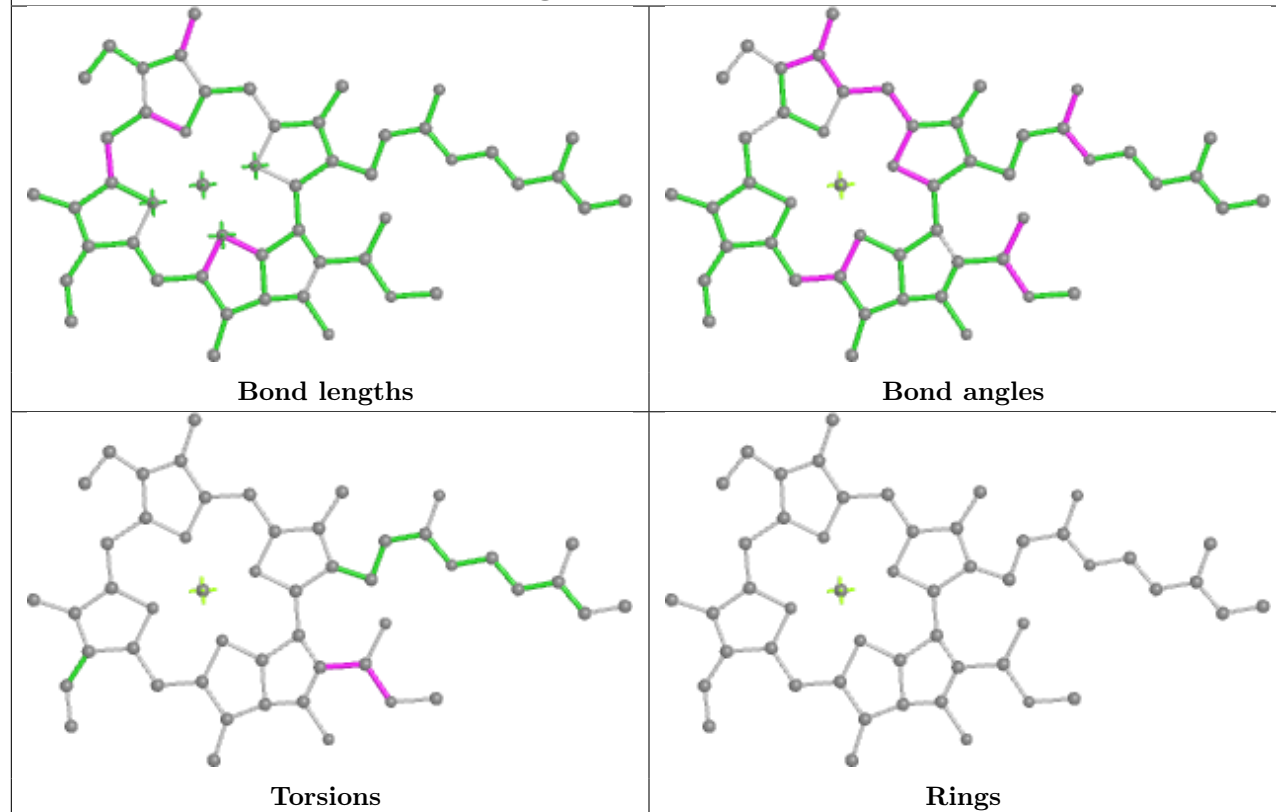
## Ligand CLA 3 312

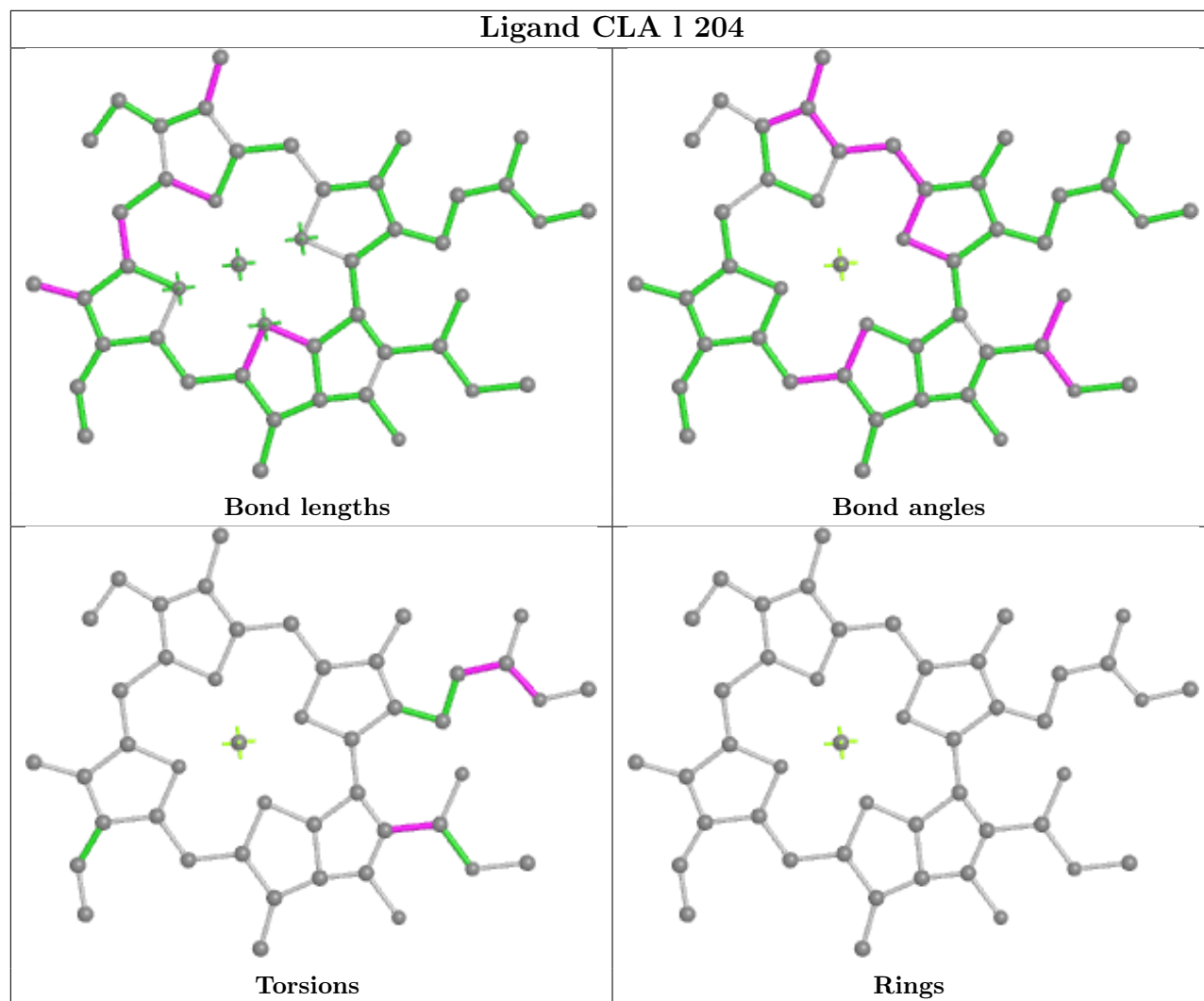
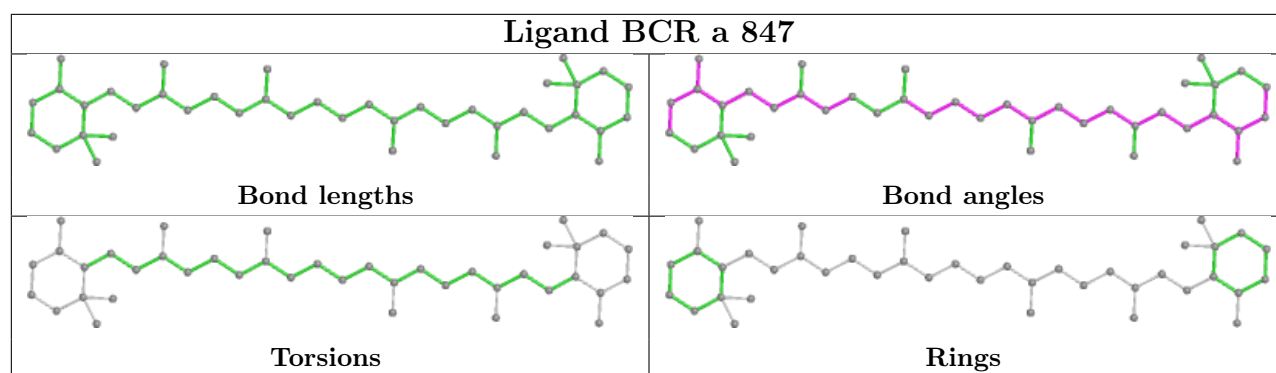


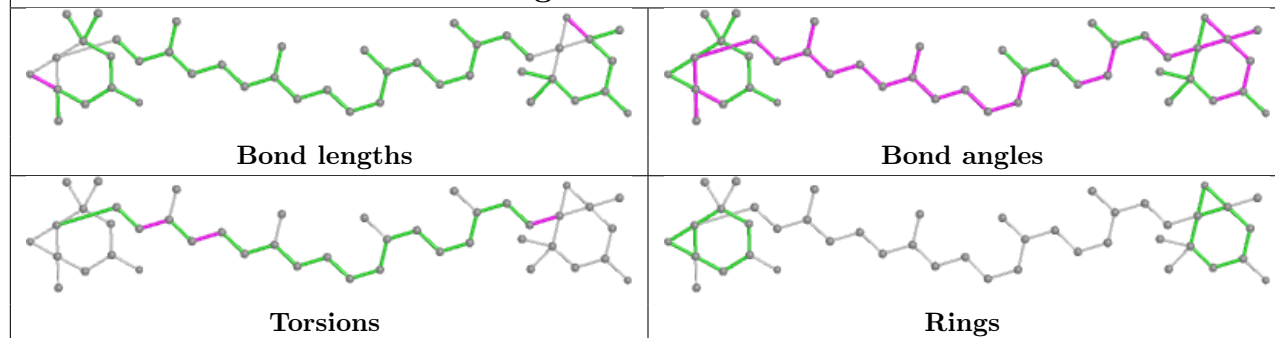
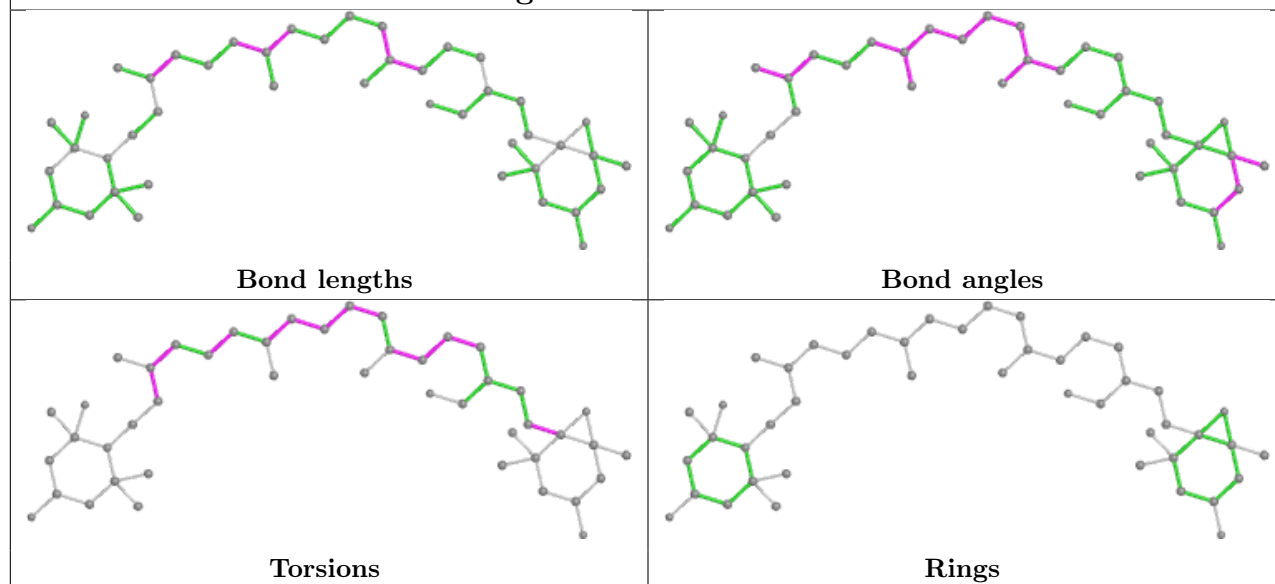
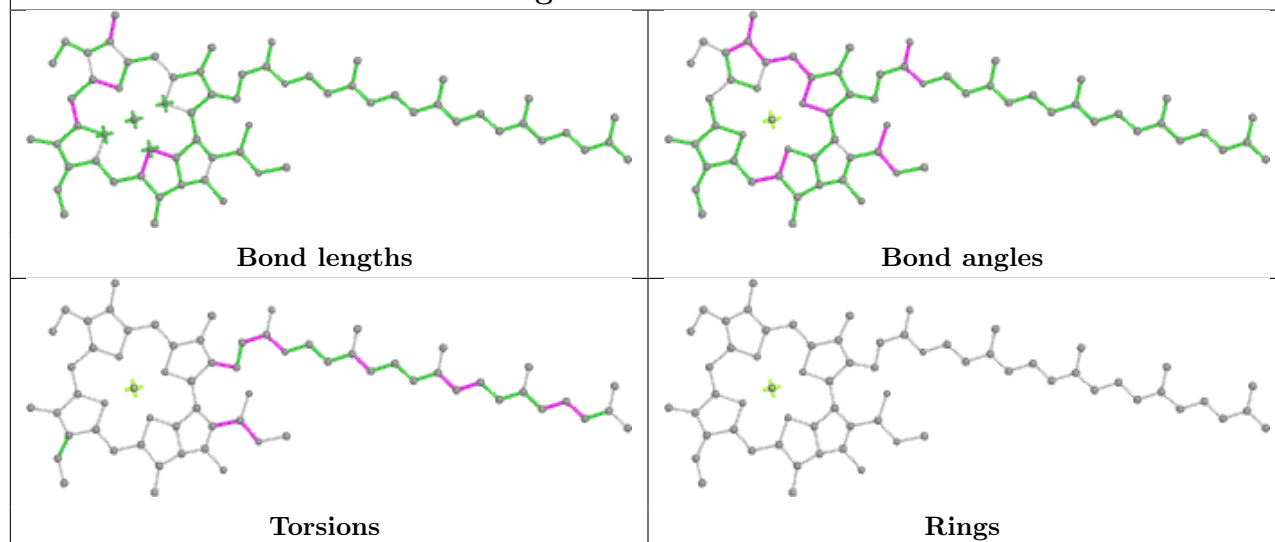
## Ligand CLA 1 308



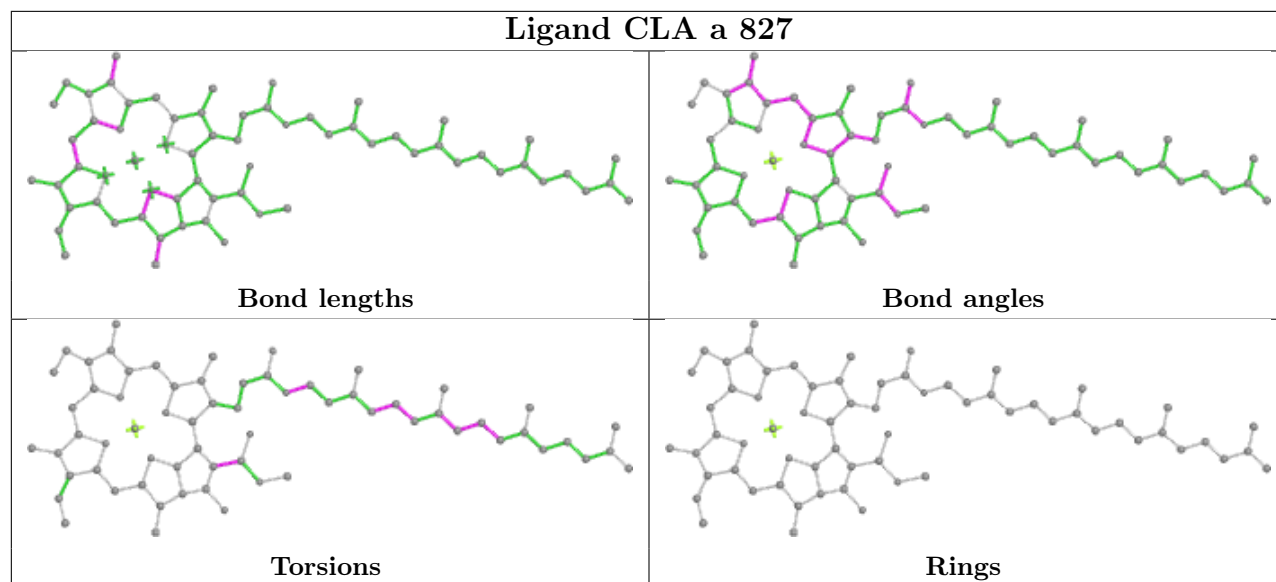
## Ligand CLA a 808



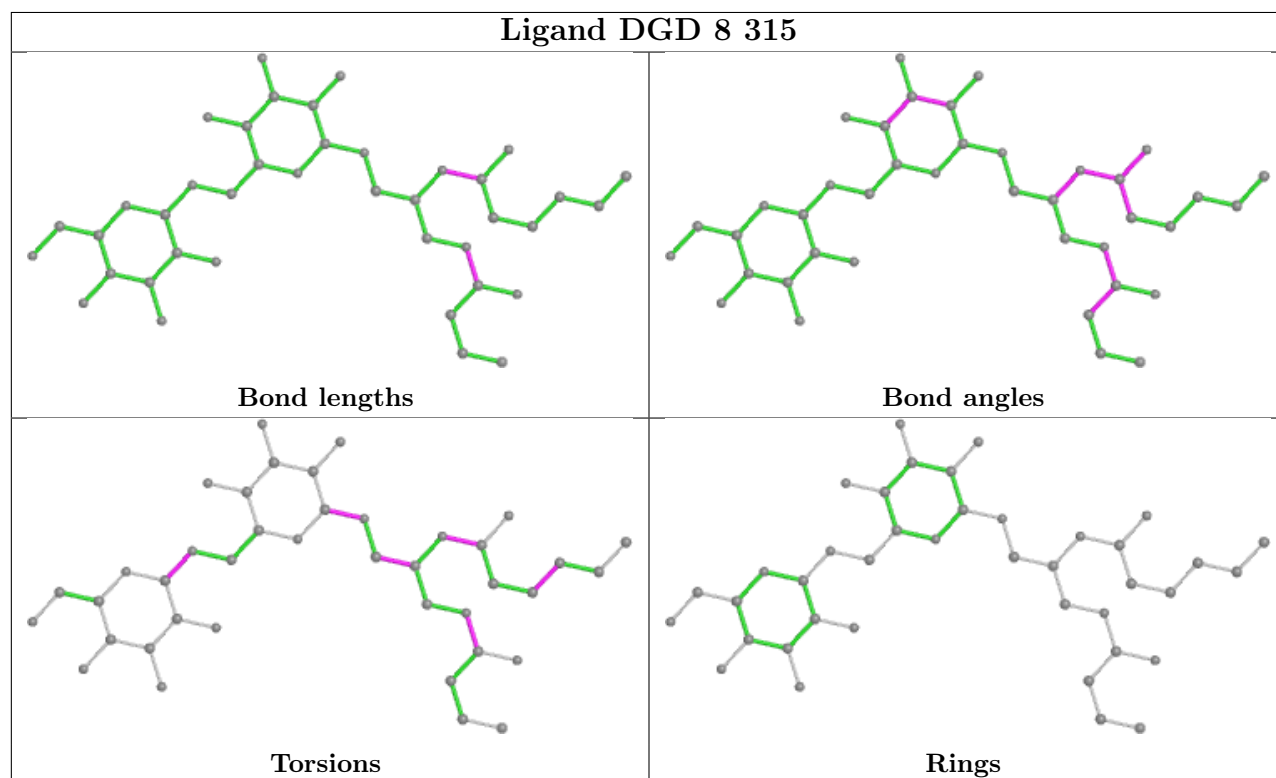


**Ligand XAT 4 301****Ligand A1L1G 7 302****Ligand CLA 4 310**

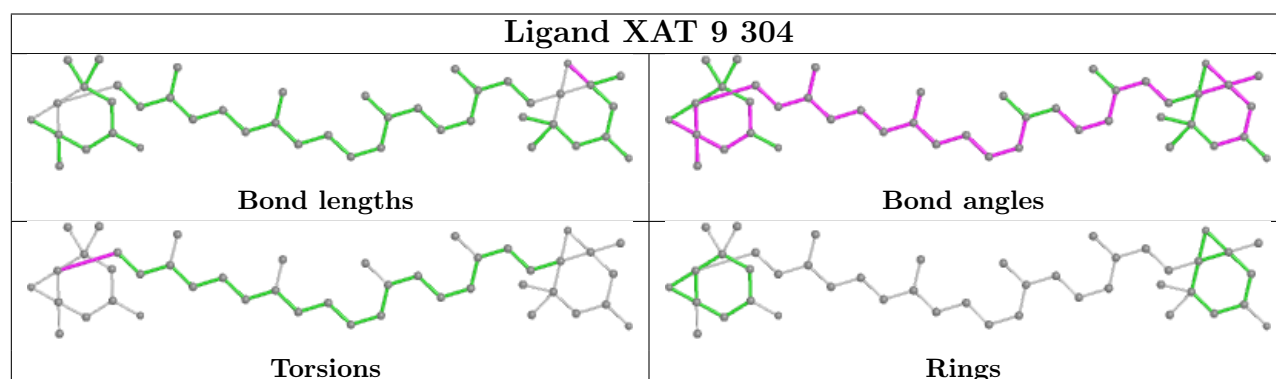
## Ligand CLA a 827



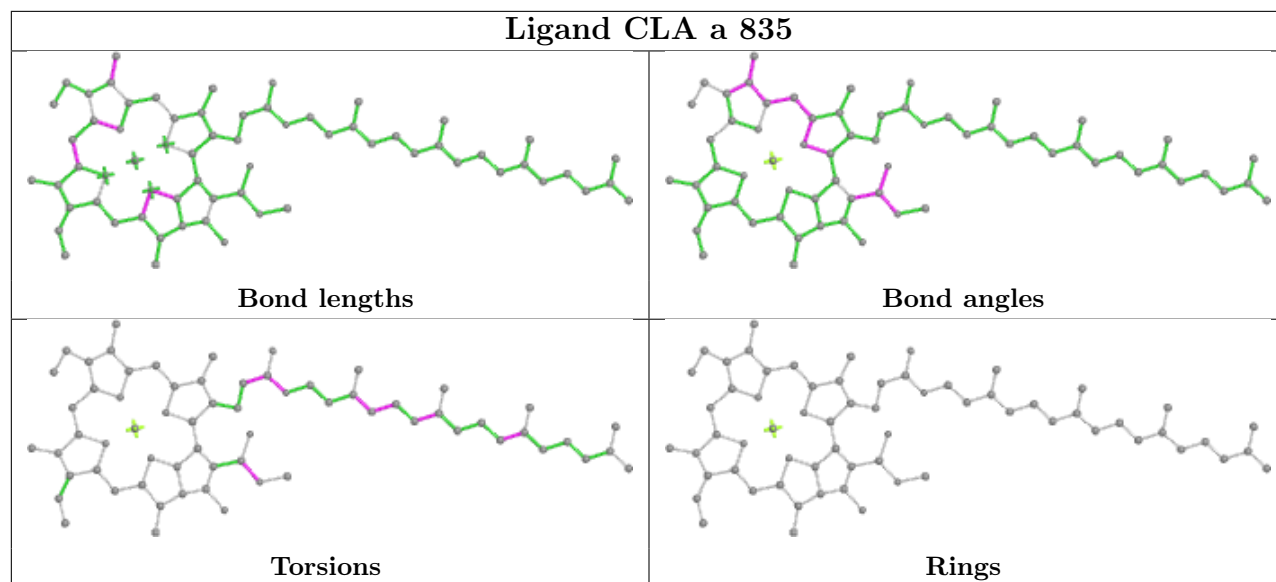
## Ligand DGD 8 315



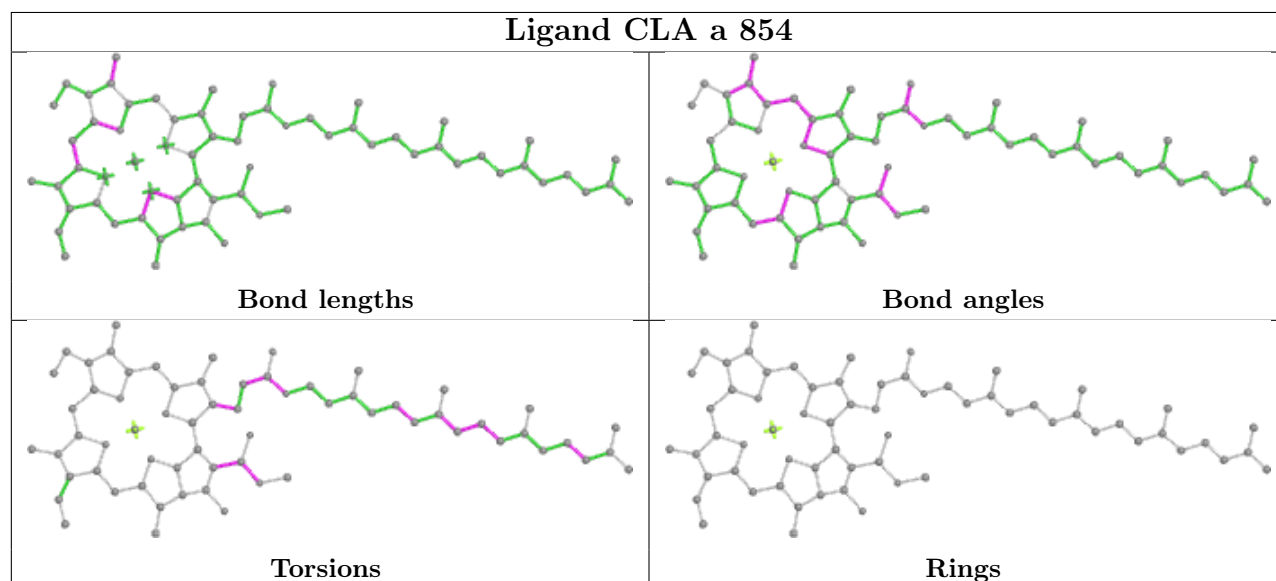
## Ligand XAT 9 304



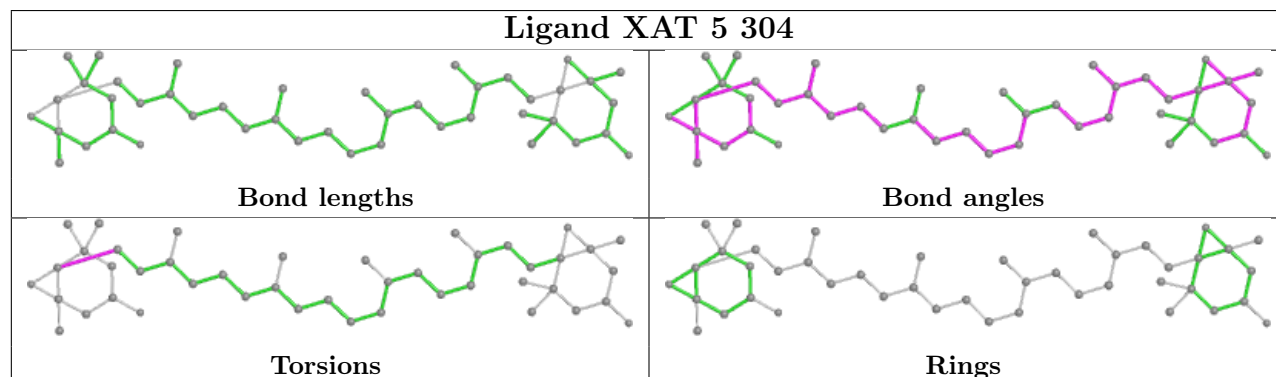
## Ligand CLA a 835

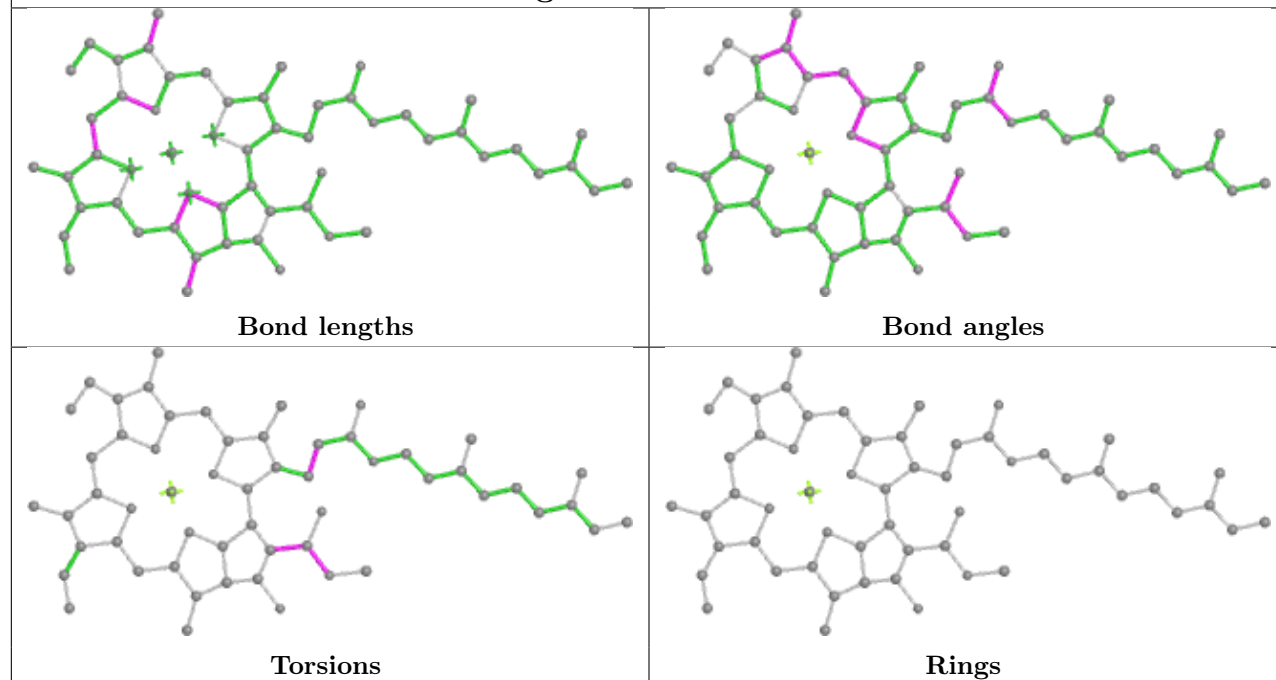
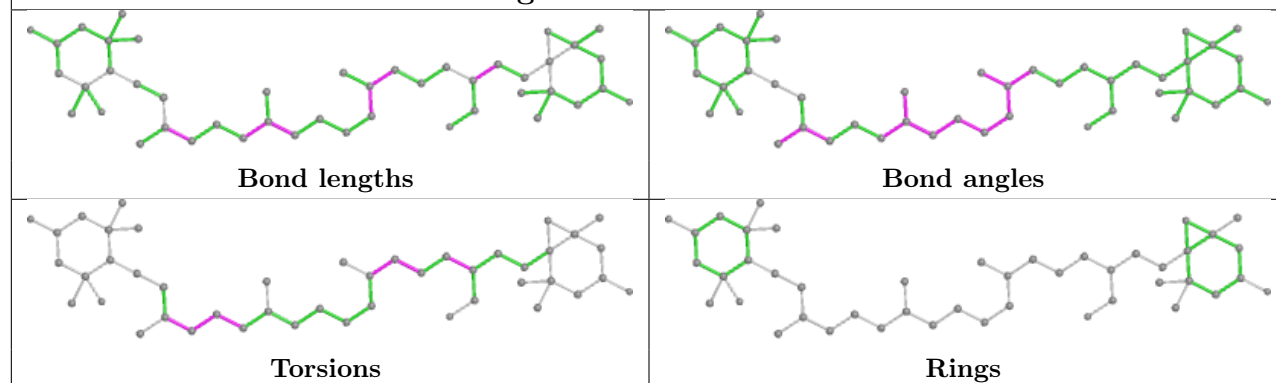
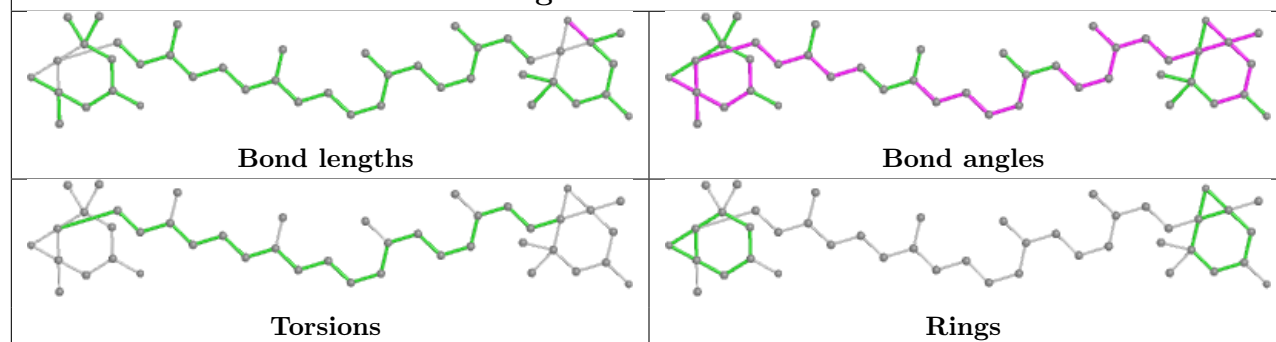


## Ligand CLA a 854

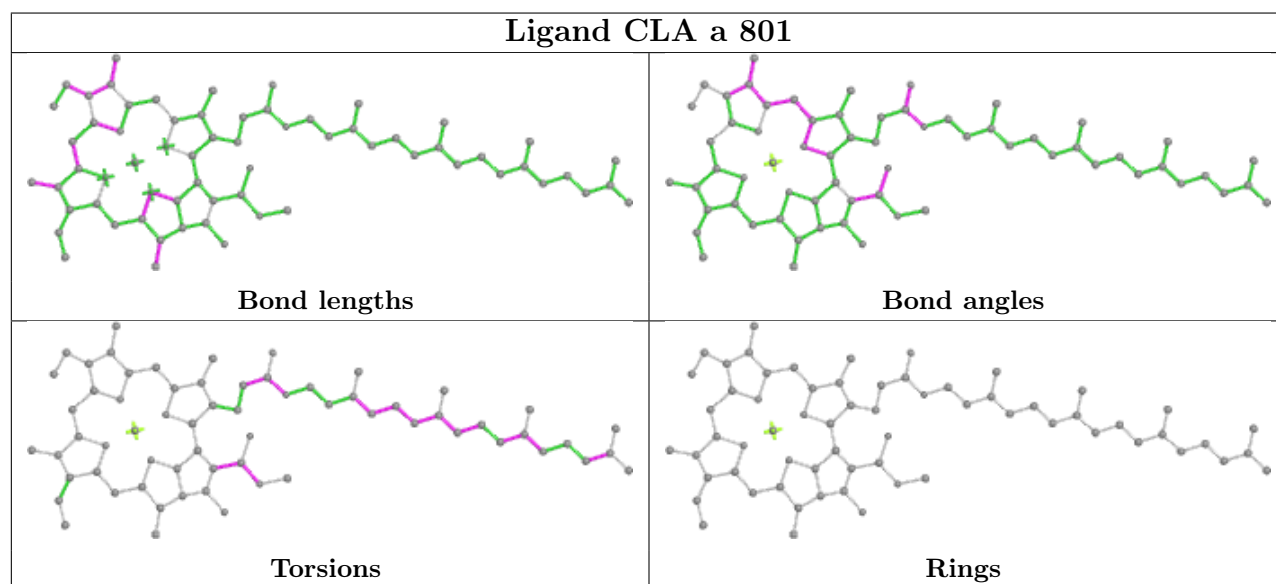
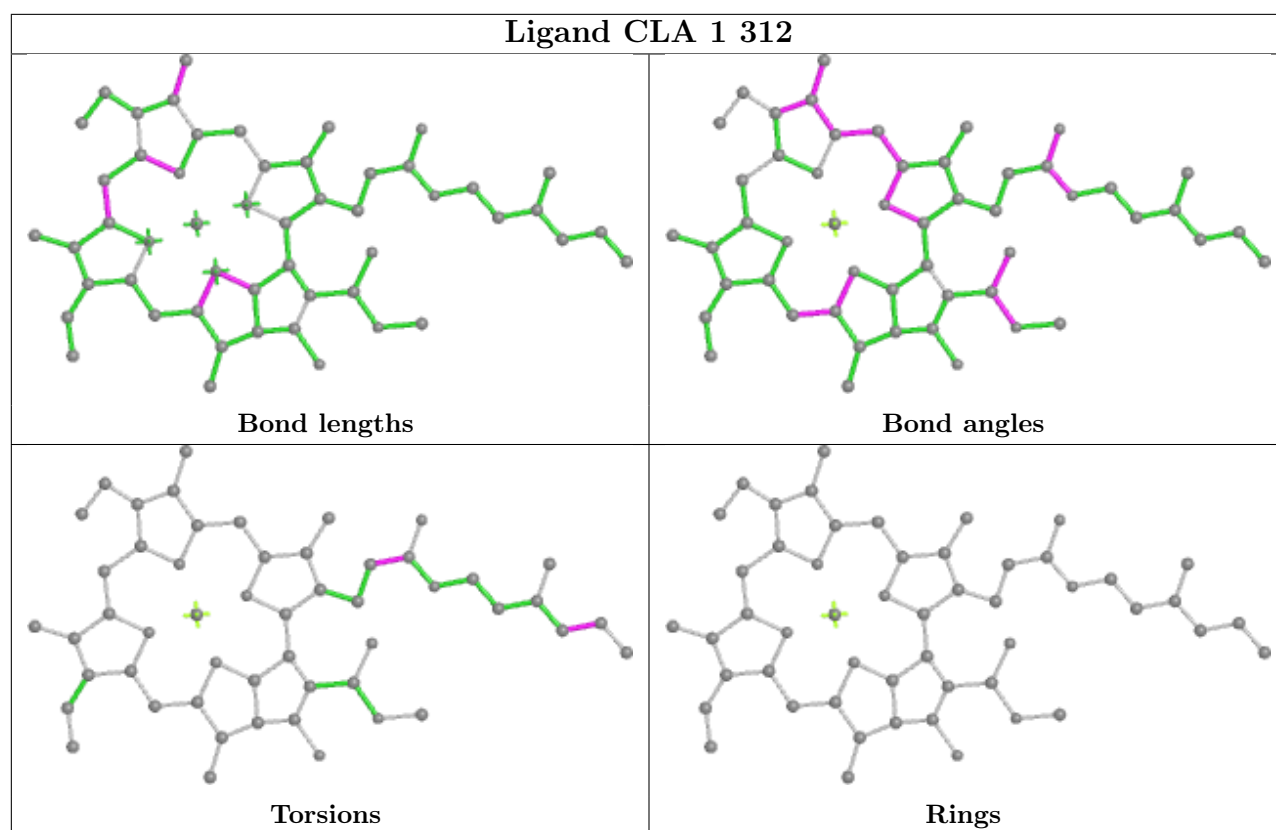


## Ligand XAT 5 304

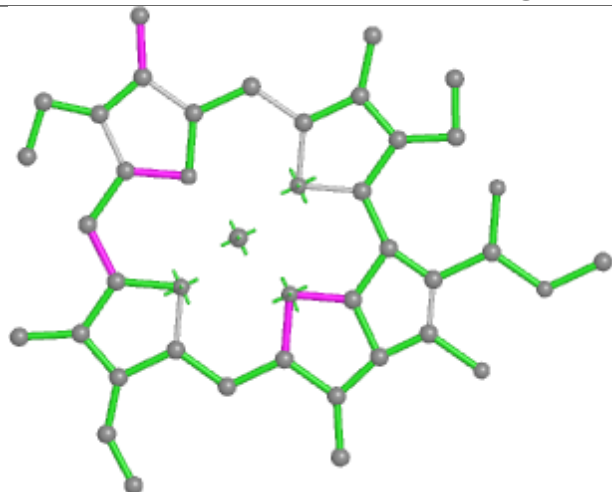


**Ligand CLA 3 309****Ligand A1L1G 5 303****Ligand XAT 2 302**

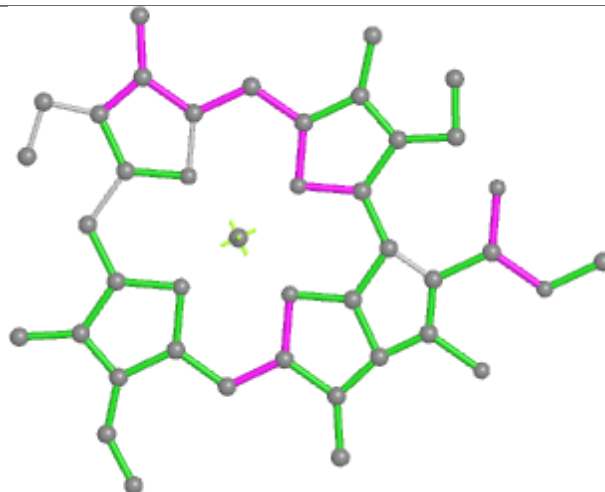




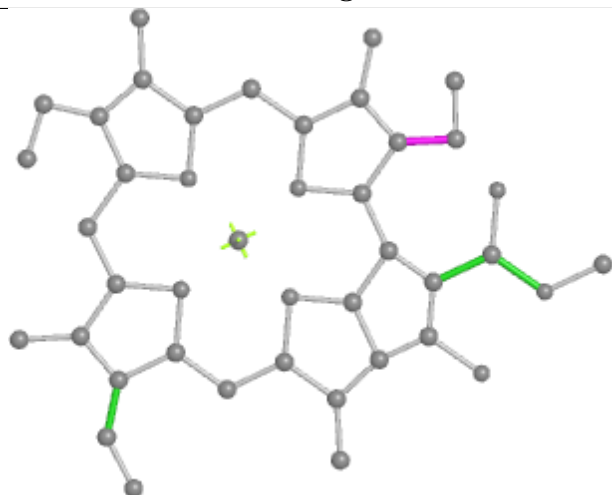
## Ligand CLA 2 315



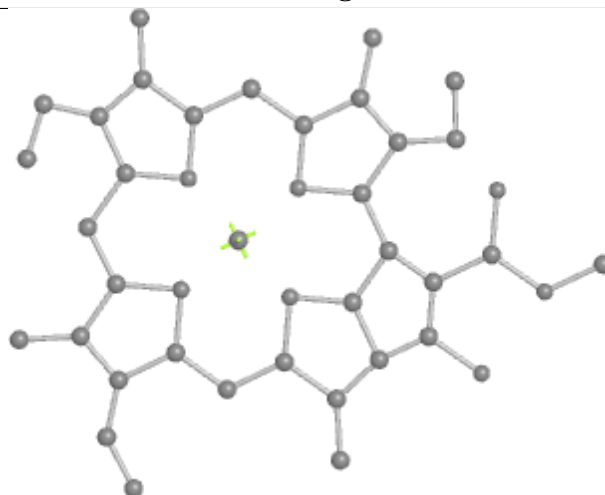
Bond lengths



Bond angles

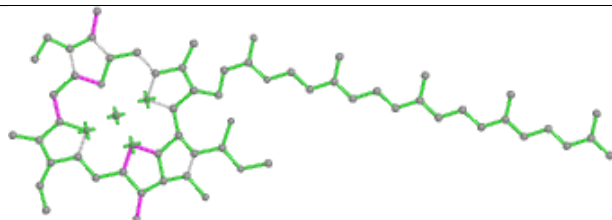


Torsions

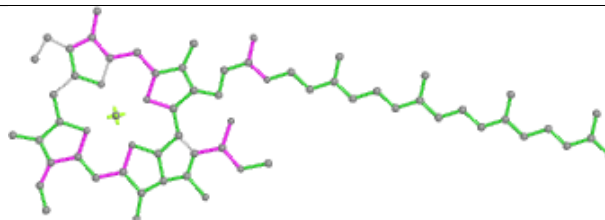


Rings

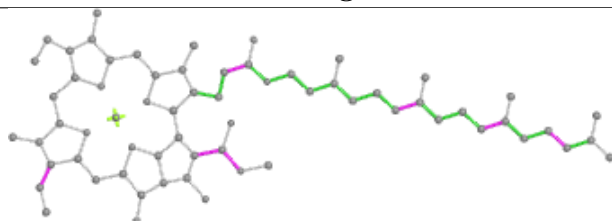
## Ligand CLA b 804



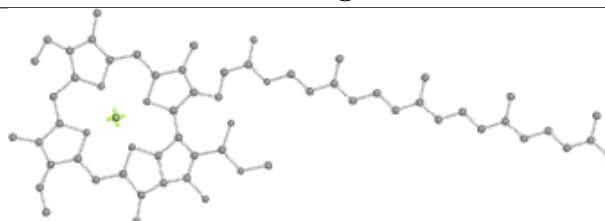
Bond lengths



Bond angles

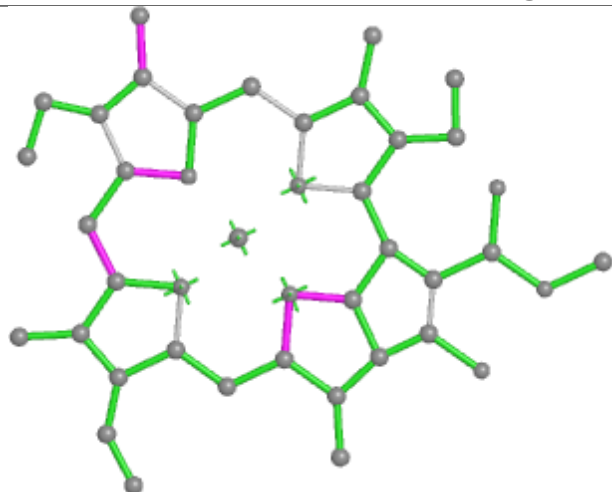


Torsions

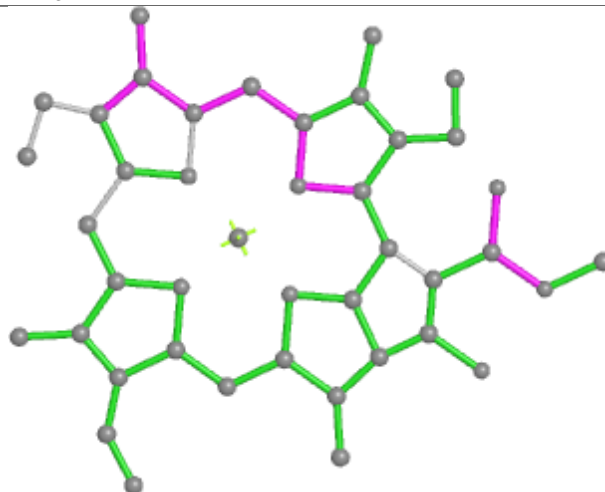


Rings

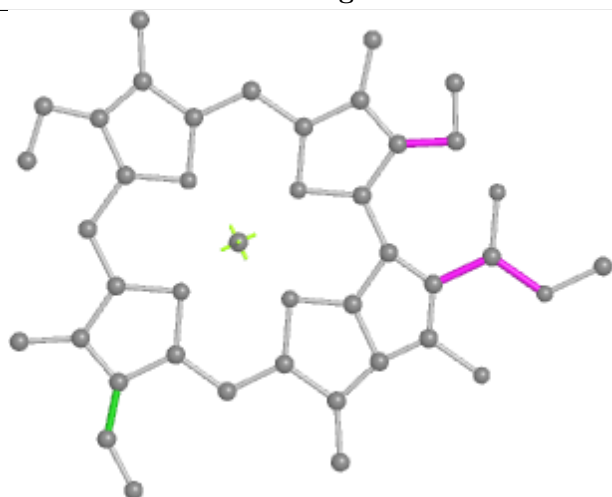
## Ligand CLA j 103



Bond lengths



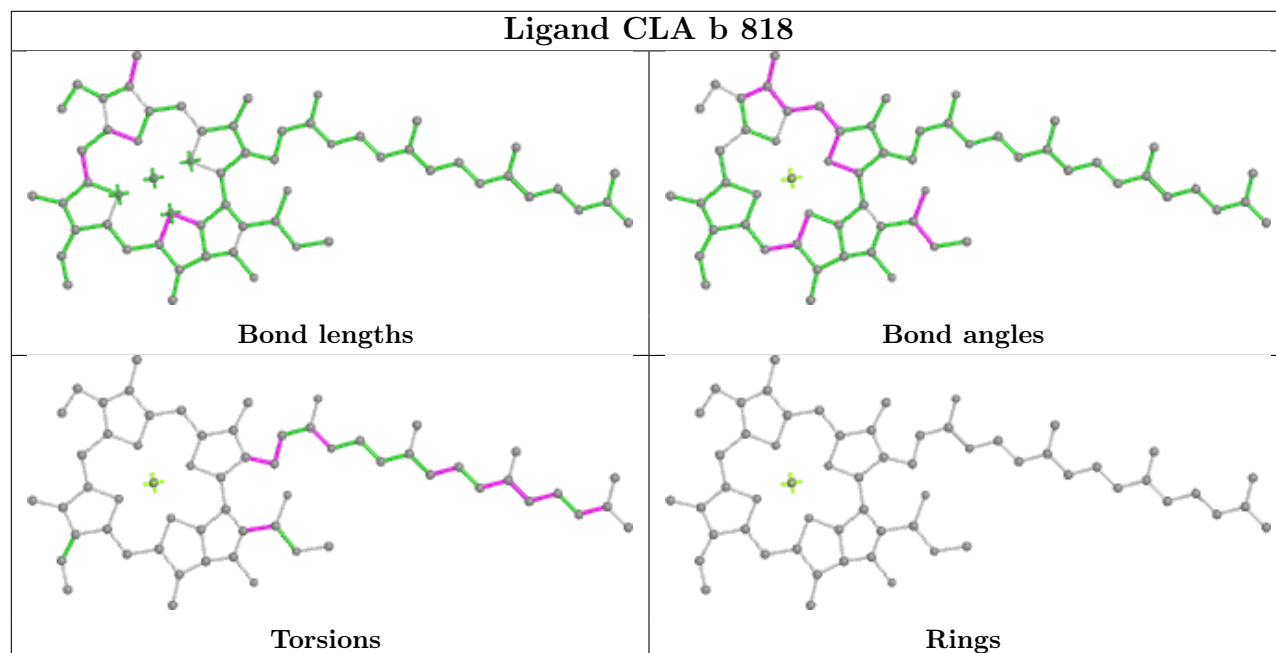
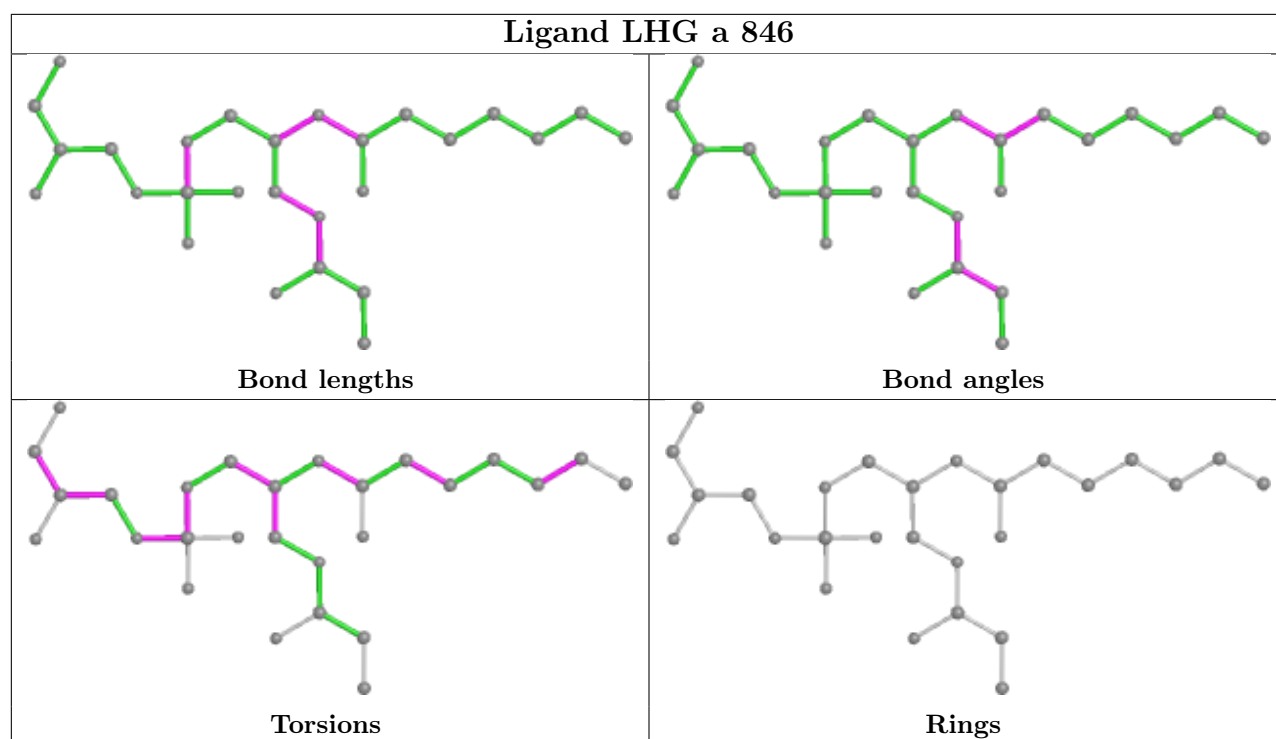
Bond angles



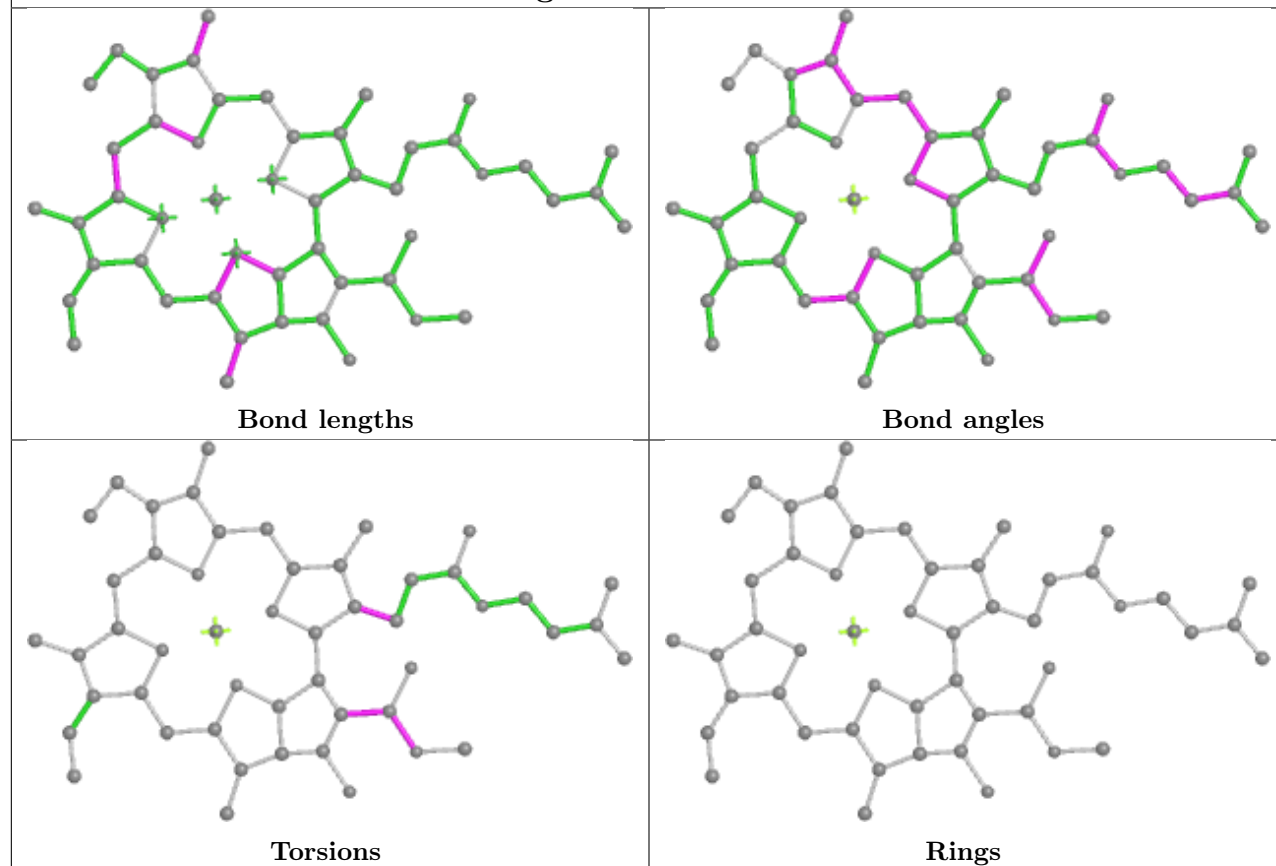
Torsions



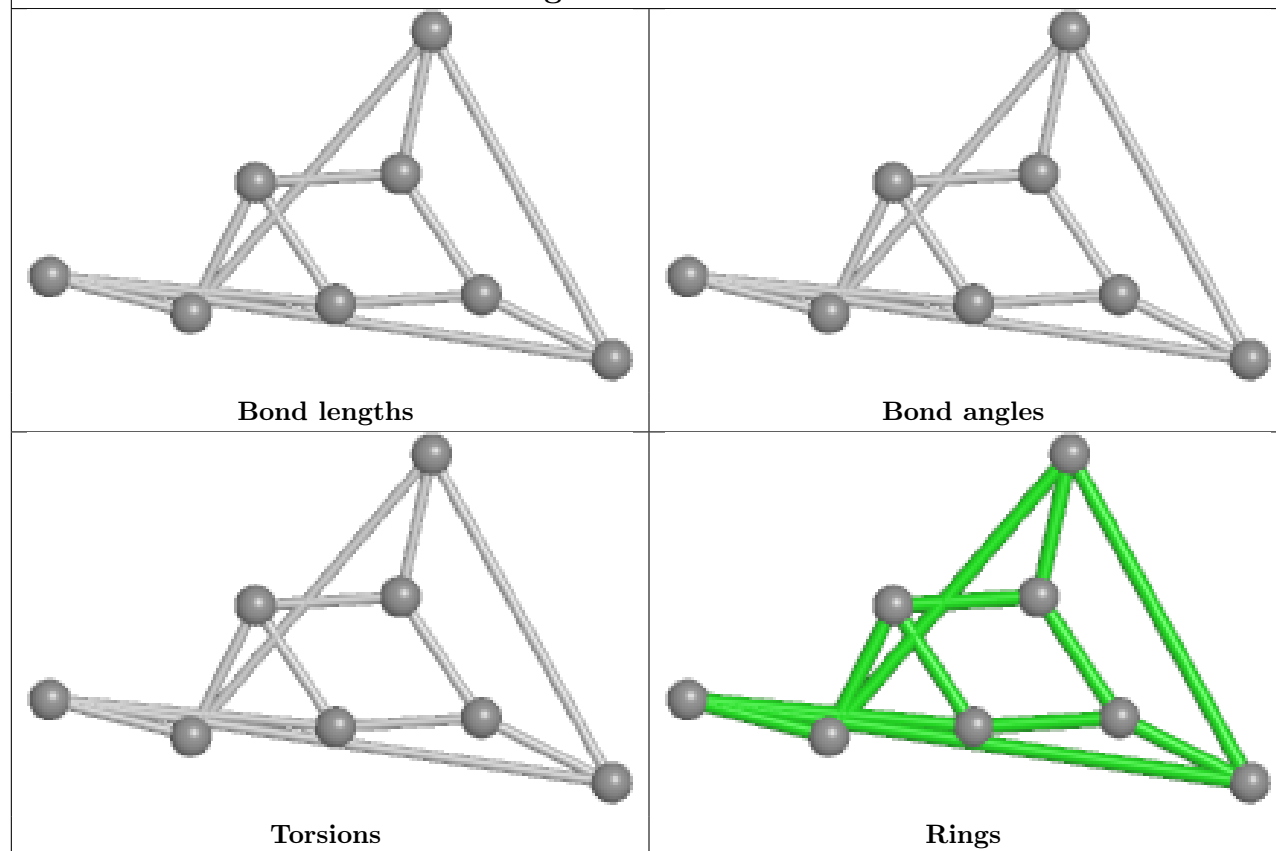
Rings

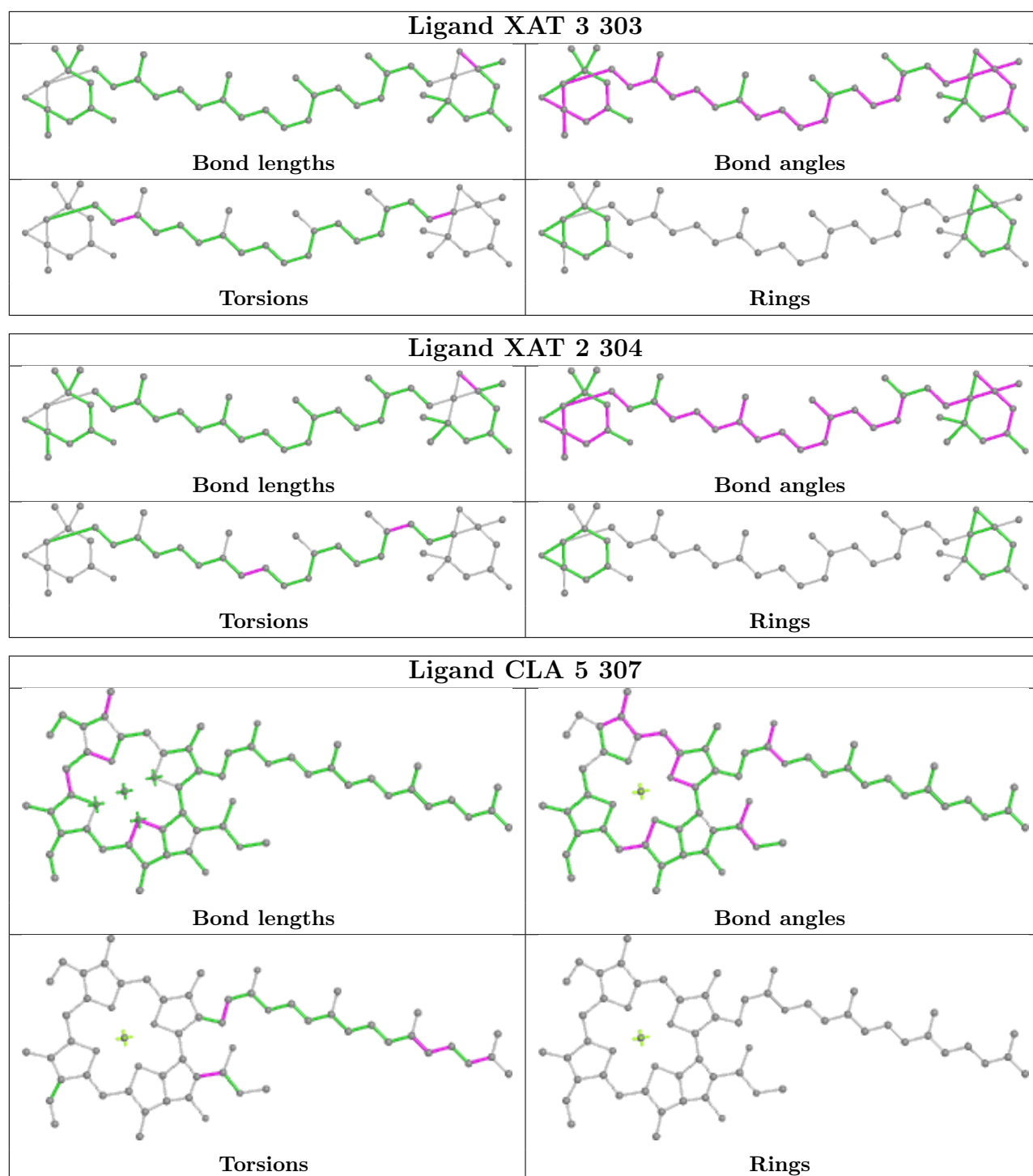


## Ligand CLA a 832

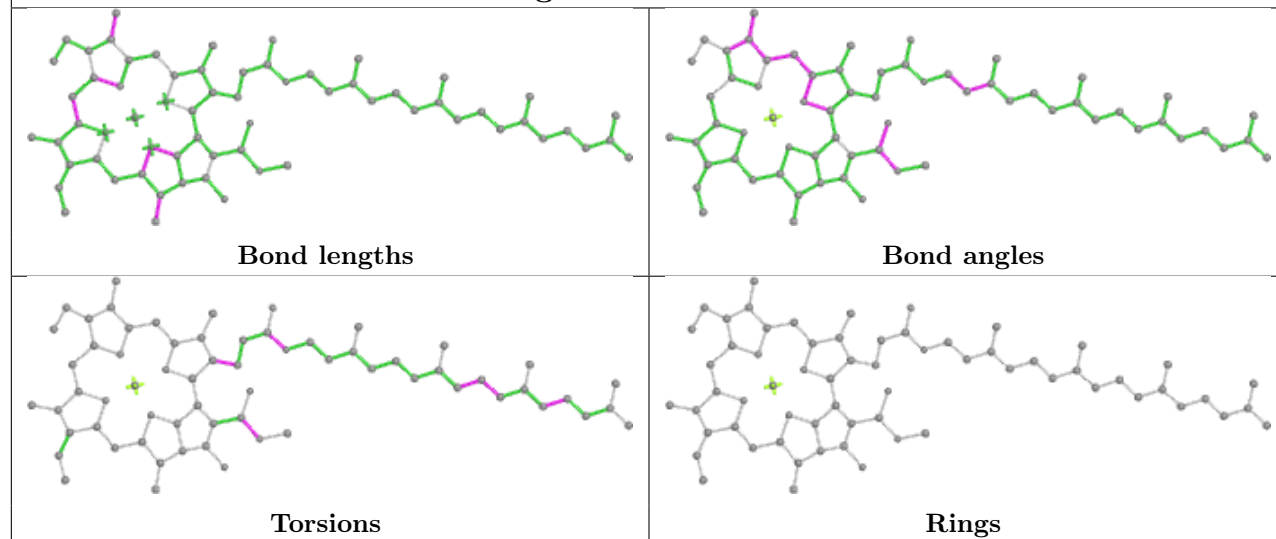


## Ligand SF4 c 101

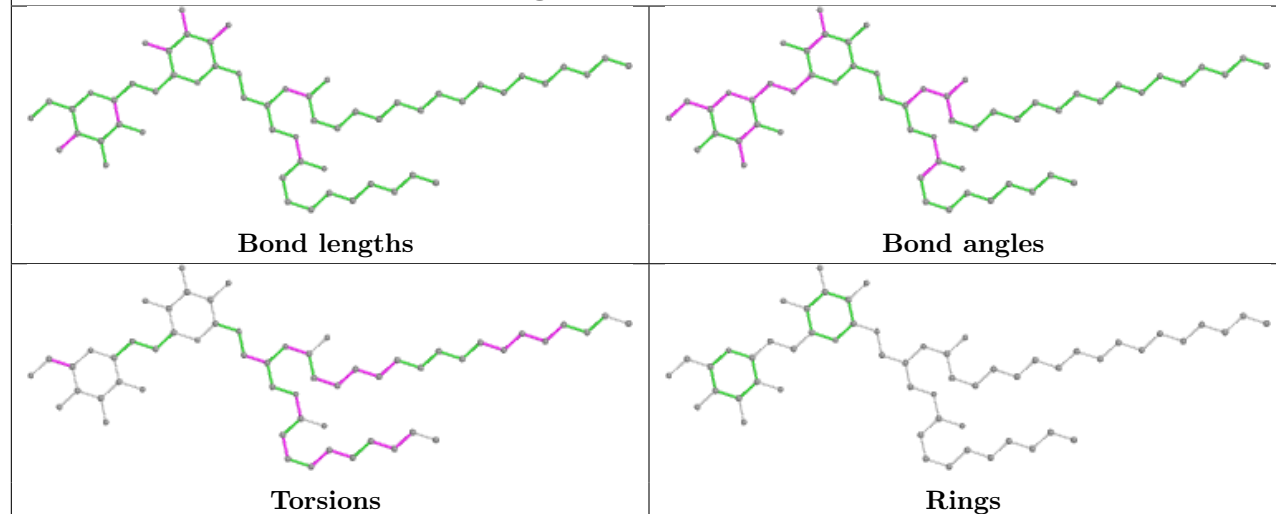




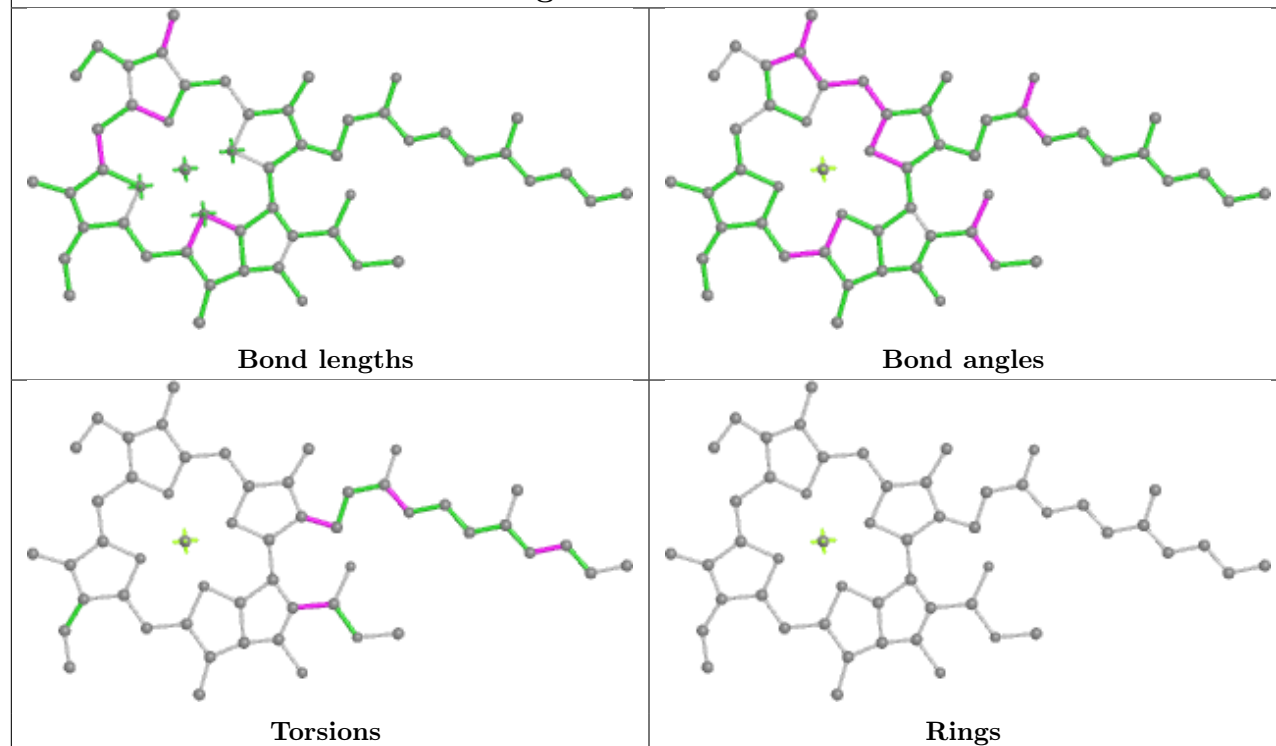
## Ligand CLA h 203



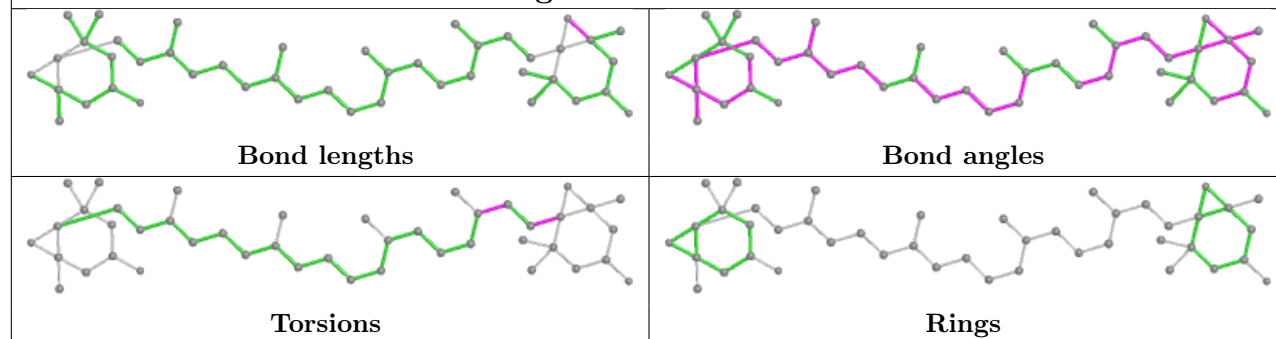
## Ligand DGD b 848



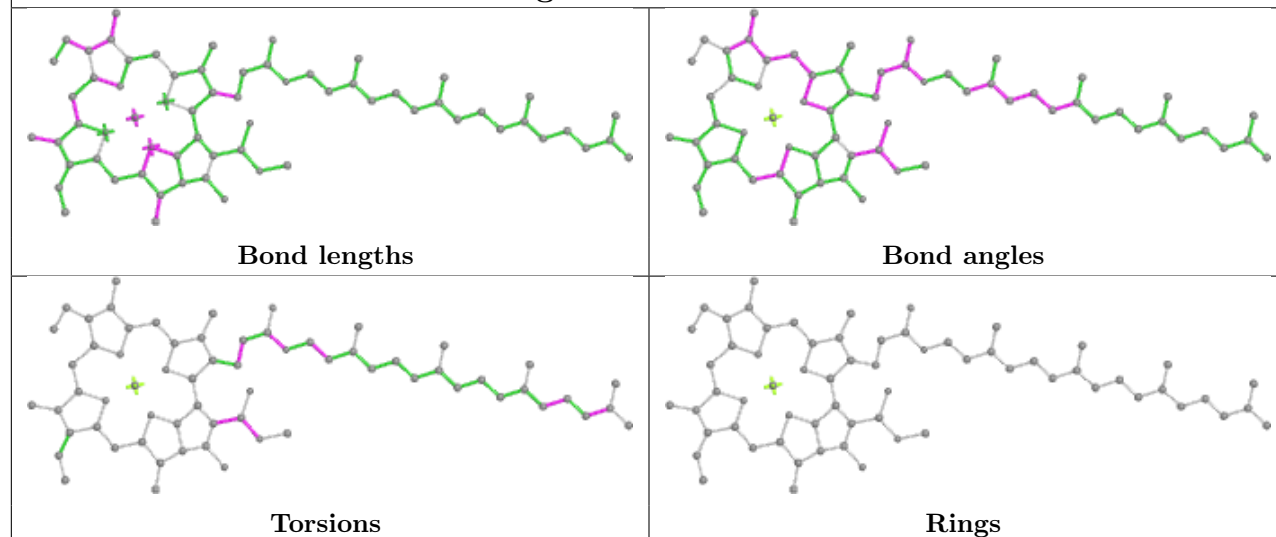
## Ligand CLA 4 313



## Ligand XAT 5 301

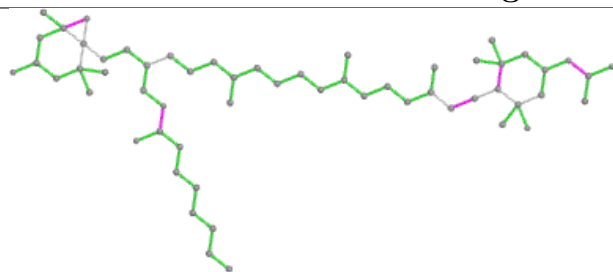


## Ligand CLA a 806

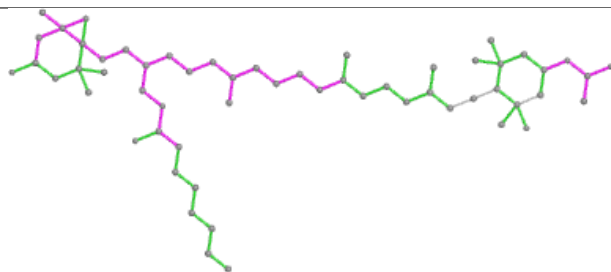




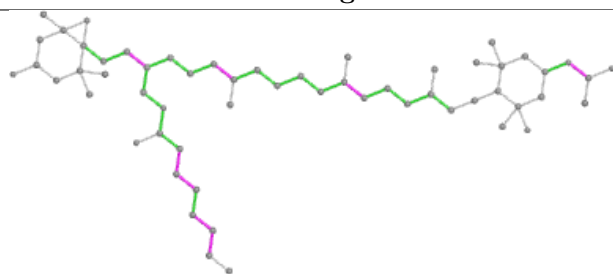
## Ligand A1L1F 1 304



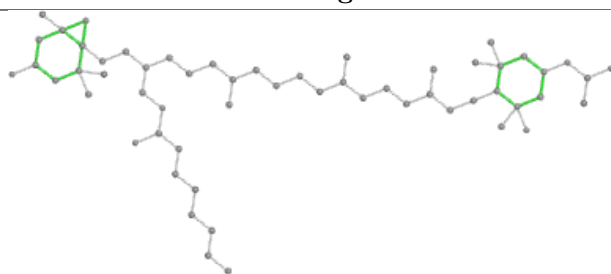
Bond lengths



Bond angles

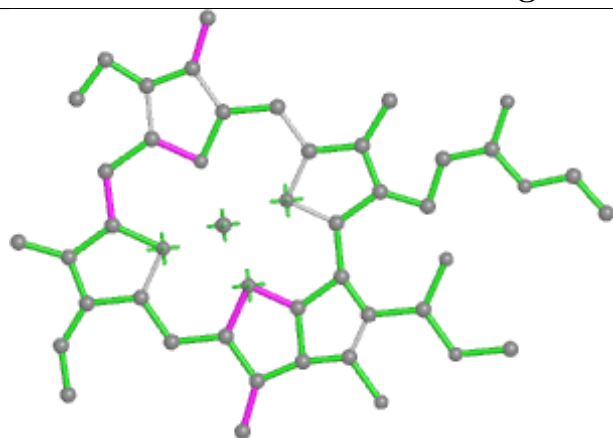


Torsions

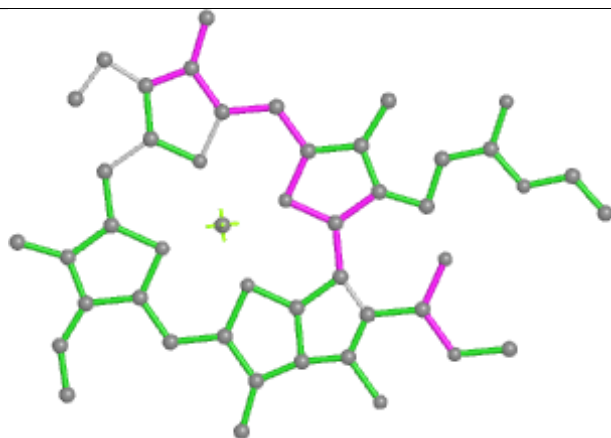


Rings

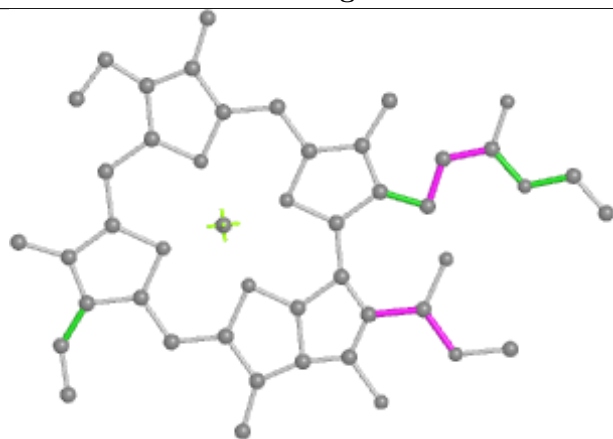
## Ligand CLA 2 307



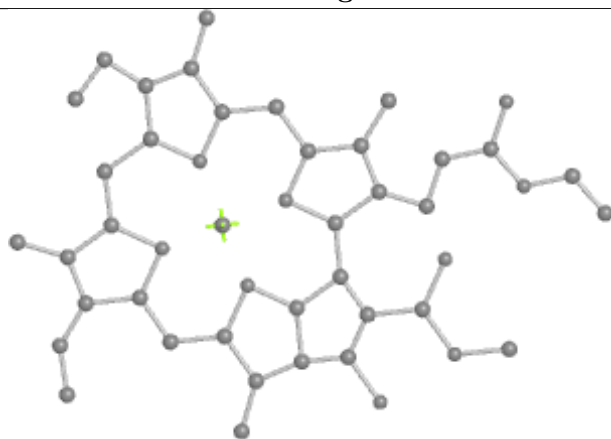
Bond lengths



Bond angles

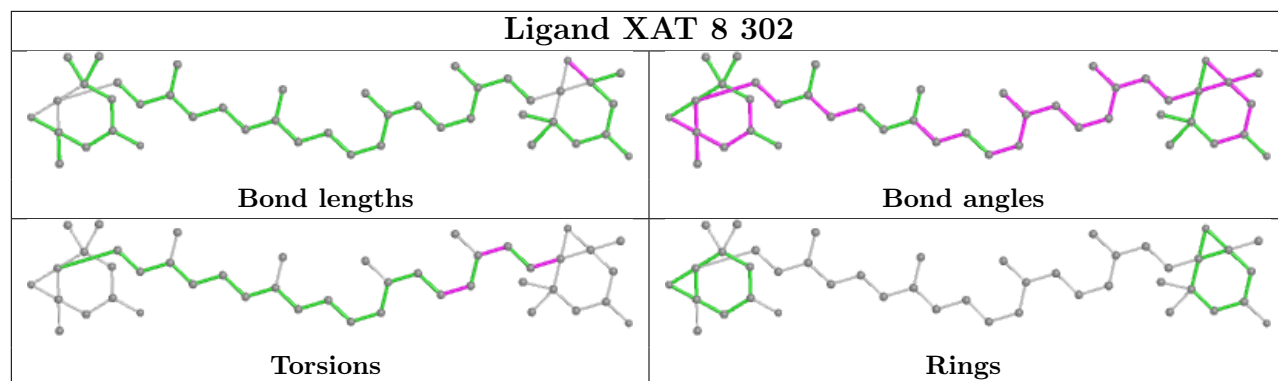


Torsions

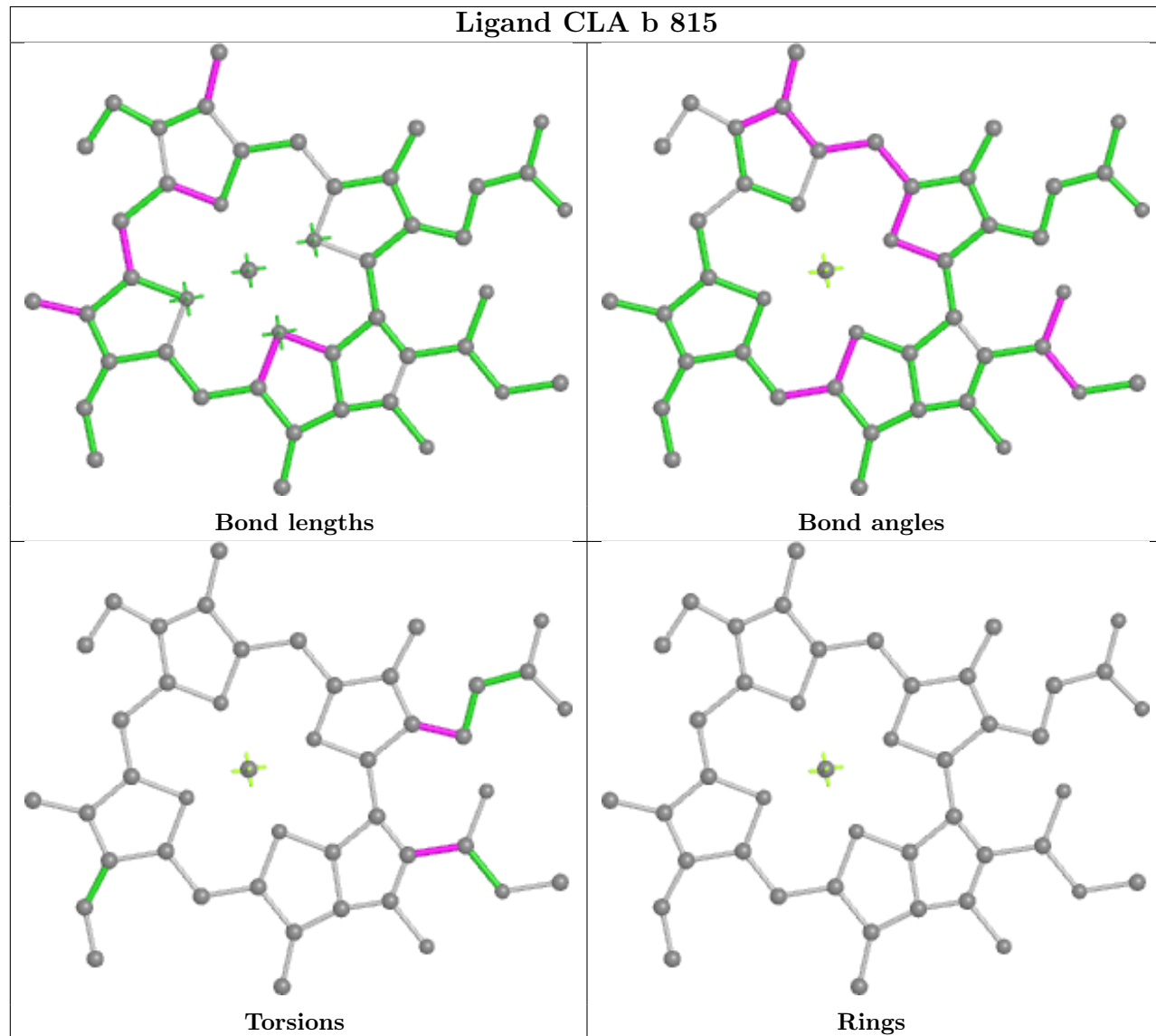


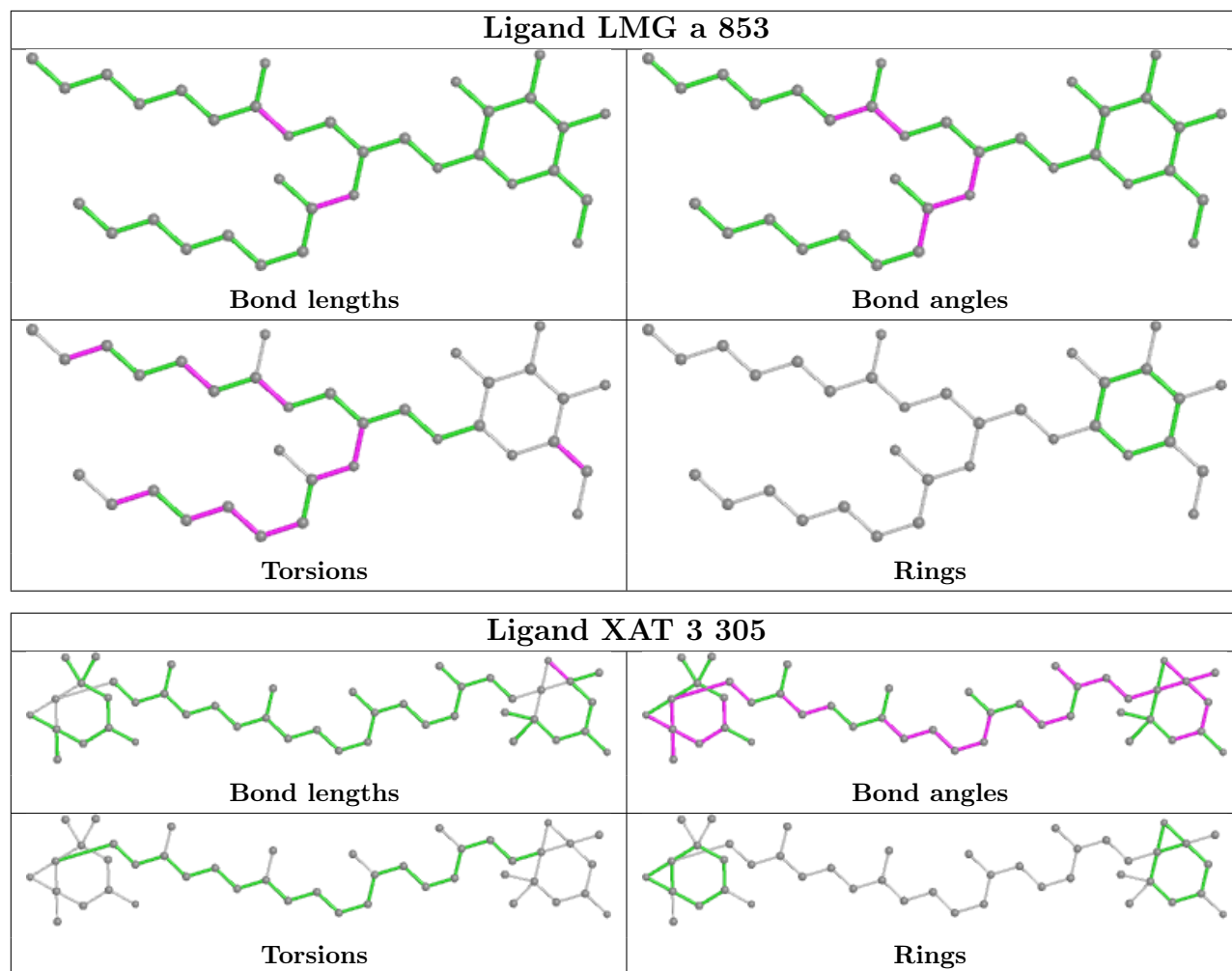
Rings

## Ligand XAT 8 302

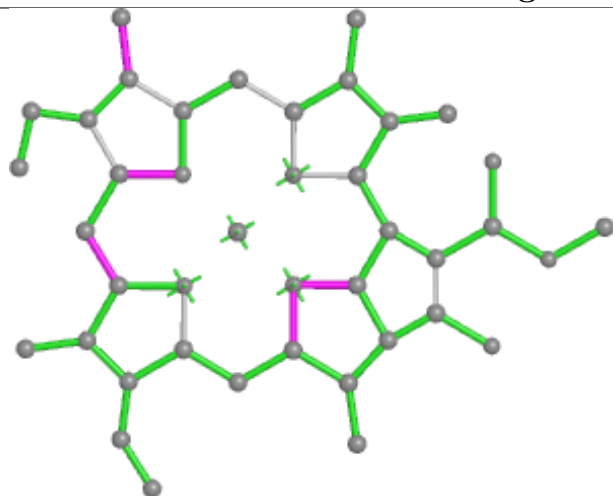


## Ligand CLA b 815

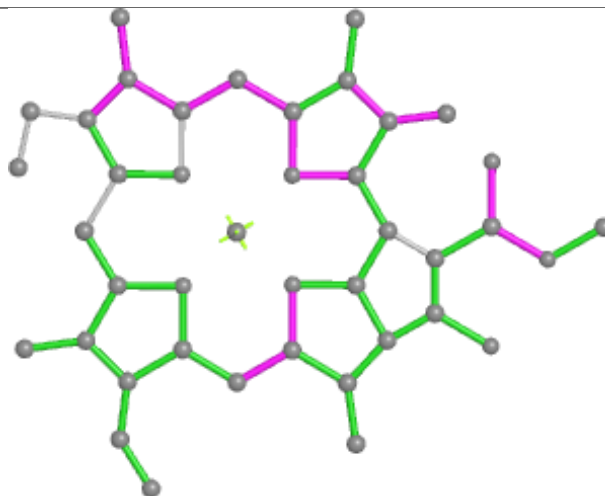




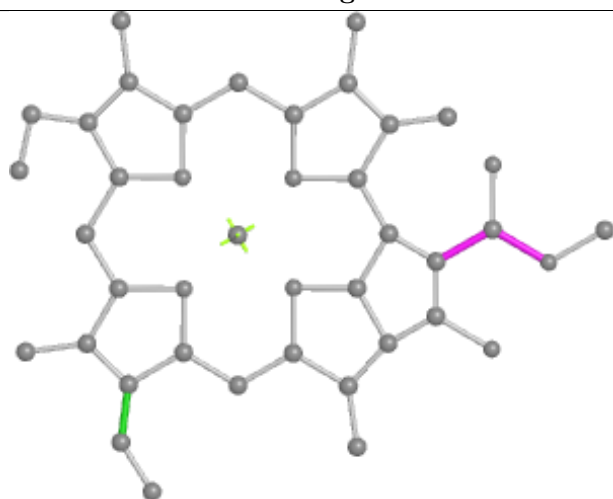
## Ligand CLA 2 313



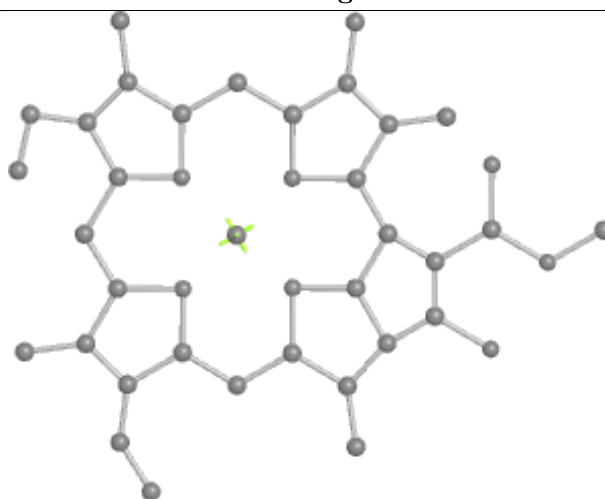
Bond lengths



Bond angles

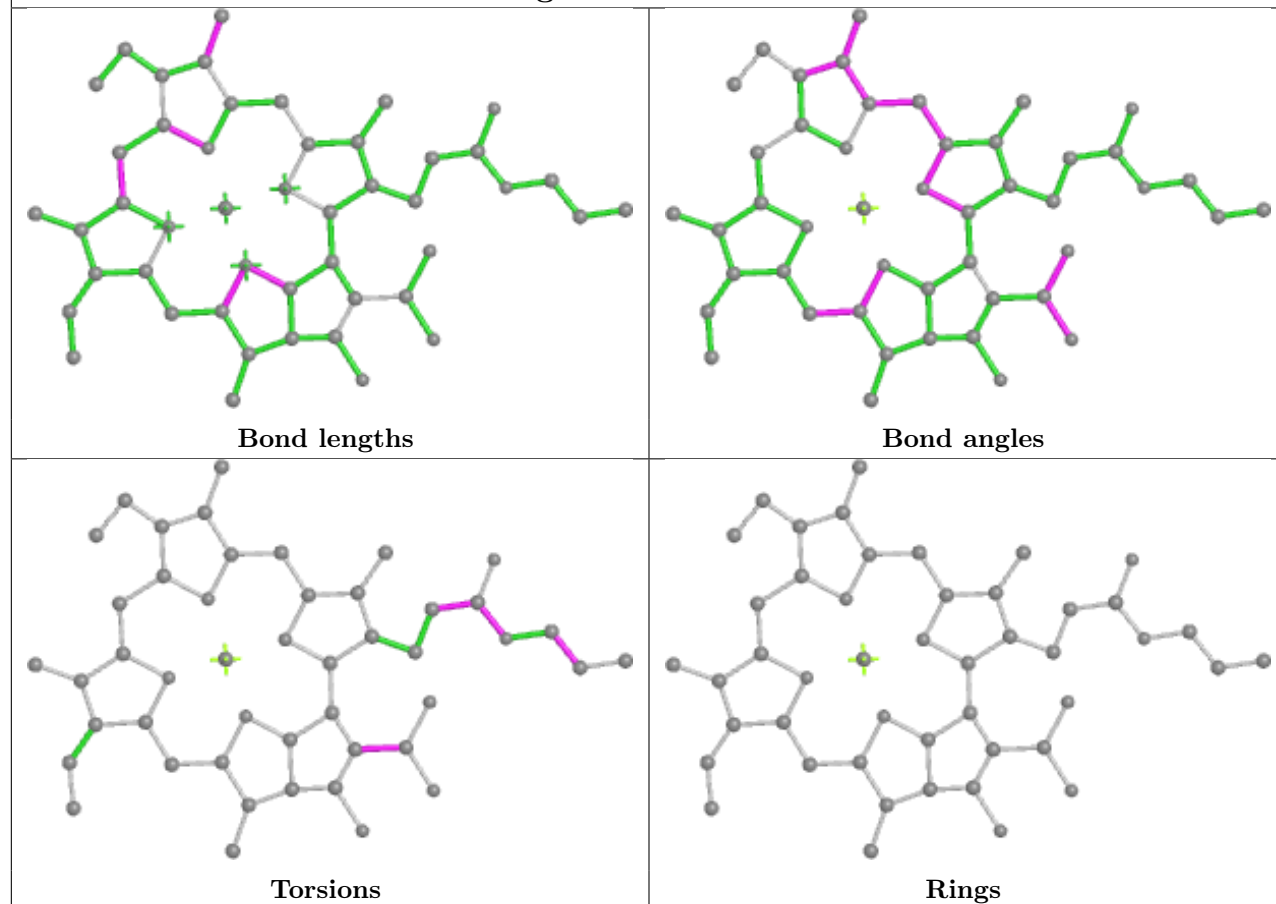


Torsions

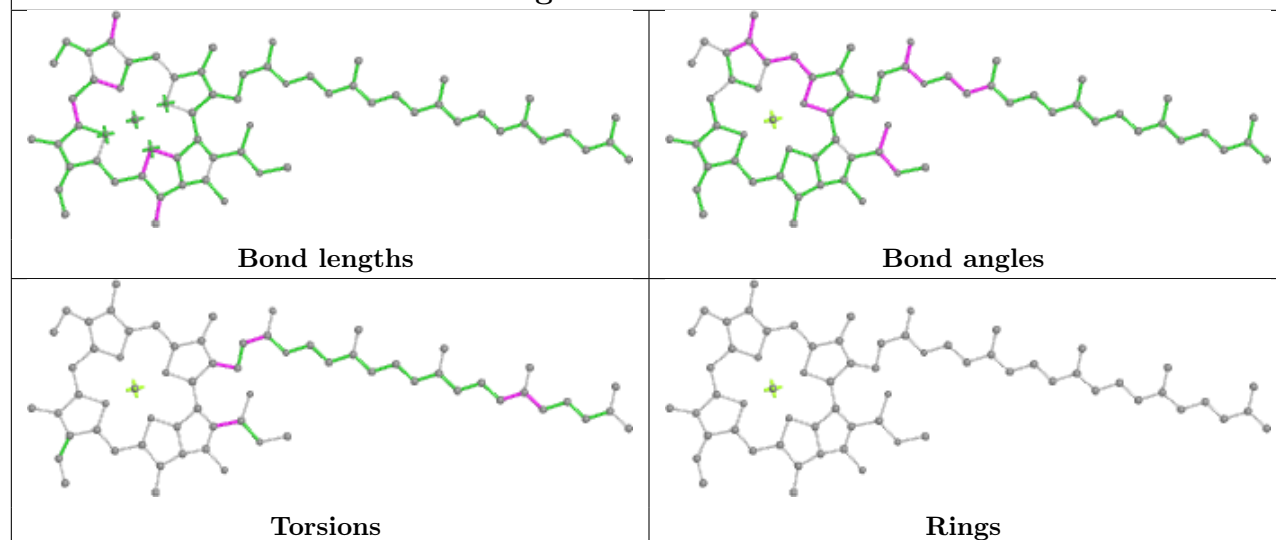


Rings

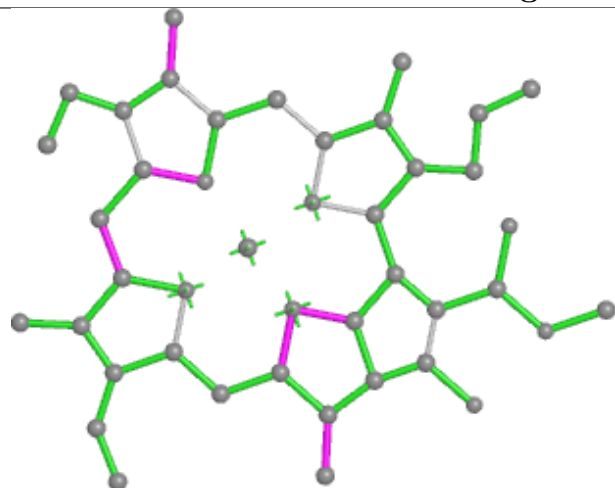
## Ligand CLA 7 309



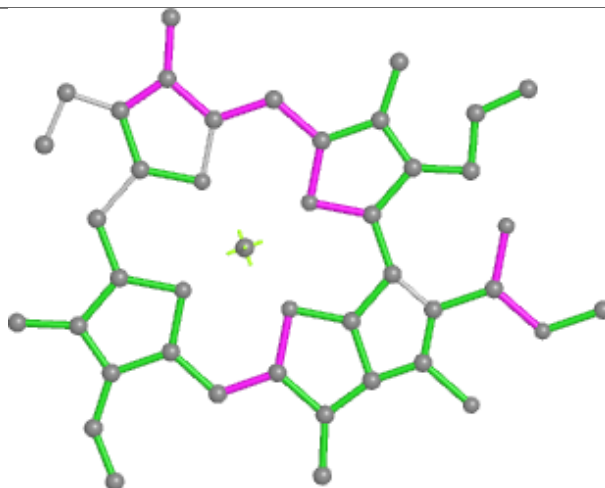
## Ligand CLA b 837



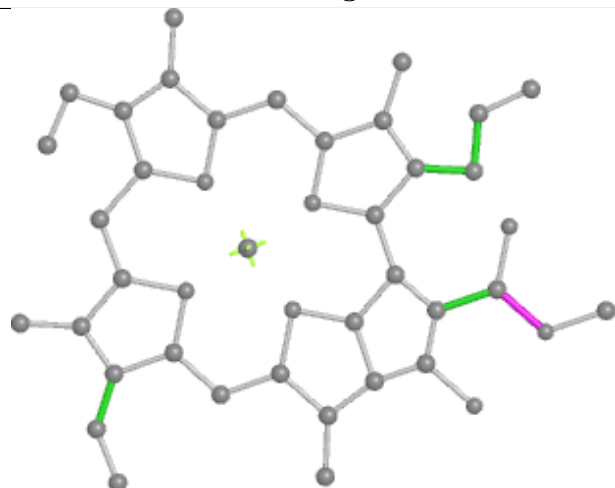
## Ligand CLA 8 305



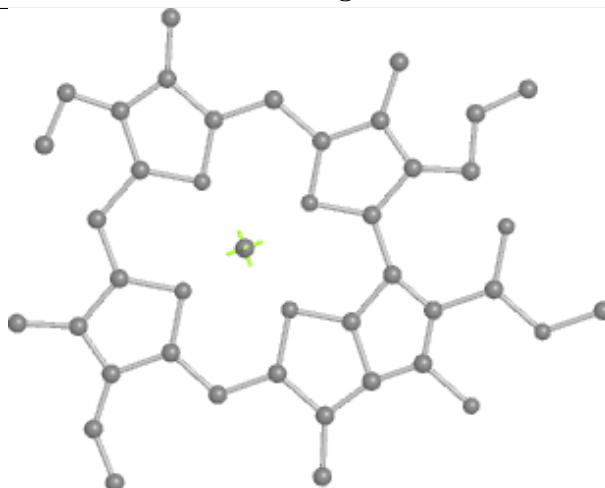
Bond lengths



Bond angles

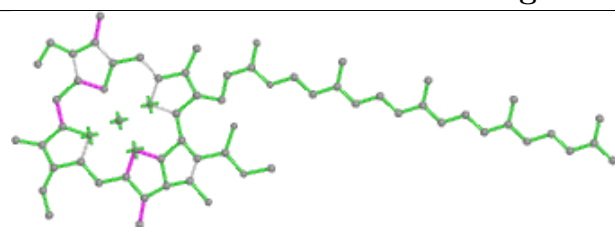


Torsions

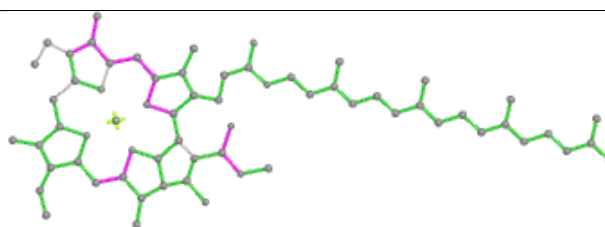


Rings

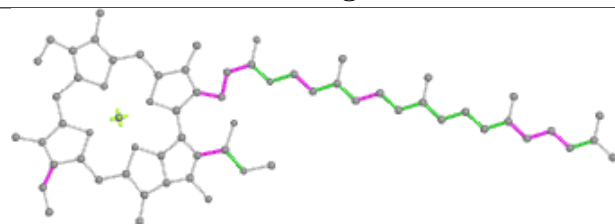
## Ligand CLA b 832



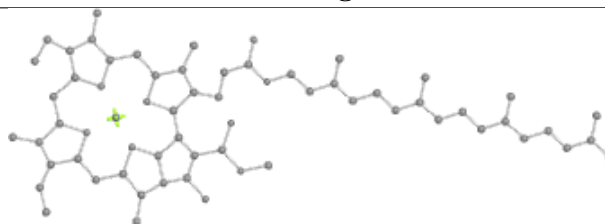
Bond lengths



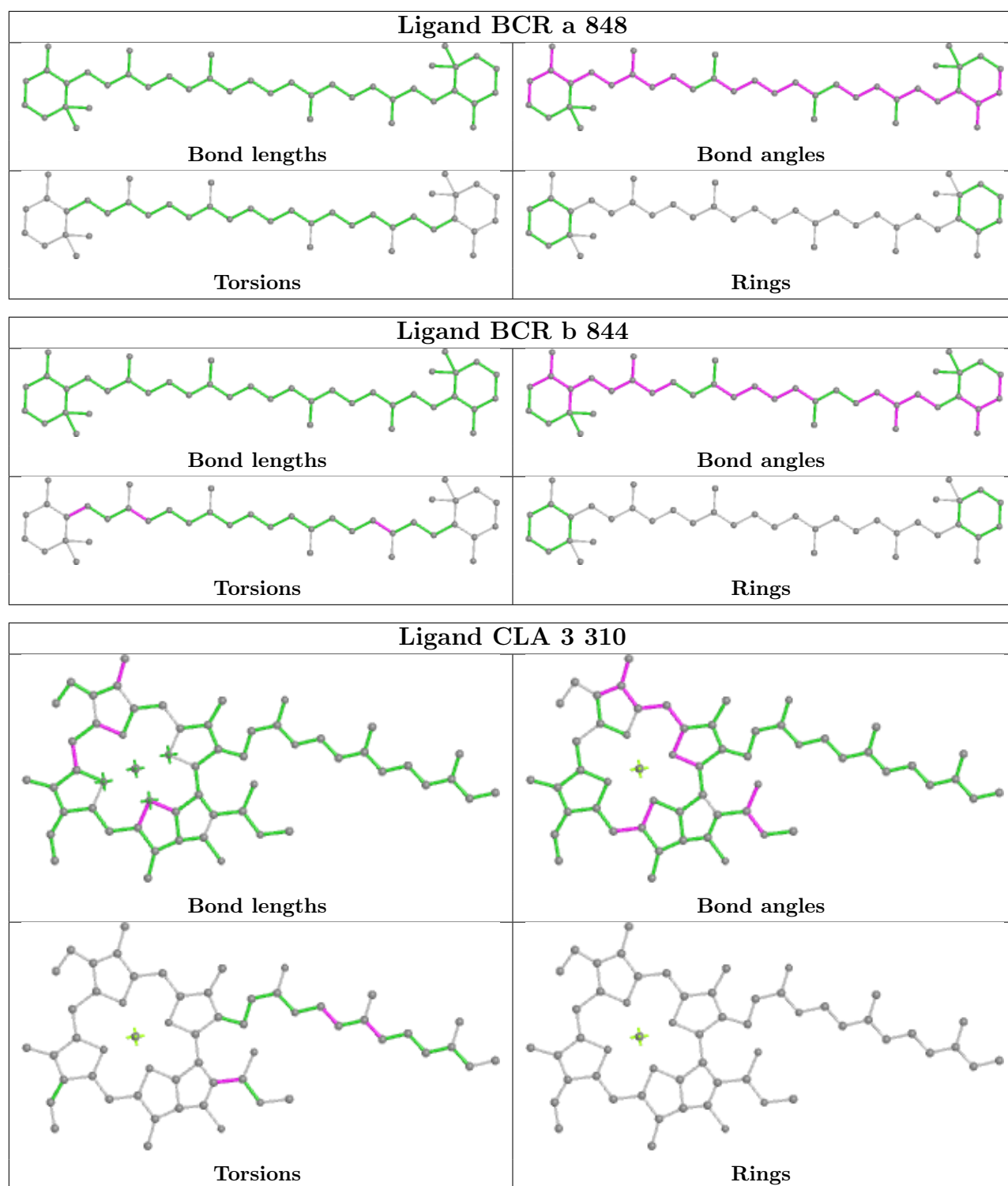
Bond angles



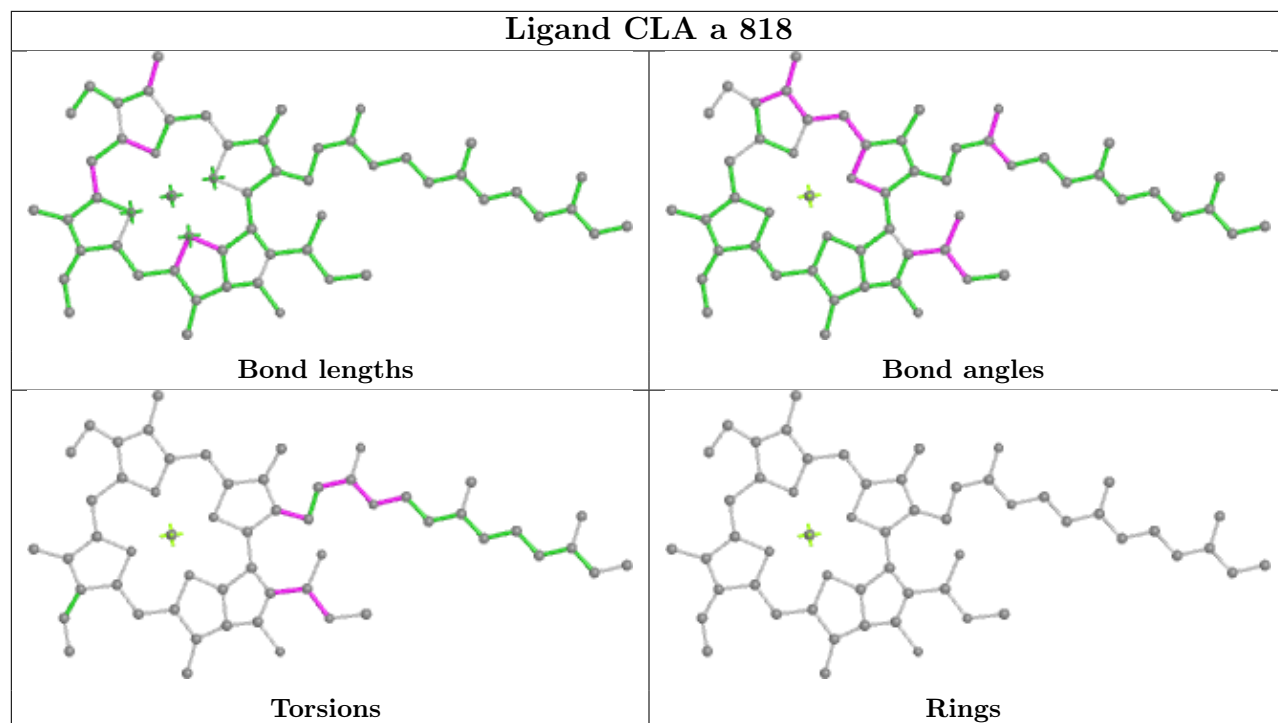
Torsions



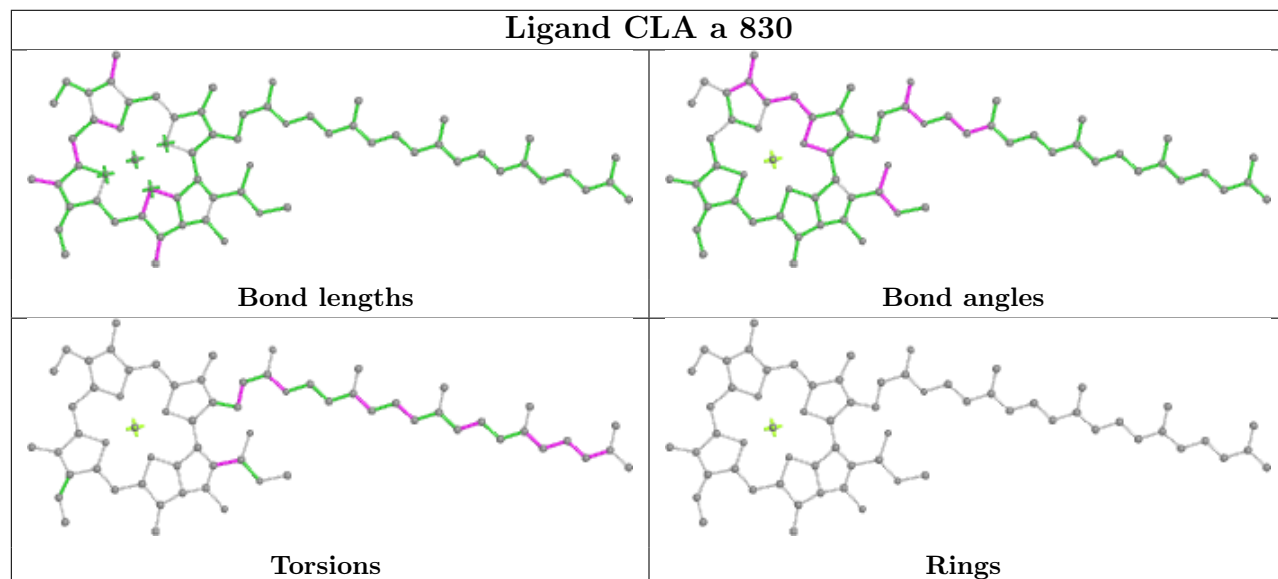
Rings



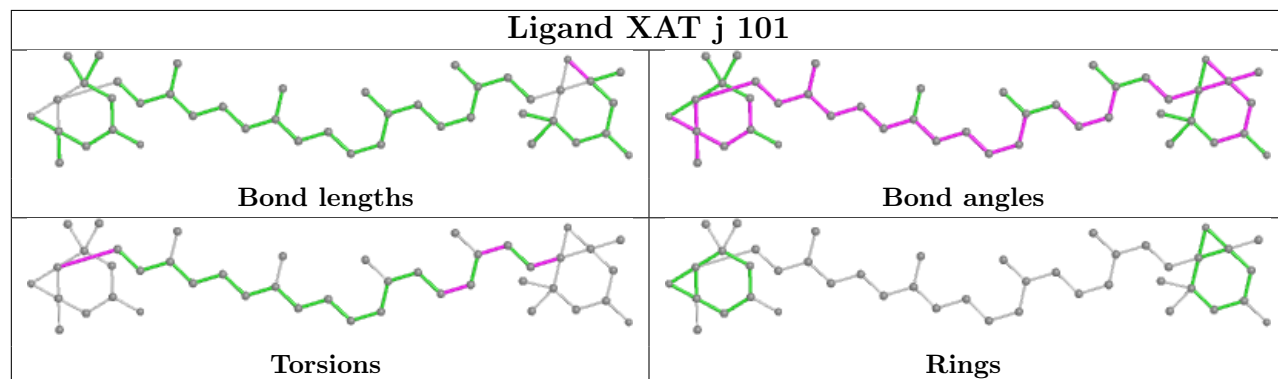
## Ligand CLA a 818



## Ligand CLA a 830

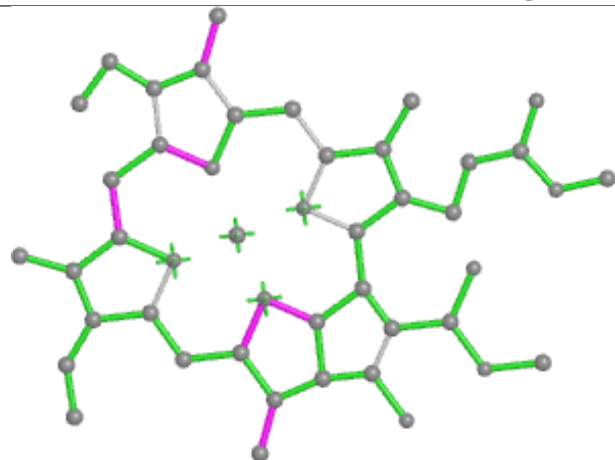


## Ligand XAT j 101

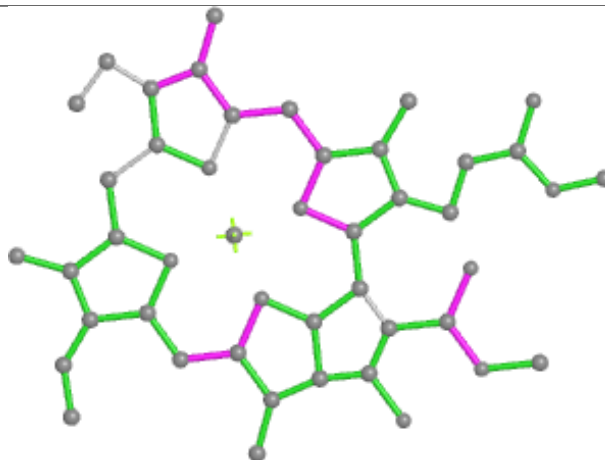




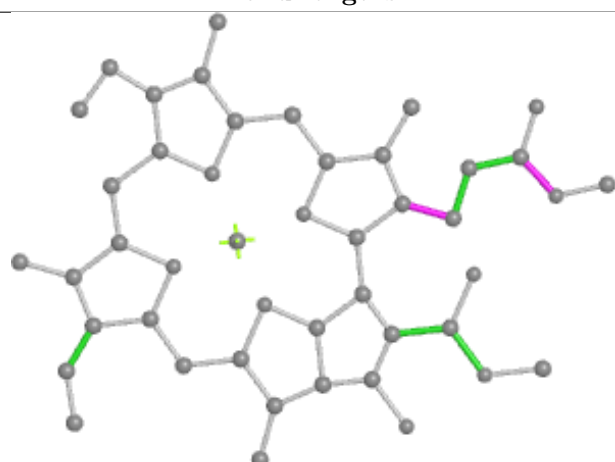
## Ligand CLA 4 312



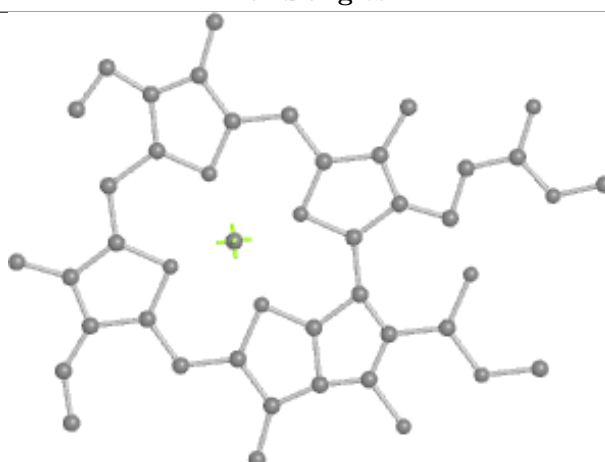
Bond lengths



Bond angles

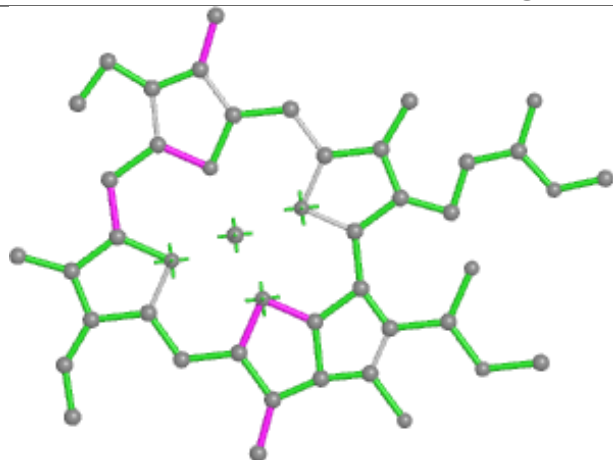


Torsions

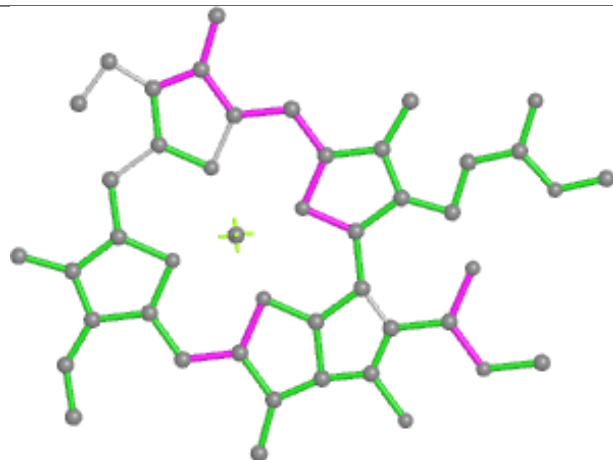


Rings

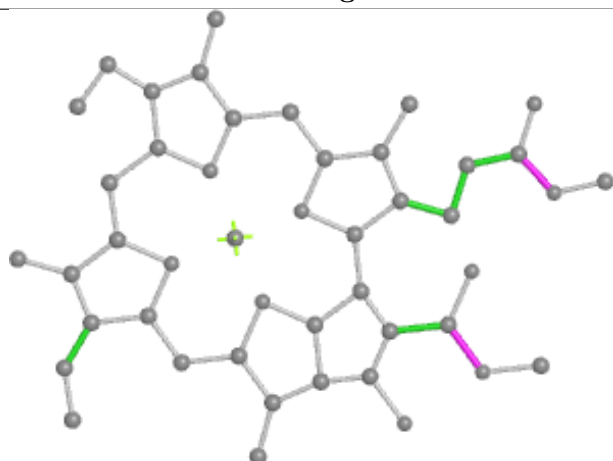
## Ligand CLA 5 305



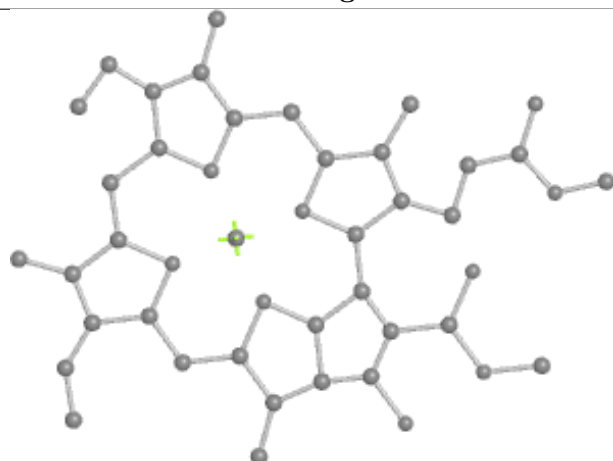
Bond lengths



Bond angles

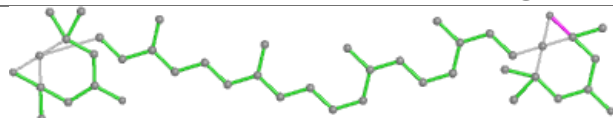


Torsions

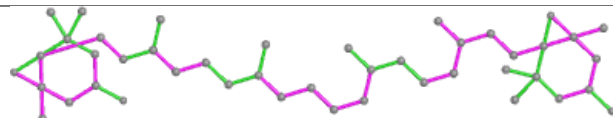


Rings

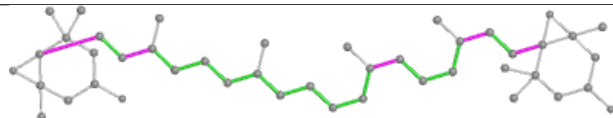
## Ligand XAT 7 303



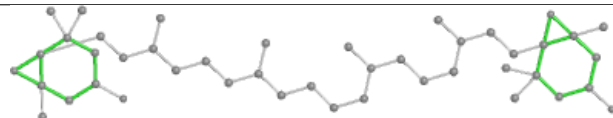
Bond lengths



Bond angles

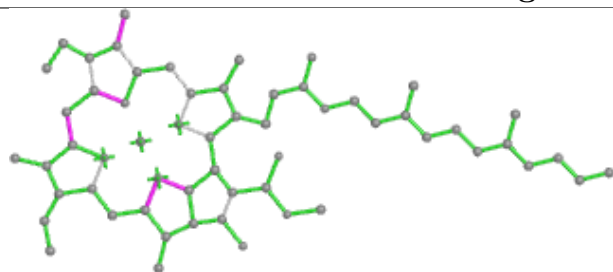


Torsions

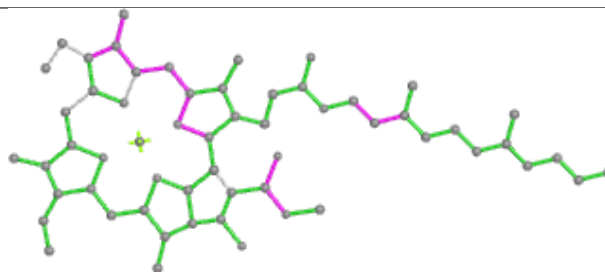


Rings

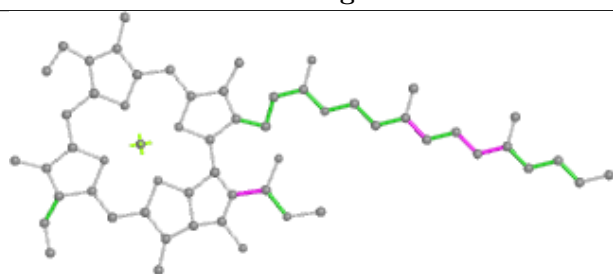
## Ligand CLA a 802



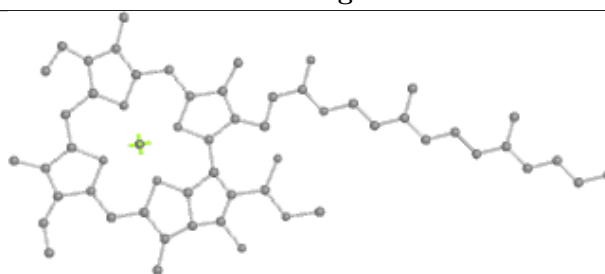
Bond lengths



Bond angles

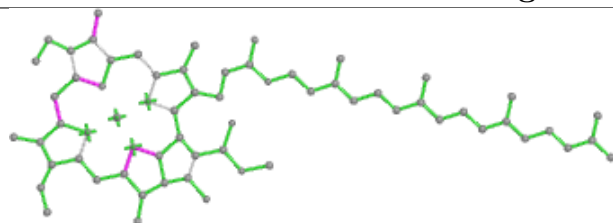


Torsions

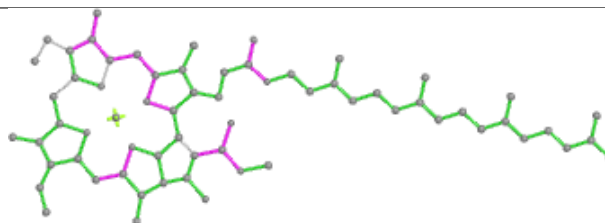


Rings

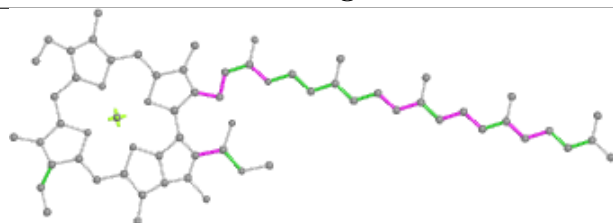
## Ligand CLA a 809



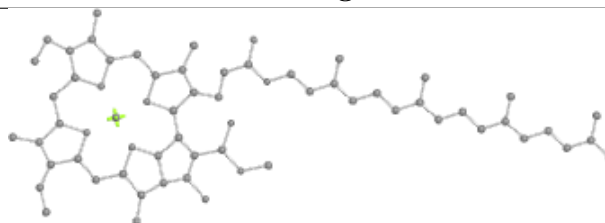
Bond lengths



Bond angles

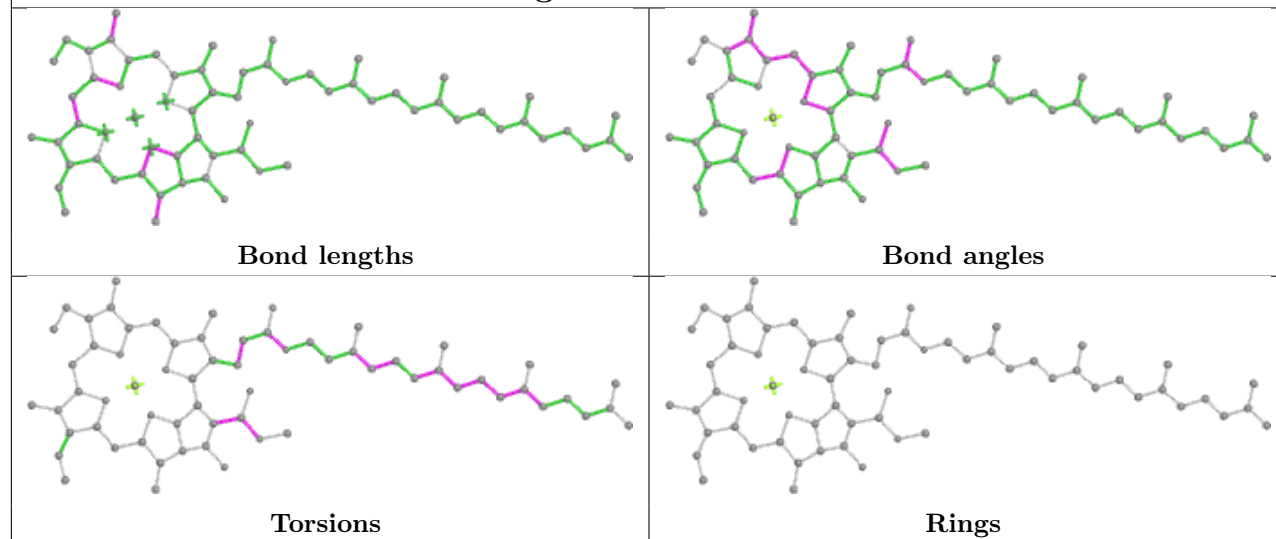


Torsions

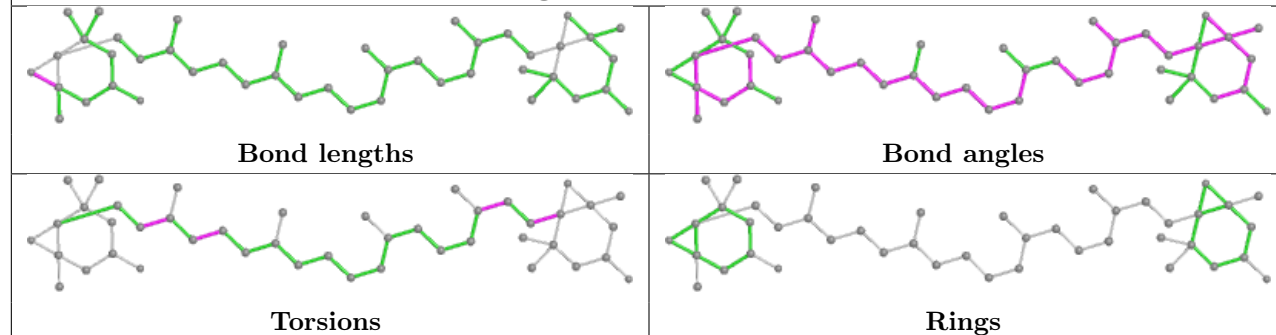


Rings

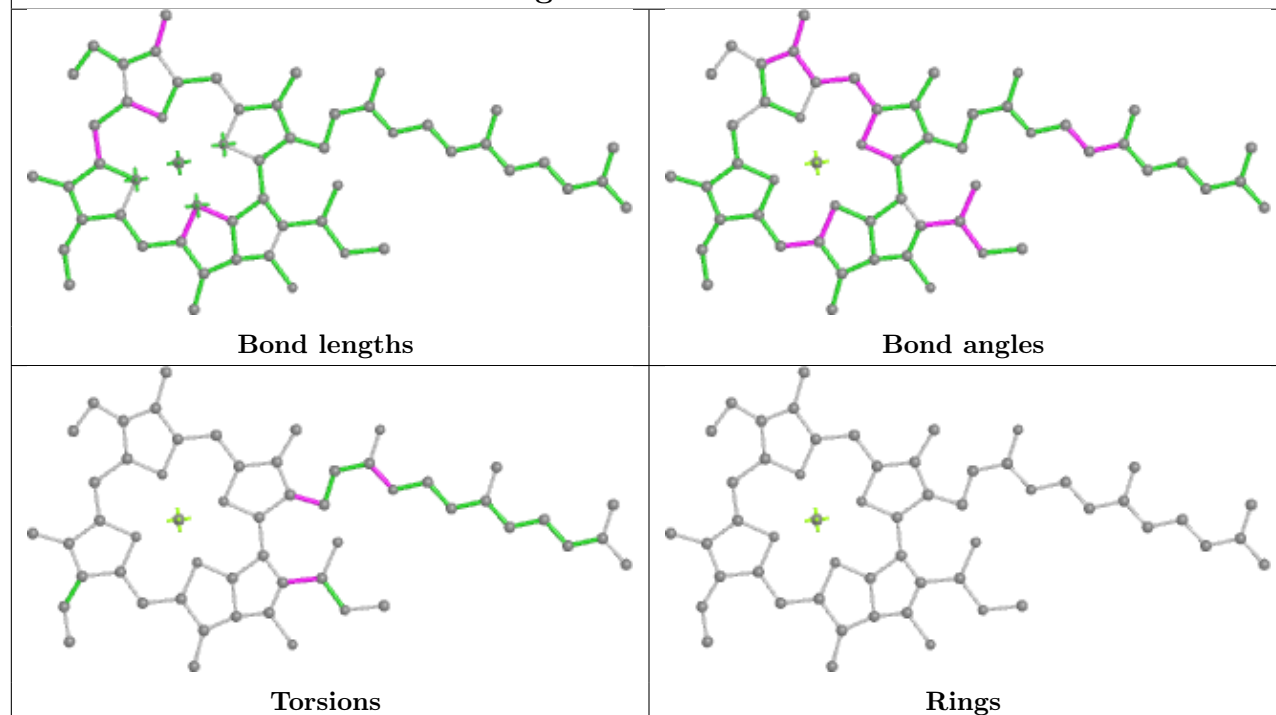
## Ligand CLA b 802

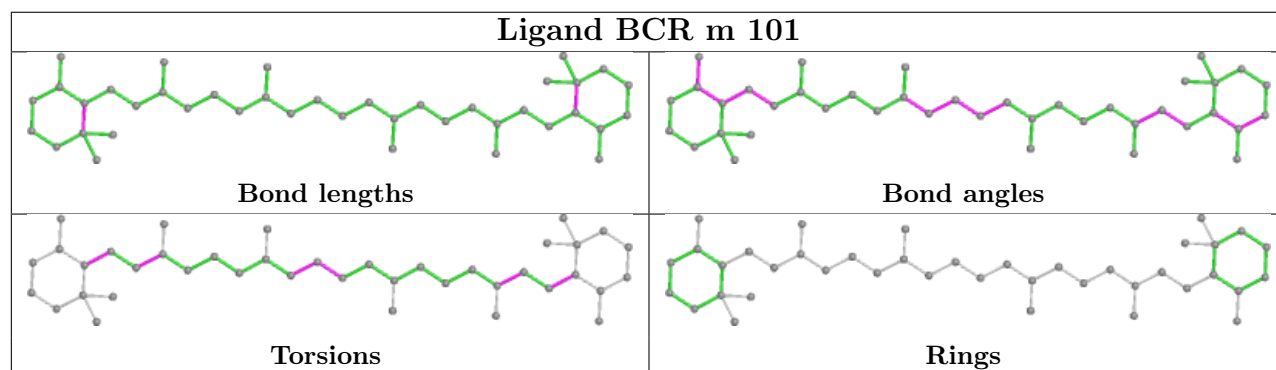
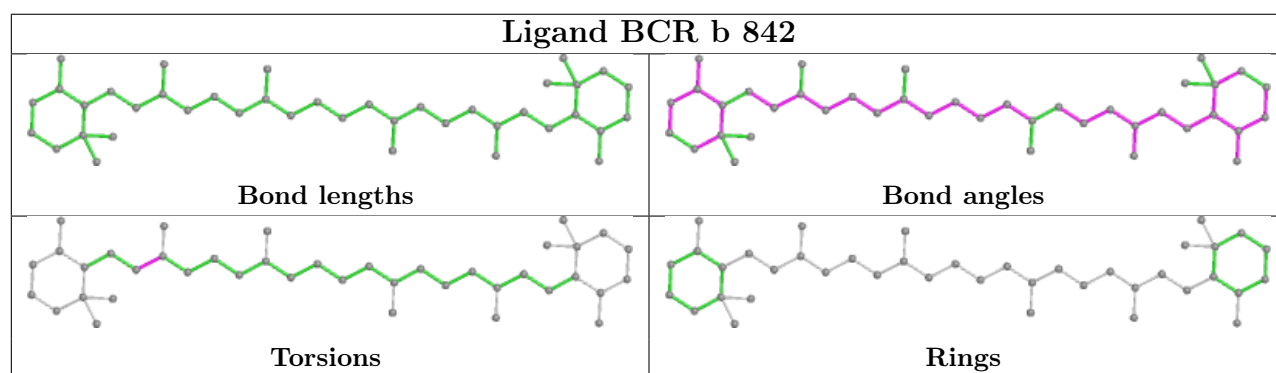
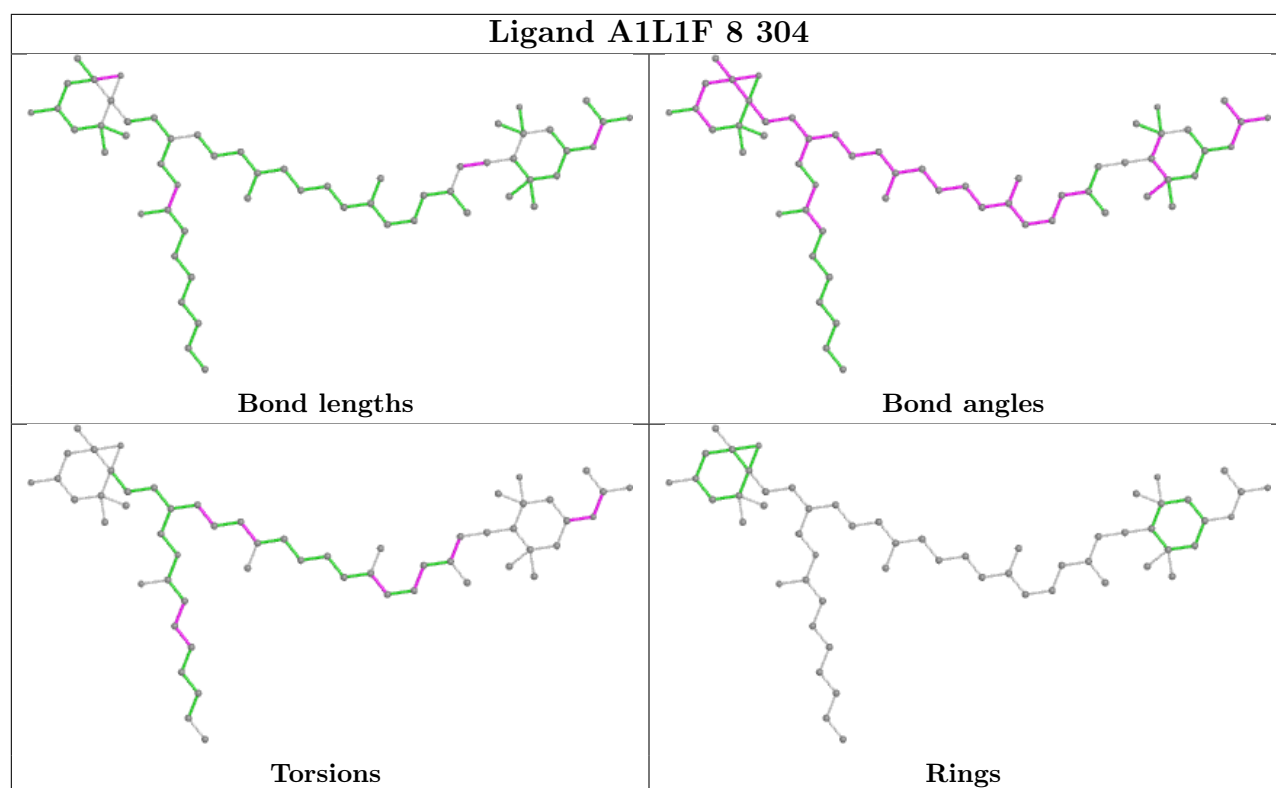


## Ligand XAT 7 301

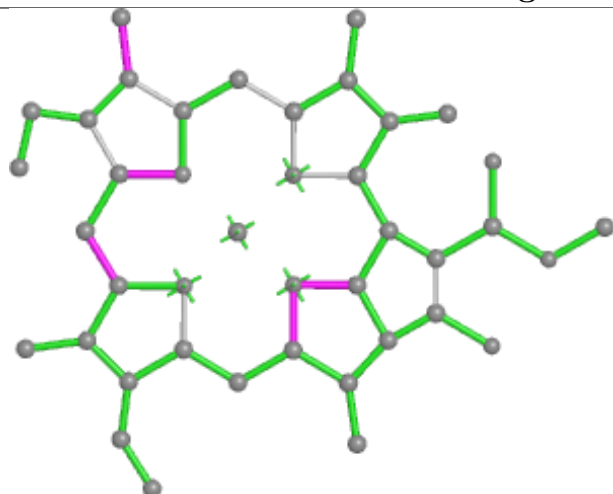


## Ligand CLA b 816

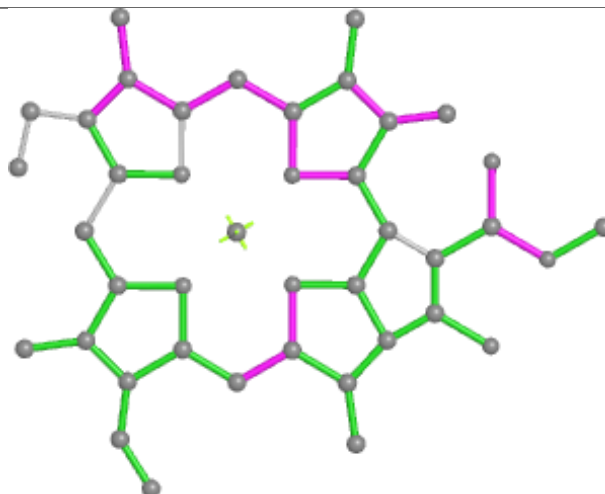




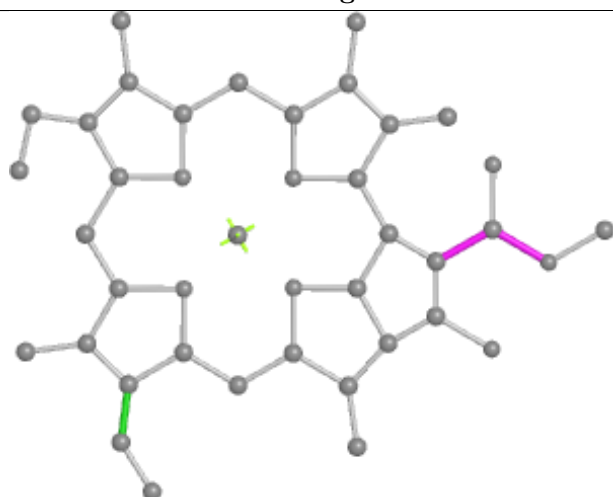
## Ligand CLA 4 315



Bond lengths



Bond angles

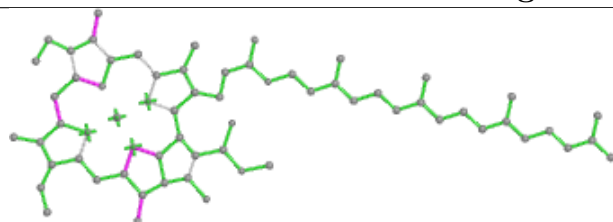


Torsions

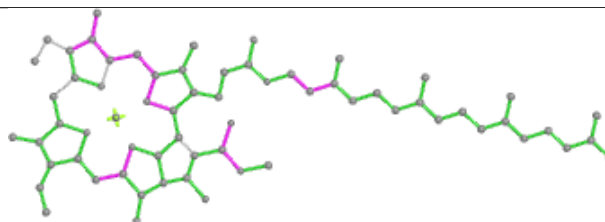


Rings

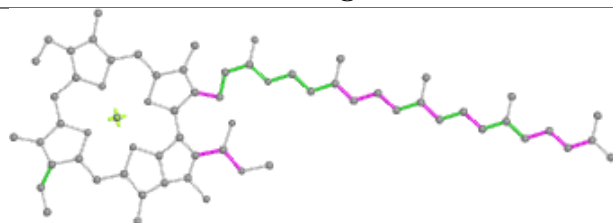
## Ligand CLA b 813



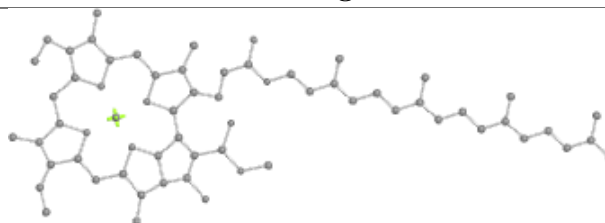
Bond lengths



Bond angles

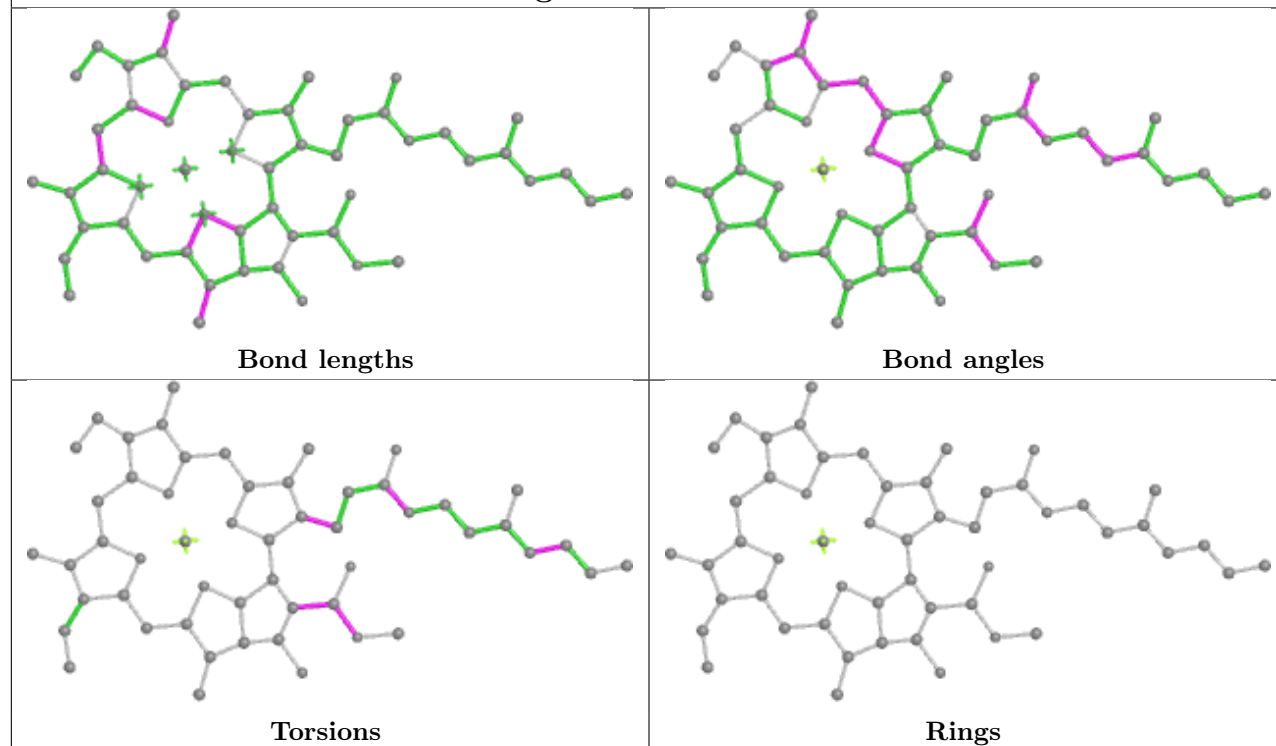


Torsions

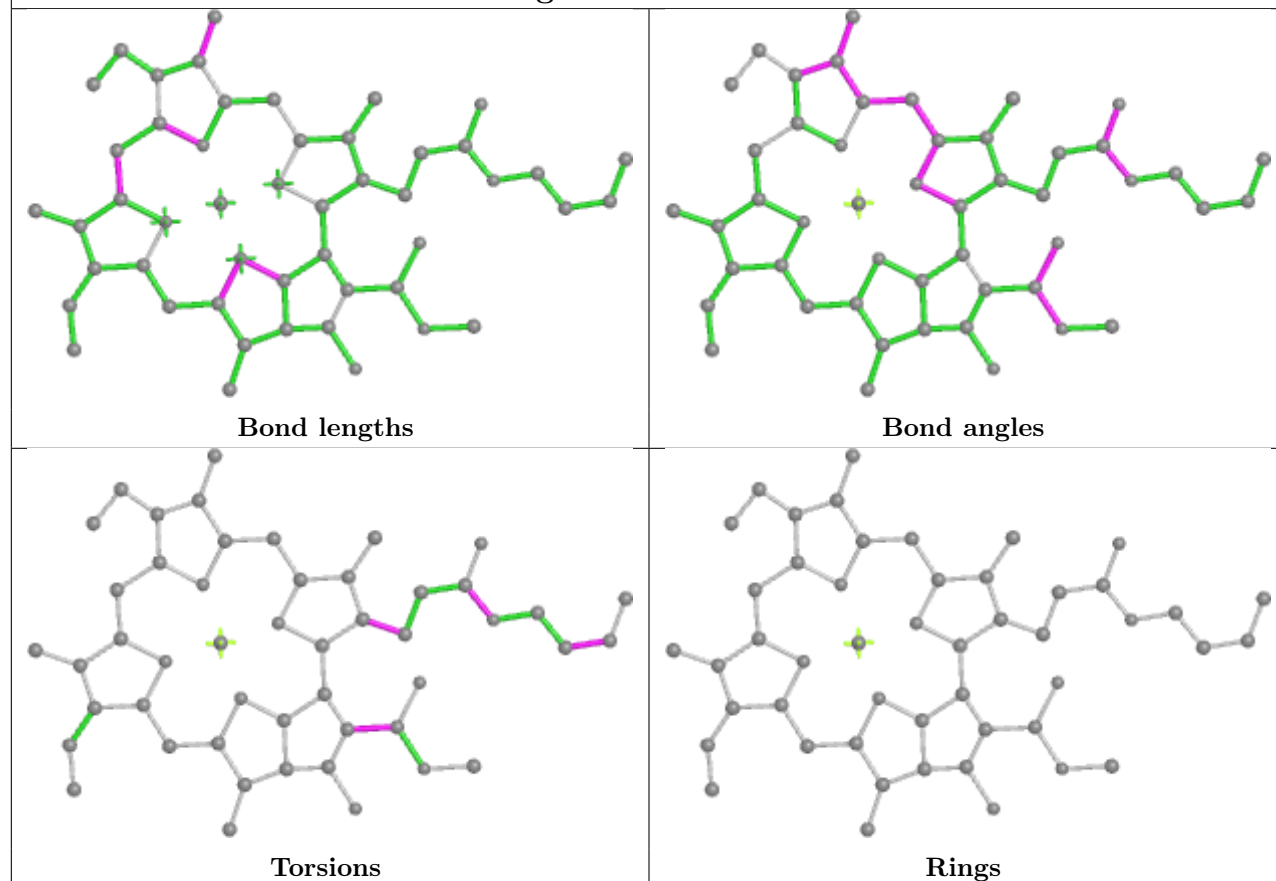


Rings

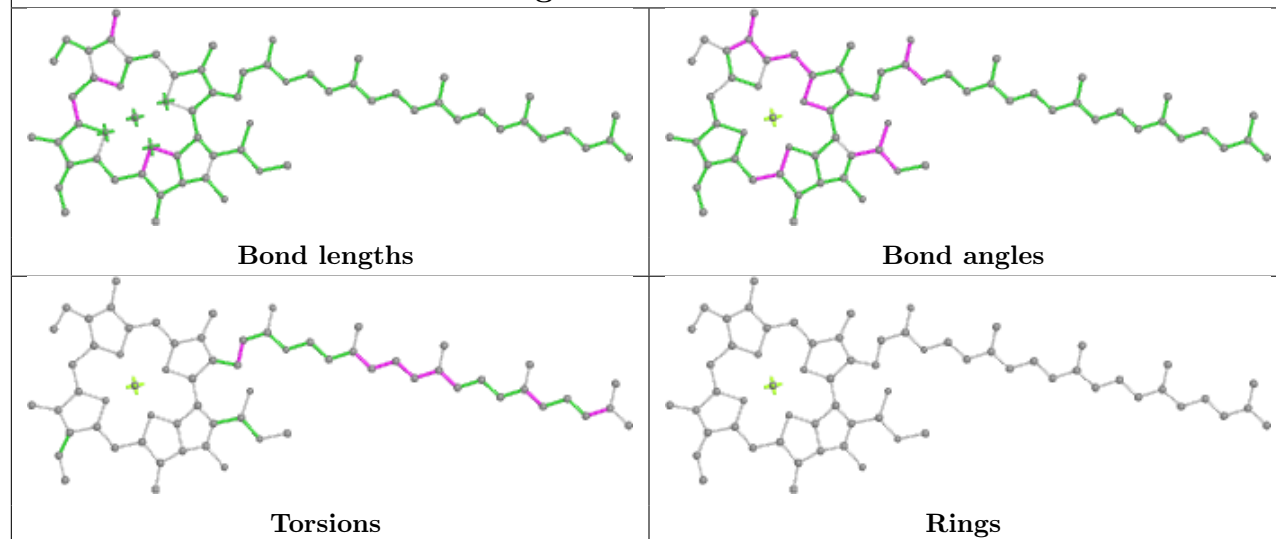
## Ligand CLA b 823



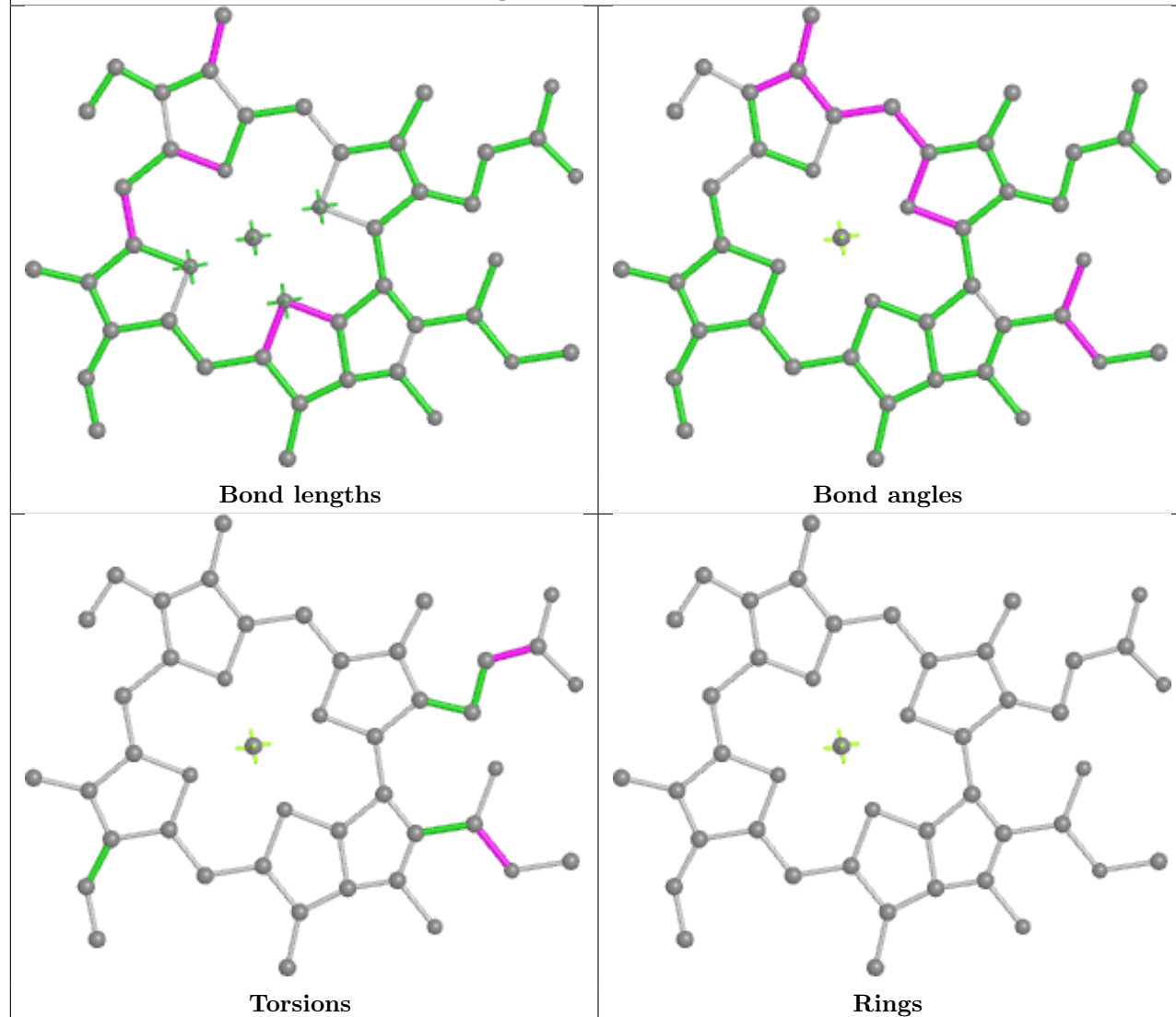
## Ligand CLA a 823



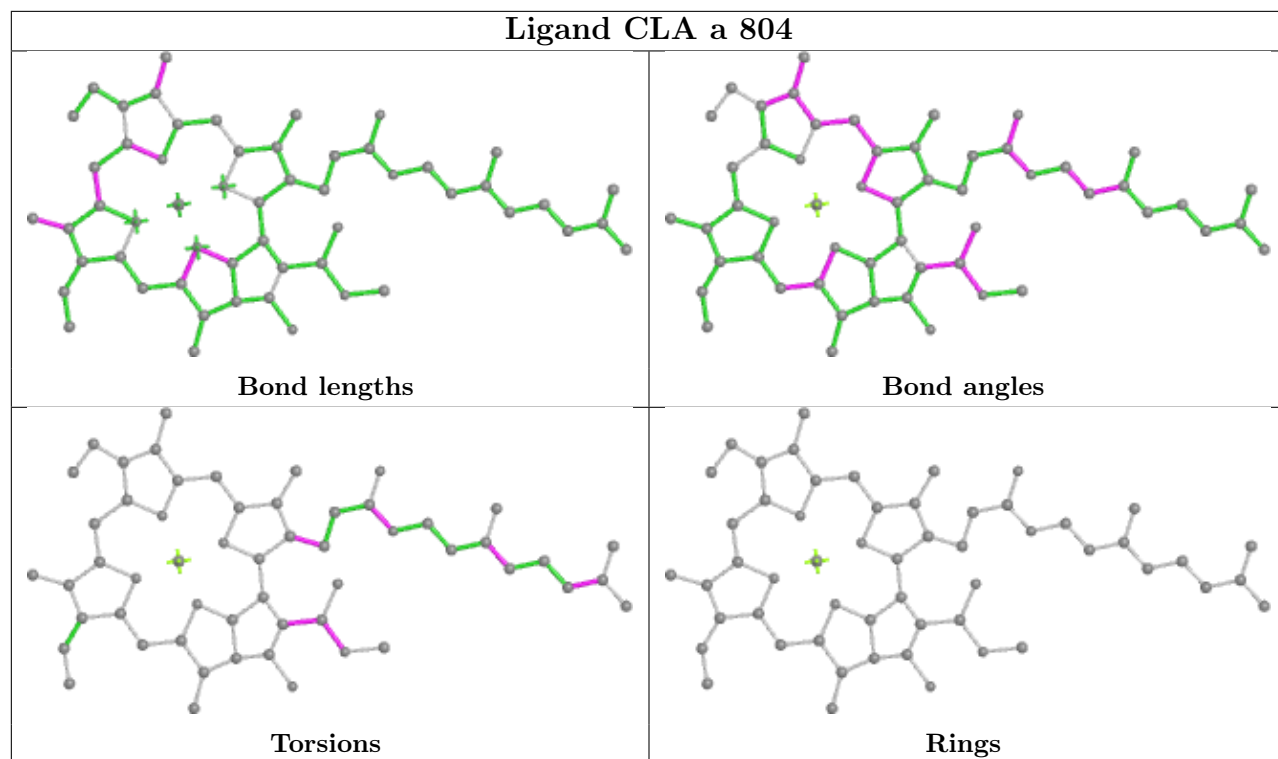
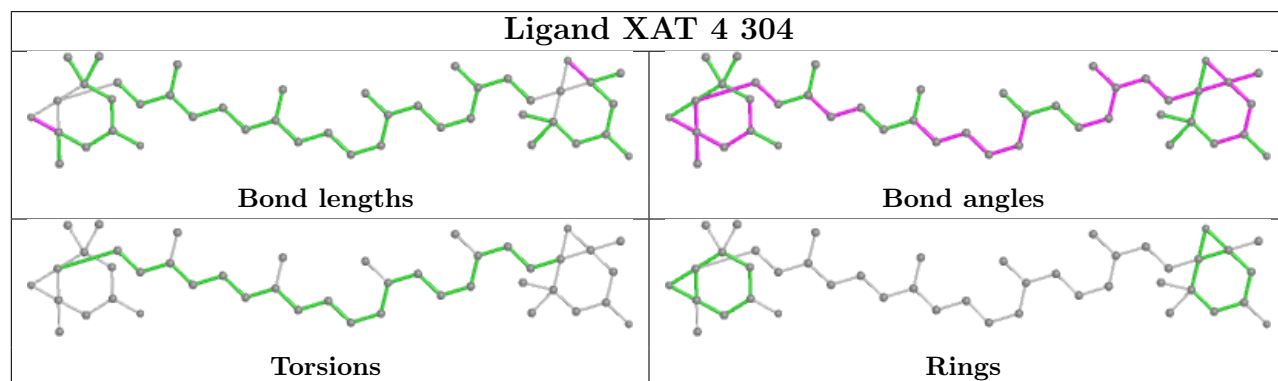
## Ligand CLA b 808



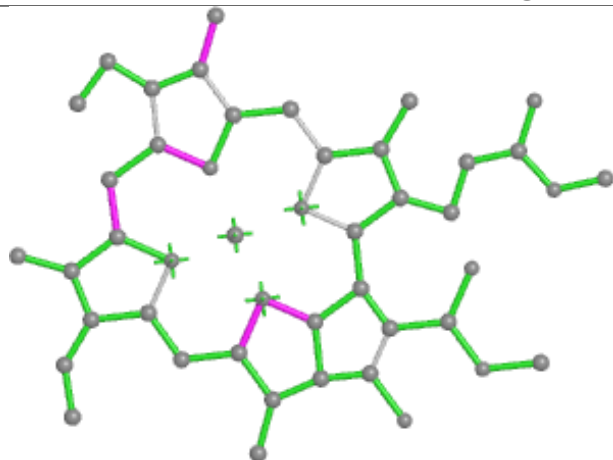
## Ligand CLA 5 313



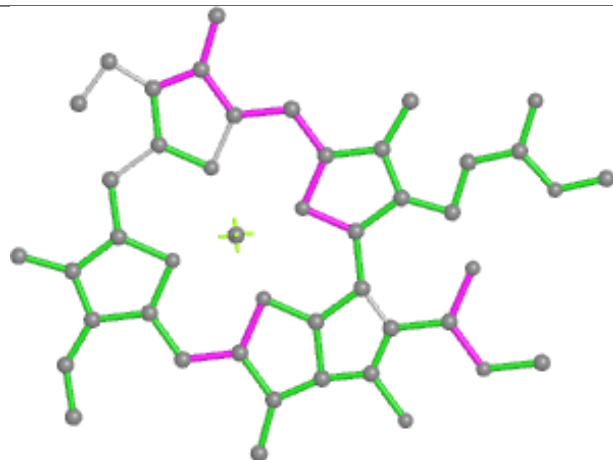


**Ligand CLA a 804****Ligand XAT 4 304**

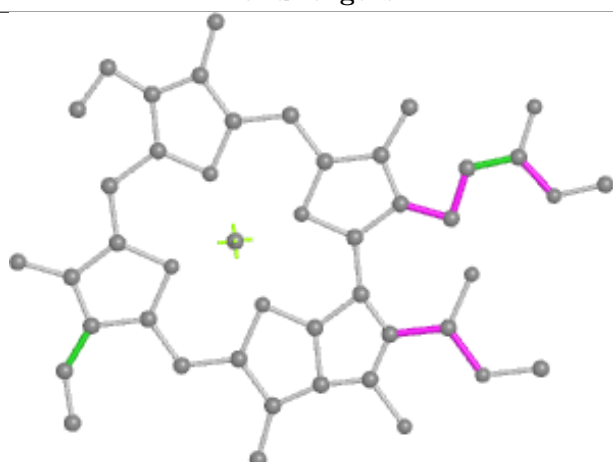
## Ligand CLA 4 316



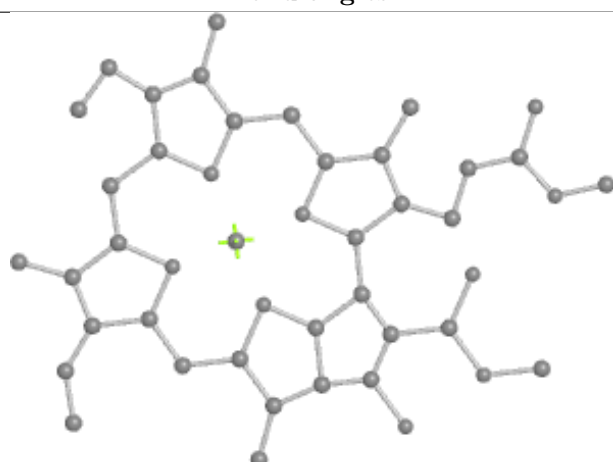
Bond lengths



Bond angles

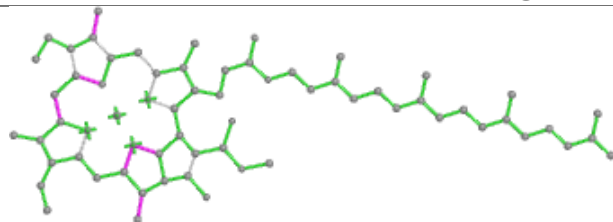


Torsions

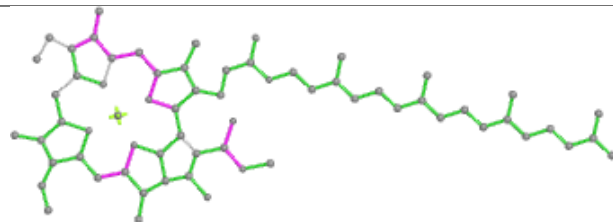


Rings

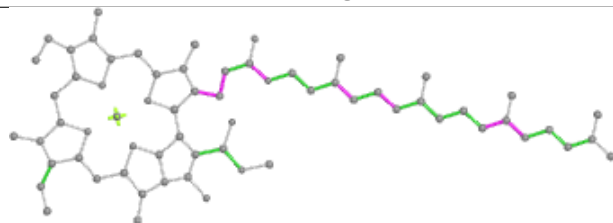
## Ligand CLA b 828



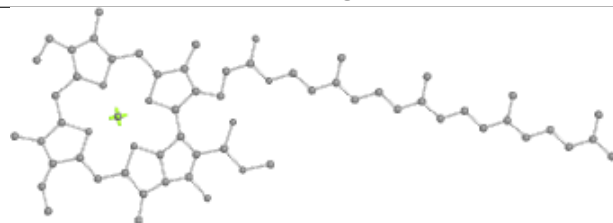
Bond lengths



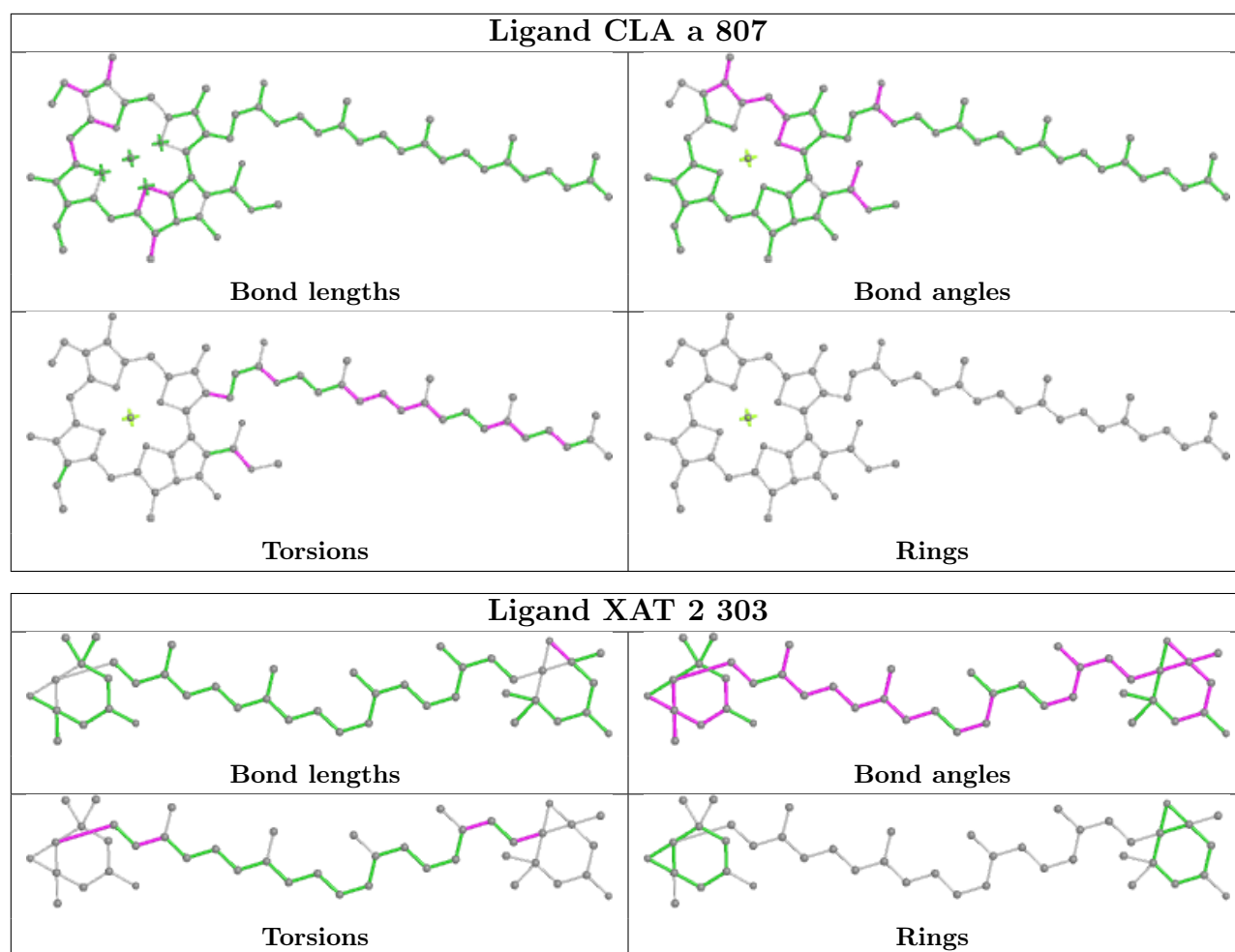
Bond angles

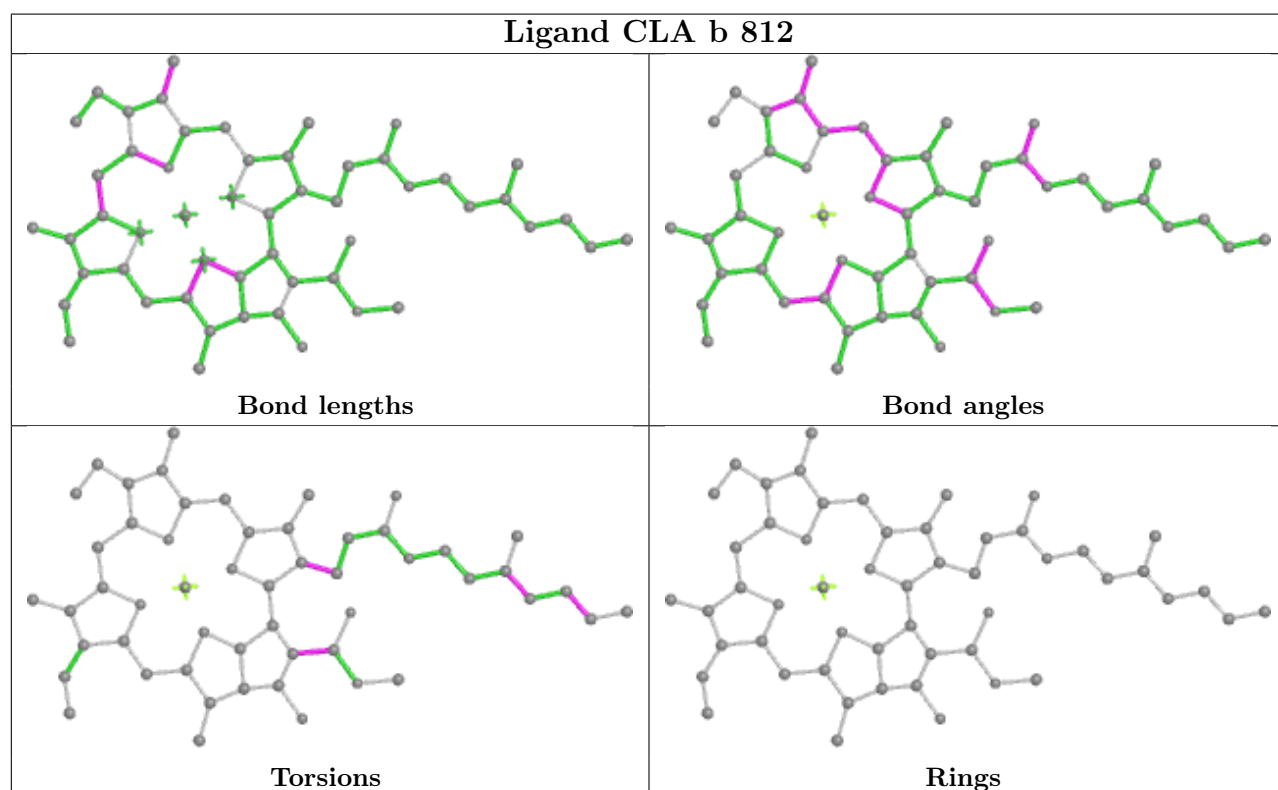
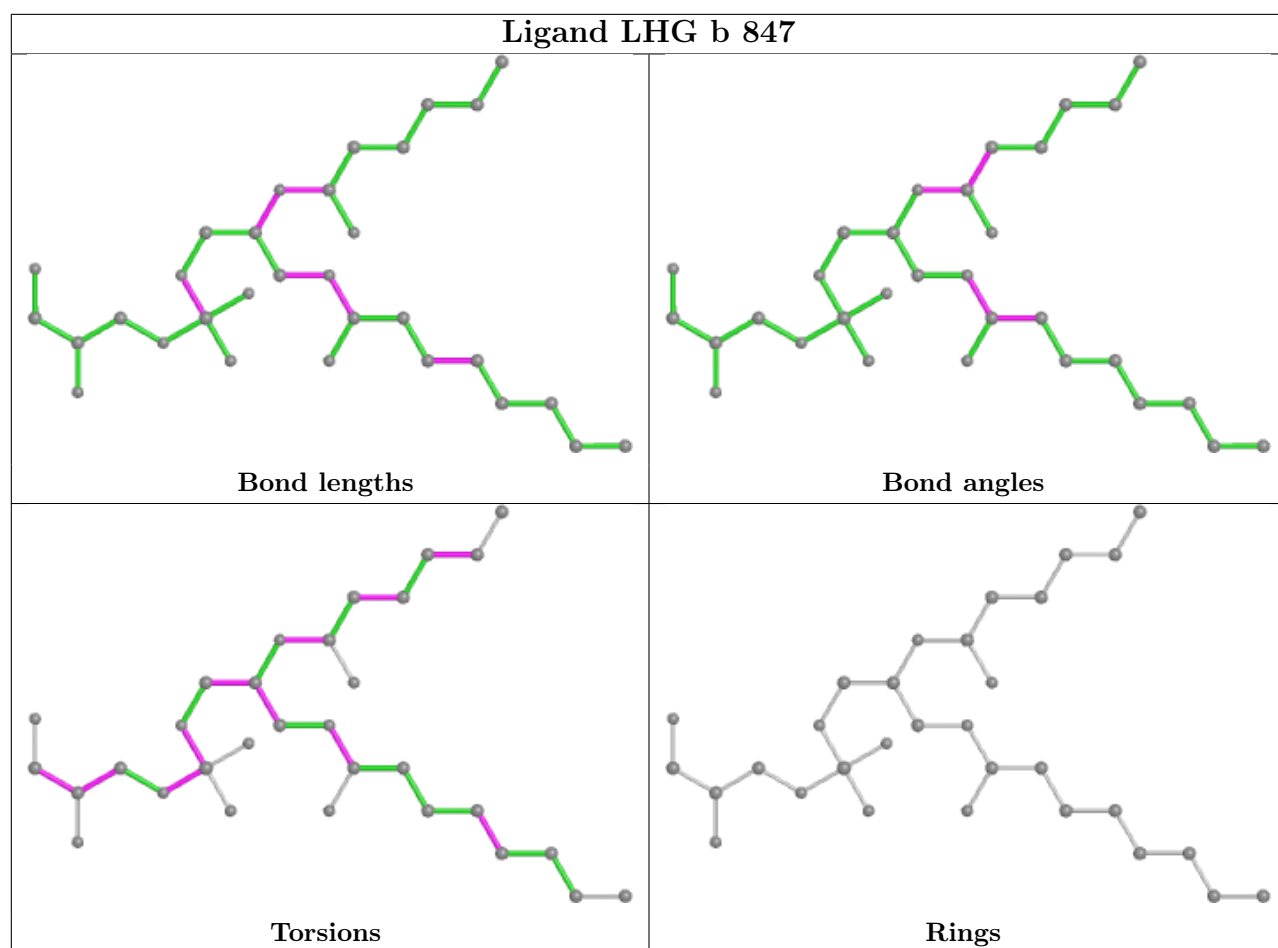


Torsions

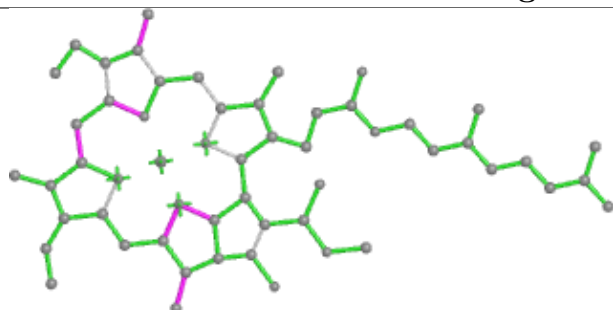


Rings

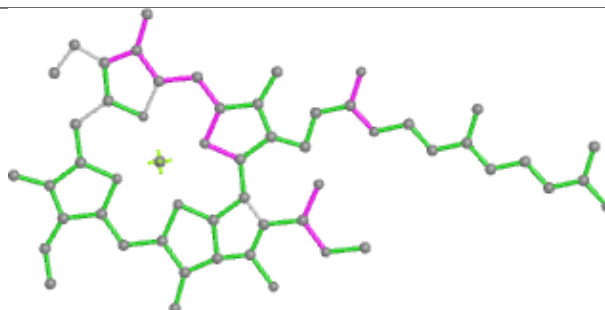




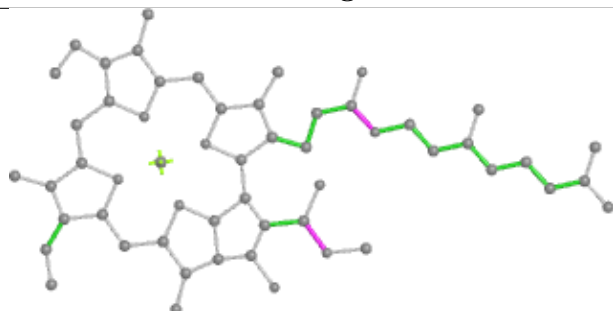
## Ligand CLA 5 308



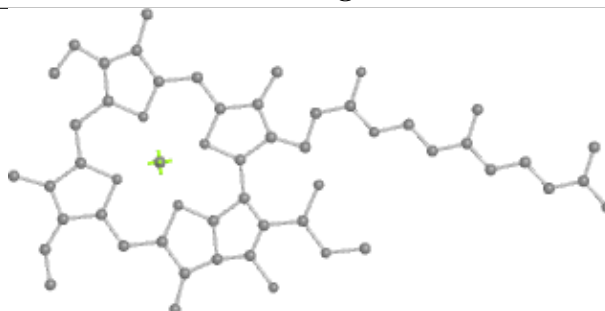
Bond lengths



Bond angles

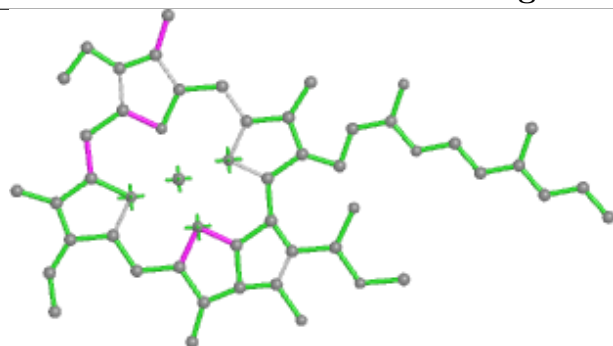


Torsions

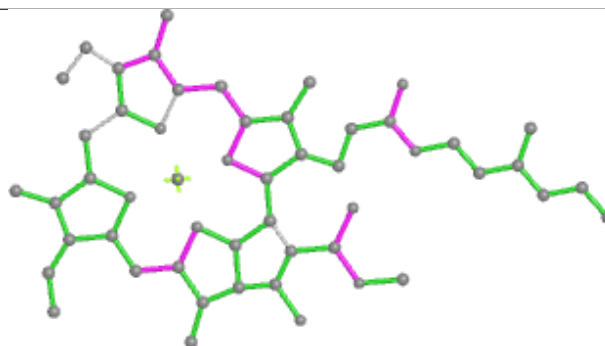


Rings

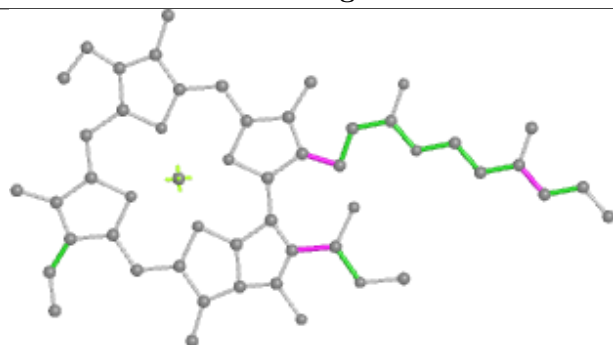
## Ligand CLA 5 314



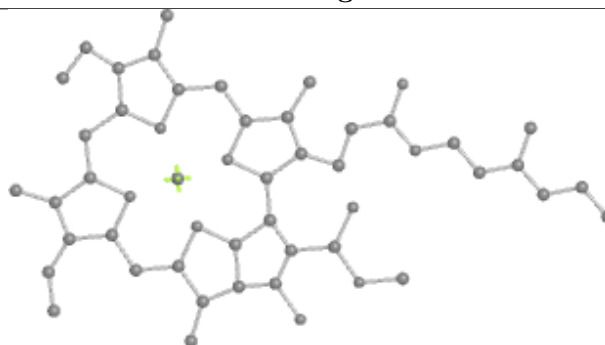
Bond lengths



Bond angles

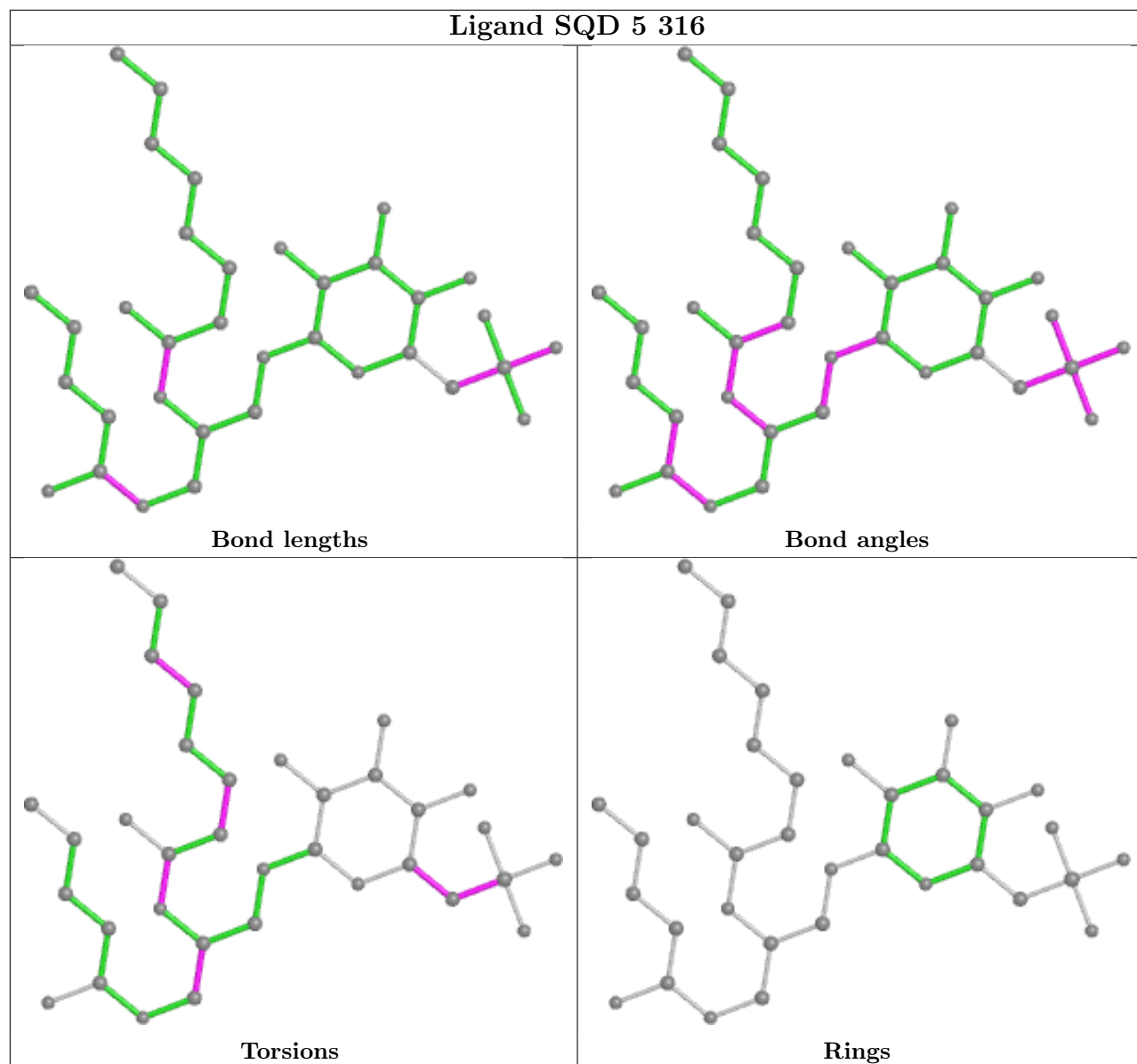


Torsions

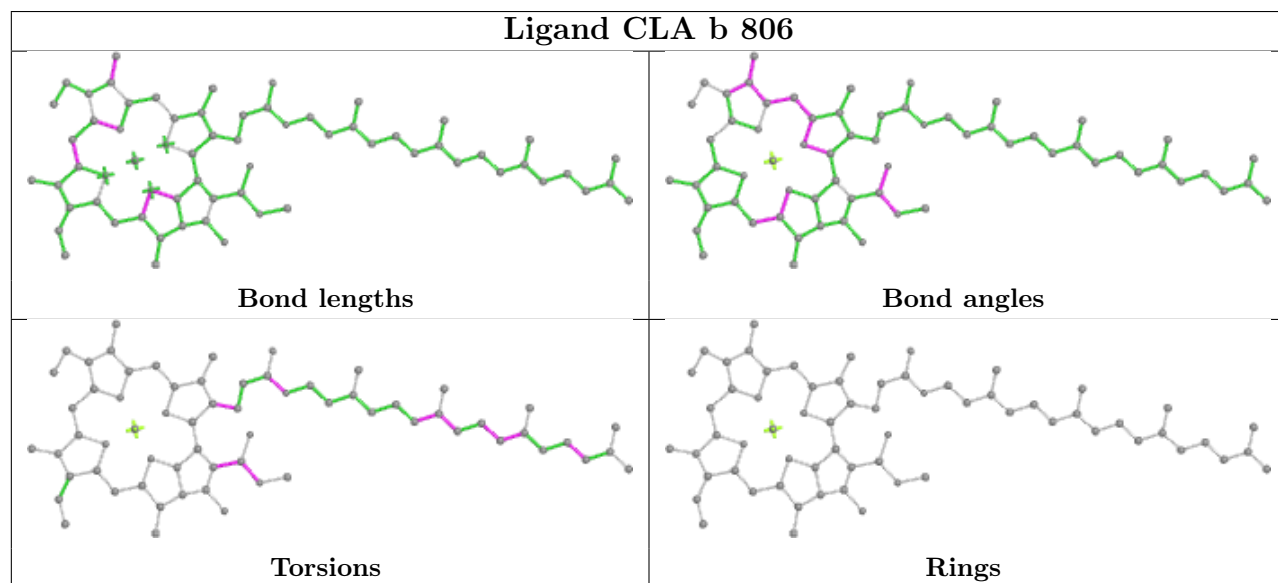


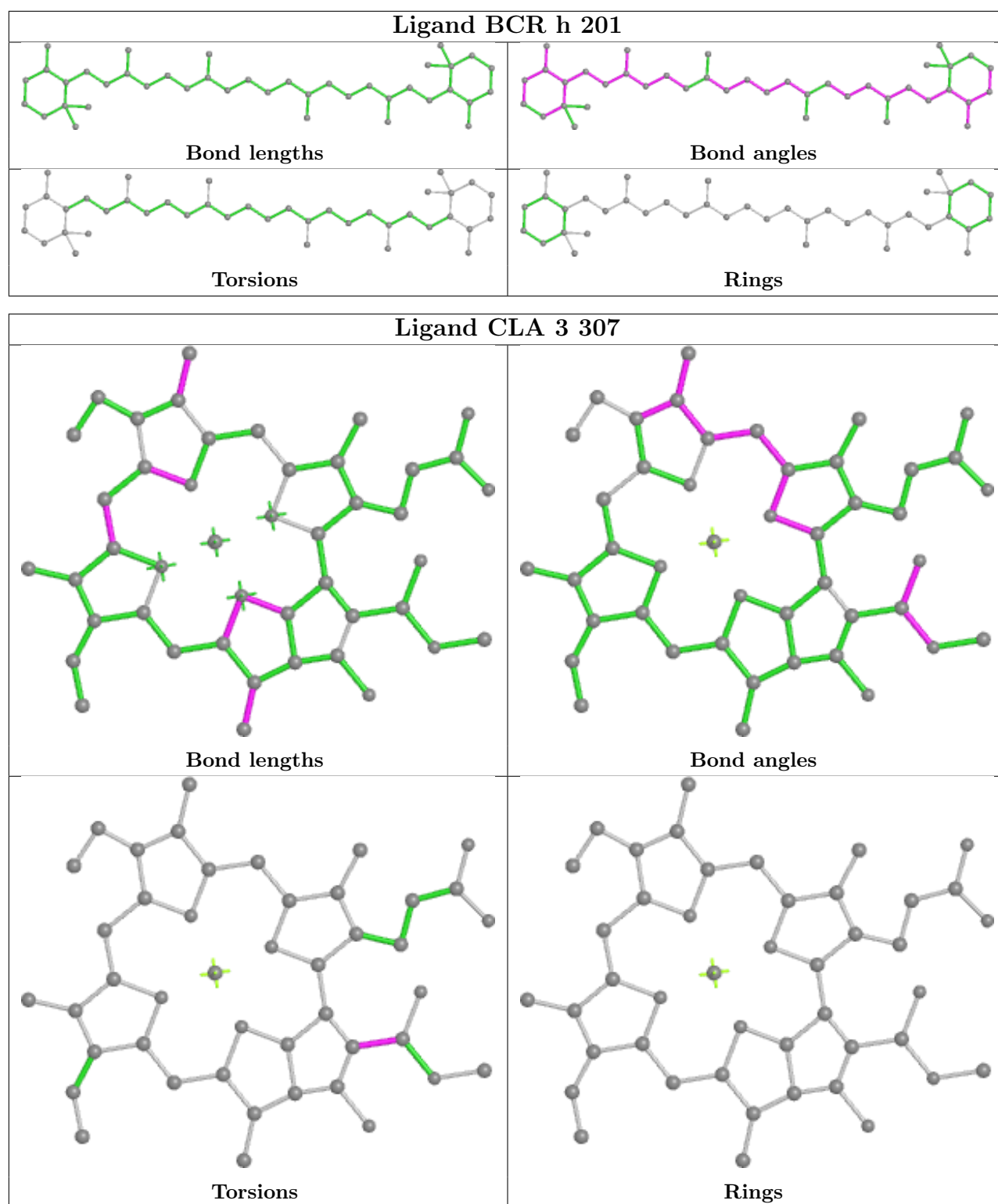
Rings

## Ligand SQD 5 316



## Ligand CLA b 806





## 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.



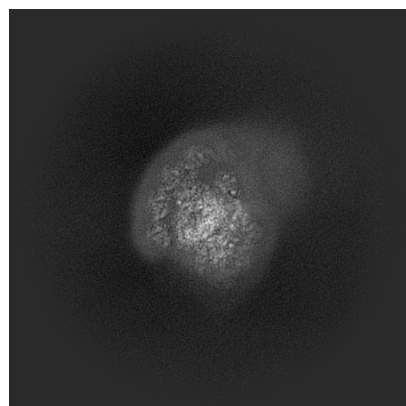
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60286. These allow visual inspection of the internal detail of the map and identification of artifacts.

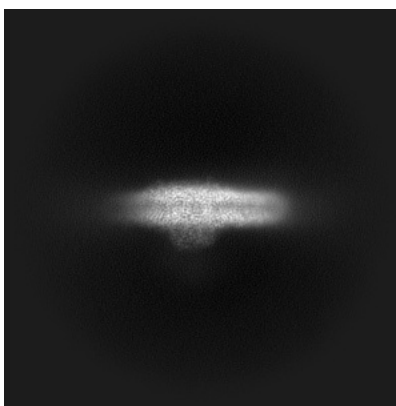
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

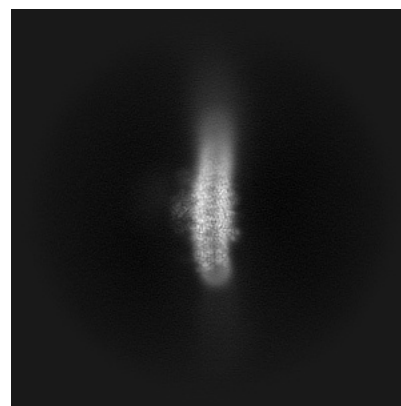
#### 6.1.1 Primary map



X

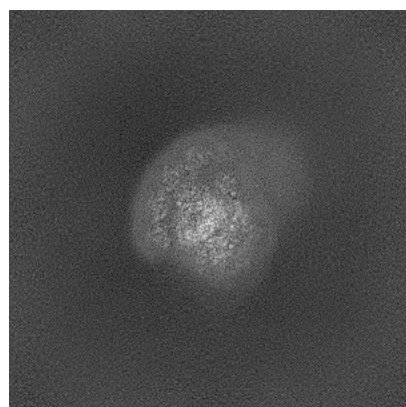


Y

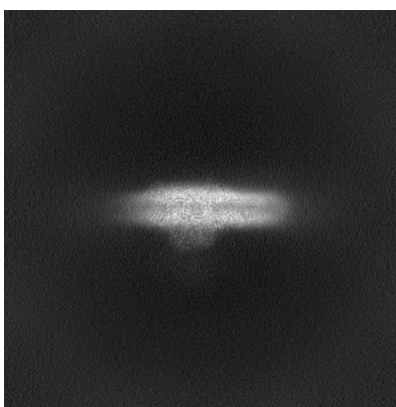


Z

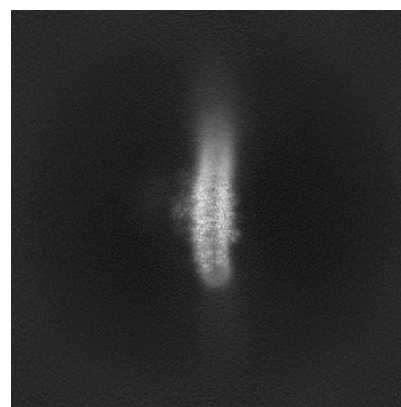
#### 6.1.2 Raw map



X



Y

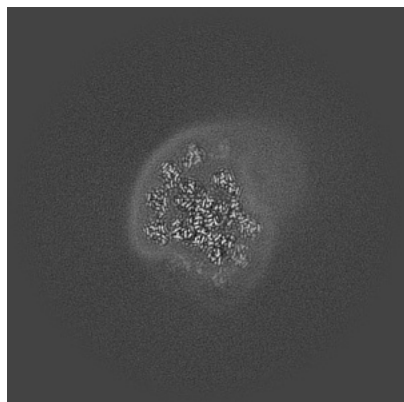


Z

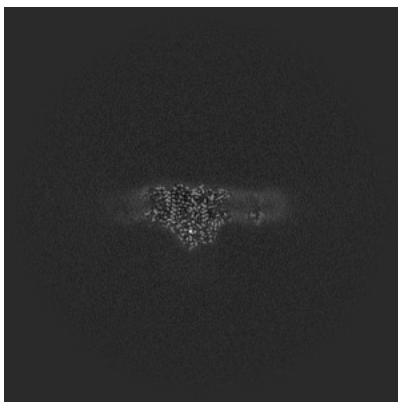
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

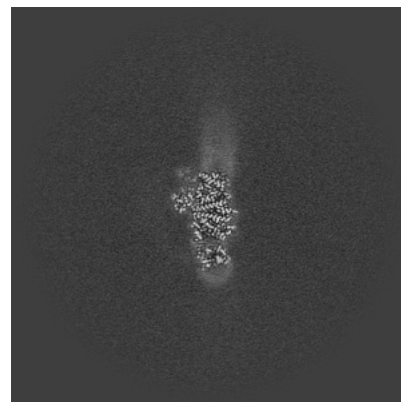
### 6.2.1 Primary map



X Index: 256

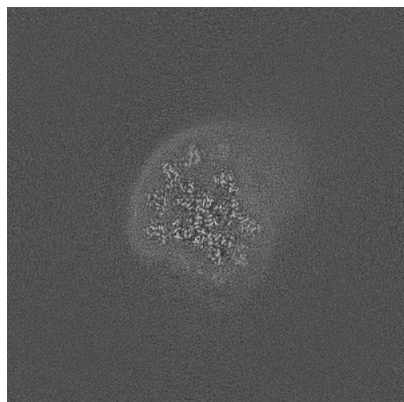


Y Index: 256

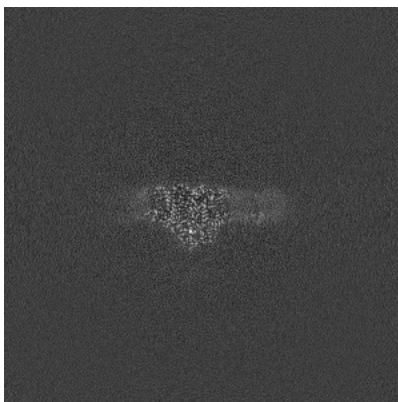


Z Index: 256

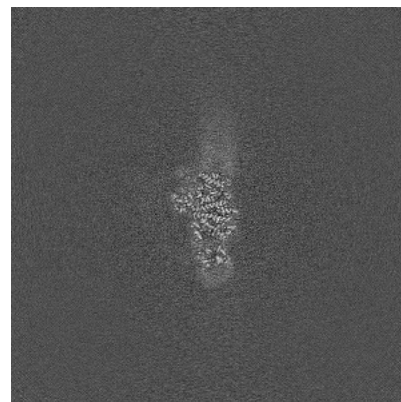
### 6.2.2 Raw map



X Index: 256



Y Index: 256

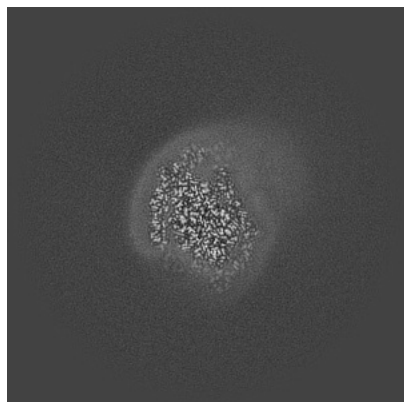


Z Index: 256

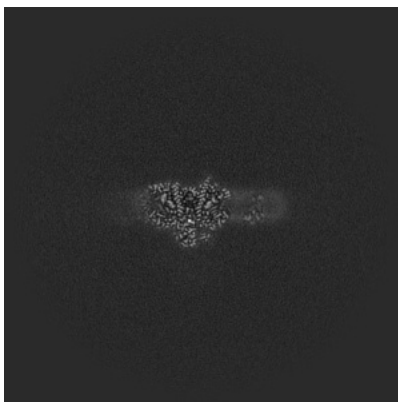
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

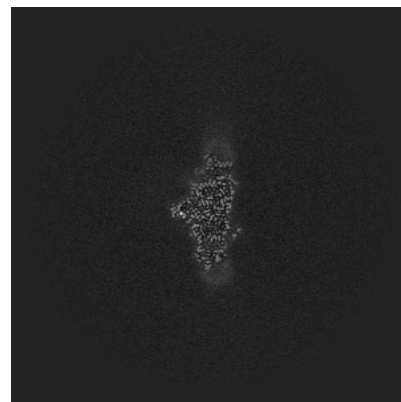
### 6.3.1 Primary map



X Index: 268

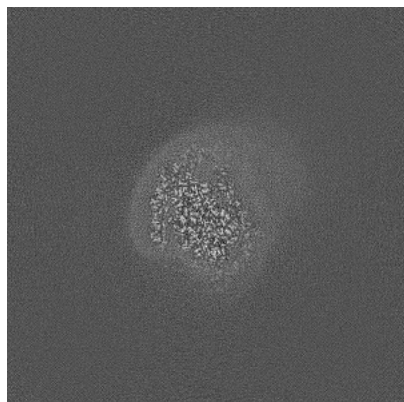


Y Index: 251



Z Index: 234

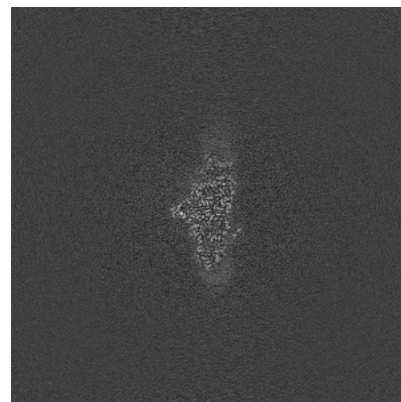
### 6.3.2 Raw map



X Index: 268



Y Index: 251

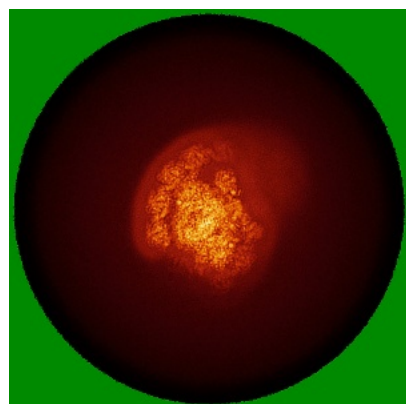


Z Index: 234

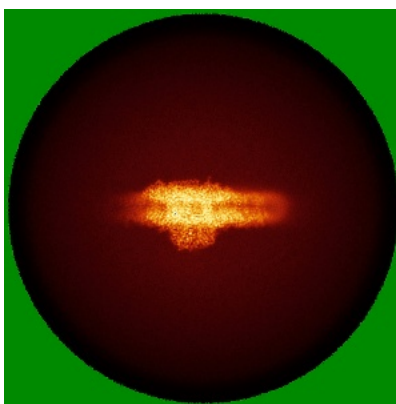
The images above show the largest variance slices of the map in three orthogonal directions.

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

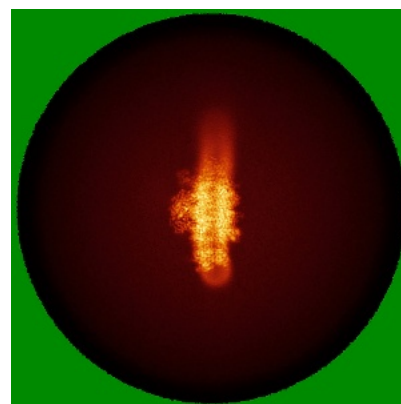
### 6.4.1 Primary map



X

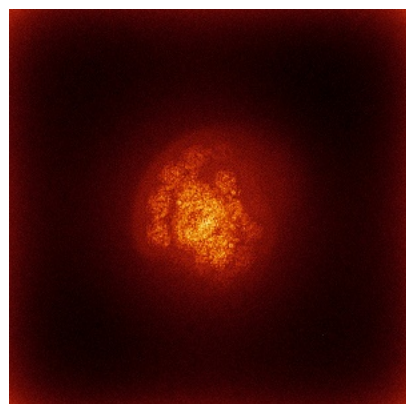


Y

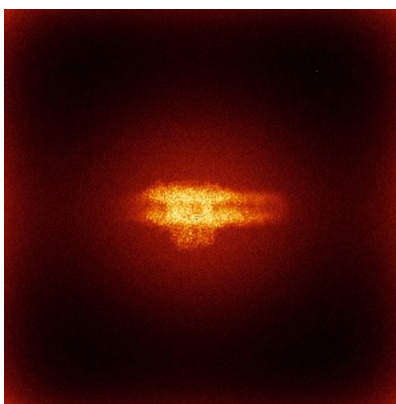


Z

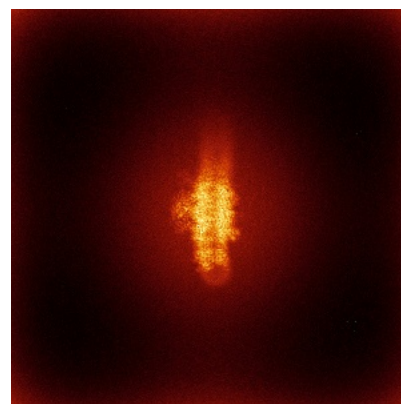
### 6.4.2 Raw map



X



Y



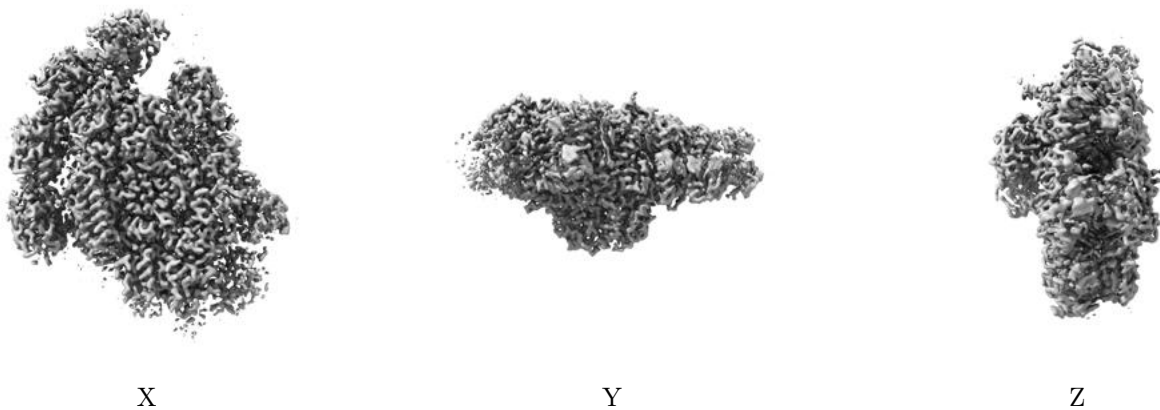
Z

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



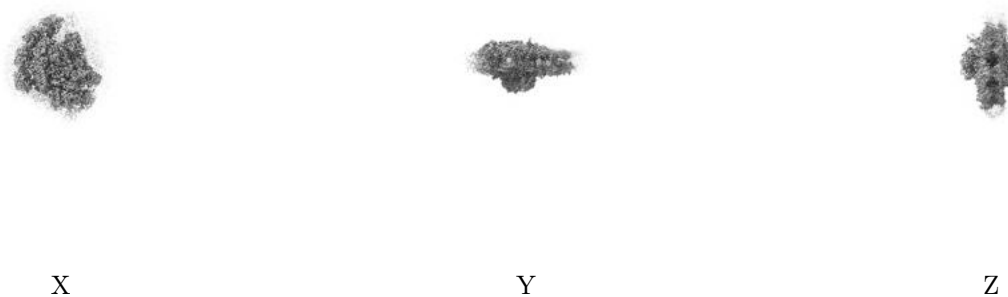
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.295. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

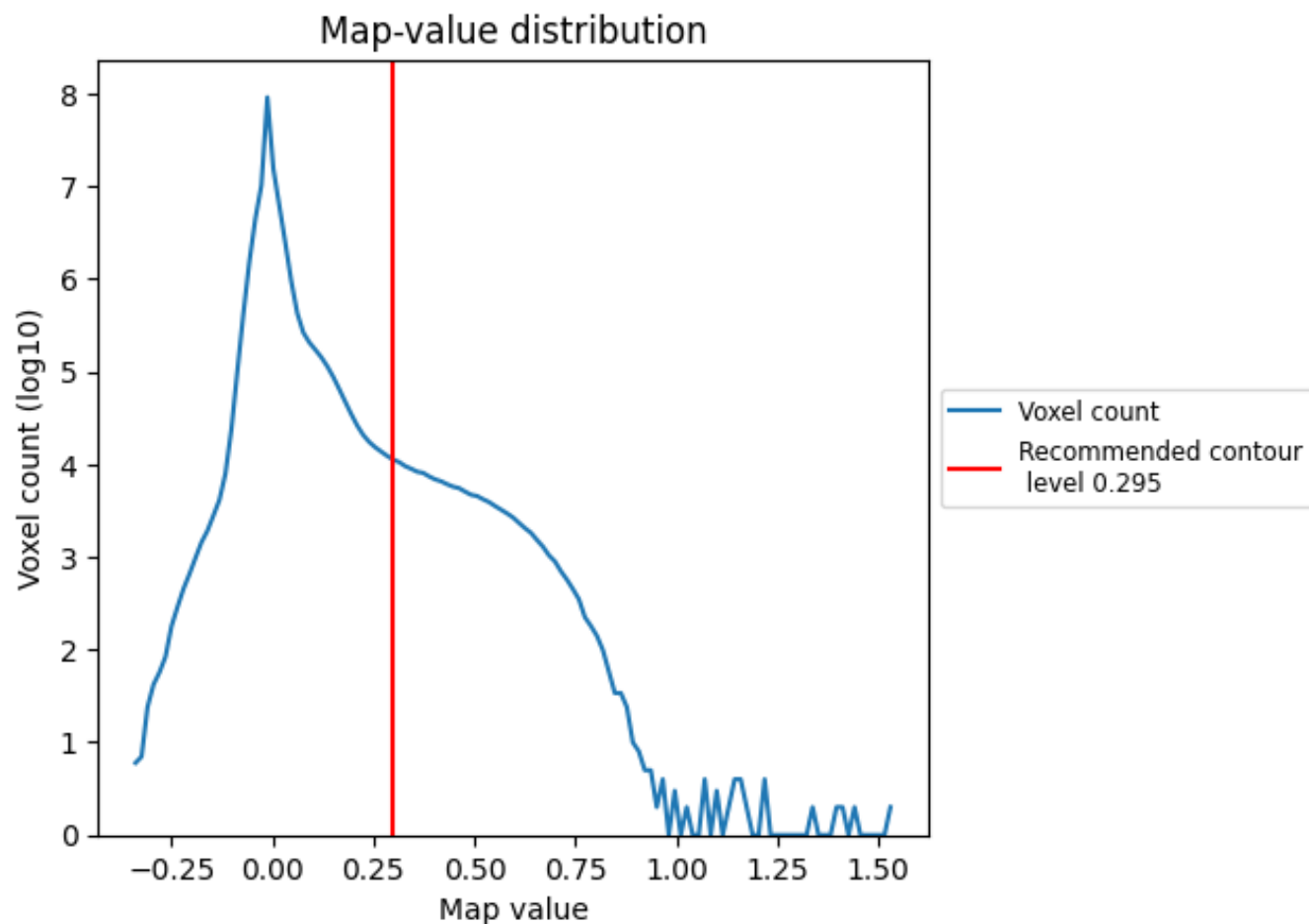
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

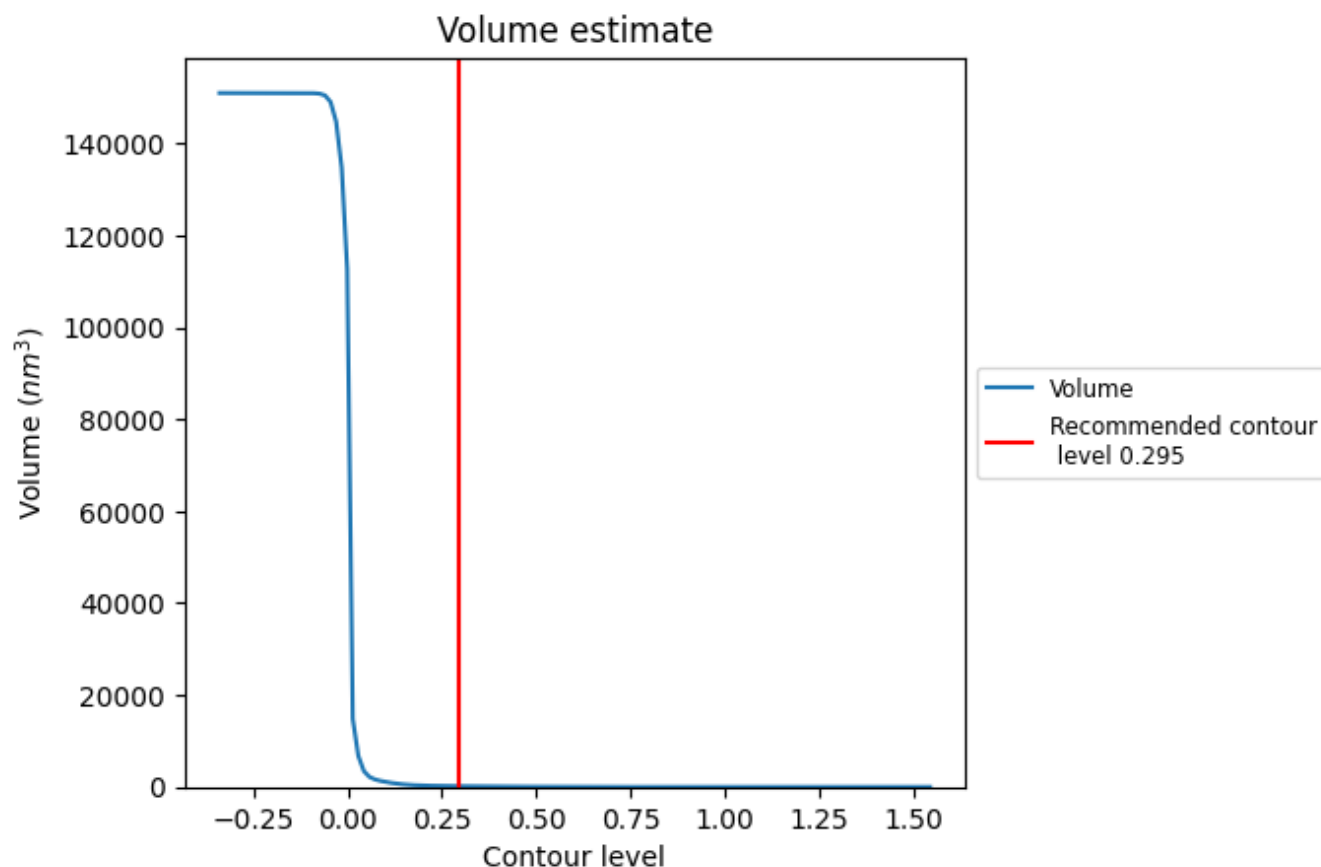
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

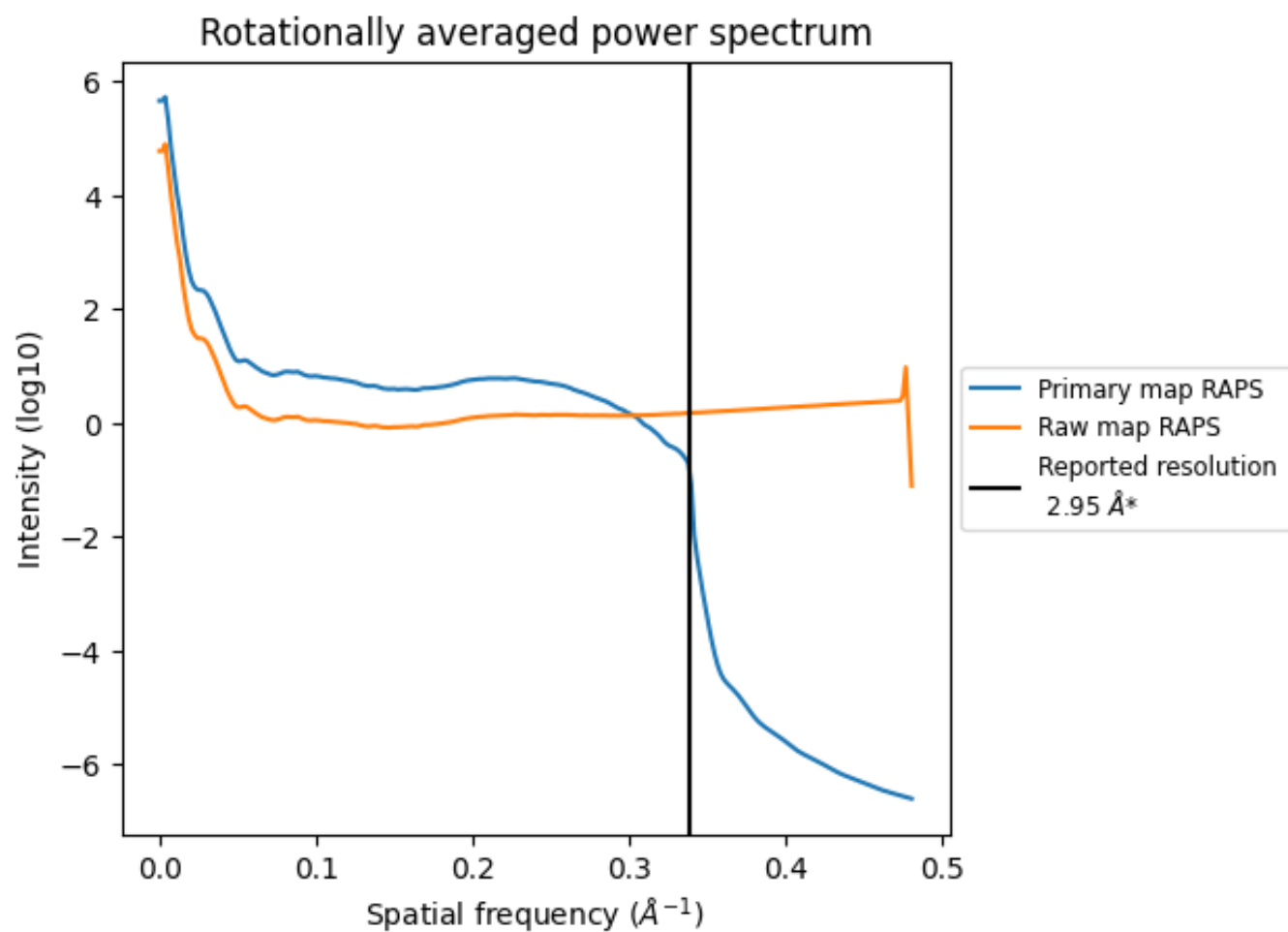
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164  $\text{nm}^3$ ; this corresponds to an approximate mass of 149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



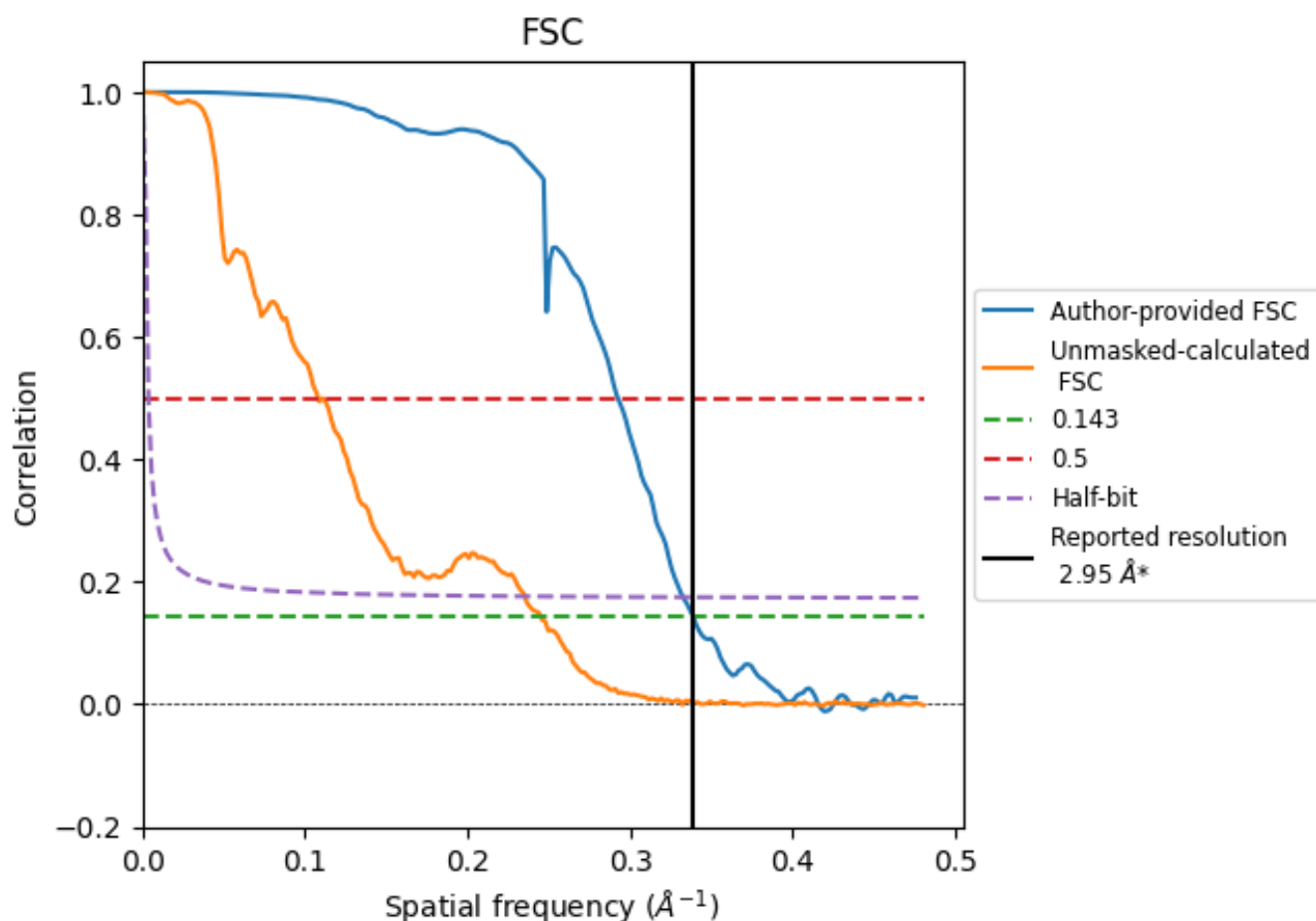
\*Reported resolution corresponds to spatial frequency of 0.339  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.339 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

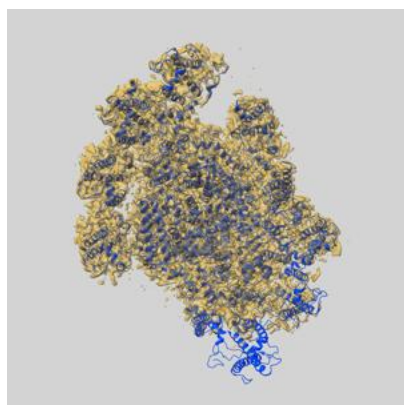
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.42	3.00
Unmasked-calculated*	4.08	9.24	4.25

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 2.95 by more than 10 %

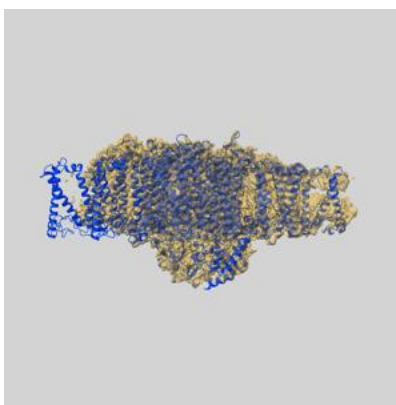
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60286 and PDB model 8ZOA. Per-residue inclusion information can be found in section 3 on page 30.

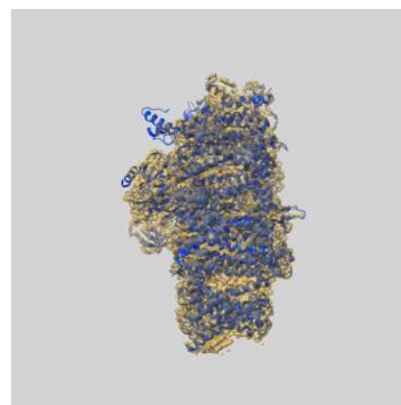
### 9.1 Map-model overlay [i](#)



X



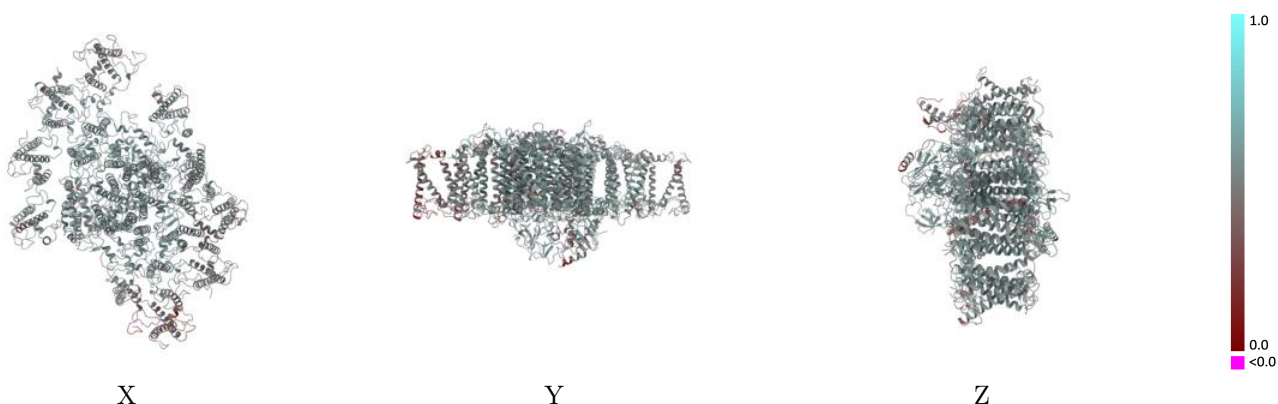
Y



Z

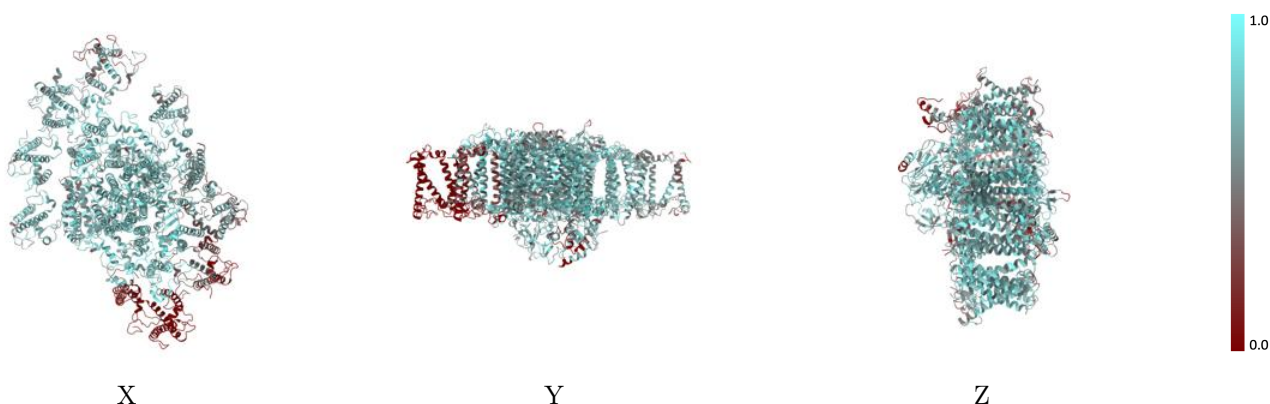
The images above show the 3D surface view of the map at the recommended contour level 0.295 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



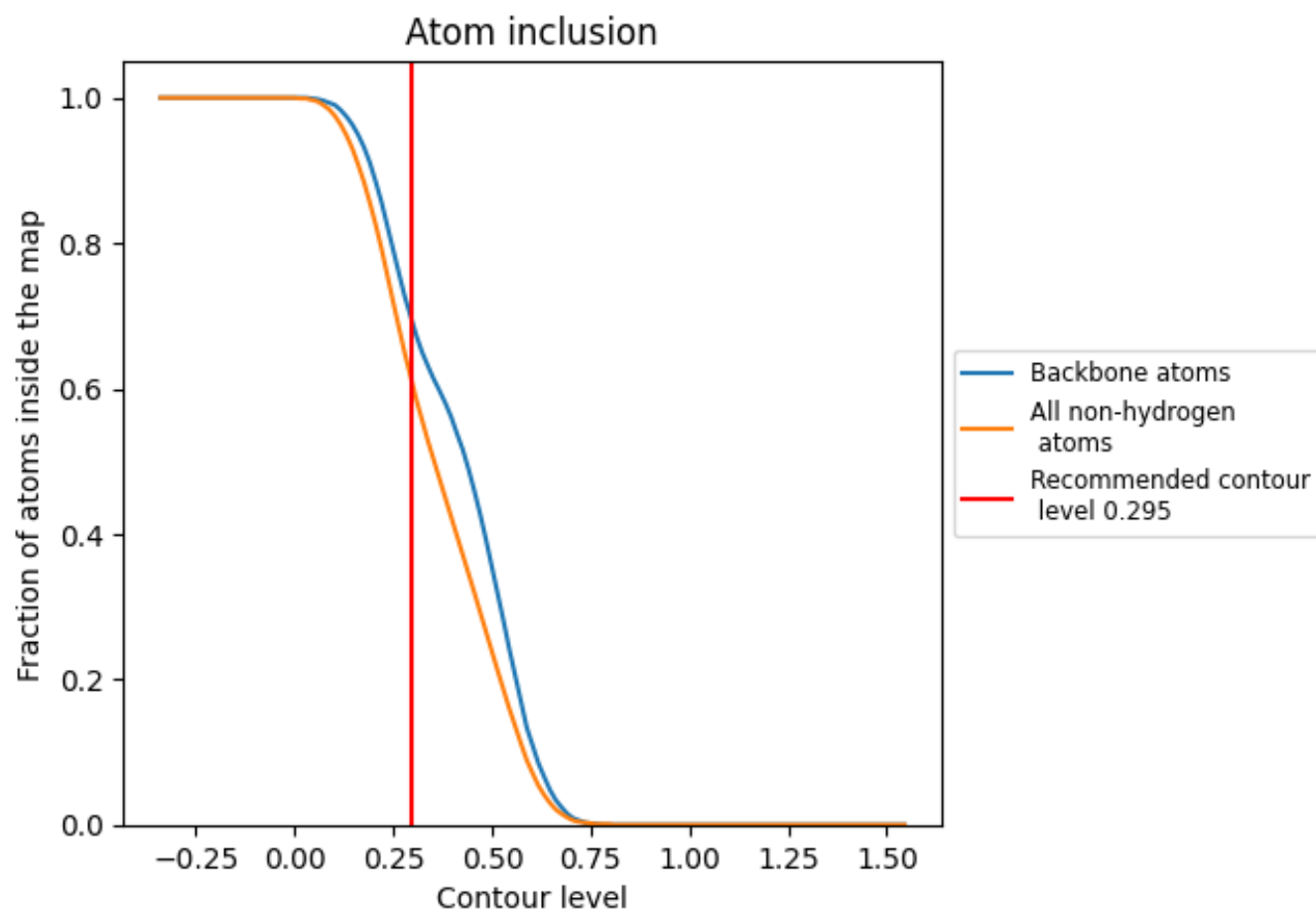
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.295).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6140</div>	<div><div></div>0.5290</div>
1	<div><div></div>0.6330</div>	<div><div></div>0.5250</div>
2	<div><div></div>0.4790</div>	<div><div></div>0.4640</div>
3	<div><div></div>0.6590</div>	<div><div></div>0.5320</div>
4	<div><div></div>0.6850</div>	<div><div></div>0.5340</div>
5	<div><div></div>0.6530</div>	<div><div></div>0.5180</div>
7	<div><div></div>0.0110</div>	<div><div></div>0.3890</div>
8	<div><div></div>0.2650</div>	<div><div></div>0.4850</div>
9	<div><div></div>0.4640</div>	<div><div></div>0.4980</div>
a	<div><div></div>0.7450</div>	<div><div></div>0.5690</div>
b	<div><div></div>0.7440</div>	<div><div></div>0.5620</div>
c	<div><div></div>0.7780</div>	<div><div></div>0.5450</div>
d	<div><div></div>0.6890</div>	<div><div></div>0.5510</div>
e	<div><div></div>0.6530</div>	<div><div></div>0.5370</div>
f	<div><div></div>0.6770</div>	<div><div></div>0.5320</div>
g	<div><div></div>0.4180</div>	<div><div></div>0.4380</div>
h	<div><div></div>0.0880</div>	<div><div></div>0.4680</div>
i	<div><div></div>0.6840</div>	<div><div></div>0.5390</div>
j	<div><div></div>0.7160</div>	<div><div></div>0.5590</div>
l	<div><div></div>0.6510</div>	<div><div></div>0.5180</div>
m	<div><div></div>0.6600</div>	<div><div></div>0.5110</div>

