



## Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 07:08 PM JST

PDB ID : 8ZOD / pdb\_00008zod  
EMDB ID : EMD-60289  
Title : Structure of the canthaxanthin mutant PSI-5VCPI supercomplex in Nan-  
nochloropsis oceanica  
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.  
Deposited on : 2024-05-28  
Resolution : 2.88 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

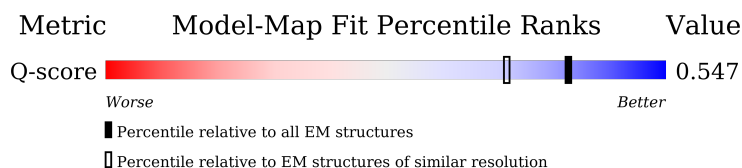
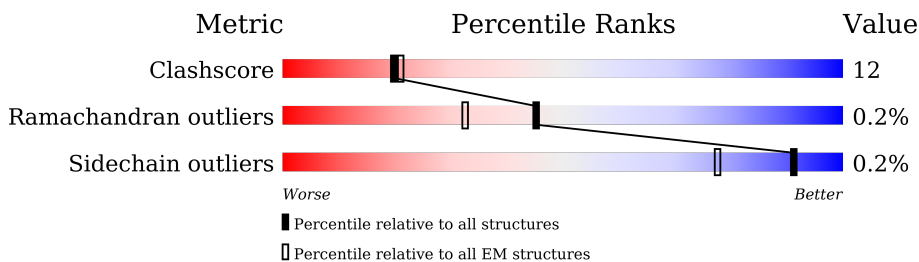
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.88 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	12111 ( 2.38 - 3.38 )

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>10%</div> <div>52%</div> <div>18%</div> <div>31%</div> </div>
2	4	202	<div> <div>10%</div> <div>72%</div> <div>11%</div> <div>17%</div> </div>
3	3	220	<div> <div>10%</div> <div>66%</div> <div>15%</div> <div>20%</div> </div>
4	2	223	<div> <div>45%</div> <div>68%</div> <div>15%</div> <div>17%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	1	208	
6	a	745	
7	b	737	
8	d	136	
9	e	67	
10	f	185	
11	i	45	
12	j	41	
13	l	172	
14	m	30	
15	g	55	
16	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
19	CLA	1	305	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	2	306	X	-	-	-
19	CLA	2	307	X	-	-	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	313	X	-	-	-
19	CLA	2	314	X	-	-	-
19	CLA	2	315	X	-	-	-
19	CLA	2	316	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	3	315	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	314	X	-	-	-
19	CLA	4	315	X	-	-	-
19	CLA	4	316	X	-	-	-
19	CLA	4	317	X	-	-	-
19	CLA	5	305	X	-	-	-
19	CLA	5	306	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	315	X	-	-	-
19	CLA	a	801	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	814	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	838	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	844	X	-	-	-
19	CLA	a	854	X	-	-	-
19	CLA	b	801	X	-	-	-
19	CLA	b	802	X	-	-	-
19	CLA	b	803	X	-	-	-
19	CLA	b	804	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	805	X	-	-	-
19	CLA	b	806	X	-	-	-
19	CLA	b	807	X	-	-	-
19	CLA	b	808	X	-	-	-
19	CLA	b	809	X	-	-	-
19	CLA	b	810	X	-	-	-
19	CLA	b	811	X	-	-	-
19	CLA	b	812	X	-	-	-
19	CLA	b	813	X	-	-	-
19	CLA	b	814	X	-	-	-
19	CLA	b	815	X	-	-	-
19	CLA	b	816	X	-	-	-
19	CLA	b	817	X	-	-	-
19	CLA	b	818	X	-	-	-
19	CLA	b	819	X	-	-	-
19	CLA	b	820	X	-	-	-
19	CLA	b	821	X	-	-	-
19	CLA	b	822	X	-	-	-
19	CLA	b	823	X	-	-	-
19	CLA	b	824	X	-	-	-
19	CLA	b	825	X	-	-	-
19	CLA	b	826	X	-	-	-
19	CLA	b	827	X	-	-	-
19	CLA	b	828	X	-	-	-
19	CLA	b	829	X	-	-	-
19	CLA	b	830	X	-	-	-
19	CLA	b	831	X	-	-	-
19	CLA	b	832	X	-	-	-
19	CLA	b	833	X	-	-	-
19	CLA	b	834	X	-	-	-
19	CLA	b	835	X	-	-	-
19	CLA	b	836	X	-	-	-
19	CLA	b	837	X	-	-	-
19	CLA	b	838	X	-	-	-
19	CLA	b	839	X	-	-	-
19	CLA	b	840	X	-	-	-
19	CLA	b	841	X	-	-	-
19	CLA	f	802	X	-	-	-
19	CLA	f	803	X	-	-	-
19	CLA	i	102	X	-	-	-
19	CLA	j	102	X	-	-	-
19	CLA	j	103	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
19	CLA	l	204	X	-	-	-
27	SF4	c	102	-	-	X	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34630 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		

- Molecule 3 is a protein called VCPI-3.

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

- Molecule 4 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 5 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called PSI subunit V.

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

- Molecule 14 is a protein called PsaM.

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

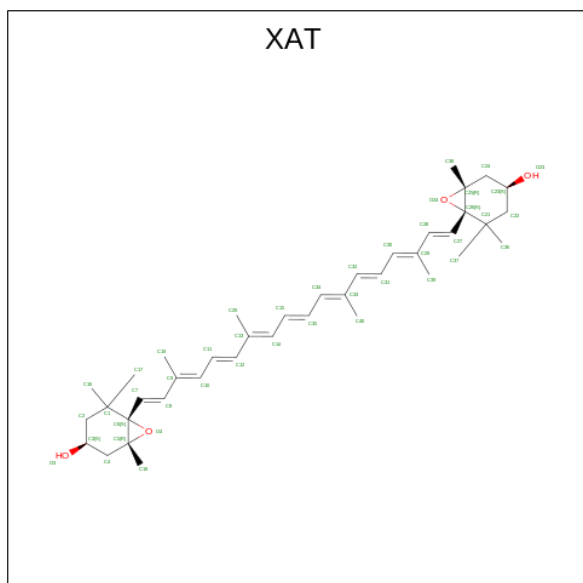
- Molecule 15 is a protein called PsaS.

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

- Molecule 16 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 17 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).



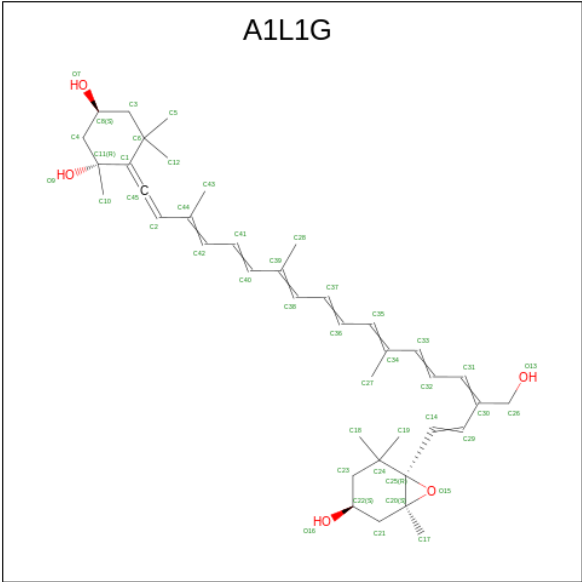
Mol	Chain	Residues	Atoms			AltConf
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	

*Continued on next page...*

*Continued from previous page...*

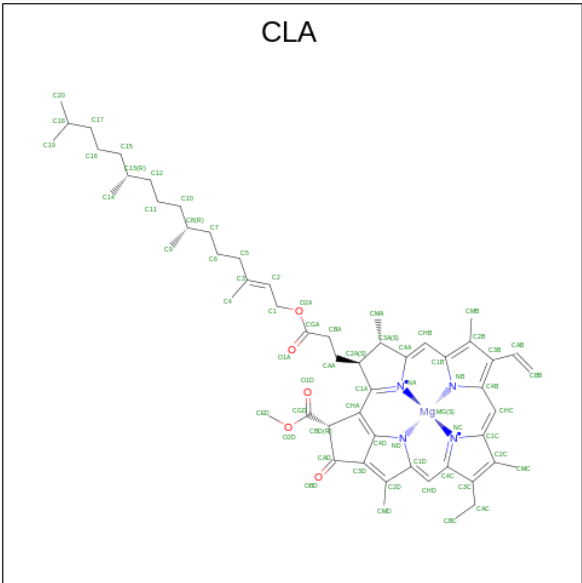
Mol	Chain	Residues	Atoms			AltConf
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	a	1	Total	C	O	0
			44	40	4	
17	j	1	Total	C	O	0
			44	40	4	

- Molecule 18 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			AltConf
18	5	1	Total	C	O	0
			45	40	5	
18	3	1	Total	C	O	0
			45	40	5	
18	3	1	Total	C	O	0
			45	40	5	
18	1	1	Total	C	O	0
			45	40	5	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	4	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
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	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
19	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

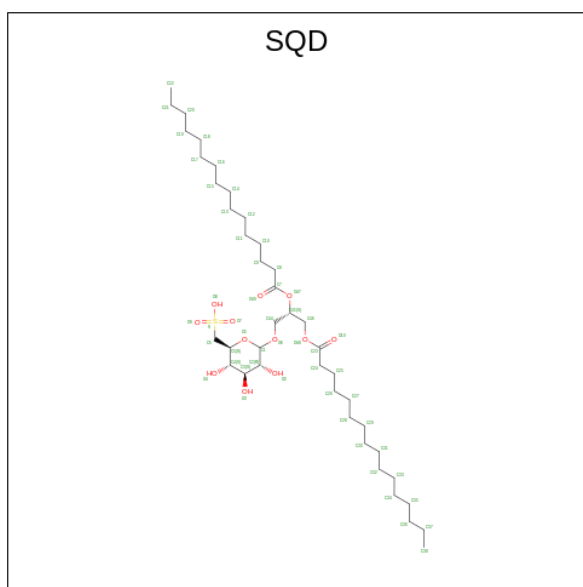
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

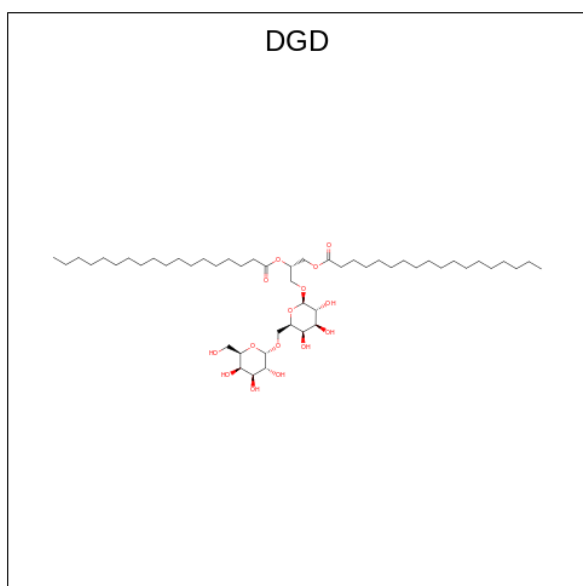
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 20 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
20	5	1	Total	C	O	S	0
			35	22	12	1	
20	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 21 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
21	4	1	Total	C	O	0
			40	25	15	

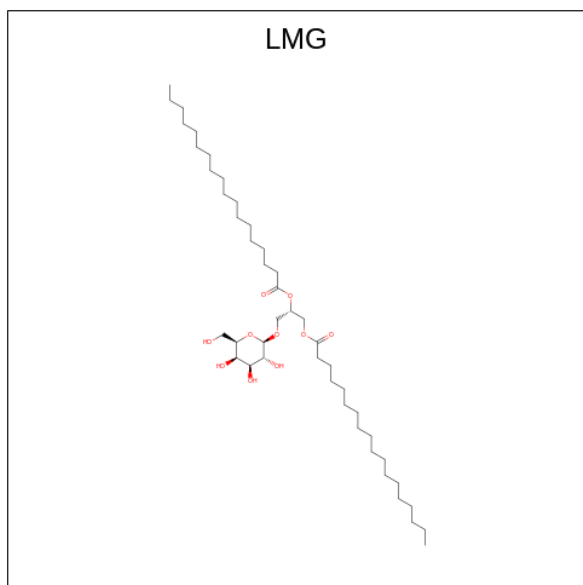
*Continued on next page...*



Continued from previous page...

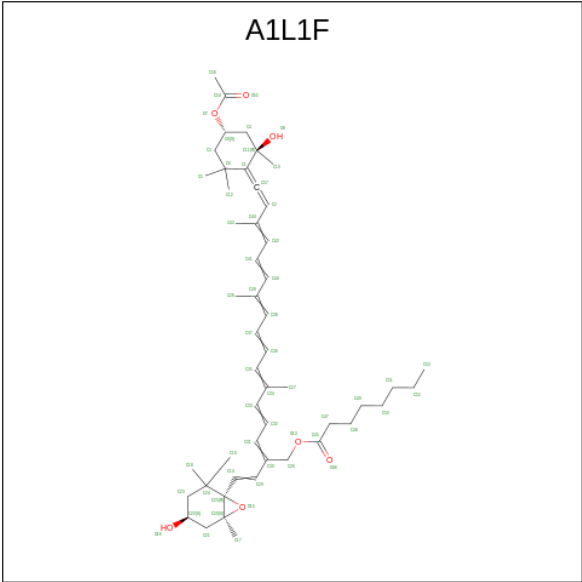
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			57	42	15	

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



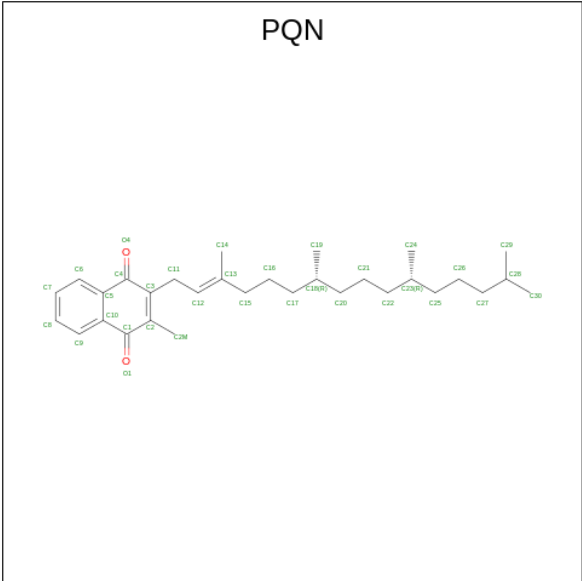
Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	C	O	0
			35	25	10	
22	a	1	Total	C	O	0
			34	24	10	
22	j	1	Total	C	O	0
			32	22	10	

- Molecule 23 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-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-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula:  $C_{50}H_{72}O_7$ ) (labeled as "Ligand of Interest" by depositor).



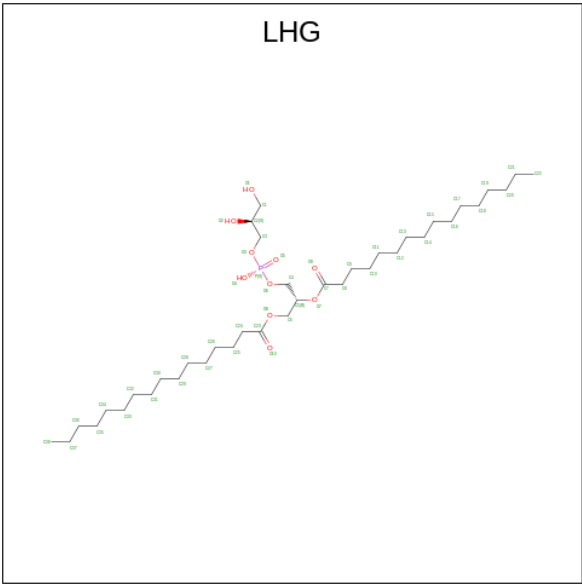
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			57	50	7	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



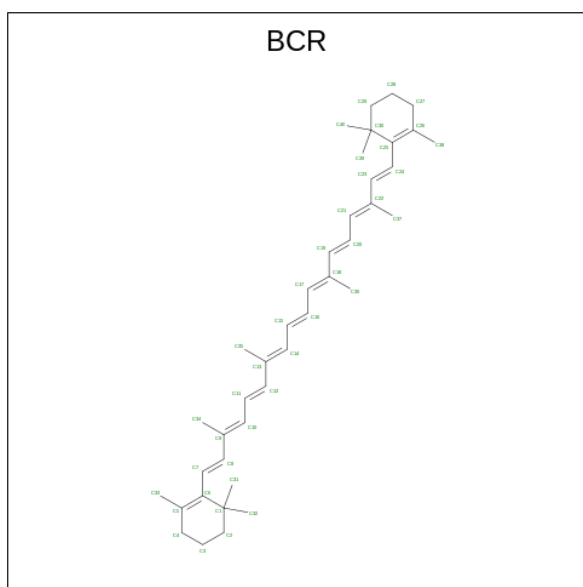
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			33	31	2	
24	b	1	Total	C	O	0
			33	31	2	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
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	
25	m	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



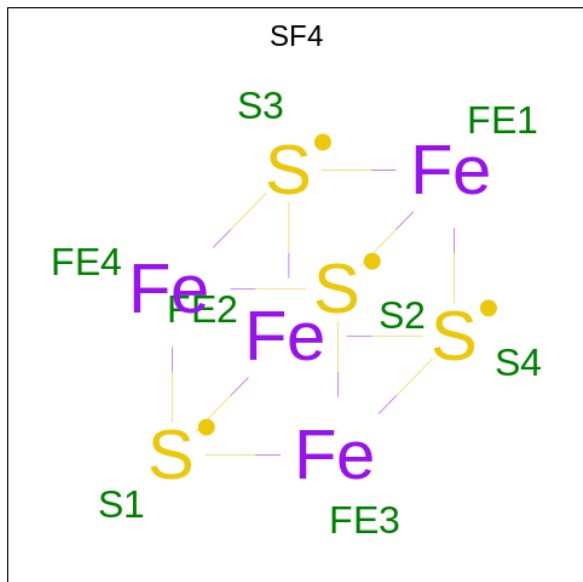
Mol	Chain	Residues	Atoms	AltConf
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C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

Continued on next page...

Continued from previous page...

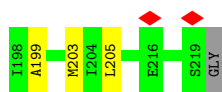
Mol	Chain	Residues	Atoms	AltConf
26	i	1	Total C 40 40	0
26	j	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	m	1	Total C 40 40	0

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).

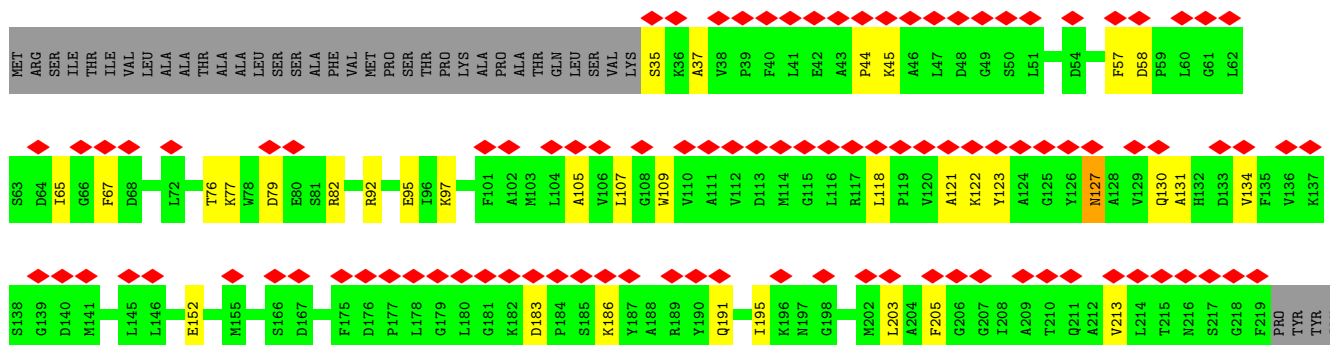
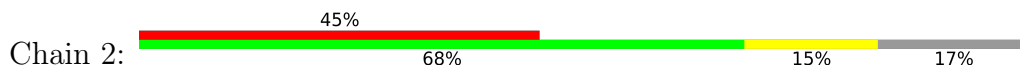


Mol	Chain	Residues	Atoms	AltConf
27	a	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0

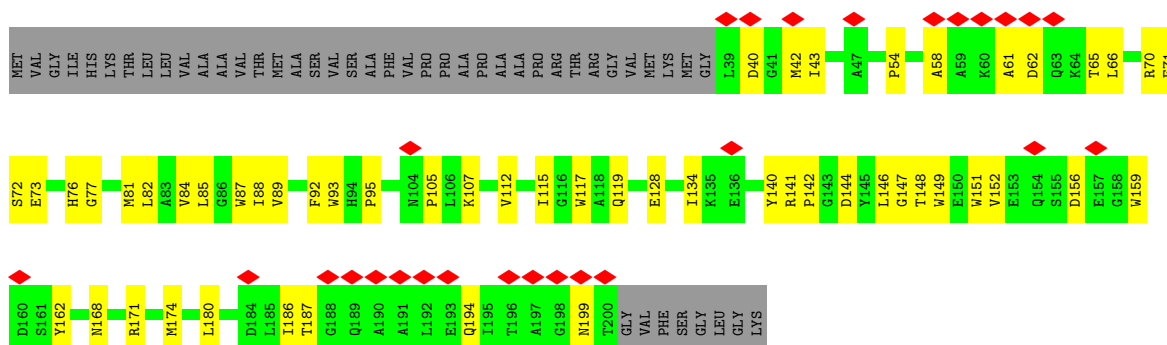




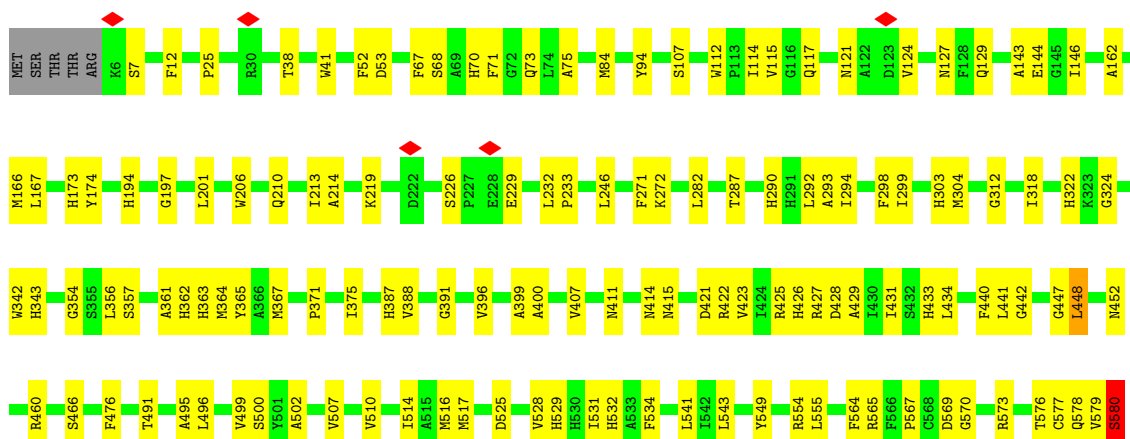
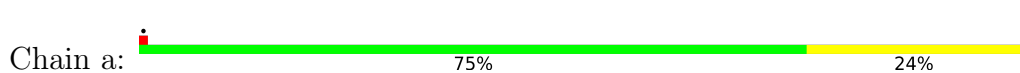
• Molecule 4: VCPI-2

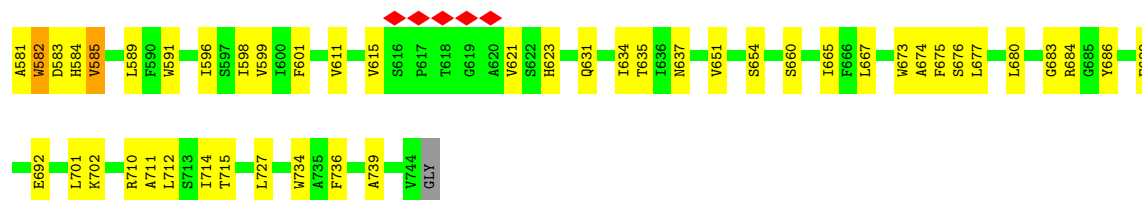


• Molecule 5: VCPI-1

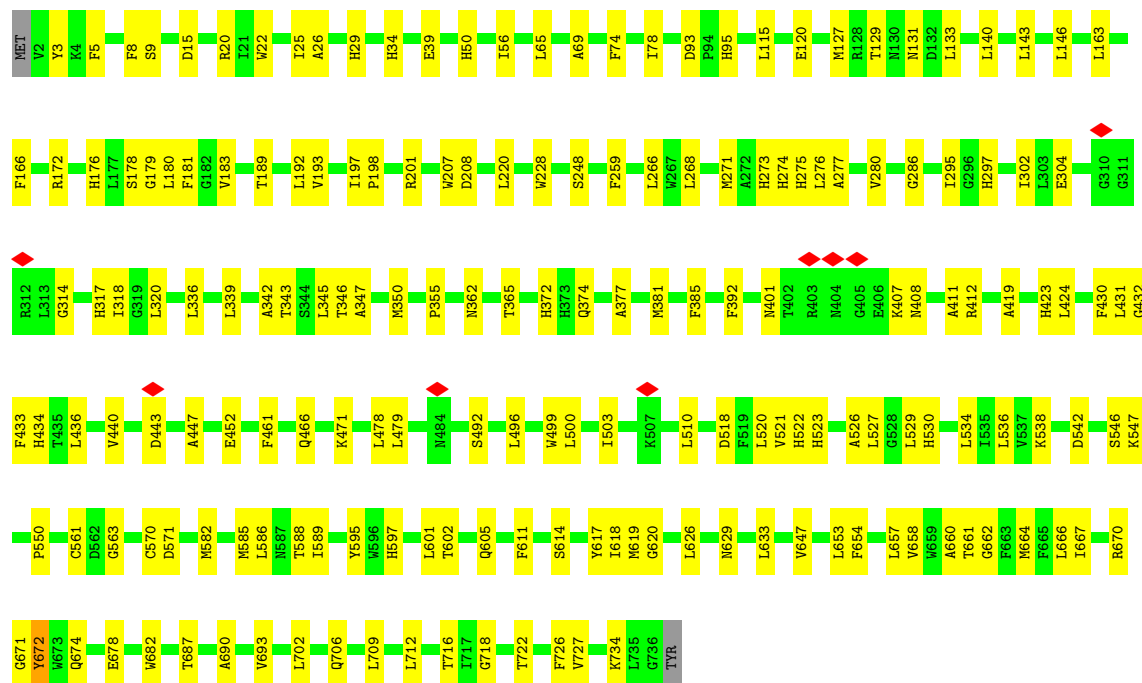
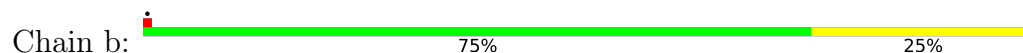


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

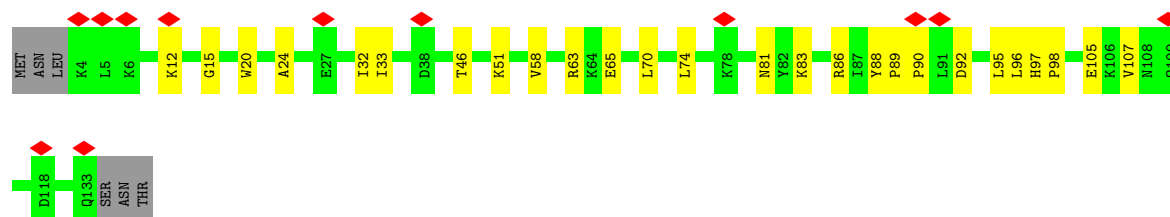
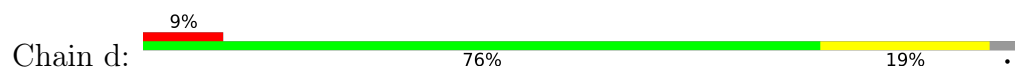




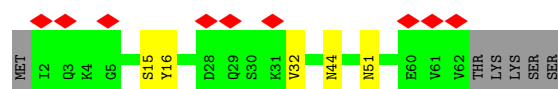
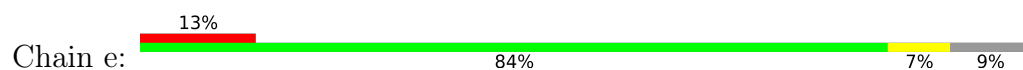
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 8: Photosystem I reaction center subunit II

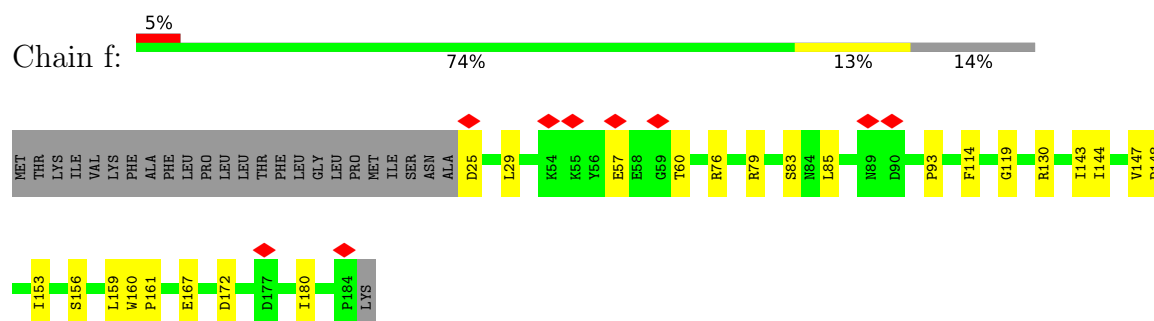


• Molecule 9: Photosystem I reaction center subunit IV

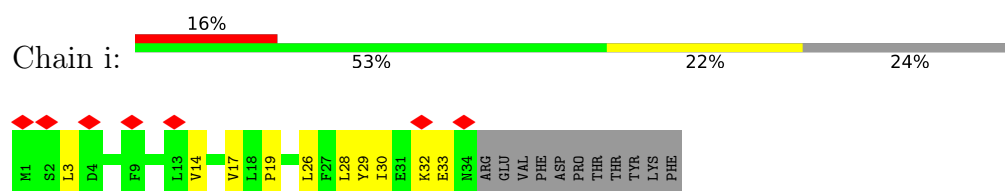




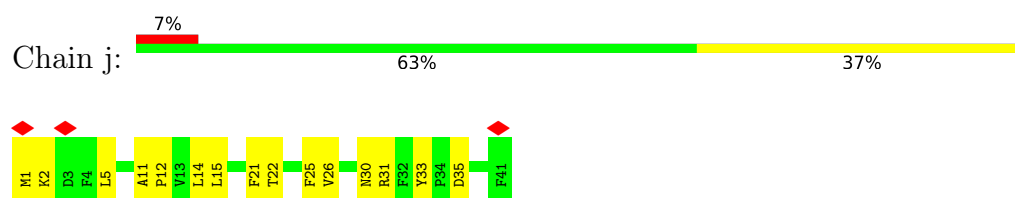
- Molecule 10: Photosystem I reaction center subunit III



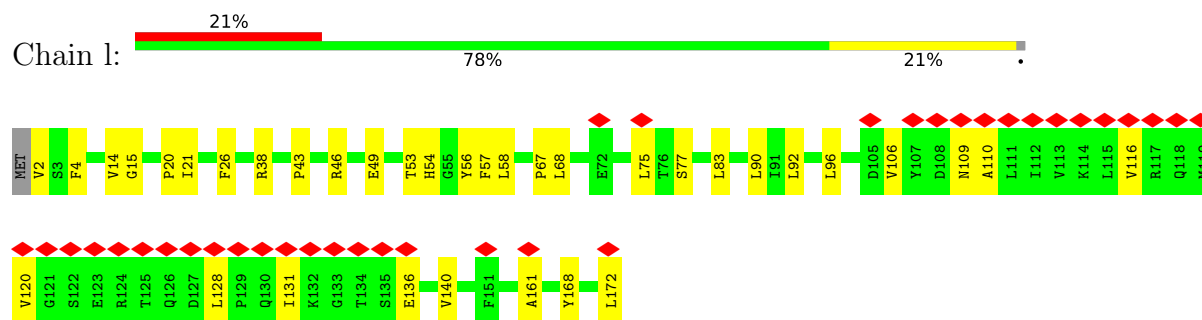
- Molecule 11: Photosystem I reaction center subunit VIII



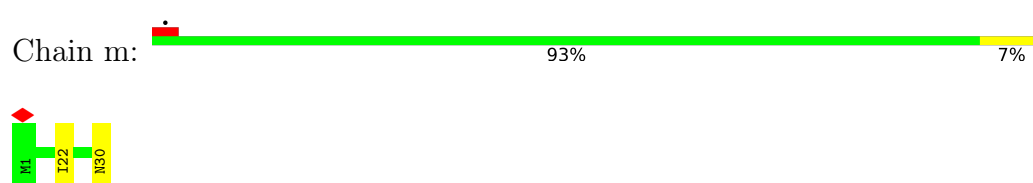
- Molecule 12: Photosystem I reaction center subunit IX



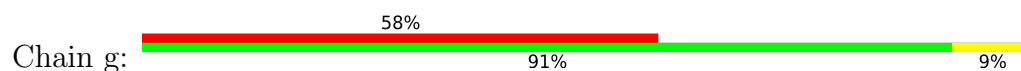
- Molecule 13: PSI subunit V

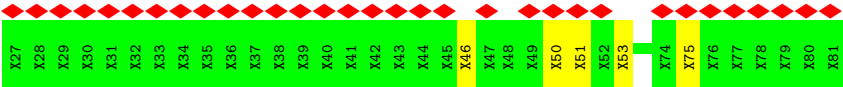


- Molecule 14: PsaM



- Molecule 15: PsaS





• Molecule 16: Photosystem I iron-sulfur center



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61296	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	1.724	Depositor
Minimum map value	-0.410	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.333	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: A1L1G, XAT, LMG, BCR, A1L1F, CLA, DGD, LHG, PQN, SF4, SQD

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	4	0.17	0/1298	0.32	0/1761
3	3	0.12	0/1350	0.27	0/1821
4	2	0.14	0/1405	0.36	0/1904
5	1	0.13	0/1293	0.33	0/1759
6	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
7	b	0.20	0/6080	0.32	1/8302 (0.0%)
8	d	0.12	0/1040	0.32	0/1402
9	e	0.09	0/502	0.20	0/681
10	f	0.14	0/1297	0.31	0/1762
11	i	0.14	0/278	0.33	0/378
12	j	0.15	0/351	0.36	0/478
13	l	0.14	0/1315	0.31	0/1796
14	m	0.09	0/210	0.28	0/288
16	c	0.13	0/606	0.34	0/822
All	All	0.20	3/24402 (0.0%)	0.32	5/33196 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	580	SER	CA-C	-7.01	1.43	1.52
6	a	581	ALA	CA-C	-5.42	1.45	1.52
6	a	582	TRP	CA-C	-5.04	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	581	ALA	N-CA-C	-8.62	102.52	113.72
6	a	448	LEU	N-CA-C	-6.13	104.15	111.69
6	a	584	HIS	N-CA-C	-5.84	106.50	113.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	672	TYR	N-CA-C	-5.61	106.28	113.23
6	a	585	VAL	N-CA-C	-5.07	105.46	112.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	37	0
2	4	1268	0	1288	22	0
3	3	1324	0	1340	22	0
4	2	1372	0	1347	22	0
5	1	1262	0	1237	39	0
6	a	5827	0	5697	140	0
7	b	5865	0	5710	152	0
8	d	1014	0	1015	20	0
9	e	494	0	495	5	0
10	f	1266	0	1262	21	0
11	i	271	0	292	12	0
12	j	339	0	342	21	0
13	l	1283	0	1278	26	0
14	m	210	0	226	2	0
15	g	275	0	62	3	0
16	c	596	0	583	19	0
17	1	88	0	112	6	0
17	2	220	0	280	24	0
17	3	176	0	224	15	0
17	4	220	0	280	28	0
17	5	132	0	168	18	0
17	a	44	0	56	4	0
17	j	44	0	56	5	0
18	1	45	0	0	1	0
18	3	90	0	0	0	0
18	5	45	0	0	1	0
19	1	547	0	508	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	544	0	452	10	0
19	3	458	0	378	10	0
19	4	613	0	522	30	0
19	5	563	0	472	22	0
19	a	2579	0	2562	139	0
19	b	2475	0	2536	129	0
19	f	117	0	115	1	0
19	i	62	0	63	5	0
19	j	100	0	86	8	0
19	l	148	0	123	3	0
20	1	45	0	54	2	0
20	5	35	0	34	1	0
21	4	40	0	38	11	0
21	b	57	0	72	5	0
22	2	35	0	40	2	0
22	a	34	0	38	11	0
22	j	32	0	34	6	0
23	1	57	0	0	2	0
24	a	33	0	46	3	0
24	b	33	0	46	2	0
25	a	75	0	93	6	0
25	b	31	0	32	0	0
25	m	46	0	65	3	0
26	a	160	0	224	14	0
26	b	320	0	448	30	0
26	f	80	0	112	13	0
26	i	40	0	56	2	0
26	j	40	0	56	8	0
26	l	80	0	112	13	0
26	m	40	0	56	1	0
27	a	8	0	0	0	0
27	c	16	0	0	2	0
All	All	34630	0	34141	839	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 12.

All (839) 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)
2:4:193:ALA:HB1	21:4:318:DGD:HE62	1.13	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:193:ALA:HB1	21:4:318:DGD:C6E	1.84	1.07
21:4:318:DGD:O4E	21:4:318:DGD:O5E	1.61	1.06
17:5:302:XAT:H12	19:5:307:CLA:HAB	1.53	0.90
17:2:303:XAT:H32	19:2:308:CLA:HAB	1.52	0.89
19:a:806:CLA:O1A	19:a:814:CLA:HBA1	1.81	0.79
6:a:531:ILE:HD12	19:a:801:CLA:H172	1.63	0.78
19:b:826:CLA:HMA1	26:b:847:BCR:H17C	1.66	0.78
2:4:193:ALA:CB	21:4:318:DGD:HE62	2.07	0.77
17:4:303:XAT:H12	19:4:308:CLA:HAB	1.67	0.75
17:2:303:XAT:H181	19:2:314:CLA:HBB1	1.70	0.73
19:1:312:CLA:HHC	19:1:312:CLA:HBB1	1.69	0.73
19:4:317:CLA:H2A	21:4:318:DGD:HE62	1.73	0.71
5:1:43:ILE:O	5:1:70:ARG:NH2	2.25	0.70
26:a:847:BCR:H362	26:a:848:BCR:H21C	1.73	0.70
19:b:807:CLA:H151	19:b:829:CLA:HBB2	1.74	0.70
19:b:834:CLA:H72	26:b:847:BCR:H391	1.72	0.69
12:j:22:THR:HA	12:j:25:PHE:CE1	2.28	0.69
7:b:273:HIS:HD1	19:b:818:CLA:HAB	1.58	0.69
10:f:167:GLU:HG3	10:f:172:ASP:HB3	1.73	0.69
6:a:569:ASP:OD2	6:a:573:ARG:NH2	2.27	0.68
19:a:804:CLA:HED1	12:j:15:LEU:HD22	1.76	0.68
1:5:179:LEU:HD12	10:f:159:LEU:HD11	1.75	0.67
5:1:194:GLN:HG3	5:1:199:ASN:HB3	1.77	0.67
6:a:363:HIS:ND1	19:a:819:CLA:OBD	2.26	0.67
7:b:295:ILE:HG13	19:b:821:CLA:HED1	1.77	0.67
17:4:302:XAT:H14	19:4:310:CLA:H12	1.76	0.67
12:j:31:ARG:HD3	17:j:101:XAT:H222	1.78	0.66
5:1:70:ARG:NH1	5:1:73:GLU:OE1	2.28	0.66
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.66
17:4:303:XAT:H193	19:4:308:CLA:H142	1.78	0.66
5:1:146:LEU:HD13	19:a:844:CLA:H91	1.77	0.65
7:b:9:SER:HB2	21:b:851:DGD:HE62	1.78	0.65
11:i:29:TYR:HA	11:i:32:LYS:HE2	1.79	0.65
19:4:317:CLA:HAA2	21:4:318:DGD:HE5	1.77	0.65
19:b:824:CLA:HBB1	19:b:838:CLA:H151	1.79	0.65
10:f:25:ASP:N	10:f:29:LEU:O	2.30	0.65
6:a:112:TRP:HB3	17:j:101:XAT:H373	1.77	0.64
19:a:834:CLA:H142	26:b:848:BCR:H15C	1.79	0.64
7:b:304:GLU:HG2	7:b:318:ILE:HG13	1.78	0.64
17:3:305:XAT:H32	19:3:313:CLA:HAB	1.80	0.64
19:a:808:CLA:HMB2	26:j:104:BCR:HC8	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:197:GLY:O	6:a:201:LEU:HB2	1.97	0.64
12:j:21:PHE:HA	19:j:103:CLA:HBB2	1.80	0.64
10:f:79:ARG:NH1	12:j:35:ASP:O	2.30	0.63
7:b:336:LEU:HD21	19:b:830:CLA:HAB	1.78	0.63
19:b:814:CLA:H121	19:b:819:CLA:H72	1.79	0.63
6:a:114:ILE:HB	17:j:101:XAT:H372	1.81	0.63
7:b:129:THR:HG22	7:b:131:ASN:H	1.63	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
6:a:684:ARG:H	7:b:570:CYS:HB2	1.64	0.63
7:b:424:LEU:HD13	7:b:534:LEU:HA	1.81	0.63
1:5:130:PHE:CE1	17:5:302:XAT:O24	2.52	0.63
7:b:115:LEU:HA	7:b:365:THR:HG22	1.80	0.63
17:4:305:XAT:H363	17:3:301:XAT:H10	1.80	0.63
6:a:356:LEU:HD11	19:a:820:CLA:H71	1.79	0.63
6:a:589:LEU:HD21	19:a:831:CLA:HBC1	1.81	0.62
12:j:26:VAL:HG11	26:j:104:BCR:H24C	1.81	0.62
17:4:304:XAT:H32	19:4:313:CLA:HAB	1.80	0.62
6:a:362:HIS:HA	6:a:365:TYR:CE1	2.33	0.62
8:d:12:LYS:HB2	8:d:51:LYS:HB3	1.82	0.62
19:b:831:CLA:HAB	19:b:838:CLA:HBB2	1.82	0.62
8:d:86:ARG:HB2	8:d:96:LEU:HD11	1.82	0.62
6:a:298:PHE:CE1	19:a:822:CLA:HAB	2.35	0.61
1:5:225:ILE:HG22	19:5:314:CLA:HAB	1.82	0.61
17:5:302:XAT:H162	19:5:307:CLA:H2	1.82	0.61
20:5:316:SQD:H2	17:4:301:XAT:H373	1.82	0.61
7:b:15:ASP:HB3	7:b:20:ARG:HB2	1.82	0.61
19:4:317:CLA:H2A	21:4:318:DGD:C6E	2.30	0.61
7:b:660:ALA:HB3	19:b:804:CLA:HBB2	1.83	0.61
6:a:298:PHE:HE1	19:a:822:CLA:HAB	1.64	0.61
8:d:88:TYR:HB2	8:d:92:ASP:HB2	1.81	0.61
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.61
19:b:832:CLA:HBC3	26:f:804:BCR:H362	1.83	0.61
23:1:304:A1L1F:C2	19:a:844:CLA:H11	2.31	0.61
4:2:76:THR:O	4:2:82:ARG:NH1	2.33	0.60
6:a:162:ALA:O	6:a:166:MET:HG2	2.00	0.60
3:3:92:HIS:HB3	3:3:197:MET:SD	2.42	0.60
19:a:818:CLA:C3D	22:a:853:LMG:HC91	2.30	0.60
7:b:561:CYS:SG	7:b:563:GLY:N	2.71	0.60
6:a:167:LEU:HD11	19:a:810:CLA:H193	1.83	0.60
3:3:199:ALA:O	3:3:203:MET:HG3	2.01	0.60
5:1:186:ILE:HG13	5:1:187:THR:HG23	1.83	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:833:CLA:HBC2	19:a:840:CLA:HMC2	1.83	0.60
7:b:412:ARG:NH2	19:b:831:CLA:O1D	2.35	0.60
4:2:44:PRO:HG3	4:2:58:ASP:HB3	1.83	0.60
6:a:53:ASP:OD2	6:a:343:HIS:NE2	2.35	0.60
1:5:111:TRP:NE1	19:5:308:CLA:O1A	2.33	0.59
5:1:72:SER:O	5:1:76:HIS:ND1	2.28	0.59
13:l:38:ARG:O	13:l:46:ARG:NH2	2.35	0.59
18:1:301:A1L1G:C18	19:1:306:CLA:HAC2	2.32	0.59
6:a:429:ALA:O	6:a:433:HIS:ND1	2.31	0.59
2:4:185:PHE:CZ	17:4:303:XAT:H30	2.37	0.59
3:3:83:TYR:OH	3:3:163:ARG:NH1	2.35	0.59
6:a:121:ASN:HB3	6:a:129:GLN:HB3	1.83	0.59
2:4:170:MET:HE1	19:4:313:CLA:H43	1.84	0.59
19:a:804:CLA:ND	12:j:12:PRO:HG3	2.17	0.59
17:2:303:XAT:H363	19:2:308:CLA:H2	1.84	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
19:3:312:CLA:H42	26:a:848:BCR:H272	1.85	0.58
6:a:507:VAL:HG22	6:a:517:MET:HG3	1.85	0.58
7:b:74:PHE:O	7:b:78:ILE:HG12	2.04	0.58
7:b:29:HIS:ND1	19:b:807:CLA:O1A	2.28	0.58
19:a:826:CLA:HBA1	19:a:830:CLA:H193	1.86	0.58
7:b:69:ALA:HB2	7:b:133:LEU:HB2	1.86	0.58
17:5:301:XAT:H14	19:5:309:CLA:H12	1.86	0.58
19:a:820:CLA:H92	19:a:830:CLA:H91	1.84	0.58
1:5:112:LEU:HD22	19:5:307:CLA:H12	1.86	0.58
3:3:87:GLU:OE2	3:3:163:ARG:NH2	2.31	0.57
6:a:517:MET:HE1	6:a:623:HIS:NE2	2.19	0.57
19:b:804:CLA:CGA	19:b:804:CLA:H3A	2.34	0.57
19:b:805:CLA:H18	11:i:14:VAL:HG22	1.86	0.57
1:5:155:VAL:HG21	19:5:309:CLA:HAA2	1.86	0.57
7:b:39:GLU:HB3	7:b:163:LEU:HD11	1.87	0.57
26:b:843:BCR:H23C	26:b:850:BCR:H323	1.86	0.57
26:f:801:BCR:HC32	19:j:102:CLA:H43	1.86	0.57
19:a:818:CLA:C1D	22:a:853:LMG:H291	2.34	0.57
7:b:93:ASP:OD1	7:b:95:HIS:ND1	2.33	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
6:a:107:SER:HB2	6:a:124:VAL:HG11	1.85	0.57
6:a:7:SER:H	6:a:12:PHE:HE2	1.53	0.57
19:a:802:CLA:CGA	19:a:802:CLA:H3A	2.35	0.57
22:a:853:LMG:H112	22:a:853:LMG:C9	2.35	0.57
22:a:853:LMG:H112	22:a:853:LMG:O8	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:693:VAL:HG11	19:b:801:CLA:HAB	1.87	0.57
3:3:86:ARG:NH1	3:3:89:GLU:OE1	2.38	0.56
3:3:182:PHE:HZ	19:3:313:CLA:HED3	1.70	0.56
6:a:70:HIS:ND1	19:a:814:CLA:OBD	2.31	0.56
6:a:292:LEU:HD21	19:a:818:CLA:CAB	2.34	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
6:a:651:VAL:HG22	6:a:739:ALA:HB3	1.87	0.56
7:b:178:SER:HB3	7:b:286:GLY:HA3	1.86	0.56
6:a:114:ILE:HG13	6:a:115:VAL:HG13	1.86	0.56
6:a:324:GLY:HA3	25:a:846:LHG:HC32	1.87	0.56
7:b:582:MET:HG3	7:b:712:LEU:HD21	1.87	0.56
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.56
19:a:818:CLA:CHD	22:a:853:LMG:H291	2.36	0.56
19:a:841:CLA:H72	26:f:801:BCR:H17C	1.88	0.56
19:b:822:CLA:HHB	19:b:823:CLA:H2	1.88	0.56
11:i:26:LEU:HD13	26:l:205:BCR:HC8	1.86	0.56
8:d:97:HIS:HB3	8:d:98:PRO:HD3	1.86	0.56
3:3:48:LEU:HD13	3:3:51:LEU:HD12	1.87	0.56
4:2:35:SER:OG	4:2:37:ALA:O	2.22	0.56
17:2:303:XAT:C36	19:2:308:CLA:H2	2.35	0.56
6:a:598:ILE:HG13	19:a:801:CLA:H192	1.86	0.56
6:a:734:TRP:NE1	19:a:829:CLA:O1A	2.36	0.56
13:l:54:HIS:HA	13:l:57:PHE:CE2	2.41	0.56
6:a:213:ILE:HG23	6:a:233:PRO:HB3	1.87	0.55
6:a:290:HIS:HB2	19:a:819:CLA:C1B	2.37	0.55
6:a:660:SER:HB2	7:b:447:ALA:HB1	1.88	0.55
2:4:185:PHE:CE2	17:4:303:XAT:H30	2.42	0.55
6:a:651:VAL:HG21	6:a:736:PHE:HA	1.88	0.55
19:a:841:CLA:H92	26:f:801:BCR:H15C	1.88	0.55
7:b:521:VAL:HG21	7:b:595:TYR:HB2	1.89	0.55
19:a:822:CLA:HBC3	19:a:828:CLA:H172	1.88	0.55
5:1:115:ILE:O	5:1:119:GLN:NE2	2.40	0.55
9:e:32:VAL:HG11	16:c:35:LYS:HD3	1.89	0.55
13:l:92:LEU:HB3	26:l:205:BCR:H401	1.88	0.55
19:a:854:CLA:H112	12:j:14:LEU:HD22	1.88	0.55
6:a:441:LEU:HB3	6:a:534:PHE:HB2	1.88	0.55
5:1:88:ILE:HG22	5:1:92:PHE:HE1	1.71	0.55
19:a:825:CLA:H12	26:a:849:BCR:H14C	1.88	0.55
7:b:5:PHE:HB2	11:i:30:ILE:HA	1.89	0.55
16:c:15:THR:HG22	16:c:28:MET:HG3	1.89	0.55
18:5:303:A1L1G:C41	19:5:312:CLA:HMC1	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:136:VAL:HG22	19:4:312:CLA:HMA1	1.87	0.54
6:a:388:VAL:HG12	6:a:596:ILE:HG23	1.89	0.54
7:b:317:HIS:HB3	7:b:320:LEU:HD12	1.89	0.54
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.54
6:a:197:GLY:HA3	19:a:814:CLA:HBB1	1.89	0.54
6:a:573:ARG:HG3	16:c:78:GLY:HA3	1.90	0.54
6:a:219:LYS:HD3	6:a:246:LEU:HB3	1.90	0.54
6:a:591:TRP:HE1	19:b:804:CLA:C1D	2.21	0.54
8:d:105:GLU:HG2	16:c:19:ARG:HB3	1.88	0.54
6:a:210:GLN:HA	6:a:214:ALA:HB3	1.89	0.54
6:a:667:LEU:HD11	7:b:619:MET:HB2	1.89	0.54
19:a:820:CLA:HAB	19:a:820:CLA:H8	1.90	0.54
7:b:22:TRP:CG	7:b:706:GLN:HE22	2.26	0.54
19:b:806:CLA:HBA1	19:b:814:CLA:HBA1	1.87	0.54
2:4:140:SER:OG	12:j:1:MET:SD	2.57	0.53
7:b:140:LEU:HG	26:b:845:BCR:H382	1.90	0.53
2:4:121:LEU:HD23	2:4:124:ILE:HD12	1.90	0.53
6:a:702:LYS:HB3	10:f:130:ARG:HD3	1.89	0.53
7:b:443:ASP:OD1	7:b:617:TYR:HB2	2.08	0.53
19:b:824:CLA:HBB2	19:b:841:CLA:H52	1.90	0.53
12:j:14:LEU:HD21	22:j:105:LMG:H141	1.89	0.53
2:4:83:ILE:HD11	17:4:302:XAT:H362	1.90	0.53
19:a:829:CLA:H101	26:j:104:BCR:H341	1.89	0.53
7:b:633:LEU:HD22	7:b:726:PHE:HA	1.90	0.53
5:1:61:ALA:HB1	5:1:65:THR:HB	1.90	0.53
19:a:835:CLA:O2D	19:a:835:CLA:H2A	2.09	0.53
7:b:355:PRO:HG3	19:b:819:CLA:HBA1	1.90	0.53
19:a:825:CLA:HMA3	19:a:844:CLA:HAB	1.91	0.53
19:4:317:CLA:O2D	21:4:318:DGD:HE61	2.09	0.53
19:a:831:CLA:H42	25:a:845:LHG:H251	1.90	0.53
19:a:810:CLA:HAB	19:j:102:CLA:HMD2	1.91	0.53
7:b:419:ALA:O	7:b:423:HIS:ND1	2.40	0.53
19:b:830:CLA:H42	21:b:851:DGD:HB42	1.91	0.53
15:g:51:UNK:O	15:g:53:UNK:N	2.42	0.53
6:a:411:ASN:ND2	6:a:414:ASN:OD1	2.37	0.52
7:b:709:LEU:HD11	21:b:851:DGD:HB41	1.90	0.52
19:b:801:CLA:H101	19:b:801:CLA:HBB1	1.91	0.52
8:d:63:ARG:NH2	8:d:65:GLU:OE1	2.41	0.52
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.91	0.52
2:4:81:CYS:HB3	2:4:178:GLY:HA3	1.91	0.52
19:a:809:CLA:CHC	19:a:810:CLA:HMD2	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:l:38:ARG:NH1	13:l:49:GLU:OE1	2.40	0.52
7:b:661:THR:O	7:b:664:MET:HB3	2.08	0.52
8:d:95:LEU:HD22	15:g:75:UNK:HA	1.91	0.52
1:5:143:TYR:OH	19:5:310:CLA:OBD	2.23	0.52
19:a:834:CLA:H151	24:b:842:PQN:H202	1.91	0.52
7:b:718:GLY:O	7:b:722:THR:HG22	2.09	0.52
10:f:85:LEU:HD13	10:f:93:PRO:HB3	1.92	0.52
4:2:121:ALA:O	4:2:122:LYS:HG2	2.10	0.52
16:c:11:CYS:SG	16:c:39:ILE:HG13	2.50	0.52
7:b:208:ASP:OD1	7:b:208:ASP:N	2.43	0.52
17:5:302:XAT:C16	19:5:307:CLA:H2	2.39	0.51
3:3:79:GLY:O	3:3:158:ARG:NH1	2.43	0.51
6:a:577:CYS:O	7:b:671:GLY:HA3	2.11	0.51
19:a:827:CLA:H93	19:a:840:CLA:H52	1.92	0.51
16:c:58:CYS:SG	16:c:63:LEU:HA	2.51	0.51
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.51
8:d:33:ILE:HG22	8:d:58:VAL:HG22	1.92	0.51
19:a:818:CLA:HHC	19:a:818:CLA:HBB1	1.93	0.51
7:b:342:ALA:O	7:b:346:THR:HG23	2.11	0.51
7:b:662:GLY:O	7:b:666:LEU:HG	2.11	0.51
2:4:193:ALA:O	21:4:318:DGD:O6E	2.28	0.51
19:b:837:CLA:HBC3	26:f:804:BCR:H401	1.91	0.51
5:1:77:GLY:O	5:1:81:MET:HG3	2.09	0.51
5:1:85:LEU:HB3	19:1:308:CLA:HMC2	1.92	0.51
6:a:396:VAL:HG11	6:a:589:LEU:HG	1.91	0.51
7:b:189:THR:HG21	7:b:276:LEU:HB2	1.91	0.51
7:b:274:HIS:HB2	19:b:818:CLA:C1B	2.41	0.51
19:b:837:CLA:HBC3	26:f:804:BCR:H292	1.91	0.51
23:1:304:A1L1F:C56	25:a:846:LHG:H241	2.41	0.51
7:b:26:ALA:HA	19:b:830:CLA:H43	1.93	0.51
19:5:312:CLA:CGA	19:5:312:CLA:H3A	2.41	0.51
7:b:273:HIS:ND1	19:b:818:CLA:HAB	2.25	0.51
10:f:160:TRP:CD1	10:f:161:PRO:HD3	2.46	0.51
22:a:853:LMG:H131	22:a:853:LMG:H292	1.93	0.51
10:f:143:ILE:HG13	10:f:144:ILE:HG13	1.92	0.51
7:b:602:THR:HG21	7:b:611:PHE:HB2	1.93	0.51
17:4:303:XAT:C16	19:4:308:CLA:H2	2.41	0.50
3:3:93:CYS:HB3	3:3:193:GLY:HA3	1.93	0.50
7:b:179:GLY:O	7:b:183:VAL:HB	2.10	0.50
6:a:431:ILE:HG13	6:a:549:TYR:HE1	1.74	0.50
6:a:460:ARG:NH2	19:a:835:CLA:O1D	2.44	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:434:HIS:CD2	26:b:852:BCR:H333	2.46	0.50
17:5:301:XAT:H193	19:5:310:CLA:HBA2	1.94	0.50
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.50
19:b:824:CLA:HAB	19:b:831:CLA:HMD1	1.93	0.50
19:b:807:CLA:H52	21:b:851:DGD:HB72	1.92	0.50
13:l:106:VAL:H	13:l:140:VAL:HG23	1.77	0.50
6:a:440:PHE:HE2	19:a:839:CLA:HAB	1.76	0.50
19:b:833:CLA:HBB2	26:f:801:BCR:HC41	1.94	0.50
4:2:77:LYS:O	4:2:79:ASP:N	2.43	0.49
6:a:422:ARG:O	6:a:426:HIS:ND1	2.41	0.49
19:b:812:CLA:H72	19:b:813:CLA:HBC3	1.92	0.49
4:2:107:LEU:HB3	19:2:310:CLA:HMC2	1.94	0.49
5:1:112:VAL:HB	5:1:117:TRP:NE1	2.27	0.49
19:a:818:CLA:CHD	19:a:819:CLA:HBB2	2.43	0.49
7:b:25:ILE:HG12	26:l:205:BCR:H312	1.94	0.49
6:a:565:ARG:HG2	6:a:715:THR:HG21	1.93	0.49
22:a:853:LMG:C11	22:a:853:LMG:HC92	2.41	0.49
16:c:13:GLY:O	16:c:38:GLN:NE2	2.44	0.49
16:c:17:CYS:HB3	27:c:102:SF4:S4	2.52	0.49
6:a:615:VAL:HG22	6:a:621:VAL:HG22	1.95	0.49
7:b:3:TYR:HB2	11:i:33:GLU:HA	1.95	0.49
7:b:266:LEU:HD22	19:b:818:CLA:HBA1	1.94	0.49
19:4:309:CLA:HAC1	19:4:316:CLA:HAB	1.95	0.49
4:2:183:ASP:O	4:2:186:LYS:N	2.44	0.49
7:b:518:ASP:OD2	7:b:595:TYR:OH	2.23	0.49
19:a:818:CLA:O1A	22:a:853:LMG:O10	2.30	0.49
7:b:478:LEU:HG	7:b:479:LEU:HG	1.93	0.49
16:c:17:CYS:SG	16:c:18:VAL:N	2.85	0.49
6:a:423:VAL:HA	6:a:426:HIS:CE1	2.47	0.49
19:a:803:CLA:H2	7:b:657:LEU:HD22	1.95	0.49
1:5:171:GLU:HG3	19:5:311:CLA:NB	2.28	0.49
3:3:78:VAL:HG12	3:3:78:VAL:O	2.13	0.49
6:a:554:ARG:HB2	7:b:678:GLU:OE1	2.13	0.49
19:a:802:CLA:H41	7:b:436:LEU:HD22	1.95	0.49
7:b:722:THR:HG23	19:b:803:CLA:O1D	2.11	0.49
26:b:852:BCR:H23C	12:j:33:TYR:CD2	2.47	0.49
15:g:46:UNK:O	15:g:50:UNK:N	2.45	0.49
3:3:203:MET:HE2	17:3:305:XAT:O4	2.13	0.49
6:a:712:LEU:N	24:a:843:PQN:O4	2.45	0.49
7:b:443:ASP:OD1	7:b:618:ILE:N	2.46	0.48
13:l:43:PRO:HD3	13:l:136:GLU:CD	2.38	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:292:LEU:HD12	19:a:816:CLA:HMC3	1.95	0.48
6:a:425:ARG:NH2	8:d:15:GLY:O	2.44	0.48
7:b:407:LYS:HB3	7:b:411:ALA:HB3	1.95	0.48
7:b:492:SER:HA	7:b:496:LEU:HD12	1.94	0.48
17:5:304:XAT:C10	19:5:315:CLA:HBC3	2.43	0.48
3:3:145:ILE:O	3:3:149:ILE:HG12	2.13	0.48
19:a:832:CLA:HAB	19:a:840:CLA:HBB2	1.96	0.48
7:b:595:TYR:CZ	19:b:836:CLA:HBC3	2.49	0.48
7:b:65:LEU:HD11	26:b:845:BCR:H281	1.95	0.48
7:b:526:ALA:O	7:b:530:HIS:ND1	2.37	0.48
7:b:597:HIS:CE1	7:b:601:LEU:HD11	2.48	0.48
9:e:51:ASN:CG	16:c:61:ASP:HB2	2.39	0.48
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.48
19:3:308:CLA:HED2	19:3:308:CLA:H2A	1.94	0.48
6:a:674:ALA:HB3	19:a:802:CLA:HBB2	1.94	0.48
2:4:184:ALA:HA	19:4:315:CLA:HBB1	1.95	0.48
19:3:308:CLA:H2A	19:3:308:CLA:CED	2.44	0.48
6:a:637:ASN:HB2	7:b:653:LEU:HD11	1.94	0.48
19:b:811:CLA:H202	13:l:90:LEU:HD22	1.96	0.48
2:4:159:ASN:C	2:4:161:ALA:H	2.20	0.48
3:3:81:ASP:N	3:3:81:ASP:OD1	2.46	0.48
5:1:144:ASP:OD2	5:1:148:THR:OG1	2.23	0.48
19:a:820:CLA:H203	19:a:828:CLA:H3A	1.96	0.48
7:b:670:ARG:C	7:b:672:TYR:H	2.22	0.48
26:b:852:BCR:H23C	12:j:33:TYR:HD2	1.78	0.48
11:i:26:LEU:HD22	26:l:205:BCR:H323	1.94	0.48
7:b:8:PHE:HB2	7:b:34:HIS:CG	2.49	0.48
19:b:824:CLA:H2A	19:b:824:CLA:HED3	1.95	0.48
8:d:95:LEU:HD11	8:d:98:PRO:HD2	1.95	0.48
19:i:102:CLA:H142	19:i:102:CLA:H111	1.61	0.48
13:l:109:ASN:OD1	13:l:110:ALA:N	2.35	0.48
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.48
4:2:92:ARG:NH1	4:2:95:GLU:OE1	2.47	0.48
5:1:88:ILE:HG22	5:1:92:PHE:CE1	2.49	0.48
7:b:271:MET:O	7:b:275:HIS:ND1	2.47	0.48
7:b:432:GLY:HA2	7:b:527:LEU:HD22	1.96	0.48
19:a:825:CLA:H71	19:a:840:CLA:H62	1.96	0.48
7:b:176:HIS:O	7:b:180:LEU:HB3	2.14	0.48
19:b:839:CLA:HAB	24:b:842:PQN:H172	1.96	0.48
19:b:841:CLA:H141	19:b:841:CLA:H161	1.74	0.48
6:a:127:ASN:HD21	10:f:60:THR:HG21	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:290:HIS:HB2	19:a:819:CLA:CHB	2.44	0.47
11:i:26:LEU:HB3	26:l:205:BCR:H323	1.96	0.47
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.47
6:a:514:ILE:HD11	6:a:621:VAL:HG13	1.96	0.47
19:b:840:CLA:H13	26:i:101:BCR:H19C	1.95	0.47
17:2:305:XAT:H35	17:2:305:XAT:H401	1.74	0.47
6:a:38:THR:HB	6:a:710:ARG:HG3	1.97	0.47
6:a:114:ILE:HG23	6:a:115:VAL:HG22	1.96	0.47
7:b:166:PHE:O	7:b:172:ARG:NH2	2.46	0.47
7:b:297:HIS:HB3	7:b:302:ILE:HD11	1.97	0.47
7:b:538:LYS:O	7:b:542:ASP:HB2	2.14	0.47
26:b:845:BCR:H311	26:b:845:BCR:HC8	1.97	0.47
25:m:101:LHG:H321	25:m:101:LHG:H291	1.66	0.47
5:1:42:MET:HE1	5:1:66:LEU:HD22	1.95	0.47
7:b:586:LEU:HD21	7:b:716:THR:HG23	1.96	0.47
19:b:825:CLA:H193	19:b:825:CLA:H141	1.95	0.47
6:a:400:ALA:HB2	6:a:585:VAL:HG11	1.96	0.47
22:a:853:LMG:C9	22:a:853:LMG:C11	2.91	0.47
19:b:822:CLA:CHB	19:b:823:CLA:H2	2.44	0.47
19:2:316:CLA:C2C	22:2:317:LMG:H111	2.44	0.47
6:a:354:GLY:HA2	6:a:391:GLY:HA2	1.97	0.47
7:b:127:MET:HE1	26:b:845:BCR:H282	1.97	0.47
7:b:452:GLU:OE2	10:f:76:ARG:NE	2.42	0.47
19:b:802:CLA:H93	19:b:802:CLA:H112	1.70	0.47
19:b:811:CLA:HBA2	13:l:67:PRO:HG3	1.97	0.47
19:b:838:CLA:H101	19:b:838:CLA:H13	1.78	0.47
12:j:2:LYS:O	22:j:105:LMG:HC61	2.13	0.47
1:5:130:PHE:HE1	17:5:302:XAT:O24	1.94	0.47
19:4:317:CLA:CGD	21:4:318:DGD:HE61	2.45	0.47
6:a:502:ALA:HB2	6:a:516:MET:HE2	1.97	0.47
6:a:712:LEU:HD21	24:a:843:PQN:H151	1.96	0.47
19:a:841:CLA:H61	19:b:833:CLA:H42	1.95	0.47
7:b:143:LEU:HD23	7:b:146:LEU:HD12	1.97	0.47
7:b:181:PHE:HE2	19:b:820:CLA:HAB	1.78	0.47
19:b:831:CLA:HAB	19:b:838:CLA:CBB	2.44	0.47
19:b:839:CLA:H192	19:b:839:CLA:H162	1.73	0.47
8:d:20:TRP:CZ2	13:l:14:VAL:HG12	2.50	0.47
12:j:5:LEU:HB3	22:j:105:LMG:HC72	1.96	0.47
4:2:118:LEU:N	19:2:310:CLA:OBD	2.47	0.47
6:a:287:THR:HG23	19:a:820:CLA:HMA3	1.96	0.47
19:a:829:CLA:HBB1	19:a:829:CLA:HMB1	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:372:HIS:HB2	19:b:828:CLA:C1B	2.45	0.47
7:b:412:ARG:HH21	19:b:831:CLA:CGD	2.27	0.47
7:b:433:PHE:HZ	26:f:801:BCR:H372	1.80	0.47
7:b:687:THR:HG23	7:b:690:ALA:HB3	1.97	0.47
19:b:811:CLA:H71	13:l:83:LEU:HG	1.97	0.47
8:d:83:LYS:HG2	8:d:98:PRO:HG2	1.97	0.47
6:a:686:TYR:OH	19:a:802:CLA:OBD	2.22	0.47
19:a:827:CLA:H13	19:a:827:CLA:H172	1.77	0.47
7:b:277:ALA:HA	19:b:817:CLA:HMC2	1.96	0.47
7:b:385:PHE:HB3	7:b:536:LEU:HB3	1.97	0.47
1:5:96:VAL:HG12	19:5:307:CLA:OBD	2.15	0.47
2:4:185:PHE:CZ	17:4:303:XAT:H28	2.50	0.47
4:2:105:ALA:HB1	17:2:303:XAT:H161	1.97	0.47
19:b:807:CLA:H192	19:b:807:CLA:H161	1.72	0.46
19:b:819:CLA:HBA2	19:b:819:CLA:H3A	1.37	0.46
11:i:28:LEU:O	11:i:32:LYS:HG3	2.15	0.46
19:1:306:CLA:H93	19:1:306:CLA:H61	1.70	0.46
6:a:68:SER:OG	6:a:174:TYR:HB2	2.14	0.46
19:b:839:CLA:H41	19:b:839:CLA:H62	1.71	0.46
17:3:303:XAT:H35	17:3:303:XAT:H401	1.79	0.46
17:2:303:XAT:H11	17:2:303:XAT:H191	1.66	0.46
19:a:854:CLA:H142	19:a:854:CLA:H111	1.80	0.46
17:3:305:XAT:H35	17:3:305:XAT:H401	1.77	0.46
4:2:191:GLN:O	4:2:195:ILE:HD12	2.15	0.46
5:1:84:VAL:O	5:1:88:ILE:HG12	2.14	0.46
6:a:570:GLY:O	6:a:576:THR:OG1	2.32	0.46
19:a:801:CLA:H61	19:a:803:CLA:O1D	2.16	0.46
19:a:834:CLA:CAD	26:l:201:BCR:H10C	2.45	0.46
19:b:818:CLA:H41	19:b:834:CLA:HAA2	1.97	0.46
19:b:823:CLA:HHC	19:b:841:CLA:HED1	1.98	0.46
4:2:65:ILE:HG22	4:2:67:PHE:H	1.80	0.46
5:1:62:ASP:OD1	5:1:62:ASP:N	2.49	0.46
6:a:114:ILE:O	6:a:117:GLN:HG2	2.16	0.46
19:a:819:CLA:H3A	19:a:819:CLA:HBA2	1.53	0.46
7:b:50:HIS:HE1	19:b:806:CLA:H171	1.81	0.46
6:a:476:PHE:HB3	19:a:838:CLA:H11	1.96	0.46
19:a:818:CLA:NC	22:a:853:LMG:H302	2.31	0.46
19:b:839:CLA:H12	26:l:205:BCR:H15C	1.98	0.46
5:1:89:VAL:O	5:1:93:TRP:N	2.49	0.46
17:a:852:XAT:H15	17:a:852:XAT:H201	1.67	0.46
19:j:102:CLA:NB	26:j:104:BCR:H281	2.30	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:303:XAT:H35	17:4:303:XAT:H401	1.84	0.46
19:a:804:CLA:H41	19:a:841:CLA:HMC1	1.98	0.46
19:a:854:CLA:H143	22:j:105:LMG:H142	1.97	0.46
19:b:814:CLA:H141	19:b:814:CLA:H161	1.77	0.46
19:b:826:CLA:HAA2	19:b:827:CLA:OBD	2.16	0.46
19:b:840:CLA:HBA1	19:b:840:CLA:H3A	1.59	0.46
1:5:116:GLU:HB2	19:5:307:CLA:C1B	2.46	0.46
6:a:375:ILE:HG21	6:a:510:VAL:HB	1.96	0.46
7:b:268:LEU:HD23	7:b:271:MET:HE3	1.98	0.46
22:j:105:LMG:H292	22:j:105:LMG:H111	1.98	0.46
5:1:140:TYR:OH	5:1:142:PRO:O	2.25	0.46
6:a:25:PRO:HB2	6:a:41:TRP:HH2	1.81	0.46
6:a:665:ILE:HG23	19:a:809:CLA:H171	1.99	0.46
19:a:806:CLA:H72	26:a:848:BCR:HC8	1.98	0.46
7:b:392:PHE:CE2	26:b:847:BCR:HC42	2.51	0.46
13:l:168:TYR:O	13:l:172:LEU:HB2	2.16	0.46
1:5:124:MET:HE3	19:5:312:CLA:HMC2	1.98	0.45
17:4:305:XAT:H15	17:4:305:XAT:H201	1.71	0.45
3:3:179:PRO:C	3:3:181:LYS:H	2.24	0.45
5:1:105:PRO:C	5:1:107:LYS:H	2.24	0.45
6:a:282:LEU:HD21	6:a:367:MET:HB3	1.98	0.45
6:a:677:LEU:HB2	19:a:802:CLA:HMC2	1.97	0.45
19:a:822:CLA:H12	19:a:825:CLA:HBA2	1.98	0.45
4:2:131:ALA:HA	4:2:134:VAL:HG12	1.98	0.45
26:b:844:BCR:H11C	26:b:844:BCR:H341	1.76	0.45
17:5:302:XAT:H11	17:5:302:XAT:H191	1.65	0.45
17:4:302:XAT:H30	19:4:310:CLA:H151	1.98	0.45
19:3:310:CLA:H61	19:3:310:CLA:H41	1.86	0.45
5:1:141:ARG:HD3	5:1:149:TRP:HB3	1.99	0.45
19:b:812:CLA:H51	19:b:813:CLA:H43	1.97	0.45
10:f:119:GLY:HA3	10:f:160:TRP:CE2	2.51	0.45
12:j:26:VAL:CG1	26:j:104:BCR:H403	2.47	0.45
3:3:121:GLN:HA	3:3:124:VAL:HG12	1.99	0.45
5:1:73:GLU:HB2	19:1:306:CLA:C1B	2.45	0.45
7:b:339:LEU:O	7:b:343:THR:HG22	2.16	0.45
19:b:824:CLA:HBA1	26:b:846:BCR:H16C	1.98	0.45
10:f:143:ILE:O	12:j:11:ALA:N	2.48	0.45
17:4:305:XAT:H11	17:4:305:XAT:H191	1.81	0.45
6:a:144:GLU:HG2	6:a:206:TRP:HH2	1.80	0.45
7:b:466:GLN:NE2	19:b:836:CLA:OBD	2.34	0.45
19:b:811:CLA:H141	19:b:811:CLA:H162	1.75	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:232:HIS:HE1	17:5:304:XAT:H14	1.81	0.45
17:2:303:XAT:H15	17:2:303:XAT:H201	1.79	0.45
6:a:312:GLY:HA2	19:a:823:CLA:HMD2	1.99	0.45
19:b:833:CLA:H18	26:f:804:BCR:H17C	1.97	0.45
17:2:302:XAT:H15	17:2:302:XAT:H201	1.82	0.45
6:a:71:PHE:HD1	6:a:166:MET:HE3	1.82	0.45
6:a:304:MET:HG3	19:a:823:CLA:C3C	2.47	0.45
6:a:466:SER:HG	6:a:631:GLN:HE22	1.64	0.45
7:b:228:TRP:HZ3	26:b:850:BCR:H363	1.81	0.45
19:b:813:CLA:H62	19:b:813:CLA:H41	1.62	0.45
19:b:824:CLA:HHB	19:b:841:CLA:O1D	2.16	0.45
6:a:407:VAL:HG11	6:a:564:PHE:N	2.32	0.45
7:b:605:GLN:HE21	7:b:734:LYS:HB3	1.82	0.45
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.45
17:4:304:XAT:H35	17:4:304:XAT:H401	1.80	0.45
17:3:304:XAT:H15	17:3:304:XAT:H201	1.78	0.45
17:2:303:XAT:H31	17:2:303:XAT:H391	1.70	0.45
17:1:303:XAT:H183	19:1:308:CLA:C2B	2.47	0.45
1:5:164:PHE:HE1	19:f:802:CLA:H121	1.81	0.45
17:4:305:XAT:H391	17:4:305:XAT:H31	1.62	0.45
19:4:311:CLA:H2A	19:4:311:CLA:O2D	2.17	0.45
19:1:312:CLA:HMA2	20:1:315:SQD:H141	1.99	0.45
19:a:835:CLA:H61	26:l:201:BCR:H363	1.99	0.45
19:b:825:CLA:H41	19:b:825:CLA:H62	1.79	0.45
8:d:20:TRP:HB2	8:d:24:ALA:HB3	1.99	0.45
1:5:106:PHE:HB2	10:f:148:PRO:HG3	1.99	0.44
2:4:37:SER:HB3	2:4:45:ARG:HA	1.98	0.44
17:3:304:XAT:H35	17:3:304:XAT:H401	1.68	0.44
19:2:316:CLA:C1C	22:2:317:LMG:H111	2.46	0.44
20:1:315:SQD:H311	20:1:315:SQD:H282	1.84	0.44
6:a:683:GLY:HA3	7:b:571:ASP:HB2	1.99	0.44
7:b:50:HIS:ND1	19:b:814:CLA:OBD	2.38	0.44
7:b:259:PHE:CZ	7:b:510:LEU:HD12	2.53	0.44
7:b:280:VAL:HG21	19:b:817:CLA:HAB	1.98	0.44
26:b:845:BCR:H24C	26:b:845:BCR:H371	1.70	0.44
11:i:14:VAL:O	11:i:19:PRO:HD2	2.17	0.44
13:l:68:LEU:O	13:l:77:SER:OG	2.24	0.44
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.44
3:3:133:PRO:HB2	17:3:301:XAT:H23	2.00	0.44
17:2:302:XAT:H401	17:2:302:XAT:H35	1.71	0.44
5:1:156:ASP:OD2	13:l:2:VAL:N	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:801:CLA:CED	19:a:801:CLA:HAA2	2.46	0.44
10:f:79:ARG:O	10:f:83:SER:HB2	2.17	0.44
2:4:170:MET:CE	19:4:313:CLA:H12	2.47	0.44
17:2:303:XAT:H35	17:2:303:XAT:H401	1.71	0.44
5:1:40:ASP:HB2	5:1:42:MET:HG3	1.98	0.44
19:a:801:CLA:HED2	19:a:801:CLA:HBD	1.48	0.44
4:2:97:LYS:NZ	4:2:152:GLU:OE1	2.38	0.44
6:a:73:GLN:HG2	19:a:806:CLA:H3A	2.00	0.44
6:a:342:TRP:CD1	19:a:826:CLA:H192	2.51	0.44
6:a:447:GLY:HA3	19:a:835:CLA:HAB	1.98	0.44
19:a:826:CLA:HMB3	19:a:826:CLA:HBB1	1.99	0.44
7:b:172:ARG:HB2	19:b:814:CLA:HBC2	2.00	0.44
7:b:343:THR:HG23	7:b:377:ALA:HB2	2.00	0.44
19:b:811:CLA:H112	19:i:102:CLA:HAB	1.99	0.44
19:b:821:CLA:HBA2	19:b:821:CLA:H3A	1.33	0.44
19:b:836:CLA:H12	19:b:837:CLA:O1A	2.18	0.44
2:4:59:PHE:HE1	19:4:306:CLA:HBC3	1.83	0.44
6:a:367:MET:HG2	6:a:500:SER:HB2	1.99	0.44
6:a:580:SER:HB2	6:a:582:TRP:H	1.82	0.44
6:a:686:TYR:CE1	7:b:538:LYS:HD2	2.52	0.44
19:a:803:CLA:H151	19:b:811:CLA:HBC3	1.97	0.44
19:a:812:CLA:H142	19:a:812:CLA:H112	1.85	0.44
19:b:808:CLA:H93	19:b:808:CLA:H61	1.71	0.44
19:b:814:CLA:H143	19:b:825:CLA:H51	1.99	0.44
8:d:81:ASN:H	8:d:81:ASN:ND2	2.16	0.44
16:c:3:HIS:HB2	16:c:48:CYS:SG	2.56	0.44
5:1:95:PRO:HD2	19:1:308:CLA:HMD3	1.99	0.44
19:a:813:CLA:H62	19:a:813:CLA:H41	1.85	0.44
7:b:654:PHE:O	7:b:658:VAL:HG23	2.17	0.44
19:b:839:CLA:H161	13:l:92:LEU:HD21	1.99	0.44
26:b:843:BCR:H15C	26:b:843:BCR:H351	1.73	0.44
17:5:302:XAT:H383	19:5:309:CLA:C2B	2.48	0.44
17:2:305:XAT:H15	17:2:305:XAT:H201	1.78	0.44
6:a:532:HIS:CE1	6:a:599:VAL:HA	2.53	0.44
6:a:578:GLN:HA	6:a:583:ASP:OD2	2.18	0.44
19:a:829:CLA:H91	19:a:831:CLA:H192	2.00	0.44
19:a:834:CLA:H201	26:l:205:BCR:H343	1.98	0.44
7:b:682:TRP:NE1	13:l:15:GLY:O	2.43	0.44
26:b:852:BCR:H20C	26:b:852:BCR:H361	1.76	0.44
10:f:160:TRP:CG	10:f:161:PRO:HD3	2.52	0.44
17:j:101:XAT:H35	17:j:101:XAT:H401	1.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:59:PRO:HD2	27:c:102:SF4:S2	2.58	0.44
3:3:189:GLU:HB2	19:3:313:CLA:C1B	2.47	0.44
4:2:118:LEU:HB2	4:2:123:TYR:HD2	1.83	0.44
5:1:152:VAL:HG11	5:1:159:TRP:CD1	2.53	0.44
5:1:171:ARG:HA	5:1:174:MET:HE3	2.00	0.44
22:a:853:LMG:H112	22:a:853:LMG:HC92	1.98	0.44
7:b:678:GLU:HG2	16:c:81:TYR:HE1	1.81	0.44
19:b:818:CLA:HBA2	19:b:818:CLA:H3A	1.26	0.44
10:f:153:ILE:O	10:f:156:SER:OG	2.31	0.44
26:j:104:BCR:H341	26:j:104:BCR:H11C	1.72	0.44
13:l:116:VAL:HG11	13:l:128:LEU:C	2.42	0.44
25:m:101:LHG:H272	25:m:101:LHG:H302	1.86	0.44
17:4:302:XAT:H11	17:4:302:XAT:H191	1.89	0.44
4:2:127:ASN:OD1	4:2:130:GLN:N	2.46	0.44
17:1:302:XAT:H31	17:1:302:XAT:H391	1.88	0.44
6:a:52:PHE:CD2	19:a:806:CLA:HMC2	2.53	0.44
6:a:415:ASN:O	6:a:421:ASP:HB2	2.18	0.44
6:a:442:GLY:HA3	19:b:804:CLA:O1A	2.18	0.44
6:a:701:LEU:HD12	19:a:841:CLA:HMA2	2.00	0.44
7:b:302:ILE:HD13	19:b:823:CLA:HMD2	2.00	0.44
7:b:526:ALA:HB2	19:b:837:CLA:HMA1	2.00	0.44
19:b:826:CLA:H3A	19:b:826:CLA:HBA2	1.72	0.44
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.43
2:4:85:MET:HE3	2:4:177:ASN:HB3	2.00	0.43
19:a:807:CLA:H43	25:a:845:LHG:H252	2.00	0.43
7:b:26:ALA:HB1	21:b:851:DGD:O1B	2.17	0.43
7:b:520:LEU:HD23	7:b:520:LEU:HA	1.88	0.43
10:f:57:GLU:O	10:f:60:THR:OG1	2.32	0.43
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.43
19:a:806:CLA:H162	19:a:806:CLA:H141	1.59	0.43
7:b:518:ASP:O	7:b:522:HIS:ND1	2.38	0.43
19:b:805:CLA:H162	19:b:805:CLA:H141	1.67	0.43
16:c:54:CYS:SG	16:c:55:GLU:N	2.91	0.43
19:4:310:CLA:C1A	19:4:310:CLA:CGA	2.96	0.43
6:a:194:HIS:HE1	19:a:826:CLA:H72	1.83	0.43
6:a:565:ARG:HD2	25:a:845:LHG:HC61	2.00	0.43
19:a:822:CLA:OBD	19:a:824:CLA:HMD3	2.19	0.43
19:a:826:CLA:H202	19:a:826:CLA:H162	1.79	0.43
19:a:831:CLA:H92	19:a:831:CLA:H61	1.70	0.43
6:a:84:MET:SD	19:a:829:CLA:HED1	2.58	0.43
6:a:517:MET:HE2	6:a:611:VAL:HA	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:807:CLA:H2	19:b:807:CLA:H62	1.79	0.43
9:e:16:TYR:CD2	9:e:44:ASN:HA	2.54	0.43
11:i:17:VAL:HG21	19:i:102:CLA:HMC2	2.01	0.43
13:l:96:LEU:HG	26:l:205:BCR:H24C	2.01	0.43
2:4:183:LEU:HD11	19:4:308:CLA:HAC1	2.00	0.43
7:b:201:ARG:HG2	7:b:248:SER:HB2	1.99	0.43
26:b:847:BCR:H15C	26:b:847:BCR:H351	1.85	0.43
12:j:30:ASN:ND2	19:j:102:CLA:O1A	2.47	0.43
19:a:844:CLA:C1C	25:a:846:LHG:HC31	2.48	0.43
17:a:852:XAT:H35	17:a:852:XAT:H401	1.85	0.43
7:b:172:ARG:HD2	19:b:825:CLA:OBD	2.18	0.43
19:b:841:CLA:H161	19:b:841:CLA:H192	1.82	0.43
19:j:103:CLA:O1D	19:j:103:CLA:H2A	2.18	0.43
17:4:301:XAT:H11	17:4:301:XAT:H191	1.86	0.43
5:1:171:ARG:HA	5:1:174:MET:CE	2.49	0.43
7:b:220:LEU:HD23	7:b:220:LEU:HA	1.87	0.43
7:b:350:MET:HE2	7:b:350:MET:HB3	1.89	0.43
19:b:807:CLA:H161	19:b:807:CLA:H102	2.01	0.43
19:b:814:CLA:H161	19:b:814:CLA:H192	1.76	0.43
19:5:307:CLA:HBC1	17:4:301:XAT:H383	2.01	0.43
17:2:304:XAT:H11	17:2:304:XAT:H191	1.89	0.43
5:1:128:GLU:HG3	17:1:302:XAT:H372	2.01	0.43
5:1:151:TRP:CH2	13:l:20:PRO:HA	2.54	0.43
5:1:168:ASN:HA	5:1:171:ARG:HD2	2.01	0.43
6:a:94:TYR:OH	6:a:146:ILE:O	2.24	0.43
19:a:833:CLA:H72	19:l:203:CLA:H12	2.00	0.43
7:b:207:TRP:HE1	19:b:815:CLA:H11	1.84	0.43
26:f:804:BCR:H11C	26:f:804:BCR:H341	1.73	0.43
3:3:103:ILE:HD11	17:3:304:XAT:H363	2.01	0.43
4:2:205:PHE:CD2	17:2:303:XAT:H12	2.54	0.43
19:2:310:CLA:H192	19:2:310:CLA:H162	1.71	0.43
5:1:58:ALA:HB1	5:1:66:LEU:HD21	2.00	0.43
5:1:82:LEU:HD11	19:1:311:CLA:HBC1	2.01	0.43
7:b:274:HIS:HB2	19:b:818:CLA:CHB	2.48	0.43
7:b:440:VAL:HG12	19:j:102:CLA:HAC1	2.01	0.43
7:b:547:LYS:NZ	9:e:15:SER:O	2.45	0.43
19:b:801:CLA:H91	19:b:801:CLA:H111	1.70	0.43
16:c:25:VAL:HG21	16:c:48:CYS:HA	2.00	0.43
17:4:304:XAT:H15	17:4:304:XAT:H201	1.87	0.43
3:3:56:ASN:HB3	3:3:82:LEU:HD22	2.01	0.43
17:2:301:XAT:H401	17:2:301:XAT:H35	1.75	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:555:LEU:HD11	7:b:674:GLN:HB3	2.01	0.43
7:b:140:LEU:HD23	7:b:143:LEU:HD12	2.01	0.43
7:b:345:LEU:CD1	19:b:827:CLA:HAA1	2.49	0.43
7:b:424:LEU:HG	19:b:838:CLA:CBB	2.48	0.43
7:b:626:LEU:HD22	19:b:803:CLA:HMD3	2.01	0.43
19:i:102:CLA:H91	19:i:102:CLA:H112	1.69	0.43
17:5:304:XAT:H15	17:5:304:XAT:H201	1.76	0.42
19:4:317:CLA:H92	19:4:317:CLA:H62	1.83	0.42
19:a:807:CLA:H92	19:a:807:CLA:H61	1.69	0.42
19:a:841:CLA:HED3	19:a:841:CLA:H2A	2.01	0.42
19:a:807:CLA:H102	19:a:807:CLA:H161	2.00	0.42
19:a:820:CLA:CAD	19:a:830:CLA:H41	2.48	0.42
26:a:848:BCR:H15C	26:a:848:BCR:H351	1.78	0.42
7:b:529:LEU:HD23	7:b:588:THR:HG21	2.00	0.42
2:4:193:ALA:HB1	21:4:318:DGD:O5E	2.16	0.42
19:4:309:CLA:HED2	19:4:309:CLA:HBD	1.83	0.42
6:a:727:LEU:HD22	19:a:842:CLA:HMA3	2.01	0.42
7:b:500:LEU:HA	7:b:503:ILE:HG22	2.02	0.42
8:d:88:TYR:HB3	8:d:89:PRO:HD2	2.01	0.42
12:j:12:PRO:HB2	17:j:101:XAT:H21	2.01	0.42
1:5:98:PHE:HE1	19:5:305:CLA:HBC3	1.84	0.42
17:5:301:XAT:H15	17:5:301:XAT:H201	1.85	0.42
17:5:301:XAT:H35	17:5:301:XAT:H401	1.77	0.42
19:4:306:CLA:CHA	19:4:306:CLA:HBA1	2.48	0.42
19:4:309:CLA:H3A	19:4:309:CLA:HBA1	1.77	0.42
6:a:75:ALA:HB2	6:a:166:MET:HB2	2.01	0.42
6:a:271:PHE:HE2	6:a:495:ALA:HB2	1.84	0.42
6:a:689:GLU:OE2	7:b:546:SER:OG	2.30	0.42
19:a:810:CLA:HBB1	26:j:104:BCR:H23C	2.00	0.42
8:d:32:ILE:HG21	8:d:70:LEU:HD23	2.00	0.42
3:3:172:PRO:HD2	17:3:305:XAT:H242	2.00	0.42
6:a:452:ASN:HD22	6:a:634:ILE:HB	1.85	0.42
7:b:381:MET:HE1	26:b:847:BCR:H352	2.02	0.42
19:b:817:CLA:CHD	19:b:818:CLA:HBB2	2.49	0.42
19:j:102:CLA:H111	19:j:102:CLA:H91	1.83	0.42
6:a:361:ALA:HB2	6:a:387:HIS:HB2	2.01	0.42
19:a:803:CLA:O1A	19:a:803:CLA:H3A	2.19	0.42
19:a:831:CLA:H93	19:a:842:CLA:HED3	2.01	0.42
7:b:347:ALA:HB3	7:b:374:GLN:HE21	1.85	0.42
19:b:827:CLA:HED1	26:b:847:BCR:H21C	2.02	0.42
26:b:845:BCR:HC7	26:b:845:BCR:H331	1.91	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:304:XAT:H35	17:5:304:XAT:H401	1.80	0.42
17:2:305:XAT:H31	17:2:305:XAT:H391	1.71	0.42
6:a:143:ALA:HB2	6:a:371:PRO:HD2	2.00	0.42
19:a:804:CLA:C4D	12:j:12:PRO:HG3	2.50	0.42
26:a:850:BCR:H20C	26:a:850:BCR:H361	1.80	0.42
7:b:56:ILE:HD11	26:m:102:BCR:HC7	2.02	0.42
7:b:647:VAL:HG21	19:b:809:CLA:HAC1	2.00	0.42
19:b:815:CLA:H61	19:b:815:CLA:H2	1.77	0.42
19:b:836:CLA:H51	19:b:836:CLA:H11	1.73	0.42
19:b:840:CLA:H61	19:b:840:CLA:H92	1.73	0.42
12:j:14:LEU:CD2	22:j:105:LMG:H141	2.49	0.42
13:l:53:THR:HG22	19:l:202:CLA:C1B	2.49	0.42
17:3:304:XAT:H12	19:3:309:CLA:HAB	2.01	0.42
17:1:303:XAT:H35	17:1:303:XAT:H401	1.85	0.42
6:a:567:PRO:HB3	6:a:714:ILE:HB	2.00	0.42
19:a:807:CLA:H161	19:a:807:CLA:H192	1.82	0.42
19:a:823:CLA:CHD	17:a:852:XAT:H183	2.49	0.42
26:a:849:BCR:H15C	26:a:849:BCR:H351	1.79	0.42
26:a:849:BCR:H24C	26:a:849:BCR:H371	1.86	0.42
7:b:120:GLU:OE2	7:b:362:ASN:ND2	2.39	0.42
7:b:220:LEU:HD21	26:b:843:BCR:H391	2.01	0.42
19:b:805:CLA:H2	19:b:805:CLA:H61	1.62	0.42
19:b:817:CLA:CBB	26:b:850:BCR:H14C	2.50	0.42
26:l:201:BCR:H352	19:l:203:CLA:HAB	2.02	0.42
16:c:32:ASP:OD1	16:c:32:ASP:N	2.53	0.42
6:a:272:LYS:HG2	6:a:496:LEU:HD12	2.02	0.42
6:a:364:MET:HE1	19:a:830:CLA:CAD	2.49	0.42
6:a:440:PHE:CE2	19:a:839:CLA:HAB	2.55	0.42
6:a:680:LEU:HB3	7:b:667:ILE:HG12	2.02	0.42
26:a:849:BCR:H20C	26:a:849:BCR:H361	1.89	0.42
26:b:843:BCR:H11C	26:b:843:BCR:H341	1.74	0.42
2:4:75:GLU:OE1	2:4:148:ARG:NH2	2.47	0.42
17:4:303:XAT:H163	19:4:308:CLA:H2	2.02	0.42
4:2:205:PHE:HE1	17:2:303:XAT:H162	1.84	0.42
17:2:305:XAT:H11	17:2:305:XAT:H191	1.90	0.42
6:a:290:HIS:O	6:a:294:ILE:HG12	2.20	0.42
6:a:601:PHE:CZ	19:a:801:CLA:HED3	2.55	0.42
6:a:684:ARG:NH1	6:a:711:ALA:O	2.52	0.42
6:a:692:GLU:CD	7:b:547:LYS:HB2	2.44	0.42
19:a:806:CLA:H202	19:a:806:CLA:H161	1.70	0.42
19:a:840:CLA:H72	26:a:850:BCR:H373	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:192:LEU:HA	7:b:192:LEU:HD23	1.83	0.42
7:b:597:HIS:CE1	7:b:727:VAL:HG23	2.54	0.42
19:b:802:CLA:HMA1	19:b:803:CLA:H161	2.02	0.42
19:1:306:CLA:H3A	19:1:306:CLA:O2A	2.20	0.41
6:a:491:THR:OG1	19:a:836:CLA:OBD	2.32	0.41
6:a:525:ASP:HA	6:a:528:VAL:HG12	2.01	0.41
19:a:816:CLA:C4B	17:a:852:XAT:H242	2.50	0.41
19:a:840:CLA:H112	19:a:840:CLA:H152	1.80	0.41
7:b:197:ILE:HB	7:b:198:PRO:HD3	2.02	0.41
7:b:585:MET:O	7:b:589:ILE:HG12	2.20	0.41
19:b:828:CLA:H13	19:b:830:CLA:H141	2.02	0.41
8:d:70:LEU:O	8:d:74:LEU:HG	2.19	0.41
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
17:5:301:XAT:H31	17:5:301:XAT:H391	1.88	0.41
6:a:67:PHE:HE2	6:a:173:HIS:CG	2.38	0.41
6:a:399:ALA:HB1	6:a:543:LEU:HB3	2.02	0.41
6:a:427:ARG:NH2	8:d:46:THR:O	2.53	0.41
19:a:805:CLA:H61	19:a:805:CLA:H41	1.91	0.41
19:a:834:CLA:H142	26:b:848:BCR:H17C	2.01	0.41
7:b:430:PHE:O	7:b:434:HIS:ND1	2.40	0.41
19:b:801:CLA:H141	19:b:801:CLA:H161	1.63	0.41
13:l:75:LEU:HD23	13:l:75:LEU:HA	1.89	0.41
4:2:109:TRP:CE3	17:2:303:XAT:H22	2.54	0.41
4:2:203:LEU:HD13	17:2:301:XAT:C10	2.50	0.41
5:1:162:TYR:CE2	19:a:844:CLA:HBD	2.56	0.41
6:a:293:ALA:HB1	19:a:818:CLA:HBC2	2.02	0.41
19:a:826:CLA:HMD2	19:a:826:CLA:H143	2.03	0.41
19:a:839:CLA:H141	19:a:839:CLA:H161	1.68	0.41
7:b:471:LYS:HB2	7:b:471:LYS:HE2	1.89	0.41
19:b:836:CLA:HBB1	19:b:836:CLA:HMB1	2.02	0.41
10:f:114:PHE:HB2	26:f:801:BCR:C32	2.49	0.41
17:5:302:XAT:H15	17:5:302:XAT:H201	1.74	0.41
5:1:54:PRO:HD2	17:1:303:XAT:H242	2.02	0.41
19:1:311:CLA:H72	13:l:21:ILE:HG12	2.02	0.41
7:b:193:VAL:O	7:b:198:PRO:HD3	2.20	0.41
7:b:314:GLY:HA3	7:b:412:ARG:HD2	2.02	0.41
7:b:702:LEU:HD22	7:b:706:GLN:NE2	2.35	0.41
19:4:307:CLA:HBD	19:4:314:CLA:OBD	2.20	0.41
17:3:303:XAT:H15	17:3:303:XAT:H201	1.79	0.41
17:2:301:XAT:H31	17:2:301:XAT:H391	1.72	0.41
5:1:147:GLY:HA2	5:1:149:TRP:CZ3	2.55	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:310:CLA:H41	19:1:310:CLA:H62	1.80	0.41
6:a:194:HIS:ND1	19:a:826:CLA:OBD	2.48	0.41
6:a:357:SER:HB2	19:a:830:CLA:HMC2	2.01	0.41
26:a:847:BCR:H24C	26:a:847:BCR:H371	1.92	0.41
19:b:801:CLA:H51	19:b:839:CLA:H102	2.01	0.41
17:3:301:XAT:H201	17:3:301:XAT:H15	1.79	0.41
19:a:834:CLA:H143	19:a:834:CLA:H161	1.93	0.41
7:b:342:ALA:HB2	19:b:825:CLA:H43	2.02	0.41
19:b:809:CLA:C4A	19:b:809:CLA:HBA2	2.50	0.41
19:b:825:CLA:H52	19:b:825:CLA:H12	1.85	0.41
26:l:205:BCR:H15C	26:l:205:BCR:H351	1.74	0.41
1:5:149:VAL:HG22	17:5:304:XAT:H182	2.02	0.41
4:2:57:PHE:CZ	17:2:305:XAT:H172	2.55	0.41
6:a:232:LEU:HD23	6:a:232:LEU:HA	1.92	0.41
6:a:356:LEU:HB2	19:a:828:CLA:H41	2.02	0.41
6:a:434:LEU:HG	6:a:541:LEU:HB2	2.03	0.41
6:a:651:VAL:O	6:a:654:SER:OG	2.29	0.41
19:a:841:CLA:HAA2	19:b:832:CLA:HMB1	2.02	0.41
24:a:843:PQN:H211	24:a:843:PQN:H252	1.82	0.41
7:b:181:PHE:CE2	19:b:820:CLA:HAB	2.56	0.41
10:f:114:PHE:HB2	26:f:801:BCR:H321	2.02	0.41
17:4:303:XAT:H11	17:4:303:XAT:H191	1.74	0.41
19:a:806:CLA:H52	26:a:848:BCR:HC8	2.03	0.41
19:a:818:CLA:OBD	19:a:837:CLA:HED2	2.21	0.41
19:a:820:CLA:H3A	19:a:820:CLA:HBA2	1.48	0.41
19:a:828:CLA:H2	19:a:828:CLA:H61	1.78	0.41
7:b:433:PHE:CZ	26:f:801:BCR:H372	2.56	0.41
11:i:3:LEU:HD23	11:i:3:LEU:HA	1.92	0.41
17:4:305:XAT:H363	17:3:301:XAT:C10	2.49	0.41
17:2:304:XAT:H31	17:2:304:XAT:H391	1.85	0.41
5:1:71:GLU:HG2	5:1:142:PRO:O	2.20	0.41
5:1:87:TRP:CG	5:1:180:LEU:HD13	2.56	0.41
19:1:310:CLA:H111	19:1:310:CLA:H71	1.89	0.41
6:a:226:SER:OG	6:a:229:GLU:HG2	2.21	0.41
6:a:499:VAL:HG12	19:a:819:CLA:H11	2.03	0.41
6:a:675:PHE:HZ	19:a:842:CLA:HBC2	1.86	0.41
7:b:346:THR:HG21	19:b:829:CLA:HHD	2.03	0.41
7:b:547:LYS:HE2	10:f:180:ILE:HD11	2.03	0.41
7:b:585:MET:HE3	7:b:585:MET:HB3	1.83	0.41
19:b:802:CLA:H122	19:b:802:CLA:H162	1.60	0.41
19:b:804:CLA:HBC2	19:b:804:CLA:HHD	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:813:CLA:H3A	19:b:813:CLA:HBA2	1.61	0.41
19:b:827:CLA:HMB2	19:b:834:CLA:HBA1	2.03	0.41
26:b:845:BCR:H15C	26:b:845:BCR:H351	1.78	0.41
9:e:51:ASN:ND2	16:c:61:ASP:HB2	2.35	0.41
11:i:29:TYR:HE1	14:m:30:ASN:HD21	1.67	0.41
17:1:302:XAT:H11	17:1:302:XAT:H191	1.86	0.41
6:a:318:ILE:O	6:a:322:HIS:ND1	2.54	0.41
6:a:342:TRP:HB3	19:a:806:CLA:HAC1	2.02	0.41
7:b:499:TRP:CD1	19:b:834:CLA:HED2	2.57	0.41
7:b:629:ASN:HA	7:b:734:LYS:HE2	2.02	0.41
19:b:822:CLA:H12	19:b:823:CLA:H52	2.03	0.41
8:d:107:VAL:HG21	16:c:38:GLN:HB3	2.01	0.41
4:2:92:ARG:NH2	19:2:308:CLA:HED3	2.36	0.40
6:a:452:ASN:HB3	6:a:635:THR:HG22	2.04	0.40
6:a:529:HIS:CG	19:a:839:CLA:HED2	2.56	0.40
7:b:523:HIS:CE1	26:b:852:BCR:H322	2.56	0.40
7:b:614:SER:O	7:b:620:GLY:HA3	2.21	0.40
26:j:104:BCR:H20C	26:j:104:BCR:H361	1.91	0.40
13:l:56:TYR:CD2	13:l:161:ALA:HB2	2.56	0.40
14:m:22:ILE:HD12	25:m:101:LHG:H312	2.02	0.40
17:4:303:XAT:H383	19:4:310:CLA:C2B	2.51	0.40
19:3:312:CLA:H11	19:3:312:CLA:H51	1.89	0.40
6:a:673:TRP:O	6:a:676:SER:OG	2.32	0.40
26:a:847:BCR:H20C	26:a:847:BCR:H361	1.80	0.40
7:b:401:ASN:HB3	7:b:408:ASN:OD1	2.22	0.40
7:b:431:LEU:HD11	19:b:837:CLA:HMB1	2.03	0.40
19:b:815:CLA:CHA	19:b:815:CLA:HBA1	2.49	0.40
19:b:840:CLA:H111	19:b:840:CLA:H152	1.87	0.40
26:b:852:BCR:H11C	26:b:852:BCR:H341	1.73	0.40
26:i:101:BCR:H11C	26:i:101:BCR:H341	1.86	0.40
26:l:205:BCR:H20C	26:l:205:BCR:H361	1.91	0.40
17:4:301:XAT:H35	17:4:301:XAT:H401	1.66	0.40
17:4:302:XAT:H35	17:4:302:XAT:H401	1.76	0.40
19:4:307:CLA:H41	19:4:307:CLA:H61	1.86	0.40
3:3:106:VAL:HG11	19:3:311:CLA:HED1	2.03	0.40
3:3:205:LEU:HD12	3:3:205:LEU:HA	1.86	0.40
6:a:299:ILE:O	6:a:303:HIS:ND1	2.53	0.40
19:a:820:CLA:H122	19:a:820:CLA:H161	1.83	0.40
19:a:828:CLA:H152	19:a:840:CLA:H191	2.03	0.40
19:a:829:CLA:O1D	19:a:830:CLA:HMA1	2.21	0.40
26:a:847:BCR:H15C	26:a:847:BCR:H351	1.84	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:850:BCR:H361	26:b:850:BCR:H20C	1.88	0.40
8:d:89:PRO:HB2	8:d:90:PRO:HD3	2.03	0.40
19:i:102:CLA:H41	19:i:102:CLA:H62	1.88	0.40
19:5:308:CLA:CBB	19:5:315:CLA:HAB	2.51	0.40
17:4:304:XAT:H30	19:4:313:CLA:H71	2.02	0.40
19:4:317:CLA:HMB3	17:3:301:XAT:H392	2.03	0.40
6:a:226:SER:HG	6:a:229:GLU:HG2	1.86	0.40
19:a:825:CLA:H62	19:a:825:CLA:H41	1.84	0.40
7:b:339:LEU:HD11	19:b:806:CLA:H51	2.04	0.40
10:f:147:VAL:HG22	12:j:14:LEU:HD11	2.04	0.40
13:l:54:HIS:O	13:l:58:LEU:HB2	2.22	0.40
1:5:98:PHE:CD2	19:5:305:CLA:HMD2	2.56	0.40
5:1:134:ILE:HD11	13:l:26:PHE:HA	2.03	0.40
19:a:828:CLA:H122	19:a:828:CLA:H162	1.66	0.40
7:b:461:PHE:HB2	19:b:837:CLA:CAD	2.52	0.40
7:b:550:PRO:HD2	16:c:62:PHE:CE1	2.57	0.40
19:b:834:CLA:H61	19:b:834:CLA:H102	1.98	0.40
13:l:4:PHE:HB3	13:l:20:PRO:HG3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	49
3	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
4	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	25
5	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
6	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
8	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
9	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
10	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
11	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
12	j	39/41 (95%)	39 (100%)	0	0	100	100
13	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	32
14	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3012/3336 (90%)	2834 (94%)	171 (6%)	7 (0%)	45	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	45	LYS
13	1	120	VAL
4	2	127	ASN
4	2	213	VAL
6	a	580	SER
13	1	131	ILE
2	4	146	SER

### 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	4	133/159 (84%)	133 (100%)	0	100	100
3	3	136/164 (83%)	136 (100%)	0	100	100
4	2	134/172 (78%)	134 (100%)	0	100	100
5	1	128/165 (78%)	128 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	a	607/613 (99%)	603 (99%)	4 (1%)	81	93
7	b	599/602 (100%)	599 (100%)	0	100	100
8	d	107/113 (95%)	107 (100%)	0	100	100
9	e	56/62 (90%)	56 (100%)	0	100	100
10	f	138/162 (85%)	138 (100%)	0	100	100
11	i	32/43 (74%)	32 (100%)	0	100	100
12	j	36/36 (100%)	36 (100%)	0	100	100
13	l	130/141 (92%)	130 (100%)	0	100	100
14	m	21/24 (88%)	21 (100%)	0	100	100
16	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2457/2706 (91%)	2453 (100%)	4 (0%)	91	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	a	428	ASP
6	a	448	LEU
6	a	579	VAL
6	a	580	SER

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	3	156	GLN
3	3	169	ASN
3	3	211	HIS
5	1	63	GLN
5	1	119	GLN
5	1	132	ASN
5	1	194	GLN
6	a	127	ASN
6	a	186	ASN
6	a	435	ASN
7	b	80	ASN
7	b	112	ASN
7	b	169	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	b	234	ASN
7	b	326	ASN
7	b	605	GLN
7	b	629	ASN
8	d	7	GLN
10	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](#)

207 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	$\# Z  > 2$
19	CLA	a	837	6	45,53,73	1.79	5 (11%)	52,89,113	1.59	7 (13%)
19	CLA	i	102	-	62,70,73	1.55	6 (9%)	72,109,113	1.38	8 (11%)
22	LMG	2	317	-	35,35,55	1.09	2 (5%)	43,43,63	1.31	4 (9%)
19	CLA	a	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	6 (7%)
17	XAT	3	305	-	39,47,47	0.88	1 (2%)	54,74,74	2.57	16 (29%)
19	CLA	5	314	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	a	815	-	45,53,73	1.78	5 (11%)	52,89,113	1.58	8 (15%)
19	CLA	b	832	-	49,57,73	1.69	5 (10%)	55,93,113	1.56	8 (14%)
21	DGD	4	318	-	41,41,67	1.06	2 (4%)	55,55,81	1.82	6 (10%)
17	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
19	CLA	b	804	-	65,73,73	1.45	5 (7%)	76,113,113	1.54	12 (15%)
20	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
26	BCR	b	845	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
17	XAT	4	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.56	17 (31%)
19	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
19	CLA	j	102	-	58,66,73	1.59	6 (10%)	67,104,113	1.42	8 (11%)
19	CLA	2	312	-	47,55,73	1.74	6 (12%)	54,91,113	1.57	7 (12%)
19	CLA	b	819	-	60,68,73	1.56	5 (8%)	70,107,113	1.40	7 (10%)
19	CLA	4	314	2	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
19	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
19	CLA	a	805	19	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
19	CLA	b	828	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
27	SF4	c	102	-	0,12,12	-	-	-	-	-
26	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	15 (26%)
19	CLA	3	314	3	47,55,73	1.73	6 (12%)	54,91,113	1.56	6 (11%)
19	CLA	b	824	-	53,61,73	1.63	6 (11%)	61,98,113	1.47	8 (13%)
26	BCR	m	102	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
19	CLA	a	854	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
19	CLA	2	311	-	58,66,73	1.58	5 (8%)	67,104,113	1.42	7 (10%)
19	CLA	b	840	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
19	CLA	a	825	-	55,63,73	1.63	5 (9%)	64,101,113	1.46	8 (12%)
19	CLA	b	805	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
26	BCR	l	205	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
19	CLA	5	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.58	7 (13%)
19	CLA	b	813	-	53,61,73	1.64	6 (11%)	61,98,113	1.50	8 (13%)
19	CLA	a	812	19	62,70,73	1.52	6 (9%)	72,109,113	1.45	8 (11%)
19	CLA	b	826	-	64,72,73	1.49	6 (9%)	74,111,113	1.45	8 (10%)
19	CLA	5	311	-	51,59,73	1.67	6 (11%)	59,96,113	1.53	9 (15%)
19	CLA	b	827	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
19	CLA	1	308	5	65,73,73	1.47	5 (7%)	76,113,113	1.42	9 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	2	308	4	54,62,73	1.64	5 (9%)	62,99,113	1.44	8 (12%)
26	BCR	b	844	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
19	CLA	1	204	-	46,54,73	1.76	6 (13%)	53,90,113	1.58	7 (13%)
19	CLA	1	309	5	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
19	CLA	b	814	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
19	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
19	CLA	b	835	-	53,61,73	1.68	6 (11%)	61,98,113	1.50	9 (14%)
19	CLA	1	305	-	61,69,73	1.56	5 (8%)	71,108,113	1.39	7 (9%)
26	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	21 (37%)
18	A1L1G	3	306	-	38,47,47	1.44	6 (15%)	49,71,71	1.50	9 (18%)
19	CLA	a	806	-	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)
19	CLA	a	816	-	50,58,73	1.68	6 (12%)	58,95,113	1.57	9 (15%)
27	SF4	c	101	-	0,12,12	-	-	-	-	-
19	CLA	2	306	-	41,50,73	1.84	6 (14%)	46,85,113	1.56	6 (13%)
19	CLA	a	807	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	5	312	-	52,60,73	1.65	5 (9%)	60,97,113	1.55	9 (15%)
19	CLA	a	811	-	56,64,73	1.59	5 (8%)	65,102,113	1.47	8 (12%)
19	CLA	a	844	25	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
19	CLA	b	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	3	309	3	56,64,73	1.59	6 (10%)	65,102,113	1.45	7 (10%)
19	CLA	a	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
19	CLA	5	308	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	7 (10%)
19	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	9 (11%)
22	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.16	3 (7%)
19	CLA	2	315	-	42,50,73	1.86	5 (11%)	48,85,113	1.55	7 (14%)
19	CLA	1	307	-	54,62,73	1.62	5 (9%)	62,99,113	1.51	8 (12%)
19	CLA	4	313	-	53,61,73	1.66	5 (9%)	61,98,113	1.49	8 (13%)
19	CLA	3	311	-	50,58,73	1.70	5 (10%)	58,95,113	1.53	9 (15%)
22	LMG	j	105	-	32,32,55	1.13	2 (6%)	40,40,63	1.14	3 (7%)
19	CLA	5	306	20	45,53,73	1.79	5 (11%)	52,89,113	1.57	6 (11%)
24	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
19	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
17	XAT	3	301	-	39,47,47	0.91	2 (5%)	54,74,74	2.55	18 (33%)
19	CLA	2	309	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	7 (13%)
19	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	8 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	5	307	1	60,68,73	1.54	5 (8%)	70,107,113	1.42	8 (11%)
19	CLA	3	310	-	56,64,73	1.60	5 (8%)	65,102,113	1.45	7 (10%)
25	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.98	2 (4%)
26	BCR	b	852	-	41,41,41	0.73	0	56,56,56	2.05	15 (26%)
17	XAT	2	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.71	19 (35%)
19	CLA	a	817	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
19	CLA	b	839	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
17	XAT	4	305	-	39,47,47	0.92	1 (2%)	54,74,74	2.74	19 (35%)
19	CLA	b	821	-	50,58,73	1.70	6 (12%)	58,95,113	1.58	10 (17%)
26	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.05	16 (28%)
19	CLA	a	824	-	46,54,73	1.78	6 (13%)	53,90,113	1.49	7 (13%)
17	XAT	4	302	-	39,47,47	0.90	0	54,74,74	2.57	20 (37%)
19	CLA	a	842	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	a	829	-	62,70,73	1.52	5 (8%)	72,109,113	1.40	8 (11%)
19	CLA	b	829	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
17	XAT	3	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.62	19 (35%)
19	CLA	b	809	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
17	XAT	5	304	-	39,47,47	0.89	0	54,74,74	2.86	22 (40%)
19	CLA	3	312	3	59,67,73	1.57	6 (10%)	68,105,113	1.43	7 (10%)
19	CLA	b	808	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	9 (11%)
19	CLA	b	831	-	41,49,73	1.84	6 (14%)	47,84,113	1.64	8 (17%)
19	CLA	b	825	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	7 (9%)
26	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
17	XAT	1	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.52	19 (35%)
17	XAT	2	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.50	18 (33%)
17	XAT	4	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.63	18 (33%)
19	CLA	4	306	2	45,53,73	1.81	5 (11%)	52,89,113	1.58	7 (13%)
17	XAT	3	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.59	20 (37%)
19	CLA	3	315	3	46,54,73	1.78	6 (13%)	53,90,113	1.51	7 (13%)
19	CLA	a	809	6	65,73,73	1.45	5 (7%)	76,113,113	1.43	9 (11%)
19	CLA	l	202	-	42,50,73	1.83	5 (11%)	48,85,113	1.63	7 (14%)
19	CLA	b	836	-	58,66,73	1.56	6 (10%)	67,104,113	1.52	9 (13%)
19	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	9 (14%)
19	CLA	4	310	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
19	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	XAT	2	304	-	39,47,47	0.89	0	54,74,74	2.54	20 (37%)
19	CLA	3	307	3	45,53,73	1.80	6 (13%)	52,89,113	1.56	6 (11%)
19	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
17	XAT	1	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.59	15 (27%)
26	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.93	18 (32%)
19	CLA	f	803	10	52,60,73	1.67	5 (9%)	60,97,113	1.49	8 (13%)
17	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)
19	CLA	a	801	-	65,73,73	1.50	9 (13%)	76,113,113	1.37	7 (9%)
26	BCR	i	101	-	41,41,41	0.74	0	56,56,56	2.14	14 (25%)
19	CLA	2	307	-	47,55,73	1.73	5 (10%)	54,91,113	1.64	7 (12%)
19	CLA	b	816	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
19	CLA	b	833	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
19	CLA	b	812	-	54,62,73	1.67	7 (12%)	67,100,113	1.50	9 (13%)
19	CLA	a	814	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
19	CLA	a	838	-	51,59,73	1.65	6 (11%)	59,96,113	1.56	9 (15%)
19	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.42	8 (12%)
19	CLA	b	817	-	55,63,73	1.62	5 (9%)	64,101,113	1.46	9 (14%)
19	CLA	b	802	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
19	CLA	b	822	-	51,59,73	1.64	5 (9%)	59,96,113	1.57	9 (15%)
19	CLA	4	312	-	46,54,73	1.77	6 (13%)	53,90,113	1.52	7 (13%)
19	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	10 (13%)
19	CLA	3	308	-	47,55,73	1.74	5 (10%)	54,91,113	1.56	8 (14%)
19	CLA	1	314	-	45,53,73	1.80	5 (11%)	52,89,113	1.56	6 (11%)
19	CLA	4	309	-	50,58,73	1.68	5 (10%)	58,95,113	1.56	8 (13%)
19	CLA	a	819	-	54,62,73	1.63	5 (9%)	62,99,113	1.46	7 (11%)
26	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
19	CLA	4	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.56	7 (13%)
24	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.20	4 (9%)
19	CLA	a	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
17	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.58	19 (35%)
19	CLA	b	811	-	65,73,73	1.45	5 (7%)	76,113,113	1.44	8 (10%)
19	CLA	4	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
19	CLA	j	103	12	42,50,73	1.82	5 (11%)	48,85,113	1.64	6 (12%)
19	CLA	3	313	-	52,60,73	1.67	5 (9%)	60,97,113	1.52	9 (15%)
19	CLA	a	813	-	54,62,73	1.64	5 (9%)	62,99,113	1.44	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
19	CLA	a	808	-	51,59,73	1.71	5 (9%)	59,96,113	1.50	8 (13%)
19	CLA	b	806	-	65,73,73	1.46	5 (7%)	76,113,113	1.44	7 (9%)
19	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.53	7 (10%)
19	CLA	2	316	4	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
19	CLA	b	820	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
19	CLA	4	317	-	55,63,73	1.63	5 (9%)	64,101,113	1.46	7 (10%)
19	CLA	b	823	-	60,68,73	1.55	6 (10%)	70,107,113	1.38	7 (10%)
19	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
19	CLA	4	307	-	56,64,73	1.62	6 (10%)	65,102,113	1.43	8 (12%)
19	CLA	a	834	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	9 (11%)
25	LHG	m	101	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
19	CLA	a	802	-	58,66,73	1.55	5 (8%)	67,104,113	1.50	7 (10%)
19	CLA	a	826	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	6 (7%)
19	CLA	b	815	-	55,63,73	1.60	6 (10%)	64,101,113	1.56	7 (10%)
19	CLA	4	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
25	LHG	a	846	19	26,26,48	1.28	5 (19%)	29,32,54	1.21	2 (6%)
26	BCR	j	104	-	41,41,41	0.74	0	56,56,56	2.08	17 (30%)
17	XAT	2	305	-	39,47,47	0.92	1 (2%)	54,74,74	2.43	18 (33%)
17	XAT	j	101	-	39,47,47	0.88	0	54,74,74	2.73	18 (33%)
25	LHG	b	849	19	30,30,48	1.34	6 (20%)	33,36,54	1.15	2 (6%)
19	CLA	a	804	-	55,63,73	1.63	6 (10%)	64,101,113	1.55	10 (15%)
23	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
19	CLA	b	830	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
26	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	18 (32%)
17	XAT	4	303	-	39,47,47	0.89	0	54,74,74	2.57	18 (33%)
19	CLA	4	315	2	41,49,73	1.88	5 (12%)	47,84,113	1.66	8 (17%)
19	CLA	b	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
26	BCR	b	846	-	41,41,41	0.72	0	56,56,56	1.97	20 (35%)
19	CLA	a	810	6	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
19	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
19	CLA	2	314	-	56,64,73	1.61	7 (12%)	65,102,113	1.44	7 (10%)
18	A1L1G	5	303	-	38,47,47	1.42	6 (15%)	49,71,71	1.45	7 (14%)
19	CLA	5	305	1	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
19	CLA	a	832	-	50,58,73	1.69	6 (12%)	58,95,113	1.53	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	b	843	-	41,41,41	0.70	0	56,56,56	2.29	20 (35%)
19	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.38	8 (10%)
19	CLA	5	309	1	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
19	CLA	b	841	25	65,73,73	1.52	5 (7%)	76,113,113	1.36	8 (10%)
19	CLA	l	203	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	8 (11%)
19	CLA	a	823	-	49,57,73	1.67	5 (10%)	55,93,113	1.61	7 (12%)
19	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)
19	CLA	1	310	5	65,73,73	1.51	5 (7%)	76,113,113	1.35	8 (10%)
19	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
19	CLA	b	810	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)
19	CLA	b	818	-	59,67,73	1.55	5 (8%)	68,105,113	1.50	9 (13%)
18	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
18	A1L1G	3	302	-	38,47,47	1.48	6 (15%)	49,71,71	1.38	7 (14%)
19	CLA	5	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.55	7 (13%)
19	CLA	1	312	5	52,60,73	1.71	5 (9%)	60,97,113	1.48	8 (13%)
21	DGD	b	851	-	58,58,67	1.14	7 (12%)	72,72,81	1.53	10 (13%)
26	BCR	a	850	-	41,41,41	0.73	0	56,56,56	2.16	15 (26%)
26	BCR	a	849	-	41,41,41	0.73	0	56,56,56	2.17	20 (35%)
19	CLA	b	807	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
19	CLA	b	838	-	65,73,73	1.52	6 (9%)	76,113,113	1.33	8 (10%)
27	SF4	a	851	-	0,12,12	-	-	-	-	-
17	XAT	5	302	-	39,47,47	0.93	2 (5%)	54,74,74	2.58	20 (37%)
19	CLA	2	313	4	41,49,73	1.84	5 (12%)	47,84,113	1.69	8 (17%)
19	CLA	a	830	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	5	313	1	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
20	SQD	5	316	19	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	837	6	1/1/11/20	4/13/91/115	-
19	CLA	i	102	-	1/1/14/20	9/34/112/115	-
22	LMG	2	317	-	-	11/30/50/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	803	-	1/1/15/20	3/37/115/115	-
17	XAT	3	305	-	-	0/31/93/93	0/4/4/4
19	CLA	5	314	-	1/1/12/20	4/22/100/115	-
19	CLA	a	815	-	1/1/11/20	2/13/91/115	-
19	CLA	b	832	-	1/1/11/20	6/18/96/115	-
21	DGD	4	318	-	-	10/29/69/95	0/2/2/2
19	CLA	b	804	-	1/1/15/20	10/37/115/115	-
17	XAT	2	303	-	-	6/31/93/93	0/4/4/4
20	SQD	1	315	-	-	19/40/60/69	0/1/1/1
26	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	CLA	a	821	-	1/1/11/20	2/13/91/115	-
17	XAT	4	304	-	-	0/31/93/93	0/4/4/4
19	CLA	j	102	-	1/1/13/20	16/29/107/115	-
19	CLA	2	312	-	1/1/11/20	4/16/94/115	-
19	CLA	b	819	-	1/1/14/20	14/31/109/115	-
19	CLA	4	314	2	1/1/11/20	3/13/91/115	-
19	CLA	a	827	-	1/1/15/20	8/37/115/115	-
19	CLA	a	805	19	1/1/13/20	6/25/103/115	-
19	CLA	b	828	-	1/1/15/20	14/37/115/115	-
27	SF4	c	102	-	-	-	0/6/5/5
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2
19	CLA	3	314	3	1/1/11/20	7/16/94/115	-
19	CLA	b	824	-	1/1/12/20	8/23/101/115	-
26	BCR	m	102	-	-	9/29/63/63	0/2/2/2
19	CLA	a	828	-	1/1/15/20	9/37/115/115	-
19	CLA	a	854	-	1/1/15/20	13/37/115/115	-
19	CLA	2	311	-	1/1/13/20	5/29/107/115	-
19	CLA	b	840	-	1/1/15/20	17/37/115/115	-
19	CLA	a	825	-	1/1/13/20	8/25/103/115	-
19	CLA	b	805	-	1/1/15/20	12/37/115/115	-
26	BCR	l	205	-	-	8/29/63/63	0/2/2/2
19	CLA	5	315	-	1/1/11/20	5/15/93/115	-
19	CLA	b	813	-	1/1/12/20	6/23/101/115	-
19	CLA	a	812	19	1/1/14/20	9/34/112/115	-
19	CLA	b	826	-	1/1/14/20	6/36/114/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	5	311	-	1/1/12/20	8/21/99/115	-
19	CLA	b	827	-	1/1/15/20	5/37/115/115	-
19	CLA	1	308	5	1/1/15/20	13/37/115/115	-
19	CLA	2	308	4	1/1/12/20	5/24/102/115	-
26	BCR	b	844	-	-	2/29/63/63	0/2/2/2
19	CLA	l	204	-	1/1/11/20	4/15/93/115	-
19	CLA	1	309	5	1/1/11/20	6/15/93/115	-
19	CLA	b	814	-	1/1/15/20	14/37/115/115	-
19	CLA	1	313	-	1/1/10/20	3/8/86/115	-
19	CLA	b	835	-	1/1/12/20	8/23/101/115	-
19	CLA	1	305	-	1/1/14/20	10/33/111/115	-
26	BCR	b	847	-	-	1/29/63/63	0/2/2/2
19	CLA	a	806	-	1/1/15/20	12/37/115/115	-
18	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
19	CLA	a	816	-	1/1/12/20	5/19/97/115	-
27	SF4	c	101	-	-	-	0/6/5/5
19	CLA	2	306	-	1/1/10/20	2/9/87/115	-
19	CLA	a	807	-	1/1/15/20	18/37/115/115	-
19	CLA	5	312	-	1/1/12/20	0/22/100/115	-
19	CLA	a	811	-	1/1/13/20	8/27/105/115	-
19	CLA	a	844	25	1/1/15/20	16/37/115/115	-
19	CLA	b	834	-	1/1/15/20	14/37/115/115	-
19	CLA	3	309	3	1/1/13/20	5/27/105/115	-
19	CLA	a	839	-	1/1/15/20	15/37/115/115	-
19	CLA	5	308	-	1/1/13/20	4/25/103/115	-
19	CLA	a	841	-	1/1/15/20	15/37/115/115	-
22	LMG	a	853	-	-	13/29/49/70	0/1/1/1
19	CLA	2	315	-	1/1/10/20	1/10/88/115	-
19	CLA	1	307	-	1/1/12/20	6/24/102/115	-
19	CLA	4	313	-	1/1/12/20	6/23/101/115	-
19	CLA	3	311	-	1/1/12/20	4/19/97/115	-
22	LMG	j	105	-	-	11/27/47/70	0/1/1/1
19	CLA	5	306	20	1/1/11/20	7/13/91/115	-
24	PQN	a	843	-	-	5/23/43/43	0/2/2/2
19	CLA	f	802	-	1/1/15/20	13/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	XAT	3	301	-	-	3/31/93/93	0/4/4/4
19	CLA	2	309	-	1/1/11/20	4/15/93/115	-
19	CLA	a	831	-	1/1/15/20	11/37/115/115	-
19	CLA	5	307	1	1/1/14/20	7/31/109/115	-
19	CLA	3	310	-	1/1/13/20	4/27/105/115	-
25	LHG	a	845	-	-	27/52/52/53	-
26	BCR	b	852	-	-	5/29/63/63	0/2/2/2
17	XAT	2	301	-	-	3/31/93/93	0/4/4/4
19	CLA	a	817	-	1/1/11/20	6/13/91/115	-
19	CLA	b	839	-	1/1/15/20	14/37/115/115	-
17	XAT	4	305	-	-	4/31/93/93	0/4/4/4
19	CLA	b	821	-	1/1/12/20	7/19/97/115	-
26	BCR	f	804	-	-	4/29/63/63	0/2/2/2
19	CLA	a	824	-	1/1/11/20	4/15/93/115	-
17	XAT	4	302	-	-	0/31/93/93	0/4/4/4
19	CLA	a	842	-	1/1/15/20	9/37/115/115	-
19	CLA	a	829	-	1/1/14/20	15/34/112/115	-
19	CLA	b	829	-	1/1/15/20	11/37/115/115	-
17	XAT	3	304	-	-	3/31/93/93	0/4/4/4
19	CLA	b	809	-	1/1/15/20	11/37/115/115	-
19	CLA	3	312	3	1/1/13/20	9/30/108/115	-
17	XAT	5	304	-	-	1/31/93/93	0/4/4/4
19	CLA	b	808	-	1/1/15/20	12/37/115/115	-
19	CLA	b	831	-	1/1/10/20	1/8/86/115	-
19	CLA	b	825	-	1/1/15/20	14/37/115/115	-
26	BCR	b	850	-	-	2/29/63/63	0/2/2/2
17	XAT	1	303	-	-	0/31/93/93	0/4/4/4
17	XAT	2	302	-	-	0/31/93/93	0/4/4/4
17	XAT	4	301	-	-	4/31/93/93	0/4/4/4
19	CLA	4	306	2	1/1/11/20	7/13/91/115	-
19	CLA	3	315	3	1/1/11/20	8/15/93/115	-
19	CLA	a	809	6	1/1/15/20	15/37/115/115	-
17	XAT	3	303	-	-	3/31/93/93	0/4/4/4
19	CLA	1	202	-	1/1/10/20	2/10/88/115	-
19	CLA	b	836	-	1/1/13/20	11/29/107/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	311	-	1/1/12/20	6/23/101/115	-
19	CLA	4	310	-	1/1/15/20	16/37/115/115	-
19	CLA	b	837	-	1/1/15/20	8/37/115/115	-
19	CLA	3	307	3	1/1/11/20	1/13/91/115	-
17	XAT	2	304	-	-	3/31/93/93	0/4/4/4
19	CLA	b	801	-	1/1/15/20	20/37/115/115	-
17	XAT	1	302	-	-	0/31/93/93	0/4/4/4
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2
19	CLA	f	803	10	1/1/12/20	2/22/100/115	-
17	XAT	a	852	-	-	7/31/93/93	0/4/4/4
19	CLA	a	801	-	1/1/15/20	22/37/115/115	-
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
19	CLA	2	307	-	1/1/11/20	6/16/94/115	-
19	CLA	b	816	-	1/1/11/20	3/13/91/115	-
19	CLA	b	833	-	1/1/15/20	13/37/115/115	-
19	CLA	b	812	-	1/1/13/20	5/25/101/115	-
19	CLA	a	814	-	1/1/15/20	20/37/115/115	-
19	CLA	a	838	-	1/1/12/20	6/21/99/115	-
19	CLA	a	818	-	1/1/13/20	11/27/105/115	-
19	CLA	b	817	-	1/1/13/20	4/25/103/115	-
19	CLA	b	802	-	1/1/15/20	17/37/115/115	-
19	CLA	b	822	-	1/1/12/20	2/21/99/115	-
19	CLA	4	312	-	1/1/11/20	4/15/93/115	-
19	CLA	1	306	-	1/1/15/20	15/37/115/115	-
19	CLA	3	308	-	1/1/11/20	5/16/94/115	-
19	CLA	1	314	-	1/1/11/20	5/13/91/115	-
19	CLA	4	309	-	1/1/12/20	7/19/97/115	-
19	CLA	a	819	-	1/1/12/20	4/24/102/115	-
26	BCR	b	848	-	-	2/29/63/63	0/2/2/2
19	CLA	4	311	-	1/1/11/20	8/15/93/115	-
24	PQN	b	842	-	-	1/23/43/43	0/2/2/2
19	CLA	a	836	-	1/1/12/20	6/19/97/115	-
17	XAT	5	301	-	-	3/31/93/93	0/4/4/4
19	CLA	b	811	-	1/1/15/20	17/37/115/115	-
19	CLA	4	316	-	1/1/11/20	7/15/93/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	j	103	12	1/1/10/20	5/10/88/115	-
19	CLA	3	313	-	1/1/12/20	1/22/100/115	-
19	CLA	a	813	-	1/1/12/20	10/24/102/115	-
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
19	CLA	a	808	-	1/1/12/20	3/21/99/115	-
19	CLA	b	806	-	1/1/15/20	16/37/115/115	-
19	CLA	a	833	-	1/1/13/20	2/25/103/115	-
19	CLA	2	316	4	1/1/11/20	5/15/93/115	-
19	CLA	b	820	-	1/1/13/20	3/25/103/115	-
19	CLA	4	317	-	1/1/13/20	7/25/103/115	-
19	CLA	b	823	-	1/1/14/20	7/31/109/115	-
19	CLA	a	822	-	1/1/15/20	5/37/115/115	-
19	CLA	4	307	-	1/1/13/20	7/27/105/115	-
19	CLA	a	834	-	1/1/15/20	7/37/115/115	-
25	LHG	m	101	-	-	28/50/50/53	-
19	CLA	a	802	-	1/1/13/20	7/29/107/115	-
19	CLA	a	826	-	1/1/15/20	9/37/115/115	-
19	CLA	b	815	-	1/1/13/20	13/25/103/115	-
19	CLA	4	308	-	1/1/15/20	14/37/115/115	-
25	LHG	a	846	19	-	16/31/31/53	-
26	BCR	j	104	-	-	4/29/63/63	0/2/2/2
17	XAT	2	305	-	-	2/31/93/93	0/4/4/4
17	XAT	j	101	-	-	5/31/93/93	0/4/4/4
25	LHG	b	849	19	-	20/35/35/53	-
19	CLA	a	804	-	1/1/13/20	10/25/103/115	-
23	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
19	CLA	b	830	-	1/1/15/20	10/37/115/115	-
26	BCR	l	201	-	-	4/29/63/63	0/2/2/2
19	CLA	4	315	2	1/1/10/20	5/8/86/115	-
19	CLA	b	803	-	1/1/15/20	18/37/115/115	-
17	XAT	4	303	-	-	3/31/93/93	0/4/4/4
26	BCR	b	846	-	-	0/29/63/63	0/2/2/2
19	CLA	a	810	6	1/1/15/20	13/37/115/115	-
19	CLA	a	835	-	1/1/15/20	12/37/115/115	-
19	CLA	2	314	-	1/1/13/20	13/27/105/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	5	305	1	1/1/11/20	4/15/93/115	-
19	CLA	a	832	-	1/1/12/20	5/19/97/115	-
18	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2
19	CLA	a	840	-	1/1/15/20	8/37/115/115	-
19	CLA	5	309	1	1/1/15/20	14/37/115/115	-
19	CLA	b	841	25	1/1/15/20	9/37/115/115	-
19	CLA	l	203	-	1/1/14/20	6/31/109/115	-
19	CLA	a	823	-	1/1/11/20	7/18/96/115	-
19	CLA	a	820	-	1/1/15/20	15/37/115/115	-
19	CLA	1	310	5	1/1/15/20	18/37/115/115	-
19	CLA	2	310	-	1/1/15/20	14/37/115/115	-
19	CLA	b	810	-	1/1/15/20	16/37/115/115	-
19	CLA	b	818	-	1/1/13/20	10/30/108/115	-
19	CLA	5	310	-	1/1/11/20	6/15/93/115	-
18	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
19	CLA	1	312	5	1/1/12/20	3/22/100/115	-
18	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
21	DGD	b	851	-	-	20/46/86/95	0/2/2/2
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
19	CLA	b	807	-	1/1/15/20	19/37/115/115	-
19	CLA	b	838	-	1/1/15/20	8/37/115/115	-
27	SF4	a	851	-	-	-	0/6/5/5
17	XAT	5	302	-	-	3/31/93/93	0/4/4/4
19	CLA	2	313	4	1/1/10/20	4/8/86/115	-
19	CLA	a	830	-	1/1/15/20	15/37/115/115	-
19	CLA	5	313	1	1/1/11/20	5/13/91/115	-
20	SQD	5	316	19	-	11/30/50/69	0/1/1/1

All (912) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	312	CLA	C4B-NB	7.99	1.42	1.35
19	a	818	CLA	C4B-NB	7.76	1.42	1.35
19	a	840	CLA	C4B-NB	7.74	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	315	CLA	C4B-NB	7.73	1.42	1.35
19	4	315	CLA	C4B-NB	7.72	1.42	1.35
19	b	838	CLA	C4B-NB	7.70	1.42	1.35
19	5	313	CLA	C4B-NB	7.68	1.42	1.35
19	4	306	CLA	C4B-NB	7.68	1.42	1.35
19	1	309	CLA	C4B-NB	7.67	1.42	1.35
19	1	314	CLA	C4B-NB	7.66	1.42	1.35
19	a	842	CLA	C4B-NB	7.66	1.42	1.35
19	1	305	CLA	C4B-NB	7.65	1.42	1.35
19	b	821	CLA	C4B-NB	7.65	1.42	1.35
19	3	315	CLA	C4B-NB	7.64	1.42	1.35
19	i	102	CLA	C4B-NB	7.63	1.42	1.35
19	4	307	CLA	C4B-NB	7.63	1.42	1.35
19	a	808	CLA	C4B-NB	7.62	1.42	1.35
19	b	835	CLA	C4B-NB	7.61	1.42	1.35
19	a	825	CLA	C4B-NB	7.61	1.42	1.35
19	b	830	CLA	C4B-NB	7.60	1.42	1.35
19	f	803	CLA	C4B-NB	7.60	1.42	1.35
24	a	843	PQN	C3-C2	7.58	1.49	1.35
19	a	831	CLA	C4B-NB	7.58	1.42	1.35
19	4	317	CLA	C4B-NB	7.58	1.42	1.35
19	b	802	CLA	C4B-NB	7.57	1.42	1.35
19	j	102	CLA	C4B-NB	7.57	1.42	1.35
19	4	311	CLA	C4B-NB	7.57	1.42	1.35
19	b	840	CLA	C4B-NB	7.56	1.41	1.35
19	b	801	CLA	C4B-NB	7.55	1.41	1.35
19	4	314	CLA	C4B-NB	7.55	1.41	1.35
19	3	311	CLA	C4B-NB	7.55	1.41	1.35
19	a	804	CLA	C4B-NB	7.55	1.41	1.35
19	2	312	CLA	C4B-NB	7.54	1.41	1.35
19	a	824	CLA	C4B-NB	7.54	1.41	1.35
19	b	841	CLA	C4B-NB	7.54	1.41	1.35
19	2	308	CLA	C4B-NB	7.54	1.41	1.35
19	4	310	CLA	C4B-NB	7.54	1.41	1.35
19	4	312	CLA	C4B-NB	7.54	1.41	1.35
19	4	313	CLA	C4B-NB	7.54	1.41	1.35
19	4	316	CLA	C4B-NB	7.54	1.41	1.35
19	1	202	CLA	C4B-NB	7.54	1.41	1.35
19	2	311	CLA	C4B-NB	7.53	1.41	1.35
19	5	310	CLA	C4B-NB	7.53	1.41	1.35
19	a	817	CLA	C4B-NB	7.53	1.41	1.35
19	b	827	CLA	C4B-NB	7.53	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	813	CLA	C4B-NB	7.53	1.41	1.35
19	2	314	CLA	C4B-NB	7.52	1.41	1.35
19	a	805	CLA	C4B-NB	7.52	1.41	1.35
19	5	305	CLA	C4B-NB	7.51	1.41	1.35
19	2	310	CLA	C4B-NB	7.51	1.41	1.35
19	b	837	CLA	C4B-NB	7.50	1.41	1.35
19	3	313	CLA	C4B-NB	7.50	1.41	1.35
19	5	306	CLA	C4B-NB	7.49	1.41	1.35
19	5	315	CLA	C4B-NB	7.49	1.41	1.35
19	1	313	CLA	C4B-NB	7.49	1.41	1.35
19	1	310	CLA	C4B-NB	7.49	1.41	1.35
19	b	829	CLA	C4B-NB	7.49	1.41	1.35
19	a	820	CLA	C4B-NB	7.49	1.41	1.35
19	b	805	CLA	C4B-NB	7.49	1.41	1.35
19	3	310	CLA	C4B-NB	7.48	1.41	1.35
19	a	841	CLA	C4B-NB	7.48	1.41	1.35
19	a	829	CLA	C4B-NB	7.47	1.41	1.35
19	b	828	CLA	C4B-NB	7.47	1.41	1.35
19	3	307	CLA	C4B-NB	7.47	1.41	1.35
19	2	309	CLA	C4B-NB	7.46	1.41	1.35
19	2	316	CLA	C4B-NB	7.46	1.41	1.35
19	a	822	CLA	C4B-NB	7.46	1.41	1.35
19	b	825	CLA	C4B-NB	7.46	1.41	1.35
19	b	817	CLA	C4B-NB	7.46	1.41	1.35
19	3	312	CLA	C4B-NB	7.45	1.41	1.35
19	b	823	CLA	C4B-NB	7.45	1.41	1.35
19	5	309	CLA	C4B-NB	7.45	1.41	1.35
19	f	802	CLA	C4B-NB	7.45	1.41	1.35
19	b	804	CLA	C4B-NB	7.45	1.41	1.35
19	b	819	CLA	C4B-NB	7.45	1.41	1.35
19	b	808	CLA	C4B-NB	7.44	1.41	1.35
19	a	854	CLA	C4B-NB	7.44	1.41	1.35
19	4	309	CLA	C4B-NB	7.44	1.41	1.35
19	1	307	CLA	C4B-NB	7.44	1.41	1.35
19	b	815	CLA	C4B-NB	7.43	1.41	1.35
19	a	834	CLA	C4B-NB	7.43	1.41	1.35
19	3	308	CLA	C4B-NB	7.43	1.41	1.35
19	b	832	CLA	C4B-NB	7.43	1.41	1.35
19	a	810	CLA	C4B-NB	7.43	1.41	1.35
19	b	812	CLA	C4B-NB	7.42	1.41	1.35
19	a	837	CLA	C4B-NB	7.42	1.41	1.35
19	b	834	CLA	C4B-NB	7.42	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	812	CLA	C4B-NB	7.41	1.41	1.35
19	2	306	CLA	C4B-NB	7.41	1.41	1.35
19	j	103	CLA	C4B-NB	7.40	1.41	1.35
19	a	826	CLA	C4B-NB	7.40	1.41	1.35
24	b	842	PQN	C3-C2	7.40	1.48	1.35
19	2	313	CLA	C4B-NB	7.39	1.41	1.35
19	a	827	CLA	C4B-NB	7.39	1.41	1.35
19	a	830	CLA	C4B-NB	7.38	1.41	1.35
19	5	307	CLA	C4B-NB	7.38	1.41	1.35
19	l	203	CLA	C4B-NB	7.37	1.41	1.35
19	a	816	CLA	C4B-NB	7.37	1.41	1.35
19	l	204	CLA	C4B-NB	7.36	1.41	1.35
19	b	809	CLA	C4B-NB	7.36	1.41	1.35
19	5	311	CLA	C4B-NB	7.36	1.41	1.35
19	a	821	CLA	C4B-NB	7.36	1.41	1.35
19	1	306	CLA	C4B-NB	7.35	1.41	1.35
19	1	308	CLA	C4B-NB	7.34	1.41	1.35
19	a	836	CLA	C4B-NB	7.34	1.41	1.35
19	b	833	CLA	C4B-NB	7.34	1.41	1.35
19	a	811	CLA	C4B-NB	7.34	1.41	1.35
19	a	835	CLA	C4B-NB	7.34	1.41	1.35
19	b	803	CLA	C4B-NB	7.34	1.41	1.35
19	b	810	CLA	C4B-NB	7.33	1.41	1.35
19	a	815	CLA	C4B-NB	7.33	1.41	1.35
19	a	832	CLA	C4B-NB	7.33	1.41	1.35
19	a	839	CLA	C4B-NB	7.33	1.41	1.35
19	3	309	CLA	C4B-NB	7.33	1.41	1.35
19	b	839	CLA	C4B-NB	7.33	1.41	1.35
19	a	823	CLA	C4B-NB	7.32	1.41	1.35
19	a	844	CLA	C4B-NB	7.32	1.41	1.35
19	a	803	CLA	C4B-NB	7.32	1.41	1.35
19	5	312	CLA	C4B-NB	7.31	1.41	1.35
19	5	308	CLA	C4B-NB	7.30	1.41	1.35
19	b	816	CLA	C4B-NB	7.29	1.41	1.35
19	5	314	CLA	C4B-NB	7.28	1.41	1.35
19	b	814	CLA	C4B-NB	7.28	1.41	1.35
19	b	820	CLA	C4B-NB	7.28	1.41	1.35
19	a	819	CLA	C4B-NB	7.27	1.41	1.35
19	a	833	CLA	C4B-NB	7.26	1.41	1.35
19	b	831	CLA	C4B-NB	7.26	1.41	1.35
19	3	314	CLA	C4B-NB	7.25	1.41	1.35
19	a	802	CLA	C4B-NB	7.25	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	814	CLA	C4B-NB	7.24	1.41	1.35
19	b	826	CLA	C4B-NB	7.24	1.41	1.35
19	b	824	CLA	C4B-NB	7.24	1.41	1.35
19	b	813	CLA	C4B-NB	7.24	1.41	1.35
19	1	311	CLA	C4B-NB	7.23	1.41	1.35
19	a	807	CLA	C4B-NB	7.23	1.41	1.35
19	b	836	CLA	C4B-NB	7.21	1.41	1.35
19	b	806	CLA	C4B-NB	7.20	1.41	1.35
19	a	801	CLA	C4B-NB	7.20	1.41	1.35
19	a	838	CLA	C4B-NB	7.20	1.41	1.35
19	2	307	CLA	C4B-NB	7.19	1.41	1.35
19	b	818	CLA	C4B-NB	7.18	1.41	1.35
19	b	807	CLA	C4B-NB	7.17	1.41	1.35
19	a	828	CLA	C4B-NB	7.16	1.41	1.35
19	b	822	CLA	C4B-NB	7.16	1.41	1.35
19	4	308	CLA	C4B-NB	7.16	1.41	1.35
19	a	809	CLA	C4B-NB	7.13	1.41	1.35
19	b	811	CLA	C4B-NB	7.13	1.41	1.35
19	a	806	CLA	C4B-NB	6.04	1.40	1.35
24	b	842	PQN	C10-C5	4.83	1.48	1.40
24	a	843	PQN	C10-C5	4.82	1.48	1.40
20	5	316	SQD	O8-S	4.62	1.64	1.47
20	1	315	SQD	O8-S	4.59	1.63	1.47
23	1	304	A1L1F	O7-C54	4.48	1.45	1.35
20	1	315	SQD	O48-C23	4.31	1.45	1.33
22	a	853	LMG	O8-C28	4.26	1.45	1.33
20	5	316	SQD	O48-C23	4.22	1.45	1.33
23	1	304	A1L1F	O13-C45	4.22	1.45	1.33
20	1	315	SQD	O47-C7	4.17	1.46	1.34
22	a	853	LMG	O7-C10	4.13	1.46	1.34
22	j	105	LMG	O8-C28	4.10	1.45	1.33
20	5	316	SQD	O47-C7	4.08	1.45	1.34
19	a	806	CLA	C4D-ND	-4.08	1.32	1.37
22	2	317	LMG	O8-C28	4.06	1.45	1.33
21	4	318	DGD	O1G-C1A	4.03	1.45	1.33
19	2	313	CLA	C1D-ND	4.00	1.42	1.37
21	b	851	DGD	O2G-C1B	3.99	1.45	1.34
19	b	827	CLA	C1D-ND	3.96	1.42	1.37
19	a	804	CLA	C1D-ND	3.96	1.42	1.37
21	b	851	DGD	O1G-C1A	3.95	1.44	1.33
19	1	310	CLA	C1D-ND	3.94	1.42	1.37
22	2	317	LMG	O7-C10	3.94	1.45	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	837	CLA	C1D-ND	3.93	1.42	1.37
19	3	308	CLA	C1D-ND	3.93	1.42	1.37
19	5	308	CLA	C1D-ND	3.92	1.42	1.37
19	3	314	CLA	C1D-ND	3.92	1.42	1.37
18	1	301	A1L1G	C38-C39	3.91	1.41	1.35
22	j	105	LMG	O7-C10	3.90	1.45	1.34
19	3	313	CLA	C1D-ND	3.90	1.42	1.37
19	a	828	CLA	C1D-ND	3.90	1.42	1.37
19	1	312	CLA	C1D-ND	3.89	1.42	1.37
19	5	310	CLA	C1D-ND	3.89	1.42	1.37
19	4	307	CLA	C1D-ND	3.89	1.42	1.37
19	a	840	CLA	C1D-ND	3.89	1.42	1.37
19	4	316	CLA	C1D-ND	3.89	1.42	1.37
19	2	307	CLA	C1D-ND	3.89	1.42	1.37
19	5	314	CLA	C1D-ND	3.88	1.42	1.37
19	a	814	CLA	C1D-ND	3.88	1.42	1.37
19	j	103	CLA	C1D-ND	3.88	1.42	1.37
19	a	839	CLA	C1D-ND	3.87	1.42	1.37
19	4	314	CLA	C1D-ND	3.87	1.42	1.37
19	5	311	CLA	C1D-ND	3.87	1.42	1.37
19	5	305	CLA	C1D-ND	3.87	1.42	1.37
19	2	314	CLA	C1D-ND	3.86	1.42	1.37
19	b	834	CLA	C1D-ND	3.86	1.42	1.37
19	b	825	CLA	C1D-ND	3.85	1.42	1.37
19	a	825	CLA	C1D-ND	3.85	1.42	1.37
19	4	315	CLA	C1D-ND	3.85	1.42	1.37
19	l	204	CLA	C1D-ND	3.84	1.42	1.37
19	b	819	CLA	C1D-ND	3.84	1.42	1.37
19	b	840	CLA	C1D-ND	3.84	1.42	1.37
19	b	821	CLA	C1D-ND	3.84	1.42	1.37
19	a	816	CLA	C1D-ND	3.84	1.42	1.37
19	3	311	CLA	C1D-ND	3.84	1.42	1.37
19	3	315	CLA	C1D-ND	3.84	1.42	1.37
19	2	315	CLA	C1D-ND	3.84	1.42	1.37
19	b	841	CLA	C1D-ND	3.83	1.42	1.37
19	2	312	CLA	C1D-ND	3.83	1.42	1.37
19	l	202	CLA	C1D-ND	3.83	1.42	1.37
21	4	318	DGD	O2G-C1B	3.83	1.45	1.34
19	b	839	CLA	C1D-ND	3.83	1.42	1.37
19	3	312	CLA	C1D-ND	3.83	1.42	1.37
19	a	811	CLA	C1D-ND	3.83	1.42	1.37
19	2	311	CLA	C1D-ND	3.82	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	309	CLA	C1D-ND	3.82	1.42	1.37
19	b	816	CLA	C1D-ND	3.82	1.42	1.37
19	a	829	CLA	C1D-ND	3.82	1.42	1.37
19	a	815	CLA	C1D-ND	3.81	1.42	1.37
19	2	306	CLA	C1D-ND	3.81	1.42	1.37
19	b	836	CLA	C1D-ND	3.81	1.42	1.37
19	1	307	CLA	C1D-ND	3.81	1.42	1.37
19	a	835	CLA	C1D-ND	3.81	1.42	1.37
19	b	818	CLA	C1D-ND	3.81	1.42	1.37
19	4	310	CLA	C1D-ND	3.80	1.42	1.37
19	3	310	CLA	C1D-ND	3.80	1.42	1.37
19	b	835	CLA	C1D-ND	3.80	1.42	1.37
19	a	832	CLA	C1D-ND	3.80	1.42	1.37
19	5	309	CLA	C1D-ND	3.80	1.42	1.37
19	4	317	CLA	C1D-ND	3.80	1.42	1.37
19	b	813	CLA	C1D-ND	3.80	1.42	1.37
19	4	312	CLA	C1D-ND	3.80	1.42	1.37
19	a	809	CLA	C1D-ND	3.80	1.42	1.37
19	a	842	CLA	C1D-ND	3.80	1.42	1.37
19	a	826	CLA	C1D-ND	3.79	1.42	1.37
19	f	802	CLA	C1D-ND	3.79	1.42	1.37
19	a	836	CLA	C1D-ND	3.79	1.42	1.37
19	a	813	CLA	C1D-ND	3.79	1.42	1.37
19	b	805	CLA	C1D-ND	3.79	1.42	1.37
19	a	838	CLA	C1D-ND	3.79	1.42	1.37
19	5	315	CLA	C1D-ND	3.79	1.42	1.37
19	1	314	CLA	C1D-ND	3.78	1.42	1.37
19	b	820	CLA	C1D-ND	3.78	1.42	1.37
19	a	844	CLA	C1D-ND	3.78	1.42	1.37
19	b	832	CLA	C1D-ND	3.78	1.42	1.37
19	i	102	CLA	C1D-ND	3.78	1.42	1.37
19	2	308	CLA	C1D-ND	3.78	1.42	1.37
19	4	309	CLA	C1D-ND	3.78	1.42	1.37
19	a	817	CLA	C1D-ND	3.77	1.42	1.37
19	4	306	CLA	C1D-ND	3.77	1.42	1.37
19	b	807	CLA	C1D-ND	3.77	1.42	1.37
19	f	803	CLA	C1D-ND	3.77	1.42	1.37
19	a	824	CLA	C1D-ND	3.77	1.42	1.37
18	1	301	A1L1G	C35-C34	3.76	1.40	1.35
19	a	854	CLA	C1D-ND	3.76	1.42	1.37
19	5	306	CLA	C1D-ND	3.76	1.42	1.37
19	a	834	CLA	C1D-ND	3.76	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	309	CLA	C1D-ND	3.76	1.42	1.37
19	b	814	CLA	C1D-ND	3.76	1.42	1.37
19	4	313	CLA	C1D-ND	3.76	1.42	1.37
19	a	822	CLA	C1D-ND	3.76	1.42	1.37
19	a	808	CLA	C1D-ND	3.76	1.42	1.37
19	a	819	CLA	C1D-ND	3.75	1.42	1.37
19	5	313	CLA	C1D-ND	3.75	1.42	1.37
19	a	841	CLA	C1D-ND	3.75	1.42	1.37
19	5	312	CLA	C1D-ND	3.75	1.42	1.37
19	b	817	CLA	C1D-ND	3.75	1.42	1.37
19	3	309	CLA	C1D-ND	3.75	1.42	1.37
19	b	822	CLA	C1D-ND	3.75	1.42	1.37
19	1	306	CLA	C1D-ND	3.75	1.42	1.37
19	a	807	CLA	C1D-ND	3.75	1.42	1.37
19	1	311	CLA	C1D-ND	3.75	1.42	1.37
19	1	308	CLA	C1D-ND	3.74	1.42	1.37
19	b	815	CLA	C1D-ND	3.74	1.42	1.37
19	b	829	CLA	C1D-ND	3.74	1.42	1.37
19	b	808	CLA	C1D-ND	3.74	1.42	1.37
19	b	830	CLA	C1D-ND	3.74	1.42	1.37
19	b	838	CLA	C1D-ND	3.74	1.42	1.37
19	b	828	CLA	C1D-ND	3.73	1.42	1.37
19	a	805	CLA	C1D-ND	3.73	1.42	1.37
19	a	823	CLA	C1D-ND	3.73	1.42	1.37
19	4	308	CLA	C1D-ND	3.73	1.42	1.37
19	1	305	CLA	C1D-ND	3.73	1.42	1.37
18	3	302	A1L1G	C35-C34	3.73	1.40	1.35
19	b	811	CLA	C1D-ND	3.73	1.42	1.37
19	b	823	CLA	C1D-ND	3.73	1.42	1.37
19	3	307	CLA	C1D-ND	3.72	1.42	1.37
19	a	821	CLA	C1D-ND	3.72	1.42	1.37
19	b	801	CLA	C1D-ND	3.72	1.42	1.37
19	a	818	CLA	C1D-ND	3.72	1.42	1.37
19	a	820	CLA	C1D-ND	3.72	1.42	1.37
19	b	826	CLA	C1D-ND	3.71	1.42	1.37
19	a	831	CLA	C1D-ND	3.71	1.42	1.37
19	a	827	CLA	C1D-ND	3.70	1.42	1.37
19	1	313	CLA	C1D-ND	3.70	1.42	1.37
19	a	810	CLA	C1D-ND	3.70	1.42	1.37
19	j	102	CLA	C1D-ND	3.70	1.42	1.37
19	a	812	CLA	C1D-ND	3.69	1.42	1.37
19	b	809	CLA	C1D-ND	3.69	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	307	CLA	C1D-ND	3.68	1.42	1.37
19	1	203	CLA	C1D-ND	3.66	1.42	1.37
19	b	810	CLA	C1D-ND	3.66	1.42	1.37
19	2	310	CLA	C1D-ND	3.66	1.42	1.37
19	a	830	CLA	C1D-ND	3.66	1.42	1.37
19	a	803	CLA	C1D-ND	3.66	1.42	1.37
19	b	837	CLA	C1D-ND	3.65	1.42	1.37
19	b	802	CLA	C1D-ND	3.64	1.42	1.37
18	3	302	A1L1G	C38-C39	3.64	1.40	1.35
19	2	316	CLA	C1D-ND	3.64	1.42	1.37
18	3	306	A1L1G	C38-C39	3.62	1.40	1.35
26	m	102	BCR	C1-C6	-3.62	1.48	1.53
19	a	802	CLA	C1D-ND	3.61	1.42	1.37
19	b	806	CLA	C1D-ND	3.61	1.42	1.37
19	4	311	CLA	C1D-ND	3.60	1.42	1.37
19	b	824	CLA	C1D-ND	3.60	1.42	1.37
19	b	812	CLA	C1D-ND	3.60	1.42	1.37
19	b	833	CLA	C1D-ND	3.58	1.42	1.37
19	b	803	CLA	C1D-ND	3.58	1.42	1.37
23	1	304	A1L1F	C57-C2	-3.57	1.26	1.32
18	5	303	A1L1G	C38-C39	3.54	1.40	1.35
19	a	801	CLA	C1D-ND	3.54	1.42	1.37
19	b	831	CLA	C1D-ND	3.53	1.42	1.37
18	5	303	A1L1G	C35-C34	3.50	1.40	1.35
19	b	812	CLA	CAB-C3B	-3.48	1.44	1.51
19	a	833	CLA	C1D-ND	3.47	1.42	1.37
18	3	306	A1L1G	C35-C34	3.45	1.40	1.35
18	3	302	A1L1G	C42-C44	3.44	1.40	1.35
19	4	313	CLA	CHC-C1C	3.35	1.43	1.35
19	b	817	CLA	CHC-C1C	3.27	1.43	1.35
19	a	802	CLA	CHC-C1C	3.26	1.43	1.35
19	b	839	CLA	CHC-C1C	3.25	1.43	1.35
19	i	102	CLA	CHC-C1C	3.25	1.43	1.35
19	a	822	CLA	CHC-C1C	3.25	1.43	1.35
19	b	804	CLA	C1D-ND	3.25	1.41	1.37
19	2	308	CLA	CHC-C1C	3.25	1.43	1.35
19	a	818	CLA	CHC-C1C	3.24	1.43	1.35
19	4	312	CLA	CHC-C1C	3.23	1.43	1.35
19	b	812	CLA	CHC-C1C	3.23	1.43	1.35
19	b	815	CLA	CHC-C1C	3.22	1.43	1.35
19	a	819	CLA	CHC-C1C	3.22	1.43	1.35
19	1	308	CLA	CHC-C1C	3.22	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	804	CLA	CHC-C1C	3.22	1.43	1.35
19	a	820	CLA	CHC-C1C	3.21	1.43	1.35
19	b	805	CLA	CHC-C1C	3.21	1.43	1.35
19	b	837	CLA	CHC-C1C	3.21	1.43	1.35
19	a	813	CLA	CHC-C1C	3.21	1.43	1.35
19	a	826	CLA	CHC-C1C	3.20	1.43	1.35
19	5	315	CLA	CHC-C1C	3.20	1.43	1.35
19	b	826	CLA	CHC-C1C	3.20	1.43	1.35
19	b	836	CLA	CHC-C1C	3.20	1.43	1.35
19	2	315	CLA	CHC-C1C	3.20	1.43	1.35
19	2	309	CLA	CHC-C1C	3.20	1.43	1.35
19	1	310	CLA	CHC-C1C	3.20	1.43	1.35
19	b	814	CLA	CHC-C1C	3.20	1.43	1.35
19	5	311	CLA	CHC-C1C	3.20	1.43	1.35
19	a	841	CLA	CHC-C1C	3.19	1.43	1.35
19	b	829	CLA	CHC-C1C	3.19	1.43	1.35
19	5	312	CLA	CHC-C1C	3.19	1.43	1.35
19	3	315	CLA	CHC-C1C	3.19	1.43	1.35
19	a	808	CLA	CHC-C1C	3.19	1.43	1.35
19	b	813	CLA	CHC-C1C	3.19	1.43	1.35
19	b	835	CLA	CHC-C1C	3.19	1.43	1.35
19	5	313	CLA	CHC-C1C	3.19	1.43	1.35
19	a	829	CLA	CHC-C1C	3.19	1.43	1.35
19	b	806	CLA	CHC-C1C	3.19	1.43	1.35
19	a	827	CLA	CHC-C1C	3.18	1.43	1.35
19	5	314	CLA	CHC-C1C	3.18	1.43	1.35
19	b	816	CLA	CHC-C1C	3.18	1.43	1.35
19	4	308	CLA	CHC-C1C	3.18	1.43	1.35
19	a	837	CLA	CHC-C1C	3.18	1.43	1.35
19	1	309	CLA	CHC-C1C	3.18	1.43	1.35
19	a	854	CLA	CHC-C1C	3.18	1.43	1.35
19	b	809	CLA	CHC-C1C	3.18	1.43	1.35
19	b	818	CLA	CHC-C1C	3.18	1.43	1.35
19	a	809	CLA	CHC-C1C	3.18	1.43	1.35
19	3	313	CLA	CHC-C1C	3.18	1.43	1.35
19	1	312	CLA	CHC-C1C	3.18	1.43	1.35
19	5	309	CLA	CHC-C1C	3.18	1.43	1.35
19	3	307	CLA	CHC-C1C	3.18	1.43	1.35
19	3	311	CLA	CHC-C1C	3.17	1.43	1.35
19	5	306	CLA	CHC-C1C	3.17	1.43	1.35
19	b	838	CLA	CHC-C1C	3.17	1.43	1.35
19	b	802	CLA	CHC-C1C	3.17	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	307	CLA	CHC-C1C	3.17	1.43	1.35
19	a	844	CLA	CHC-C1C	3.17	1.43	1.35
19	a	833	CLA	CHC-C1C	3.17	1.43	1.35
19	2	311	CLA	CHC-C1C	3.17	1.43	1.35
19	b	832	CLA	CHC-C1C	3.17	1.43	1.35
19	2	316	CLA	CHC-C1C	3.17	1.43	1.35
19	3	309	CLA	CHC-C1C	3.16	1.43	1.35
19	b	834	CLA	CHC-C1C	3.16	1.43	1.35
19	a	815	CLA	CHC-C1C	3.16	1.43	1.35
19	b	807	CLA	CHC-C1C	3.16	1.43	1.35
19	b	833	CLA	CHC-C1C	3.16	1.43	1.35
19	4	314	CLA	CHC-C1C	3.16	1.43	1.35
19	1	311	CLA	CHC-C1C	3.16	1.43	1.35
19	a	828	CLA	CHC-C1C	3.16	1.43	1.35
19	1	314	CLA	CHC-C1C	3.16	1.43	1.35
19	4	315	CLA	CHC-C1C	3.16	1.43	1.35
19	2	313	CLA	CHC-C1C	3.16	1.43	1.35
19	4	309	CLA	CHC-C1C	3.16	1.43	1.35
19	a	814	CLA	CHC-C1C	3.16	1.43	1.35
19	l	202	CLA	CHC-C1C	3.16	1.43	1.35
19	a	811	CLA	CHC-C1C	3.15	1.43	1.35
19	j	102	CLA	CHC-C1C	3.15	1.43	1.35
19	a	828	CLA	C4D-ND	-3.15	1.33	1.37
19	l	204	CLA	CHC-C1C	3.15	1.43	1.35
19	5	310	CLA	CHC-C1C	3.15	1.43	1.35
19	b	824	CLA	CHC-C1C	3.15	1.43	1.35
19	4	310	CLA	CHC-C1C	3.15	1.43	1.35
19	a	805	CLA	CHC-C1C	3.15	1.43	1.35
19	a	816	CLA	CHC-C1C	3.15	1.43	1.35
19	a	842	CLA	CHC-C1C	3.15	1.43	1.35
19	a	839	CLA	CHC-C1C	3.15	1.43	1.35
19	a	832	CLA	CHC-C1C	3.15	1.43	1.35
19	b	831	CLA	CHC-C1C	3.15	1.43	1.35
19	f	803	CLA	CHC-C1C	3.15	1.43	1.35
19	a	803	CLA	CHC-C1C	3.15	1.43	1.35
19	l	203	CLA	CHC-C1C	3.15	1.43	1.35
19	2	312	CLA	CHC-C1C	3.15	1.43	1.35
19	4	317	CLA	CHC-C1C	3.14	1.43	1.35
19	4	307	CLA	CHC-C1C	3.14	1.43	1.35
19	a	824	CLA	CHC-C1C	3.14	1.43	1.35
19	b	828	CLA	CHC-C1C	3.14	1.43	1.35
19	5	305	CLA	CHC-C1C	3.14	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	840	CLA	CHC-C1C	3.14	1.43	1.35
19	b	804	CLA	CHC-C1C	3.14	1.43	1.35
19	a	817	CLA	CHC-C1C	3.14	1.43	1.35
19	b	841	CLA	CHC-C1C	3.14	1.43	1.35
19	a	834	CLA	CHC-C1C	3.14	1.43	1.35
19	a	812	CLA	CHC-C1C	3.14	1.43	1.35
19	5	307	CLA	CHC-C1C	3.14	1.43	1.35
19	3	312	CLA	CHC-C1C	3.13	1.43	1.35
19	2	310	CLA	CHC-C1C	3.13	1.43	1.35
19	b	818	CLA	C4D-ND	-3.13	1.33	1.37
19	1	313	CLA	CHC-C1C	3.13	1.43	1.35
19	3	314	CLA	CHC-C1C	3.13	1.43	1.35
19	4	306	CLA	CHC-C1C	3.13	1.43	1.35
19	a	825	CLA	CHC-C1C	3.12	1.43	1.35
19	3	310	CLA	CHC-C1C	3.12	1.43	1.35
19	f	802	CLA	CHC-C1C	3.12	1.43	1.35
19	a	830	CLA	CHC-C1C	3.12	1.43	1.35
19	b	822	CLA	CHC-C1C	3.12	1.43	1.35
19	a	836	CLA	CHC-C1C	3.12	1.43	1.35
19	1	305	CLA	CHC-C1C	3.12	1.43	1.35
19	4	308	CLA	C4D-ND	-3.12	1.33	1.37
19	2	314	CLA	CHC-C1C	3.12	1.43	1.35
19	b	823	CLA	CHC-C1C	3.12	1.43	1.35
19	b	803	CLA	CHC-C1C	3.12	1.43	1.35
19	a	823	CLA	CHC-C1C	3.12	1.43	1.35
26	m	102	BCR	C30-C25	-3.11	1.49	1.53
19	a	838	CLA	CHC-C1C	3.11	1.42	1.35
19	3	309	CLA	C4D-ND	-3.11	1.33	1.37
19	b	821	CLA	CHC-C1C	3.11	1.42	1.35
19	2	306	CLA	CHC-C1C	3.11	1.42	1.35
19	a	821	CLA	CHC-C1C	3.11	1.42	1.35
19	5	308	CLA	CHC-C1C	3.10	1.42	1.35
19	4	316	CLA	CHC-C1C	3.10	1.42	1.35
19	b	801	CLA	CHC-C1C	3.10	1.42	1.35
19	3	308	CLA	CHC-C1C	3.10	1.42	1.35
19	b	820	CLA	CHC-C1C	3.10	1.42	1.35
19	b	827	CLA	C4D-ND	-3.10	1.33	1.37
19	b	841	CLA	C4D-ND	-3.10	1.33	1.37
19	b	825	CLA	CHC-C1C	3.09	1.42	1.35
19	5	307	CLA	C4D-ND	-3.09	1.33	1.37
19	a	835	CLA	CHC-C1C	3.09	1.42	1.35
19	1	306	CLA	CHC-C1C	3.09	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	810	CLA	CHC-C1C	3.09	1.42	1.35
19	4	311	CLA	CHC-C1C	3.09	1.42	1.35
19	a	830	CLA	C4D-ND	-3.09	1.33	1.37
19	b	820	CLA	C4D-ND	-3.09	1.33	1.37
19	a	803	CLA	C4D-ND	-3.09	1.33	1.37
19	b	808	CLA	CHC-C1C	3.09	1.42	1.35
19	b	811	CLA	CHC-C1C	3.08	1.42	1.35
19	5	312	CLA	C4D-ND	-3.07	1.33	1.37
19	l	203	CLA	C4D-ND	-3.07	1.33	1.37
19	a	801	CLA	CHC-C1C	3.07	1.42	1.35
19	b	823	CLA	C4D-ND	-3.06	1.33	1.37
19	a	807	CLA	CHC-C1C	3.06	1.42	1.35
19	2	307	CLA	CHC-C1C	3.05	1.42	1.35
19	j	103	CLA	CHC-C1C	3.05	1.42	1.35
19	b	830	CLA	CMB-C2B	-3.05	1.45	1.51
19	b	833	CLA	C4D-ND	-3.04	1.33	1.37
19	b	827	CLA	CHC-C1C	3.04	1.42	1.35
19	b	810	CLA	CHC-C1C	3.04	1.42	1.35
19	a	854	CLA	C4D-ND	-3.04	1.33	1.37
19	b	814	CLA	C4D-ND	-3.03	1.33	1.37
19	b	836	CLA	C4D-ND	-3.03	1.33	1.37
19	b	817	CLA	C4D-ND	-3.03	1.33	1.37
19	b	819	CLA	CHC-C1C	3.03	1.42	1.35
19	l	311	CLA	C4D-ND	-3.03	1.33	1.37
19	l	305	CLA	C4D-ND	-3.03	1.33	1.37
19	a	827	CLA	C4D-ND	-3.03	1.33	1.37
19	a	807	CLA	C4D-ND	-3.03	1.33	1.37
19	a	819	CLA	C4D-ND	-3.02	1.33	1.37
19	b	831	CLA	C4D-ND	-3.02	1.33	1.37
19	a	829	CLA	C4D-ND	-3.02	1.33	1.37
19	l	204	CLA	C4D-ND	-3.02	1.33	1.37
19	2	308	CLA	C4D-ND	-3.02	1.33	1.37
19	a	831	CLA	CMB-C2B	-3.02	1.45	1.51
19	i	102	CLA	C4D-ND	-3.02	1.33	1.37
19	4	309	CLA	C4D-ND	-3.01	1.33	1.37
19	b	826	CLA	C4D-ND	-3.01	1.33	1.37
19	j	102	CLA	C4D-ND	-3.01	1.33	1.37
19	a	808	CLA	C4D-ND	-3.00	1.33	1.37
19	a	801	CLA	C4D-ND	-3.00	1.33	1.37
19	b	811	CLA	C4D-ND	-3.00	1.33	1.37
19	a	814	CLA	C4D-ND	-2.99	1.33	1.37
19	3	313	CLA	C4D-ND	-2.98	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	310	CLA	C4D-ND	-2.98	1.33	1.37
19	a	834	CLA	C4D-ND	-2.98	1.33	1.37
19	b	829	CLA	C4D-ND	-2.97	1.33	1.37
19	a	812	CLA	C4D-ND	-2.97	1.33	1.37
19	b	812	CLA	C4D-ND	-2.97	1.33	1.37
19	b	839	CLA	C4D-ND	-2.97	1.33	1.37
19	b	806	CLA	C4D-ND	-2.97	1.33	1.37
19	3	311	CLA	C4D-ND	-2.96	1.33	1.37
19	1	310	CLA	C4D-ND	-2.96	1.33	1.37
19	b	830	CLA	CHC-C1C	2.96	1.42	1.35
19	5	308	CLA	C4D-ND	-2.96	1.33	1.37
19	a	831	CLA	CHC-C1C	2.96	1.42	1.35
19	4	310	CLA	C4D-ND	-2.96	1.33	1.37
19	a	824	CLA	C4D-ND	-2.96	1.33	1.37
19	1	309	CLA	C4D-ND	-2.96	1.33	1.37
19	b	835	CLA	C4D-ND	-2.95	1.33	1.37
19	5	311	CLA	C4D-ND	-2.95	1.33	1.37
19	a	825	CLA	C4D-ND	-2.95	1.33	1.37
19	b	807	CLA	C4D-ND	-2.95	1.33	1.37
19	b	824	CLA	C4D-ND	-2.95	1.33	1.37
19	a	811	CLA	C4D-ND	-2.95	1.33	1.37
19	4	312	CLA	C4D-ND	-2.95	1.33	1.37
19	1	202	CLA	C4D-ND	-2.95	1.33	1.37
19	b	808	CLA	C4D-ND	-2.95	1.33	1.37
19	b	813	CLA	C4D-ND	-2.95	1.33	1.37
19	5	309	CLA	C4D-ND	-2.94	1.33	1.37
19	5	313	CLA	C4D-ND	-2.94	1.33	1.37
19	2	309	CLA	C4D-ND	-2.94	1.33	1.37
19	a	822	CLA	C4D-ND	-2.94	1.33	1.37
19	a	815	CLA	C4D-ND	-2.94	1.33	1.37
19	b	821	CLA	C4D-ND	-2.93	1.33	1.37
19	b	837	CLA	C4D-ND	-2.93	1.33	1.37
19	a	806	CLA	CHC-C1C	2.93	1.42	1.35
20	5	316	SQD	C6-S	-2.93	1.66	1.77
19	a	833	CLA	C4D-ND	-2.92	1.33	1.37
19	4	316	CLA	C4D-ND	-2.92	1.33	1.37
19	5	306	CLA	C4D-ND	-2.92	1.33	1.37
19	a	832	CLA	C4D-ND	-2.92	1.33	1.37
19	a	842	CLA	C4D-ND	-2.92	1.33	1.37
19	2	316	CLA	C4D-ND	-2.92	1.33	1.37
19	a	810	CLA	C4D-ND	-2.92	1.33	1.37
19	a	838	CLA	C4D-ND	-2.91	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	840	CLA	CHC-C1C	2.91	1.42	1.35
19	a	816	CLA	C4D-ND	-2.91	1.33	1.37
19	a	844	CLA	C4D-ND	-2.91	1.33	1.37
19	a	831	CLA	C4D-ND	-2.91	1.33	1.37
19	b	816	CLA	C4D-ND	-2.91	1.33	1.37
19	b	838	CLA	C4D-ND	-2.91	1.33	1.37
19	3	314	CLA	C4D-ND	-2.91	1.33	1.37
19	a	836	CLA	C4D-ND	-2.90	1.33	1.37
19	4	313	CLA	C4D-ND	-2.90	1.33	1.37
19	a	804	CLA	C4D-ND	-2.90	1.33	1.37
19	b	819	CLA	C4D-ND	-2.90	1.33	1.37
19	b	801	CLA	C4D-ND	-2.90	1.33	1.37
19	a	837	CLA	C4D-ND	-2.90	1.33	1.37
19	4	306	CLA	C4D-ND	-2.89	1.33	1.37
19	b	803	CLA	C4D-ND	-2.89	1.33	1.37
19	b	802	CLA	C4D-ND	-2.89	1.33	1.37
19	b	834	CLA	C4D-ND	-2.89	1.33	1.37
19	b	822	CLA	C4D-ND	-2.89	1.33	1.37
19	5	315	CLA	C4D-ND	-2.89	1.33	1.37
19	a	826	CLA	C4D-ND	-2.89	1.33	1.37
19	a	809	CLA	C4D-ND	-2.89	1.33	1.37
19	b	825	CLA	C4D-ND	-2.89	1.33	1.37
19	2	310	CLA	C4D-ND	-2.89	1.33	1.37
19	a	805	CLA	C4D-ND	-2.89	1.33	1.37
20	1	315	SQD	C6-S	-2.89	1.66	1.77
19	a	802	CLA	C4D-ND	-2.88	1.33	1.37
19	f	802	CLA	C4D-ND	-2.88	1.33	1.37
19	a	839	CLA	C4D-ND	-2.88	1.33	1.37
18	1	301	A1L1G	C42-C44	2.88	1.39	1.35
19	2	311	CLA	C4D-ND	-2.88	1.33	1.37
19	a	813	CLA	C4D-ND	-2.88	1.33	1.37
19	f	803	CLA	C4D-ND	-2.87	1.33	1.37
19	b	828	CLA	C4D-ND	-2.87	1.33	1.37
19	a	821	CLA	C4D-ND	-2.87	1.33	1.37
19	4	314	CLA	C4D-ND	-2.86	1.33	1.37
19	4	317	CLA	C4D-ND	-2.86	1.33	1.37
19	a	820	CLA	C4D-ND	-2.86	1.33	1.37
19	1	306	CLA	C4D-ND	-2.86	1.33	1.37
19	j	103	CLA	C4D-ND	-2.86	1.33	1.37
25	a	845	LHG	C26-C25	-2.86	1.35	1.51
19	b	805	CLA	C4D-ND	-2.86	1.33	1.37
19	b	840	CLA	C4D-ND	-2.85	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	313	CLA	C4D-ND	-2.85	1.33	1.37
19	a	818	CLA	C4D-ND	-2.85	1.33	1.37
19	a	841	CLA	C4D-ND	-2.85	1.33	1.37
19	3	312	CLA	C4D-ND	-2.85	1.33	1.37
19	a	823	CLA	C4D-ND	-2.85	1.33	1.37
19	2	312	CLA	C4D-ND	-2.84	1.33	1.37
19	1	312	CLA	C4D-ND	-2.84	1.33	1.37
25	m	101	LHG	C26-C25	-2.84	1.35	1.51
19	2	313	CLA	C4D-ND	-2.84	1.33	1.37
19	1	308	CLA	C4D-ND	-2.84	1.33	1.37
19	3	307	CLA	C4D-ND	-2.84	1.33	1.37
19	b	810	CLA	C4D-ND	-2.84	1.33	1.37
19	a	835	CLA	C4D-ND	-2.84	1.33	1.37
19	b	809	CLA	C4D-ND	-2.83	1.33	1.37
19	2	315	CLA	C4D-ND	-2.83	1.33	1.37
19	4	315	CLA	C4D-ND	-2.83	1.33	1.37
25	b	849	LHG	C26-C25	-2.82	1.35	1.51
19	1	307	CLA	C4D-ND	-2.81	1.33	1.37
19	a	817	CLA	C4D-ND	-2.81	1.33	1.37
19	5	310	CLA	C4D-ND	-2.81	1.33	1.37
19	3	315	CLA	C4D-ND	-2.81	1.33	1.37
19	5	314	CLA	C4D-ND	-2.81	1.33	1.37
19	a	840	CLA	C4D-ND	-2.81	1.33	1.37
19	2	307	CLA	C4D-ND	-2.81	1.33	1.37
19	b	815	CLA	C4D-ND	-2.80	1.33	1.37
19	2	306	CLA	C4D-ND	-2.80	1.33	1.37
19	b	832	CLA	C4D-ND	-2.80	1.33	1.37
19	2	314	CLA	C4D-ND	-2.79	1.33	1.37
19	4	307	CLA	C4D-ND	-2.77	1.33	1.37
19	5	305	CLA	C4D-ND	-2.76	1.33	1.37
19	4	311	CLA	C4D-ND	-2.75	1.33	1.37
19	a	806	CLA	CMB-C2B	-2.75	1.45	1.51
19	b	830	CLA	C4D-ND	-2.74	1.33	1.37
19	3	308	CLA	C4D-ND	-2.74	1.33	1.37
19	a	801	CLA	CMB-C2B	-2.70	1.46	1.51
19	b	820	CLA	CMB-C2B	-2.70	1.46	1.51
18	5	303	A1L1G	C42-C44	2.67	1.39	1.35
19	1	314	CLA	C4D-ND	-2.67	1.34	1.37
19	b	801	CLA	CMB-C2B	-2.64	1.46	1.51
19	b	840	CLA	CMB-C2B	-2.64	1.46	1.51
19	b	810	CLA	CMB-C2B	-2.64	1.46	1.51
18	5	303	A1L1G	C33-C34	-2.63	1.40	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	804	CLA	C4D-ND	-2.62	1.34	1.37
19	2	307	CLA	CMB-C2B	-2.62	1.46	1.51
18	3	306	A1L1G	C40-C39	-2.61	1.40	1.45
18	3	306	A1L1G	C42-C44	2.60	1.39	1.35
18	3	306	A1L1G	C33-C34	-2.60	1.40	1.45
19	b	831	CLA	CMB-C2B	-2.60	1.46	1.51
19	2	310	CLA	CMB-C2B	-2.59	1.46	1.51
19	4	311	CLA	CMB-C2B	-2.58	1.46	1.51
19	a	832	CLA	CMB-C2B	-2.58	1.46	1.51
19	a	836	CLA	CMB-C2B	-2.57	1.46	1.51
19	b	818	CLA	CMB-C2B	-2.55	1.46	1.51
19	b	835	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	820	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	819	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	803	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	829	CLA	CMB-C2B	-2.53	1.46	1.51
19	4	317	CLA	CMB-C2B	-2.52	1.46	1.51
18	3	302	A1L1G	C33-C34	-2.52	1.40	1.45
19	3	307	CLA	CMB-C2B	-2.51	1.46	1.51
19	a	802	CLA	CMB-C2B	-2.49	1.46	1.51
19	l	203	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	806	CLA	CMD-C2D	-2.49	1.45	1.50
19	a	808	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	824	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	822	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	825	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	837	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	806	CLA	C1D-ND	2.48	1.40	1.37
18	1	301	A1L1G	C33-C34	-2.48	1.40	1.45
19	4	313	CLA	CMB-C2B	-2.48	1.46	1.51
18	5	303	A1L1G	C40-C39	-2.48	1.40	1.45
19	5	312	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	1	307	CLA	CMB-C2B	-2.46	1.46	1.51
19	l	202	CLA	CMB-C2B	-2.45	1.46	1.51
19	a	817	CLA	CMB-C2B	-2.45	1.46	1.51
19	l	204	CLA	CMB-C2B	-2.45	1.46	1.51
19	b	841	CLA	CMB-C2B	-2.45	1.46	1.51
18	3	302	A1L1G	C40-C39	-2.45	1.40	1.45
19	b	826	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	810	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	842	CLA	CMB-C2B	-2.44	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	305	CLA	CMB-C2B	-2.44	1.46	1.51
19	1	312	CLA	CMB-C2B	-2.43	1.46	1.51
19	1	309	CLA	CMB-C2B	-2.43	1.46	1.51
19	a	840	CLA	CMB-C2B	-2.43	1.46	1.51
19	2	314	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	830	CLA	CMD-C2D	-2.43	1.45	1.50
19	a	818	CLA	CMB-C2B	-2.43	1.46	1.51
19	a	854	CLA	CMB-C2B	-2.42	1.46	1.51
19	1	310	CLA	CMB-C2B	-2.42	1.46	1.51
19	4	312	CLA	CMB-C2B	-2.42	1.46	1.51
19	b	812	CLA	CMB-C2B	-2.42	1.46	1.51
19	5	315	CLA	CMB-C2B	-2.42	1.46	1.51
19	2	309	CLA	CMB-C2B	-2.41	1.46	1.51
19	3	308	CLA	CMB-C2B	-2.41	1.46	1.51
19	2	306	CLA	CMB-C2B	-2.41	1.46	1.51
19	1	314	CLA	CMB-C2B	-2.41	1.46	1.51
19	j	103	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	813	CLA	CMB-C2B	-2.41	1.46	1.51
19	1	313	CLA	CMB-C2B	-2.41	1.46	1.51
19	a	815	CLA	CMB-C2B	-2.41	1.46	1.51
19	3	314	CLA	CMB-C2B	-2.40	1.46	1.51
18	3	302	A1L1G	C29-C30	-2.40	1.40	1.45
19	j	102	CLA	CMB-C2B	-2.40	1.46	1.51
19	4	315	CLA	CMB-C2B	-2.40	1.46	1.51
19	3	311	CLA	CMB-C2B	-2.40	1.46	1.51
19	b	839	CLA	CMB-C2B	-2.40	1.46	1.51
19	3	315	CLA	CMB-C2B	-2.40	1.46	1.51
19	5	307	CLA	CMB-C2B	-2.40	1.46	1.51
19	2	316	CLA	CMB-C2B	-2.39	1.46	1.51
19	i	102	CLA	CMB-C2B	-2.39	1.46	1.51
19	3	313	CLA	CMB-C2B	-2.39	1.46	1.51
19	a	838	CLA	CMB-C2B	-2.39	1.46	1.51
19	a	834	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	823	CLA	CMB-C2B	-2.39	1.46	1.51
19	1	311	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	816	CLA	CMB-C2B	-2.39	1.46	1.51
19	2	315	CLA	CMB-C2B	-2.39	1.46	1.51
19	3	309	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	837	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	838	CLA	CMB-C2B	-2.39	1.46	1.51
19	5	306	CLA	CMB-C2B	-2.38	1.46	1.51
19	5	313	CLA	CMB-C2B	-2.38	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	841	CLA	CMB-C2B	-2.38	1.46	1.51
19	5	308	CLA	CMB-C2B	-2.38	1.46	1.51
19	2	311	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	849	LHG	O8-C6	-2.38	1.39	1.45
19	4	316	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	801	CLA	CMD-C2D	-2.38	1.45	1.50
19	a	833	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	827	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	812	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	835	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	828	CLA	CMB-C2B	-2.38	1.46	1.51
19	4	314	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	802	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	806	CLA	CMC-C2C	-2.37	1.45	1.50
19	b	814	CLA	CMB-C2B	-2.37	1.46	1.51
19	5	310	CLA	CMB-C2B	-2.37	1.46	1.51
19	3	312	CLA	CMB-C2B	-2.37	1.46	1.51
19	5	309	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	819	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	813	CLA	CMB-C2B	-2.37	1.46	1.51
19	f	803	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	807	CLA	CMB-C2B	-2.37	1.46	1.51
19	5	305	CLA	CMB-C2B	-2.37	1.46	1.51
19	b	821	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	804	CLA	CMB-C2B	-2.37	1.46	1.51
19	b	808	CLA	CMB-C2B	-2.37	1.46	1.51
25	a	846	LHG	O8-C6	-2.37	1.39	1.45
19	f	802	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	830	CLA	CMC-C2C	-2.37	1.45	1.50
19	a	821	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	849	LHG	O8-C23	2.36	1.40	1.33
19	b	806	CLA	CMB-C2B	-2.36	1.46	1.51
19	a	839	CLA	CMB-C2B	-2.36	1.46	1.51
19	b	822	CLA	CMB-C2B	-2.36	1.46	1.51
19	2	312	CLA	CMB-C2B	-2.36	1.46	1.51
19	a	825	CLA	CMB-C2B	-2.36	1.46	1.51
19	5	314	CLA	CMB-C2B	-2.35	1.46	1.51
19	4	307	CLA	CMB-C2B	-2.35	1.46	1.51
19	1	306	CLA	CMB-C2B	-2.35	1.46	1.51
19	1	308	CLA	CMB-C2B	-2.35	1.46	1.51
19	4	306	CLA	CMB-C2B	-2.35	1.46	1.51
19	b	824	CLA	CMB-C2B	-2.35	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	313	CLA	CMB-C2B	-2.34	1.46	1.51
19	4	309	CLA	CMB-C2B	-2.34	1.46	1.51
19	3	310	CLA	CMB-C2B	-2.34	1.46	1.51
25	m	101	LHG	O8-C23	2.34	1.40	1.33
19	b	815	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	814	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	828	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	816	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	823	CLA	CMB-C2B	-2.34	1.46	1.51
19	4	311	CLA	CMD-C2D	-2.33	1.45	1.50
19	a	805	CLA	CMB-C2B	-2.33	1.46	1.51
19	4	310	CLA	CMB-C2B	-2.33	1.46	1.51
25	a	845	LHG	O8-C6	-2.33	1.39	1.45
19	a	806	CLA	C3B-C2B	-2.33	1.37	1.40
19	2	308	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	827	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	806	CLA	C3B-CAB	-2.33	1.43	1.47
19	b	834	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	811	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	803	CLA	CMB-C2B	-2.33	1.46	1.51
19	5	311	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	829	CLA	CMB-C2B	-2.33	1.46	1.51
19	4	308	CLA	CMB-C2B	-2.32	1.46	1.51
19	b	805	CLA	CMB-C2B	-2.32	1.46	1.51
25	m	101	LHG	O8-C6	-2.32	1.39	1.45
19	b	836	CLA	CMB-C2B	-2.32	1.46	1.51
25	m	101	LHG	O7-C7	2.32	1.40	1.34
19	a	830	CLA	CMB-C2B	-2.32	1.46	1.51
19	b	807	CLA	CMB-C2B	-2.31	1.46	1.51
19	b	817	CLA	CMB-C2B	-2.31	1.46	1.51
19	b	832	CLA	CMB-C2B	-2.31	1.46	1.51
23	1	304	A1L1F	C6-C1	-2.31	1.50	1.54
19	b	811	CLA	CMB-C2B	-2.30	1.46	1.51
19	a	826	CLA	CMB-C2B	-2.30	1.46	1.51
25	a	845	LHG	O8-C23	2.30	1.40	1.33
19	a	844	CLA	CMB-C2B	-2.30	1.46	1.51
19	a	809	CLA	CMB-C2B	-2.29	1.46	1.51
18	1	301	A1L1G	C40-C39	-2.29	1.41	1.45
25	a	846	LHG	O8-C23	2.28	1.40	1.33
25	a	845	LHG	O7-C7	2.28	1.40	1.34
18	3	306	A1L1G	C29-C30	-2.28	1.40	1.45
25	a	846	LHG	O7-C5	-2.28	1.40	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	833	CLA	CMB-C2B	-2.27	1.46	1.51
25	a	846	LHG	O7-C7	2.26	1.40	1.34
18	5	303	A1L1G	C29-C30	-2.26	1.40	1.45
25	b	849	LHG	O7-C7	2.24	1.40	1.34
23	1	304	A1L1F	O15-C20	-2.23	1.43	1.46
19	b	831	CLA	CMD-C2D	-2.23	1.46	1.50
18	1	301	A1L1G	C29-C30	-2.23	1.40	1.45
25	a	845	LHG	O7-C5	-2.23	1.41	1.46
25	b	849	LHG	O7-C5	-2.23	1.41	1.46
19	b	823	CLA	CMD-C2D	-2.22	1.46	1.50
19	b	809	CLA	CMD-C2D	-2.22	1.46	1.50
19	a	801	CLA	C3B-CAB	-2.20	1.43	1.47
19	a	806	CLA	CAA-C2A	-2.19	1.50	1.54
19	a	824	CLA	CMD-C2D	-2.19	1.46	1.50
19	3	307	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	824	CLA	CMD-C2D	-2.17	1.46	1.50
25	m	101	LHG	O7-C5	-2.17	1.41	1.46
19	a	801	CLA	CMC-C2C	-2.17	1.46	1.50
17	4	304	XAT	O24-C25	-2.17	1.43	1.46
17	1	302	XAT	O4-C5	-2.16	1.43	1.46
19	5	305	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	810	CLA	CMD-C2D	-2.16	1.46	1.50
17	4	301	XAT	O24-C25	-2.15	1.43	1.46
19	a	830	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	804	CLA	CMC-C2C	-2.14	1.46	1.50
19	a	828	CLA	CMC-C2C	-2.14	1.46	1.50
19	b	804	CLA	CMB-C2B	-2.14	1.47	1.51
19	b	803	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	829	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	838	CLA	CMD-C2D	-2.12	1.46	1.50
17	3	301	XAT	O24-C25	-2.12	1.43	1.46
21	b	851	DGD	O3D-C3D	-2.12	1.38	1.43
19	2	310	CLA	CMD-C2D	-2.12	1.46	1.50
17	3	305	XAT	O4-C5	-2.11	1.43	1.46
21	b	851	DGD	O4D-C4D	-2.11	1.38	1.43
19	b	801	CLA	CMD-C2D	-2.11	1.46	1.50
17	2	302	XAT	O4-C5	-2.11	1.43	1.46
19	b	839	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	815	CLA	CMD-C2D	-2.10	1.46	1.50
21	b	851	DGD	C1E-C2E	2.10	1.58	1.52
19	a	806	CLA	MG-ND	-2.10	2.01	2.05
19	a	812	CLA	CMD-C2D	-2.09	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	832	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	842	CLA	CMD-C2D	-2.09	1.46	1.50
17	5	301	XAT	O4-C5	-2.08	1.43	1.46
19	a	803	CLA	C3B-CAB	-2.08	1.43	1.47
19	b	812	CLA	CMD-C2D	-2.07	1.46	1.50
25	m	101	LHG	P-O6	2.07	1.67	1.59
25	b	849	LHG	P-O6	2.07	1.67	1.59
19	2	316	CLA	CMD-C2D	-2.07	1.46	1.50
17	5	302	XAT	O4-C5	-2.07	1.43	1.46
19	a	821	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	816	CLA	CMC-C2C	-2.07	1.46	1.50
17	5	302	XAT	O24-C25	-2.07	1.43	1.46
19	1	313	CLA	CMD-C2D	-2.06	1.46	1.50
17	1	303	XAT	O4-C5	-2.06	1.43	1.46
25	a	845	LHG	P-O6	2.06	1.67	1.59
19	b	826	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	852	XAT	O4-C5	-2.06	1.43	1.46
19	i	102	CLA	CMD-C2D	-2.06	1.46	1.50
17	4	305	XAT	O4-C5	-2.06	1.43	1.46
19	a	816	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	826	CLA	CMD-C2D	-2.05	1.46	1.50
19	3	309	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	827	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	834	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	839	CLA	CMD-C2D	-2.05	1.46	1.50
19	1	309	CLA	CMD-C2D	-2.04	1.46	1.50
17	3	303	XAT	O4-C5	-2.04	1.43	1.46
17	2	303	XAT	O4-C5	-2.04	1.43	1.46
19	a	801	CLA	C3B-C2B	-2.04	1.37	1.40
19	b	820	CLA	CMD-C2D	-2.04	1.46	1.50
19	4	308	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	803	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	809	CLA	CMC-C2C	-2.03	1.46	1.50
17	a	852	XAT	O24-C25	-2.03	1.43	1.46
17	2	301	XAT	O4-C5	-2.03	1.43	1.46
19	a	807	CLA	CMD-C2D	-2.03	1.46	1.50
19	2	306	CLA	CMD-C2D	-2.03	1.46	1.50
19	3	314	CLA	CMD-C2D	-2.03	1.46	1.50
19	b	834	CLA	CMD-C2D	-2.03	1.46	1.50
19	b	835	CLA	CMD-C2D	-2.03	1.46	1.50
21	b	851	DGD	O4E-C4E	-2.03	1.38	1.43
19	2	314	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)
19	b	836	CLA	CMD-C2D	-2.03	1.46	1.50
19	l	204	CLA	CMC-C2C	-2.02	1.46	1.50
21	b	851	DGD	O2D-C2D	-2.02	1.38	1.43
17	2	305	XAT	O4-C5	-2.02	1.43	1.46
19	3	315	CLA	CMD-C2D	-2.02	1.46	1.50
17	3	304	XAT	O24-C25	-2.02	1.43	1.46
19	b	807	CLA	CMD-C2D	-2.02	1.46	1.50
19	4	312	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	808	CLA	CMD-C2D	-2.02	1.46	1.50
19	2	312	CLA	CMD-C2D	-2.02	1.46	1.50
19	j	102	CLA	CMD-C2D	-2.02	1.46	1.50
19	4	307	CLA	CMD-C2D	-2.02	1.46	1.50
19	4	314	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	838	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	810	CLA	CMD-C2D	-2.01	1.46	1.50
25	a	846	LHG	P-O6	2.01	1.67	1.59
19	b	821	CLA	CMD-C2D	-2.01	1.46	1.50
19	2	314	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	813	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	814	CLA	CMD-C2D	-2.01	1.46	1.50
19	b	802	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	304	XAT	O4-C5	-2.01	1.43	1.46
19	5	311	CLA	CMD-C2D	-2.00	1.46	1.50
19	3	312	CLA	CMD-C2D	-2.00	1.46	1.50
19	l	203	CLA	CMC-C2C	-2.00	1.46	1.50
17	3	301	XAT	O4-C5	-2.00	1.43	1.46
19	a	807	CLA	C3B-CAB	-2.00	1.43	1.47

All (1940) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	318	DGD	C6E-C5E-C4E	-9.39	91.01	113.00
23	1	304	A1L1F	C17-C20-C25	-8.08	108.73	122.26
23	1	304	A1L1F	O15-C20-C21	7.27	118.84	113.38
19	b	840	CLA	C4A-NA-C1A	7.27	109.97	106.71
19	a	806	CLA	C4A-NA-C1A	7.25	109.97	106.71
19	l	203	CLA	C4A-NA-C1A	7.23	109.96	106.71
17	5	304	XAT	C38-C25-C24	7.20	122.38	114.28
17	3	305	XAT	C38-C25-C24	7.20	122.38	114.28
17	1	303	XAT	C38-C25-C24	7.18	122.36	114.28
17	4	305	XAT	C38-C25-C24	7.17	122.35	114.28
19	b	803	CLA	C4A-NA-C1A	7.15	109.92	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	101	XAT	C38-C25-C24	7.12	122.28	114.28
19	a	823	CLA	C4A-NA-C1A	7.09	109.89	106.71
19	b	809	CLA	C4A-NA-C1A	7.08	109.89	106.71
17	a	852	XAT	C15-C14-C13	-7.08	117.21	127.31
19	4	310	CLA	C4A-NA-C1A	7.06	109.88	106.71
19	a	835	CLA	C4A-NA-C1A	7.05	109.88	106.71
19	a	810	CLA	C4A-NA-C1A	7.02	109.86	106.71
17	5	304	XAT	C18-C5-C4	7.00	122.16	114.28
19	a	826	CLA	C4A-NA-C1A	7.00	109.85	106.71
19	a	833	CLA	C4A-NA-C1A	6.99	109.85	106.71
19	a	821	CLA	C4A-NA-C1A	6.99	109.85	106.71
26	f	801	BCR	C24-C23-C22	-6.97	115.70	126.23
17	4	304	XAT	C38-C25-C24	6.97	122.12	114.28
19	j	103	CLA	C4A-NA-C1A	6.96	109.84	106.71
17	3	304	XAT	C38-C25-C24	6.96	122.11	114.28
19	a	828	CLA	C4A-NA-C1A	6.93	109.82	106.71
19	b	821	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	4	316	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	b	801	CLA	C4A-NA-C1A	6.89	109.80	106.71
17	5	301	XAT	C38-C25-C26	-6.88	110.73	122.26
19	b	806	CLA	C4A-NA-C1A	6.87	109.79	106.71
19	b	822	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	2	301	XAT	C18-C5-C6	-6.86	110.76	122.26
19	b	805	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	1	302	XAT	C38-C25-C24	6.86	121.99	114.28
17	5	304	XAT	C6-C7-C8	-6.84	111.53	125.99
19	2	316	CLA	C4A-NA-C1A	6.84	109.78	106.71
19	1	308	CLA	C4A-NA-C1A	6.84	109.78	106.71
19	b	815	CLA	C4A-NA-C1A	6.84	109.78	106.71
19	4	317	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	b	811	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	f	802	CLA	C4A-NA-C1A	6.82	109.77	106.71
17	4	305	XAT	C38-C25-C26	-6.81	110.84	122.26
19	b	828	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	b	813	CLA	C4A-NA-C1A	6.80	109.76	106.71
17	a	852	XAT	C38-C25-C24	6.80	121.93	114.28
17	4	303	XAT	C38-C25-C24	6.79	121.92	114.28
19	1	306	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	a	807	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	b	825	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	a	801	CLA	C4A-NA-C1A	6.79	109.76	106.71
17	2	304	XAT	C38-C25-C24	6.79	121.91	114.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	825	CLA	C4A-NA-C1A	6.78	109.75	106.71
17	3	304	XAT	C38-C25-C26	-6.78	110.90	122.26
19	4	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	a	840	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	b	808	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	l	204	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	5	310	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	a	812	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	b	810	CLA	C4A-NA-C1A	6.76	109.74	106.71
19	a	841	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	4	315	CLA	C4A-NA-C1A	6.74	109.74	106.71
19	3	314	CLA	C4A-NA-C1A	6.74	109.74	106.71
19	2	311	CLA	C4A-NA-C1A	6.74	109.74	106.71
19	a	838	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	a	817	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	b	807	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	b	837	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	3	313	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	a	831	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	2	304	XAT	C18-C5-C4	6.70	121.82	114.28
17	4	302	XAT	C38-C25-C24	6.70	121.82	114.28
19	a	805	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	a	839	CLA	C4A-NA-C1A	6.70	109.72	106.71
17	5	304	XAT	C18-C5-C6	-6.69	111.05	122.26
19	2	312	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	3	303	XAT	C38-C25-C24	6.69	121.80	114.28
19	3	308	CLA	C4A-NA-C1A	6.69	109.71	106.71
19	5	306	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	5	311	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	a	809	CLA	C4A-NA-C1A	6.67	109.71	106.71
19	3	312	CLA	C4A-NA-C1A	6.67	109.70	106.71
17	2	301	XAT	C18-C5-C4	6.67	121.78	114.28
19	a	834	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	5	313	CLA	C4A-NA-C1A	6.66	109.70	106.71
17	3	304	XAT	C18-C5-C6	-6.66	111.10	122.26
17	j	101	XAT	C38-C25-C26	-6.66	111.11	122.26
19	1	305	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	b	833	CLA	C4A-NA-C1A	6.65	109.69	106.71
26	i	101	BCR	C24-C23-C22	-6.64	116.20	126.23
17	3	301	XAT	C18-C5-C4	6.64	121.75	114.28
19	5	314	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	j	102	CLA	C4A-NA-C1A	6.62	109.68	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	811	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	5	312	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	l	202	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	a	837	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	4	301	XAT	C31-C30-C29	-6.60	117.89	127.31
19	4	307	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	f	803	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	5	302	XAT	C18-C5-C6	-6.59	111.21	122.26
17	5	301	XAT	C38-C25-C24	6.59	121.69	114.28
19	a	844	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	4	306	CLA	C4A-NA-C1A	6.58	109.66	106.71
17	4	301	XAT	C18-C5-C4	6.58	121.68	114.28
19	a	842	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	a	804	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	2	313	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	4	314	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	b	816	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	a	829	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	b	823	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	2	303	XAT	C18-C5-C6	-6.53	111.31	122.26
19	2	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	a	832	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	4	301	XAT	C18-C5-C6	-6.53	111.32	122.26
19	1	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	4	303	XAT	C18-C5-C6	-6.53	111.32	122.26
19	a	808	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	a	854	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	5	308	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	a	827	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	5	304	XAT	C38-C25-C26	-6.51	111.35	122.26
19	b	824	CLA	C4A-NA-C1A	6.50	109.63	106.71
17	4	302	XAT	C18-C5-C4	6.49	121.59	114.28
19	4	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
17	3	305	XAT	C38-C25-C26	-6.49	111.39	122.26
19	5	315	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	b	814	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	3	309	CLA	C4A-NA-C1A	6.48	109.62	106.71
17	2	305	XAT	C18-C5-C6	-6.48	111.40	122.26
19	a	836	CLA	C4A-NA-C1A	6.48	109.62	106.71
17	4	303	XAT	C38-C25-C26	-6.47	111.41	122.26
26	a	850	BCR	C24-C23-C22	-6.47	116.46	126.23
19	2	309	CLA	C4A-NA-C1A	6.47	109.61	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	XAT	C38-C25-C26	-6.46	111.44	122.26
19	a	819	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	3	311	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	a	830	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	2	304	XAT	C18-C5-C6	-6.45	111.45	122.26
17	2	304	XAT	C38-C25-C26	-6.45	111.45	122.26
19	i	102	CLA	C4A-NA-C1A	6.45	109.60	106.71
19	a	822	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	b	834	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	1	313	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	b	836	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	3	303	XAT	C18-C5-C6	-6.42	111.50	122.26
17	j	101	XAT	C18-C5-C6	-6.42	111.50	122.26
17	3	301	XAT	C18-C5-C6	-6.42	111.51	122.26
19	3	310	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	b	832	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	3	315	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	b	827	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	2	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	5	302	XAT	C26-C27-C28	-6.40	112.46	125.99
19	1	312	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	b	819	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	j	101	XAT	C18-C5-C4	6.38	121.46	114.28
19	a	814	CLA	C4A-NA-C1A	6.38	109.58	106.71
19	a	816	CLA	C4A-NA-C1A	6.38	109.58	106.71
19	2	306	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	1	310	CLA	C4A-NA-C1A	6.38	109.57	106.71
17	1	302	XAT	C38-C25-C26	-6.38	111.57	122.26
19	b	826	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	b	839	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	2	302	XAT	C38-C25-C24	6.37	121.45	114.28
19	3	307	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	3	303	XAT	C38-C25-C26	-6.37	111.59	122.26
19	a	818	CLA	C4A-NA-C1A	6.36	109.56	106.71
17	3	305	XAT	C18-C5-C4	6.35	121.43	114.28
17	4	304	XAT	C18-C5-C6	-6.35	111.62	122.26
17	4	302	XAT	C18-C5-C6	-6.35	111.63	122.26
17	2	303	XAT	C38-C25-C24	6.35	121.42	114.28
19	b	820	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	5	305	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	1	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	4	308	CLA	C4A-NA-C1A	6.33	109.55	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	309	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	1	309	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	2	315	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	a	815	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	b	835	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	4	305	XAT	C31-C30-C29	-6.32	118.29	127.31
17	1	302	XAT	C18-C5-C4	6.32	121.39	114.28
19	4	312	CLA	C4A-NA-C1A	6.31	109.55	106.71
17	4	305	XAT	C18-C5-C6	-6.31	111.68	122.26
19	2	310	CLA	C4A-NA-C1A	6.30	109.54	106.71
17	1	302	XAT	C18-C5-C6	-6.29	111.72	122.26
19	5	307	CLA	C4A-NA-C1A	6.29	109.53	106.71
17	2	302	XAT	C18-C5-C6	-6.29	111.72	122.26
17	4	303	XAT	C18-C5-C4	6.28	121.34	114.28
19	a	813	CLA	C4A-NA-C1A	6.28	109.53	106.71
17	3	303	XAT	C18-C5-C4	6.28	121.34	114.28
17	3	304	XAT	C18-C5-C4	6.28	121.34	114.28
19	1	311	CLA	C4A-NA-C1A	6.27	109.53	106.71
17	4	302	XAT	C38-C25-C26	-6.27	111.75	122.26
26	i	101	BCR	C20-C21-C22	-6.27	118.36	127.31
19	a	824	CLA	C4A-NA-C1A	6.27	109.52	106.71
17	3	305	XAT	C18-C5-C6	-6.27	111.76	122.26
19	b	841	CLA	C4A-NA-C1A	6.26	109.52	106.71
17	a	852	XAT	C38-C25-C26	-6.26	111.77	122.26
17	3	301	XAT	C38-C25-C26	-6.26	111.77	122.26
17	1	303	XAT	C18-C5-C6	-6.25	111.78	122.26
17	4	304	XAT	C38-C25-C26	-6.25	111.79	122.26
19	a	802	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	2	301	XAT	C38-C25-C24	6.24	121.30	114.28
17	1	303	XAT	C38-C25-C26	-6.22	111.83	122.26
19	b	830	CLA	C4A-NA-C1A	6.21	109.50	106.71
17	5	301	XAT	C18-C5-C6	-6.21	111.85	122.26
17	2	302	XAT	C38-C25-C26	-6.19	111.89	122.26
17	4	304	XAT	C18-C5-C4	6.18	121.23	114.28
19	b	829	CLA	C4A-NA-C1A	6.18	109.48	106.71
19	b	812	CLA	C4A-NA-C1A	6.17	109.48	106.71
17	3	301	XAT	C38-C25-C24	6.15	121.20	114.28
17	5	302	XAT	C38-C25-C24	6.13	121.18	114.28
17	a	852	XAT	C26-C27-C28	-6.12	113.06	125.99
19	a	820	CLA	C4A-NA-C1A	6.11	109.45	106.71
17	1	303	XAT	C18-C5-C4	6.10	121.14	114.28
19	b	838	CLA	C4A-NA-C1A	6.10	109.45	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	301	XAT	C31-C30-C29	-6.06	118.66	127.31
19	b	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
17	2	301	XAT	C38-C25-C26	-6.05	112.13	122.26
17	2	305	XAT	C18-C5-C4	6.04	121.08	114.28
17	4	305	XAT	C18-C5-C4	6.03	121.06	114.28
19	b	818	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	4	313	CLA	C4A-NA-C1A	5.99	109.40	106.71
17	2	302	XAT	C18-C5-C4	5.97	121.00	114.28
26	b	843	BCR	C7-C8-C9	-5.95	117.24	126.23
19	b	817	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	2	308	CLA	C4A-NA-C1A	5.94	109.38	106.71
17	5	304	XAT	C26-C27-C28	-5.92	113.47	125.99
17	5	302	XAT	C18-C5-C4	5.91	120.93	114.28
17	5	301	XAT	C18-C5-C4	5.86	120.87	114.28
17	j	101	XAT	C6-C7-C8	-5.86	113.61	125.99
19	b	831	CLA	C4A-NA-C1A	5.86	109.34	106.71
26	b	852	BCR	C16-C17-C18	-5.86	118.95	127.31
19	b	802	CLA	C4A-NA-C1A	5.84	109.33	106.71
17	2	303	XAT	C18-C5-C4	5.80	120.80	114.28
17	5	302	XAT	C38-C25-C26	-5.79	112.56	122.26
17	4	301	XAT	C35-C34-C33	-5.73	119.13	127.31
26	a	850	BCR	C20-C21-C22	-5.70	119.17	127.31
26	f	801	BCR	C16-C17-C18	-5.65	119.25	127.31
17	4	301	XAT	C38-C25-C24	5.64	120.63	114.28
17	5	302	XAT	C11-C10-C9	-5.64	119.26	127.31
23	1	304	A1L1F	O15-C20-C17	5.64	121.81	115.06
26	b	845	BCR	C24-C23-C22	-5.63	117.73	126.23
26	b	843	BCR	C11-C10-C9	-5.61	119.31	127.31
26	b	845	BCR	C7-C8-C9	-5.51	117.91	126.23
26	b	847	BCR	C16-C17-C18	-5.49	119.48	127.31
26	j	104	BCR	C28-C27-C26	-5.44	104.37	114.08
17	3	301	XAT	C6-C7-C8	-5.44	114.50	125.99
26	f	801	BCR	C20-C21-C22	-5.42	119.58	127.31
17	3	304	XAT	C35-C34-C33	-5.40	119.60	127.31
26	f	804	BCR	C15-C14-C13	-5.38	119.64	127.31
17	2	303	XAT	C35-C34-C33	-5.36	119.65	127.31
26	b	845	BCR	C33-C5-C6	-5.34	118.53	124.53
26	b	843	BCR	C3-C4-C5	-5.34	104.55	114.08
17	a	852	XAT	C18-C5-C6	-5.33	113.33	122.26
17	2	303	XAT	C31-C30-C29	-5.32	119.72	127.31
17	4	301	XAT	C38-C25-C26	-5.31	113.35	122.26
19	a	803	CLA	C4A-NA-C1A	5.31	109.09	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	303	XAT	C26-C27-C28	-5.29	114.81	125.99
17	4	305	XAT	C15-C14-C13	-5.28	119.77	127.31
26	b	843	BCR	C15-C14-C13	-5.28	119.77	127.31
21	b	851	DGD	O2G-C1B-C2B	5.28	122.88	111.50
26	a	849	BCR	C3-C4-C5	-5.27	104.67	114.08
17	4	304	XAT	C26-C27-C28	-5.26	114.87	125.99
17	2	305	XAT	C31-C30-C29	-5.25	119.82	127.31
17	a	852	XAT	C18-C5-C4	5.24	120.17	114.28
17	2	303	XAT	C11-C10-C9	-5.23	119.84	127.31
17	a	852	XAT	C6-C7-C8	-5.23	114.93	125.99
17	2	301	XAT	C35-C34-C33	-5.22	119.87	127.31
17	2	302	XAT	C35-C34-C33	-5.21	119.87	127.31
26	l	201	BCR	C7-C8-C9	-5.21	118.36	126.23
17	2	304	XAT	C6-C7-C8	-5.20	115.01	125.99
17	j	101	XAT	C26-C27-C28	-5.16	115.08	125.99
26	l	205	BCR	C24-C23-C22	-5.14	118.47	126.23
26	b	846	BCR	C3-C4-C5	-5.12	104.94	114.08
17	2	305	XAT	C35-C34-C33	-5.06	120.09	127.31
26	a	847	BCR	C16-C17-C18	-5.05	120.10	127.31
17	3	305	XAT	C26-C27-C28	-5.04	115.33	125.99
17	1	302	XAT	C35-C34-C33	-5.04	120.12	127.31
17	5	301	XAT	C26-C27-C28	-5.01	115.41	125.99
17	1	302	XAT	C26-C27-C28	-4.99	115.44	125.99
17	4	304	XAT	C6-C7-C8	-4.99	115.44	125.99
26	a	850	BCR	C16-C17-C18	-4.97	120.22	127.31
26	b	852	BCR	C11-C10-C9	-4.97	120.22	127.31
17	3	305	XAT	C6-C7-C8	-4.96	115.50	125.99
26	b	852	BCR	C20-C21-C22	-4.95	120.24	127.31
26	f	804	BCR	C11-C10-C9	-4.94	120.25	127.31
17	2	301	XAT	C15-C14-C13	-4.93	120.27	127.31
17	1	303	XAT	C6-C7-C8	-4.91	115.60	125.99
26	a	849	BCR	C16-C17-C18	-4.91	120.31	127.31
26	j	104	BCR	C11-C10-C9	-4.87	120.36	127.31
17	2	305	XAT	C6-C7-C8	-4.86	115.71	125.99
17	2	301	XAT	C6-C7-C8	-4.86	115.72	125.99
17	4	303	XAT	C11-C10-C9	-4.84	120.40	127.31
17	j	101	XAT	C11-C10-C9	-4.84	120.41	127.31
17	5	302	XAT	C15-C14-C13	-4.81	120.44	127.31
17	1	302	XAT	C6-C7-C8	-4.81	115.83	125.99
26	b	852	BCR	C38-C26-C25	-4.80	119.14	124.53
26	l	205	BCR	C15-C14-C13	-4.80	120.47	127.31
26	b	850	BCR	C16-C17-C18	-4.77	120.51	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	831	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
17	5	304	XAT	C15-C14-C13	-4.75	120.53	127.31
26	i	101	BCR	C16-C17-C18	-4.75	120.53	127.31
19	b	830	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
17	4	302	XAT	C26-C27-C28	-4.73	115.99	125.99
26	b	852	BCR	C7-C8-C9	-4.70	119.13	126.23
17	3	303	XAT	C26-C27-C28	-4.68	116.09	125.99
17	4	302	XAT	C6-C7-C8	-4.67	116.11	125.99
19	b	818	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
17	4	302	XAT	C35-C34-C33	-4.63	120.70	127.31
17	3	304	XAT	C6-C7-C8	-4.62	116.22	125.99
26	b	848	BCR	C16-C17-C18	-4.60	120.74	127.31
17	5	301	XAT	C35-C34-C33	-4.57	120.79	127.31
17	2	305	XAT	C15-C14-C13	-4.54	120.82	127.31
26	b	844	BCR	C7-C8-C9	-4.54	119.37	126.23
17	4	305	XAT	C26-C27-C28	-4.54	116.40	125.99
26	b	844	BCR	C11-C10-C9	-4.53	120.84	127.31
17	3	303	XAT	C6-C7-C8	-4.49	116.49	125.99
17	2	302	XAT	C6-C7-C8	-4.49	116.49	125.99
17	3	305	XAT	C35-C34-C33	-4.47	120.93	127.31
17	2	304	XAT	C26-C27-C28	-4.46	116.55	125.99
19	a	802	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
21	b	851	DGD	O5D-C6D-C5D	-4.44	100.83	109.05
26	a	850	BCR	C15-C14-C13	-4.41	121.01	127.31
26	a	848	BCR	C15-C14-C13	-4.41	121.02	127.31
26	a	848	BCR	C16-C17-C18	-4.40	121.03	127.31
26	b	845	BCR	C16-C17-C18	-4.38	121.06	127.31
22	2	317	LMG	O7-C10-C11	4.38	120.94	111.50
26	j	104	BCR	C15-C14-C13	-4.37	121.07	127.31
26	a	849	BCR	C15-C14-C13	-4.37	121.07	127.31
26	b	843	BCR	C16-C17-C18	-4.37	121.08	127.31
26	b	848	BCR	C33-C5-C6	-4.36	119.64	124.53
21	4	318	DGD	O6E-C5E-C6E	4.34	117.23	106.44
17	3	303	XAT	C35-C34-C33	-4.34	121.12	127.31
19	b	836	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
17	j	101	XAT	C35-C34-C33	-4.31	121.15	127.31
17	3	303	XAT	C15-C14-C13	-4.31	121.16	127.31
19	2	307	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
17	5	304	XAT	C35-C34-C33	-4.30	121.18	127.31
17	4	301	XAT	C6-C7-C8	-4.29	116.92	125.99
26	j	104	BCR	C16-C17-C18	-4.29	121.19	127.31
19	a	826	CLA	CMB-C2B-C1B	-4.27	121.90	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	304	XAT	C31-C30-C29	-4.26	121.23	127.31
19	a	844	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
19	4	313	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
19	a	833	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
26	b	844	BCR	C15-C14-C13	-4.24	121.25	127.31
19	b	826	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
17	4	304	XAT	C35-C34-C33	-4.23	121.27	127.31
26	b	845	BCR	C15-C14-C13	-4.23	121.27	127.31
25	a	845	LHG	O7-C7-C8	4.22	120.60	111.50
26	f	804	BCR	C24-C23-C22	-4.22	119.85	126.23
23	1	304	A1L1F	C37-C38-C39	-4.22	121.29	127.31
19	a	809	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
17	3	301	XAT	C15-C14-C13	-4.22	121.29	127.31
21	4	318	DGD	O2G-C1B-C2B	4.22	120.59	111.50
24	b	842	PQN	C11-C12-C13	-4.22	119.77	126.79
17	2	305	XAT	C38-C25-C24	4.20	119.01	114.28
19	3	310	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
19	a	820	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
17	4	305	XAT	C35-C34-C33	-4.18	121.35	127.31
26	b	847	BCR	C24-C23-C22	-4.18	119.92	126.23
23	1	304	A1L1F	O7-C54-C56	4.17	118.76	111.09
19	a	806	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	j	104	BCR	C7-C8-C9	-4.17	119.94	126.23
19	a	829	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	l	205	BCR	C20-C21-C22	-4.17	121.36	127.31
19	a	823	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	b	850	BCR	C33-C5-C6	-4.16	119.85	124.53
26	l	201	BCR	C15-C14-C13	-4.16	121.37	127.31
19	b	815	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
26	l	201	BCR	C33-C5-C6	-4.16	119.86	124.53
26	b	846	BCR	C16-C17-C18	-4.15	121.38	127.31
23	1	304	A1L1F	C17-C20-C21	4.13	118.93	114.28
17	3	304	XAT	C15-C14-C13	-4.13	121.42	127.31
22	a	853	LMG	O7-C10-C11	4.12	120.38	111.50
26	f	804	BCR	C7-C8-C9	-4.11	120.02	126.23
26	b	847	BCR	C20-C21-C22	-4.11	121.44	127.31
17	5	301	XAT	C11-C10-C9	-4.11	121.45	127.31
19	a	816	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
19	1	307	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
19	b	833	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	a	850	BCR	C38-C26-C25	-4.09	119.94	124.53
26	f	801	BCR	C3-C4-C5	-4.08	106.78	114.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	849	LHG	O7-C7-C8	4.08	120.30	111.50
26	b	847	BCR	C7-C8-C9	-4.06	120.10	126.23
19	a	803	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
26	b	847	BCR	C16-C15-C14	-4.05	115.17	123.47
26	l	205	BCR	C38-C26-C25	-4.05	119.98	124.53
19	b	811	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
19	a	804	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
17	4	301	XAT	C15-C14-C13	-4.04	121.55	127.31
19	2	308	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
19	b	822	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
19	a	805	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
26	a	848	BCR	C11-C10-C9	-4.03	121.56	127.31
26	b	843	BCR	C28-C27-C26	-4.03	106.89	114.08
19	5	307	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
19	b	806	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
26	a	847	BCR	C38-C26-C25	-4.01	120.03	124.53
19	5	311	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
17	3	301	XAT	C35-C34-C33	-4.00	121.60	127.31
19	b	810	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
19	b	827	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
19	a	839	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
19	4	308	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
17	4	305	XAT	C6-C7-C8	-3.98	117.57	125.99
26	b	847	BCR	C28-C27-C26	-3.98	106.98	114.08
25	a	846	LHG	O7-C7-C8	3.97	120.06	111.50
26	f	804	BCR	C33-C5-C6	-3.97	120.07	124.53
26	i	101	BCR	C7-C8-C9	-3.97	120.24	126.23
25	m	101	LHG	O7-C7-C8	3.97	120.05	111.50
19	b	807	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
22	j	105	LMG	O7-C10-C11	3.96	120.03	111.50
19	b	832	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
26	b	847	BCR	C15-C14-C13	-3.95	121.67	127.31
17	4	305	XAT	C11-C10-C9	-3.95	121.67	127.31
17	a	852	XAT	C31-C30-C29	-3.95	121.67	127.31
19	3	309	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
17	1	303	XAT	C26-C27-C28	-3.93	117.68	125.99
19	1	308	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
19	a	838	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
19	a	822	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
26	l	201	BCR	C11-C10-C9	-3.93	121.70	127.31
19	b	814	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
19	5	312	CLA	CMB-C2B-C1B	-3.91	122.45	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	305	XAT	C27-C28-C29	-3.91	119.46	125.53
19	b	802	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
17	4	303	XAT	C15-C14-C13	-3.91	121.73	127.31
17	2	302	XAT	C31-C30-C29	-3.91	121.73	127.31
26	a	847	BCR	C20-C21-C22	-3.90	121.74	127.31
19	b	817	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
19	4	309	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
17	j	101	XAT	C15-C14-C13	-3.90	121.74	127.31
19	f	802	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
17	2	303	XAT	C15-C14-C13	-3.90	121.75	127.31
19	b	804	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
19	a	815	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
17	2	302	XAT	C15-C14-C13	-3.89	121.75	127.31
19	2	310	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
26	l	205	BCR	C33-C5-C6	-3.88	120.18	124.53
19	l	202	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
26	f	804	BCR	C20-C21-C22	-3.87	121.79	127.31
18	1	301	A1L1G	C37-C36-C35	3.86	131.38	123.47
26	f	804	BCR	C38-C26-C25	-3.86	120.19	124.53
19	b	816	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
19	2	312	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
18	3	306	A1L1G	C36-C37-C38	3.85	131.36	123.47
26	l	205	BCR	C16-C17-C18	-3.85	121.82	127.31
26	l	201	BCR	C16-C17-C18	-3.85	121.82	127.31
19	a	827	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
19	5	314	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	b	818	CLA	CMB-C2B-C3B	3.84	131.87	124.68
17	2	302	XAT	C26-C27-C28	-3.83	117.90	125.99
19	a	811	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
19	l	203	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
26	f	804	BCR	C16-C17-C18	-3.82	121.86	127.31
19	b	805	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
19	2	313	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
26	a	849	BCR	C28-C27-C26	-3.81	107.28	114.08
19	1	306	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
26	b	848	BCR	C15-C14-C13	-3.80	121.89	127.31
19	b	825	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
17	5	301	XAT	C15-C14-C13	-3.79	121.91	127.31
19	b	828	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
19	5	315	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	a	814	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
17	1	303	XAT	C35-C34-C33	-3.76	121.94	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	309	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
20	1	315	SQD	O47-C7-C8	3.75	119.58	111.50
19	a	812	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
19	1	310	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
26	b	846	BCR	C15-C14-C13	-3.75	121.96	127.31
26	j	104	BCR	C20-C21-C22	-3.75	121.96	127.31
18	5	303	A1L1G	C36-C37-C38	3.75	131.15	123.47
19	b	831	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	a	806	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
26	f	801	BCR	C16-C15-C14	-3.73	115.82	123.47
26	a	850	BCR	C33-C5-C6	-3.73	120.34	124.53
19	a	830	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
17	a	852	XAT	C35-C34-C33	-3.71	122.02	127.31
19	3	313	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
19	1	311	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	b	844	BCR	C3-C4-C5	-3.71	107.46	114.08
17	2	303	XAT	C26-C27-C28	-3.70	118.17	125.99
19	3	311	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
19	a	803	CLA	CMB-C2B-C3B	3.70	131.60	124.68
17	3	301	XAT	C26-C27-C28	-3.70	118.18	125.99
17	3	301	XAT	C31-C30-C29	-3.69	122.05	127.31
19	a	826	CLA	CMB-C2B-C3B	3.69	131.57	124.68
19	a	828	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
19	b	804	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
19	b	835	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
19	b	839	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
19	a	837	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
17	2	301	XAT	C27-C28-C29	-3.67	119.84	125.53
17	2	303	XAT	C6-C7-C8	-3.66	118.25	125.99
19	a	821	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
19	b	836	CLA	CMB-C2B-C3B	3.66	131.52	124.68
19	b	821	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
19	5	309	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
26	a	849	BCR	C20-C21-C22	-3.64	122.11	127.31
19	a	802	CLA	CMB-C2B-C3B	3.64	131.50	124.68
19	b	829	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	b	850	BCR	C7-C8-C9	-3.63	120.76	126.23
19	b	813	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
26	b	847	BCR	C3-C4-C5	-3.61	107.62	114.08
19	4	310	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
19	2	307	CLA	CMB-C2B-C3B	3.61	131.43	124.68
17	4	302	XAT	C35-C15-C14	-3.60	116.10	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	302	XAT	C11-C10-C9	-3.60	122.18	127.31
26	a	847	BCR	C33-C5-C6	-3.59	120.49	124.53
26	a	849	BCR	C11-C10-C9	-3.59	122.18	127.31
19	a	829	CLA	CMB-C2B-C3B	3.59	131.40	124.68
19	b	837	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
19	a	844	CLA	CMB-C2B-C3B	3.58	131.37	124.68
19	b	812	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
19	a	809	CLA	CMB-C2B-C3B	3.58	131.37	124.68
19	b	812	CLA	CAB-C3B-C4B	-3.57	122.98	128.46
19	b	819	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
19	a	833	CLA	CMB-C2B-C3B	3.56	131.34	124.68
19	b	808	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
19	b	834	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
19	a	808	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
19	a	835	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
19	b	823	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
26	b	844	BCR	C33-C5-C6	-3.55	120.54	124.53
19	l	204	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	b	815	CLA	CMB-C2B-C3B	3.55	131.31	124.68
19	b	826	CLA	CMB-C2B-C3B	3.54	131.31	124.68
19	4	313	CLA	CMB-C2B-C3B	3.54	131.30	124.68
17	4	303	XAT	C35-C34-C33	-3.54	122.26	127.31
26	l	205	BCR	C11-C10-C9	-3.54	122.26	127.31
26	l	205	BCR	C3-C4-C5	-3.53	107.78	114.08
19	3	310	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	i	101	BCR	C33-C5-C6	-3.52	120.57	124.53
26	a	847	BCR	C15-C14-C13	-3.52	122.29	127.31
19	a	813	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
19	a	832	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	1	312	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	b	804	CLA	CHB-C4A-NA	3.51	129.36	124.51
26	i	101	BCR	C28-C27-C26	-3.51	107.82	114.08
26	b	850	BCR	C38-C26-C25	-3.50	120.59	124.53
19	a	823	CLA	CMB-C2B-C3B	3.50	131.23	124.68
20	5	316	SQD	O47-C7-C8	3.50	119.05	111.50
17	1	303	XAT	C15-C14-C13	-3.50	122.31	127.31
19	a	806	CLA	CAA-CBA-CGA	-3.50	103.03	113.25
19	3	314	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
26	a	847	BCR	C7-C8-C9	-3.50	120.95	126.23
19	4	314	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
19	b	811	CLA	CMB-C2B-C3B	3.49	131.21	124.68
26	b	846	BCR	C24-C23-C22	-3.49	120.96	126.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	842	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
19	b	833	CLA	CMB-C2B-C3B	3.49	131.20	124.68
19	5	305	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
17	4	302	XAT	C11-C10-C9	-3.48	122.34	127.31
19	4	317	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
19	3	307	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
19	a	807	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
19	5	306	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	a	849	BCR	C4-C5-C6	-3.47	117.69	122.73
18	3	302	A1L1G	C36-C37-C38	3.47	130.58	123.47
19	b	802	CLA	CMB-C2B-C3B	3.47	131.17	124.68
19	4	315	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
19	b	827	CLA	CMB-C2B-C3B	3.46	131.16	124.68
26	a	848	BCR	C24-C23-C22	-3.46	121.00	126.23
19	a	819	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
19	a	817	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
19	1	305	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
19	a	841	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
19	a	805	CLA	CMB-C2B-C3B	3.45	131.14	124.68
19	a	818	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
18	5	303	A1L1G	C28-C39-C38	-3.44	118.10	122.92
19	5	308	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
19	1	309	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
19	a	806	CLA	CMB-C2B-C3B	3.44	131.12	124.68
25	a	846	LHG	O8-C23-C24	3.44	120.40	111.38
17	3	303	XAT	C11-C10-C9	-3.44	122.40	127.31
18	3	302	A1L1G	C37-C36-C35	3.44	130.52	123.47
19	5	313	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	3	315	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
17	2	304	XAT	C11-C10-C9	-3.44	122.41	127.31
19	4	312	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	b	820	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	b	824	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
17	2	305	XAT	C24-C23-C22	-3.43	104.14	110.77
19	b	809	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
19	i	102	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	1	301	A1L1G	C27-C34-C35	-3.43	118.12	122.92
17	2	304	XAT	C31-C30-C29	-3.43	122.42	127.31
19	1	313	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	2	308	CLA	CMB-C2B-C3B	3.43	131.09	124.68
19	4	306	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
26	a	849	BCR	C7-C8-C9	-3.43	121.06	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	847	BCR	C24-C23-C22	-3.42	121.06	126.23
19	a	831	CLA	CMB-C2B-C3B	3.42	131.08	124.68
19	2	314	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
19	4	316	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
17	3	305	XAT	C15-C14-C13	-3.42	122.43	127.31
19	a	816	CLA	CMB-C2B-C3B	3.42	131.08	124.68
18	3	302	A1L1G	C28-C39-C38	-3.42	118.13	122.92
19	3	308	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	j	102	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	b	806	CLA	CMB-C2B-C3B	3.42	131.07	124.68
19	f	803	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
26	a	848	BCR	C20-C21-C22	-3.41	122.44	127.31
19	a	840	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
18	3	306	A1L1G	C27-C34-C35	-3.41	118.15	122.92
19	1	307	CLA	CMB-C2B-C3B	3.41	131.05	124.68
26	a	847	BCR	C11-C10-C9	-3.41	122.45	127.31
19	2	311	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
19	2	306	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
19	1	314	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
19	b	822	CLA	CMB-C2B-C3B	3.40	131.04	124.68
17	5	302	XAT	C6-C7-C8	-3.40	118.81	125.99
19	b	838	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	5	311	CLA	CMB-C2B-C3B	3.40	131.03	124.68
19	a	820	CLA	CMB-C2B-C3B	3.39	131.03	124.68
19	a	810	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
17	5	301	XAT	C7-C8-C9	-3.39	120.27	125.53
26	a	849	BCR	C24-C23-C22	-3.39	121.11	126.23
18	1	301	A1L1G	C28-C39-C38	-3.39	118.18	122.92
19	2	315	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
19	4	308	CLA	CMB-C2B-C3B	3.38	131.01	124.68
19	j	103	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	b	832	CLA	CMB-C2B-C3B	3.38	131.00	124.68
19	2	316	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
19	a	825	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
23	1	304	A1L1F	C8-O7-C54	-3.38	111.61	117.90
19	a	854	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
18	5	303	A1L1G	C37-C36-C35	3.37	130.38	123.47
19	a	804	CLA	CMB-C2B-C3B	3.37	130.98	124.68
19	b	807	CLA	CMB-C2B-C3B	3.37	130.97	124.68
19	b	830	CLA	CMB-C2B-C3B	3.37	130.97	124.68
19	3	309	CLA	CMB-C2B-C3B	3.36	130.97	124.68
19	5	307	CLA	CMB-C2B-C3B	3.36	130.97	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	302	A1L1G	C27-C34-C35	-3.36	118.22	122.92
18	3	306	A1L1G	C28-C39-C38	-3.36	118.22	122.92
19	4	307	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
17	5	301	XAT	C6-C7-C8	-3.35	118.90	125.99
17	j	101	XAT	C10-C11-C12	-3.35	112.75	123.22
26	a	847	BCR	C3-C4-C5	-3.35	108.09	114.08
19	a	834	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
19	b	804	CLA	CMB-C2B-C3B	3.35	130.94	124.68
26	b	847	BCR	C10-C11-C12	-3.34	112.79	123.22
19	b	814	CLA	CMB-C2B-C3B	3.34	130.93	124.68
18	5	303	A1L1G	C27-C34-C35	-3.33	118.25	122.92
24	a	843	PQN	C14-C13-C15	3.33	120.88	115.27
26	b	850	BCR	C11-C10-C9	-3.33	122.56	127.31
19	5	310	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
17	1	303	XAT	C31-C30-C29	-3.33	122.56	127.31
19	a	824	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
18	1	301	A1L1G	C36-C37-C38	3.32	130.28	123.47
21	b	851	DGD	C2G-O2G-C1B	-3.31	109.63	117.79
17	1	303	XAT	C24-C23-C22	-3.31	104.38	110.77
26	i	101	BCR	C15-C14-C13	-3.31	122.58	127.31
17	4	301	XAT	C11-C10-C9	-3.31	122.59	127.31
19	4	311	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
19	a	838	CLA	CMB-C2B-C3B	3.31	130.86	124.68
19	a	839	CLA	CMB-C2B-C3B	3.30	130.86	124.68
19	b	801	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
19	f	802	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	a	827	CLA	CMB-C2B-C3B	3.30	130.84	124.68
19	1	308	CLA	CMB-C2B-C3B	3.29	130.83	124.68
19	5	312	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
19	b	817	CLA	CMB-C2B-C3B	3.28	130.82	124.68
17	4	303	XAT	C6-C7-C8	-3.28	119.06	125.99
17	5	304	XAT	C24-C23-C22	-3.28	104.44	110.77
26	a	850	BCR	C7-C8-C9	-3.27	121.29	126.23
19	4	309	CLA	CMB-C2B-C3B	3.27	130.80	124.68
26	j	104	BCR	C24-C23-C22	-3.27	121.30	126.23
26	i	101	BCR	C11-C10-C9	-3.26	122.65	127.31
19	5	314	CLA	CMB-C2B-C3B	3.26	130.78	124.68
17	5	304	XAT	C4-C3-C2	-3.26	104.48	110.77
19	3	312	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
26	l	201	BCR	C38-C26-C25	-3.25	120.88	124.53
18	1	301	A1L1G	C43-C44-C42	-3.24	118.38	122.92
19	a	815	CLA	CMB-C2B-C3B	3.24	130.74	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	312	CLA	CMB-C2B-C3B	3.24	130.73	124.68
19	j	103	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
17	5	301	XAT	C24-C23-C22	-3.23	104.54	110.77
19	b	841	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
17	3	304	XAT	C26-C27-C28	-3.23	119.17	125.99
19	b	809	CLA	O2A-CGA-O1A	-3.22	115.45	123.59
26	a	848	BCR	C33-C5-C6	-3.22	120.91	124.53
23	1	304	A1L1F	C14-C29-C30	-3.22	119.80	125.47
19	b	816	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	b	852	BCR	C24-C23-C22	-3.21	121.38	126.23
19	5	312	CLA	CMB-C2B-C3B	3.21	130.68	124.68
19	b	828	CLA	CMB-C2B-C3B	3.21	130.68	124.68
19	2	313	CLA	CMB-C2B-C3B	3.21	130.68	124.68
17	4	304	XAT	C15-C14-C13	-3.20	122.74	127.31
19	b	805	CLA	CMB-C2B-C3B	3.20	130.67	124.68
17	a	852	XAT	C10-C11-C12	-3.20	113.22	123.22
19	b	825	CLA	CMB-C2B-C3B	3.20	130.67	124.68
19	b	821	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
19	a	828	CLA	CMB-C2B-C3B	3.20	130.66	124.68
19	a	836	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
19	a	822	CLA	CMB-C2B-C3B	3.20	130.66	124.68
19	a	835	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
19	1	306	CLA	CMB-C2B-C3B	3.19	130.64	124.68
18	1	301	A1L1G	C33-C34-C35	3.19	123.83	118.94
17	1	302	XAT	C15-C14-C13	-3.18	122.77	127.31
18	3	306	A1L1G	C37-C36-C35	3.18	129.99	123.47
17	a	852	XAT	C11-C10-C9	-3.18	122.77	127.31
26	a	850	BCR	C11-C10-C9	-3.18	122.77	127.31
19	5	315	CLA	CMB-C2B-C3B	3.18	130.63	124.68
19	a	814	CLA	CMB-C2B-C3B	3.18	130.63	124.68
26	b	846	BCR	C20-C21-C22	-3.18	122.77	127.31
18	5	303	A1L1G	C40-C39-C38	3.17	123.81	118.94
19	2	309	CLA	CMB-C2B-C3B	3.17	130.61	124.68
17	4	303	XAT	C24-C23-C22	-3.17	104.66	110.77
17	2	301	XAT	C11-C10-C9	-3.16	122.80	127.31
19	a	812	CLA	CMB-C2B-C3B	3.16	130.59	124.68
26	l	201	BCR	C24-C23-C22	-3.16	121.46	126.23
19	1	310	CLA	CMB-C2B-C3B	3.16	130.58	124.68
26	b	844	BCR	C16-C17-C18	-3.15	122.81	127.31
19	l	202	CLA	CMB-C2B-C3B	3.15	130.58	124.68
17	3	304	XAT	C11-C10-C9	-3.15	122.81	127.31
19	a	830	CLA	CMB-C2B-C3B	3.15	130.57	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	840	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
19	a	811	CLA	CMB-C2B-C3B	3.15	130.57	124.68
19	a	804	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
26	a	848	BCR	C3-C4-C5	-3.15	108.45	114.08
19	b	810	CLA	CMB-C2B-C3B	3.14	130.56	124.68
26	a	848	BCR	C38-C26-C25	-3.14	121.00	124.53
17	4	304	XAT	C24-C23-C22	-3.14	104.71	110.77
19	1	311	CLA	CMB-C2B-C3B	3.14	130.55	124.68
19	a	803	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
17	3	303	XAT	C24-C23-C22	-3.14	104.72	110.77
19	b	833	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	2	301	XAT	C26-C27-C28	-3.12	119.39	125.99
19	a	818	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	b	848	BCR	C10-C11-C12	-3.12	113.49	123.22
26	b	852	BCR	C33-C5-C6	-3.11	121.03	124.53
19	5	309	CLA	CMB-C2B-C3B	3.11	130.50	124.68
19	1	313	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
21	4	318	DGD	O1G-C1A-C2A	3.11	121.67	111.91
26	a	849	BCR	C33-C5-C4	3.10	119.58	113.62
19	3	313	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	b	846	BCR	C33-C5-C4	3.09	119.56	113.62
19	l	203	CLA	CMB-C2B-C3B	3.09	130.46	124.68
26	b	846	BCR	C38-C26-C25	-3.09	121.06	124.53
19	a	837	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	3	306	A1L1G	C40-C39-C38	3.09	123.68	118.94
19	4	311	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	a	852	XAT	C35-C15-C14	-3.08	117.16	123.47
26	a	849	BCR	C38-C26-C25	-3.08	121.07	124.53
19	b	831	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	b	821	CLA	CMB-C2B-C3B	3.08	130.44	124.68
18	1	301	A1L1G	C40-C39-C38	3.08	123.66	118.94
19	a	809	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
26	b	843	BCR	C20-C21-C22	-3.07	122.93	127.31
18	3	302	A1L1G	C33-C34-C35	3.07	123.65	118.94
19	2	310	CLA	CMB-C2B-C3B	3.07	130.42	124.68
19	b	813	CLA	CMB-C2B-C3B	3.07	130.41	124.68
19	4	316	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
17	4	304	XAT	C35-C15-C14	-3.06	117.20	123.47
19	b	809	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	b	802	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
19	3	308	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
26	l	205	BCR	C8-C7-C6	-3.06	118.62	127.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	801	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
19	4	307	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
19	a	821	CLA	CMB-C2B-C3B	3.05	130.38	124.68
17	2	303	XAT	C19-C9-C10	-3.05	118.65	122.92
17	5	301	XAT	C31-C30-C29	-3.05	122.96	127.31
17	3	304	XAT	C4-C3-C2	-3.05	104.89	110.77
26	a	848	BCR	C8-C7-C6	-3.04	118.68	127.20
17	1	302	XAT	C31-C30-C29	-3.03	122.98	127.31
19	3	311	CLA	CMB-C2B-C3B	3.03	130.35	124.68
26	b	850	BCR	C15-C14-C13	-3.03	122.99	127.31
19	a	807	CLA	CMB-C2B-C3B	3.03	130.34	124.68
19	b	808	CLA	CMB-C2B-C3B	3.03	130.34	124.68
17	a	852	XAT	C31-C32-C33	-3.02	117.93	126.42
18	3	306	A1L1G	C43-C44-C42	-3.02	118.69	122.92
26	f	801	BCR	C8-C7-C6	-3.02	118.72	127.20
26	b	847	BCR	C11-C10-C9	-3.02	123.00	127.31
19	b	837	CLA	CMB-C2B-C3B	3.02	130.33	124.68
19	b	839	CLA	CMB-C2B-C3B	3.02	130.32	124.68
19	b	817	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	a	831	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	3	302	A1L1G	C40-C39-C38	3.00	123.55	118.94
17	4	305	XAT	C24-C23-C22	-3.00	104.97	110.77
19	a	835	CLA	CMB-C2B-C3B	3.00	130.30	124.68
19	b	835	CLA	CMB-C2B-C3B	3.00	130.29	124.68
26	b	850	BCR	C16-C15-C14	-3.00	117.34	123.47
19	b	823	CLA	CMB-C2B-C3B	3.00	130.28	124.68
17	3	305	XAT	C4-C3-C2	-3.00	104.99	110.77
19	1	314	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
19	b	803	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	b	808	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
19	b	815	CLA	CHB-C4A-NA	2.98	128.64	124.51
19	l	204	CLA	CMB-C2B-C3B	2.98	130.26	124.68
19	4	310	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	b	834	CLA	CMB-C2B-C3B	2.98	130.25	124.68
21	b	851	DGD	O3E-C3E-C2E	-2.98	103.47	110.35
26	b	848	BCR	C8-C7-C6	-2.97	118.85	127.20
19	b	819	CLA	CMB-C2B-C3B	2.97	130.24	124.68
18	5	303	A1L1G	C33-C34-C35	2.97	123.50	118.94
19	b	835	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	812	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	b	837	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
17	4	301	XAT	C31-C32-C33	-2.97	118.08	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	306	A1L1G	C33-C34-C35	2.97	123.49	118.94
19	a	830	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
19	4	308	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	5	308	CLA	CMB-C2B-C3B	2.95	130.20	124.68
26	a	850	BCR	C28-C27-C26	-2.95	108.81	114.08
19	3	314	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	4	309	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
17	3	305	XAT	C31-C30-C29	-2.94	123.11	127.31
19	a	839	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	b	846	BCR	C8-C7-C6	-2.94	118.95	127.20
19	b	825	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	2	309	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	3	301	XAT	C4-C3-C2	-2.93	105.11	110.77
26	b	852	BCR	C16-C15-C14	-2.93	117.47	123.47
17	4	304	XAT	C4-C3-C2	-2.93	105.11	110.77
19	1	311	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	3	305	XAT	C24-C23-C22	-2.93	105.12	110.77
19	3	309	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
19	a	808	CLA	CMB-C2B-C3B	2.92	130.15	124.68
19	b	815	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
19	2	313	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
17	1	302	XAT	C35-C15-C14	-2.92	117.49	123.47
18	5	303	A1L1G	C43-C44-C42	-2.92	118.83	122.92
26	b	844	BCR	C38-C26-C25	-2.92	121.25	124.53
19	b	840	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	a	817	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	b	830	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
17	4	303	XAT	C30-C31-C32	-2.92	114.12	123.22
19	b	819	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
17	2	304	XAT	C24-C23-C22	-2.91	105.15	110.77
19	a	812	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	b	841	CLA	CMB-C2B-C3B	2.91	130.12	124.68
19	a	840	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	5	304	XAT	C5-C4-C3	-2.91	106.99	112.75
20	5	316	SQD	C44-O6-C1	-2.91	108.06	113.74
26	b	845	BCR	C38-C26-C25	-2.90	121.27	124.53
17	1	302	XAT	C4-C3-C2	-2.90	105.17	110.77
17	4	302	XAT	C24-C23-C22	-2.90	105.17	110.77
19	3	307	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	4	312	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	2	303	XAT	C4-C3-C2	-2.90	105.18	110.77
19	2	316	CLA	O2D-CGD-O1D	-2.90	118.17	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	l	202	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	b	818	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
26	a	848	BCR	C7-C8-C9	-2.90	121.86	126.23
19	1	313	CLA	CMB-C2B-C3B	2.90	130.09	124.68
19	5	315	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	b	824	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	b	827	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	4	314	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	a	813	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	5	302	XAT	C24-C23-C22	-2.89	105.20	110.77
19	b	805	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	b	806	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	b	829	CLA	CMB-C2B-C3B	2.88	130.07	124.68
19	4	317	CLA	CMB-C2B-C3B	2.88	130.07	124.68
19	5	307	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	f	801	BCR	C20-C19-C18	-2.88	118.32	126.42
19	j	102	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
17	2	305	XAT	C11-C10-C9	-2.88	123.20	127.31
19	a	810	CLA	CMB-C2B-C3B	2.88	130.07	124.68
19	a	820	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	b	847	BCR	C33-C5-C6	-2.88	121.29	124.53
19	2	310	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	a	819	CLA	CMB-C2B-C3B	2.87	130.06	124.68
19	a	841	CLA	CMB-C2B-C3B	2.87	130.06	124.68
19	a	837	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	b	838	CLA	CMB-C2B-C3B	2.87	130.05	124.68
19	1	309	CLA	CMB-C2B-C3B	2.87	130.05	124.68
19	3	307	CLA	CMB-C2B-C3B	2.87	130.04	124.68
19	a	832	CLA	CMB-C2B-C3B	2.87	130.04	124.68
17	1	302	XAT	C24-C23-C22	-2.87	105.23	110.77
26	b	850	BCR	C23-C24-C25	-2.87	119.15	127.20
19	3	308	CLA	CMB-C2B-C3B	2.87	130.04	124.68
19	2	314	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
19	5	309	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
26	f	801	BCR	C33-C5-C6	-2.86	121.31	124.53
17	a	852	XAT	C24-C23-C22	-2.86	105.25	110.77
19	1	305	CLA	CMB-C2B-C3B	2.86	130.02	124.68
19	2	307	CLA	CHB-C4A-NA	2.85	128.46	124.51
19	b	804	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
19	b	809	CLA	CMB-C2B-C3B	2.85	130.01	124.68
26	b	848	BCR	C15-C16-C17	-2.85	117.64	123.47
19	5	312	CLA	O2D-CGD-CBD	2.85	116.33	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	315	CLA	CMB-C2B-C3B	2.85	130.01	124.68
18	3	302	A1L1G	C43-C44-C42	-2.85	118.93	122.92
19	1	312	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	5	305	CLA	CMB-C2B-C3B	2.85	130.00	124.68
17	4	302	XAT	C4-C3-C2	-2.85	105.28	110.77
19	a	823	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
17	2	304	XAT	C4-C3-C2	-2.84	105.28	110.77
19	a	816	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	a	825	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	2	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	a	817	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	4	301	XAT	C4-C3-C2	-2.84	105.29	110.77
19	b	839	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	j	102	CLA	CMB-C2B-C3B	2.84	129.98	124.68
21	4	318	DGD	O5E-C6E-C5E	-2.83	101.57	111.29
17	1	303	XAT	C4-C3-C2	-2.83	105.30	110.77
19	b	838	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	3	303	XAT	C4-C3-C2	-2.83	105.30	110.77
17	5	302	XAT	C35-C34-C33	-2.83	123.27	127.31
19	1	307	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	a	825	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	1	314	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	b	846	BCR	C4-C5-C6	-2.83	118.62	122.73
19	a	826	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	b	828	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	b	845	BCR	C34-C9-C10	-2.83	118.96	122.92
19	a	833	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	a	802	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
19	a	811	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
19	a	827	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	5	310	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	1	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	f	803	CLA	CMB-C2B-C3B	2.82	129.95	124.68
19	a	832	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	a	813	CLA	CMB-C2B-C3B	2.82	129.95	124.68
17	j	101	XAT	C4-C3-C2	-2.81	105.34	110.77
19	3	311	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	j	104	BCR	C38-C26-C27	2.81	119.02	113.62
17	5	304	XAT	C19-C9-C8	2.81	122.50	118.08
17	4	304	XAT	C11-C10-C9	-2.81	123.31	127.31
19	4	312	CLA	CMB-C2B-C3B	2.80	129.93	124.68
19	5	306	CLA	CMB-C2B-C3B	2.80	129.92	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	848	BCR	C21-C20-C19	-2.80	114.47	123.22
18	1	301	A1L1G	C20-C21-C22	-2.80	107.20	112.75
19	j	103	CLA	CMB-C2B-C3B	2.80	129.92	124.68
19	a	841	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	1	310	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	a	842	CLA	CMB-C2B-C3B	2.80	129.92	124.68
19	3	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	a	834	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	4	313	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	a	805	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
21	b	851	DGD	O1G-C1A-C2A	2.80	120.68	111.91
19	2	316	CLA	CMB-C2B-C3B	2.79	129.91	124.68
19	1	306	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
19	b	822	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
17	3	304	XAT	C24-C23-C22	-2.79	105.38	110.77
19	b	832	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	3	314	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	a	840	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	2	301	XAT	C4-C3-C2	-2.79	105.39	110.77
19	b	841	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	a	836	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	a	821	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	2	308	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	a	815	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	1	203	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	4	306	CLA	CMB-C2B-C3B	2.78	129.89	124.68
19	5	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	b	843	BCR	C33-C5-C4	2.78	118.96	113.62
19	3	312	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	2	311	CLA	CMB-C2B-C3B	2.78	129.88	124.68
19	a	803	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	a	844	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	2	317	LMG	O8-C28-C29	2.78	120.62	111.91
19	3	315	CLA	CMB-C2B-C3B	2.78	129.87	124.68
23	1	304	A1L1F	C20-C21-C22	-2.77	107.26	112.75
24	b	842	PQN	C16-C15-C13	-2.77	106.18	113.45
19	b	801	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	2	315	CLA	CMB-C2B-C3B	2.77	129.87	124.68
19	5	313	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	4	306	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	b	816	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	b	811	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	829	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	b	844	BCR	C21-C20-C19	-2.77	114.57	123.22
19	3	315	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	2	315	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	1	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	2	314	CLA	CMB-C2B-C3B	2.77	129.86	124.68
19	i	102	CLA	CMB-C2B-C3B	2.77	129.85	124.68
19	2	306	CLA	CMB-C2B-C3B	2.76	129.85	124.68
17	4	305	XAT	C4-C3-C2	-2.76	105.43	110.77
21	b	851	DGD	C6D-O5D-C1E	2.76	119.14	113.74
19	b	831	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	b	845	BCR	C37-C22-C21	-2.76	119.06	122.92
19	b	823	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	4	301	XAT	C26-C27-C28	-2.76	120.16	125.99
19	b	820	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	1	304	A1L1F	C36-C35-C34	-2.76	123.37	127.31
19	5	314	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	5	313	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	b	812	CLA	CMB-C2B-C3B	2.76	130.09	124.69
23	1	304	A1L1F	C26-O13-C45	2.76	121.81	115.68
26	b	845	BCR	C20-C21-C22	-2.76	123.38	127.31
19	a	820	CLA	C1-C2-C3	-2.75	121.28	126.04
26	b	843	BCR	C4-C5-C6	-2.75	118.73	122.73
19	3	312	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	a	819	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	4	316	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	a	854	CLA	CMB-C2B-C3B	2.75	129.83	124.68
17	2	305	XAT	C38-C25-C26	-2.75	117.65	122.26
19	b	820	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	b	843	BCR	C38-C26-C25	-2.75	121.44	124.53
19	b	826	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	3	303	XAT	C31-C30-C29	-2.75	123.39	127.31
19	a	828	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	4	302	XAT	C31-C30-C29	-2.74	123.39	127.31
26	a	849	BCR	C2-C1-C6	2.74	114.70	110.48
19	b	813	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	2	301	XAT	C24-C23-C22	-2.74	105.48	110.77
19	b	824	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	a	841	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	f	803	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
19	a	838	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
19	l	204	CLA	O2D-CGD-O1D	-2.73	118.49	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	315	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	3	301	XAT	C10-C11-C12	-2.73	114.69	123.22
26	a	850	BCR	C38-C26-C27	2.73	118.86	113.62
19	a	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	f	802	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	3	305	XAT	C35-C15-C14	-2.73	117.89	123.47
26	i	101	BCR	C20-C19-C18	-2.72	118.76	126.42
19	a	805	CLA	CHB-C4A-NA	2.72	128.28	124.51
17	2	302	XAT	C35-C15-C14	-2.72	117.90	123.47
19	4	314	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	2	305	XAT	C4-C3-C2	-2.72	105.52	110.77
19	4	313	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
19	4	307	CLA	CMB-C2B-C3B	2.72	129.76	124.68
19	l	203	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	b	850	BCR	C24-C23-C22	-2.72	122.13	126.23
19	2	312	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
19	b	836	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
26	j	104	BCR	C23-C24-C25	-2.71	119.58	127.20
17	2	302	XAT	C24-C23-C22	-2.71	105.53	110.77
19	a	824	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
19	5	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	5	310	CLA	CMB-C2B-C3B	2.71	129.75	124.68
26	b	845	BCR	C11-C10-C9	-2.71	123.44	127.31
26	b	843	BCR	C24-C23-C22	-2.71	122.14	126.23
22	a	853	LMG	O8-C28-C29	2.71	120.41	111.91
17	2	301	XAT	C31-C32-C33	-2.71	118.81	126.42
17	j	101	XAT	C24-C23-C22	-2.71	105.54	110.77
19	b	810	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
26	m	102	BCR	C33-C5-C6	-2.70	121.49	124.53
19	a	808	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
20	1	315	SQD	O48-C23-C24	2.70	120.38	111.91
26	b	852	BCR	C20-C19-C18	-2.69	118.85	126.42
26	b	843	BCR	C23-C24-C25	-2.69	119.64	127.20
17	1	303	XAT	C10-C11-C12	-2.69	114.81	123.22
19	a	814	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
19	a	829	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
19	b	812	CLA	CAB-C3B-C2B	2.69	129.95	124.69
17	5	304	XAT	C31-C30-C29	-2.69	123.47	127.31
26	b	850	BCR	C20-C21-C22	-2.69	123.47	127.31
19	b	801	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	j	101	XAT	C31-C30-C29	-2.69	123.48	127.31
26	b	847	BCR	C35-C13-C12	2.68	122.31	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	826	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	a	835	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	b	846	BCR	C7-C8-C9	-2.68	122.19	126.23
26	i	101	BCR	C29-C30-C25	2.68	114.60	110.48
17	j	101	XAT	C15-C35-C34	-2.68	117.99	123.47
17	5	302	XAT	C4-C3-C2	-2.68	105.60	110.77
17	3	301	XAT	C19-C9-C8	2.68	122.30	118.08
19	2	313	CLA	CAA-C2A-C3A	-2.68	109.86	116.10
17	4	302	XAT	C15-C14-C13	-2.67	123.49	127.31
19	3	312	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	4	315	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
17	3	301	XAT	C27-C28-C29	-2.67	121.38	125.53
26	b	846	BCR	C10-C11-C12	-2.67	114.88	123.22
25	m	101	LHG	O8-C23-C24	2.67	120.28	111.91
19	a	822	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	j	101	XAT	C31-C32-C33	-2.67	118.92	126.42
20	5	316	SQD	O48-C23-C24	2.67	120.28	111.91
19	4	310	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
19	5	314	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	b	842	PQN	C2M-C2-C3	-2.67	120.05	124.40
17	5	304	XAT	C10-C11-C12	-2.66	114.90	123.22
19	b	806	CLA	CHB-C4A-NA	2.66	128.20	124.51
17	4	305	XAT	C31-C32-C33	-2.66	118.94	126.42
19	1	312	CLA	CMB-C2B-C3B	2.66	129.65	124.68
19	a	804	CLA	C1-C2-C3	-2.65	121.45	126.04
17	4	301	XAT	C39-C29-C30	-2.65	119.21	122.92
19	b	807	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	4	308	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
19	b	825	CLA	CHB-C4A-NA	2.65	128.17	124.51
17	5	301	XAT	C35-C15-C14	-2.64	118.06	123.47
19	5	306	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	a	810	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	a	819	CLA	CHB-C4A-NA	2.64	128.17	124.51
19	a	829	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	b	827	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	4	317	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	b	809	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	a	821	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	b	819	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	a	814	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	a	834	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
26	a	847	BCR	C16-C15-C14	-2.63	118.08	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	311	CLA	CHB-C4A-NA	2.63	128.16	124.51
19	a	807	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	4	303	XAT	C4-C3-C2	-2.63	105.69	110.77
19	b	831	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
17	3	301	XAT	C24-C23-C22	-2.63	105.69	110.77
19	4	310	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	2	304	XAT	C15-C14-C13	-2.63	123.56	127.31
17	4	303	XAT	C39-C29-C28	2.63	122.22	118.08
17	4	301	XAT	C27-C28-C29	-2.63	121.45	125.53
26	f	801	BCR	C33-C5-C4	2.63	118.66	113.62
26	b	850	BCR	C28-C27-C26	-2.62	109.39	114.08
19	a	842	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	f	801	BCR	C10-C11-C12	-2.62	115.03	123.22
19	b	811	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	b	843	BCR	C2-C1-C6	2.62	114.51	110.48
17	2	305	XAT	C31-C32-C33	-2.62	119.06	126.42
17	4	305	XAT	C39-C29-C30	-2.62	119.25	122.92
19	b	820	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
23	1	304	A1L1F	C26-C30-C31	-2.62	121.51	124.93
17	4	305	XAT	C7-C8-C9	-2.62	121.47	125.53
26	b	850	BCR	C21-C20-C19	-2.61	115.06	123.22
19	b	841	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
19	a	833	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	a	809	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	i	102	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
19	2	311	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
19	j	103	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	b	851	DGD	C1E-O6E-C5E	2.60	118.80	113.69
19	b	818	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
19	1	309	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	l	201	BCR	C20-C21-C22	-2.60	123.60	127.31
25	b	849	LHG	O8-C23-C24	2.60	120.06	111.91
19	b	809	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	j	105	LMG	O8-C28-C29	2.60	120.06	111.91
19	b	826	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
17	4	304	XAT	C31-C30-C29	-2.60	123.60	127.31
19	5	313	CLA	CHB-C4A-NA	2.60	128.10	124.51
26	a	849	BCR	C16-C15-C14	-2.60	118.16	123.47
26	b	846	BCR	C2-C1-C6	2.59	114.47	110.48
19	a	824	CLA	CMB-C2B-C3B	2.59	129.53	124.68
19	a	832	CLA	CHB-C4A-NA	2.59	128.10	124.51
19	4	317	CLA	O2D-CGD-O1D	-2.59	118.77	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	802	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
19	4	315	CLA	CAA-C2A-C3A	-2.59	110.05	116.10
26	m	102	BCR	C27-C26-C25	2.59	126.49	122.73
19	5	311	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	b	834	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	a	802	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
19	b	818	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	2	311	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	1	314	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	3	310	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	a	818	CLA	CMB-C2B-C3B	2.59	129.51	124.68
19	b	801	CLA	CMB-C2B-C3B	2.58	129.51	124.68
26	l	205	BCR	C28-C27-C26	-2.58	109.47	114.08
17	2	304	XAT	C35-C15-C14	-2.58	118.19	123.47
23	1	304	AI1F	O13-C45-C47	2.58	120.01	111.91
19	1	306	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	1	308	CLA	C1-C2-C3	-2.58	121.58	126.04
26	m	102	BCR	C15-C16-C17	-2.58	118.20	123.47
26	b	847	BCR	C38-C26-C25	-2.58	121.64	124.53
19	b	814	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	3	315	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	3	314	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	b	817	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
19	a	804	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	2	308	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	a	849	BCR	C23-C24-C25	-2.56	120.00	127.20
19	a	806	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
25	a	845	LHG	O8-C23-C24	2.56	119.95	111.91
19	l	204	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	b	848	BCR	C24-C23-C22	-2.56	122.36	126.23
19	a	854	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	b	821	CLA	C1-C2-C3	-2.56	122.61	126.75
19	a	840	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	b	814	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	2	306	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
19	a	827	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
19	4	306	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	838	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	b	847	BCR	C8-C7-C6	-2.55	120.03	127.20
20	1	315	SQD	O8-S-C6	2.55	109.81	105.74
26	b	848	BCR	C34-C9-C8	2.55	122.10	118.08
19	2	307	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(°)
19	a	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	825	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	2	302	XAT	C11-C10-C9	-2.55	123.67	127.31
19	b	803	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	4	307	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	a	820	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
19	b	813	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	3	309	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	5	311	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	1	308	CLA	CHB-C4A-NA	2.54	128.03	124.51
17	a	852	XAT	O4-C5-C4	2.54	115.29	113.38
19	2	313	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	j	104	BCR	C33-C5-C6	-2.54	121.68	124.53
19	3	313	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	a	827	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	4	314	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	b	804	CLA	CHD-C1D-ND	-2.54	122.12	124.45
17	5	304	XAT	C8-C9-C10	-2.54	115.05	118.94
19	f	802	CLA	CHB-C4A-NA	2.53	128.02	124.51
19	5	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	b	848	BCR	C20-C21-C22	-2.53	123.69	127.31
19	5	312	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	b	836	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	1	309	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
19	4	311	CLA	CMB-C2B-C3B	2.53	129.41	124.68
19	a	832	CLA	C1-C2-C3	-2.53	122.66	126.75
19	a	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	b	844	BCR	C24-C23-C22	-2.53	122.41	126.23
19	3	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
19	2	316	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	1	303	XAT	C35-C15-C14	-2.53	118.29	123.47
19	b	835	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
26	b	847	BCR	C33-C5-C4	2.53	118.47	113.62
19	b	807	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	802	CLA	CHB-C4A-NA	2.53	128.00	124.51
17	2	302	XAT	C4-C3-C2	-2.52	105.90	110.77
19	1	307	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	b	838	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
19	a	836	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	f	803	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	b	830	CLA	C2D-C1D-ND	-2.52	108.25	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	812	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	b	852	BCR	C15-C14-C13	-2.52	123.72	127.31
19	5	306	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	a	822	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	b	803	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	a	853	LMG	C8-O7-C10	-2.52	111.60	117.79
19	b	830	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
19	1	312	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	3	308	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	b	832	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	b	837	CLA	CHB-C4A-NA	2.51	127.99	124.51
26	f	804	BCR	C15-C16-C17	-2.51	118.33	123.47
19	b	821	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	5	302	XAT	C19-C9-C10	-2.51	119.40	122.92
26	l	201	BCR	C28-C27-C26	-2.51	109.59	114.08
19	a	816	CLA	CHB-C4A-NA	2.51	127.99	124.51
26	l	201	BCR	C34-C9-C10	-2.51	119.41	122.92
19	a	801	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
19	b	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	5	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	l	205	BCR	C38-C26-C27	2.51	118.43	113.62
19	a	822	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
19	a	808	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	l	205	BCR	C15-C16-C17	-2.50	118.34	123.47
19	1	310	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	b	834	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	5	304	XAT	C15-C35-C34	-2.50	118.35	123.47
19	3	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	b	822	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	l	205	BCR	C33-C5-C4	2.50	118.41	113.62
19	5	312	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	l	203	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	5	305	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	a	823	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	l	202	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	a	836	CLA	CMB-C2B-C3B	2.49	129.34	124.68
19	a	802	CLA	C1-C2-C3	-2.49	121.73	126.04
19	a	831	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
20	5	316	SQD	O7-S-C6	2.49	109.90	106.94
17	5	304	XAT	C30-C31-C32	-2.49	115.44	123.22
19	5	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	4	316	CLA	CHB-C4A-NA	2.49	127.96	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	841	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	b	823	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	2	314	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	a	828	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	b	834	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	b	840	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	2	312	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	a	814	CLA	CHD-C1D-ND	-2.48	122.17	124.45
19	a	837	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	b	821	CLA	O2D-CGD-CBD	2.48	115.68	111.27
26	j	104	BCR	C27-C26-C25	-2.48	119.13	122.73
18	3	306	A1L1G	C17-C20-C21	2.48	117.07	114.28
19	1	310	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
26	f	801	BCR	C2-C1-C6	2.48	114.29	110.48
19	2	309	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	b	820	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	a	812	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
19	a	835	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
19	b	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	a	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	a	841	CLA	C1-C2-C3	-2.47	121.76	126.04
17	5	301	XAT	C4-C3-C2	-2.47	106.00	110.77
26	b	844	BCR	C15-C16-C17	-2.47	118.41	123.47
19	a	839	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	a	820	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	b	816	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	b	808	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
19	2	311	CLA	CHB-C4A-NA	2.47	127.92	124.51
17	5	304	XAT	C39-C29-C28	2.46	121.95	118.08
26	b	843	BCR	C15-C16-C17	-2.46	118.44	123.47
19	4	313	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	b	839	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	2	315	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	4	301	XAT	C35-C15-C14	-2.46	118.44	123.47
19	l	204	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	a	815	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	b	842	PQN	C14-C13-C15	2.45	119.40	115.27
19	b	832	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
26	b	847	BCR	C39-C30-C25	-2.45	106.32	110.30
19	a	805	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	b	811	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
19	a	837	CLA	C1B-CHB-C4A	-2.44	125.28	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	851	DGD	O2G-C1B-O1B	-2.44	117.80	123.70
26	j	104	BCR	C15-C16-C17	-2.44	118.47	123.47
19	a	806	CLA	O1D-CGD-CBD	2.44	129.48	124.48
19	2	306	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	b	846	BCR	C21-C20-C19	-2.44	115.60	123.22
19	b	835	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	a	809	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	b	834	CLA	CHD-C1D-ND	-2.44	122.22	124.45
26	a	848	BCR	C33-C5-C4	2.43	118.29	113.62
19	3	310	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	b	829	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	5	308	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	f	804	BCR	C28-C27-C26	-2.43	109.74	114.08
19	a	818	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	b	814	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
26	l	201	BCR	C21-C20-C19	-2.43	115.64	123.22
19	a	807	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
17	5	302	XAT	C31-C30-C29	-2.43	123.85	127.31
26	j	104	BCR	C38-C26-C25	-2.43	121.80	124.53
19	a	832	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
19	b	826	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	a	830	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
19	4	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	b	850	BCR	C33-C5-C4	2.42	118.27	113.62
26	b	846	BCR	C33-C5-C6	-2.42	121.81	124.53
23	1	304	A1L1F	C27-C34-C33	2.42	121.89	118.08
19	3	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	a	854	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	b	806	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	a	814	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	4	302	XAT	C10-C11-C12	-2.41	115.68	123.22
19	b	828	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
26	a	850	BCR	C16-C15-C14	-2.41	118.53	123.47
19	5	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	a	836	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	a	804	CLA	O2D-CGD-CBD	2.41	115.55	111.27
19	4	309	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	1	313	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	b	828	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	a	850	BCR	C8-C7-C6	-2.41	120.44	127.20
19	b	803	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
26	b	845	BCR	C28-C27-C26	-2.41	109.78	114.08

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	831	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	2	303	XAT	C8-C9-C10	2.40	122.63	118.94
19	3	311	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	5	314	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
26	b	843	BCR	C29-C30-C25	2.40	114.17	110.48
19	4	312	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	4	312	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	b	823	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	a	840	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	b	812	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
17	3	305	XAT	C10-C11-C12	-2.40	115.74	123.22
19	4	308	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	5	309	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	b	810	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	b	843	BCR	C21-C20-C19	-2.39	115.75	123.22
19	5	307	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	a	854	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	j	102	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	2	303	XAT	C24-C23-C22	-2.39	106.16	110.77
17	3	304	XAT	C31-C32-C33	-2.39	119.71	126.42
26	b	848	BCR	C38-C26-C25	-2.39	121.85	124.53
19	3	311	CLA	C1-C2-C3	-2.39	122.89	126.75
19	a	810	CLA	C1-C2-C3	-2.39	121.91	126.04
26	b	846	BCR	C16-C15-C14	-2.39	118.59	123.47
22	j	105	LMG	C8-O7-C10	-2.39	111.92	117.79
19	a	808	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	a	842	CLA	CHB-C4A-NA	2.38	127.81	124.51
19	i	102	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	b	850	BCR	C8-C7-C6	-2.38	120.51	127.20
19	1	313	CLA	CAA-C2A-C3A	-2.38	110.54	116.10
19	b	812	CLA	CHB-C4A-NA	2.38	127.81	124.51
19	1	313	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	a	804	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	a	835	CLA	O2D-CGD-CBD	2.38	115.50	111.27
19	a	834	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	3	310	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	b	816	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
26	a	850	BCR	C10-C11-C12	-2.38	115.80	123.22
19	b	810	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	a	818	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	b	837	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	a	803	CLA	CHD-C1D-ND	-2.38	122.27	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	813	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	b	833	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	3	313	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
19	a	825	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
19	f	802	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
26	b	844	BCR	C28-C27-C26	-2.37	109.84	114.08
19	5	315	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	i	102	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	b	824	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	a	816	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	a	833	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	l	202	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	1	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	a	844	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	1	311	CLA	CHB-C4A-NA	2.37	127.78	124.51
19	a	801	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	b	839	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
26	a	847	BCR	C23-C24-C25	-2.36	120.56	127.20
19	a	839	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	2	314	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	b	817	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	4	313	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	4	315	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	1	311	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	b	819	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	5	310	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	l	203	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	a	806	CLA	C5-C3-C2	-2.36	116.34	121.12
19	a	819	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	b	825	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	b	826	CLA	CHD-C1D-ND	-2.36	122.29	124.45
19	j	102	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	1	305	CLA	CHB-C4A-NA	2.36	127.77	124.51
17	3	303	XAT	C30-C31-C32	-2.36	115.87	123.22
26	b	850	BCR	C10-C11-C12	-2.35	115.87	123.22
26	b	843	BCR	C38-C26-C27	2.35	118.14	113.62
19	1	309	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	b	807	CLA	C1-C2-C3	-2.35	121.97	126.04
19	4	311	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
26	b	852	BCR	C36-C18-C17	-2.35	119.63	122.92
19	a	827	CLA	CHD-C1D-ND	-2.35	122.29	124.45
19	b	837	CLA	CHD-C1D-ND	-2.35	122.30	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	315	CLA	CHB-C4A-NA	2.35	127.75	124.51
17	5	304	XAT	C25-C24-C23	-2.34	108.11	112.75
26	b	844	BCR	C23-C24-C25	-2.34	120.62	127.20
19	a	834	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
19	b	813	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	4	302	XAT	C30-C31-C32	-2.34	115.91	123.22
19	a	806	CLA	C6-C5-C3	-2.34	107.31	113.45
19	a	844	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	b	801	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	i	101	BCR	C37-C22-C21	-2.34	119.64	122.92
19	b	817	CLA	CHD-C1D-ND	-2.34	122.30	124.45
19	3	308	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	a	828	CLA	C1-C2-C3	-2.34	122.00	126.04
19	a	811	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	b	821	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	a	831	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	b	805	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
19	a	828	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
19	a	824	CLA	CHB-C4A-NA	2.33	127.74	124.51
26	l	201	BCR	C15-C16-C17	-2.33	118.70	123.47
19	f	803	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	f	804	BCR	C11-C12-C13	-2.33	119.88	126.42
19	b	807	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	a	801	CLA	CMB-C2B-C3B	2.32	129.03	124.68
19	a	830	CLA	C1-C2-C3	-2.32	122.02	126.04
19	5	309	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	3	315	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
26	b	843	BCR	C11-C12-C13	-2.32	119.89	126.42
23	1	304	A1L1F	C31-C32-C33	-2.32	115.97	123.22
19	4	317	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	a	848	BCR	C15-C16-C17	-2.32	118.72	123.47
19	3	314	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	i	101	BCR	C16-C15-C14	-2.32	118.72	123.47
19	a	826	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	a	847	BCR	C33-C5-C4	2.32	118.07	113.62
19	5	307	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	a	841	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
19	a	812	CLA	CHD-C1D-ND	-2.32	122.32	124.45
19	b	836	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	b	804	CLA	C3C-C4C-NC	-2.32	107.97	110.57
19	a	810	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	4	314	CLA	C1B-CHB-C4A	-2.32	125.53	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	844	BCR	C33-C5-C4	2.31	118.06	113.62
17	4	301	XAT	C40-C33-C34	-2.31	119.68	122.92
19	b	815	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	b	833	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	a	816	CLA	C1-C2-C3	-2.31	123.02	126.75
19	2	313	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	5	310	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
17	2	301	XAT	C10-C11-C12	-2.31	116.02	123.22
23	1	304	A1L1F	C37-C36-C35	-2.31	118.75	123.47
26	a	848	BCR	C10-C11-C12	-2.31	116.02	123.22
24	a	843	PQN	C11-C12-C13	-2.31	122.95	126.79
19	b	841	CLA	CHB-C4A-NA	2.31	127.70	124.51
19	4	310	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
17	5	302	XAT	O4-C5-C4	2.30	115.11	113.38
26	m	102	BCR	C8-C7-C6	-2.30	120.73	127.20
19	a	815	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	b	831	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	1	312	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	5	313	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	3	311	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	a	836	CLA	C1-C2-C3	-2.30	123.03	126.75
19	2	310	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	j	103	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	a	805	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	b	840	CLA	CMB-C2B-C3B	2.30	128.98	124.68
19	a	841	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	4	312	CLA	CHD-C1D-ND	-2.29	122.34	124.45
17	3	301	XAT	C15-C35-C34	-2.29	118.77	123.47
19	a	820	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	5	314	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
17	2	302	XAT	C10-C11-C12	-2.29	116.06	123.22
26	b	852	BCR	C23-C24-C25	-2.29	120.76	127.20
19	a	838	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
17	2	304	XAT	C35-C34-C33	-2.29	124.04	127.31
19	2	310	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
17	j	101	XAT	C39-C29-C28	2.29	121.69	118.08
17	5	301	XAT	O4-C5-C4	2.29	115.10	113.38
19	a	810	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
19	3	307	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
17	1	303	XAT	C27-C28-C29	-2.29	121.98	125.53
17	5	302	XAT	C15-C35-C34	-2.29	118.79	123.47
19	a	824	CLA	C1B-CHB-C4A	-2.29	125.59	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	817	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
26	f	804	BCR	C3-C4-C5	-2.28	110.00	114.08
19	1	307	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	5	306	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	1	305	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	4	307	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	4	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
19	2	309	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	a	842	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	b	838	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	1	303	XAT	O4-C5-C4	2.27	115.09	113.38
19	1	314	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
18	1	301	A1L1G	C17-C20-C21	2.27	116.83	114.28
19	2	306	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	b	847	BCR	C21-C20-C19	-2.27	116.14	123.22
19	b	806	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	a	805	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
26	m	102	BCR	C24-C23-C22	-2.27	122.81	126.23
19	a	823	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
26	j	104	BCR	C34-C9-C10	-2.27	119.75	122.92
19	b	833	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	1	311	CLA	CHD-C1D-ND	-2.26	122.37	124.45
19	2	312	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
17	2	302	XAT	O4-C5-C4	2.26	115.08	113.38
17	2	303	XAT	O4-C5-C4	2.26	115.08	113.38
19	b	824	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
19	5	305	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	1	304	A1L1F	O7-C54-O55	-2.26	118.47	122.96
19	a	821	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	3	304	XAT	C40-C33-C34	-2.26	119.76	122.92
19	b	803	CLA	CHB-C4A-NA	2.26	127.63	124.51
19	4	310	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
19	a	827	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
19	1	306	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	2	316	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
17	a	852	XAT	C19-C9-C8	2.25	121.63	118.08
26	l	201	BCR	C23-C24-C25	-2.25	120.87	127.20
19	4	306	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
26	f	801	BCR	C28-C27-C26	-2.25	110.06	114.08
26	a	848	BCR	C16-C15-C14	-2.25	118.86	123.47
17	3	304	XAT	C27-C28-C29	-2.25	122.04	125.53
17	4	303	XAT	O4-C5-C4	2.25	115.07	113.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	852	BCR	C38-C26-C27	2.25	117.93	113.62
19	b	822	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
19	b	841	CLA	CHD-C1D-ND	-2.24	122.39	124.45
19	a	813	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	b	810	CLA	C1-C2-C3	-2.24	122.17	126.04
19	a	825	CLA	CHD-C1D-ND	-2.24	122.39	124.45
20	1	315	SQD	O9-S-C6	2.24	109.60	106.94
19	a	829	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	a	836	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	b	847	BCR	C38-C26-C27	2.24	117.92	113.62
19	b	827	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	b	822	CLA	C1-C2-C3	-2.24	122.17	126.04
18	1	301	A1L1G	C14-C29-C30	-2.24	121.53	125.47
17	5	302	XAT	C11-C12-C13	-2.24	120.14	126.42
26	a	849	BCR	C38-C26-C27	2.23	117.91	113.62
17	2	304	XAT	C20-C13-C12	2.23	121.59	118.08
26	b	850	BCR	C37-C22-C23	2.23	121.59	118.08
26	a	848	BCR	C21-C20-C19	-2.23	116.27	123.22
19	b	804	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
19	2	311	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	b	846	BCR	C11-C10-C9	-2.23	124.13	127.31
19	b	809	CLA	O2D-CGD-CBD	2.23	115.22	111.27
19	3	313	CLA	CHD-C1D-ND	-2.22	122.41	124.45
20	5	316	SQD	C45-O47-C7	-2.22	112.32	117.79
26	b	847	BCR	C34-C9-C8	2.22	121.58	118.08
19	4	316	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
19	4	308	CLA	CHD-C1D-ND	-2.22	122.42	124.45
17	2	303	XAT	C40-C33-C34	-2.22	119.82	122.92
19	1	305	CLA	CHD-C1D-ND	-2.22	122.42	124.45
19	b	830	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	b	847	BCR	C23-C24-C25	-2.21	120.98	127.20
26	b	848	BCR	C35-C13-C12	2.21	121.56	118.08
26	f	801	BCR	C34-C9-C8	2.21	121.56	118.08
17	5	301	XAT	O24-C25-C38	2.21	117.71	115.06
19	a	818	CLA	O2D-CGD-CBD	2.21	115.20	111.27
19	5	312	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	a	850	BCR	C20-C19-C18	-2.21	120.20	126.42
17	1	303	XAT	C19-C9-C8	2.21	121.56	118.08
19	l	202	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	f	801	BCR	C35-C13-C12	2.21	121.56	118.08
19	a	822	CLA	CHD-C1D-ND	-2.21	122.42	124.45
17	4	305	XAT	O4-C5-C4	2.21	115.04	113.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	836	CLA	CAC-C3C-C4C	2.21	127.68	124.81
17	4	305	XAT	C15-C35-C34	-2.21	118.95	123.47
19	b	832	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	f	801	BCR	C15-C14-C13	-2.21	124.16	127.31
19	1	309	CLA	CHD-C1D-ND	-2.21	122.43	124.45
26	b	845	BCR	C33-C5-C4	2.21	117.85	113.62
19	a	820	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
19	a	806	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	a	849	BCR	C21-C20-C19	-2.20	116.34	123.22
19	a	806	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	b	835	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	a	813	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	b	837	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	3	303	XAT	C15-C35-C34	-2.20	118.97	123.47
19	b	819	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	2	305	XAT	C19-C9-C8	2.19	121.53	118.08
19	f	803	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	b	822	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	2	305	XAT	C15-C35-C34	-2.19	118.98	123.47
17	2	301	XAT	O4-C5-C4	2.19	115.03	113.38
19	a	819	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
19	b	829	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	3	301	XAT	C8-C9-C10	-2.19	115.58	118.94
17	5	301	XAT	C30-C31-C32	-2.19	116.38	123.22
19	5	307	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
19	1	312	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
19	b	814	CLA	C1-C2-C3	-2.19	122.26	126.04
19	j	102	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	3	312	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	2	303	XAT	C39-C29-C30	-2.18	119.87	122.92
18	3	306	A1L1G	C20-C21-C22	-2.18	108.43	112.75
19	2	308	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	a	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	5	316	SQD	O9-S-C6	2.18	109.53	106.94
19	a	815	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	3	303	XAT	O24-C25-C38	2.18	117.67	115.06
26	1	201	BCR	C29-C30-C25	2.18	113.83	110.48
19	5	311	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
19	a	808	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	b	845	BCR	C7-C6-C5	-2.17	116.20	121.46
17	3	305	XAT	C19-C9-C8	2.17	121.50	118.08
19	b	804	CLA	O1D-CGD-CBD	2.17	128.92	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	XAT	C31-C32-C33	-2.17	120.33	126.42
17	4	305	XAT	O24-C25-C38	2.16	117.65	115.06
19	a	831	CLA	O2D-CGD-CBD	2.16	115.11	111.27
19	a	801	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	b	805	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
26	a	848	BCR	C23-C24-C25	-2.16	121.13	127.20
19	3	311	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
19	1	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	m	102	BCR	C15-C14-C13	-2.16	124.22	127.31
26	a	849	BCR	C8-C7-C6	-2.16	121.13	127.20
26	l	201	BCR	C3-C4-C5	-2.16	110.22	114.08
26	b	844	BCR	C36-C18-C19	2.16	121.48	118.08
19	5	315	CLA	CHD-C1D-ND	-2.16	122.47	124.45
17	4	302	XAT	C39-C29-C28	2.16	121.48	118.08
26	b	846	BCR	C34-C9-C8	2.16	121.48	118.08
19	1	312	CLA	CHD-C1D-ND	-2.16	122.47	124.45
17	4	303	XAT	O24-C25-C38	2.16	117.64	115.06
26	b	844	BCR	C37-C22-C23	2.16	121.48	118.08
17	3	303	XAT	C35-C15-C14	-2.16	119.05	123.47
26	l	201	BCR	C39-C30-C25	-2.16	106.80	110.30
17	4	301	XAT	O4-C5-C4	2.16	115.00	113.38
26	b	844	BCR	C11-C12-C13	-2.16	120.36	126.42
19	b	840	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	a	816	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	b	802	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	b	808	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	a	834	CLA	C1-C2-C3	-2.16	122.31	126.04
26	b	850	BCR	C35-C13-C12	2.16	121.47	118.08
19	a	833	CLA	C1-C2-C3	-2.15	122.32	126.04
26	b	847	BCR	C29-C30-C25	2.15	113.80	110.48
19	a	811	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	5	309	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	2	309	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	i	102	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	5	304	XAT	O24-C25-C38	2.15	117.63	115.06
19	1	308	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
19	a	830	CLA	CHB-C4A-NA	2.15	127.48	124.51
19	a	804	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
26	i	101	BCR	C23-C22-C21	2.15	122.23	118.94
17	3	303	XAT	O4-C5-C4	2.14	114.99	113.38
24	a	843	PQN	C2M-C2-C3	-2.14	120.90	124.40
19	a	834	CLA	O2A-CGA-O1A	-2.14	118.18	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	303	XAT	C7-C8-C9	-2.14	122.20	125.53
17	a	852	XAT	C40-C33-C32	2.14	121.45	118.08
17	2	305	XAT	O4-C5-C4	2.14	114.99	113.38
19	a	844	CLA	C1-C2-C3	-2.14	122.34	126.04
17	5	302	XAT	C20-C13-C14	-2.14	119.93	122.92
19	5	312	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	b	836	CLA	C1-C2-C3	-2.14	122.35	126.04
17	2	301	XAT	C39-C29-C30	-2.13	119.94	122.92
18	1	301	A1L1G	C29-C30-C31	2.13	122.16	118.93
19	5	305	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	j	101	XAT	O4-C5-C4	2.13	114.98	113.38
26	a	849	BCR	C10-C11-C12	-2.13	116.56	123.22
19	a	831	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	b	846	BCR	C23-C24-C25	-2.13	121.22	127.20
21	b	851	DGD	O3D-C3D-C4D	-2.13	105.43	110.35
19	a	806	CLA	C6-C7-C8	-2.13	109.04	115.92
19	b	839	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	a	839	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
17	4	302	XAT	C20-C13-C12	2.13	121.43	118.08
17	j	101	XAT	O24-C25-C38	2.12	117.60	115.06
26	a	849	BCR	C15-C16-C17	-2.12	119.12	123.47
26	i	101	BCR	C10-C11-C12	-2.12	116.59	123.22
17	2	304	XAT	O24-C25-C38	2.12	117.60	115.06
22	2	317	LMG	C8-O7-C10	-2.12	112.56	117.79
19	b	840	CLA	C1-C2-C3	-2.12	122.37	126.04
26	a	847	BCR	C38-C26-C27	2.12	117.69	113.62
19	a	829	CLA	CHD-C1D-ND	-2.12	122.50	124.45
19	b	813	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	3	313	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	a	848	BCR	C34-C9-C8	2.12	121.42	118.08
26	a	847	BCR	C8-C7-C6	-2.12	121.25	127.20
19	b	838	CLA	C1-C2-C3	-2.12	122.38	126.04
19	4	307	CLA	O2D-CGD-CBD	2.12	115.03	111.27
19	b	807	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	b	816	CLA	CHD-C1D-ND	-2.12	122.51	124.45
17	3	304	XAT	O4-C5-C18	2.11	117.59	115.06
19	b	817	CLA	C1-C2-C3	-2.11	122.39	126.04
17	4	304	XAT	O4-C5-C18	2.11	117.59	115.06
26	b	846	BCR	C15-C16-C17	-2.11	119.14	123.47
19	b	823	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
17	2	304	XAT	C10-C11-C12	-2.11	116.62	123.22
17	4	301	XAT	C28-C29-C30	2.11	122.18	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	XAT	O4-C5-C18	2.11	117.59	115.06
19	b	801	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	b	824	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	f	802	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	5	307	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	j	104	BCR	C16-C15-C14	-2.11	119.15	123.47
19	b	811	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	f	804	BCR	C35-C13-C14	-2.11	119.97	122.92
26	l	201	BCR	C37-C22-C23	2.11	121.40	118.08
19	b	822	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	b	845	BCR	C8-C9-C10	2.11	122.17	118.94
17	3	301	XAT	O24-C25-C38	2.11	117.58	115.06
19	a	812	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
17	a	852	XAT	C20-C13-C14	-2.11	119.97	122.92
19	5	311	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	i	102	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
17	3	303	XAT	C39-C29-C28	2.10	121.39	118.08
19	a	844	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	a	838	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
19	b	821	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
17	a	852	XAT	O24-C25-C38	2.10	117.58	115.06
17	2	301	XAT	O24-C25-C38	2.10	117.58	115.06
26	b	848	BCR	C37-C22-C23	2.10	121.39	118.08
17	3	303	XAT	C10-C11-C12	-2.10	116.66	123.22
19	a	836	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	b	829	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	b	835	CLA	C1-C2-C3	-2.10	122.41	126.04
19	b	839	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	b	830	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	b	830	CLA	C1-C2-C3	-2.10	122.42	126.04
26	j	104	BCR	C3-C4-C5	-2.10	110.33	114.08
19	4	308	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	b	802	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	4	311	CLA	O2D-CGD-CBD	2.10	114.99	111.27
19	a	807	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	b	848	BCR	C23-C24-C25	-2.10	121.32	127.20
26	a	847	BCR	C28-C27-C26	-2.09	110.34	114.08
19	b	812	CLA	CHD-C1D-ND	-2.09	122.53	124.45
17	2	305	XAT	O4-C5-C18	2.09	117.56	115.06
17	3	303	XAT	O4-C5-C18	2.09	117.56	115.06
17	1	302	XAT	O24-C25-C38	2.09	117.56	115.06
19	b	813	CLA	O2A-CGA-O1A	-2.09	118.32	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	834	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	4	306	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	4	308	CLA	O2D-CGD-CBD	2.09	114.98	111.27
17	4	303	XAT	C35-C15-C14	-2.09	119.20	123.47
17	5	302	XAT	O4-C5-C18	2.09	117.56	115.06
19	1	307	CLA	CHD-C1D-ND	-2.09	122.54	124.45
19	2	308	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
19	4	310	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	4	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
17	5	302	XAT	O24-C25-C26	-2.08	57.23	58.96
19	4	313	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
19	a	829	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
19	b	832	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
19	a	809	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	a	827	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
19	a	809	CLA	O2D-CGD-CBD	2.08	114.97	111.27
19	a	854	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	4	309	CLA	C1-C2-C3	-2.08	123.39	126.75
17	5	304	XAT	O4-C5-C18	2.08	117.55	115.06
19	b	821	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	2	317	LMG	C4-C3-C2	-2.08	107.19	110.82
17	3	305	XAT	O24-C25-C38	2.08	117.55	115.06
17	5	302	XAT	C30-C31-C32	-2.08	116.74	123.22
19	a	817	CLA	CHD-C1D-ND	-2.08	122.55	124.45
17	4	304	XAT	O4-C5-C4	2.07	114.94	113.38
19	b	820	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	j	104	BCR	C29-C30-C25	2.07	113.67	110.48
19	1	306	CLA	C1-C2-C3	-2.07	122.46	126.04
26	b	843	BCR	C37-C22-C23	2.07	121.34	118.08
17	3	304	XAT	C35-C15-C14	-2.07	119.23	123.47
17	2	303	XAT	O24-C25-C38	2.07	117.54	115.06
17	3	301	XAT	O4-C5-C18	2.07	117.54	115.06
17	5	304	XAT	C35-C15-C14	-2.07	119.23	123.47
19	b	808	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
19	b	824	CLA	C1-C2-C3	-2.07	122.46	126.04
19	2	314	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	3	309	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
19	a	824	CLA	CHD-C1D-ND	-2.07	122.56	124.45
26	f	804	BCR	C33-C5-C4	2.07	117.58	113.62
17	a	852	XAT	C39-C29-C28	2.06	121.33	118.08
19	b	831	CLA	CMA-C3A-C2A	-2.06	111.28	116.10
19	a	825	CLA	O2A-CGA-O1A	-2.06	118.38	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	304	XAT	C40-C33-C32	2.06	121.33	118.08
19	a	837	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	2	312	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	b	852	BCR	C32-C1-C6	-2.06	106.96	110.30
17	1	303	XAT	O24-C25-C38	2.06	117.53	115.06
17	2	302	XAT	O24-C25-C38	2.06	117.52	115.06
26	b	845	BCR	C16-C15-C14	-2.06	119.25	123.47
17	2	302	XAT	C27-C28-C29	-2.06	122.33	125.53
17	4	305	XAT	O4-C5-C18	2.06	117.52	115.06
19	1	310	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	1	306	CLA	CAC-C3C-C4C	2.06	127.48	124.81
19	1	306	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	a	844	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	b	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	2	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	a	854	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
19	b	841	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
19	a	832	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	b	820	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	3	313	CLA	C1-C2-C3	-2.05	122.49	126.04
19	b	838	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	1	302	XAT	O4-C5-C18	2.05	117.52	115.06
26	a	850	BCR	C37-C22-C21	-2.05	120.05	122.92
19	a	808	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	5	301	XAT	C39-C29-C28	2.05	121.31	118.08
19	b	805	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	a	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	b	852	BCR	C34-C9-C10	-2.05	120.05	122.92
17	1	303	XAT	C11-C10-C9	-2.05	124.39	127.31
17	2	304	XAT	C15-C35-C34	-2.05	119.28	123.47
17	5	301	XAT	O4-C5-C18	2.05	117.51	115.06
19	a	842	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	b	814	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	l	204	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	a	822	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
26	a	849	BCR	C37-C22-C23	2.05	121.30	118.08
26	b	848	BCR	C33-C5-C4	2.05	117.55	113.62
19	2	307	CLA	C2A-C1A-CHA	2.05	127.44	123.86
17	3	304	XAT	O24-C25-C38	2.04	117.50	115.06
17	3	304	XAT	O4-C5-C4	2.04	114.92	113.38
19	b	830	CLA	O2D-CGD-CBD	2.04	114.90	111.27
17	4	302	XAT	O4-C5-C18	2.04	117.50	115.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	1	306	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	b	828	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	b	840	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	4	304	XAT	C19-C9-C8	2.04	121.29	118.08
17	1	303	XAT	C20-C13-C12	2.04	121.29	118.08
19	2	310	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	2	305	XAT	C10-C11-C12	-2.04	116.85	123.22
26	f	804	BCR	C8-C7-C6	-2.04	121.48	127.20
19	j	102	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	a	840	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	1	311	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	5	311	CLA	C1-C2-C3	-2.04	122.52	126.04
19	1	307	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	a	832	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	4	302	XAT	O4-C5-C4	2.04	114.91	113.38
19	f	803	CLA	C1-C2-C3	-2.04	122.52	126.04
19	a	814	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	4	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	f	804	BCR	C21-C20-C19	-2.04	116.86	123.22
26	a	848	BCR	C28-C27-C26	-2.04	110.44	114.08
19	b	818	CLA	C1-C2-C3	-2.04	122.52	126.04
19	2	315	CLA	CHD-C1D-ND	-2.03	122.58	124.45
19	4	317	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
21	b	851	DGD	O5E-C6E-C5E	-2.03	104.32	111.29
19	a	804	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	b	804	CLA	CAC-C3C-C4C	2.03	127.45	124.81
17	4	304	XAT	O24-C25-C38	2.03	117.49	115.06
19	b	803	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	b	846	BCR	C28-C27-C26	-2.03	110.45	114.08
19	f	802	CLA	C1-C2-C3	-2.03	122.53	126.04
19	b	825	CLA	CHD-C1D-ND	-2.03	122.59	124.45
20	5	316	SQD	O8-S-C6	2.03	108.98	105.74
19	a	801	CLA	O1D-CGD-CBD	2.03	128.64	124.48
19	a	838	CLA	C1-C2-C3	-2.03	122.53	126.04
19	2	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	3	305	XAT	O4-C5-C18	2.03	117.49	115.06
19	b	808	CLA	O2D-CGD-CBD	2.03	114.87	111.27
19	a	840	CLA	C1-C2-C3	-2.03	122.54	126.04
19	b	818	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	b	817	CLA	O2D-CGD-CBD	2.03	114.87	111.27
19	a	811	CLA	C1-C2-C3	-2.03	122.54	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	304	XAT	O4-C5-C18	2.03	117.48	115.06
26	a	847	BCR	C20-C19-C18	-2.02	120.73	126.42
19	a	838	CLA	CHD-C1D-ND	-2.02	122.59	124.45
19	a	830	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
17	2	301	XAT	C19-C9-C8	2.02	121.27	118.08
19	3	315	CLA	CHD-C1D-ND	-2.02	122.59	124.45
17	2	302	XAT	C19-C9-C8	2.02	121.26	118.08
19	b	804	CLA	O2D-CGD-CBD	2.02	114.86	111.27
19	a	823	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	3	311	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	b	810	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	1	315	SQD	O7-S-C6	2.02	109.34	106.94
26	l	201	BCR	C33-C5-C4	2.02	117.50	113.62
19	3	308	CLA	O2D-CGD-CBD	2.02	114.85	111.27
19	4	316	CLA	CHD-C1D-ND	-2.02	122.60	124.45
17	4	302	XAT	O24-C25-C38	2.02	117.47	115.06
19	b	815	CLA	C1-C2-C3	-2.02	122.56	126.04
19	3	308	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
21	4	318	DGD	C4D-C3D-C2D	-2.01	107.31	110.82
19	l	203	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
17	2	304	XAT	C30-C31-C32	-2.01	116.94	123.22
19	a	816	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	1	311	CLA	O2D-CGD-CBD	2.01	114.84	111.27
19	4	307	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	b	810	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	a	809	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	b	836	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	b	811	CLA	C1-C2-C3	-2.01	122.57	126.04
19	1	308	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	b	835	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	1	304	A1L1F	C25-C14-C29	-2.01	121.75	125.99
26	b	845	BCR	C1-C6-C7	2.01	121.45	115.78
19	b	826	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
17	4	303	XAT	O4-C5-C18	2.01	117.46	115.06
19	b	801	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	f	802	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	b	843	BCR	C16-C15-C14	-2.00	119.37	123.47
19	a	815	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
19	3	310	CLA	CHD-C1D-ND	-2.00	122.61	124.45

All (146) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	5	305	CLA	ND
19	5	306	CLA	ND
19	5	307	CLA	ND
19	5	308	CLA	ND
19	5	309	CLA	ND
19	5	310	CLA	ND
19	5	311	CLA	ND
19	5	312	CLA	ND
19	5	313	CLA	ND
19	5	314	CLA	ND
19	5	315	CLA	ND
19	4	306	CLA	ND
19	4	307	CLA	ND
19	4	308	CLA	ND
19	4	309	CLA	ND
19	4	310	CLA	ND
19	4	311	CLA	ND
19	4	312	CLA	ND
19	4	313	CLA	ND
19	4	314	CLA	ND
19	4	315	CLA	ND
19	4	316	CLA	ND
19	4	317	CLA	ND
19	3	307	CLA	ND
19	3	308	CLA	ND
19	3	309	CLA	ND
19	3	310	CLA	ND
19	3	311	CLA	ND
19	3	312	CLA	ND
19	3	313	CLA	ND
19	3	314	CLA	ND
19	3	315	CLA	ND
19	2	306	CLA	ND
19	2	307	CLA	ND
19	2	308	CLA	ND
19	2	309	CLA	ND
19	2	310	CLA	ND
19	2	311	CLA	ND
19	2	312	CLA	ND
19	2	313	CLA	ND
19	2	314	CLA	ND
19	2	315	CLA	ND
19	2	316	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
19	1	305	CLA	ND
19	1	306	CLA	ND
19	1	307	CLA	ND
19	1	308	CLA	ND
19	1	309	CLA	ND
19	1	310	CLA	ND
19	1	311	CLA	ND
19	1	312	CLA	ND
19	1	313	CLA	ND
19	1	314	CLA	ND
19	a	801	CLA	ND
19	a	802	CLA	ND
19	a	803	CLA	ND
19	a	804	CLA	ND
19	a	805	CLA	ND
19	a	806	CLA	ND
19	a	807	CLA	ND
19	a	808	CLA	ND
19	a	809	CLA	ND
19	a	810	CLA	ND
19	a	811	CLA	ND
19	a	812	CLA	ND
19	a	813	CLA	ND
19	a	814	CLA	ND
19	a	815	CLA	ND
19	a	816	CLA	ND
19	a	817	CLA	ND
19	a	818	CLA	ND
19	a	819	CLA	ND
19	a	820	CLA	ND
19	a	821	CLA	ND
19	a	822	CLA	ND
19	a	823	CLA	ND
19	a	824	CLA	ND
19	a	825	CLA	ND
19	a	826	CLA	ND
19	a	827	CLA	ND
19	a	828	CLA	ND
19	a	829	CLA	ND
19	a	830	CLA	ND
19	a	831	CLA	ND
19	a	832	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
19	a	833	CLA	ND
19	a	834	CLA	ND
19	a	835	CLA	ND
19	a	836	CLA	ND
19	a	837	CLA	ND
19	a	838	CLA	ND
19	a	839	CLA	ND
19	a	840	CLA	ND
19	a	841	CLA	ND
19	a	842	CLA	ND
19	a	844	CLA	ND
19	a	854	CLA	ND
19	b	801	CLA	ND
19	b	802	CLA	ND
19	b	803	CLA	ND
19	b	804	CLA	ND
19	b	805	CLA	ND
19	b	806	CLA	ND
19	b	807	CLA	ND
19	b	808	CLA	ND
19	b	809	CLA	ND
19	b	810	CLA	ND
19	b	811	CLA	ND
19	b	812	CLA	ND
19	b	813	CLA	ND
19	b	814	CLA	ND
19	b	815	CLA	ND
19	b	816	CLA	ND
19	b	817	CLA	ND
19	b	818	CLA	ND
19	b	819	CLA	ND
19	b	820	CLA	ND
19	b	821	CLA	ND
19	b	822	CLA	ND
19	b	823	CLA	ND
19	b	824	CLA	ND
19	b	825	CLA	ND
19	b	826	CLA	ND
19	b	827	CLA	ND
19	b	828	CLA	ND
19	b	829	CLA	ND
19	b	830	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
19	b	831	CLA	ND
19	b	832	CLA	ND
19	b	833	CLA	ND
19	b	834	CLA	ND
19	b	835	CLA	ND
19	b	836	CLA	ND
19	b	837	CLA	ND
19	b	838	CLA	ND
19	b	839	CLA	ND
19	b	840	CLA	ND
19	b	841	CLA	ND
19	f	802	CLA	ND
19	f	803	CLA	ND
19	i	102	CLA	ND
19	j	102	CLA	ND
19	j	103	CLA	ND
19	l	202	CLA	ND
19	l	203	CLA	ND
19	l	204	CLA	ND

All (1617) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	5	302	XAT	O4-C6-C7-C8
17	5	302	XAT	C7-C8-C9-C10
17	5	302	XAT	C7-C8-C9-C19
17	4	301	XAT	C27-C28-C29-C30
17	4	301	XAT	C27-C28-C29-C39
17	4	303	XAT	O4-C6-C7-C8
17	4	303	XAT	C7-C8-C9-C10
17	4	303	XAT	C7-C8-C9-C19
17	4	305	XAT	O24-C26-C27-C28
17	3	301	XAT	O4-C6-C7-C8
17	3	301	XAT	C27-C28-C29-C30
17	3	301	XAT	C27-C28-C29-C39
17	3	303	XAT	C27-C28-C29-C30
17	3	303	XAT	C27-C28-C29-C39
17	3	304	XAT	O24-C26-C27-C28
17	3	304	XAT	C27-C28-C29-C30
17	3	304	XAT	C27-C28-C29-C39
17	2	303	XAT	O4-C6-C7-C8
17	2	303	XAT	O24-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	2	303	XAT	C27-C28-C29-C30
17	2	303	XAT	C27-C28-C29-C39
17	2	305	XAT	C25-C26-C27-C28
17	a	852	XAT	C7-C8-C9-C10
17	a	852	XAT	C7-C8-C9-C19
17	a	852	XAT	C11-C12-C13-C14
17	a	852	XAT	C11-C12-C13-C20
17	a	852	XAT	C27-C28-C29-C30
17	a	852	XAT	C27-C28-C29-C39
17	j	101	XAT	O4-C6-C7-C8
17	j	101	XAT	C7-C8-C9-C10
17	j	101	XAT	C7-C8-C9-C19
17	j	101	XAT	O24-C26-C27-C28
18	5	303	A1L1G	C26-C30-C31-C32
18	5	303	A1L1G	C31-C32-C33-C34
18	5	303	A1L1G	C32-C33-C34-C27
18	5	303	A1L1G	C32-C33-C34-C35
18	5	303	A1L1G	C41-C42-C44-C2
18	5	303	A1L1G	C41-C42-C44-C43
18	3	302	A1L1G	C25-C14-C29-C30
18	3	302	A1L1G	C14-C29-C30-C26
18	3	302	A1L1G	C26-C30-C31-C32
18	3	302	A1L1G	C29-C30-C31-C32
18	3	302	A1L1G	C41-C42-C44-C2
18	3	302	A1L1G	C41-C42-C44-C43
18	3	306	A1L1G	C45-C2-C44-C42
18	3	306	A1L1G	C45-C2-C44-C43
18	3	306	A1L1G	O13-C26-C30-C29
18	3	306	A1L1G	C37-C38-C39-C28
18	3	306	A1L1G	C37-C38-C39-C40
18	3	306	A1L1G	C39-C40-C41-C42
18	3	306	A1L1G	C41-C42-C44-C2
18	3	306	A1L1G	C41-C42-C44-C43
18	1	301	A1L1G	C45-C2-C44-C42
18	1	301	A1L1G	C45-C2-C44-C43
18	1	301	A1L1G	O13-C26-C30-C29
18	1	301	A1L1G	C27-C34-C35-C36
18	1	301	A1L1G	C33-C34-C35-C36
18	1	301	A1L1G	C35-C36-C37-C38
18	1	301	A1L1G	C28-C39-C40-C41
18	1	301	A1L1G	C38-C39-C40-C41
18	1	301	A1L1G	C39-C40-C41-C42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	5	307	CLA	CHA-CBD-CGD-O1D
19	5	307	CLA	CHA-CBD-CGD-O2D
19	5	308	CLA	CBD-CGD-O2D-CED
19	5	309	CLA	CHA-CBD-CGD-O1D
19	5	309	CLA	CHA-CBD-CGD-O2D
19	5	309	CLA	CAD-CBD-CGD-O1D
19	5	309	CLA	CAD-CBD-CGD-O2D
19	5	310	CLA	CBD-CGD-O2D-CED
19	5	314	CLA	C1A-C2A-CAA-CBA
19	5	314	CLA	C3A-C2A-CAA-CBA
19	5	315	CLA	CBD-CGD-O2D-CED
19	5	315	CLA	O1D-CGD-O2D-CED
19	4	306	CLA	C1A-C2A-CAA-CBA
19	4	307	CLA	CHA-CBD-CGD-O2D
19	4	309	CLA	CHA-CBD-CGD-O1D
19	4	309	CLA	CHA-CBD-CGD-O2D
19	4	309	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	C1A-C2A-CAA-CBA
19	4	311	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	C1A-C2A-CAA-CBA
19	4	312	CLA	C3A-C2A-CAA-CBA
19	4	313	CLA	CHA-CBD-CGD-O1D
19	4	313	CLA	CHA-CBD-CGD-O2D
19	4	315	CLA	CHA-CBD-CGD-O1D
19	4	315	CLA	CHA-CBD-CGD-O2D
19	4	316	CLA	C2A-CAA-CBA-CGA
19	4	316	CLA	CBD-CGD-O2D-CED
19	4	317	CLA	CBD-CGD-O2D-CED
19	3	309	CLA	CHA-CBD-CGD-O1D
19	3	309	CLA	CHA-CBD-CGD-O2D
19	3	310	CLA	C2-C3-C5-C6
19	3	310	CLA	C4-C3-C5-C6
19	3	312	CLA	C1A-C2A-CAA-CBA
19	3	315	CLA	C1A-C2A-CAA-CBA
19	2	307	CLA	CBD-CGD-O2D-CED
19	2	308	CLA	CHA-CBD-CGD-O1D
19	2	308	CLA	CHA-CBD-CGD-O2D
19	2	309	CLA	CBD-CGD-O2D-CED
19	2	312	CLA	CBD-CGD-O2D-CED
19	2	313	CLA	CBD-CGD-O2D-CED
19	1	305	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	1	305	CLA	CHA-CBD-CGD-O2D
19	1	305	CLA	C11-C10-C8-C9
19	1	310	CLA	CBD-CGD-O2D-CED
19	1	311	CLA	CHA-CBD-CGD-O1D
19	1	311	CLA	CHA-CBD-CGD-O2D
19	1	313	CLA	CBD-CGD-O2D-CED
19	1	314	CLA	C1A-C2A-CAA-CBA
19	1	314	CLA	C3A-C2A-CAA-CBA
19	a	801	CLA	CHA-CBD-CGD-O1D
19	a	801	CLA	CHA-CBD-CGD-O2D
19	a	801	CLA	CBD-CGD-O2D-CED
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	805	CLA	C3A-C2A-CAA-CBA
19	a	806	CLA	CHA-CBD-CGD-O1D
19	a	806	CLA	CHA-CBD-CGD-O2D
19	a	806	CLA	O2A-C1-C2-C3
19	a	809	CLA	C1A-C2A-CAA-CBA
19	a	809	CLA	C3A-C2A-CAA-CBA
19	a	811	CLA	CHA-CBD-CGD-O1D
19	a	811	CLA	CHA-CBD-CGD-O2D
19	a	811	CLA	CBD-CGD-O2D-CED
19	a	817	CLA	C2A-CAA-CBA-CGA
19	a	818	CLA	C1A-C2A-CAA-CBA
19	a	818	CLA	C3A-C2A-CAA-CBA
19	a	818	CLA	CHA-CBD-CGD-O1D
19	a	818	CLA	CHA-CBD-CGD-O2D
19	a	819	CLA	C3A-C2A-CAA-CBA
19	a	820	CLA	C1A-C2A-CAA-CBA
19	a	820	CLA	C3A-C2A-CAA-CBA
19	a	823	CLA	C1A-C2A-CAA-CBA
19	a	823	CLA	C3A-C2A-CAA-CBA
19	a	825	CLA	CHA-CBD-CGD-O1D
19	a	825	CLA	CHA-CBD-CGD-O2D
19	a	829	CLA	C1A-C2A-CAA-CBA
19	a	829	CLA	CBD-CGD-O2D-CED
19	a	831	CLA	C2-C3-C5-C6
19	a	831	CLA	C4-C3-C5-C6
19	a	832	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C1A-C2A-CAA-CBA
19	a	838	CLA	C2-C3-C5-C6
19	a	838	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	839	CLA	C2-C3-C5-C6
19	a	839	CLA	C4-C3-C5-C6
19	a	840	CLA	CHA-CBD-CGD-O1D
19	a	840	CLA	CHA-CBD-CGD-O2D
19	a	841	CLA	CHA-CBD-CGD-O1D
19	a	841	CLA	CHA-CBD-CGD-O2D
19	a	844	CLA	CHA-CBD-CGD-O1D
19	a	844	CLA	CHA-CBD-CGD-O2D
19	a	854	CLA	C1A-C2A-CAA-CBA
19	b	803	CLA	CHA-CBD-CGD-O1D
19	b	803	CLA	CHA-CBD-CGD-O2D
19	b	803	CLA	CBD-CGD-O2D-CED
19	b	804	CLA	CBD-CGD-O2D-CED
19	b	805	CLA	C2A-CAA-CBA-CGA
19	b	806	CLA	C1A-C2A-CAA-CBA
19	b	806	CLA	C3A-C2A-CAA-CBA
19	b	806	CLA	CHA-CBD-CGD-O1D
19	b	806	CLA	CHA-CBD-CGD-O2D
19	b	806	CLA	CAD-CBD-CGD-O1D
19	b	810	CLA	C1A-C2A-CAA-CBA
19	b	810	CLA	C2A-CAA-CBA-CGA
19	b	811	CLA	C1A-C2A-CAA-CBA
19	b	811	CLA	CHA-CBD-CGD-O1D
19	b	811	CLA	CHA-CBD-CGD-O2D
19	b	811	CLA	CAD-CBD-CGD-O1D
19	b	813	CLA	C1A-C2A-CAA-CBA
19	b	813	CLA	C2-C3-C5-C6
19	b	813	CLA	C4-C3-C5-C6
19	b	815	CLA	C1A-C2A-CAA-CBA
19	b	815	CLA	CBD-CGD-O2D-CED
19	b	818	CLA	C3A-C2A-CAA-CBA
19	b	819	CLA	C1A-C2A-CAA-CBA
19	b	819	CLA	C3A-C2A-CAA-CBA
19	b	821	CLA	C1A-C2A-CAA-CBA
19	b	821	CLA	C3A-C2A-CAA-CBA
19	b	821	CLA	CHA-CBD-CGD-O1D
19	b	821	CLA	CHA-CBD-CGD-O2D
19	b	824	CLA	CHA-CBD-CGD-O1D
19	b	824	CLA	CHA-CBD-CGD-O2D
19	b	827	CLA	CHA-CBD-CGD-O1D
19	b	827	CLA	CHA-CBD-CGD-O2D
19	b	829	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	829	CLA	C3A-C2A-CAA-CBA
19	b	833	CLA	C1A-C2A-CAA-CBA
19	b	833	CLA	C3A-C2A-CAA-CBA
19	b	834	CLA	C1A-C2A-CAA-CBA
19	b	834	CLA	C3A-C2A-CAA-CBA
19	b	834	CLA	C11-C12-C13-C14
19	b	835	CLA	CBD-CGD-O2D-CED
19	b	837	CLA	CHA-CBD-CGD-O1D
19	b	837	CLA	CHA-CBD-CGD-O2D
19	b	840	CLA	C1A-C2A-CAA-CBA
19	b	840	CLA	C3A-C2A-CAA-CBA
19	b	840	CLA	CHA-CBD-CGD-O1D
19	b	840	CLA	CHA-CBD-CGD-O2D
19	b	840	CLA	CAD-CBD-CGD-O1D
19	b	840	CLA	CBD-CGD-O2D-CED
19	j	102	CLA	C1A-C2A-CAA-CBA
19	j	102	CLA	C2-C3-C5-C6
19	j	102	CLA	C4-C3-C5-C6
19	j	103	CLA	CAD-CBD-CGD-O1D
19	j	103	CLA	CAD-CBD-CGD-O2D
19	j	103	CLA	CBD-CGD-O2D-CED
19	l	202	CLA	CHA-CBD-CGD-O1D
19	l	202	CLA	CHA-CBD-CGD-O2D
19	l	203	CLA	CHA-CBD-CGD-O1D
19	l	203	CLA	CHA-CBD-CGD-O2D
19	l	203	CLA	C6-C7-C8-C9
20	5	316	SQD	O49-C7-O47-C45
20	5	316	SQD	C8-C7-O47-C45
20	5	316	SQD	C5-C6-S-O7
20	5	316	SQD	C5-C6-S-O8
20	5	316	SQD	C5-C6-S-O9
20	1	315	SQD	O5-C5-C6-S
20	1	315	SQD	C5-C6-S-O7
20	1	315	SQD	C5-C6-S-O8
20	1	315	SQD	C5-C6-S-O9
21	4	318	DGD	C2B-C1B-O2G-C2G
21	4	318	DGD	O1B-C1B-O2G-C2G
21	4	318	DGD	C2E-C1E-O5D-C6D
21	4	318	DGD	O6E-C1E-O5D-C6D
22	2	317	LMG	O1-C7-C8-O7
22	a	853	LMG	C11-C10-O7-C8
22	j	105	LMG	O9-C10-O7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	j	105	LMG	C11-C10-O7-C8
23	1	304	A1L1F	C32-C33-C34-C27
23	1	304	A1L1F	C32-C33-C34-C35
23	1	304	A1L1F	C28-C39-C40-C41
23	1	304	A1L1F	C38-C39-C40-C41
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	849	LHG	O1-C1-C2-C3
25	b	849	LHG	C1-C2-C3-O3
25	b	849	LHG	O2-C2-C3-O3
25	b	849	LHG	C3-O3-P-O5
25	b	849	LHG	C4-O6-P-O3
25	b	849	LHG	C4-O6-P-O4
25	b	849	LHG	C4-O6-P-O5
25	m	101	LHG	C1-C2-C3-O3
25	m	101	LHG	C3-O3-P-O4
25	m	101	LHG	O9-C7-O7-C5
25	m	101	LHG	C8-C7-O7-C5
26	a	850	BCR	C23-C24-C25-C26
26	b	843	BCR	C7-C8-C9-C10
26	b	843	BCR	C7-C8-C9-C34
26	b	845	BCR	C1-C6-C7-C8
26	b	845	BCR	C5-C6-C7-C8
26	i	101	BCR	C21-C22-C23-C24
26	i	101	BCR	C37-C22-C23-C24
26	j	104	BCR	C7-C8-C9-C10
26	j	104	BCR	C7-C8-C9-C34
26	m	102	BCR	C1-C6-C7-C8
26	m	102	BCR	C7-C8-C9-C34
26	m	102	BCR	C21-C22-C23-C24
26	m	102	BCR	C37-C22-C23-C24
19	5	310	CLA	O1D-CGD-O2D-CED
19	4	309	CLA	O1D-CGD-O2D-CED
19	2	314	CLA	O1D-CGD-O2D-CED
19	2	307	CLA	O1D-CGD-O2D-CED
19	2	309	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	2	313	CLA	O1D-CGD-O2D-CED
19	1	313	CLA	O1D-CGD-O2D-CED
19	a	812	CLA	O1D-CGD-O2D-CED
19	b	803	CLA	O1D-CGD-O2D-CED
19	b	835	CLA	O1D-CGD-O2D-CED
19	5	313	CLA	CBD-CGD-O2D-CED
19	4	306	CLA	CBD-CGD-O2D-CED
19	2	314	CLA	CBD-CGD-O2D-CED
19	1	309	CLA	CBD-CGD-O2D-CED
19	a	812	CLA	CBD-CGD-O2D-CED
19	i	102	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	O1A-CGA-O2A-C1
19	a	806	CLA	O1A-CGA-O2A-C1
19	b	815	CLA	O1A-CGA-O2A-C1
22	2	317	LMG	O10-C28-O8-C9
25	m	101	LHG	O10-C23-O8-C6
19	4	316	CLA	O1D-CGD-O2D-CED
19	b	804	CLA	O1D-CGD-O2D-CED
19	5	308	CLA	O1D-CGD-O2D-CED
19	4	317	CLA	O1D-CGD-O2D-CED
19	2	312	CLA	O1D-CGD-O2D-CED
19	a	801	CLA	O1D-CGD-O2D-CED
19	a	811	CLA	O1D-CGD-O2D-CED
19	a	829	CLA	O1D-CGD-O2D-CED
19	b	815	CLA	O1D-CGD-O2D-CED
19	b	840	CLA	O1D-CGD-O2D-CED
19	j	103	CLA	O1D-CGD-O2D-CED
19	1	307	CLA	CBA-CGA-O2A-C1
19	a	806	CLA	CBA-CGA-O2A-C1
19	b	815	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	C24-C23-O8-C6
19	5	305	CLA	CBD-CGD-O2D-CED
19	5	306	CLA	CBD-CGD-O2D-CED
19	5	309	CLA	CBD-CGD-O2D-CED
19	3	308	CLA	CBD-CGD-O2D-CED
19	2	316	CLA	CBD-CGD-O2D-CED
19	a	804	CLA	CBD-CGD-O2D-CED
19	a	814	CLA	CBD-CGD-O2D-CED
19	b	806	CLA	CBD-CGD-O2D-CED
19	b	820	CLA	CBD-CGD-O2D-CED
19	b	836	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	2	310	CLA	O1A-CGA-O2A-C1
19	2	311	CLA	O1A-CGA-O2A-C1
19	a	805	CLA	O1A-CGA-O2A-C1
19	a	818	CLA	O1A-CGA-O2A-C1
19	b	822	CLA	O1A-CGA-O2A-C1
19	f	802	CLA	O1A-CGA-O2A-C1
22	a	853	LMG	O10-C28-O8-C9
25	b	849	LHG	O10-C23-O8-C6
19	4	311	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	O1D-CGD-O2D-CED
19	4	311	CLA	O1D-CGD-O2D-CED
19	4	307	CLA	CBD-CGD-O2D-CED
19	a	818	CLA	CBD-CGD-O2D-CED
19	a	837	CLA	CBD-CGD-O2D-CED
22	a	853	LMG	O9-C10-O7-C8
19	1	309	CLA	CBA-CGA-O2A-C1
23	1	304	A1L1F	C56-C54-O7-C8
19	1	309	CLA	O1A-CGA-O2A-C1
19	1	204	CLA	O1A-CGA-O2A-C1
19	3	312	CLA	C3-C5-C6-C7
19	2	310	CLA	C3-C5-C6-C7
19	2	311	CLA	C3-C5-C6-C7
19	2	314	CLA	C3-C5-C6-C7
19	a	810	CLA	C3-C5-C6-C7
19	b	802	CLA	C3-C5-C6-C7
19	b	805	CLA	C3-C5-C6-C7
19	b	807	CLA	C3-C5-C6-C7
19	b	809	CLA	C3-C5-C6-C7
19	2	310	CLA	CBA-CGA-O2A-C1
19	2	311	CLA	CBA-CGA-O2A-C1
19	a	805	CLA	CBA-CGA-O2A-C1
19	a	818	CLA	CBA-CGA-O2A-C1
19	a	836	CLA	CBA-CGA-O2A-C1
19	b	822	CLA	CBA-CGA-O2A-C1
19	b	824	CLA	CBA-CGA-O2A-C1
19	f	802	CLA	CBA-CGA-O2A-C1
22	2	317	LMG	C29-C28-O8-C9
22	a	853	LMG	C29-C28-O8-C9
23	1	304	A1L1F	O55-C54-O7-C8
19	1	309	CLA	O1D-CGD-O2D-CED
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	315	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	811	CLA	CBD-CGD-O2D-CED
19	l	204	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	C4-C3-C5-C6
19	a	825	CLA	C4-C3-C5-C6
19	b	829	CLA	C4-C3-C5-C6
19	a	841	CLA	CBD-CGD-O2D-CED
19	b	824	CLA	CBD-CGD-O2D-CED
19	b	828	CLA	CBD-CGD-O2D-CED
19	a	825	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	C2A-CAA-CBA-CGA
19	b	821	CLA	C2A-CAA-CBA-CGA
19	b	834	CLA	C2A-CAA-CBA-CGA
19	b	839	CLA	C2A-CAA-CBA-CGA
19	1	307	CLA	C3-C5-C6-C7
19	1	310	CLA	C3-C5-C6-C7
19	b	819	CLA	C3-C5-C6-C7
19	4	310	CLA	CBA-CGA-O2A-C1
19	1	305	CLA	CBA-CGA-O2A-C1
19	a	807	CLA	CBA-CGA-O2A-C1
19	a	811	CLA	CBA-CGA-O2A-C1
19	b	806	CLA	CBA-CGA-O2A-C1
19	b	811	CLA	CBA-CGA-O2A-C1
19	b	819	CLA	CBA-CGA-O2A-C1
22	j	105	LMG	C29-C28-O8-C9
25	b	849	LHG	C24-C23-O8-C6
22	j	105	LMG	C12-C13-C14-C15
22	j	105	LMG	C4-C5-C6-O5
19	5	311	CLA	O1A-CGA-O2A-C1
19	1	305	CLA	O1A-CGA-O2A-C1
19	a	811	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	O1A-CGA-O2A-C1
19	b	806	CLA	O1A-CGA-O2A-C1
19	b	819	CLA	O1A-CGA-O2A-C1
22	j	105	LMG	O10-C28-O8-C9
18	3	302	A1L1G	C30-C31-C32-C33
19	4	308	CLA	CBD-CGD-O2D-CED
19	a	807	CLA	CBD-CGD-O2D-CED
19	a	810	CLA	CBD-CGD-O2D-CED
19	a	834	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	CBD-CGD-O2D-CED
19	b	841	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	i	102	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	O2-C2-C3-O3
25	m	101	LHG	O2-C2-C3-O3
19	a	812	CLA	CBA-CGA-O2A-C1
19	b	840	CLA	CBA-CGA-O2A-C1
19	a	836	CLA	O1A-CGA-O2A-C1
19	b	824	CLA	O1A-CGA-O2A-C1
19	4	306	CLA	O1D-CGD-O2D-CED
19	5	311	CLA	CBD-CGD-O2D-CED
19	b	823	CLA	CBD-CGD-O2D-CED
19	b	840	CLA	O1A-CGA-O2A-C1
22	2	317	LMG	C29-C30-C31-C32
25	a	845	LHG	C12-C13-C14-C15
21	b	851	DGD	O6E-C5E-C6E-O5E
19	5	309	CLA	C3-C5-C6-C7
19	a	807	CLA	C3-C5-C6-C7
19	a	835	CLA	C3-C5-C6-C7
19	5	311	CLA	CBA-CGA-O2A-C1
19	a	820	CLA	CBA-CGA-O2A-C1
25	a	845	LHG	C28-C29-C30-C31
19	a	807	CLA	O1A-CGA-O2A-C1
19	b	811	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	C3-C5-C6-C7
19	a	825	CLA	C2-C3-C5-C6
19	5	310	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	b	801	CLA	C2A-CAA-CBA-CGA
19	b	827	CLA	C2A-CAA-CBA-CGA
19	5	313	CLA	O1D-CGD-O2D-CED
22	a	853	LMG	O6-C5-C6-O5
22	j	105	LMG	O6-C5-C6-O5
25	a	845	LHG	C23-C24-C25-C26
19	a	804	CLA	O1D-CGD-O2D-CED
19	b	806	CLA	O1D-CGD-O2D-CED
19	b	836	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C1-C2-C3-O3
19	5	308	CLA	CBA-CGA-O2A-C1
19	3	311	CLA	CBA-CGA-O2A-C1
19	a	809	CLA	CBA-CGA-O2A-C1
19	a	839	CLA	CBA-CGA-O2A-C1
19	a	854	CLA	CBA-CGA-O2A-C1
19	b	821	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	827	CLA	CBA-CGA-O2A-C1
19	b	834	CLA	CBA-CGA-O2A-C1
19	4	315	CLA	CBD-CGD-O2D-CED
19	b	807	CLA	CBD-CGD-O2D-CED
22	a	853	LMG	C4-C5-C6-O5
19	5	305	CLA	O1D-CGD-O2D-CED
18	5	303	A1L1G	C40-C41-C42-C44
19	a	810	CLA	C13-C15-C16-C17
19	a	807	CLA	C5-C6-C7-C8
19	b	809	CLA	C5-C6-C7-C8
19	i	102	CLA	C8-C10-C11-C12
25	a	846	LHG	O2-C2-C3-O3
22	a	853	LMG	C28-C29-C30-C31
19	a	809	CLA	O1A-CGA-O2A-C1
19	a	854	CLA	O1A-CGA-O2A-C1
19	a	813	CLA	C2-C3-C5-C6
19	2	310	CLA	C11-C12-C13-C14
19	1	306	CLA	C6-C7-C8-C9
19	1	306	CLA	C11-C12-C13-C14
19	1	310	CLA	C14-C13-C15-C16
19	a	829	CLA	C11-C10-C8-C9
19	b	801	CLA	C11-C10-C8-C9
19	b	801	CLA	C14-C13-C15-C16
19	b	805	CLA	C11-C10-C8-C9
19	b	819	CLA	C11-C10-C8-C9
19	b	825	CLA	C6-C7-C8-C9
19	b	830	CLA	C14-C13-C15-C16
19	b	839	CLA	C6-C7-C8-C9
19	f	802	CLA	C11-C12-C13-C14
19	i	102	CLA	C11-C10-C8-C9
19	i	102	CLA	C11-C12-C13-C14
19	2	316	CLA	O1D-CGD-O2D-CED
19	b	807	CLA	C15-C16-C17-C18
19	2	310	CLA	C2A-CAA-CBA-CGA
17	2	301	XAT	C27-C28-C29-C39
17	2	304	XAT	C7-C8-C9-C19
18	3	306	A1L1G	C28-C39-C40-C41
26	b	852	BCR	C7-C8-C9-C34
26	l	205	BCR	C7-C8-C9-C34
26	l	205	BCR	C37-C22-C23-C24
17	2	301	XAT	C27-C28-C29-C30
18	3	306	A1L1G	C38-C39-C40-C41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	b	852	BCR	C7-C8-C9-C10
26	l	205	BCR	C7-C8-C9-C10
26	l	205	BCR	C21-C22-C23-C24
19	a	814	CLA	O1D-CGD-O2D-CED
21	b	851	DGD	C1A-C2A-C3A-C4A
19	3	311	CLA	O1A-CGA-O2A-C1
19	b	821	CLA	O1A-CGA-O2A-C1
19	a	809	CLA	C5-C6-C7-C8
19	a	834	CLA	C15-C16-C17-C18
19	b	801	CLA	C15-C16-C17-C18
23	1	304	A1L1F	C49-C50-C51-C52
19	4	316	CLA	CBA-CGA-O2A-C1
19	2	312	CLA	CBA-CGA-O2A-C1
19	b	839	CLA	CBA-CGA-O2A-C1
19	2	310	CLA	C15-C16-C17-C18
19	b	809	CLA	C8-C10-C11-C12
19	b	833	CLA	C13-C15-C16-C17
19	b	834	CLA	C13-C15-C16-C17
19	5	309	CLA	O1D-CGD-O2D-CED
19	5	308	CLA	O1A-CGA-O2A-C1
19	b	827	CLA	O1A-CGA-O2A-C1
18	3	302	A1L1G	C35-C36-C37-C38
19	5	309	CLA	C13-C15-C16-C17
19	4	308	CLA	C10-C11-C12-C13
19	1	306	CLA	C8-C10-C11-C12
19	a	802	CLA	C5-C6-C7-C8
19	a	809	CLA	C8-C10-C11-C12
19	a	814	CLA	C13-C15-C16-C17
19	a	830	CLA	C13-C15-C16-C17
19	a	831	CLA	C5-C6-C7-C8
19	b	841	CLA	C13-C15-C16-C17
19	i	102	CLA	C10-C11-C12-C13
19	l	203	CLA	C10-C11-C12-C13
22	a	853	LMG	C10-C11-C12-C13
25	a	846	LHG	C7-C8-C9-C10
25	b	849	LHG	C7-C8-C9-C10
19	1	306	CLA	C5-C6-C7-C8
19	b	814	CLA	C15-C16-C17-C18
19	b	830	CLA	C8-C10-C11-C12
19	b	824	CLA	C3-C5-C6-C7
19	3	308	CLA	O1D-CGD-O2D-CED
19	b	820	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	807	CLA	C15-C16-C17-C18
19	a	841	CLA	C5-C6-C7-C8
19	b	815	CLA	C5-C6-C7-C8
19	b	837	CLA	C5-C6-C7-C8
23	1	304	A1L1F	C45-C47-C48-C49
19	b	802	CLA	CBD-CGD-O2D-CED
19	f	802	CLA	CBD-CGD-O2D-CED
19	1	310	CLA	C11-C10-C8-C7
19	a	801	CLA	C12-C13-C15-C16
19	a	809	CLA	C12-C13-C15-C16
19	a	828	CLA	C12-C13-C15-C16
19	a	831	CLA	C11-C10-C8-C7
19	a	844	CLA	C12-C13-C15-C16
19	b	808	CLA	C12-C13-C15-C16
19	a	801	CLA	C3-C5-C6-C7
19	a	839	CLA	O1A-CGA-O2A-C1
19	b	834	CLA	O1A-CGA-O2A-C1
19	a	830	CLA	C2A-CAA-CBA-CGA
19	5	306	CLA	O1D-CGD-O2D-CED
19	a	837	CLA	O1D-CGD-O2D-CED
19	1	306	CLA	C15-C16-C17-C18
19	b	841	CLA	C10-C11-C12-C13
19	5	305	CLA	CBA-CGA-O2A-C1
19	a	826	CLA	CBD-CGD-O2D-CED
19	a	841	CLA	C15-C16-C17-C18
19	a	818	CLA	O1D-CGD-O2D-CED
18	5	303	A1L1G	C39-C40-C41-C42
18	3	302	A1L1G	C39-C40-C41-C42
19	a	801	CLA	C8-C10-C11-C12
19	a	828	CLA	C13-C15-C16-C17
19	a	828	CLA	C15-C16-C17-C18
19	a	831	CLA	C15-C16-C17-C18
19	f	802	CLA	C13-C15-C16-C17
19	b	828	CLA	CBA-CGA-O2A-C1
19	2	312	CLA	O1A-CGA-O2A-C1
19	4	307	CLA	O1D-CGD-O2D-CED
19	b	837	CLA	C8-C10-C11-C12
24	b	842	PQN	C23-C25-C26-C27
19	3	315	CLA	O1D-CGD-O2D-CED
19	a	839	CLA	C13-C15-C16-C17
19	b	801	CLA	C13-C15-C16-C17
19	b	802	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	828	CLA	C13-C15-C16-C17
19	f	802	CLA	C5-C6-C7-C8
19	l	203	CLA	C8-C10-C11-C12
25	a	845	LHG	C3-O3-P-O6
25	b	849	LHG	C3-O3-P-O6
19	4	317	CLA	CBA-CGA-O2A-C1
19	a	816	CLA	CBA-CGA-O2A-C1
19	b	802	CLA	CBA-CGA-O2A-C1
19	b	832	CLA	CBA-CGA-O2A-C1
19	b	801	CLA	C8-C10-C11-C12
19	b	811	CLA	O1D-CGD-O2D-CED
19	1	308	CLA	C4-C3-C5-C6
21	b	851	DGD	C4E-C5E-C6E-O5E
19	5	306	CLA	C2A-CAA-CBA-CGA
19	1	314	CLA	C2A-CAA-CBA-CGA
19	b	829	CLA	C2A-CAA-CBA-CGA
19	a	801	CLA	C16-C17-C18-C20
19	b	811	CLA	C16-C17-C18-C20
19	4	313	CLA	C3-C5-C6-C7
19	a	814	CLA	CBA-CGA-O2A-C1
19	a	838	CLA	CBA-CGA-O2A-C1
19	b	824	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C11-C10-C9-C8
19	3	309	CLA	O1D-CGD-O2D-CED
20	1	315	SQD	C8-C7-O47-C45
19	a	824	CLA	CBA-CGA-O2A-C1
19	b	825	CLA	C5-C6-C7-C8
19	b	830	CLA	C10-C11-C12-C13
18	3	302	A1L1G	C37-C38-C39-C28
18	3	306	A1L1G	C27-C34-C35-C36
21	4	318	DGD	C3B-C4B-C5B-C6B
21	b	851	DGD	C9B-CAB-CBB-CCB
19	a	841	CLA	O1D-CGD-O2D-CED
19	b	834	CLA	C16-C17-C18-C19
19	b	841	CLA	C16-C17-C18-C20
19	a	833	CLA	CBA-CGA-O2A-C1
19	a	844	CLA	CBA-CGA-O2A-C1
20	1	315	SQD	O49-C7-O47-C45
19	a	854	CLA	C5-C6-C7-C8
19	b	840	CLA	C5-C6-C7-C8
19	a	836	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	C27-C28-C29-C30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	835	CLA	O1D-CGD-O2D-CED
19	b	839	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C13-C14-C15-C16
19	b	828	CLA	O1D-CGD-O2D-CED
18	5	303	A1L1G	C29-C30-C31-C32
19	a	834	CLA	O1D-CGD-O2D-CED
18	3	302	A1L1G	C37-C38-C39-C40
18	3	306	A1L1G	C33-C34-C35-C36
20	1	315	SQD	C24-C23-O48-C46
25	m	101	LHG	C9-C10-C11-C12
19	4	317	CLA	O1A-CGA-O2A-C1
19	a	816	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	C4-C3-C5-C6
19	b	840	CLA	C4-C3-C5-C6
19	1	308	CLA	C2-C3-C5-C6
19	b	807	CLA	C2-C3-C5-C6
19	b	829	CLA	C2-C3-C5-C6
18	3	302	A1L1G	C14-C29-C30-C31
19	a	828	CLA	C14-C13-C15-C16
19	a	839	CLA	C6-C7-C8-C9
19	a	840	CLA	C14-C13-C15-C16
19	b	826	CLA	C11-C10-C8-C9
22	2	317	LMG	C28-C29-C30-C31
19	5	315	CLA	C2C-C3C-CAC-CBC
21	4	318	DGD	C2B-C3B-C4B-C5B
21	b	851	DGD	C4A-C5A-C6A-C7A
25	m	101	LHG	C11-C12-C13-C14
19	a	814	CLA	C10-C11-C12-C13
19	a	814	CLA	C2A-CAA-CBA-CGA
19	b	832	CLA	C2A-CAA-CBA-CGA
19	b	841	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	O1A-CGA-O2A-C1
17	2	303	XAT	C7-C8-C9-C19
18	3	302	A1L1G	C32-C33-C34-C27
26	a	850	BCR	C37-C22-C23-C24
26	f	801	BCR	C37-C22-C23-C24
21	b	851	DGD	C3B-C4B-C5B-C6B
17	2	303	XAT	C7-C8-C9-C10
18	3	302	A1L1G	C32-C33-C34-C35
26	a	850	BCR	C21-C22-C23-C24
26	f	801	BCR	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	828	CLA	C8-C10-C11-C12
24	a	843	PQN	C25-C26-C27-C28
25	m	101	LHG	C28-C29-C30-C31
19	a	814	CLA	O1A-CGA-O2A-C1
19	4	308	CLA	C16-C17-C18-C20
19	b	811	CLA	C16-C17-C18-C19
19	b	812	CLA	C6-C7-C8-C9
19	f	802	CLA	C16-C17-C18-C19
19	f	802	CLA	C16-C17-C18-C20
19	a	827	CLA	C8-C10-C11-C12
19	a	841	CLA	C8-C10-C11-C12
19	b	806	CLA	C15-C16-C17-C18
19	b	836	CLA	C5-C6-C7-C8
20	1	315	SQD	C11-C10-C9-C8
25	m	101	LHG	C14-C15-C16-C17
19	a	814	CLA	C5-C6-C7-C8
19	b	809	CLA	C10-C11-C12-C13
23	1	304	A1L1F	C47-C48-C49-C50
19	4	308	CLA	O1D-CGD-O2D-CED
19	a	807	CLA	O1D-CGD-O2D-CED
19	a	810	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	C3A-C2A-CAA-CBA
19	3	312	CLA	C3A-C2A-CAA-CBA
19	3	314	CLA	C3A-C2A-CAA-CBA
19	2	306	CLA	C3A-C2A-CAA-CBA
19	a	807	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C3A-C2A-CAA-CBA
19	a	854	CLA	C3A-C2A-CAA-CBA
19	b	810	CLA	C3A-C2A-CAA-CBA
19	b	813	CLA	C3A-C2A-CAA-CBA
19	b	815	CLA	C3A-C2A-CAA-CBA
19	f	803	CLA	C3A-C2A-CAA-CBA
19	b	832	CLA	O1A-CGA-O2A-C1
19	b	801	CLA	C16-C17-C18-C20
19	b	812	CLA	C6-C7-C8-C10
19	b	834	CLA	C16-C17-C18-C20
21	b	851	DGD	C4B-C5B-C6B-C7B
19	3	314	CLA	CBD-CGD-O2D-CED
21	b	851	DGD	C2B-C3B-C4B-C5B
18	3	306	A1L1G	C35-C36-C37-C38
26	m	102	BCR	C14-C15-C16-C17
19	b	817	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	4	310	CLA	C2-C3-C5-C6
19	a	828	CLA	C2-C3-C5-C6
19	b	840	CLA	C2-C3-C5-C6
25	a	845	LHG	O1-C1-C2-O2
25	a	846	LHG	O1-C1-C2-O2
25	b	849	LHG	O1-C1-C2-O2
19	a	844	CLA	O1A-CGA-O2A-C1
19	b	808	CLA	C5-C6-C7-C8
19	a	833	CLA	O1A-CGA-O2A-C1
19	a	838	CLA	O1A-CGA-O2A-C1
20	1	315	SQD	O10-C23-O48-C46
19	j	102	CLA	CBD-CGD-O2D-CED
19	a	818	CLA	C2-C1-O2A-CGA
19	b	808	CLA	C3-C5-C6-C7
26	a	850	BCR	C23-C24-C25-C30
26	b	844	BCR	C1-C6-C7-C8
26	b	844	BCR	C5-C6-C7-C8
26	l	201	BCR	C1-C6-C7-C8
26	l	205	BCR	C23-C24-C25-C26
26	l	205	BCR	C23-C24-C25-C30
26	m	102	BCR	C5-C6-C7-C8
19	a	823	CLA	CBA-CGA-O2A-C1
19	b	807	CLA	CBA-CGA-O2A-C1
19	b	836	CLA	CBA-CGA-O2A-C1
19	a	809	CLA	C13-C15-C16-C17
19	b	830	CLA	C15-C16-C17-C18
19	b	839	CLA	C15-C16-C17-C18
19	j	102	CLA	C8-C10-C11-C12
25	a	845	LHG	C26-C27-C28-C29
19	2	314	CLA	C11-C10-C8-C9
19	4	316	CLA	O1A-CGA-O2A-C1
19	a	840	CLA	C13-C15-C16-C17
19	b	805	CLA	C13-C15-C16-C17
19	1	310	CLA	C4-C3-C5-C6
19	a	807	CLA	C4-C3-C5-C6
19	a	828	CLA	C4-C3-C5-C6
19	3	312	CLA	C6-C7-C8-C10
19	1	305	CLA	C11-C10-C8-C7
19	1	308	CLA	C11-C10-C8-C7
19	a	801	CLA	C11-C12-C13-C15
19	a	826	CLA	C11-C10-C8-C7
19	a	829	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	839	CLA	C6-C7-C8-C10
19	a	840	CLA	C12-C13-C15-C16
19	b	802	CLA	C11-C12-C13-C15
19	b	807	CLA	C11-C12-C13-C15
19	b	810	CLA	C11-C10-C8-C7
19	b	811	CLA	C2-C3-C5-C6
19	b	838	CLA	C11-C12-C13-C15
19	b	804	CLA	C2C-C3C-CAC-CBC
19	b	810	CLA	C5-C6-C7-C8
22	2	317	LMG	C10-C11-C12-C13
19	a	825	CLA	CBA-CGA-O2A-C1
19	b	825	CLA	CBA-CGA-O2A-C1
19	4	308	CLA	C15-C16-C17-C18
19	b	833	CLA	C15-C16-C17-C18
21	b	851	DGD	CAB-CBB-CCB-CDB
19	a	811	CLA	C11-C10-C8-C7
20	1	315	SQD	C7-C8-C9-C10
19	a	806	CLA	C13-C15-C16-C17
21	b	851	DGD	C6A-C7A-C8A-C9A
19	4	307	CLA	C3-C5-C6-C7
19	5	311	CLA	O1D-CGD-O2D-CED
19	b	817	CLA	O1A-CGA-O2A-C1
21	4	318	DGD	O6D-C1D-O3G-C3G
21	b	851	DGD	C2B-C1B-O2G-C2G
25	a	846	LHG	C8-C7-O7-C5
25	b	849	LHG	O6-C4-C5-O7
19	a	808	CLA	CBD-CGD-O2D-CED
25	a	846	LHG	O9-C7-O7-C5
19	2	308	CLA	C3-C5-C6-C7
21	4	318	DGD	O1G-C1G-C2G-O2G
19	b	841	CLA	C16-C17-C18-C19
19	b	809	CLA	C15-C16-C17-C18
19	b	807	CLA	C4-C3-C5-C6
19	b	811	CLA	C4-C3-C5-C6
19	b	835	CLA	C4-C3-C5-C6
19	3	315	CLA	CBA-CGA-O2A-C1
19	a	804	CLA	C2-C3-C5-C6
19	b	803	CLA	C2-C3-C5-C6
19	4	308	CLA	C11-C12-C13-C14
19	3	312	CLA	C6-C7-C8-C9
19	2	310	CLA	C14-C13-C15-C16
19	1	308	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	1	310	CLA	C11-C10-C8-C9
19	a	807	CLA	C14-C13-C15-C16
19	a	814	CLA	C11-C10-C8-C9
19	a	826	CLA	C11-C10-C8-C9
19	a	831	CLA	C11-C10-C8-C9
19	b	802	CLA	C11-C12-C13-C14
19	b	807	CLA	C11-C12-C13-C14
19	b	807	CLA	C14-C13-C15-C16
19	b	810	CLA	C11-C10-C8-C9
19	b	819	CLA	C6-C7-C8-C9
19	b	823	CLA	C6-C7-C8-C9
19	b	825	CLA	C11-C10-C8-C9
19	b	826	CLA	C6-C7-C8-C9
19	b	838	CLA	C11-C12-C13-C14
19	4	308	CLA	C13-C15-C16-C17
19	a	806	CLA	C2A-CAA-CBA-CGA
19	a	810	CLA	C2A-CAA-CBA-CGA
19	b	833	CLA	C2A-CAA-CBA-CGA
17	5	301	XAT	C7-C8-C9-C19
19	a	823	CLA	O1A-CGA-O2A-C1
19	b	807	CLA	O1A-CGA-O2A-C1
19	5	306	CLA	C1A-C2A-CAA-CBA
19	4	313	CLA	C1A-C2A-CAA-CBA
19	3	314	CLA	C1A-C2A-CAA-CBA
19	2	306	CLA	C1A-C2A-CAA-CBA
19	1	306	CLA	C1A-C2A-CAA-CBA
19	a	807	CLA	C1A-C2A-CAA-CBA
19	a	817	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C1A-C2A-CAA-CBA
19	a	825	CLA	C1A-C2A-CAA-CBA
19	b	817	CLA	C1A-C2A-CAA-CBA
19	b	818	CLA	C1A-C2A-CAA-CBA
19	b	838	CLA	C1A-C2A-CAA-CBA
19	f	803	CLA	C1A-C2A-CAA-CBA
19	a	801	CLA	C16-C17-C18-C19
19	a	806	CLA	C16-C17-C18-C19
19	b	801	CLA	C16-C17-C18-C19
25	m	101	LHG	C29-C30-C31-C32
19	5	305	CLA	O1A-CGA-O2A-C1
19	1	305	CLA	C8-C10-C11-C12
19	a	844	CLA	C10-C11-C12-C13
19	b	810	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	m	101	LHG	C3-O3-P-O6
19	b	807	CLA	O1D-CGD-O2D-CED
19	b	823	CLA	O1D-CGD-O2D-CED
19	b	836	CLA	O1A-CGA-O2A-C1
19	b	830	CLA	C13-C15-C16-C17
25	a	845	LHG	O6-C4-C5-C6
19	5	315	CLA	C4C-C3C-CAC-CBC
21	b	851	DGD	CBB-CCB-CDB-CEB
19	a	812	CLA	C10-C11-C12-C13
19	4	315	CLA	O1D-CGD-O2D-CED
25	m	101	LHG	C12-C13-C14-C15
19	b	814	CLA	C3-C5-C6-C7
19	b	836	CLA	C2C-C3C-CAC-CBC
19	b	825	CLA	O1A-CGA-O2A-C1
19	a	822	CLA	C2A-CAA-CBA-CGA
19	a	820	CLA	C16-C17-C18-C20
19	b	815	CLA	C6-C7-C8-C10
19	a	839	CLA	C3-C5-C6-C7
19	b	801	CLA	C3-C5-C6-C7
21	4	318	DGD	O1G-C1G-C2G-C3G
25	a	845	LHG	C4-C5-C6-O8
25	b	849	LHG	C4-C5-C6-O8
19	a	829	CLA	C10-C11-C12-C13
21	b	851	DGD	C3A-C4A-C5A-C6A
22	j	105	LMG	C13-C14-C15-C16
19	a	820	CLA	C8-C10-C11-C12
23	1	304	A1L1F	C50-C51-C52-C53
25	m	101	LHG	C11-C10-C9-C8
19	5	310	CLA	CAA-CBA-CGA-O2A
25	b	849	LHG	C8-C7-O7-C5
19	a	804	CLA	C4-C3-C5-C6
19	a	820	CLA	C4-C3-C5-C6
19	b	803	CLA	C4-C3-C5-C6
19	b	839	CLA	C4-C3-C5-C6
19	a	844	CLA	C16-C17-C18-C19
19	1	311	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C13-C15-C16-C17
19	a	854	CLA	C10-C11-C12-C13
19	b	840	CLA	C13-C15-C16-C17
24	a	843	PQN	C23-C25-C26-C27
22	a	853	LMG	C14-C15-C16-C17
19	f	802	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	802	CLA	O1D-CGD-O2D-CED
19	a	829	CLA	C8-C10-C11-C12
21	b	851	DGD	CCB-CDB-CEB-CFB
19	a	835	CLA	CBA-CGA-O2A-C1
19	a	825	CLA	O1A-CGA-O2A-C1
19	3	315	CLA	CAA-CBA-CGA-O2A
19	b	819	CLA	C11-C12-C13-C14
19	1	310	CLA	C5-C6-C7-C8
19	b	837	CLA	C2C-C3C-CAC-CBC
25	a	845	LHG	C7-C8-C9-C10
19	1	308	CLA	C15-C16-C17-C18
19	a	810	CLA	C5-C6-C7-C8
19	a	826	CLA	C15-C16-C17-C18
21	4	318	DGD	C2D-C1D-O3G-C3G
19	b	804	CLA	C15-C16-C17-C18
19	b	815	CLA	C6-C7-C8-C9
19	a	801	CLA	C4-C3-C5-C6
19	b	814	CLA	C4-C3-C5-C6
19	4	308	CLA	C12-C13-C15-C16
19	1	306	CLA	C6-C7-C8-C10
19	a	807	CLA	C12-C13-C15-C16
19	a	809	CLA	C6-C7-C8-C10
19	a	810	CLA	C12-C13-C15-C16
19	a	812	CLA	C6-C7-C8-C10
19	a	820	CLA	C2-C3-C5-C6
19	a	822	CLA	C6-C7-C8-C10
19	a	830	CLA	C12-C13-C15-C16
19	a	841	CLA	C11-C10-C8-C7
19	a	844	CLA	C11-C12-C13-C15
19	b	803	CLA	C12-C13-C15-C16
19	b	807	CLA	C11-C10-C8-C7
19	b	807	CLA	C12-C13-C15-C16
19	b	811	CLA	C11-C12-C13-C15
19	b	814	CLA	C2-C3-C5-C6
19	b	819	CLA	C6-C7-C8-C10
19	b	823	CLA	C6-C7-C8-C10
19	b	825	CLA	C11-C10-C8-C7
19	b	826	CLA	C6-C7-C8-C10
19	b	828	CLA	C6-C7-C8-C10
19	b	829	CLA	C12-C13-C15-C16
19	b	834	CLA	C11-C12-C13-C15
19	b	839	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	f	802	CLA	C11-C12-C13-C15
19	4	317	CLA	C3-C5-C6-C7
19	a	801	CLA	C11-C12-C13-C14
19	a	807	CLA	C11-C12-C13-C14
19	a	809	CLA	C14-C13-C15-C16
19	a	810	CLA	C14-C13-C15-C16
19	a	822	CLA	C6-C7-C8-C9
19	a	827	CLA	C11-C10-C8-C9
19	a	830	CLA	C14-C13-C15-C16
19	a	835	CLA	C6-C7-C8-C9
19	a	841	CLA	C11-C10-C8-C9
19	a	842	CLA	C11-C12-C13-C14
19	a	844	CLA	C11-C10-C8-C9
19	a	844	CLA	C11-C12-C13-C14
19	a	844	CLA	C14-C13-C15-C16
19	b	801	CLA	C11-C12-C13-C14
19	b	803	CLA	C6-C7-C8-C9
19	b	803	CLA	C11-C10-C8-C9
19	b	808	CLA	C11-C10-C8-C9
19	b	811	CLA	C11-C12-C13-C14
19	b	829	CLA	C11-C12-C13-C14
19	b	837	CLA	C14-C13-C15-C16
19	j	102	CLA	C6-C7-C8-C9
19	4	307	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	CBA-CGA-O2A-C1
19	a	812	CLA	C8-C10-C11-C12
19	a	819	CLA	C2A-CAA-CBA-CGA
18	3	306	A1L1G	C32-C33-C34-C27
19	a	844	CLA	C16-C17-C18-C20
17	4	305	XAT	C27-C28-C29-C30
25	b	849	LHG	C9-C10-C11-C12
19	a	826	CLA	O1D-CGD-O2D-CED
19	a	836	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	C15-C16-C17-C18
19	a	824	CLA	O1A-CGA-O2A-C1
21	b	851	DGD	C2A-C1A-O1G-C1G
19	b	805	CLA	C16-C17-C18-C20
25	b	849	LHG	O6-C4-C5-C6
19	b	834	CLA	C3-C5-C6-C7
19	a	844	CLA	C15-C16-C17-C18
19	b	802	CLA	C4-C3-C5-C6
19	a	801	CLA	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	807	CLA	C2-C3-C5-C6
19	b	807	CLA	C10-C11-C12-C13
21	b	851	DGD	O1B-C1B-O2G-C2G
19	a	811	CLA	C11-C10-C8-C9
19	b	833	CLA	C3-C5-C6-C7
19	a	805	CLA	C6-C7-C8-C9
19	3	314	CLA	CBA-CGA-O2A-C1
19	1	306	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	CBA-CGA-O2A-C1
19	b	829	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	C2-C3-O3-P
19	4	311	CLA	C3A-C2A-CAA-CBA
19	3	315	CLA	C3A-C2A-CAA-CBA
19	2	314	CLA	C3A-C2A-CAA-CBA
19	a	829	CLA	C3A-C2A-CAA-CBA
19	j	102	CLA	C3A-C2A-CAA-CBA
19	j	102	CLA	C5-C6-C7-C8
19	b	813	CLA	C5-C6-C7-C8
25	a	845	LHG	C34-C35-C36-C37
19	a	805	CLA	C6-C7-C8-C10
19	a	831	CLA	CBA-CGA-O2A-C1
19	b	812	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	C5-C6-C7-C8
20	1	315	SQD	O6-C44-C45-C46
22	2	317	LMG	O1-C7-C8-C9
25	a	846	LHG	C4-C5-C6-O8
19	b	801	CLA	C5-C6-C7-C8
19	b	836	CLA	C3-C5-C6-C7
21	b	851	DGD	C7A-C8A-C9A-CAA
19	a	840	CLA	C4-C3-C5-C6
19	b	819	CLA	C11-C12-C13-C15
19	3	314	CLA	O1D-CGD-O2D-CED
19	4	317	CLA	C5-C6-C7-C8
19	a	803	CLA	C15-C16-C17-C18
19	a	827	CLA	C3-C5-C6-C7
19	a	809	CLA	C2A-CAA-CBA-CGA
22	j	105	LMG	C28-C29-C30-C31
19	a	835	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	C16-C17-C18-C19
19	b	823	CLA	C10-C11-C12-C13
19	4	307	CLA	O1A-CGA-O2A-C1
19	a	806	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	4	308	CLA	C16-C17-C18-C19
19	a	806	CLA	C16-C17-C18-C20
19	b	803	CLA	C13-C15-C16-C17
19	b	806	CLA	C10-C11-C12-C13
25	b	849	LHG	O9-C7-O7-C5
23	1	304	A1L1F	C14-C29-C30-C31
19	4	310	CLA	C11-C10-C8-C9
19	1	306	CLA	C11-C10-C8-C9
19	1	310	CLA	C6-C7-C8-C9
19	a	814	CLA	C11-C12-C13-C14
19	a	840	CLA	C11-C10-C8-C9
19	b	802	CLA	C6-C7-C8-C9
19	b	802	CLA	C11-C10-C8-C9
19	b	804	CLA	C6-C7-C8-C9
19	b	806	CLA	C6-C7-C8-C9
19	b	810	CLA	C6-C7-C8-C9
19	b	825	CLA	C11-C12-C13-C14
19	b	838	CLA	C14-C13-C15-C16
19	b	839	CLA	C11-C12-C13-C14
19	5	309	CLA	C5-C6-C7-C8
19	1	310	CLA	C16-C17-C18-C20
19	b	828	CLA	C16-C17-C18-C20
26	b	848	BCR	C5-C6-C7-C8
26	b	852	BCR	C23-C24-C25-C26
26	b	852	BCR	C23-C24-C25-C30
26	f	804	BCR	C23-C24-C25-C26
26	l	201	BCR	C5-C6-C7-C8
26	l	205	BCR	C1-C6-C7-C8
26	l	205	BCR	C5-C6-C7-C8
19	b	810	CLA	CAA-CBA-CGA-O2A
17	4	305	XAT	C27-C28-C29-C39
19	2	315	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	C1A-C2A-CAA-CBA
19	4	310	CLA	C15-C16-C17-C18
19	a	854	CLA	C8-C10-C11-C12
19	1	306	CLA	C16-C17-C18-C20
19	b	807	CLA	C5-C6-C7-C8
19	b	829	CLA	C5-C6-C7-C8
22	a	853	LMG	C12-C13-C14-C15
25	a	846	LHG	O6-C4-C5-C6
25	m	101	LHG	O6-C4-C5-C6
19	4	310	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	1	308	CLA	C11-C12-C13-C15
19	a	801	CLA	C6-C7-C8-C10
19	a	802	CLA	C6-C7-C8-C10
19	a	807	CLA	C11-C12-C13-C15
19	a	814	CLA	C6-C7-C8-C10
19	a	814	CLA	C11-C12-C13-C15
19	a	820	CLA	C11-C12-C13-C15
19	a	827	CLA	C11-C10-C8-C7
19	a	829	CLA	C6-C7-C8-C10
19	a	835	CLA	C6-C7-C8-C10
19	a	840	CLA	C2-C3-C5-C6
19	a	842	CLA	C11-C12-C13-C15
19	a	844	CLA	C11-C10-C8-C7
19	b	801	CLA	C11-C12-C13-C15
19	b	803	CLA	C6-C7-C8-C10
19	b	803	CLA	C11-C10-C8-C7
19	b	808	CLA	C11-C10-C8-C7
19	b	810	CLA	C6-C7-C8-C10
19	b	814	CLA	C11-C10-C8-C7
19	b	825	CLA	C6-C7-C8-C10
19	b	830	CLA	C12-C13-C15-C16
19	b	837	CLA	C12-C13-C15-C16
19	b	838	CLA	C12-C13-C15-C16
19	b	839	CLA	C12-C13-C15-C16
19	i	102	CLA	C11-C10-C8-C7
19	j	102	CLA	C6-C7-C8-C10
20	1	315	SQD	C9-C10-C11-C12
18	3	306	A1L1G	C40-C41-C42-C44
19	b	805	CLA	C16-C17-C18-C19
19	a	842	CLA	C8-C10-C11-C12
19	a	841	CLA	O1A-CGA-O2A-C1
19	a	827	CLA	C5-C6-C7-C8
22	2	317	LMG	C31-C32-C33-C34
19	4	313	CLA	CBA-CGA-O2A-C1
19	5	314	CLA	CAD-CBD-CGD-O2D
19	3	310	CLA	CAD-CBD-CGD-O2D
19	a	808	CLA	CAD-CBD-CGD-O2D
19	a	810	CLA	CAD-CBD-CGD-O2D
19	a	815	CLA	CAD-CBD-CGD-O2D
19	a	821	CLA	CAD-CBD-CGD-O2D
19	a	824	CLA	CAD-CBD-CGD-O2D
19	a	832	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	842	CLA	CAD-CBD-CGD-O2D
19	a	854	CLA	CAD-CBD-CGD-O2D
19	b	802	CLA	CAD-CBD-CGD-O2D
19	b	806	CLA	CAD-CBD-CGD-O2D
19	b	812	CLA	CAD-CBD-CGD-O2D
19	b	826	CLA	CAD-CBD-CGD-O2D
19	b	831	CLA	CAD-CBD-CGD-O2D
19	b	834	CLA	CAD-CBD-CGD-O2D
19	b	839	CLA	CAD-CBD-CGD-O2D
19	b	840	CLA	CAD-CBD-CGD-O2D
22	a	853	LMG	C9-C8-O7-C10
19	a	808	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	C13-C15-C16-C17
19	b	839	CLA	C13-C15-C16-C17
25	a	845	LHG	C9-C10-C11-C12
22	2	317	LMG	C33-C34-C35-C36
19	b	812	CLA	O1A-CGA-O2A-C1
19	2	307	CLA	C2A-CAA-CBA-CGA
19	2	314	CLA	C2A-CAA-CBA-CGA
19	2	310	CLA	C16-C17-C18-C19
19	b	810	CLA	C16-C17-C18-C19
19	4	307	CLA	CHA-CBD-CGD-O1D
19	3	308	CLA	CHA-CBD-CGD-O1D
19	3	308	CLA	CHA-CBD-CGD-O2D
19	2	313	CLA	CHA-CBD-CGD-O1D
19	a	809	CLA	CHA-CBD-CGD-O1D
19	a	809	CLA	CHA-CBD-CGD-O2D
19	a	814	CLA	CHA-CBD-CGD-O1D
19	a	814	CLA	CHA-CBD-CGD-O2D
19	a	823	CLA	CHA-CBD-CGD-O1D
19	a	828	CLA	CHA-CBD-CGD-O1D
19	a	831	CLA	CHA-CBD-CGD-O1D
19	a	831	CLA	CHA-CBD-CGD-O2D
19	a	837	CLA	CHA-CBD-CGD-O1D
19	a	839	CLA	CHA-CBD-CGD-O1D
19	a	839	CLA	CHA-CBD-CGD-O2D
19	b	804	CLA	CHA-CBD-CGD-O1D
19	b	804	CLA	CHA-CBD-CGD-O2D
19	b	809	CLA	CHA-CBD-CGD-O1D
19	b	809	CLA	CHA-CBD-CGD-O2D
19	b	815	CLA	CHA-CBD-CGD-O1D
19	b	830	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	830	CLA	CHA-CBD-CGD-O2D
19	b	835	CLA	CHA-CBD-CGD-O1D
19	b	835	CLA	CHA-CBD-CGD-O2D
19	b	836	CLA	CHA-CBD-CGD-O1D
19	3	314	CLA	O1A-CGA-O2A-C1
21	b	851	DGD	O1A-C1A-O1G-C1G
19	i	102	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	829	CLA	O1A-CGA-O2A-C1
19	j	102	CLA	O1D-CGD-O2D-CED
19	b	818	CLA	C10-C11-C12-C13
22	a	853	LMG	C31-C32-C33-C34
19	1	306	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	C2-C3-C5-C6
19	1	308	CLA	C11-C12-C13-C14
19	a	807	CLA	C11-C10-C8-C9
19	a	829	CLA	C6-C7-C8-C9
19	b	833	CLA	C14-C13-C15-C16
19	4	313	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	C2A-CAA-CBA-CGA
19	b	808	CLA	C2A-CAA-CBA-CGA
17	5	301	XAT	C7-C8-C9-C10
19	1	306	CLA	C3-C5-C6-C7
19	3	311	CLA	C1A-C2A-CAA-CBA
19	2	314	CLA	C1A-C2A-CAA-CBA
19	a	824	CLA	C1A-C2A-CAA-CBA
19	b	814	CLA	C1A-C2A-CAA-CBA
19	b	824	CLA	C1A-C2A-CAA-CBA
19	1	310	CLA	C16-C17-C18-C19
17	2	304	XAT	C33-C34-C35-C15
19	a	806	CLA	O1D-CGD-O2D-CED
19	1	308	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	C5-C6-C7-C8
19	2	314	CLA	C4-C3-C5-C6
19	b	835	CLA	C2-C3-C5-C6
25	a	845	LHG	C3-O3-P-O5
25	a	846	LHG	C4-O6-P-O5
25	m	101	LHG	C3-O3-P-O5
25	m	101	LHG	C4-O6-P-O5
19	2	310	CLA	C16-C17-C18-C20
19	a	830	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	3	311	CLA	C2A-CAA-CBA-CGA
20	1	315	SQD	C13-C14-C15-C16
19	b	808	CLA	C16-C17-C18-C20
25	a	846	LHG	C10-C11-C12-C13
19	5	311	CLA	C2-C3-C5-C6
19	4	315	CLA	CAD-CBD-CGD-O1D
19	1	313	CLA	CAD-CBD-CGD-O1D
19	a	806	CLA	CAD-CBD-CGD-O1D
19	a	814	CLA	CAD-CBD-CGD-O1D
19	a	828	CLA	CAD-CBD-CGD-O1D
19	a	839	CLA	CAD-CBD-CGD-O1D
19	a	844	CLA	CAD-CBD-CGD-O1D
19	b	833	CLA	CAD-CBD-CGD-O1D
19	b	836	CLA	CAD-CBD-CGD-O1D
19	b	837	CLA	CAD-CBD-CGD-O1D
19	f	802	CLA	CAD-CBD-CGD-O1D
19	b	841	CLA	C15-C16-C17-C18
19	4	312	CLA	CBA-CGA-O2A-C1
19	5	307	CLA	C11-C10-C8-C7
19	2	310	CLA	C11-C12-C13-C15
19	a	842	CLA	C12-C13-C15-C16
19	b	801	CLA	C11-C10-C8-C7
19	b	801	CLA	C12-C13-C15-C16
19	b	806	CLA	C11-C12-C13-C15
19	b	811	CLA	C3A-C2A-CAA-CBA
19	b	826	CLA	C11-C10-C8-C7
19	b	828	CLA	C11-C10-C8-C7
19	b	830	CLA	C11-C12-C13-C15
19	b	833	CLA	C12-C13-C15-C16
24	a	843	PQN	C22-C23-C25-C26
25	m	101	LHG	O6-C4-C5-O7
19	b	819	CLA	C8-C10-C11-C12
19	a	834	CLA	C5-C6-C7-C8
19	b	825	CLA	C8-C10-C11-C12
19	1	308	CLA	C16-C17-C18-C19
20	5	316	SQD	C44-C45-C46-O48
20	5	316	SQD	O47-C45-C46-O48
20	1	315	SQD	O6-C44-C45-O47
25	a	846	LHG	O7-C5-C6-O8
25	b	849	LHG	O7-C5-C6-O8
19	b	815	CLA	C3-C5-C6-C7
19	i	102	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	1	311	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	C10-C11-C12-C13
19	5	309	CLA	C6-C7-C8-C9
19	4	308	CLA	C14-C13-C15-C16
19	2	311	CLA	C11-C10-C8-C9
19	a	801	CLA	C6-C7-C8-C9
19	a	802	CLA	C6-C7-C8-C9
19	a	807	CLA	C6-C7-C8-C9
19	a	809	CLA	C6-C7-C8-C9
19	a	814	CLA	C6-C7-C8-C9
19	a	820	CLA	C11-C12-C13-C14
19	b	804	CLA	C11-C12-C13-C14
19	b	814	CLA	C11-C10-C8-C9
19	b	839	CLA	C14-C13-C15-C16
19	3	315	CLA	O1A-CGA-O2A-C1
19	2	308	CLA	C6-C7-C8-C9
19	3	308	CLA	CAA-CBA-CGA-O2A
19	a	809	CLA	C10-C11-C12-C13
19	b	840	CLA	C2C-C3C-CAC-CBC
19	b	828	CLA	C10-C11-C12-C13
18	1	301	A1L1G	C37-C38-C39-C28
25	m	101	LHG	C13-C14-C15-C16
19	a	854	CLA	CBD-CGD-O2D-CED
19	a	823	CLA	C1-C2-C3-C4
19	b	832	CLA	C1-C2-C3-C4
19	b	803	CLA	C3-C5-C6-C7
19	1	311	CLA	O1D-CGD-O2D-CED
19	a	801	CLA	CAA-CBA-CGA-O2A
19	b	833	CLA	C2C-C3C-CAC-CBC
20	1	315	SQD	C46-C45-O47-C7
19	4	317	CLA	C2A-CAA-CBA-CGA
19	1	305	CLA	C2A-CAA-CBA-CGA
19	1	308	CLA	C2A-CAA-CBA-CGA
19	a	813	CLA	C2A-CAA-CBA-CGA
19	a	821	CLA	C2A-CAA-CBA-CGA
19	b	825	CLA	C2A-CAA-CBA-CGA
19	b	828	CLA	C2A-CAA-CBA-CGA
19	b	805	CLA	CBA-CGA-O2A-C1
19	5	311	CLA	C2-C1-O2A-CGA
19	a	816	CLA	C2-C1-O2A-CGA
19	a	822	CLA	C2-C1-O2A-CGA
19	b	810	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	5	316	SQD	C7-C8-C9-C10
19	1	308	CLA	O1D-CGD-O2D-CED
19	1	311	CLA	O1A-CGA-O2A-C1
19	b	808	CLA	C16-C17-C18-C19
25	b	849	LHG	C25-C26-C27-C28
26	b	848	BCR	C1-C6-C7-C8
26	f	804	BCR	C23-C24-C25-C30
26	j	104	BCR	C1-C6-C7-C8
19	b	839	CLA	C2-C3-C5-C6
19	b	805	CLA	O1A-CGA-O2A-C1
19	b	818	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	C16-C17-C18-C19
19	b	823	CLA	C3-C5-C6-C7
19	a	839	CLA	C15-C16-C17-C18
19	b	801	CLA	O1A-CGA-O2A-C1
19	b	818	CLA	O1A-CGA-O2A-C1
25	a	846	LHG	C3-O3-P-O6
25	a	846	LHG	C4-O6-P-O3
25	m	101	LHG	C4-O6-P-O3
19	b	803	CLA	C16-C17-C18-C20
19	a	841	CLA	C4-C3-C5-C6
19	4	308	CLA	C11-C12-C13-C15
19	2	311	CLA	C11-C10-C8-C7
19	a	807	CLA	C11-C10-C8-C7
19	a	801	CLA	C14-C13-C15-C16
19	a	812	CLA	C6-C7-C8-C9
19	a	842	CLA	C14-C13-C15-C16
19	b	803	CLA	C14-C13-C15-C16
19	b	828	CLA	C11-C10-C8-C9
19	b	829	CLA	C14-C13-C15-C16
24	a	843	PQN	C24-C23-C25-C26
17	4	301	XAT	C29-C30-C31-C32
18	3	302	A1L1G	C36-C37-C38-C39
26	m	102	BCR	C13-C14-C15-C16
19	5	307	CLA	C8-C10-C11-C12
19	a	830	CLA	C15-C16-C17-C18
19	a	854	CLA	C15-C16-C17-C18
19	b	801	CLA	CBA-CGA-O2A-C1
19	5	315	CLA	CAA-CBA-CGA-O2A
19	2	314	CLA	C11-C10-C8-C7
25	a	846	LHG	C1-C2-C3-O3
19	2	314	CLA	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	828	CLA	C16-C17-C18-C19
19	b	840	CLA	C16-C17-C18-C20
19	a	813	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	CBD-CGD-O2D-CED
19	a	832	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	CBA-CGA-O2A-C1
19	5	310	CLA	CAA-CBA-CGA-O1A
17	j	101	XAT	C9-C10-C11-C12
18	3	302	A1L1G	C40-C41-C42-C44
19	a	854	CLA	O1D-CGD-O2D-CED
19	a	820	CLA	C13-C15-C16-C17
19	a	812	CLA	C3-C5-C6-C7
19	b	814	CLA	C10-C11-C12-C13
25	a	845	LHG	C25-C26-C27-C28
19	a	832	CLA	O1D-CGD-O2D-CED
19	a	810	CLA	C2-C1-O2A-CGA
19	a	814	CLA	C2-C1-O2A-CGA
19	5	309	CLA	C2A-CAA-CBA-CGA
19	2	309	CLA	C2A-CAA-CBA-CGA
19	a	803	CLA	C2A-CAA-CBA-CGA
19	b	809	CLA	C2A-CAA-CBA-CGA
19	b	811	CLA	C2A-CAA-CBA-CGA
21	b	851	DGD	O2G-C2G-C3G-O3G
19	2	310	CLA	C3A-C2A-CAA-CBA
19	b	814	CLA	C3A-C2A-CAA-CBA
19	b	832	CLA	C3A-C2A-CAA-CBA
22	2	317	LMG	O9-C10-O7-C8
19	a	802	CLA	C4-C3-C5-C6
19	5	307	CLA	C11-C10-C8-C9
19	1	310	CLA	C11-C12-C13-C14
19	a	822	CLA	C11-C10-C8-C9
19	a	829	CLA	C11-C12-C13-C14
19	a	831	CLA	C6-C7-C8-C9
19	a	844	CLA	C6-C7-C8-C9
19	a	854	CLA	C11-C10-C8-C9
19	b	808	CLA	C6-C7-C8-C9
19	a	830	CLA	C16-C17-C18-C20
19	a	839	CLA	C16-C17-C18-C20
26	b	845	BCR	C11-C10-C9-C34
26	b	845	BCR	C20-C21-C22-C37
26	f	804	BCR	C35-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	l	201	BCR	C11-C10-C9-C34
19	5	306	CLA	CAA-CBA-CGA-O1A
19	3	312	CLA	O1A-CGA-O2A-C1
19	3	315	CLA	CAA-CBA-CGA-O1A
19	1	308	CLA	C16-C17-C18-C20
19	a	801	CLA	CBA-CGA-O2A-C1
19	b	841	CLA	CBA-CGA-O2A-C1
25	a	845	LHG	C14-C15-C16-C17
19	b	818	CLA	CBD-CGD-O2D-CED
18	3	306	A1L1G	C32-C33-C34-C35
25	m	101	LHG	C15-C16-C17-C18
19	4	311	CLA	C1A-C2A-CAA-CBA
19	4	316	CLA	C1A-C2A-CAA-CBA
19	2	310	CLA	C1A-C2A-CAA-CBA
19	2	316	CLA	C1A-C2A-CAA-CBA
19	b	816	CLA	C1A-C2A-CAA-CBA
19	b	823	CLA	C1A-C2A-CAA-CBA
19	b	835	CLA	C1A-C2A-CAA-CBA
19	a	814	CLA	C11-C10-C8-C7
19	b	802	CLA	C2-C3-C5-C6
19	b	802	CLA	C12-C13-C15-C16
19	f	802	CLA	C6-C7-C8-C10
18	3	306	A1L1G	C30-C31-C32-C33
22	a	853	LMG	C11-C12-C13-C14
19	a	801	CLA	O1A-CGA-O2A-C1
19	b	841	CLA	O1A-CGA-O2A-C1
19	4	314	CLA	CAA-CBA-CGA-O1A
19	4	314	CLA	CAA-CBA-CGA-O2A
19	a	817	CLA	CAA-CBA-CGA-O1A
19	a	817	CLA	CAA-CBA-CGA-O2A
19	b	840	CLA	C4C-C3C-CAC-CBC
19	1	305	CLA	C3-C5-C6-C7
19	5	307	CLA	C2A-CAA-CBA-CGA
19	1	307	CLA	C6-C7-C8-C9
19	4	310	CLA	C13-C15-C16-C17
19	a	841	CLA	C2-C3-C5-C6
19	4	310	CLA	O1D-CGD-O2D-CED
26	b	845	BCR	C11-C10-C9-C8
26	b	845	BCR	C20-C21-C22-C23
26	f	804	BCR	C12-C13-C14-C15
26	l	201	BCR	C11-C10-C9-C8
19	5	313	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	4	306	CLA	C2A-CAA-CBA-CGA
18	1	301	A1L1G	C40-C41-C42-C44
22	2	317	LMG	C11-C10-O7-C8
19	b	818	CLA	O1D-CGD-O2D-CED
19	a	830	CLA	C4-C3-C5-C6
19	a	839	CLA	C2-C1-O2A-CGA
19	a	802	CLA	C2-C3-C5-C6
19	b	808	CLA	C14-C13-C15-C16
19	5	306	CLA	CAA-CBA-CGA-O2A
21	b	851	DGD	C1B-C2B-C3B-C4B
19	5	311	CLA	C4-C3-C5-C6
19	a	819	CLA	CAA-CBA-CGA-O2A
20	1	315	SQD	C15-C16-C17-C18
19	a	839	CLA	C2A-CAA-CBA-CGA
19	b	836	CLA	C4C-C3C-CAC-CBC
26	b	850	BCR	C23-C24-C25-C30
26	m	102	BCR	C23-C24-C25-C30
19	5	310	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	O1-C1-C2-C3
19	a	830	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	CBA-CGA-O2A-C1
17	2	304	XAT	C7-C8-C9-C10
17	a	852	XAT	C31-C32-C33-C34
19	a	804	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	C10-C11-C12-C13
19	a	813	CLA	C6-C7-C8-C9
19	5	307	CLA	C11-C12-C13-C14
19	b	814	CLA	C16-C17-C18-C19
19	5	313	CLA	CAA-CBA-CGA-O2A
19	1	314	CLA	CAA-CBA-CGA-O2A
19	a	830	CLA	CBA-CGA-O2A-C1
19	a	826	CLA	C13-C15-C16-C17
19	2	314	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	C11-C10-C8-C7
19	b	814	CLA	C5-C6-C7-C8
19	4	308	CLA	C3-C5-C6-C7
19	1	314	CLA	CAA-CBA-CGA-O1A
19	4	309	CLA	CAA-CBA-CGA-O2A
19	b	811	CLA	C8-C10-C11-C12
19	1	306	CLA	C16-C17-C18-C19
19	a	804	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	j	105	LMG	C11-C12-C13-C14
25	m	101	LHG	C35-C36-C37-C38
19	5	314	CLA	C4-C3-C5-C6
19	b	808	CLA	C4-C3-C5-C6
19	a	830	CLA	C2-C3-C5-C6
19	4	308	CLA	C6-C7-C8-C9
19	a	801	CLA	C11-C10-C8-C9
19	b	806	CLA	C11-C12-C13-C14
19	b	830	CLA	C11-C12-C13-C14
19	4	306	CLA	C3A-C2A-CAA-CBA
19	2	316	CLA	C3A-C2A-CAA-CBA
19	1	310	CLA	C3A-C2A-CAA-CBA
19	b	809	CLA	C3A-C2A-CAA-CBA
19	b	838	CLA	CAA-CBA-CGA-O2A
19	5	306	CLA	CAD-CBD-CGD-O2D
19	5	311	CLA	CAD-CBD-CGD-O2D
19	4	311	CLA	CAD-CBD-CGD-O2D
19	3	314	CLA	CAD-CBD-CGD-O2D
19	2	316	CLA	CAD-CBD-CGD-O2D
19	1	307	CLA	CAD-CBD-CGD-O2D
19	1	309	CLA	CAD-CBD-CGD-O2D
19	a	827	CLA	CAD-CBD-CGD-O2D
19	a	829	CLA	CAD-CBD-CGD-O2D
19	b	813	CLA	CAD-CBD-CGD-O2D
19	b	814	CLA	CAD-CBD-CGD-O2D
19	b	817	CLA	CAD-CBD-CGD-O2D
19	b	838	CLA	CAD-CBD-CGD-O2D
19	l	204	CLA	CAD-CBD-CGD-O2D
19	b	819	CLA	C2A-CAA-CBA-CGA
19	b	814	CLA	C13-C15-C16-C17
19	a	818	CLA	CAA-CBA-CGA-O2A
19	b	803	CLA	C10-C11-C12-C13
19	a	835	CLA	C4-C3-C5-C6
19	b	834	CLA	C4-C3-C5-C6
19	a	804	CLA	C6-C7-C8-C9
19	b	808	CLA	C2-C3-C5-C6
19	b	801	CLA	CAA-CBA-CGA-O2A
19	l	204	CLA	CAA-CBA-CGA-O2A
26	f	801	BCR	C17-C18-C19-C20
17	5	301	XAT	O4-C6-C7-C8
17	5	304	XAT	O24-C26-C27-C28
17	4	301	XAT	O4-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	4	305	XAT	O4-C6-C7-C8
17	3	303	XAT	O4-C6-C7-C8
17	2	301	XAT	O4-C6-C7-C8
17	2	305	XAT	O24-C26-C27-C28
18	3	302	A1L1G	C29-C14-C25-O15
20	1	315	SQD	O47-C7-C8-C9
24	a	843	PQN	C18-C20-C21-C22
19	4	309	CLA	O2A-C1-C2-C3
19	3	310	CLA	O2A-C1-C2-C3
19	2	314	CLA	O2A-C1-C2-C3
19	1	305	CLA	O2A-C1-C2-C3
19	a	826	CLA	O2A-C1-C2-C3
19	b	818	CLA	O2A-C1-C2-C3
19	b	833	CLA	O2A-C1-C2-C3
19	4	308	CLA	C2A-CAA-CBA-CGA
19	2	308	CLA	C2A-CAA-CBA-CGA
19	b	834	CLA	C15-C16-C17-C18
19	a	836	CLA	CAA-CBA-CGA-O2A
19	4	306	CLA	CAA-CBA-CGA-O2A
19	5	313	CLA	CHA-CBD-CGD-O1D
19	4	310	CLA	CHA-CBD-CGD-O1D
19	4	314	CLA	CHA-CBD-CGD-O2D
19	2	307	CLA	CHA-CBD-CGD-O1D
19	2	307	CLA	CHA-CBD-CGD-O2D
19	2	310	CLA	CHA-CBD-CGD-O1D
19	2	310	CLA	CHA-CBD-CGD-O2D
19	2	313	CLA	CHA-CBD-CGD-O2D
19	a	802	CLA	CHA-CBD-CGD-O1D
19	a	802	CLA	CHA-CBD-CGD-O2D
19	a	804	CLA	CHA-CBD-CGD-O1D
19	a	804	CLA	CHA-CBD-CGD-O2D
19	a	816	CLA	CHA-CBD-CGD-O1D
19	a	817	CLA	CHA-CBD-CGD-O1D
19	a	817	CLA	CHA-CBD-CGD-O2D
19	a	820	CLA	CHA-CBD-CGD-O1D
19	a	820	CLA	CHA-CBD-CGD-O2D
19	a	823	CLA	CHA-CBD-CGD-O2D
19	a	828	CLA	CHA-CBD-CGD-O2D
19	a	830	CLA	CHA-CBD-CGD-O1D
19	a	830	CLA	CHA-CBD-CGD-O2D
19	a	837	CLA	CHA-CBD-CGD-O2D
19	b	801	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	801	CLA	CHA-CBD-CGD-O2D
19	b	805	CLA	CHA-CBD-CGD-O1D
19	b	805	CLA	CHA-CBD-CGD-O2D
19	b	815	CLA	CHA-CBD-CGD-O2D
19	b	816	CLA	CHA-CBD-CGD-O1D
19	b	816	CLA	CHA-CBD-CGD-O2D
19	b	825	CLA	CHA-CBD-CGD-O1D
19	b	825	CLA	CHA-CBD-CGD-O2D
19	b	836	CLA	CHA-CBD-CGD-O2D
19	j	102	CLA	CHA-CBD-CGD-O2D
19	a	835	CLA	C2-C3-C5-C6
19	a	827	CLA	C10-C11-C12-C13
19	b	807	CLA	C16-C17-C18-C19
19	a	810	CLA	CAA-CBA-CGA-O2A
19	b	807	CLA	CAA-CBA-CGA-O2A
19	2	314	CLA	CBA-CGA-O2A-C1
19	4	312	CLA	O1A-CGA-O2A-C1
19	b	803	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	CAA-CBA-CGA-O2A
19	a	801	CLA	C11-C10-C8-C7
19	a	835	CLA	C11-C12-C13-C15
19	b	810	CLA	C2-C3-C5-C6
18	3	306	A1L1G	C14-C29-C30-C31
19	b	825	CLA	C10-C11-C12-C13
19	1	306	CLA	CAA-CBA-CGA-O2A
19	1	309	CLA	CAA-CBA-CGA-O2A
19	b	809	CLA	CAA-CBA-CGA-O2A
19	b	818	CLA	CAA-CBA-CGA-O2A
19	a	834	CLA	C11-C12-C13-C14
19	f	802	CLA	C6-C7-C8-C9
19	1	312	CLA	CAA-CBA-CGA-O2A
19	b	838	CLA	CAA-CBA-CGA-O1A
20	5	316	SQD	C4-C5-C6-S
19	a	829	CLA	C2A-CAA-CBA-CGA
19	a	841	CLA	C2A-CAA-CBA-CGA
19	b	833	CLA	CAA-CBA-CGA-O2A
25	a	845	LHG	O8-C23-C24-C25
19	4	309	CLA	CAA-CBA-CGA-O1A
19	b	818	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	CAA-CBA-CGA-O2A
19	4	306	CLA	CAA-CBA-CGA-O1A
19	a	818	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	810	CLA	CAA-CBA-CGA-O1A
20	1	315	SQD	O49-C7-C8-C9
26	i	101	BCR	C17-C18-C19-C20
19	1	310	CLA	C1A-C2A-CAA-CBA
19	a	803	CLA	C1A-C2A-CAA-CBA
19	a	804	CLA	C1A-C2A-CAA-CBA
19	a	814	CLA	C1A-C2A-CAA-CBA
19	a	815	CLA	C1A-C2A-CAA-CBA
19	b	826	CLA	C1A-C2A-CAA-CBA
19	b	832	CLA	C1A-C2A-CAA-CBA
19	j	102	CLA	C10-C11-C12-C13
19	b	820	CLA	C6-C7-C8-C9
19	b	801	CLA	CAA-CBA-CGA-O1A
19	a	827	CLA	C2-C1-O2A-CGA
19	a	829	CLA	C2-C1-O2A-CGA
19	b	807	CLA	C2-C1-O2A-CGA
19	b	835	CLA	C2-C1-O2A-CGA
19	b	804	CLA	C4C-C3C-CAC-CBC
22	j	105	LMG	C7-C8-C9-O8
19	a	826	CLA	C10-C11-C12-C13
25	m	101	LHG	C30-C31-C32-C33
19	b	803	CLA	C5-C6-C7-C8
19	3	313	CLA	C4-C3-C5-C6
25	m	101	LHG	C27-C28-C29-C30
25	a	846	LHG	C3-O3-P-O5
19	b	809	CLA	CAA-CBA-CGA-O1A
19	b	833	CLA	CAA-CBA-CGA-O1A
19	3	312	CLA	CAA-CBA-CGA-O2A
26	b	850	BCR	C23-C24-C25-C26
26	b	852	BCR	C1-C6-C7-C8
26	j	104	BCR	C5-C6-C7-C8
26	m	102	BCR	C23-C24-C25-C26
19	1	312	CLA	CAA-CBA-CGA-O1A
19	a	836	CLA	CAA-CBA-CGA-O1A
19	b	807	CLA	CAA-CBA-CGA-O1A
19	b	804	CLA	CAA-CBA-CGA-O2A
19	a	814	CLA	C16-C17-C18-C19
19	b	810	CLA	C16-C17-C18-C20
19	a	834	CLA	C10-C11-C12-C13
19	4	310	CLA	CAD-CBD-CGD-O1D
19	4	316	CLA	CAD-CBD-CGD-O1D
19	3	307	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	2	309	CLA	CAD-CBD-CGD-O1D
19	a	816	CLA	CAD-CBD-CGD-O1D
19	b	815	CLA	CAD-CBD-CGD-O1D
19	b	819	CLA	CAD-CBD-CGD-O1D
20	5	316	SQD	O5-C5-C6-S
19	a	813	CLA	CBD-CGD-O2D-CED
19	a	813	CLA	CAA-CBA-CGA-O2A
19	b	805	CLA	C11-C12-C13-C14
19	b	806	CLA	C11-C10-C8-C9
19	j	102	CLA	C11-C10-C8-C9
19	b	814	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	C8-C10-C11-C12
19	a	810	CLA	C16-C17-C18-C20
20	5	316	SQD	C10-C11-C12-C13
19	a	820	CLA	CBD-CGD-O2D-CED
19	3	309	CLA	C2A-CAA-CBA-CGA
19	4	310	CLA	CAA-CBA-CGA-O2A
19	a	826	CLA	CAA-CBA-CGA-O2A
19	5	309	CLA	C15-C16-C17-C18
19	a	801	CLA	C5-C6-C7-C8
19	a	810	CLA	CAA-CBA-CGA-O1A
19	a	813	CLA	O1D-CGD-O2D-CED
19	b	810	CLA	C4-C3-C5-C6
19	b	825	CLA	C15-C16-C17-C18
19	1	306	CLA	C3A-C2A-CAA-CBA
19	1	310	CLA	C12-C13-C15-C16
19	a	834	CLA	C11-C12-C13-C15
19	b	805	CLA	C11-C12-C13-C15
19	b	819	CLA	C11-C10-C8-C7
19	l	203	CLA	C6-C7-C8-C10
19	a	813	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	CAA-CBA-CGA-O1A
19	5	309	CLA	CAA-CBA-CGA-O2A
19	2	307	CLA	CAA-CBA-CGA-O2A
19	a	835	CLA	CAA-CBA-CGA-O2A
19	j	102	CLA	C3-C5-C6-C7
20	1	315	SQD	C12-C13-C14-C15
26	b	847	BCR	C7-C8-C9-C10
19	3	312	CLA	CAA-CBA-CGA-O1A
19	a	854	CLA	CAA-CBA-CGA-O2A
19	a	835	CLA	CAA-CBA-CGA-O1A
25	a	845	LHG	O10-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	b	839	CLA	C3-C5-C6-C7
19	5	309	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

176 monomers are involved in 518 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	837	CLA	1	0
19	i	102	CLA	5	0
22	2	317	LMG	2	0
19	a	803	CLA	4	0
17	3	305	XAT	4	0
19	5	314	CLA	1	0
19	b	832	CLA	2	0
21	4	318	DGD	11	0
17	2	303	XAT	12	0
19	b	804	CLA	5	0
20	1	315	SQD	2	0
26	b	845	BCR	7	0
17	4	304	XAT	4	0
19	j	102	CLA	6	0
19	b	819	CLA	3	0
19	4	314	CLA	1	0
19	a	827	CLA	2	0
19	a	805	CLA	1	0
19	b	828	CLA	2	0
27	c	102	SF4	2	0
26	f	801	BCR	8	0
19	b	824	CLA	6	0
26	m	102	BCR	1	0
19	a	828	CLA	6	0
19	a	854	CLA	3	0
19	b	840	CLA	4	0
19	a	825	CLA	5	0
19	b	805	CLA	3	0
26	l	205	BCR	10	0
19	5	315	CLA	2	0
19	b	813	CLA	4	0
19	a	812	CLA	1	0
19	b	826	CLA	3	0
19	5	311	CLA	1	0
19	b	827	CLA	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	308	CLA	3	0
19	2	308	CLA	4	0
26	b	844	BCR	1	0
19	b	814	CLA	7	0
26	b	847	BCR	6	0
19	a	806	CLA	8	0
19	a	816	CLA	2	0
19	a	807	CLA	4	0
19	5	312	CLA	3	0
19	a	844	CLA	5	0
19	b	834	CLA	5	0
19	3	309	CLA	1	0
19	a	839	CLA	4	0
19	5	308	CLA	2	0
19	a	841	CLA	7	0
22	a	853	LMG	11	0
19	4	313	CLA	4	0
19	3	311	CLA	1	0
22	j	105	LMG	6	0
24	a	843	PQN	3	0
19	f	802	CLA	1	0
17	3	301	XAT	5	0
19	a	831	CLA	5	0
19	5	307	CLA	7	0
19	3	310	CLA	1	0
25	a	845	LHG	3	0
26	b	852	BCR	6	0
17	2	301	XAT	3	0
19	b	839	CLA	6	0
17	4	305	XAT	5	0
19	b	821	CLA	2	0
26	f	804	BCR	5	0
19	a	824	CLA	1	0
17	4	302	XAT	5	0
19	a	842	CLA	3	0
19	a	829	CLA	6	0
19	b	829	CLA	2	0
17	3	304	XAT	4	0
19	b	809	CLA	2	0
17	5	304	XAT	5	0
19	3	312	CLA	2	0
19	b	808	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	831	CLA	5	0
19	b	825	CLA	6	0
26	b	850	BCR	4	0
17	1	303	XAT	3	0
17	2	302	XAT	2	0
17	4	301	XAT	4	0
19	4	306	CLA	2	0
17	3	303	XAT	2	0
19	a	809	CLA	2	0
19	l	202	CLA	1	0
19	b	836	CLA	5	0
19	1	311	CLA	2	0
19	4	310	CLA	4	0
19	b	837	CLA	6	0
17	2	304	XAT	2	0
19	b	801	CLA	5	0
17	1	302	XAT	3	0
26	a	848	BCR	5	0
17	a	852	XAT	4	0
19	a	801	CLA	6	0
26	i	101	BCR	2	0
19	b	833	CLA	3	0
19	b	812	CLA	2	0
19	a	814	CLA	3	0
19	a	838	CLA	1	0
19	a	818	CLA	10	0
19	b	817	CLA	4	0
19	b	802	CLA	3	0
19	b	822	CLA	3	0
19	4	312	CLA	1	0
19	1	306	CLA	4	0
19	3	308	CLA	2	0
19	4	309	CLA	3	0
19	a	819	CLA	6	0
26	b	848	BCR	2	0
19	4	311	CLA	1	0
24	b	842	PQN	2	0
19	a	836	CLA	1	0
17	5	301	XAT	5	0
19	b	811	CLA	6	0
19	4	316	CLA	1	0
19	j	103	CLA	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	313	CLA	3	0
19	a	813	CLA	1	0
26	a	847	BCR	4	0
19	a	808	CLA	1	0
19	b	806	CLA	3	0
19	a	833	CLA	2	0
19	2	316	CLA	2	0
19	b	820	CLA	2	0
19	4	317	CLA	7	0
19	b	823	CLA	5	0
19	a	822	CLA	5	0
19	4	307	CLA	2	0
19	a	834	CLA	6	0
25	m	101	LHG	3	0
19	a	802	CLA	5	0
19	a	826	CLA	7	0
19	b	815	CLA	3	0
19	4	308	CLA	5	0
25	a	846	LHG	3	0
26	j	104	BCR	8	0
17	2	305	XAT	5	0
17	j	101	XAT	5	0
19	a	804	CLA	4	0
23	1	304	A1L1F	2	0
19	b	830	CLA	4	0
26	l	201	BCR	3	0
17	4	303	XAT	10	0
19	4	315	CLA	1	0
19	b	803	CLA	3	0
26	b	846	BCR	1	0
19	a	810	CLA	4	0
19	a	835	CLA	4	0
19	2	314	CLA	1	0
18	5	303	A1L1G	1	0
19	5	305	CLA	2	0
19	a	832	CLA	1	0
26	b	843	BCR	4	0
19	a	840	CLA	7	0
19	5	309	CLA	3	0
19	b	841	CLA	5	0
19	l	203	CLA	2	0
19	a	823	CLA	3	0

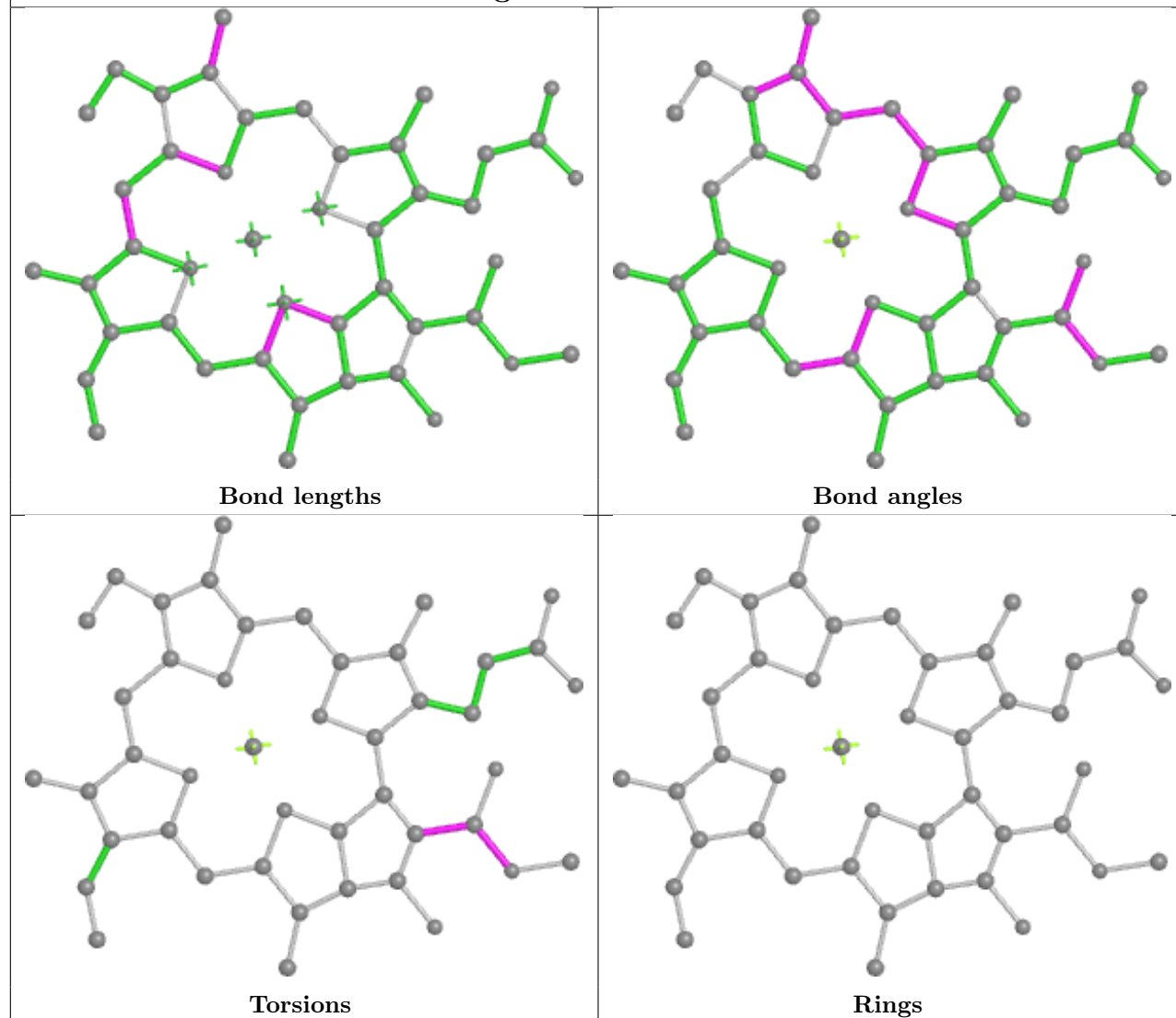
*Continued on next page...*

*Continued from previous page...*

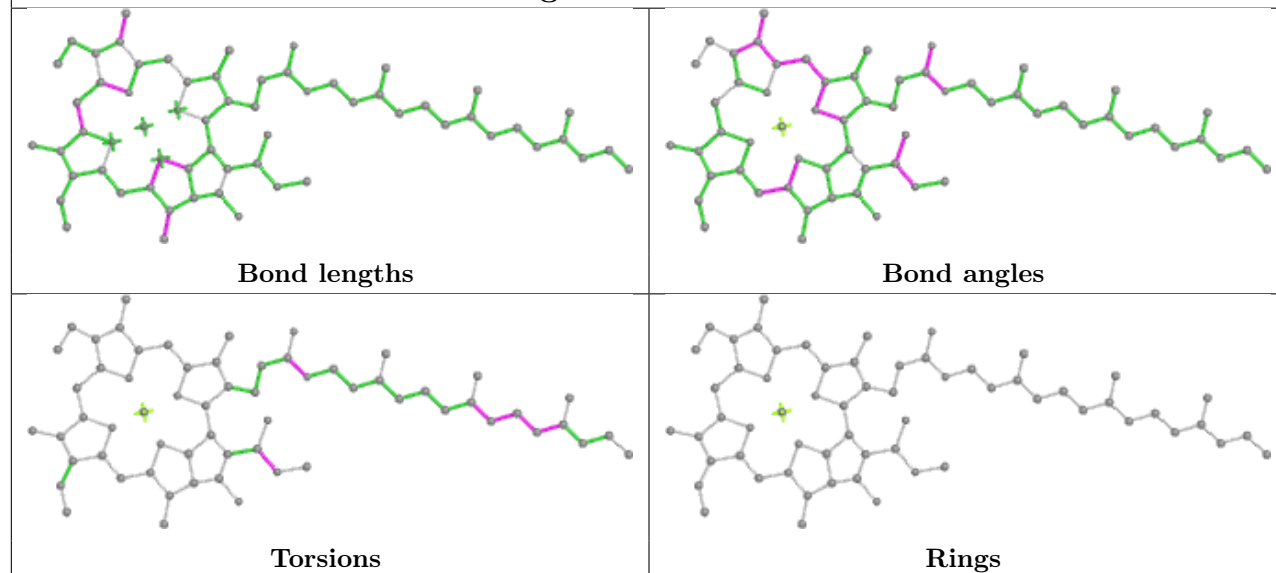
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	820	CLA	8	0
19	1	310	CLA	2	0
19	2	310	CLA	3	0
19	b	818	CLA	8	0
18	1	301	A1L1G	1	0
19	5	310	CLA	2	0
19	1	312	CLA	2	0
21	b	851	DGD	5	0
26	a	850	BCR	2	0
26	a	849	BCR	4	0
19	b	807	CLA	6	0
19	b	838	CLA	5	0
17	5	302	XAT	8	0
19	a	830	CLA	6	0
20	5	316	SQD	1	0

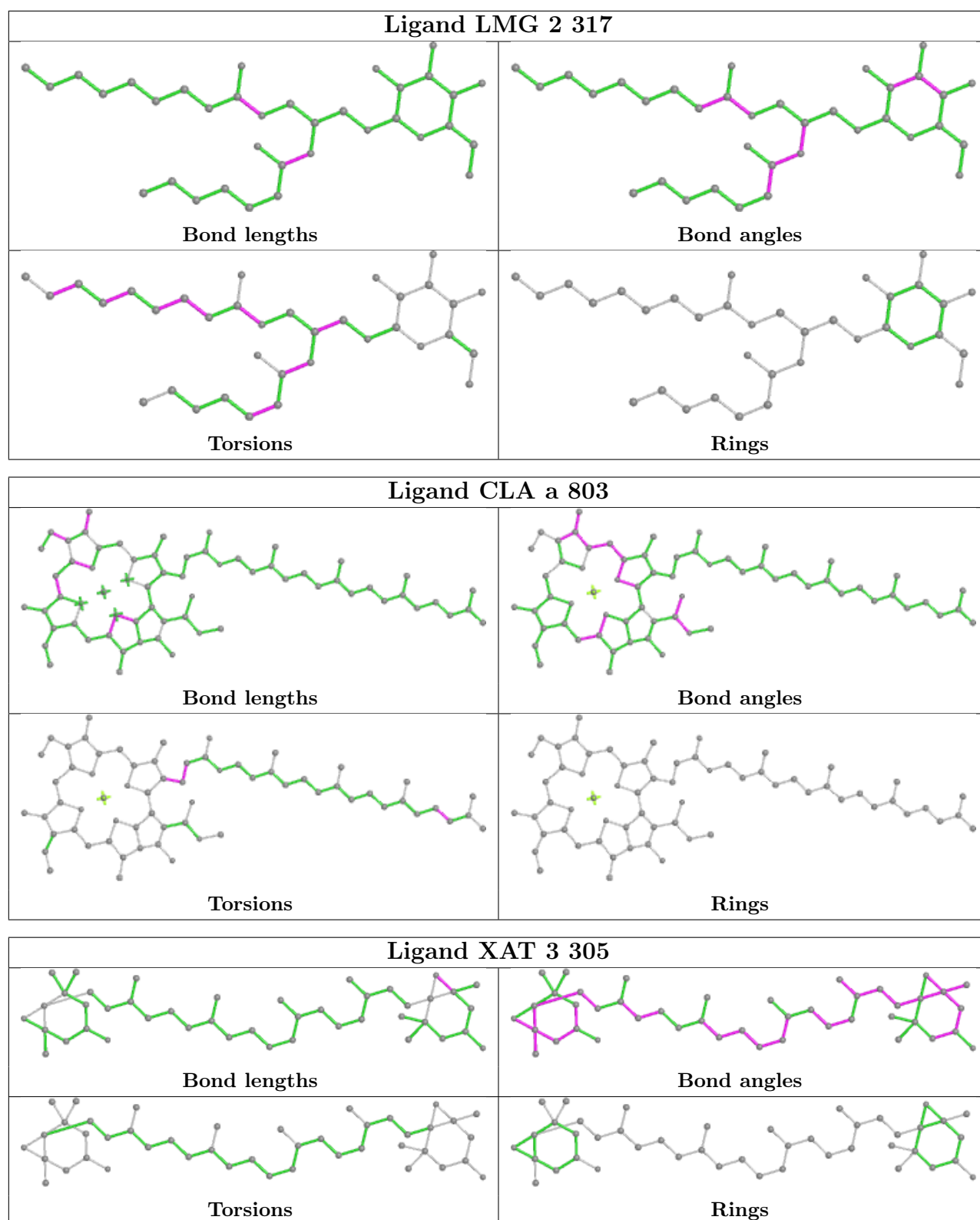
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

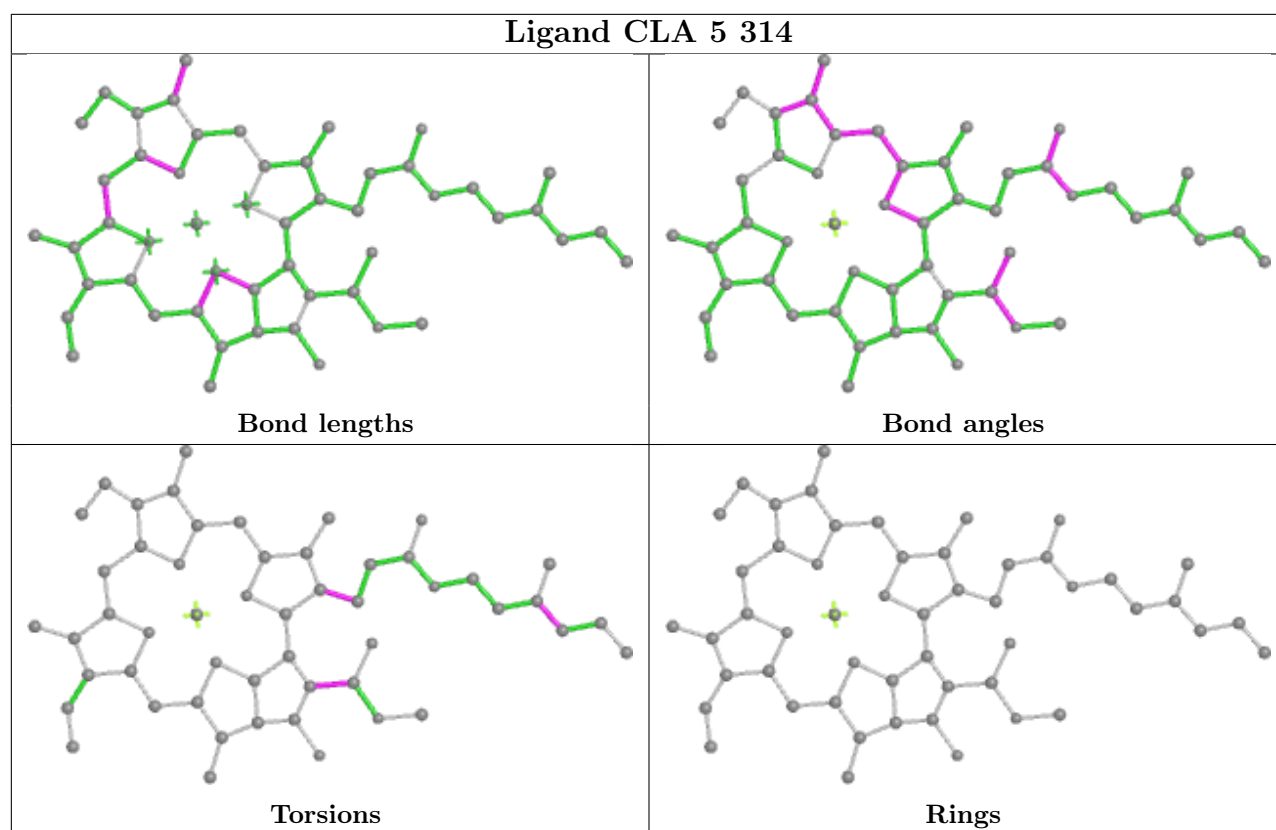
## Ligand CLA a 837



## Ligand CLA i 102

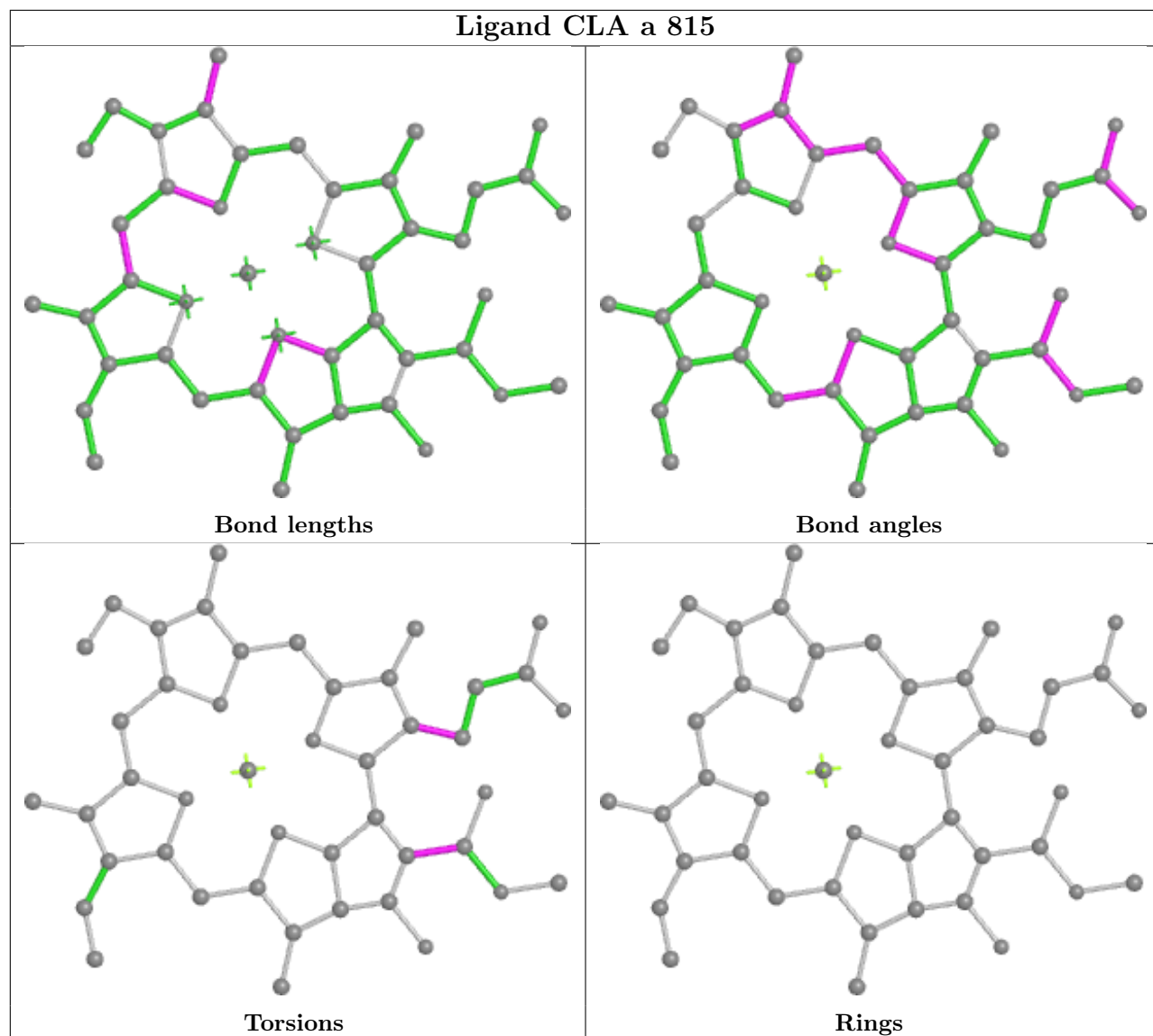


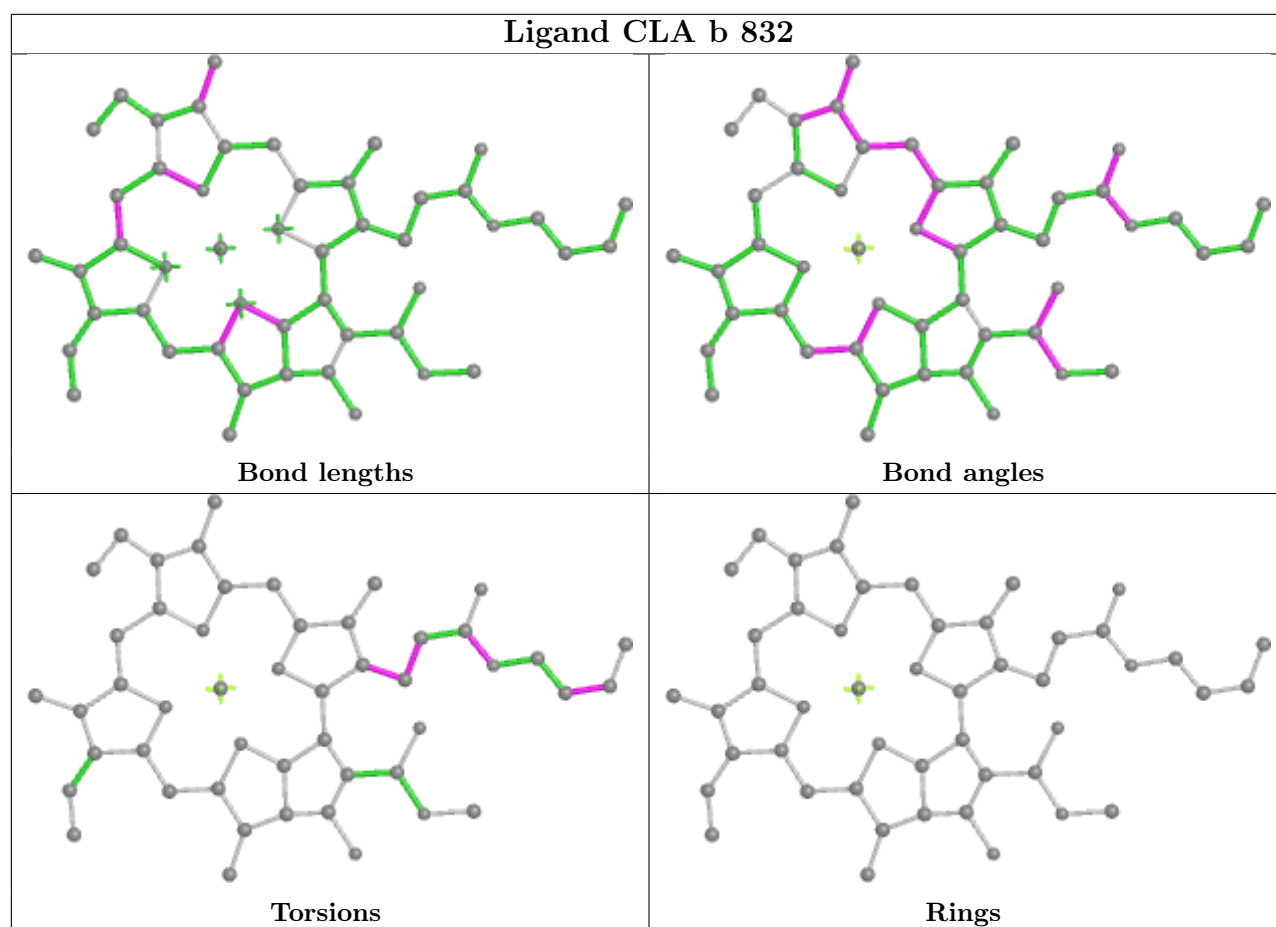


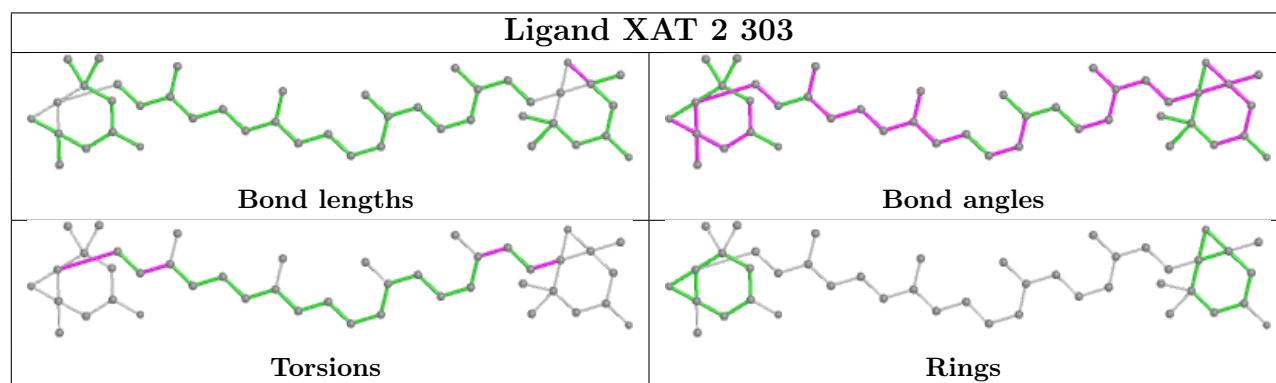
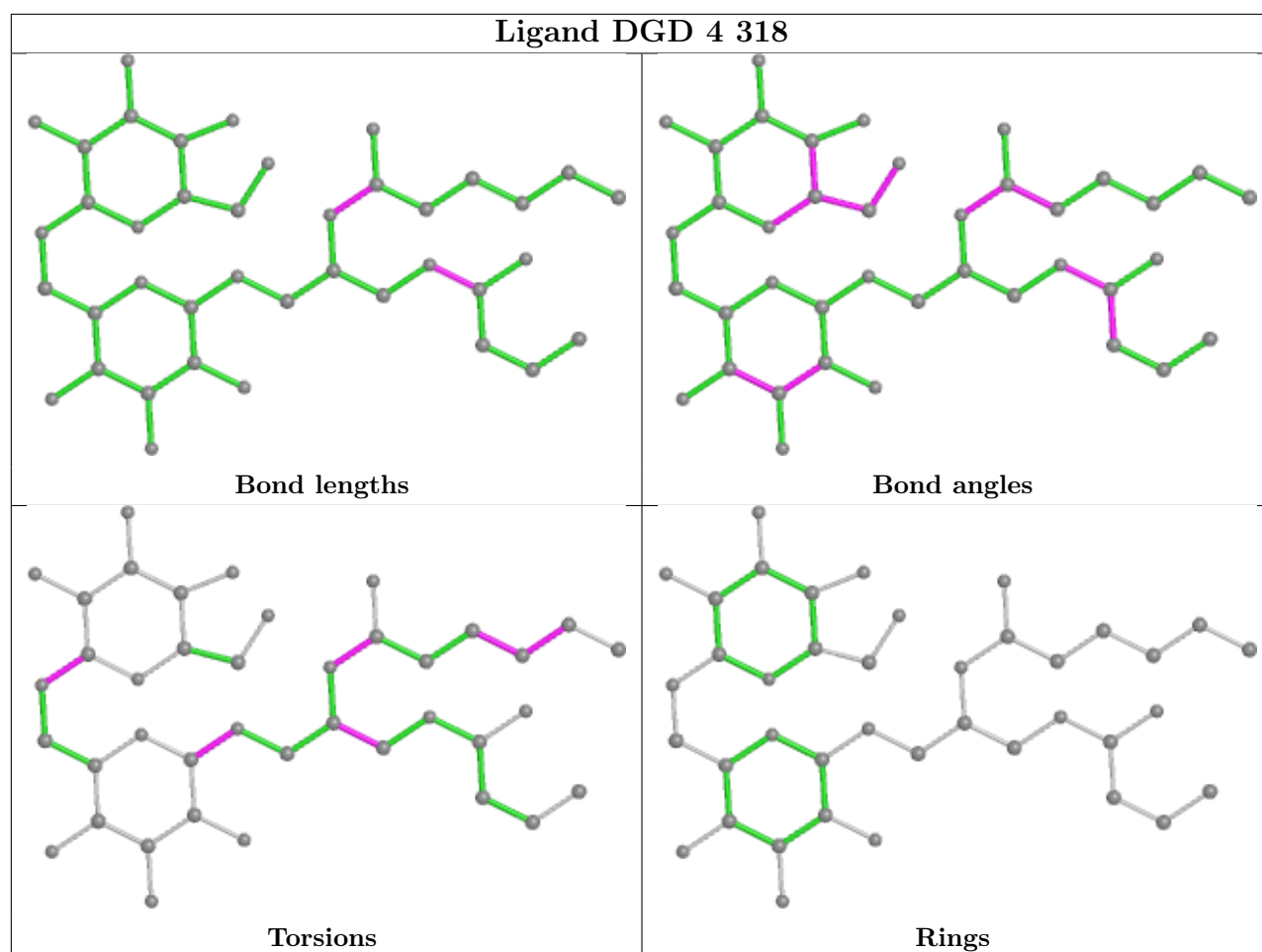




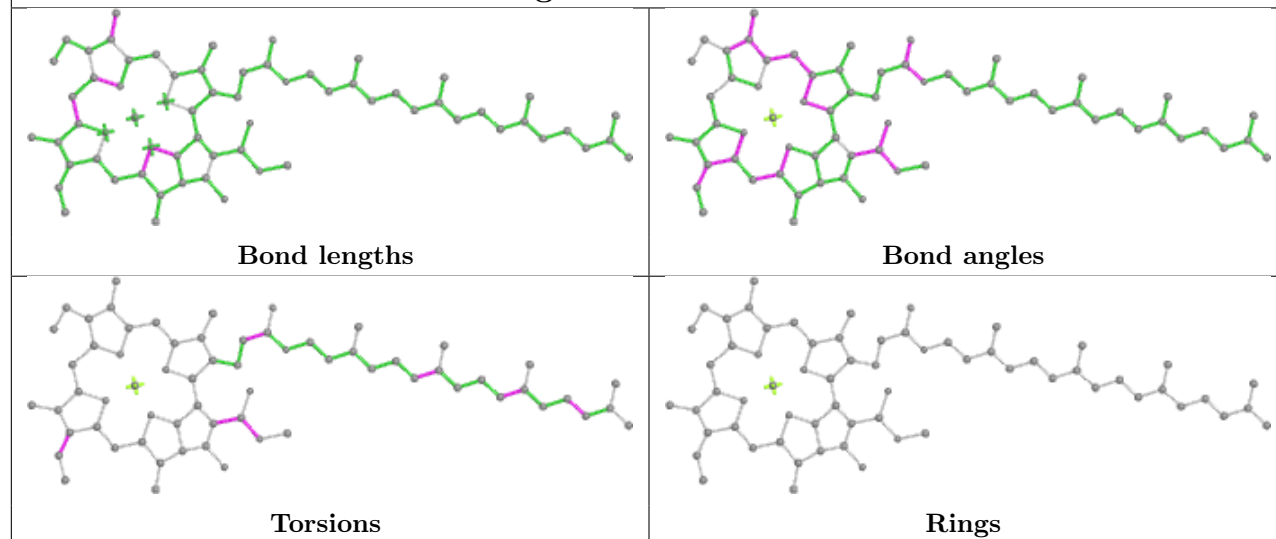
## Ligand CLA a 815



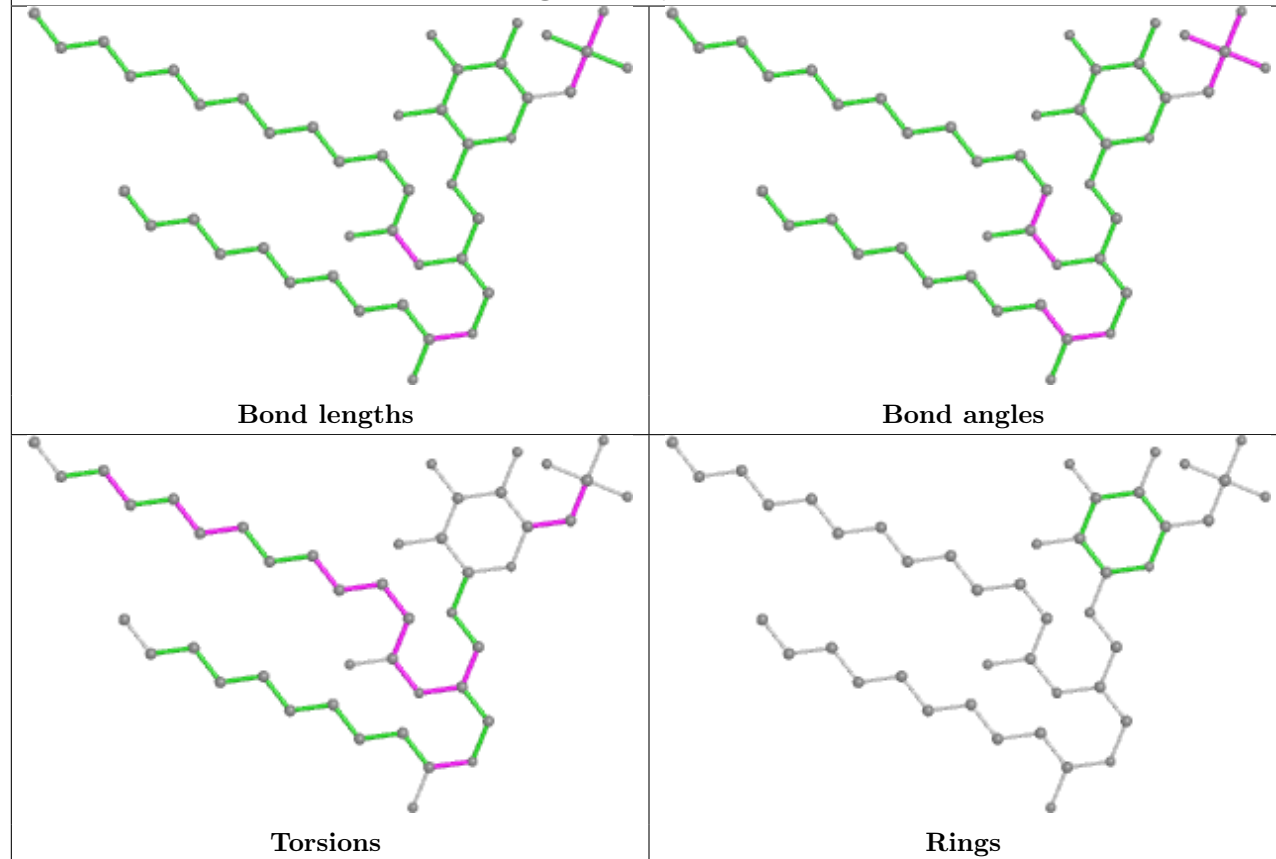


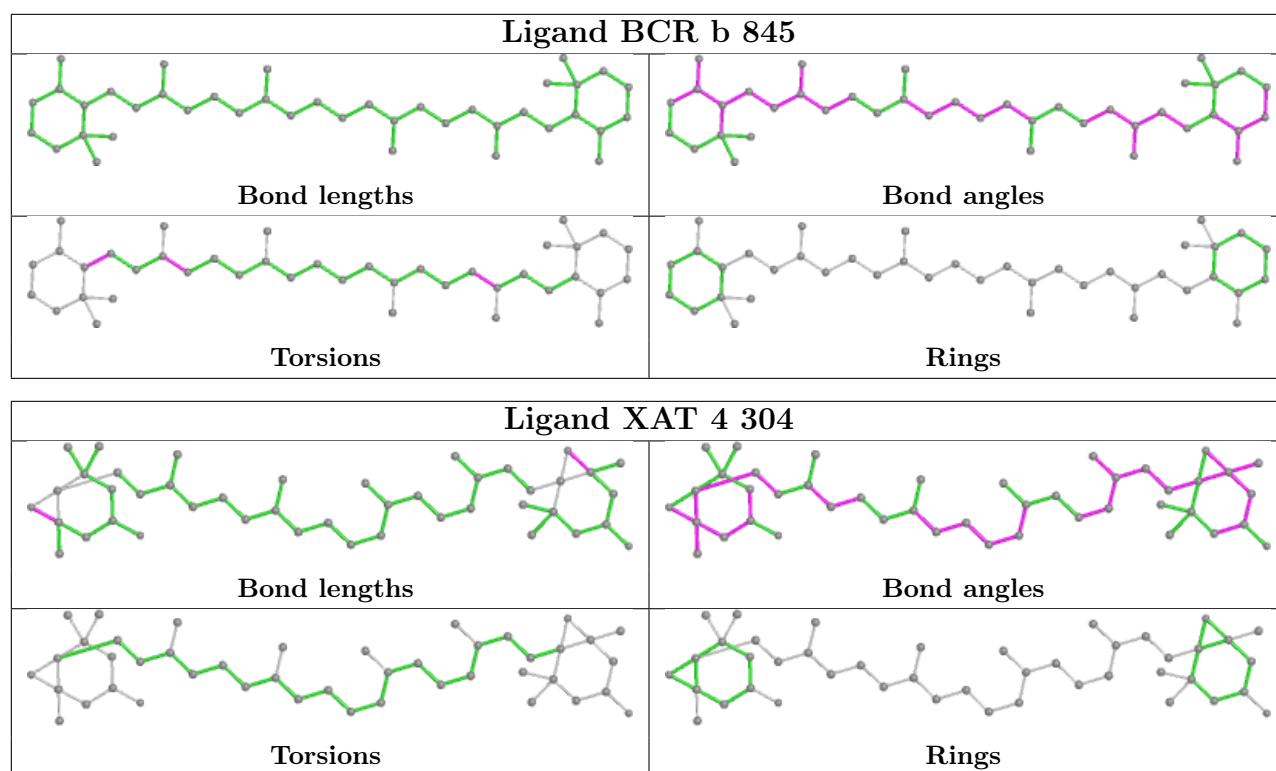


## Ligand CLA b 804

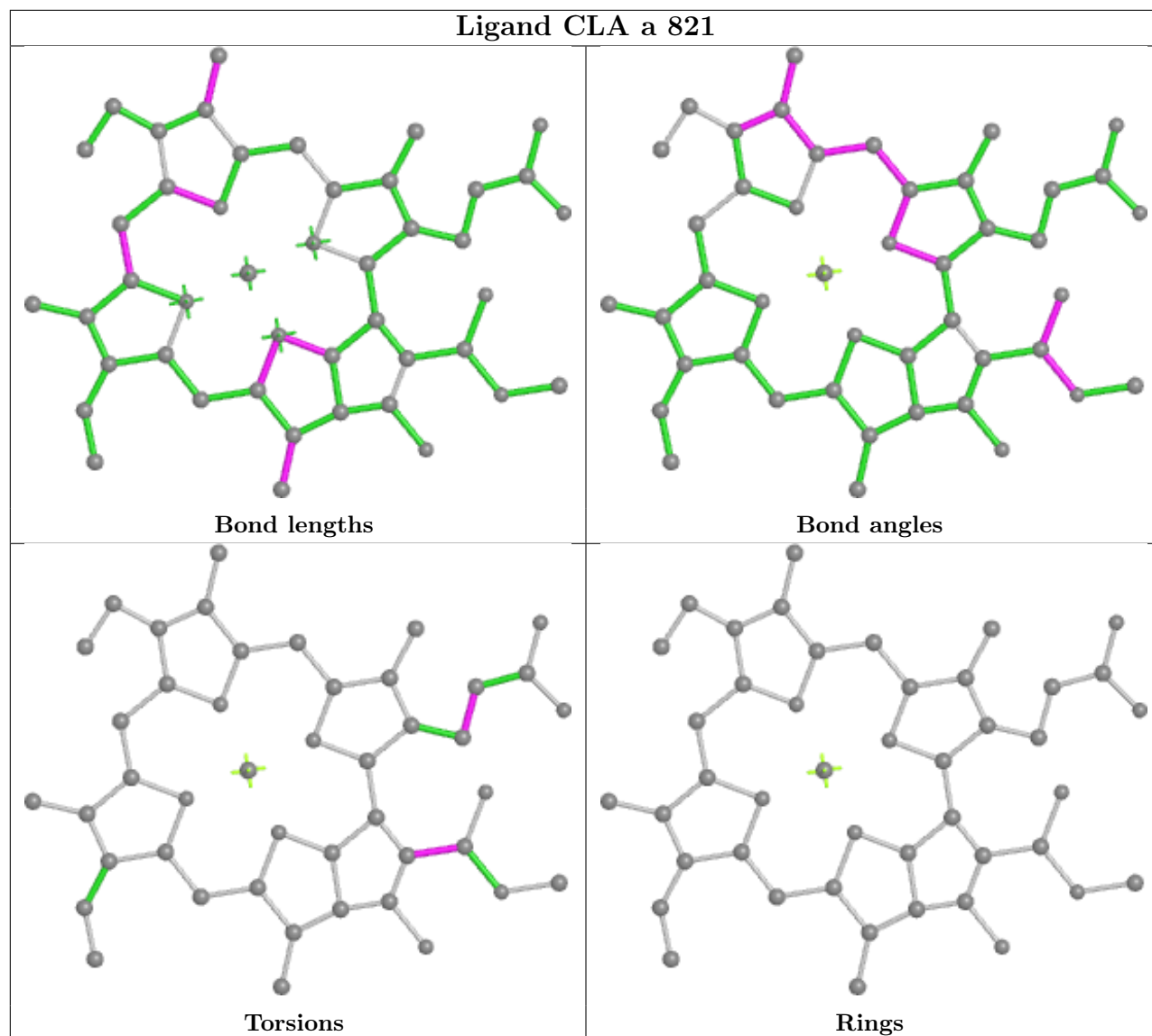


## Ligand SQD 1 315

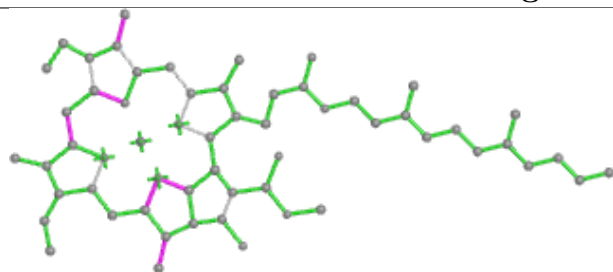




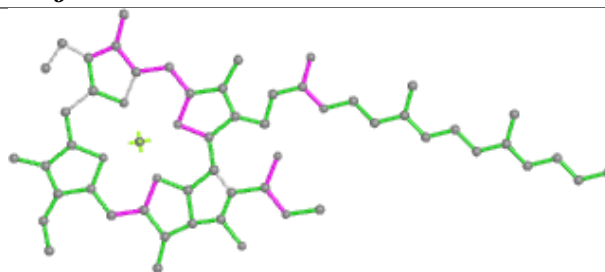
## Ligand CLA a 821



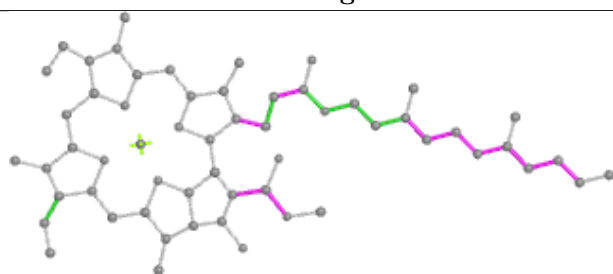
## Ligand CLA j 102



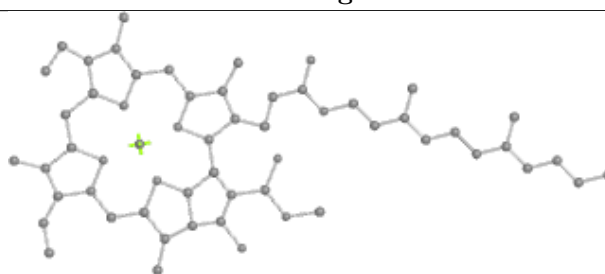
Bond lengths



Bond angles

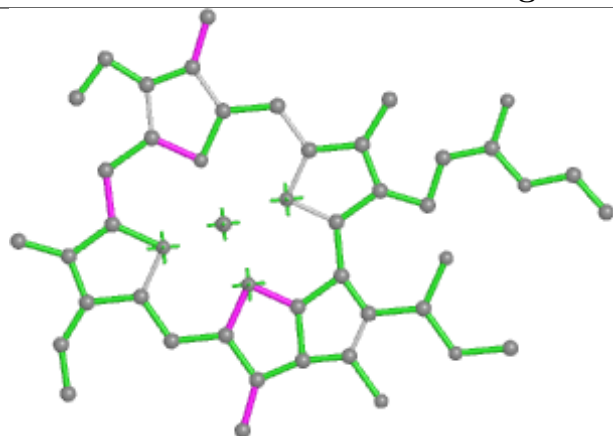


Torsions

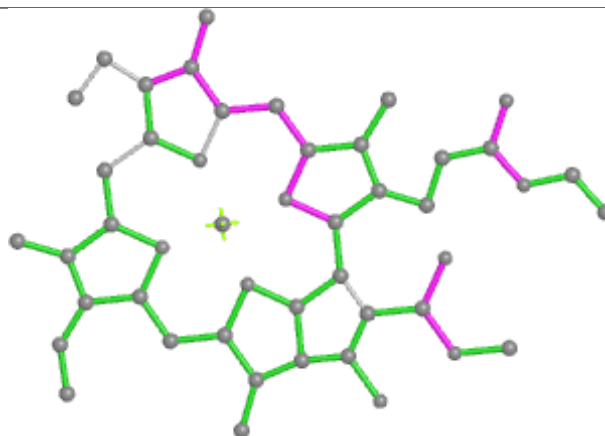


Rings

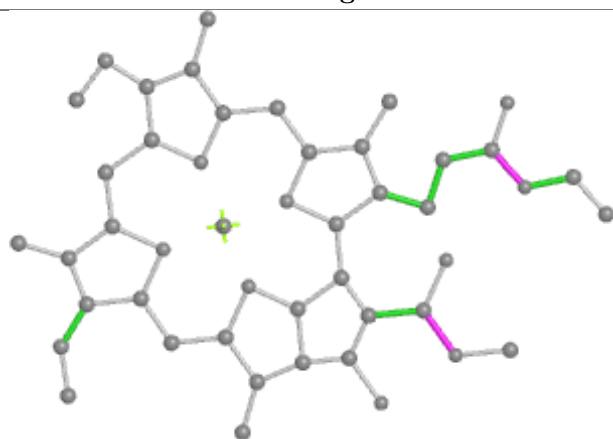
## Ligand CLA 2 312



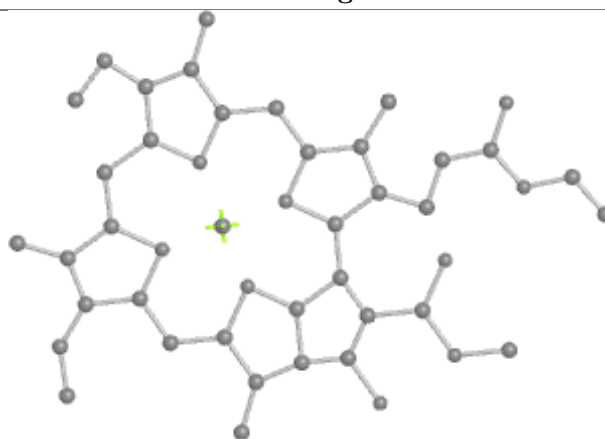
Bond lengths



Bond angles

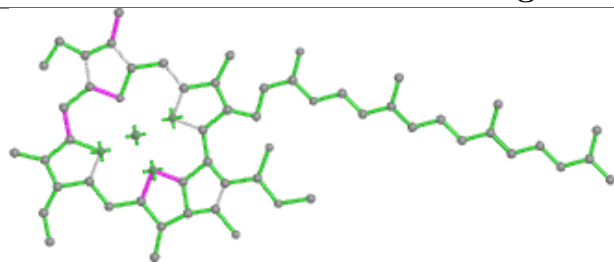


Torsions

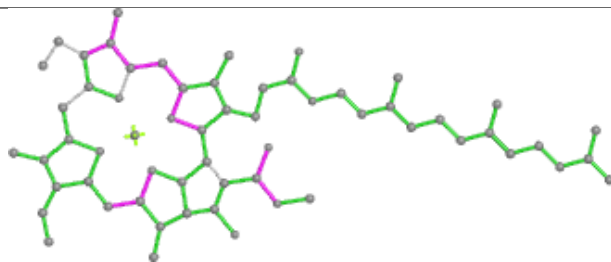


Rings

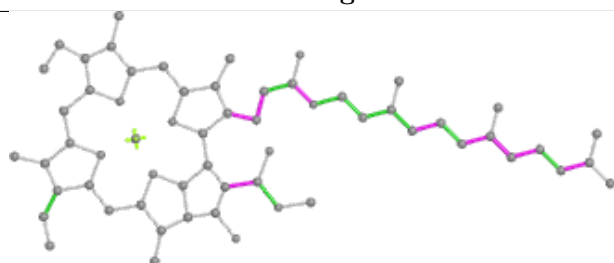
## Ligand CLA b 819



Bond lengths



Bond angles

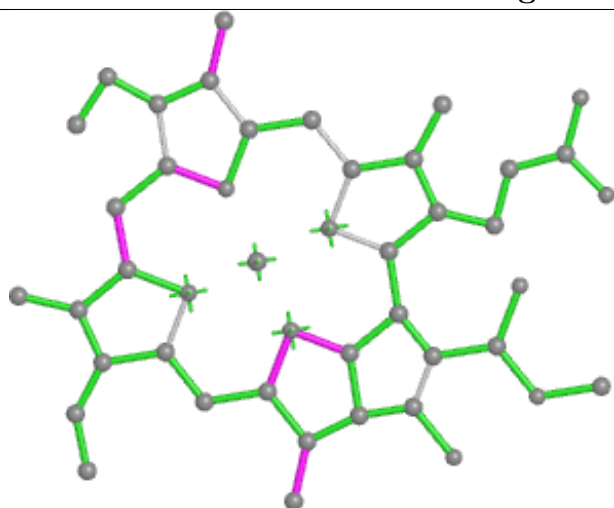


Torsions

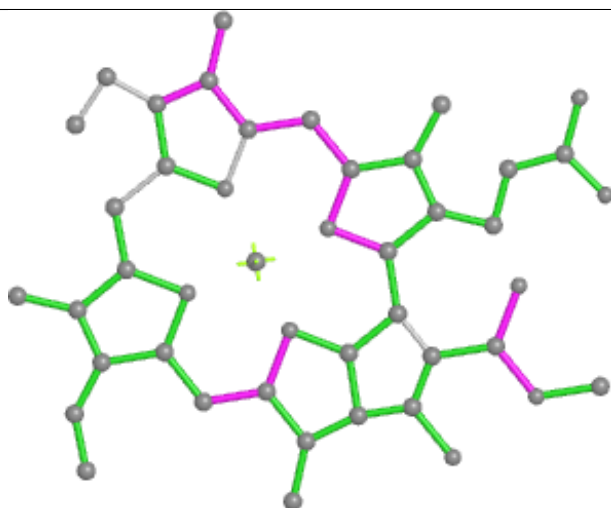


Rings

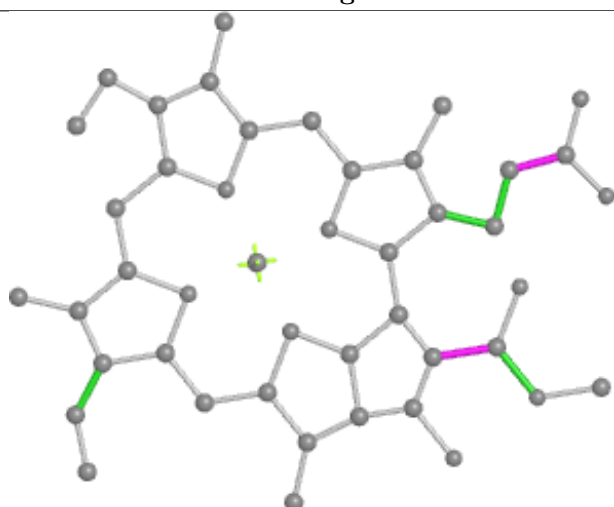
## Ligand CLA 4 314



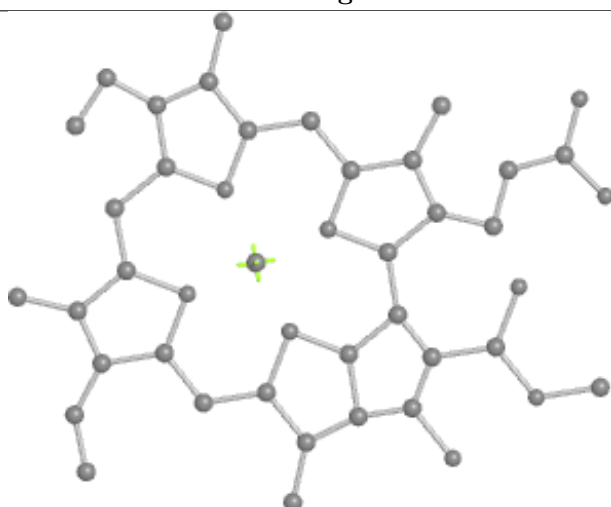
Bond lengths



Bond angles



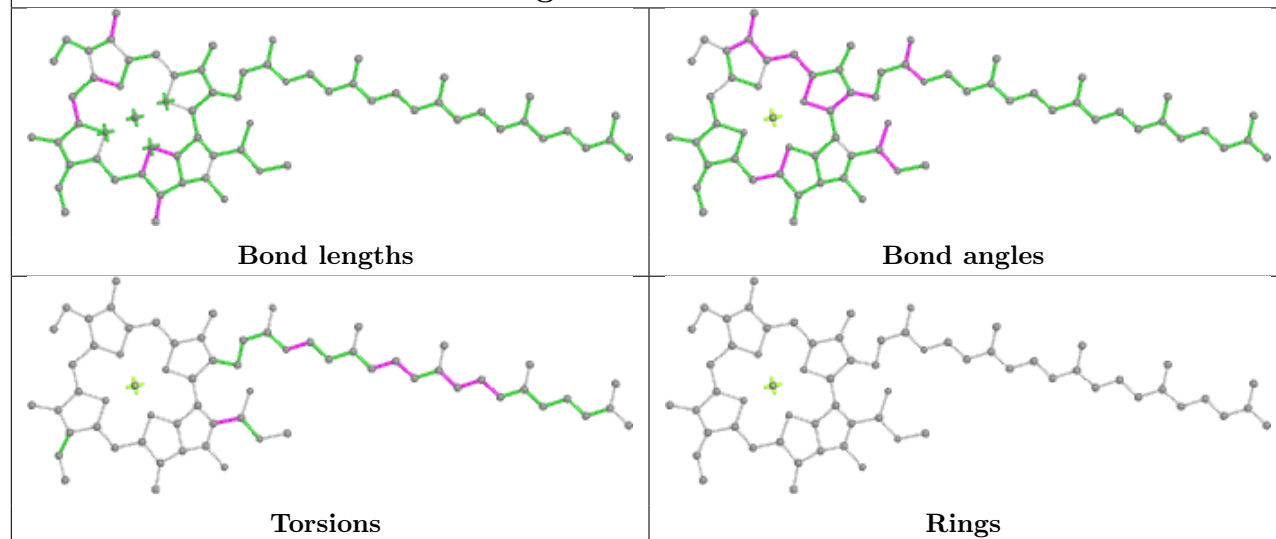
Torsions



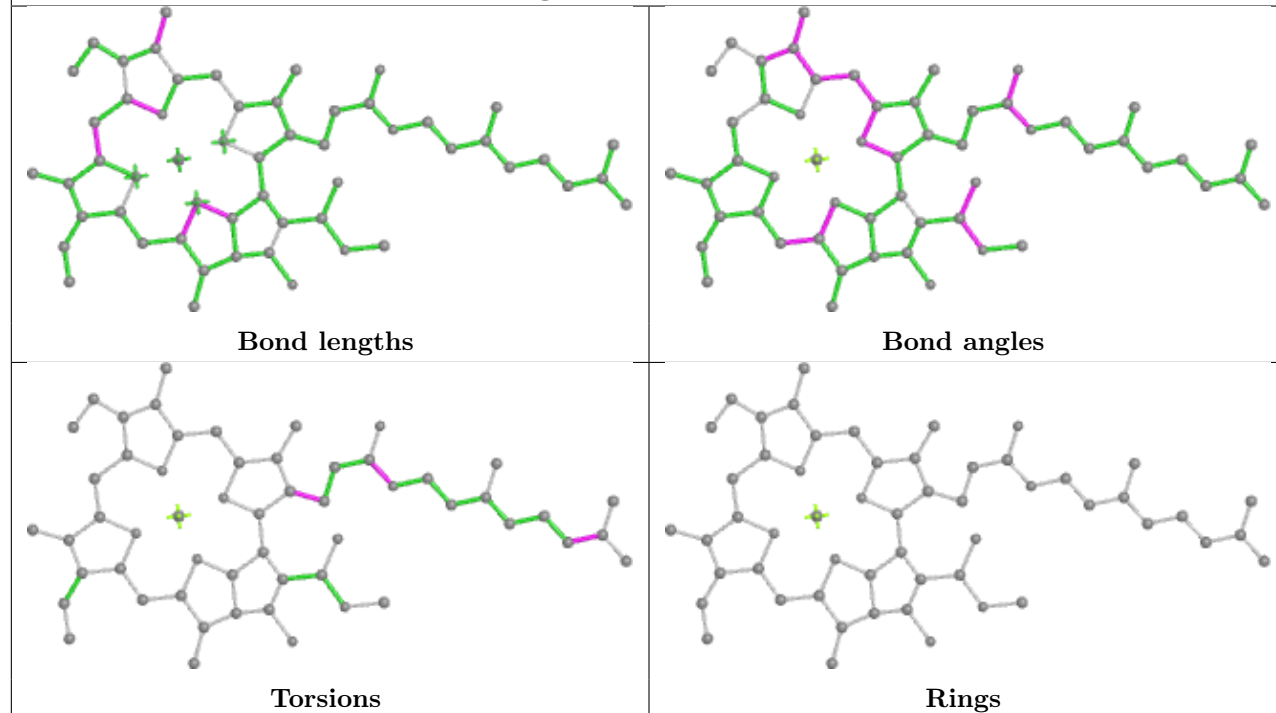
Rings



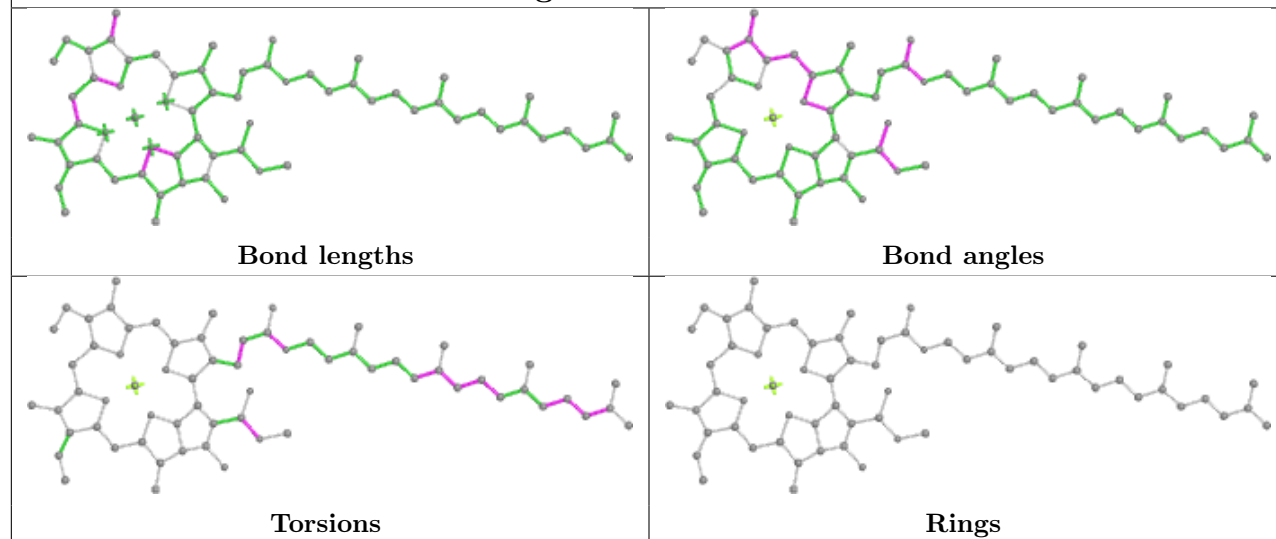
## Ligand CLA a 827



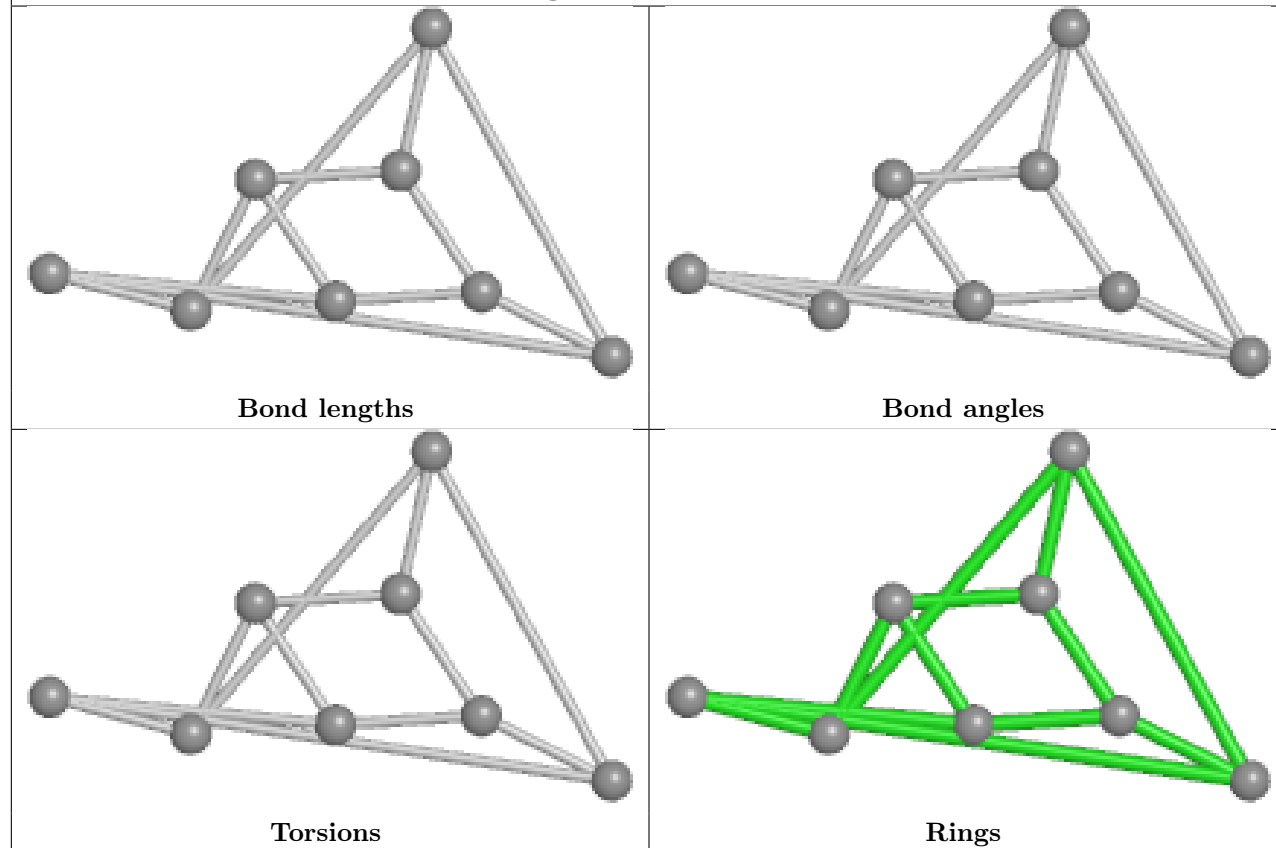
## Ligand CLA a 805

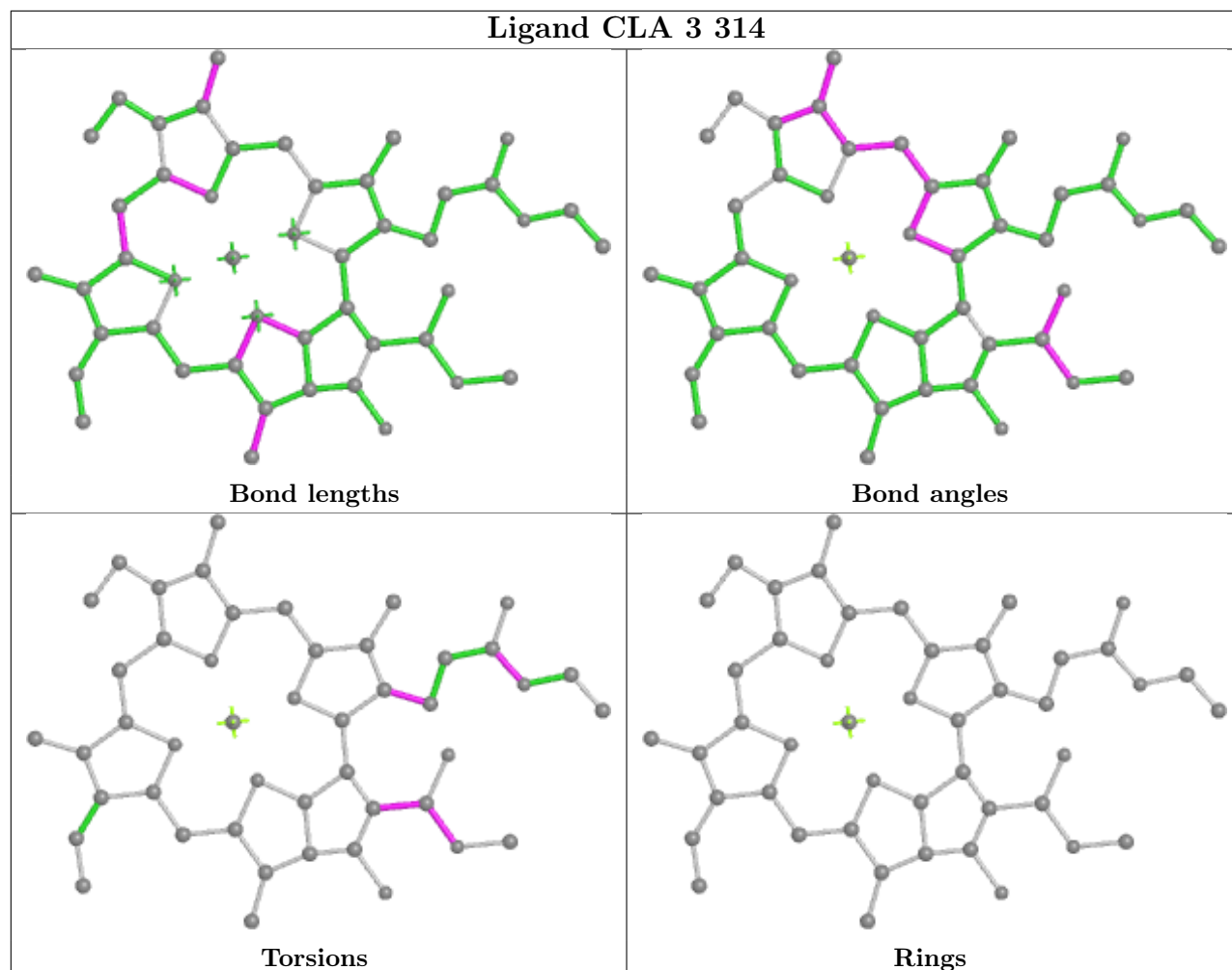
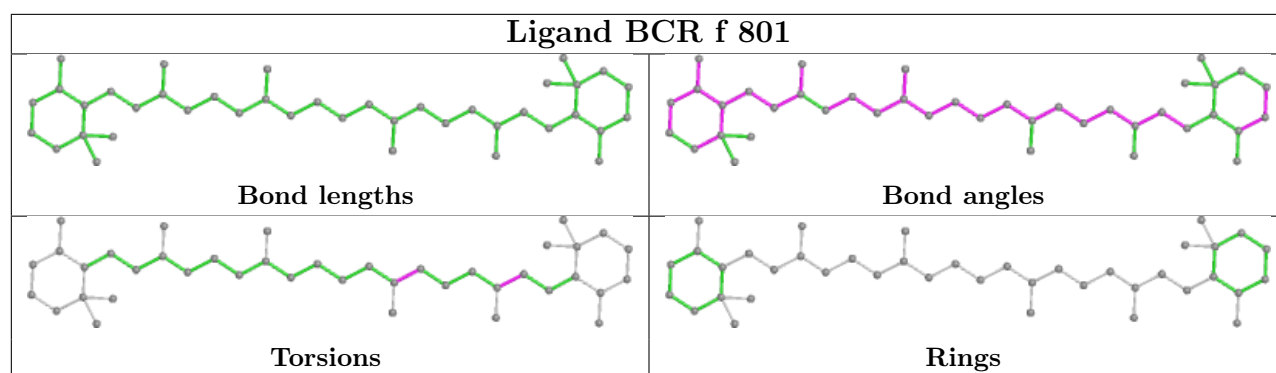


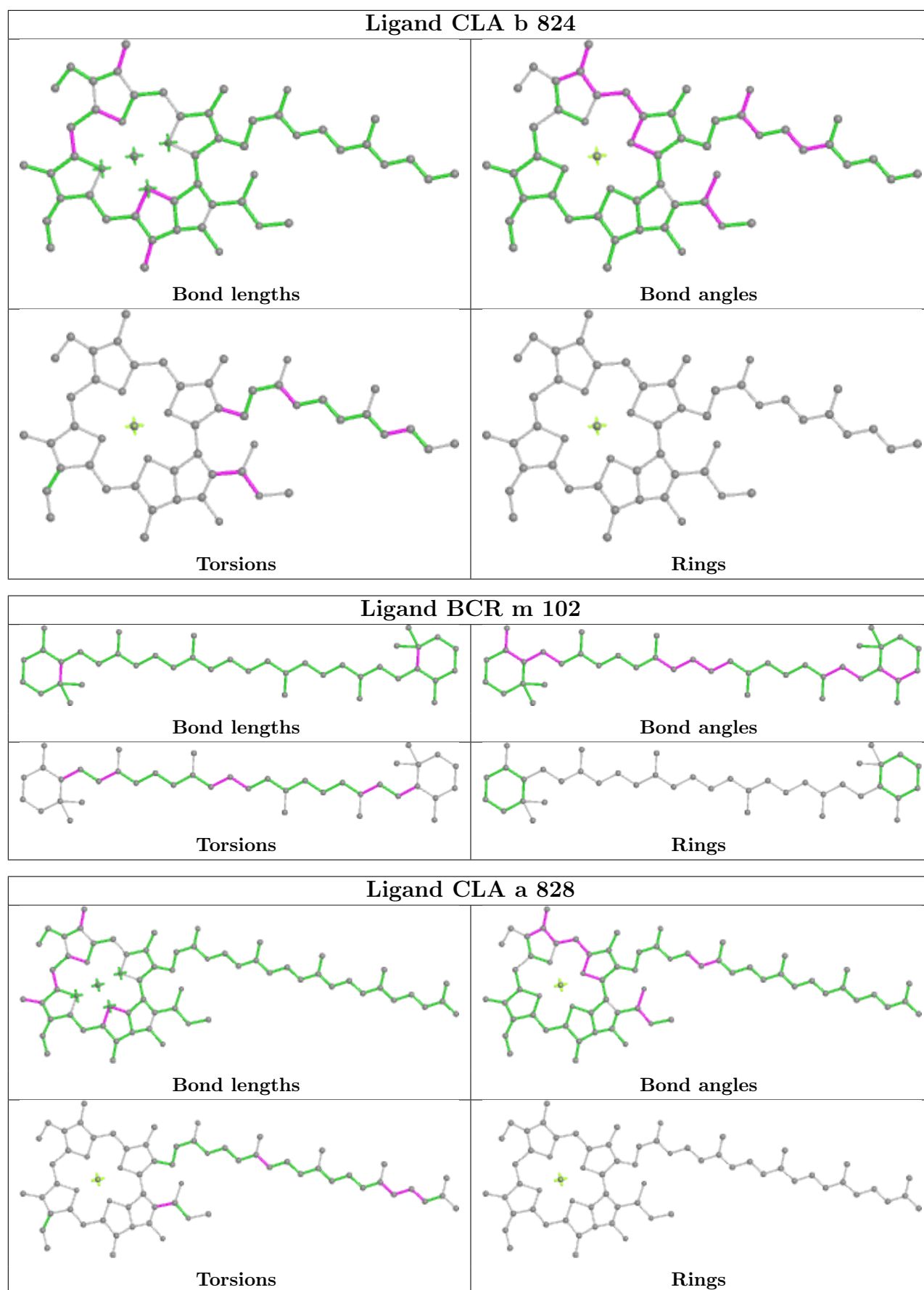
## Ligand CLA b 828



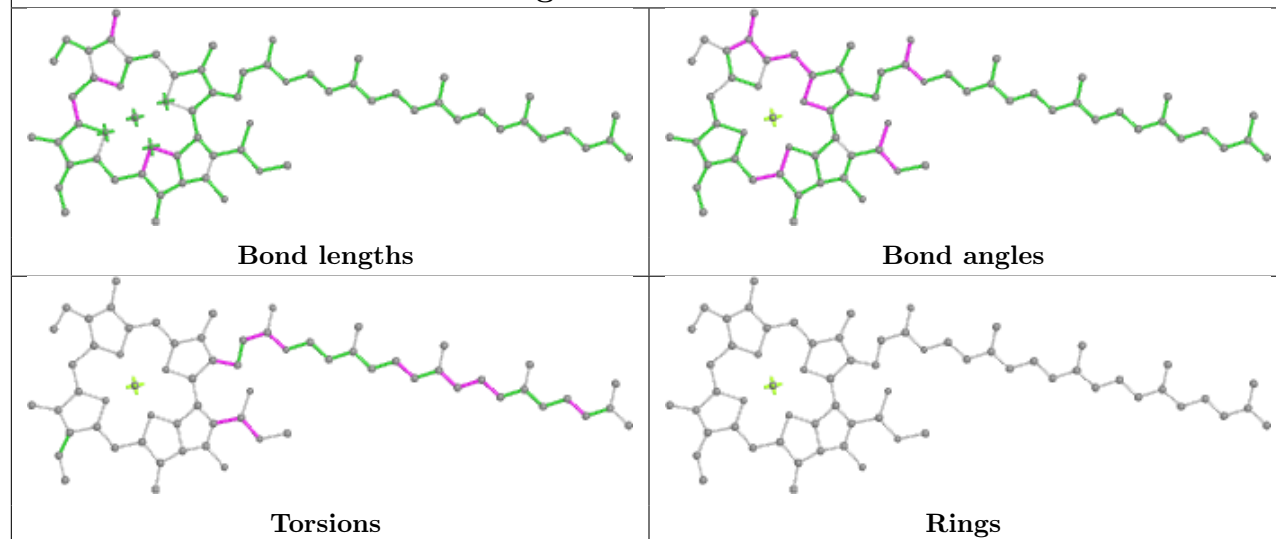
## Ligand SF4 c 102



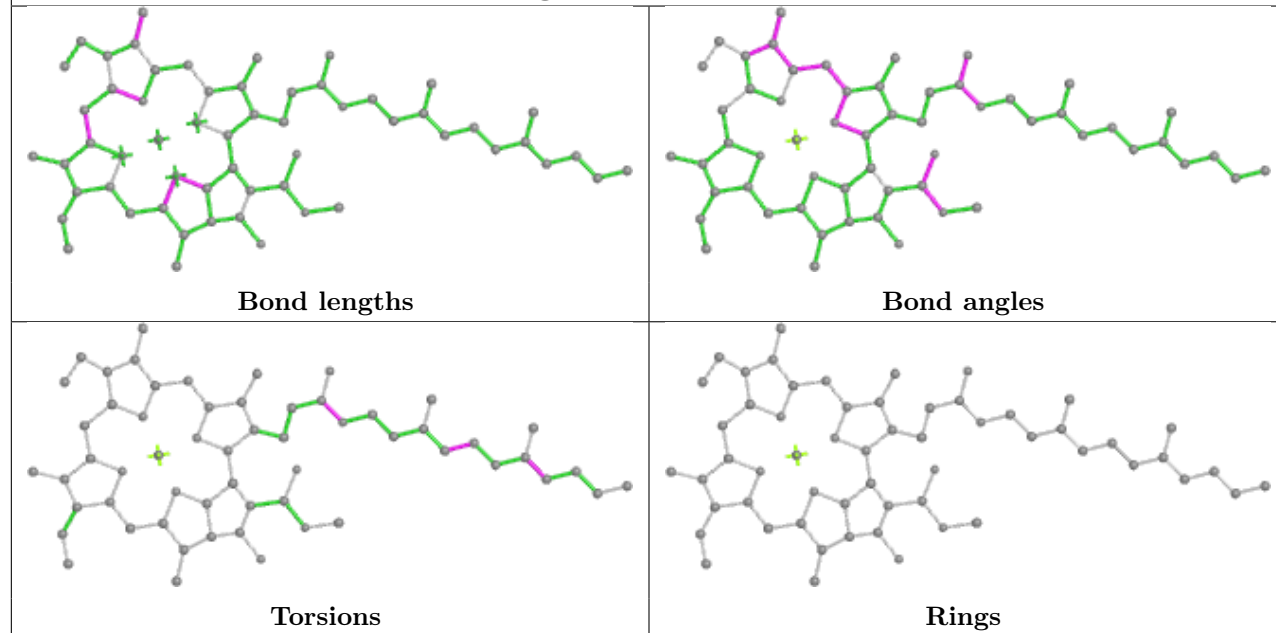




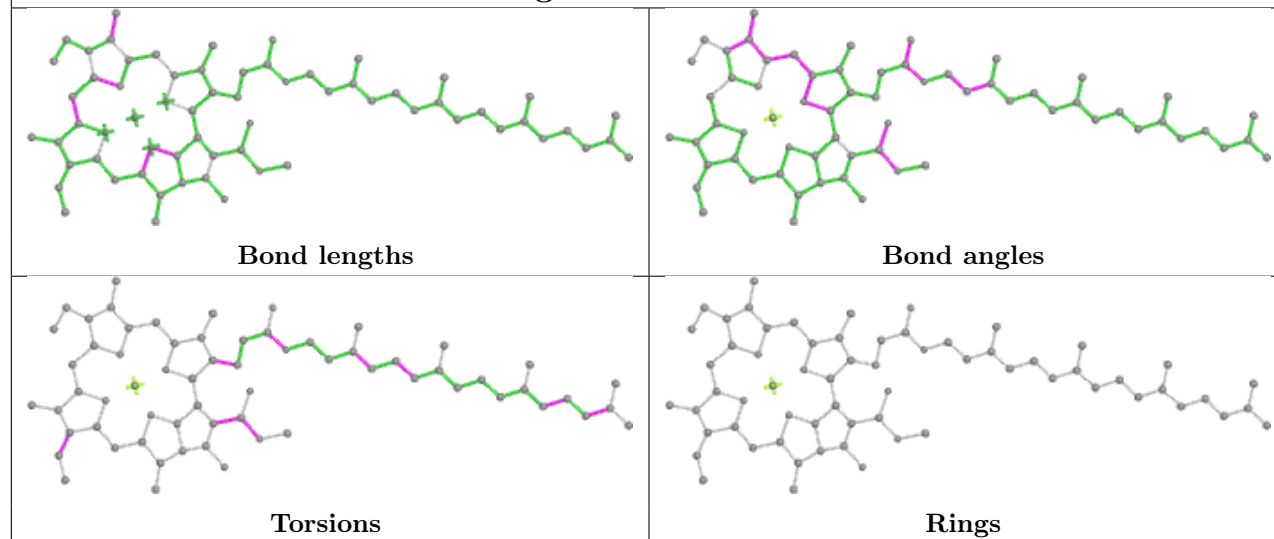
## Ligand CLA a 854



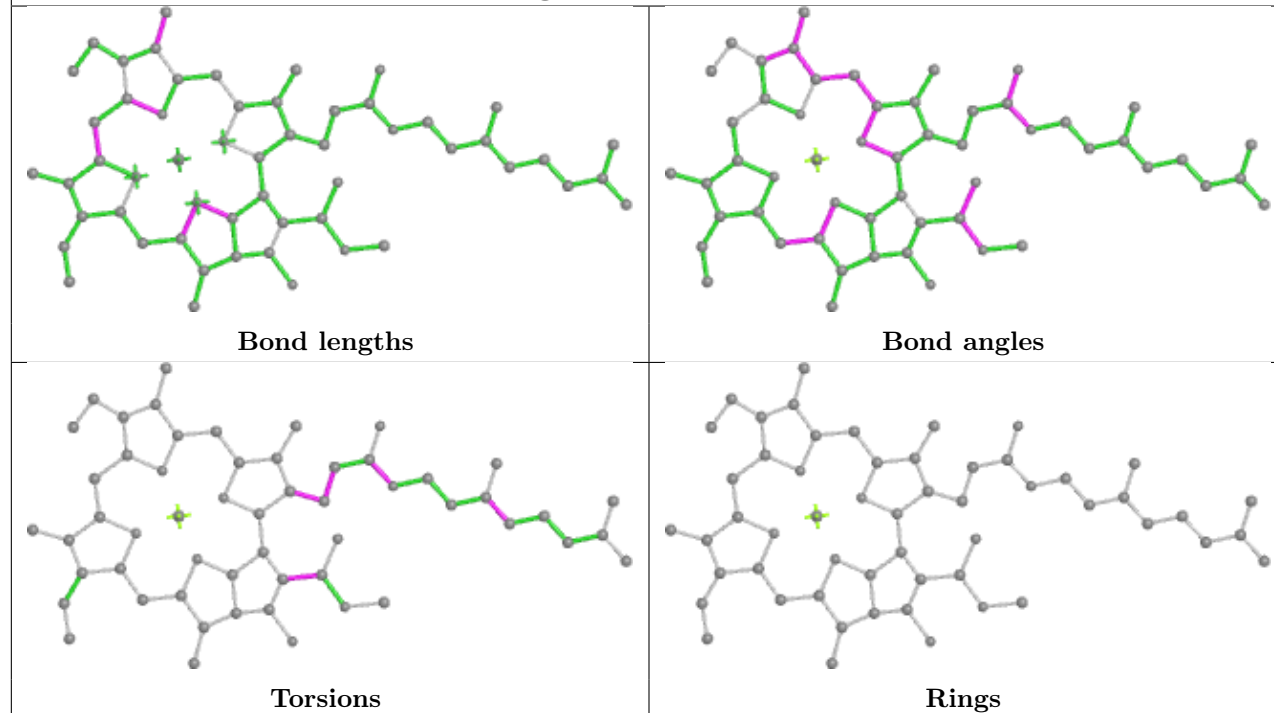
## Ligand CLA 2 311

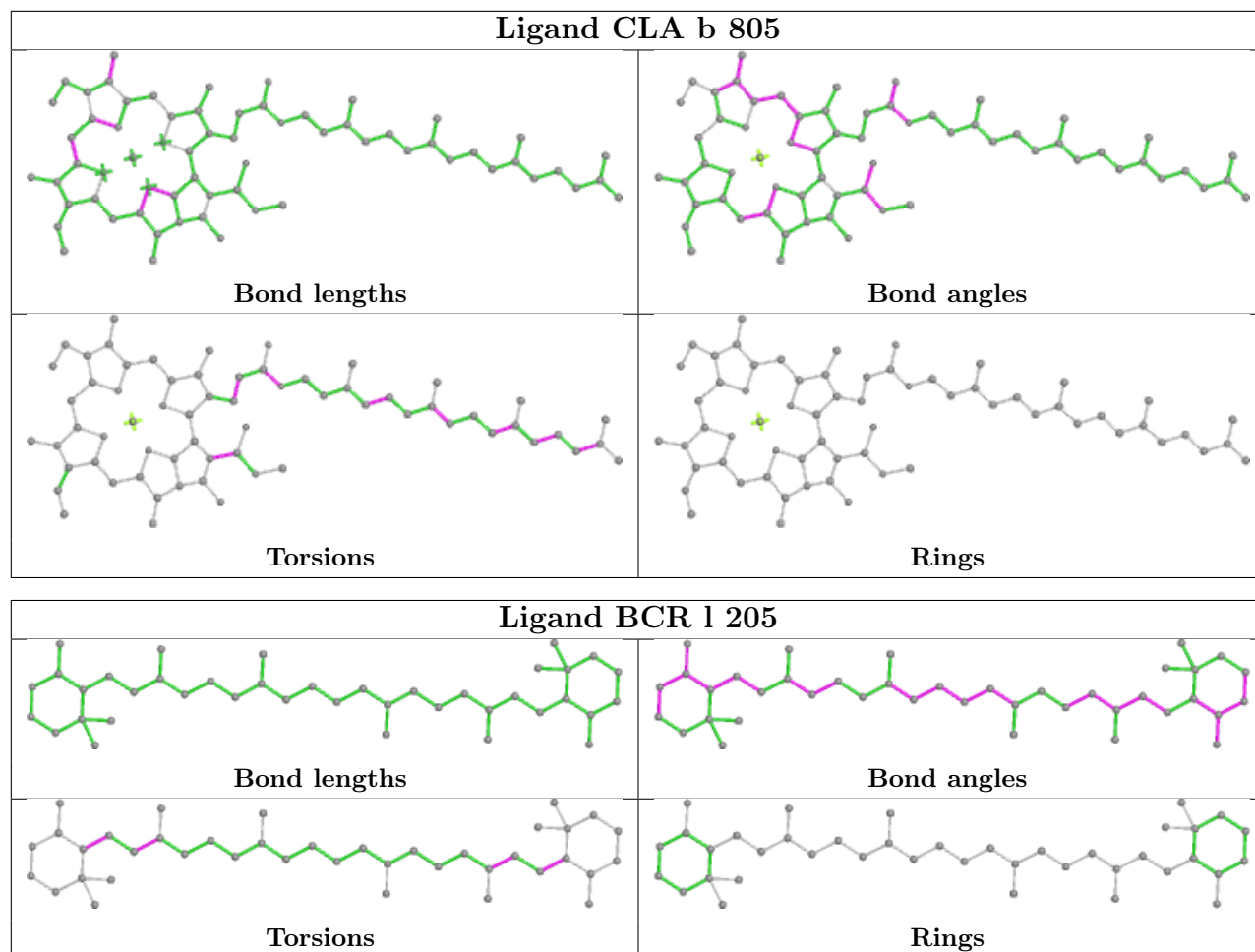


## Ligand CLA b 840

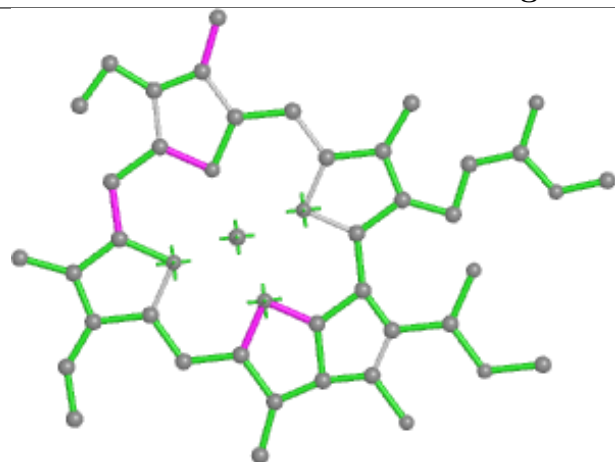


## Ligand CLA a 825

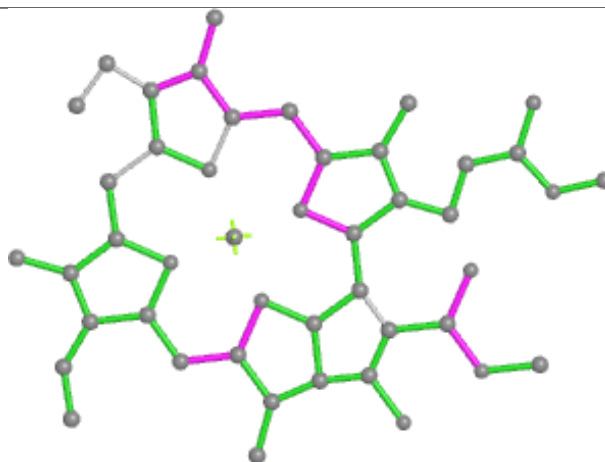




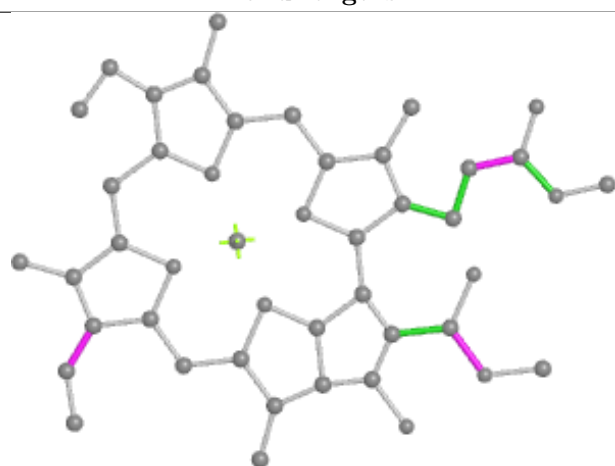
## Ligand CLA 5 315



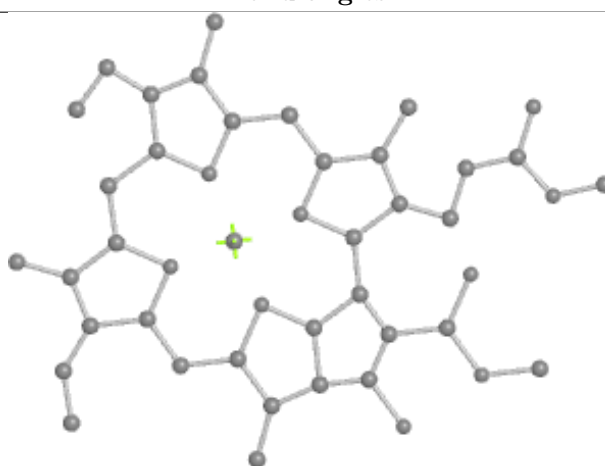
Bond lengths



Bond angles



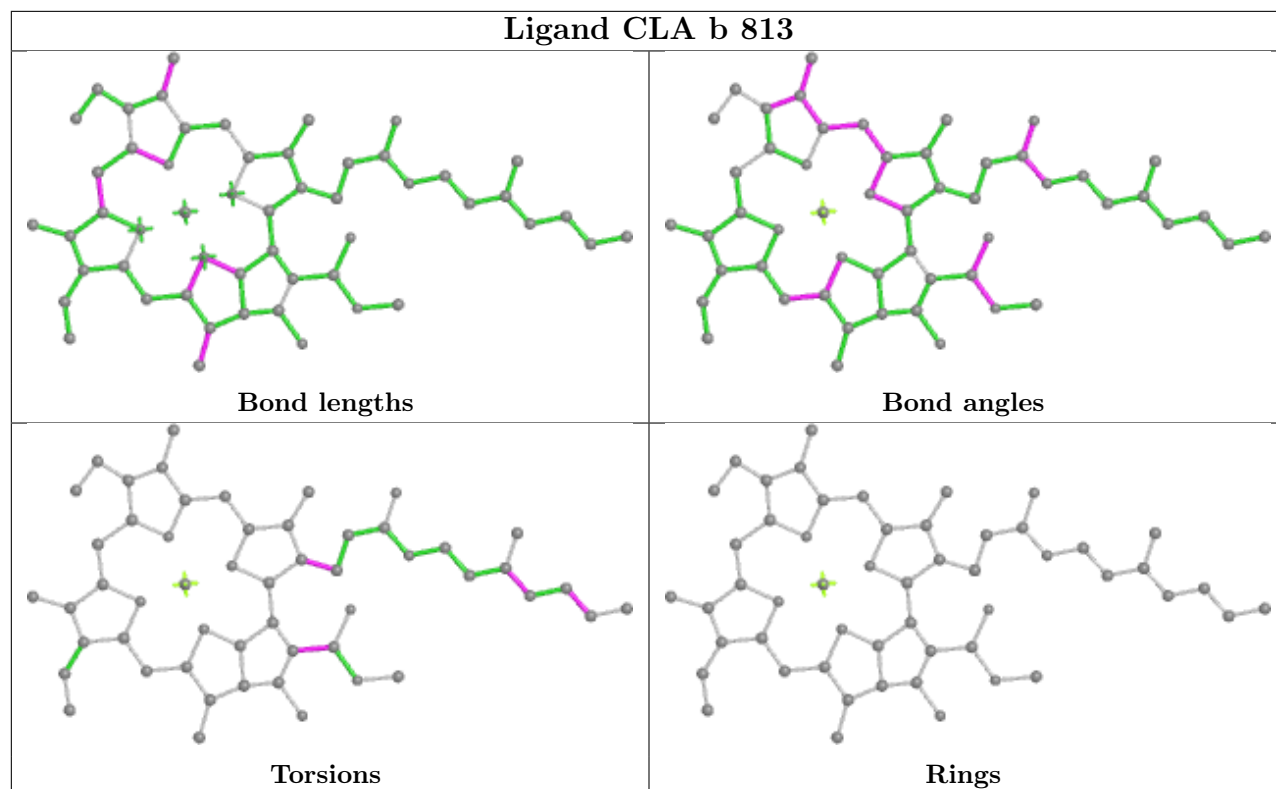
Torsions



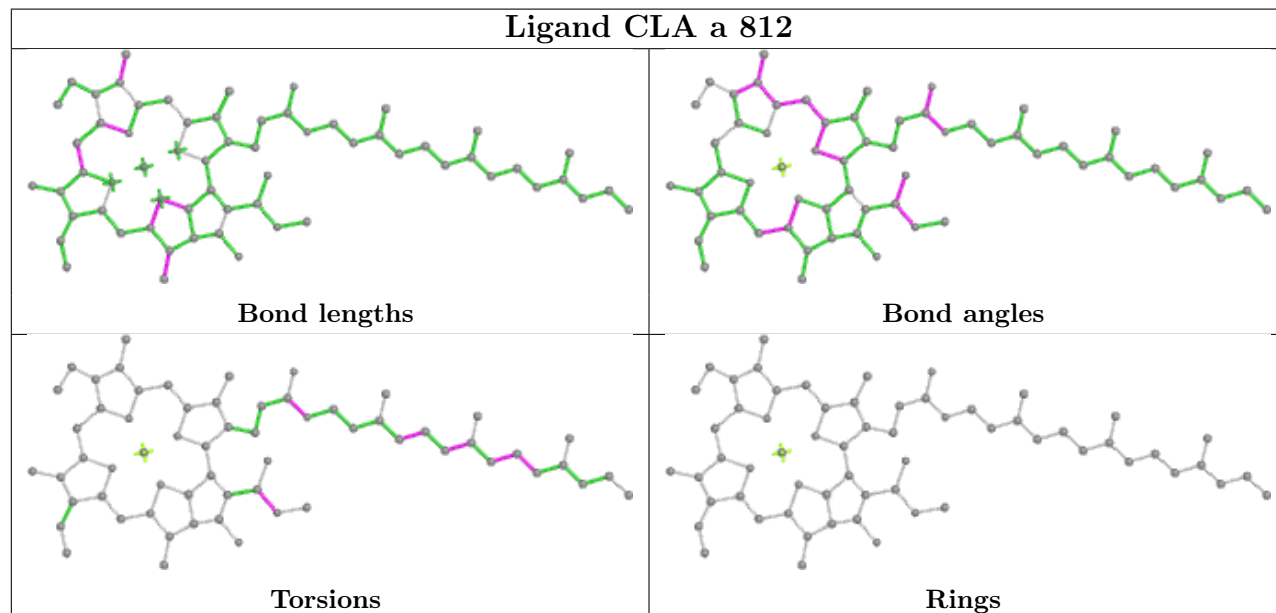
Rings

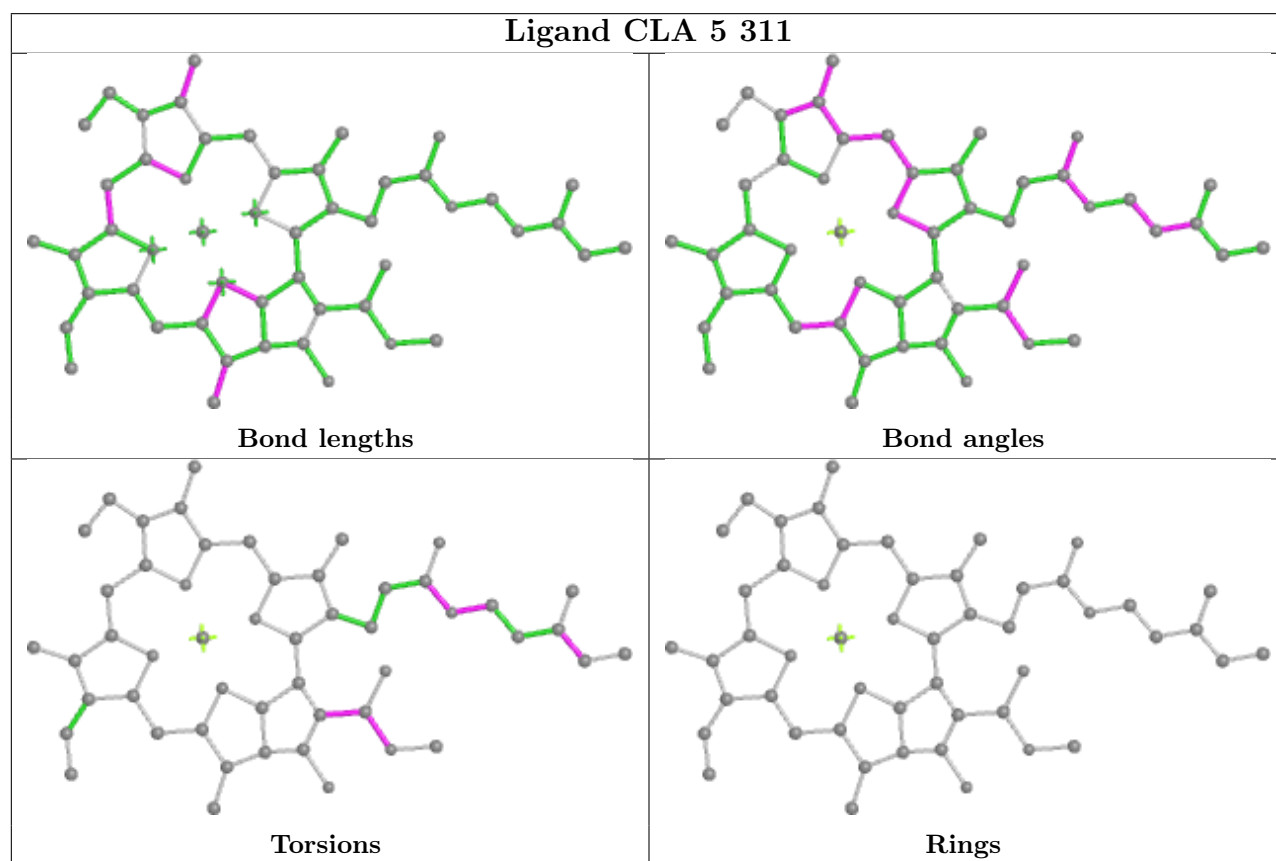
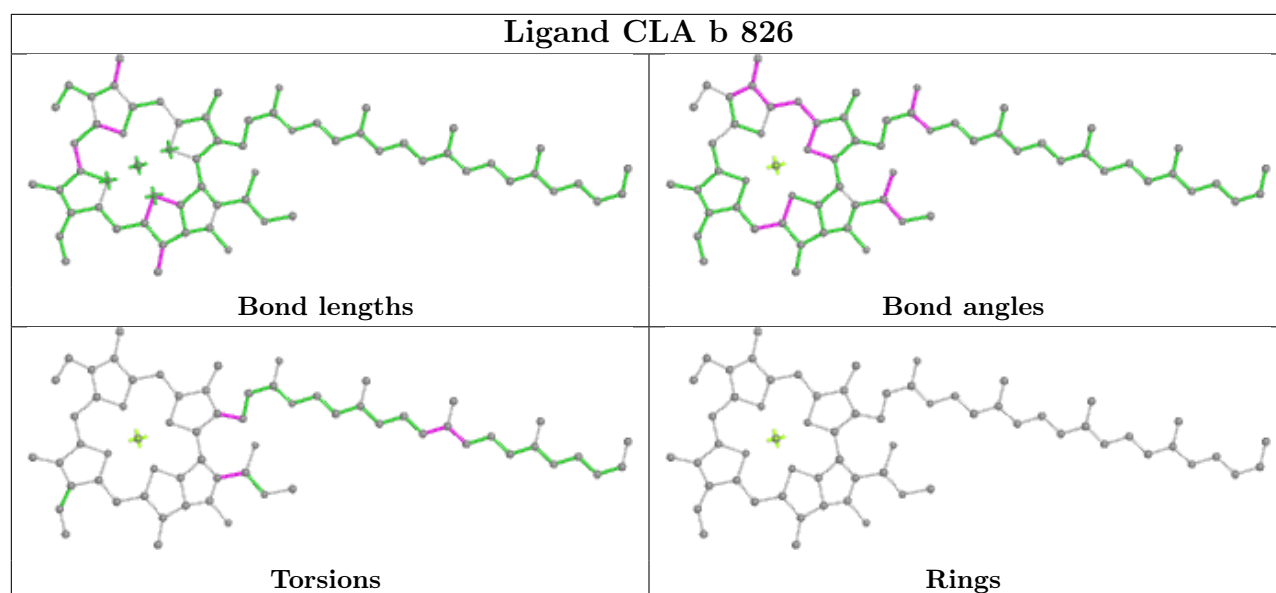


## Ligand CLA b 813

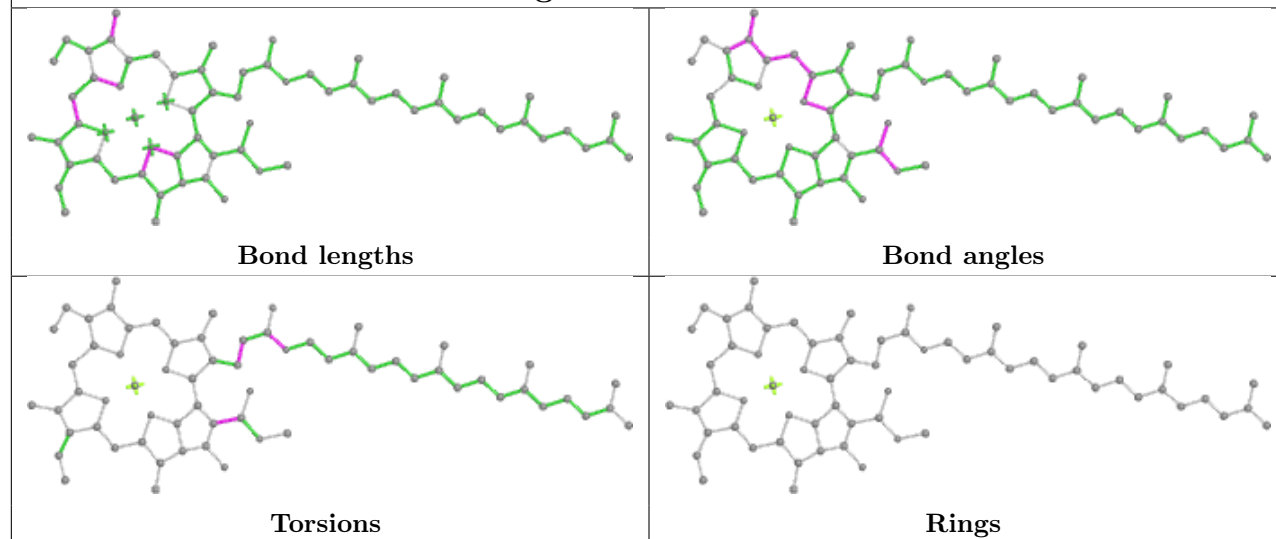


## Ligand CLA a 812

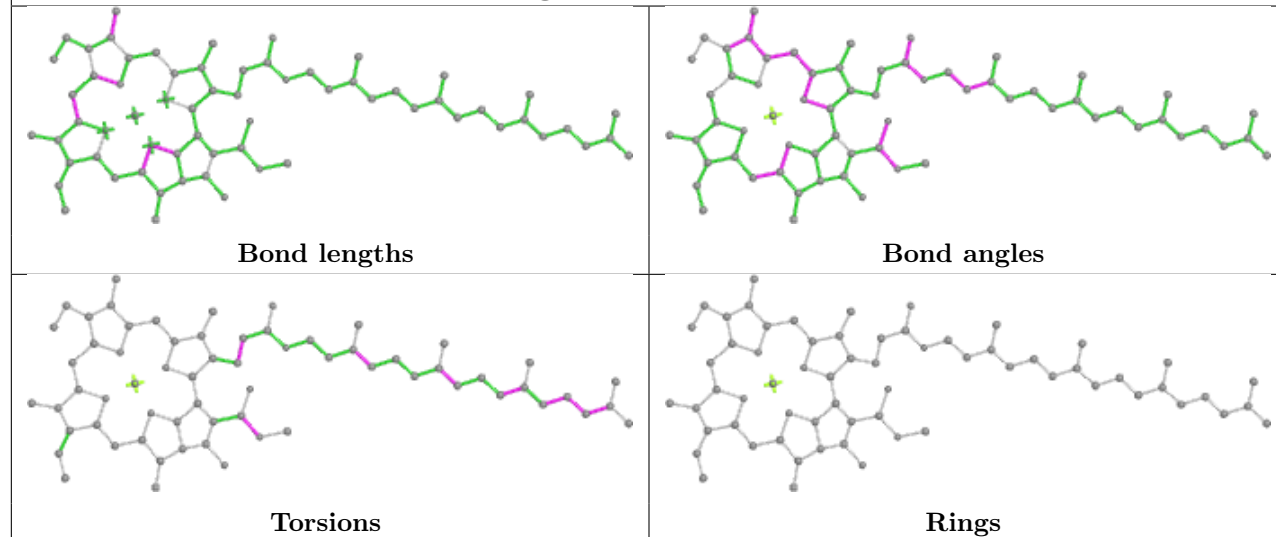




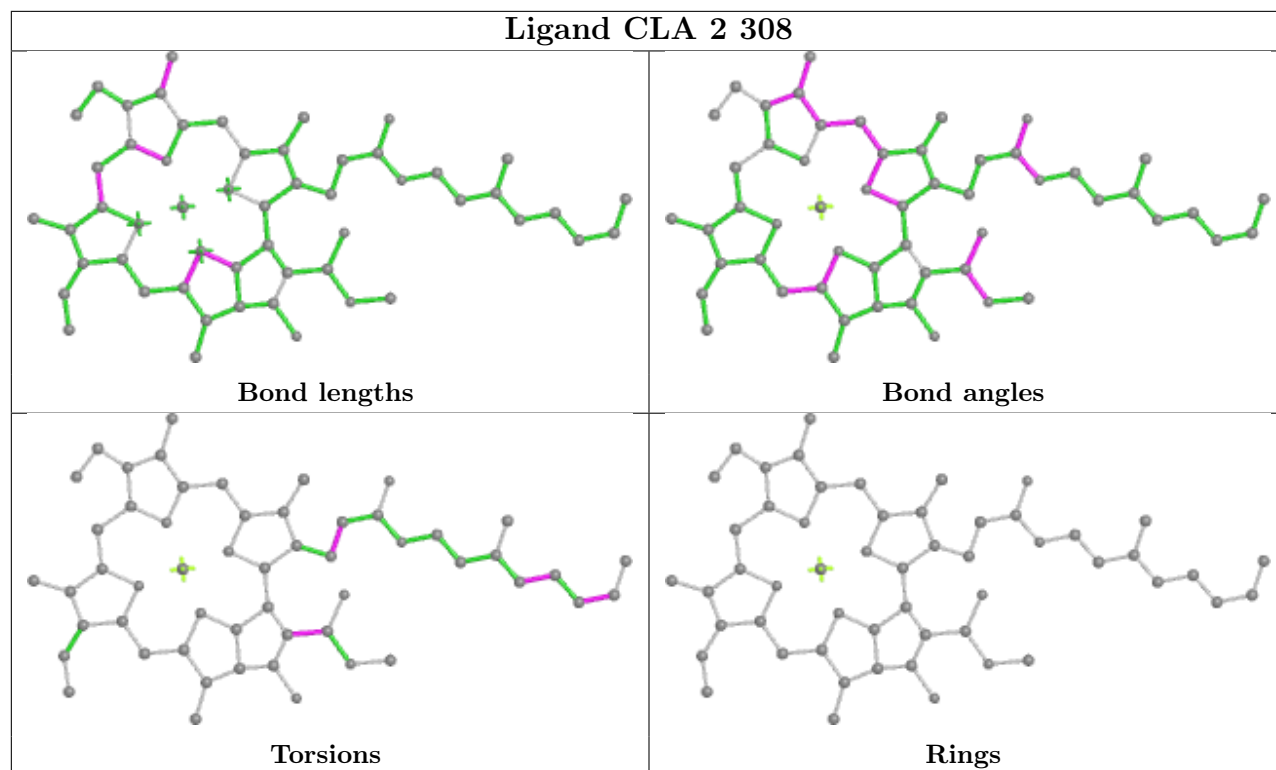
## Ligand CLA b 827



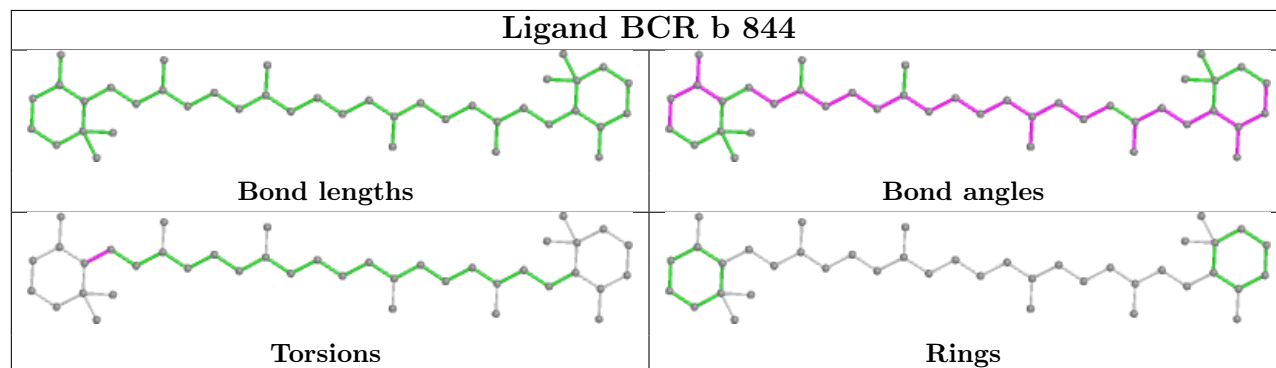
## Ligand CLA 1 308



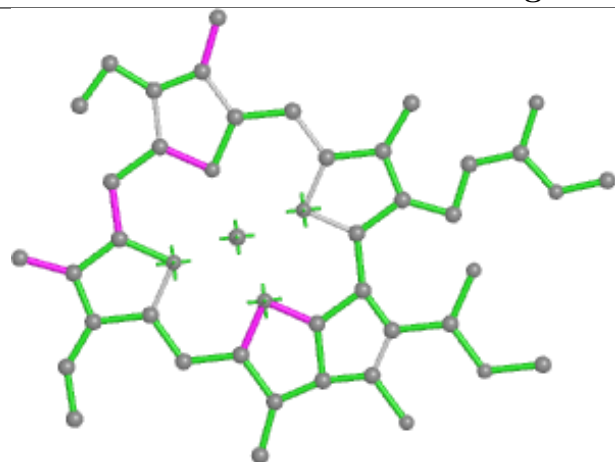
## Ligand CLA 2 308



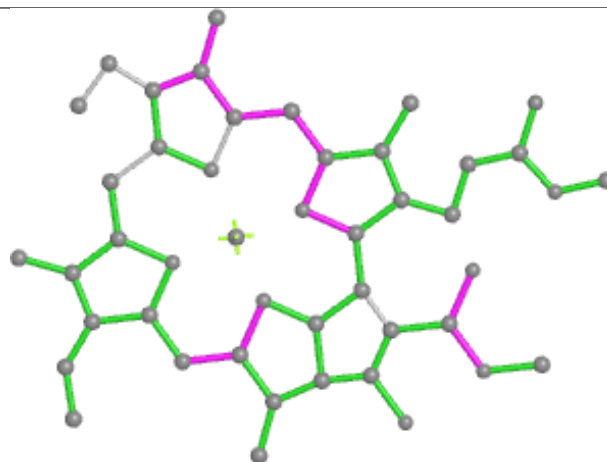
## Ligand BCR b 844



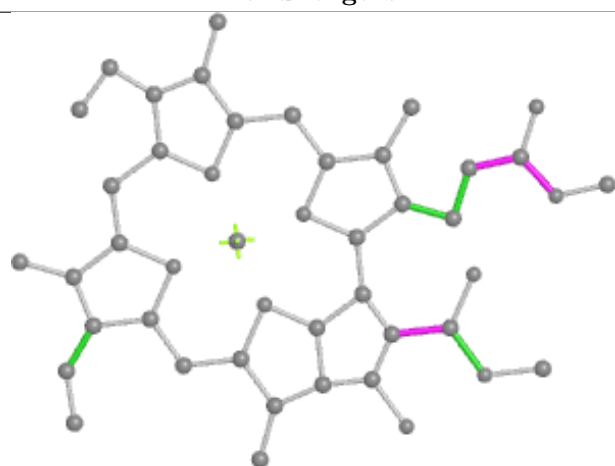
## Ligand CLA 1 204



Bond lengths



Bond angles

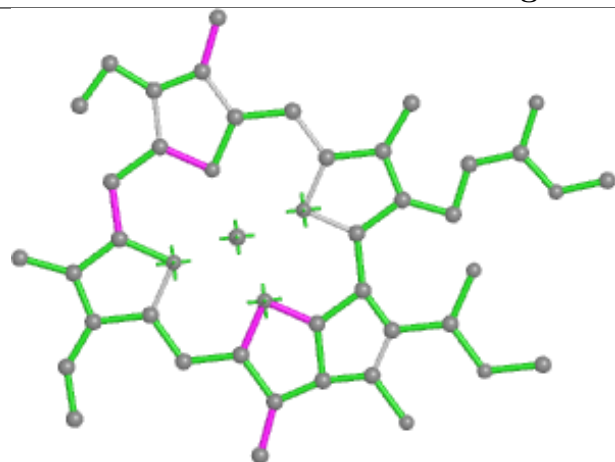


Torsions

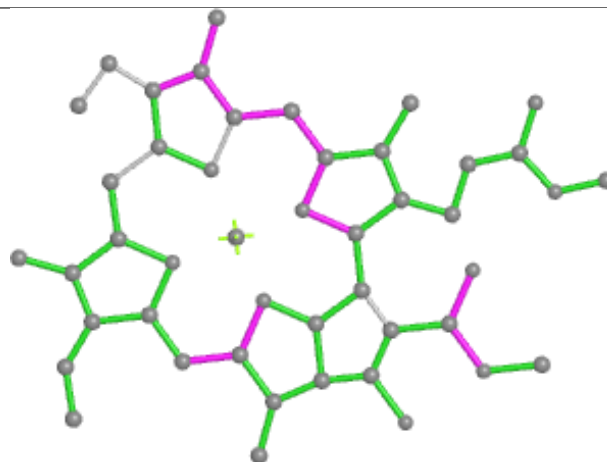


Rings

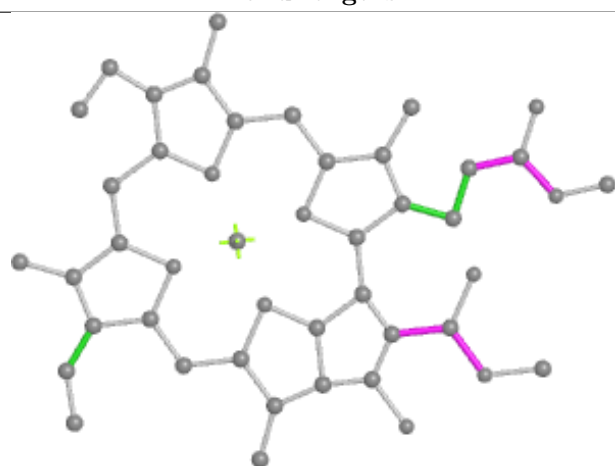
## Ligand CLA 1 309



Bond lengths



Bond angles

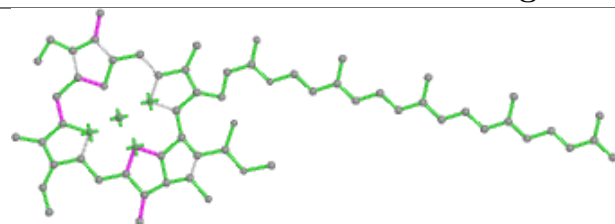


Torsions

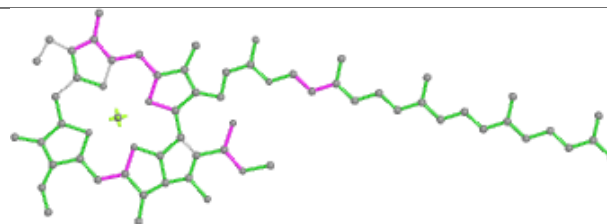


Rings

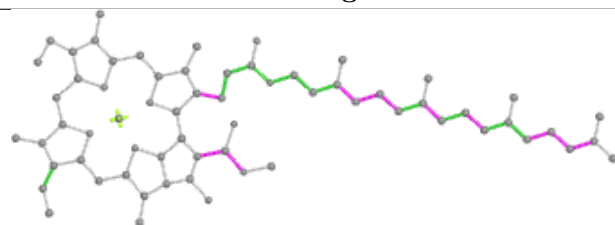
## Ligand CLA b 814



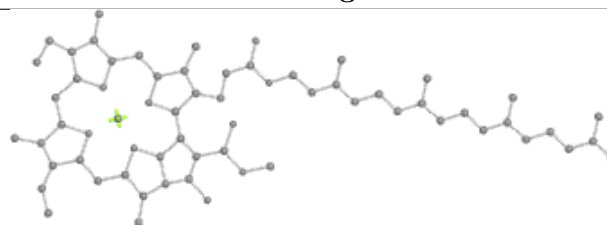
Bond lengths



Bond angles

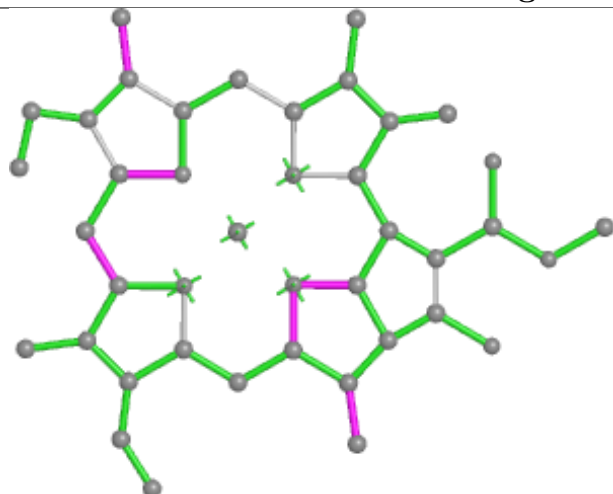


Torsions

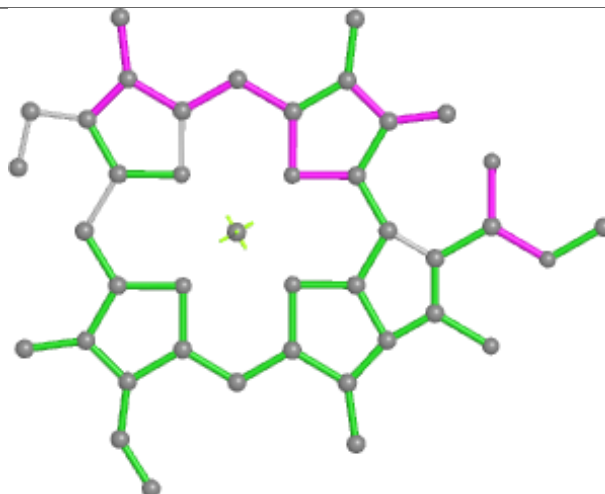


Rings

## Ligand CLA 1 313



Bond lengths



Bond angles

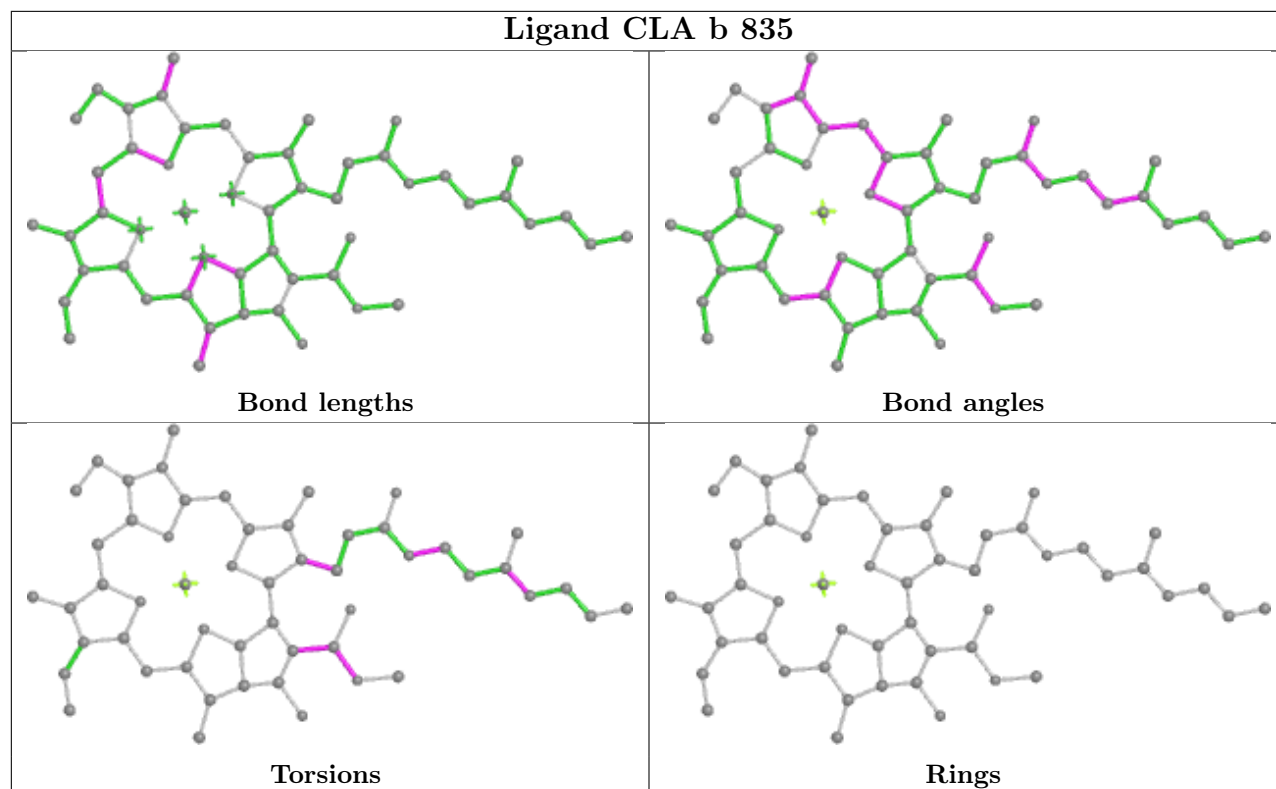


Torsions

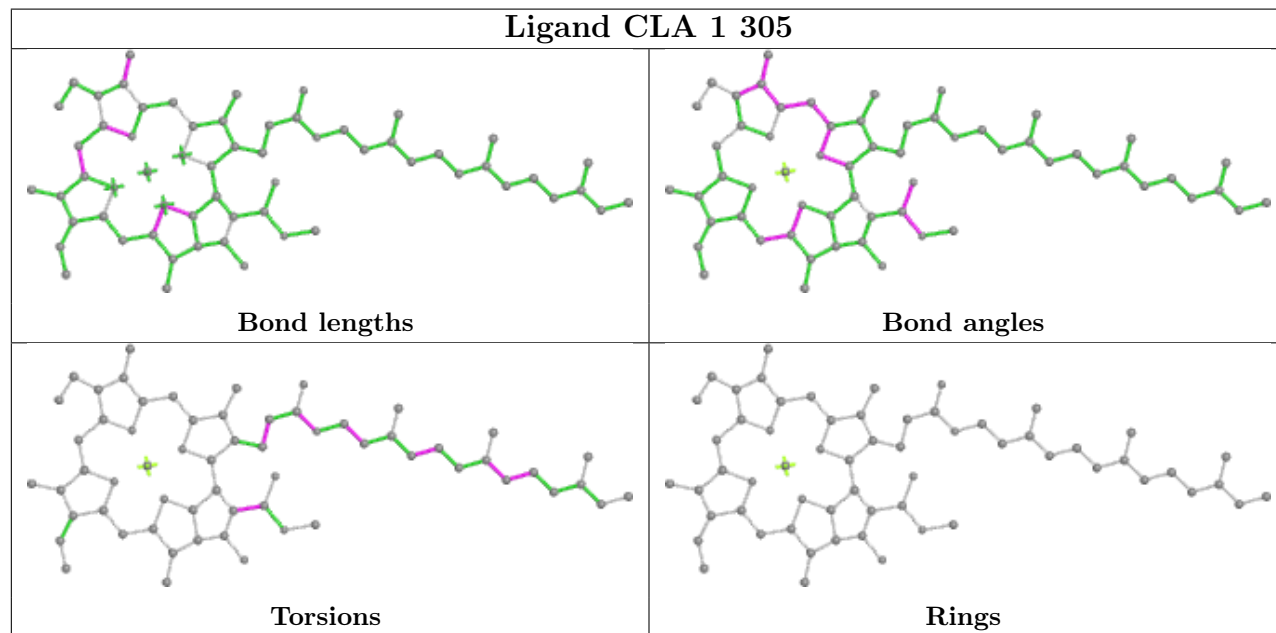


Rings

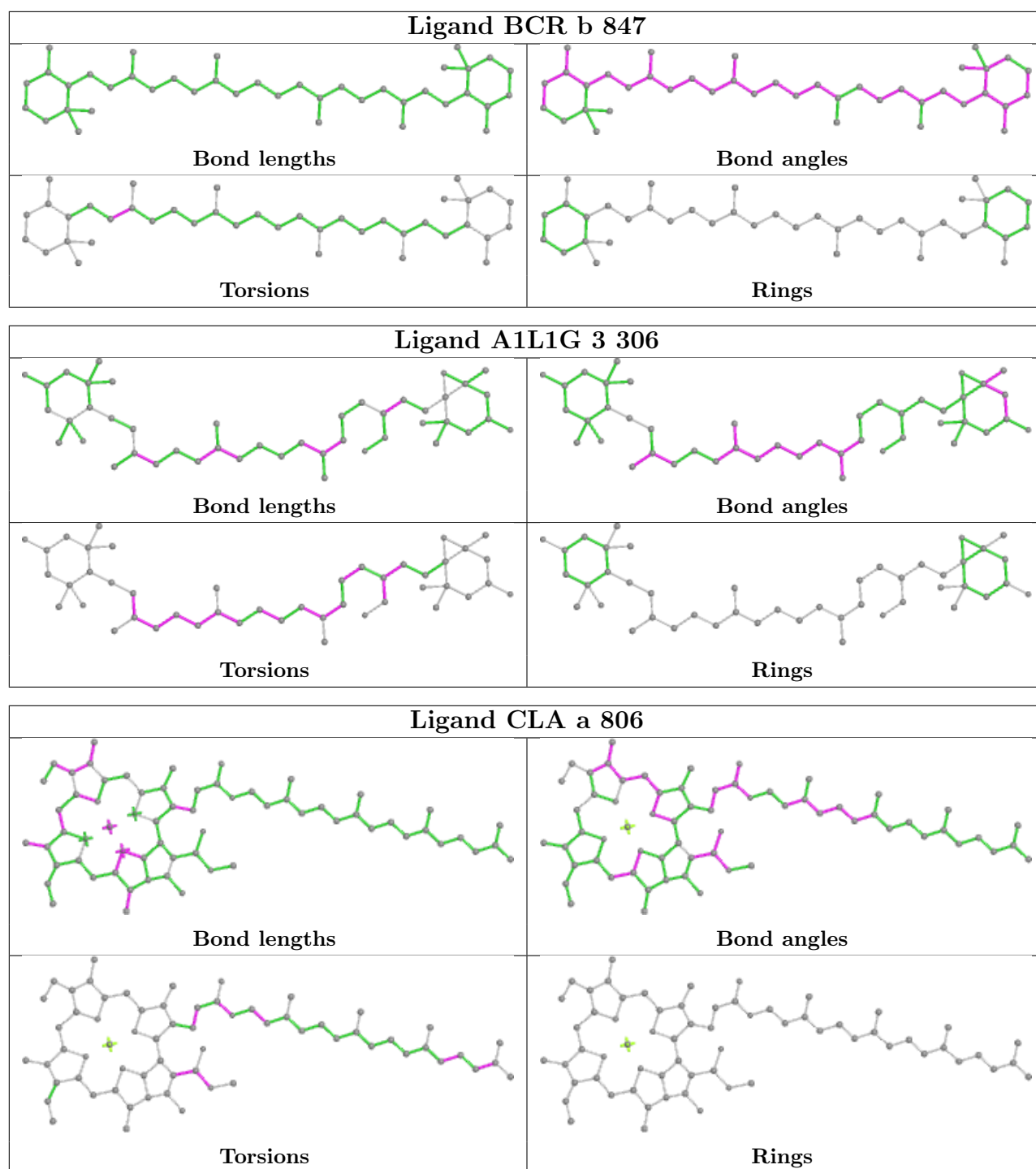
## Ligand CLA b 835



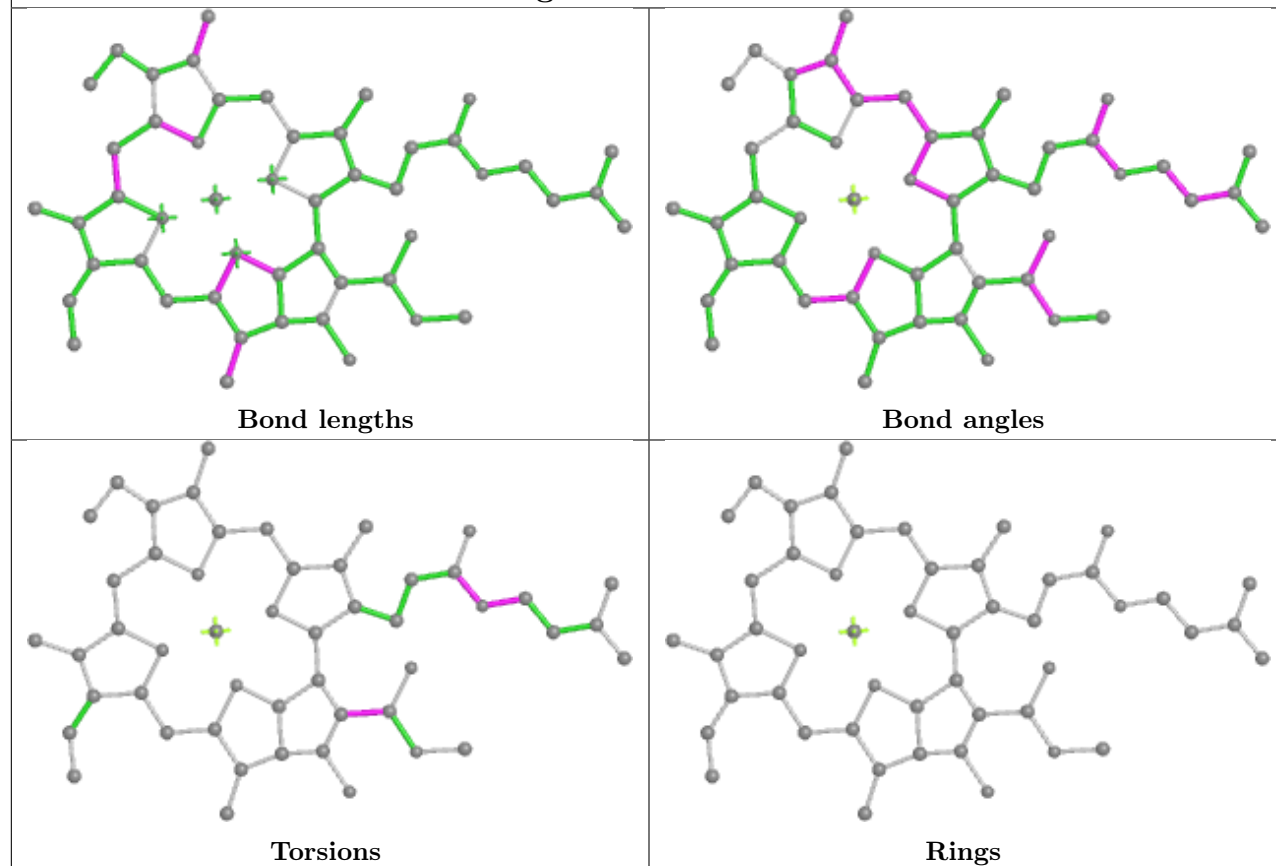
## Ligand CLA 1 305



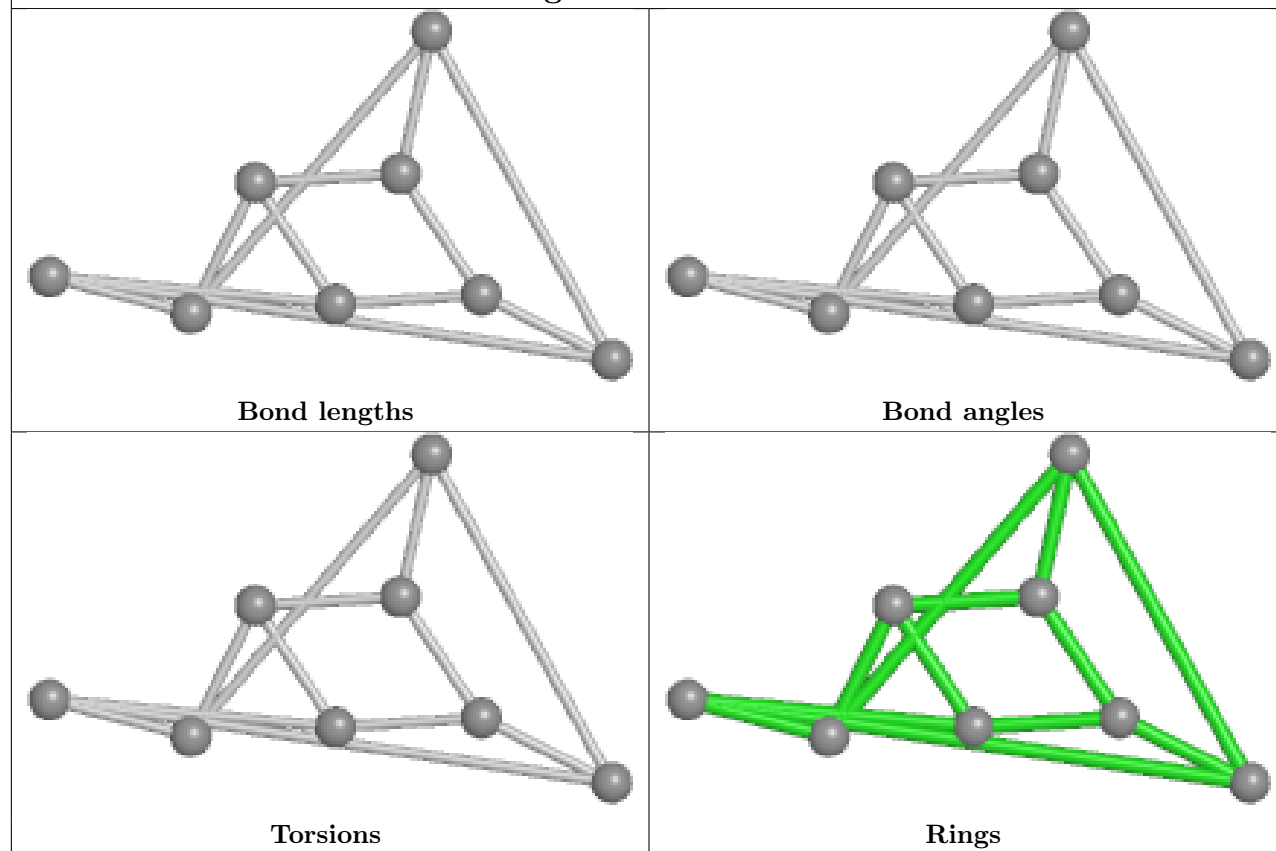




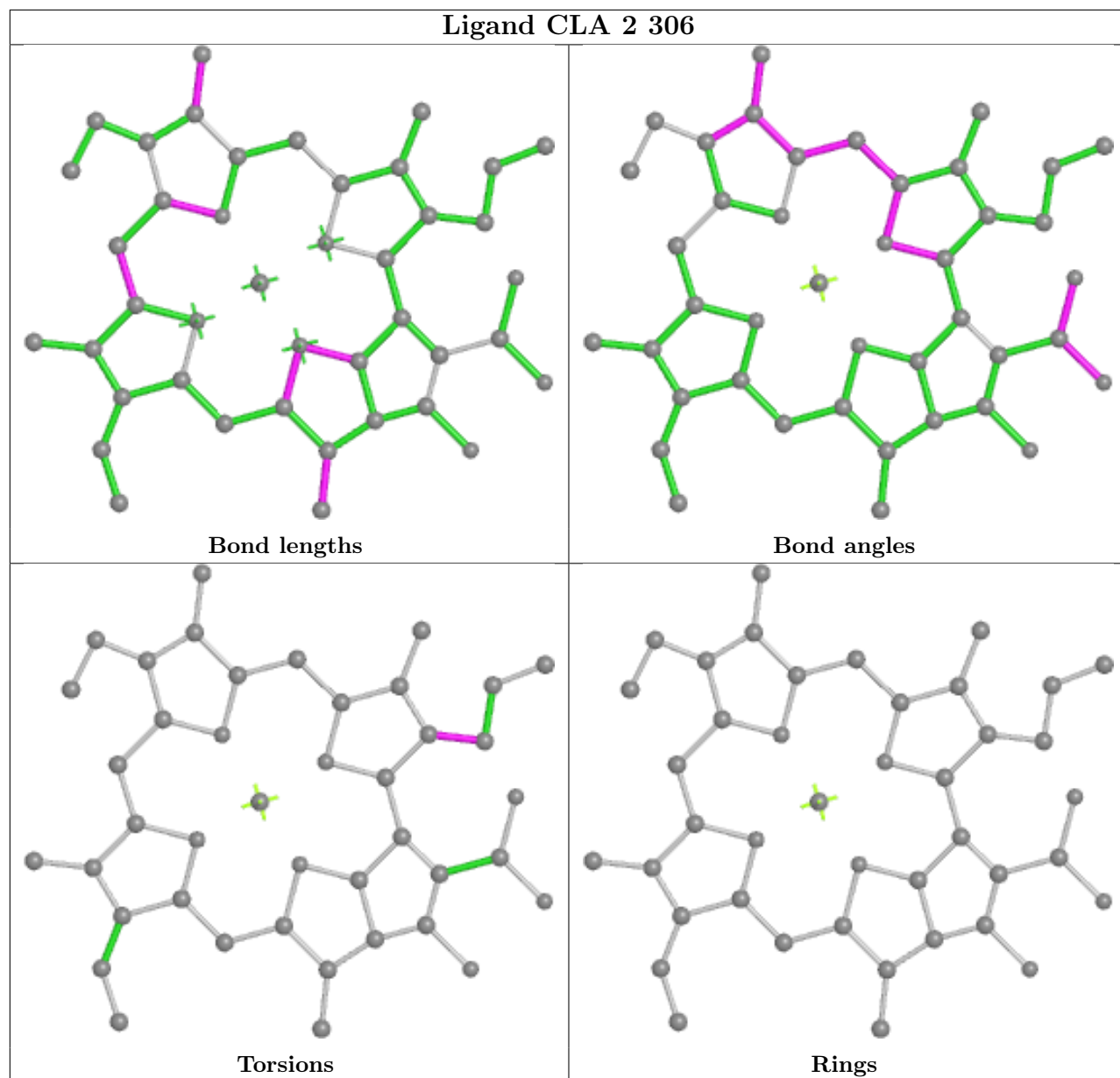
## Ligand CLA a 816



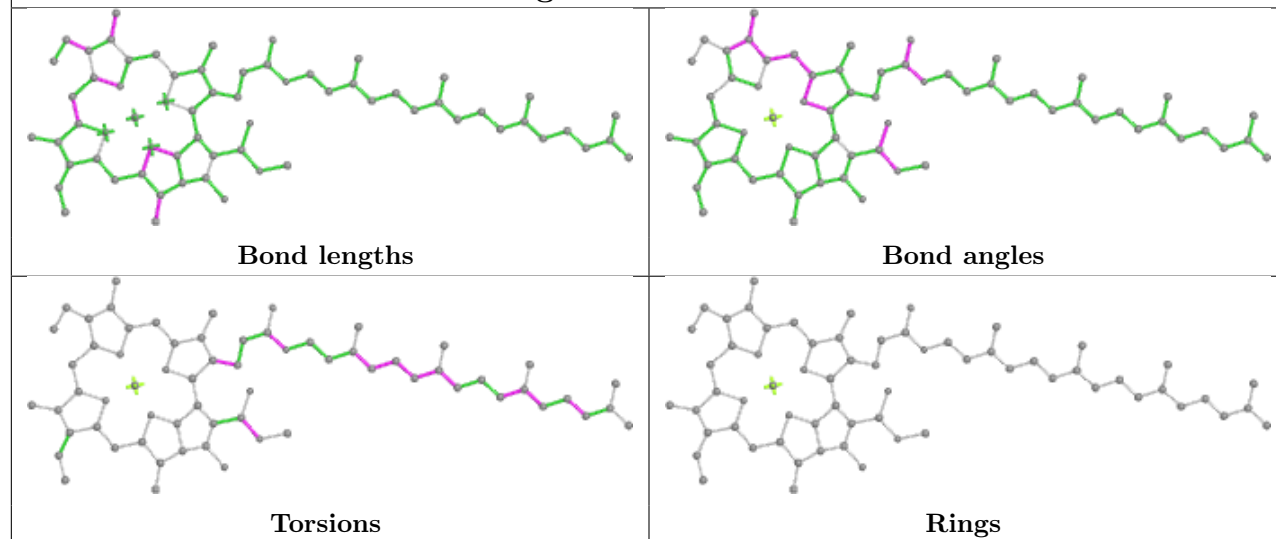
## Ligand SF4 c 101



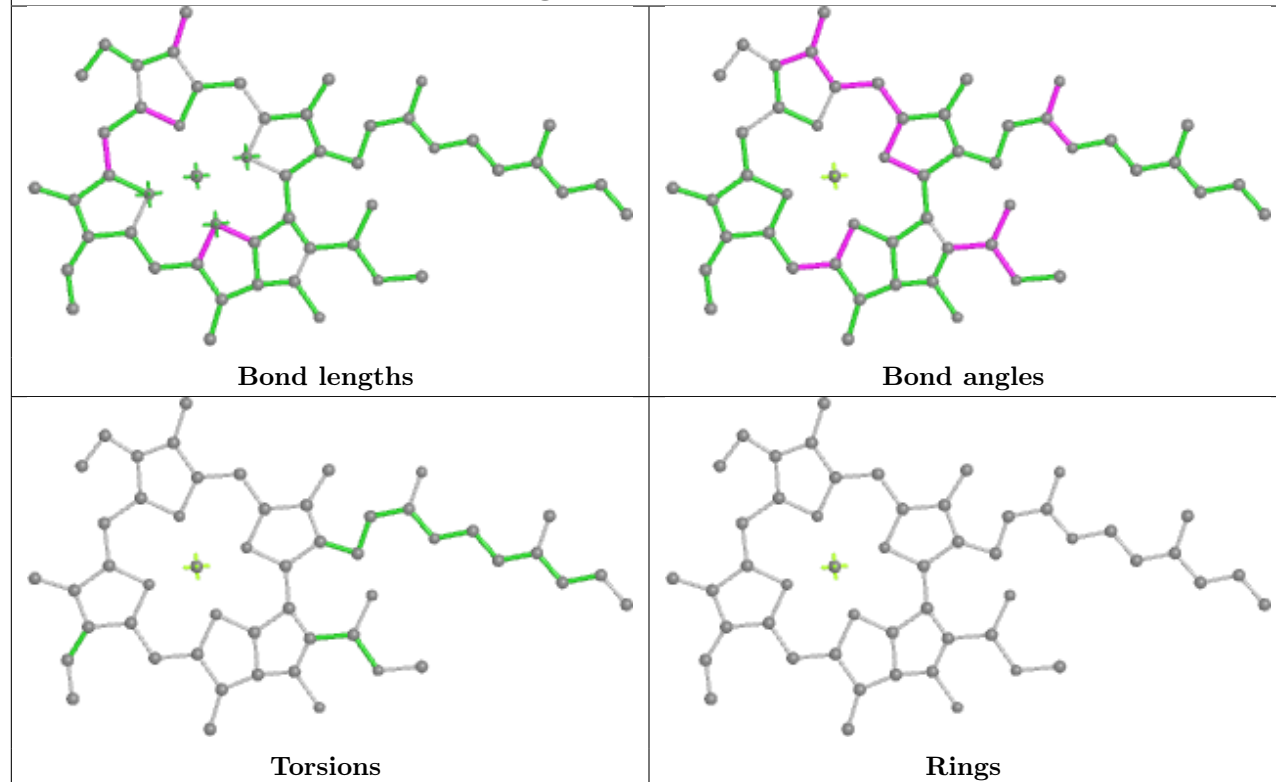
## Ligand CLA 2 306



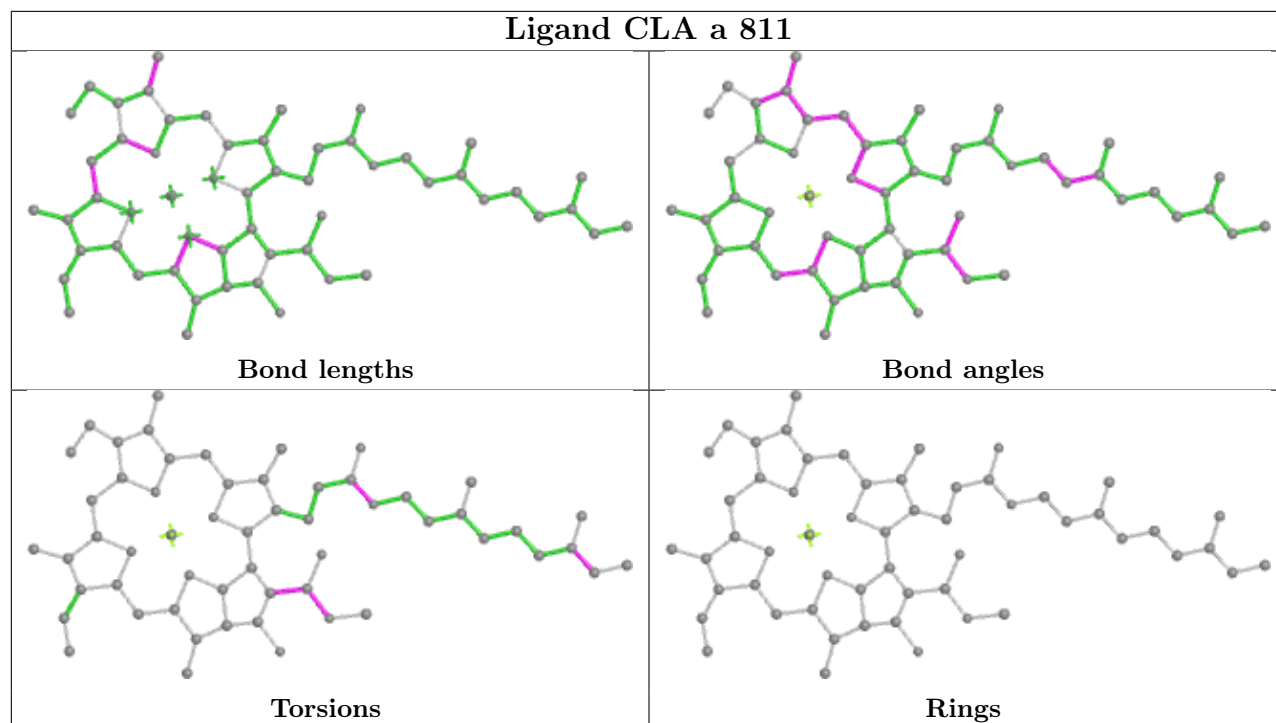
## Ligand CLA a 807



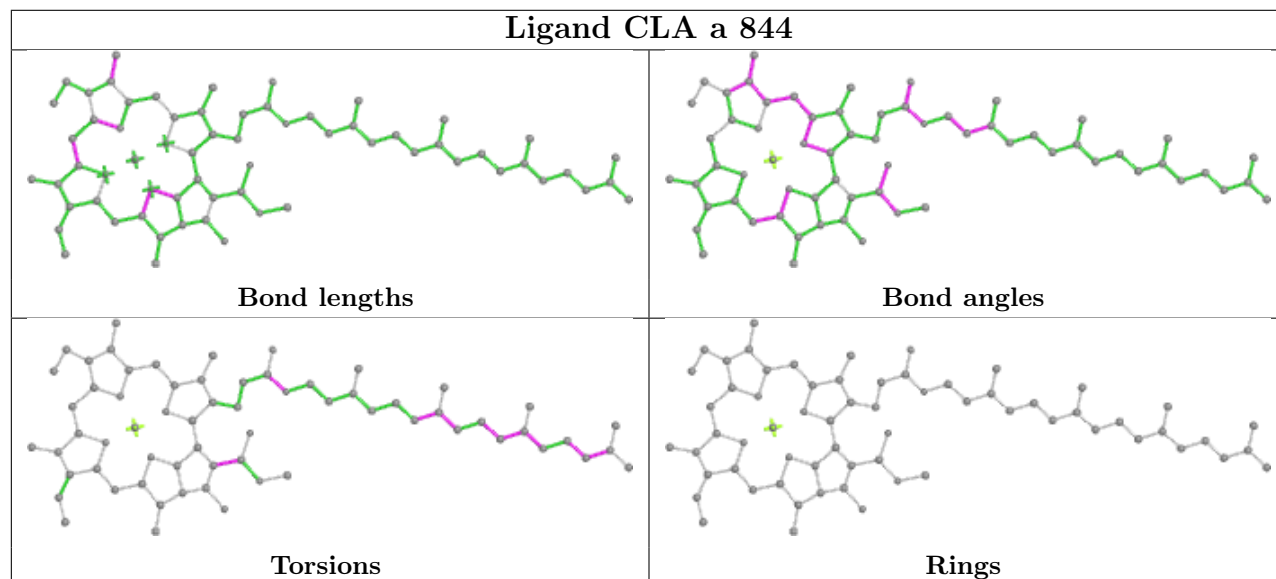
## Ligand CLA 5 312



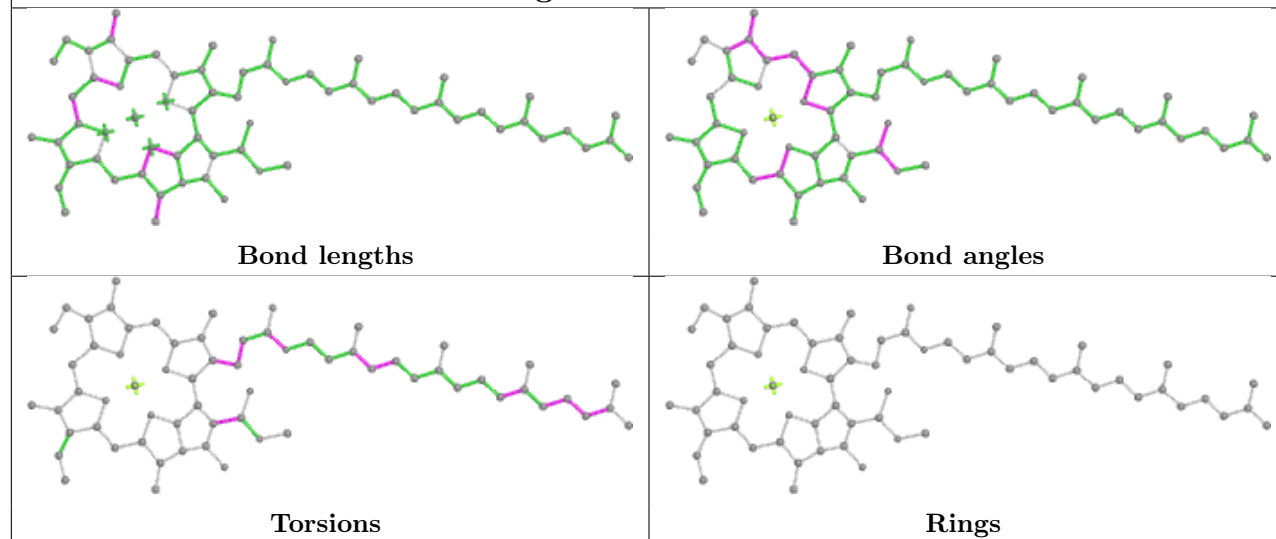
## Ligand CLA a 811



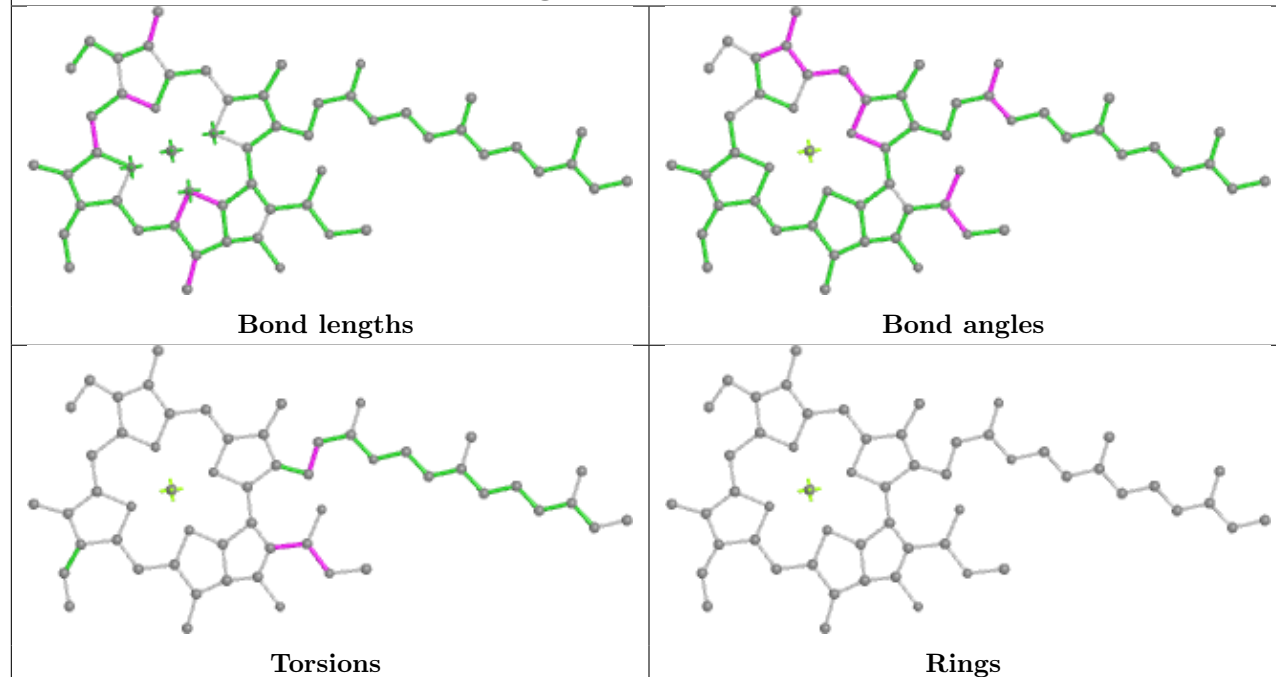
## Ligand CLA a 844



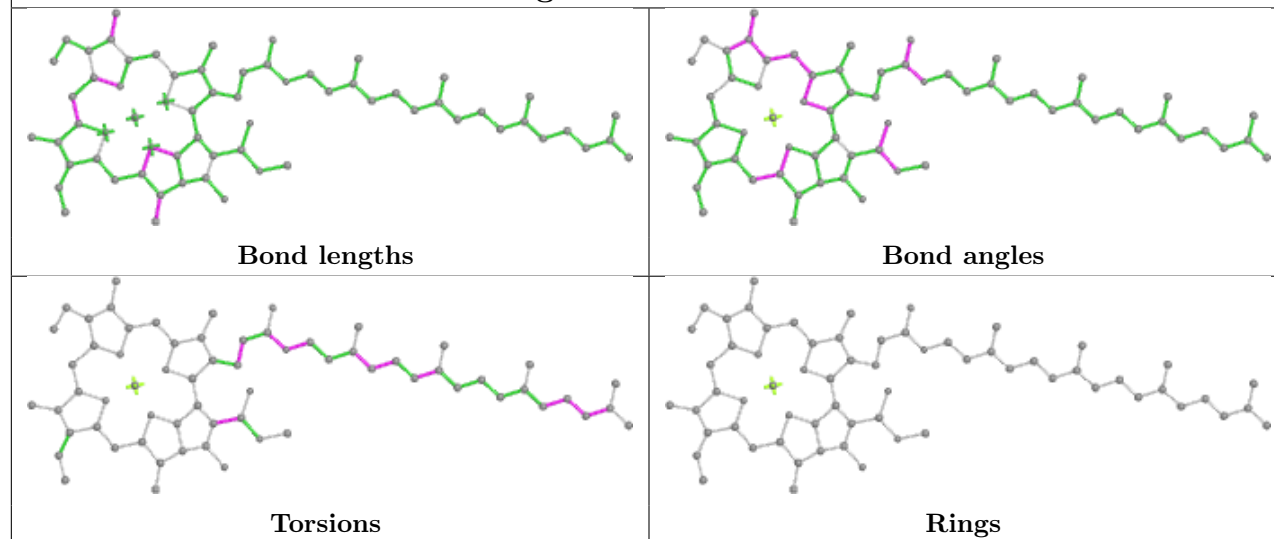
## Ligand CLA b 834



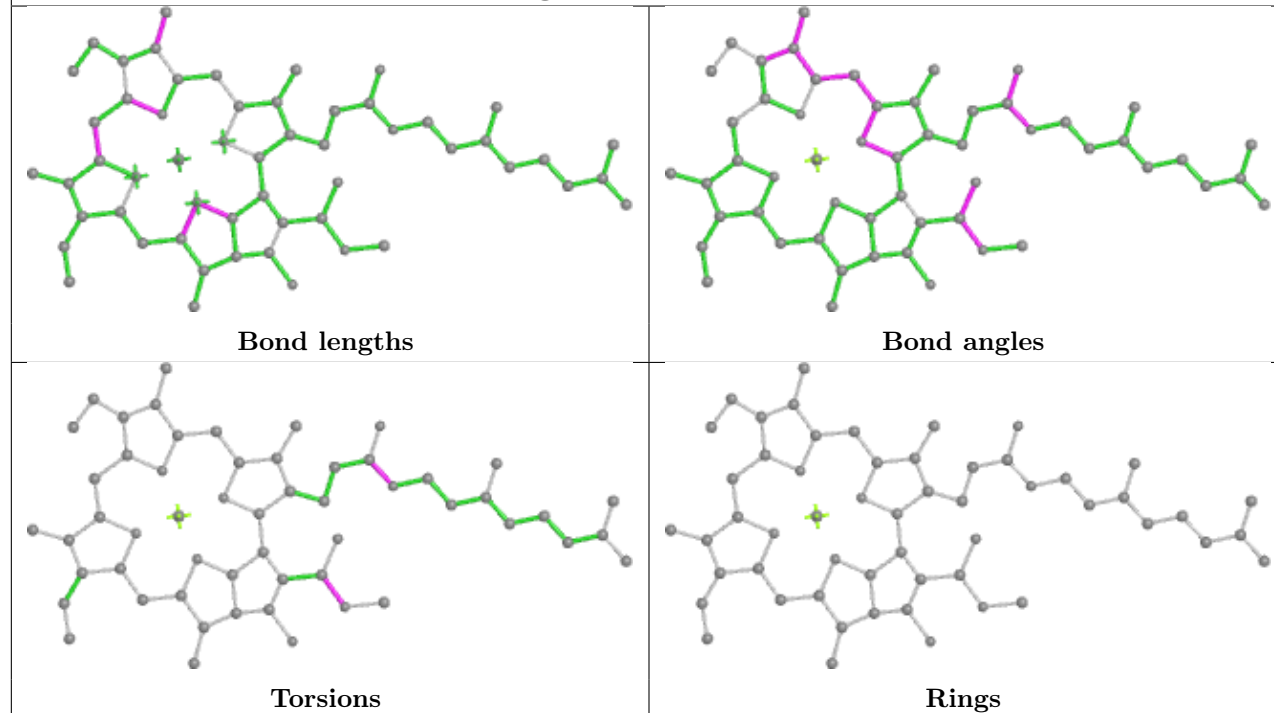
## Ligand CLA 3 309

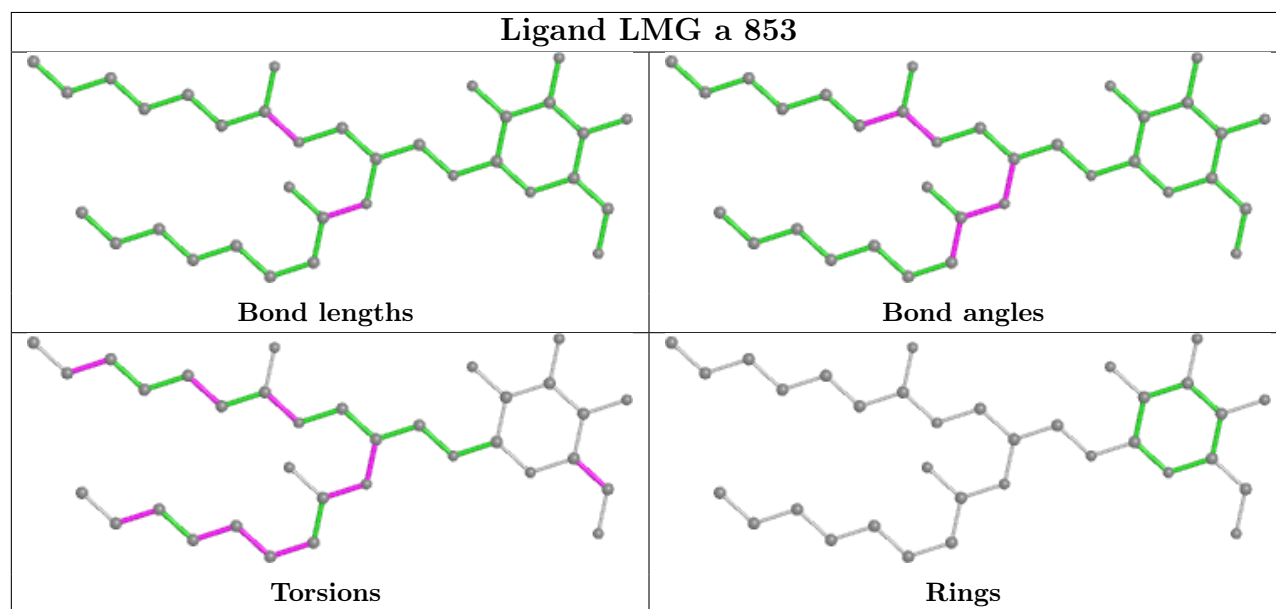
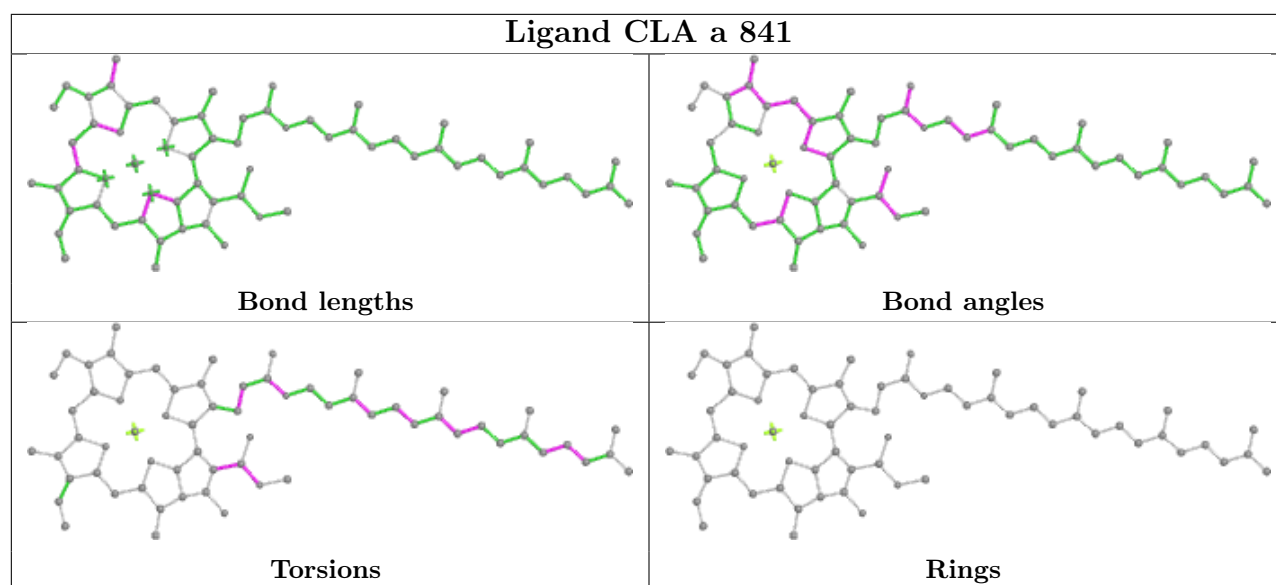


## Ligand CLA a 839



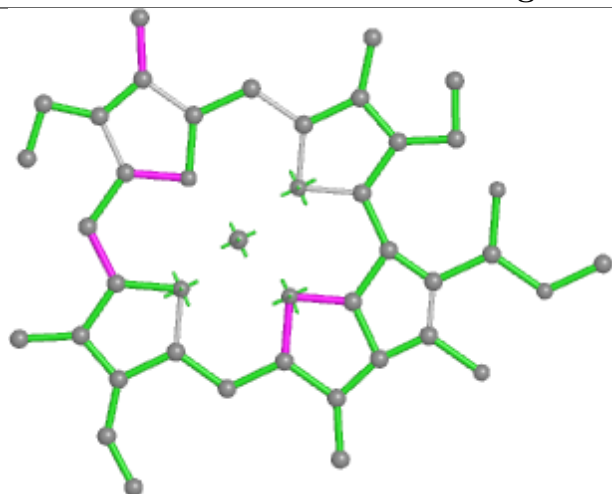
## Ligand CLA 5 308



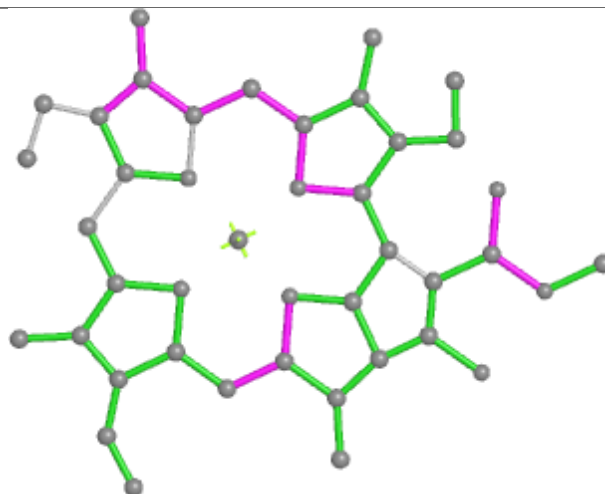




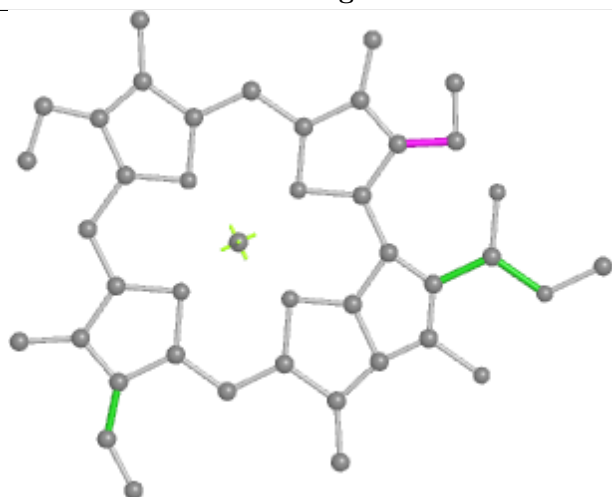
## Ligand CLA 2 315



Bond lengths



Bond angles

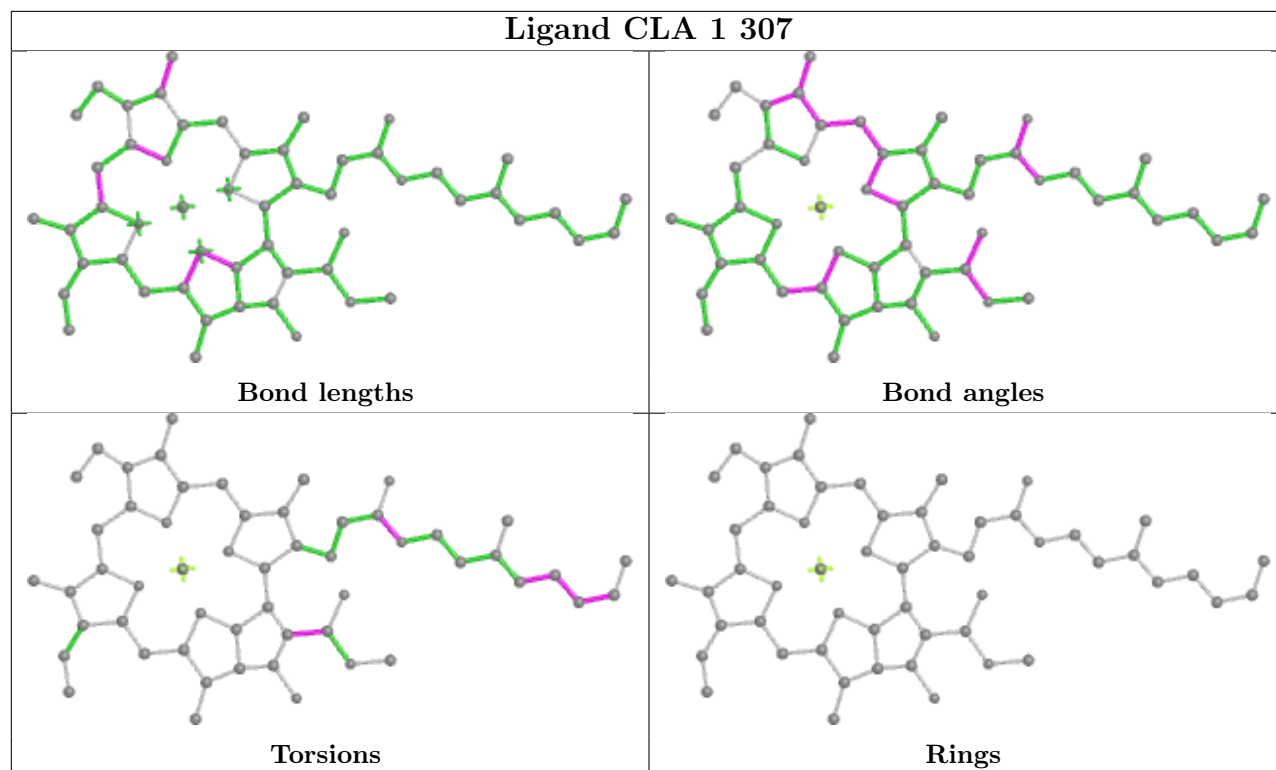


Torsions

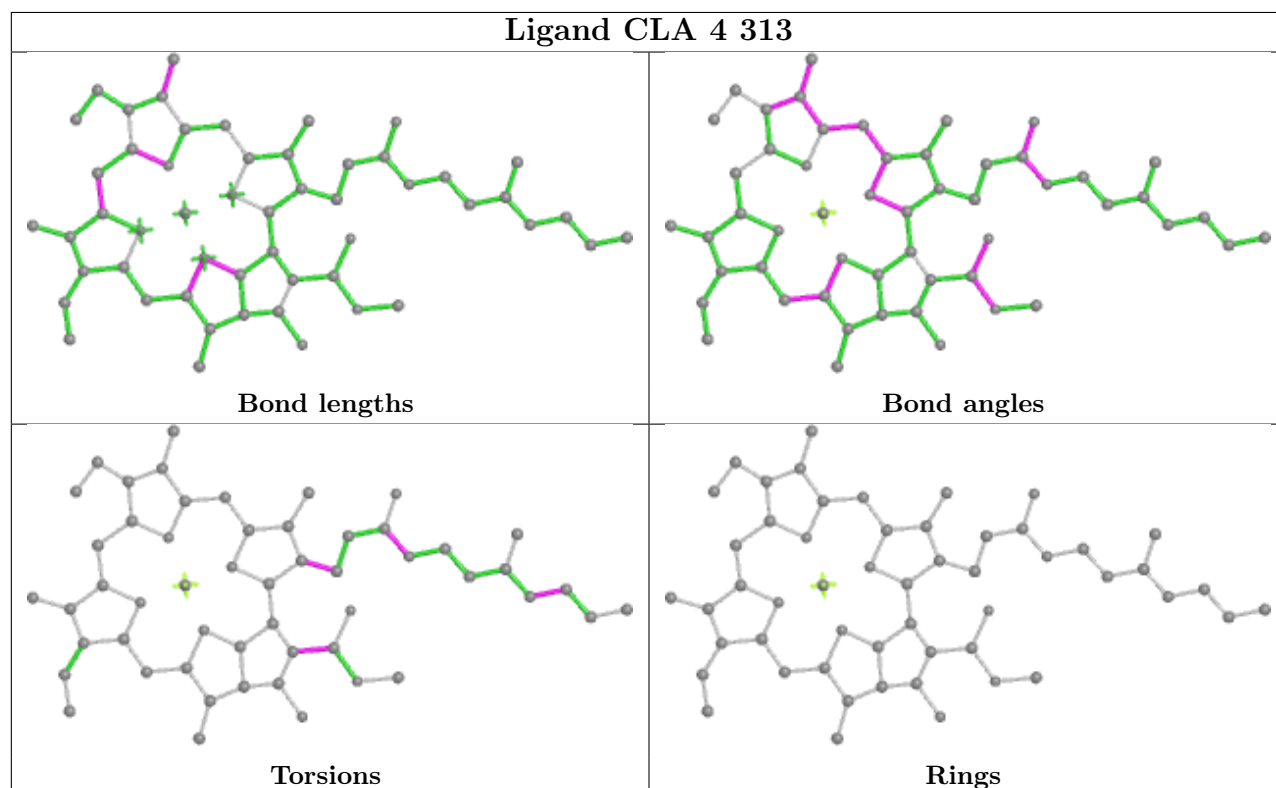


Rings

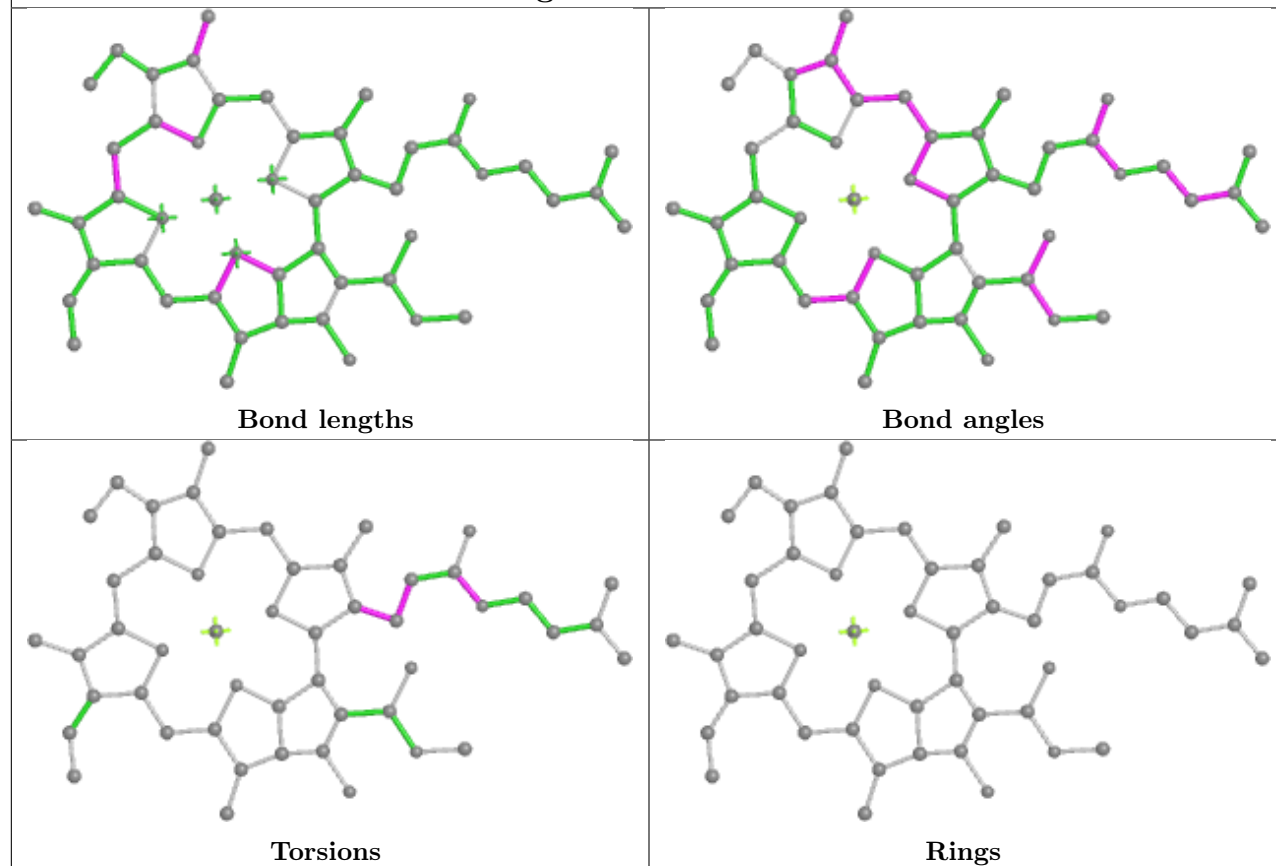
## Ligand CLA 1 307



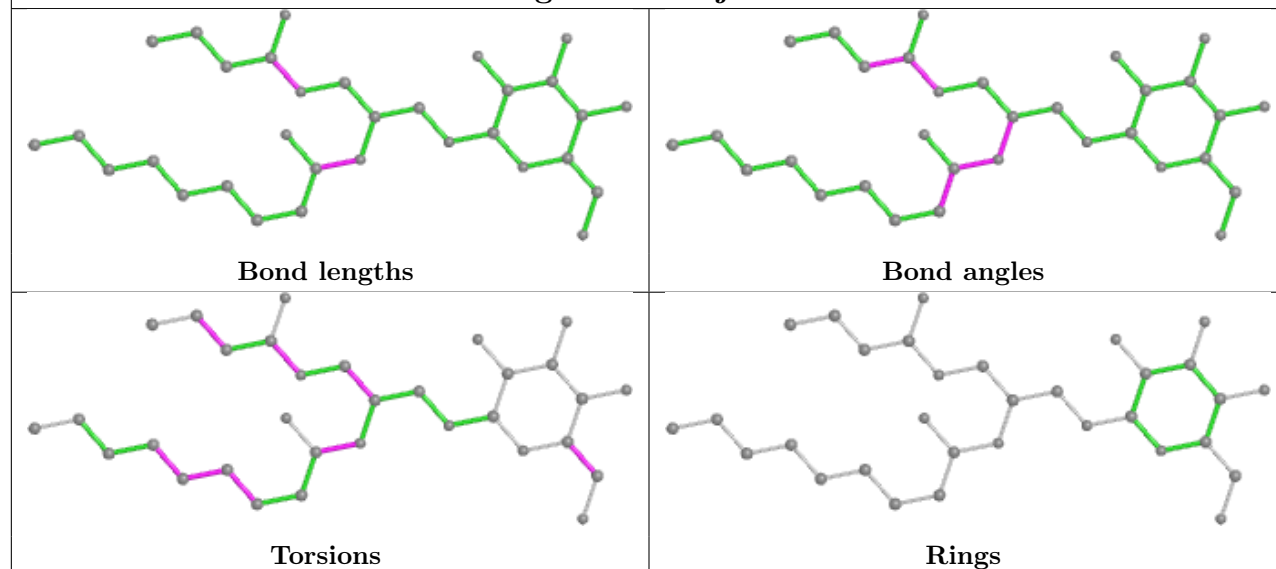
## Ligand CLA 4 313



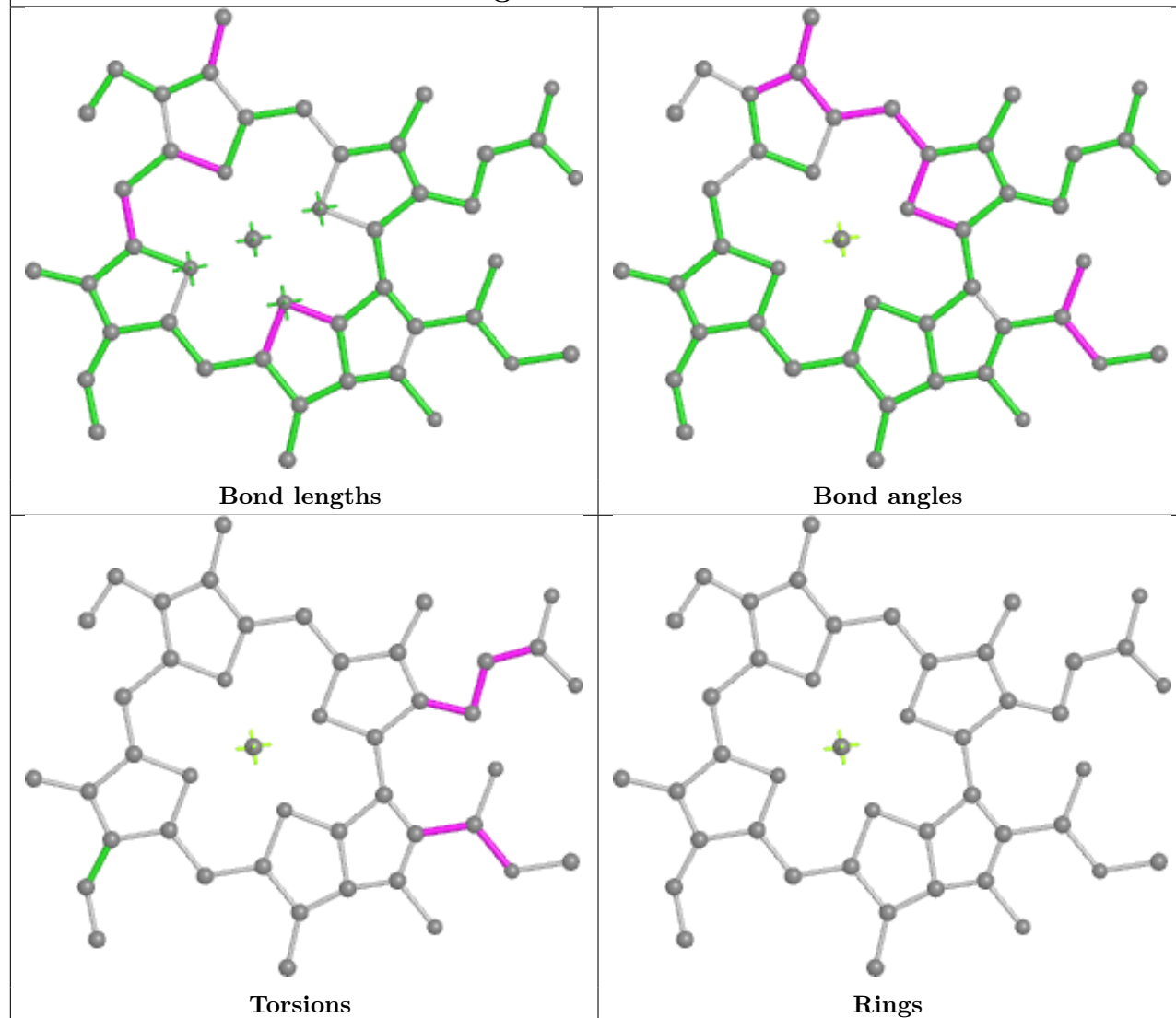
## Ligand CLA 3 311



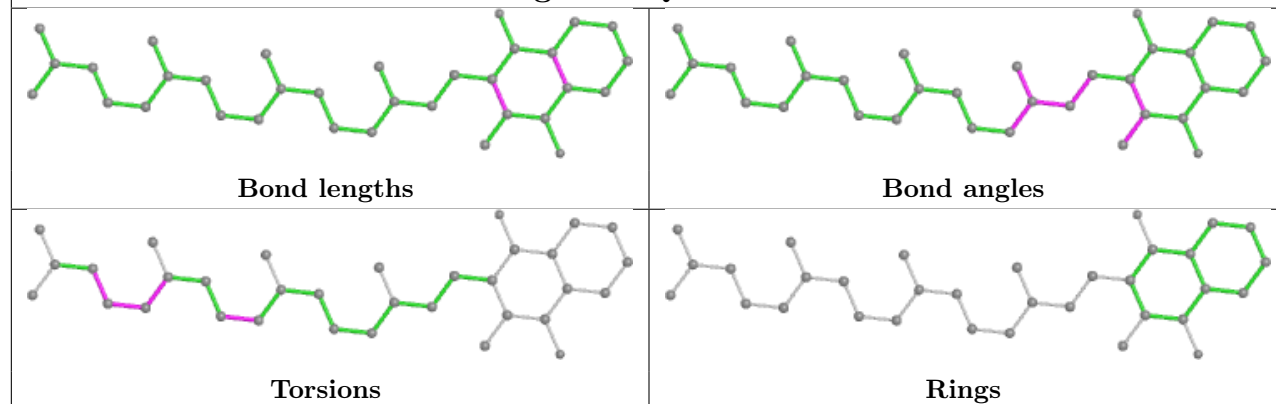
## Ligand LMG j 105

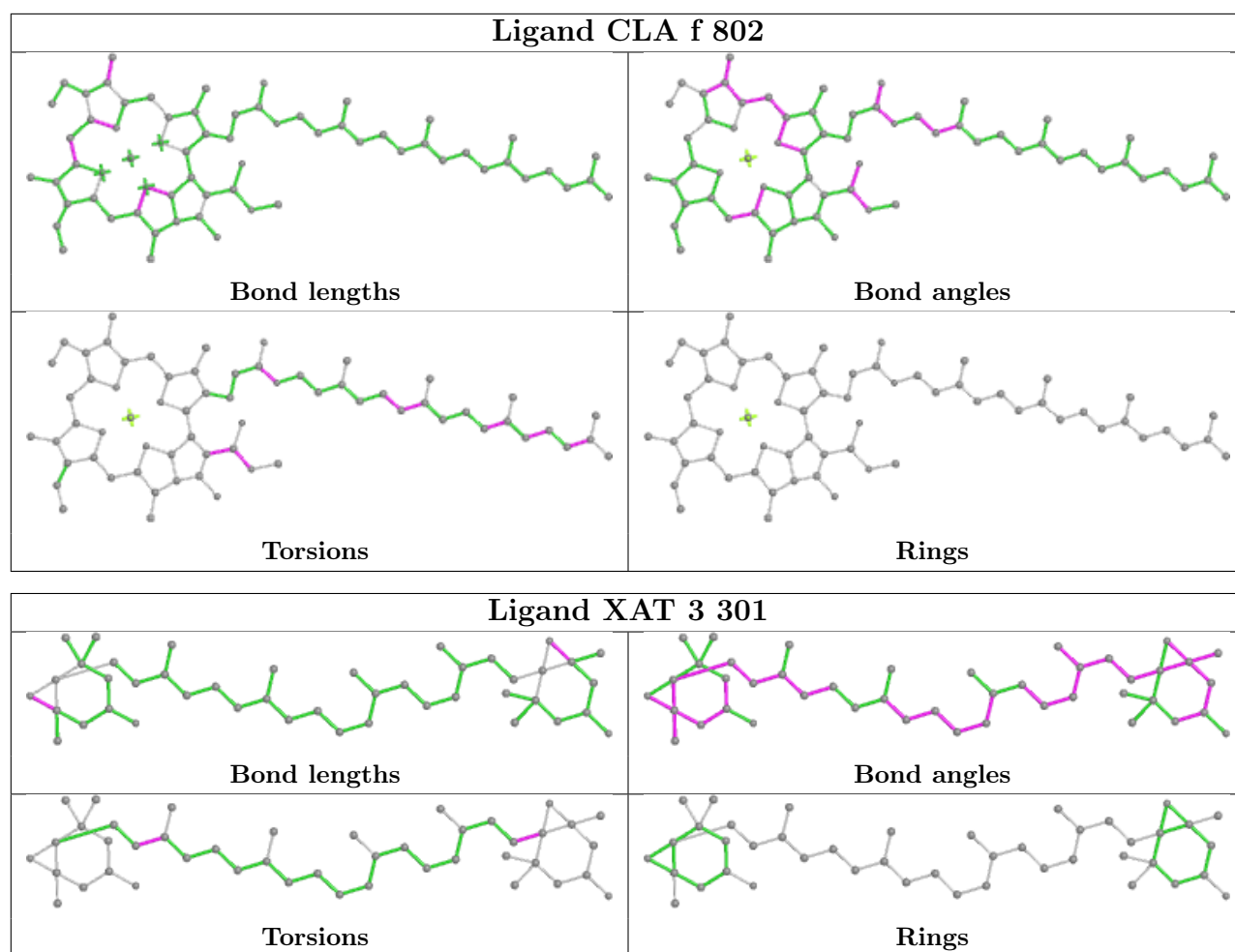


## Ligand CLA 5 306

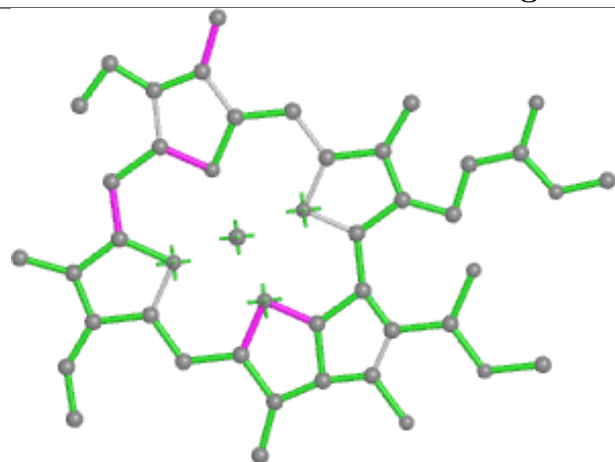


## Ligand PQN a 843

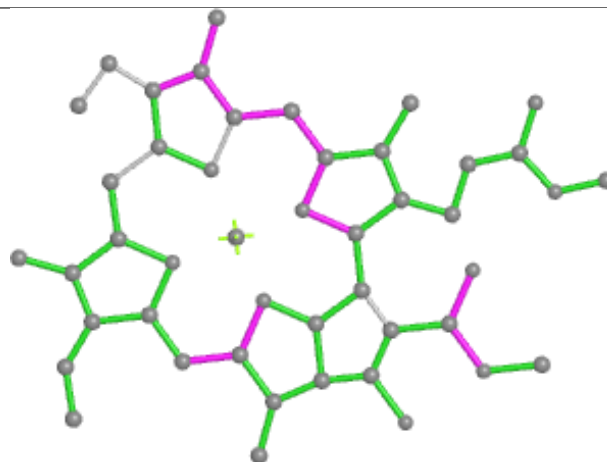




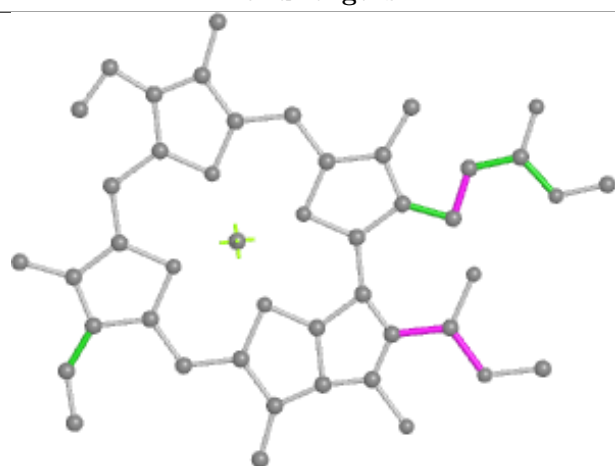
## Ligand CLA 2 309



Bond lengths



Bond angles

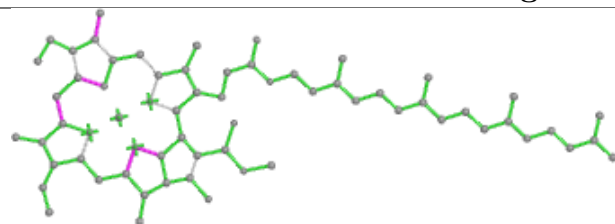


Torsions

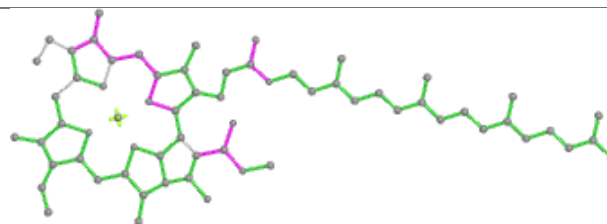


Rings

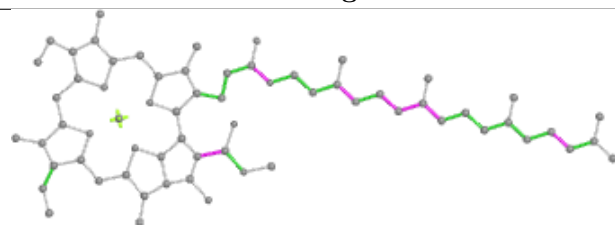
## Ligand CLA a 831



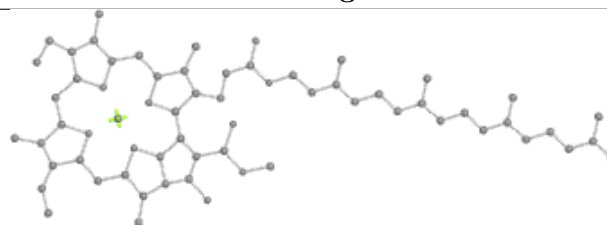
Bond lengths



Bond angles

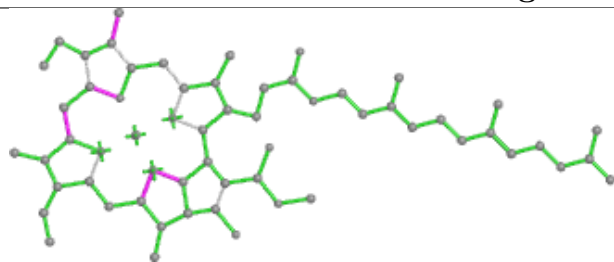


Torsions

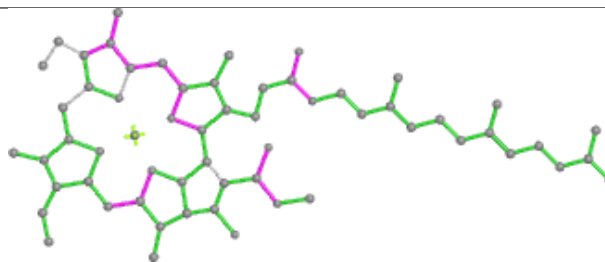


Rings

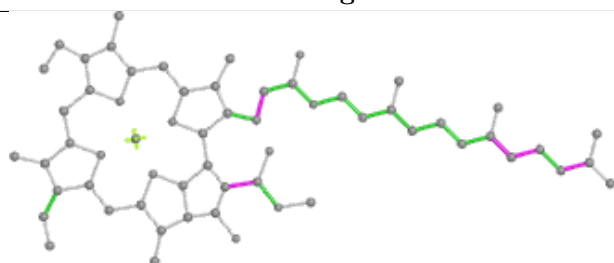
## Ligand CLA 5 307



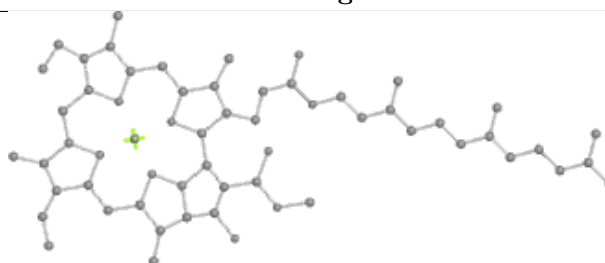
Bond lengths



Bond angles

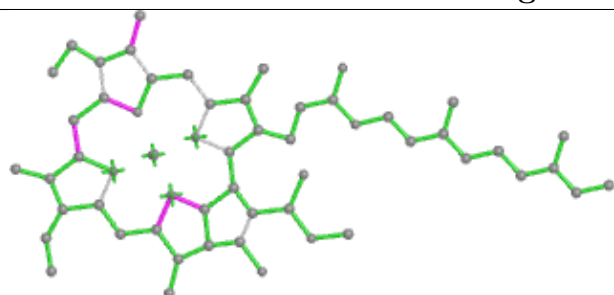


Torsions

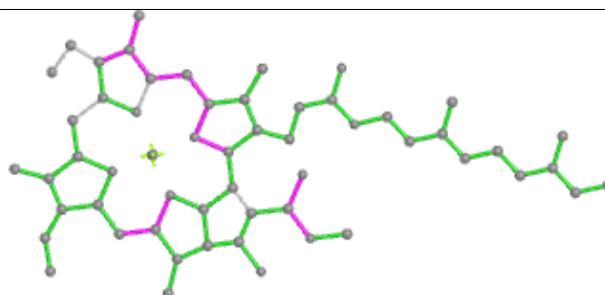


Rings

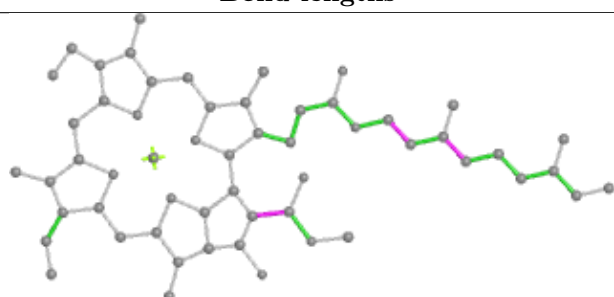
## Ligand CLA 3 310



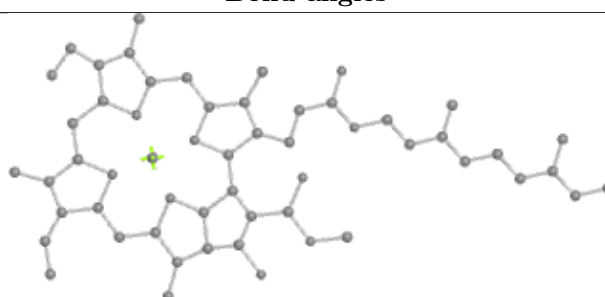
Bond lengths



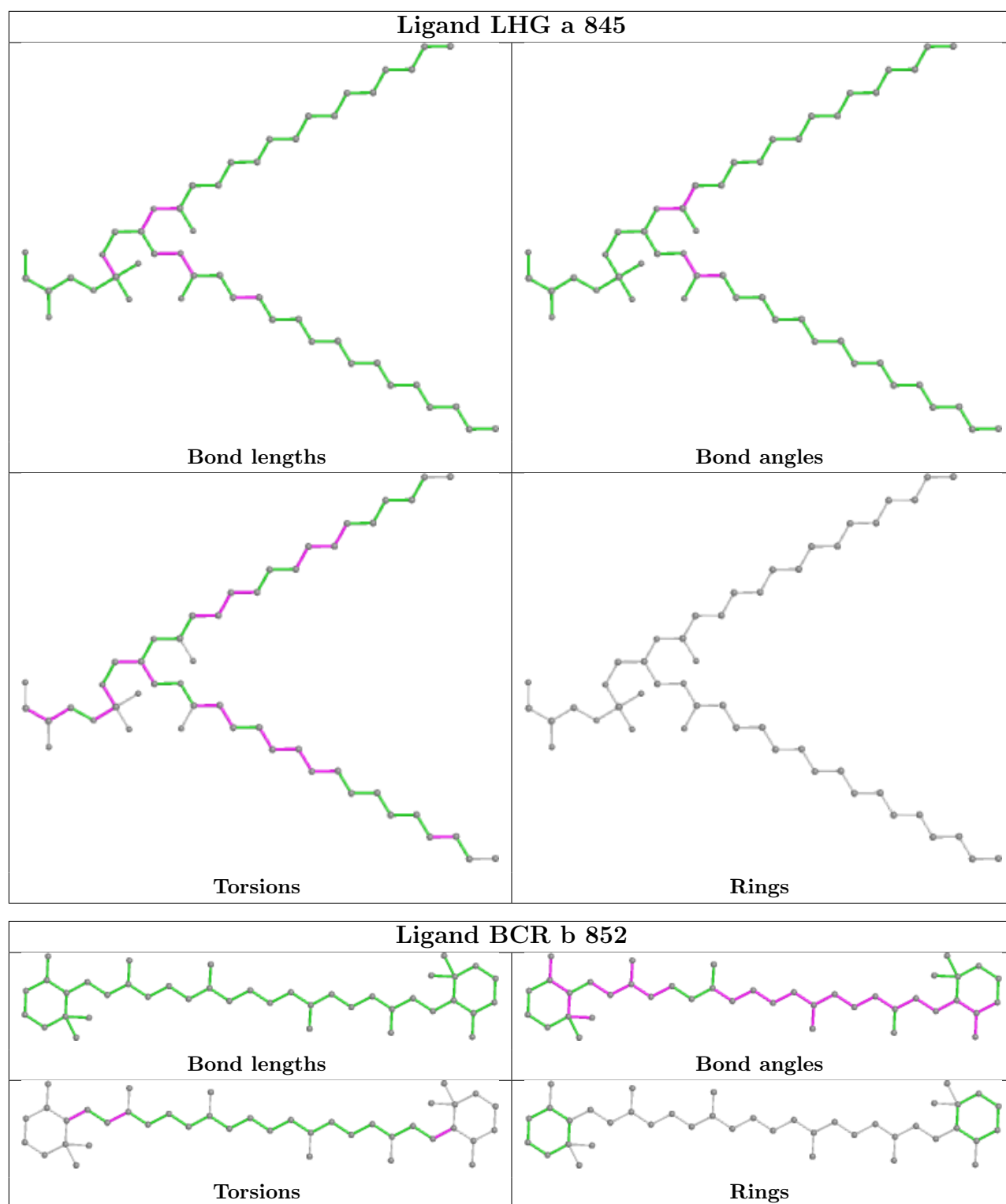
Bond angles



Torsions

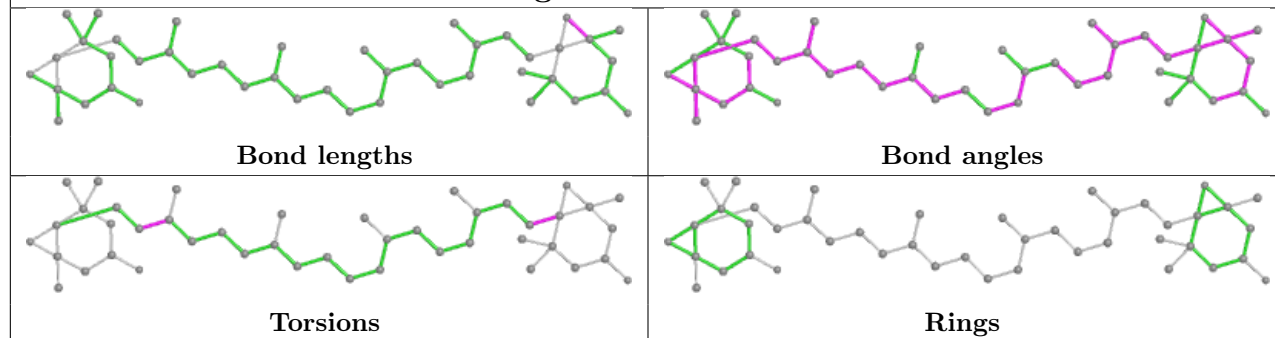


Rings

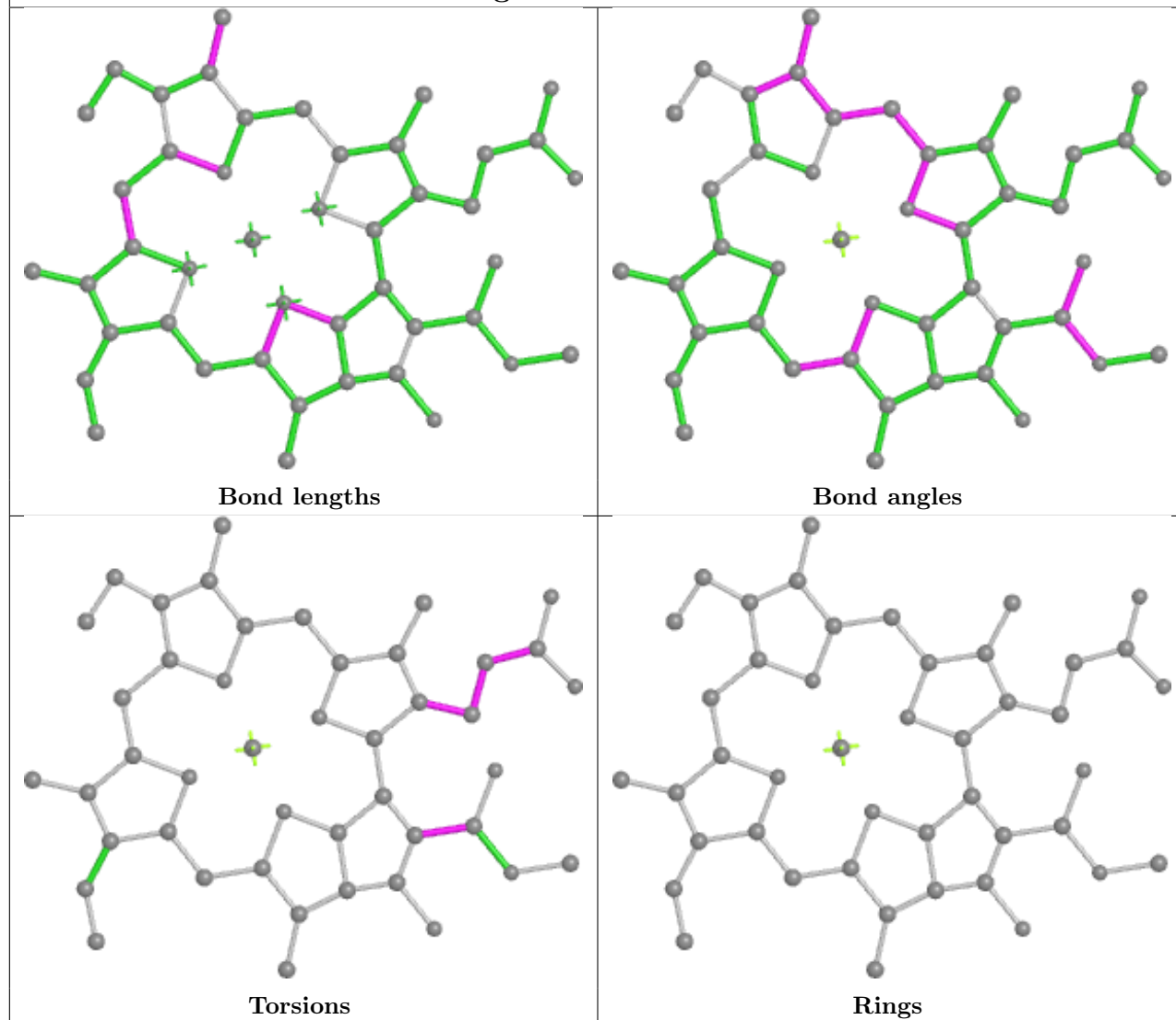


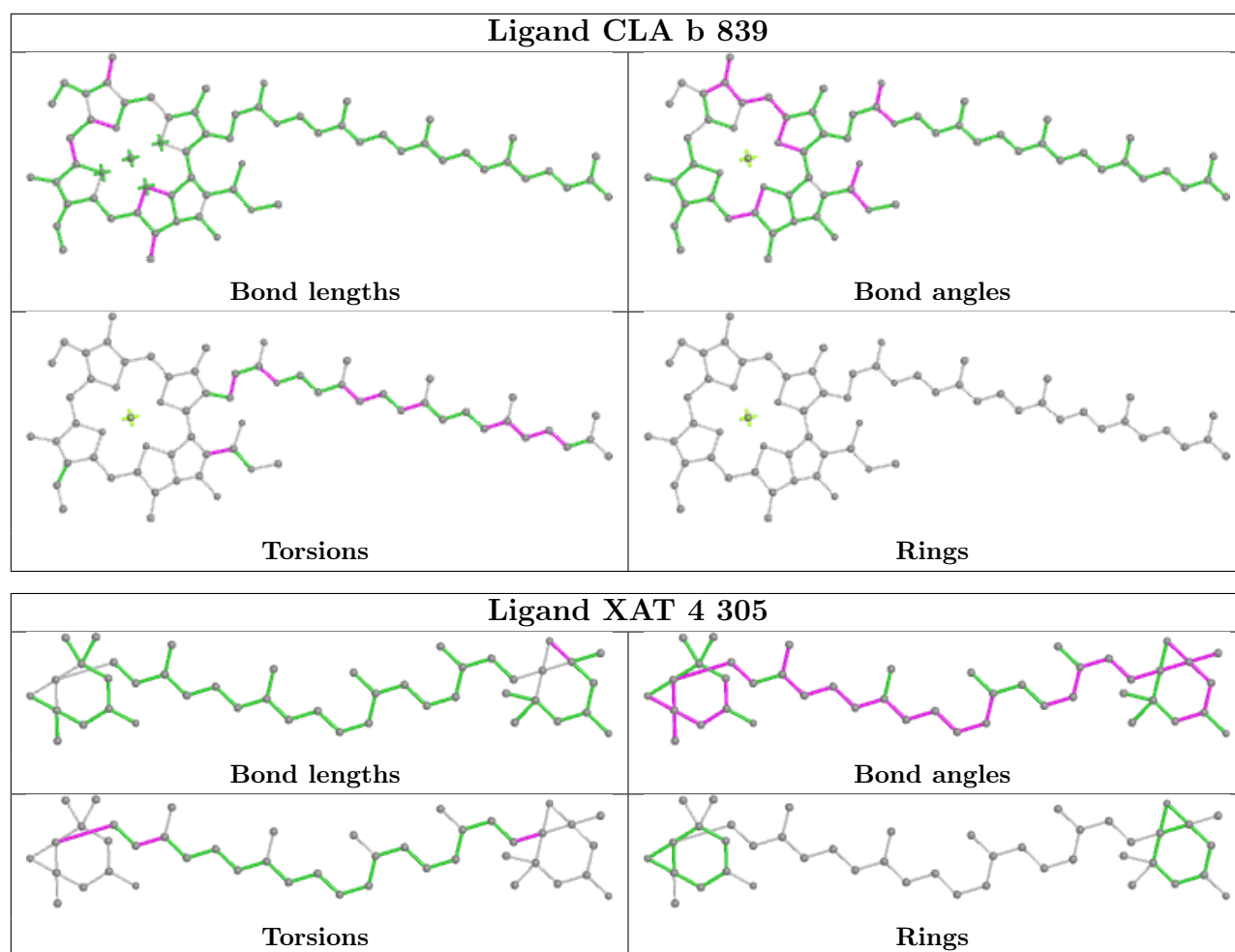


## Ligand XAT 2 301

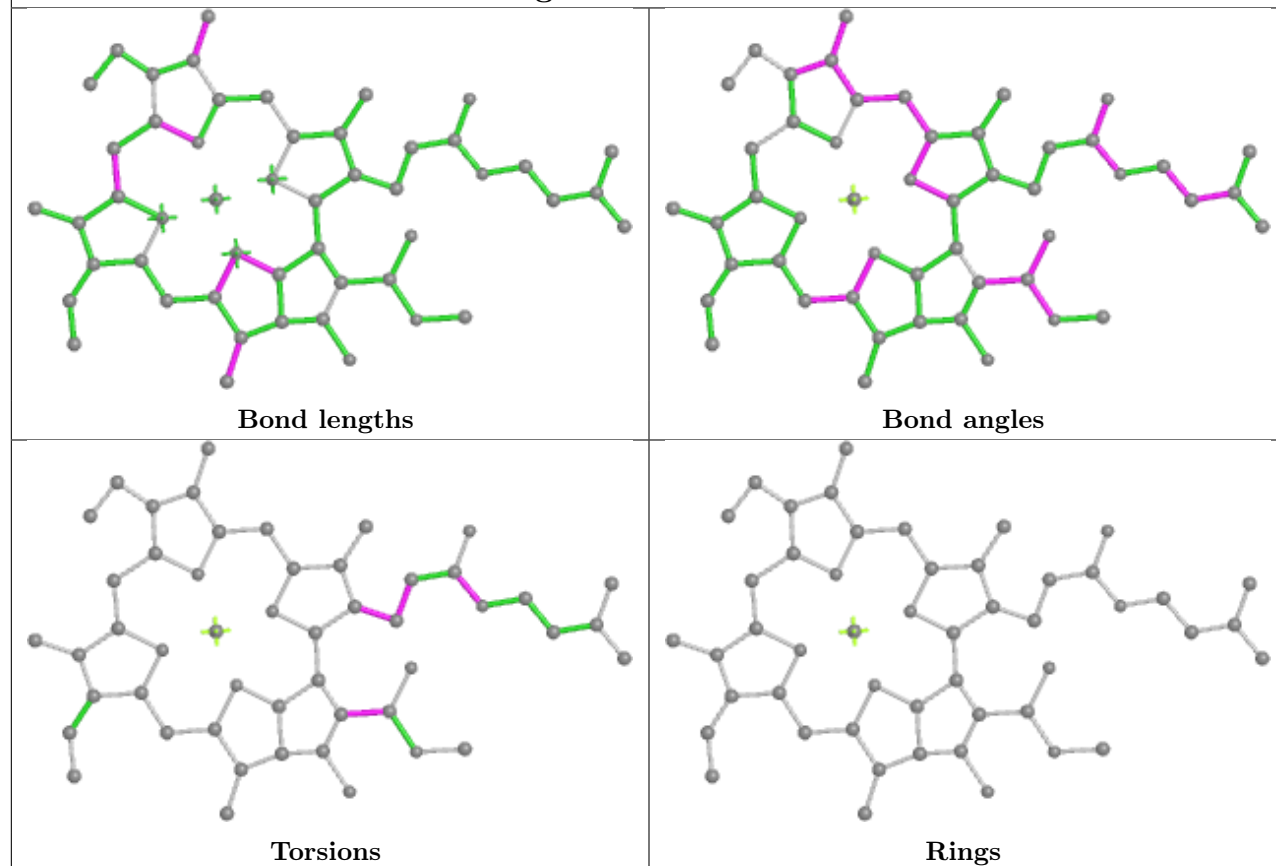


## Ligand CLA a 817

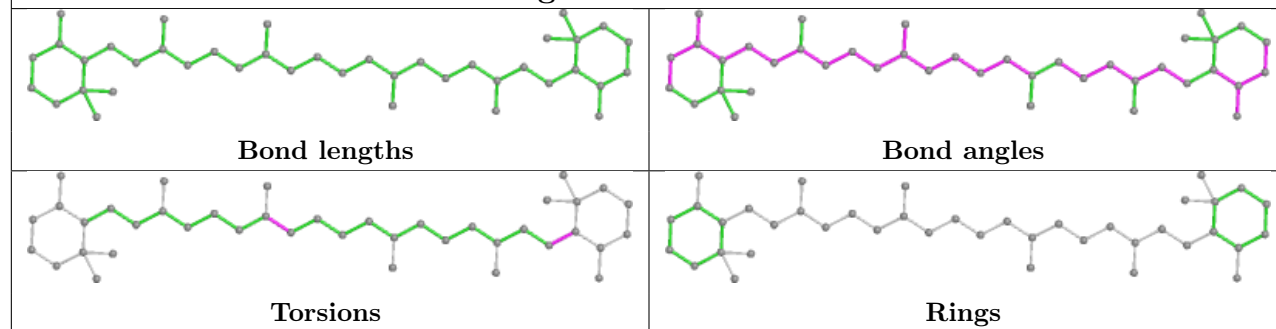




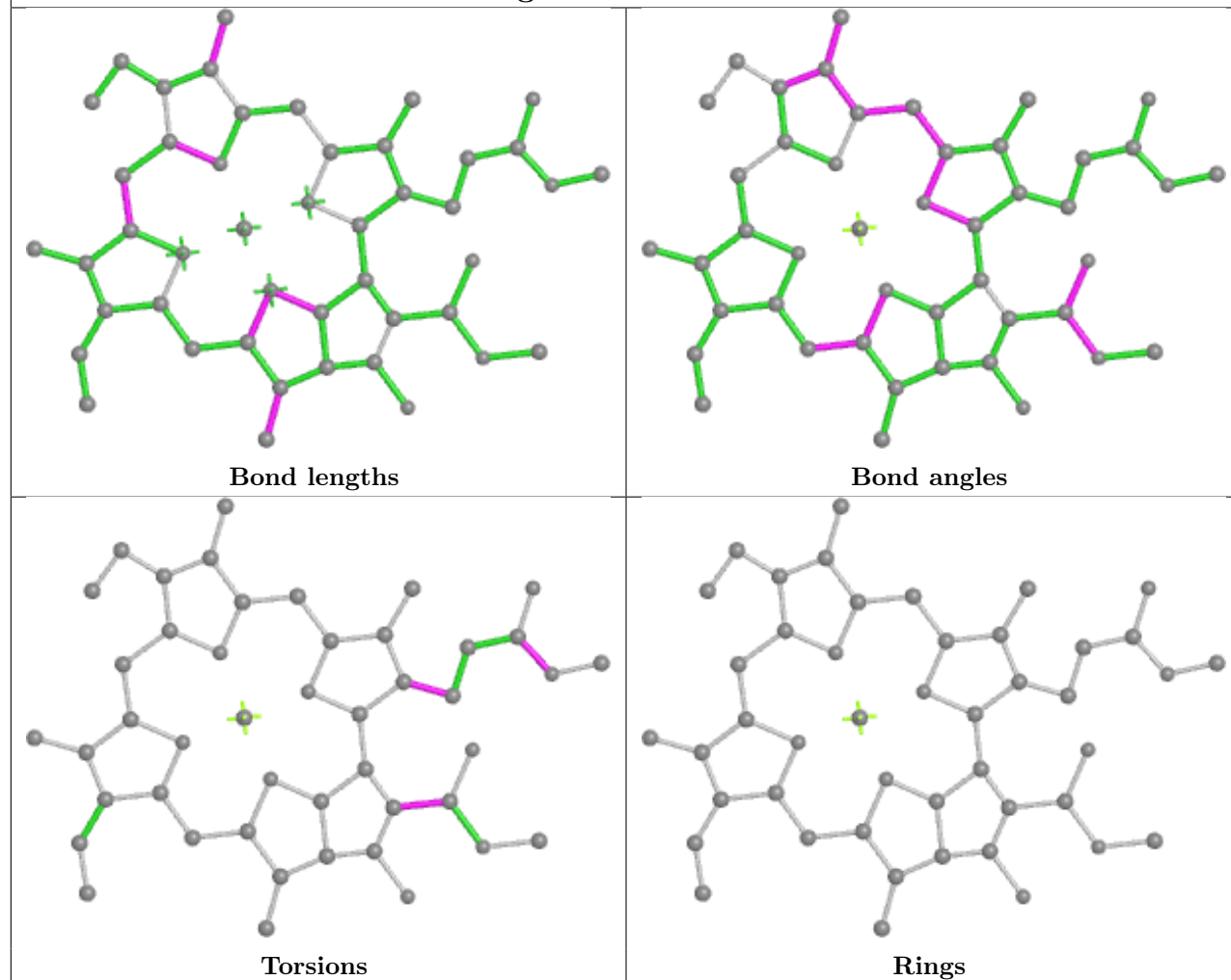
## Ligand CLA b 821



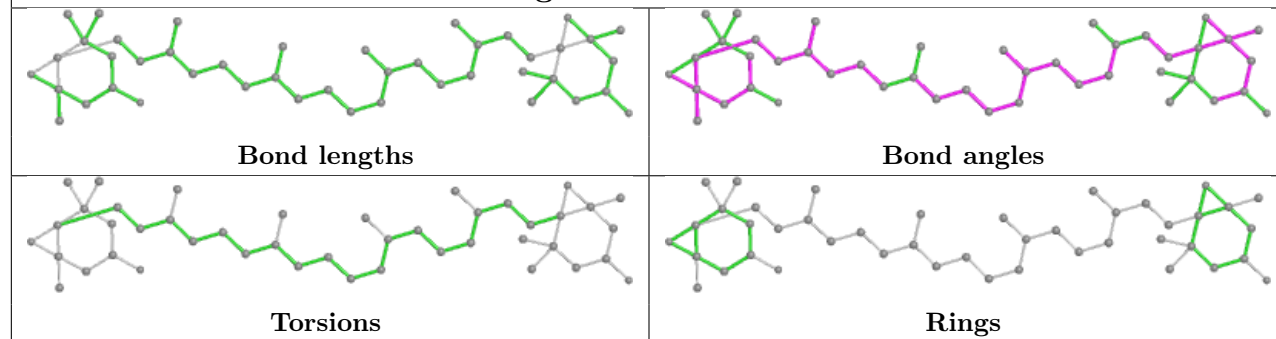
## Ligand BCR f 804

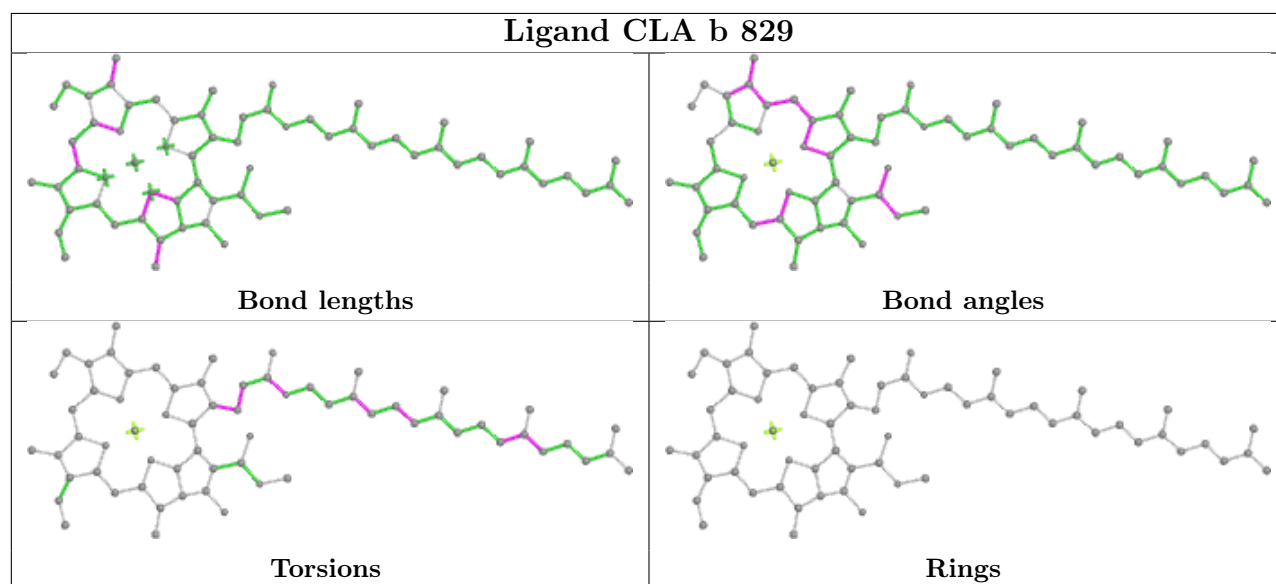
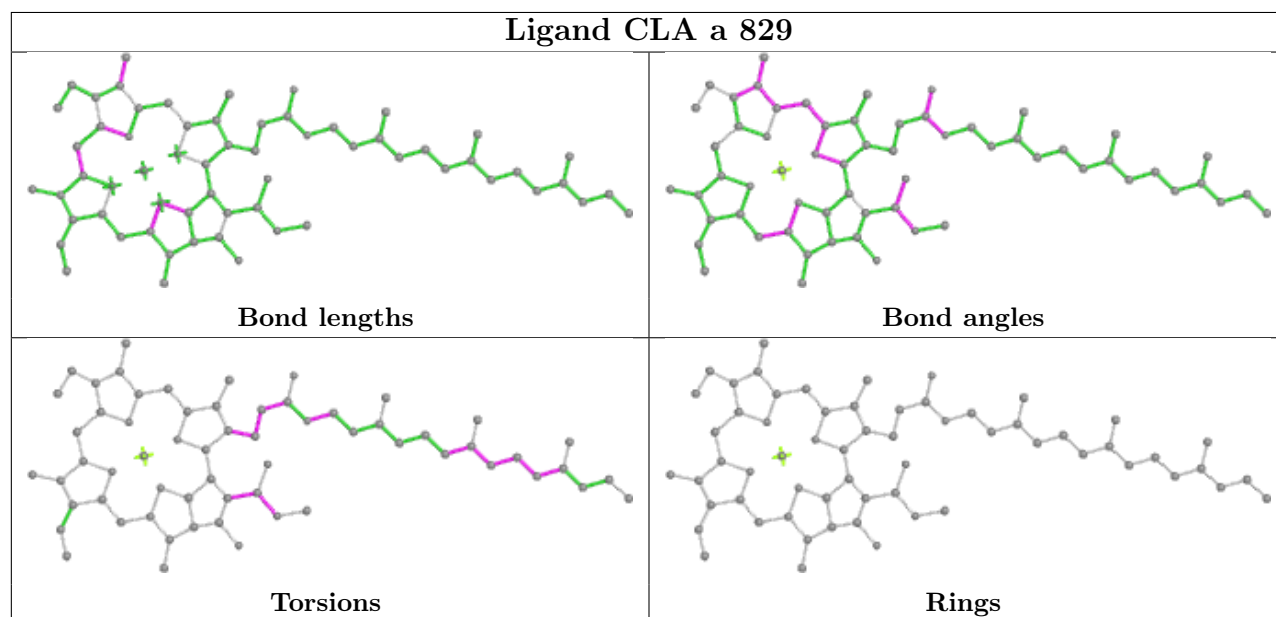
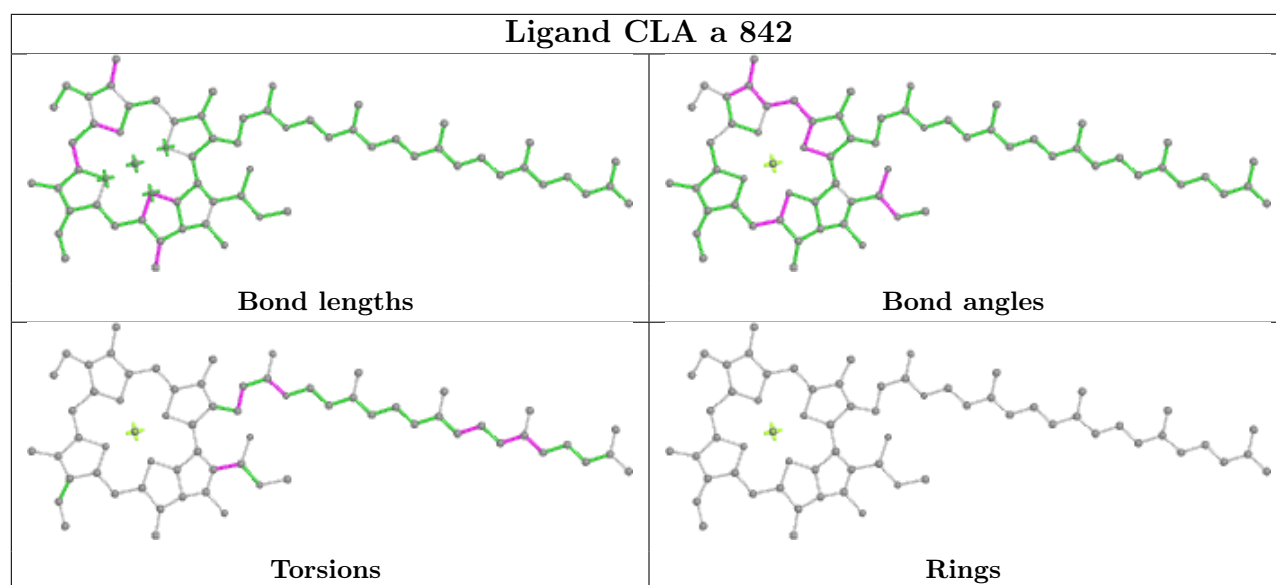


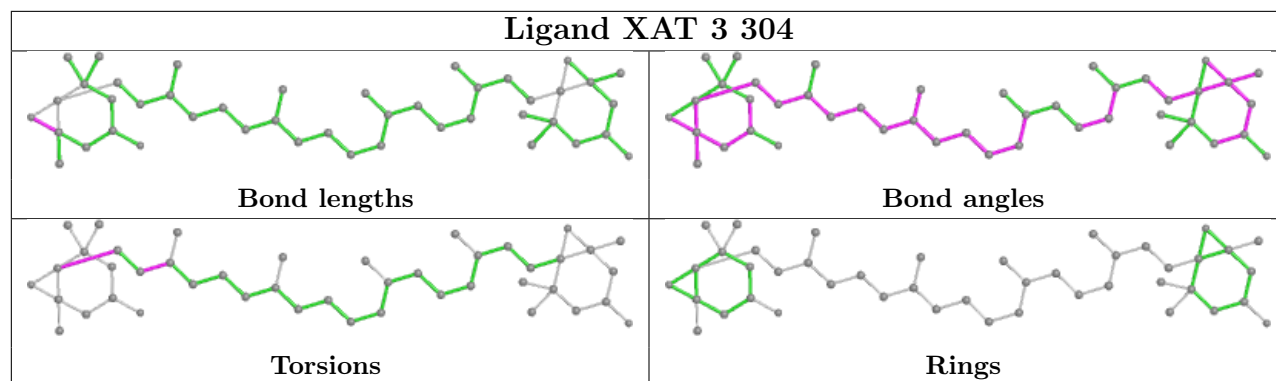
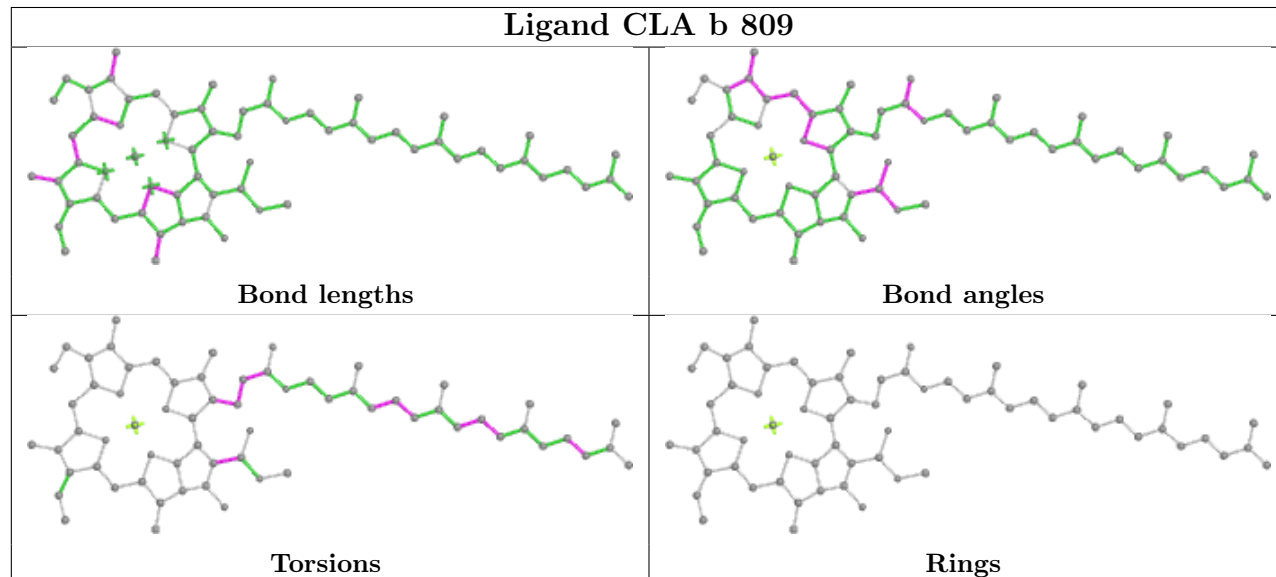
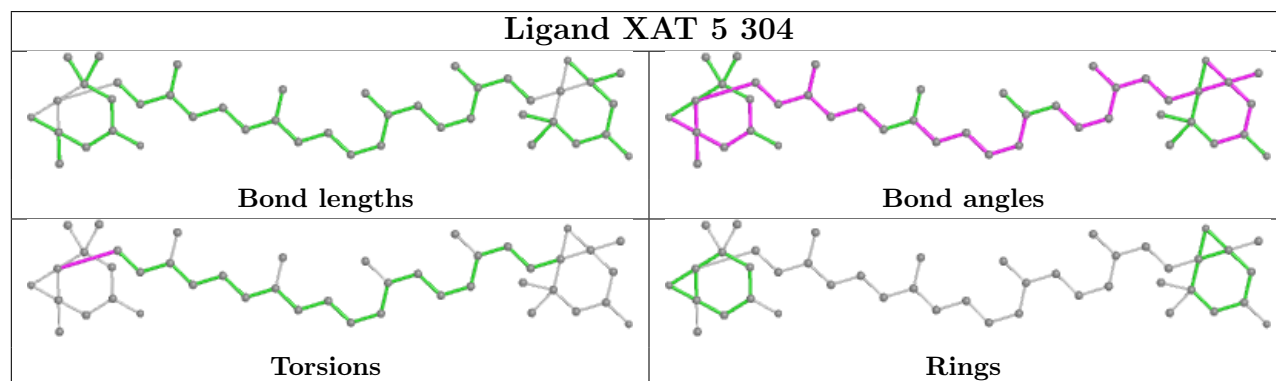
## Ligand CLA a 824

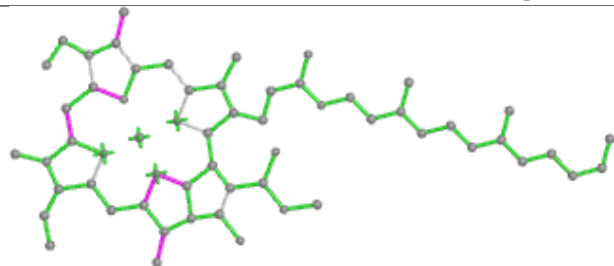


## Ligand XAT 4 302

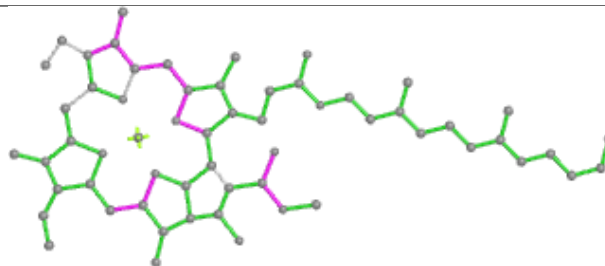




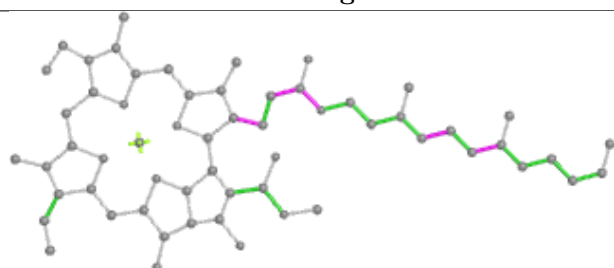
**Ligand XAT 3 304****Ligand CLA b 809****Ligand XAT 5 304**

**Ligand CLA 3 312**

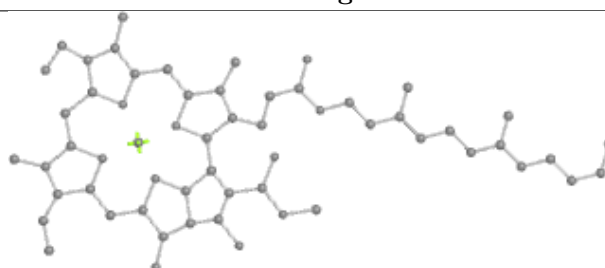
Bond lengths



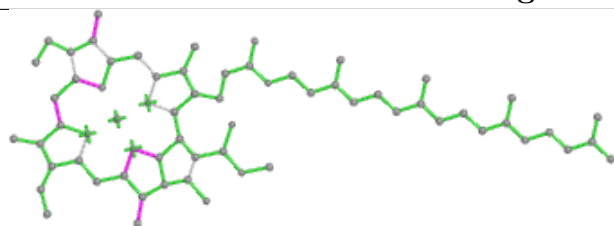
Bond angles



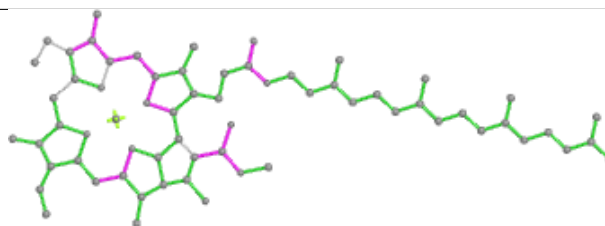
Torsions



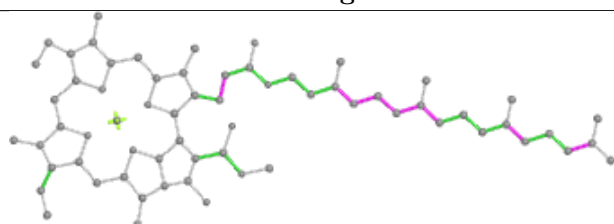
Rings

**Ligand CLA b 808**

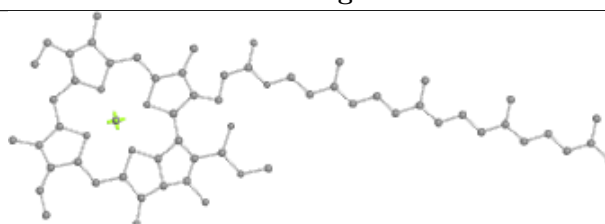
Bond lengths



Bond angles

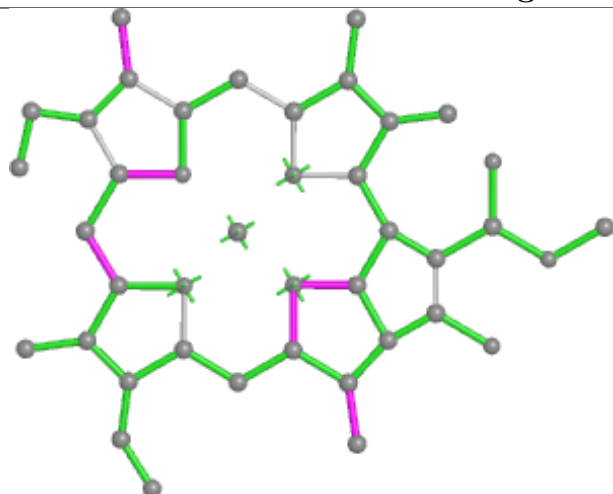


Torsions

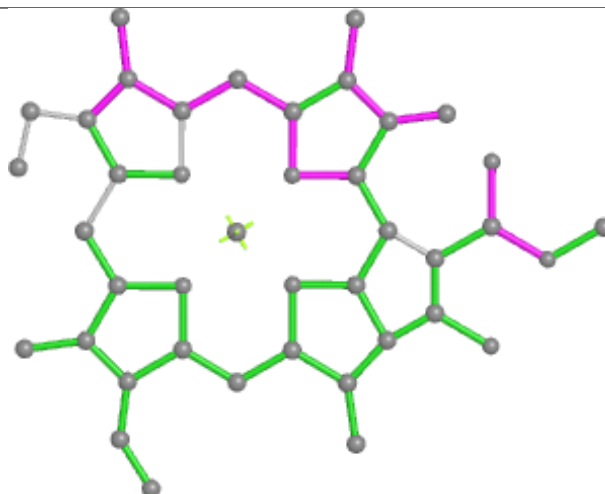


Rings

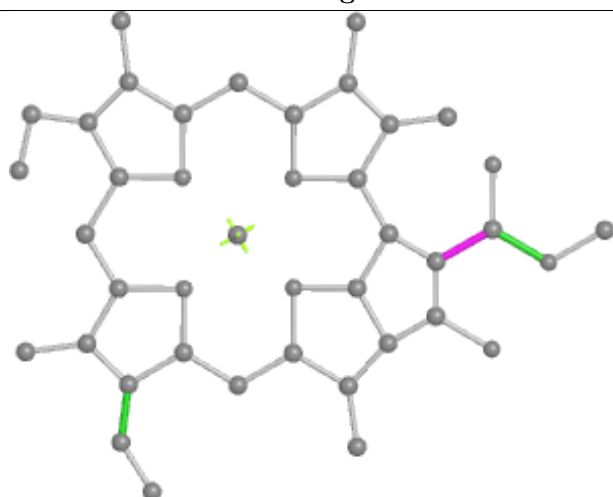
## Ligand CLA b 831



Bond lengths



Bond angles

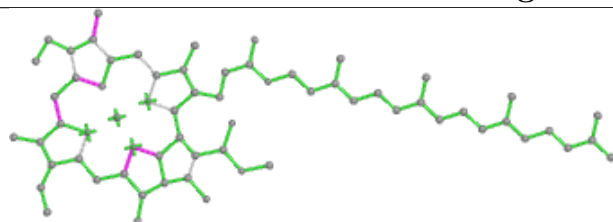


Torsions

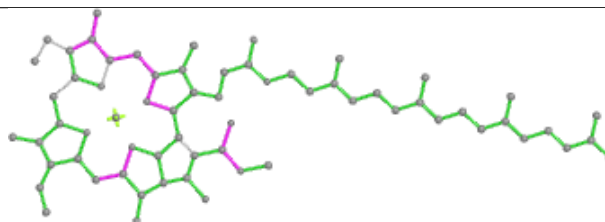


Rings

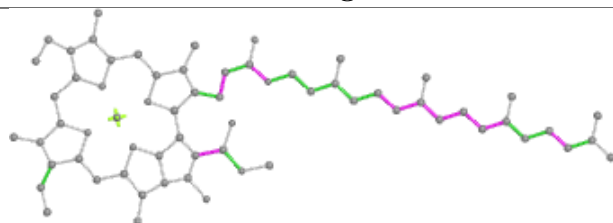
## Ligand CLA b 825



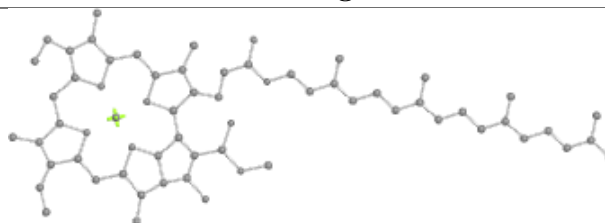
Bond lengths



Bond angles

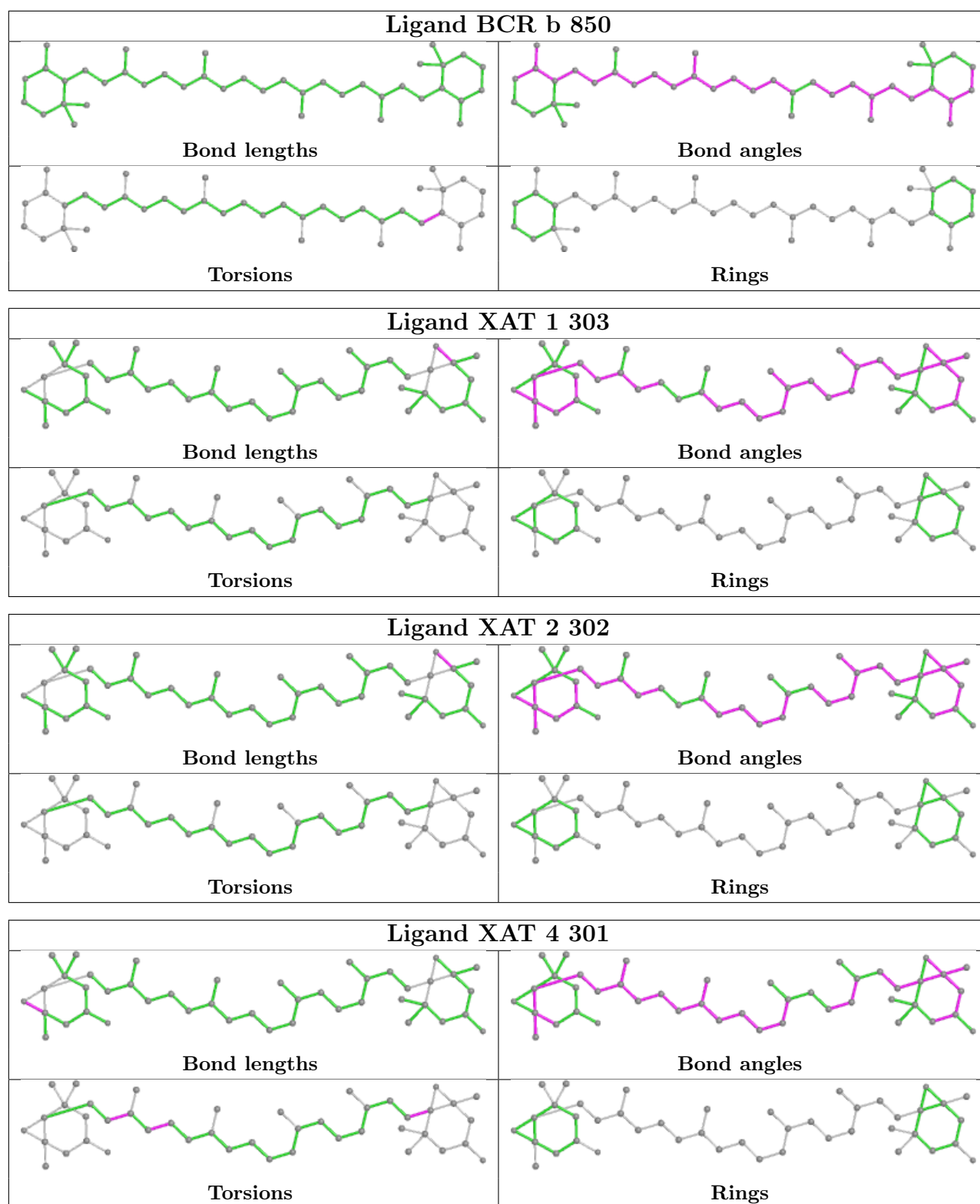


Torsions

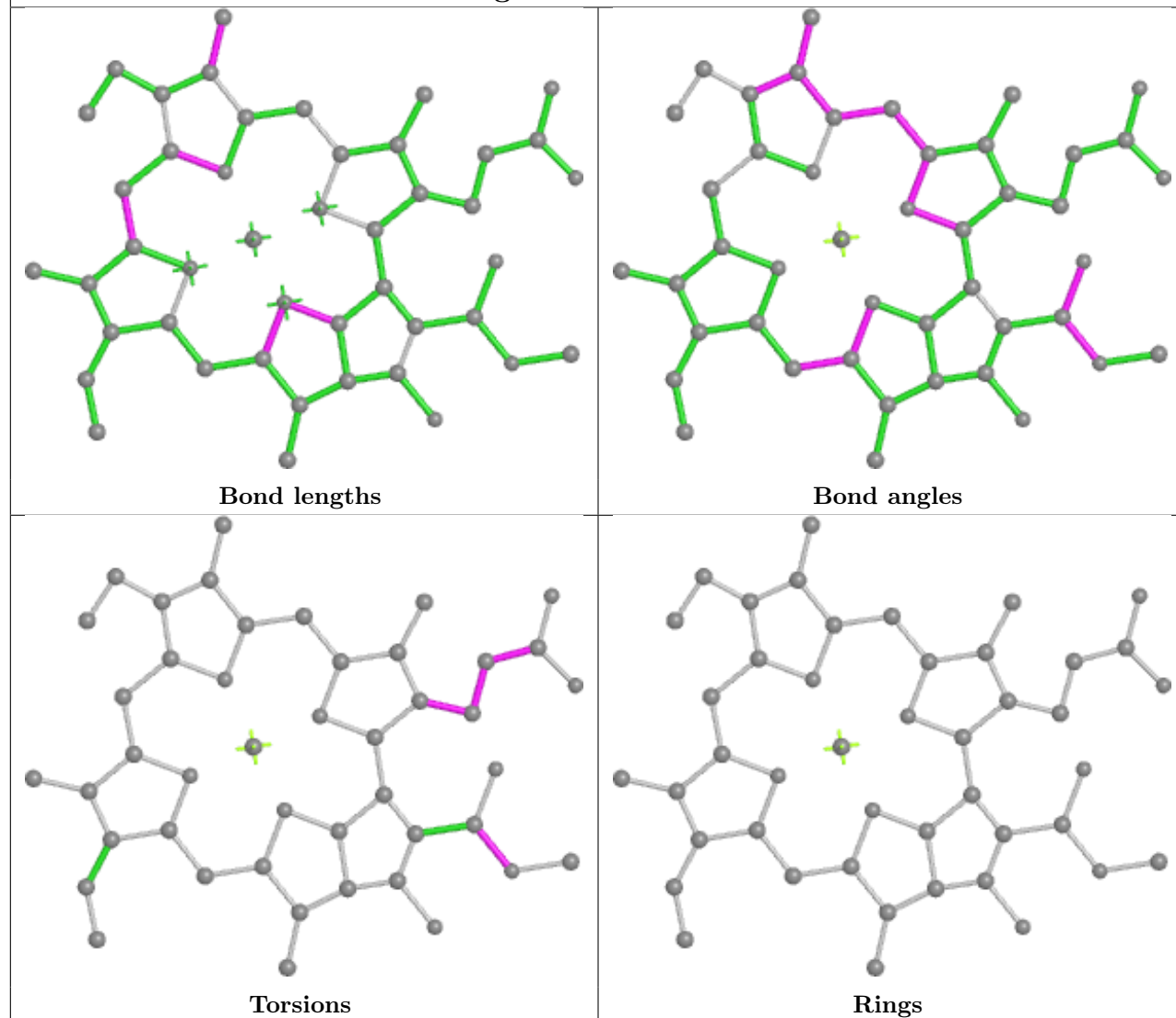


Rings

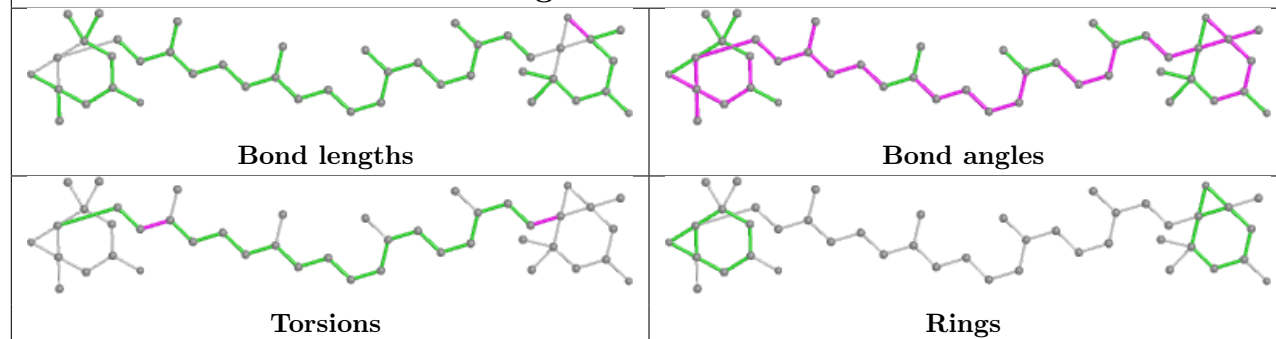




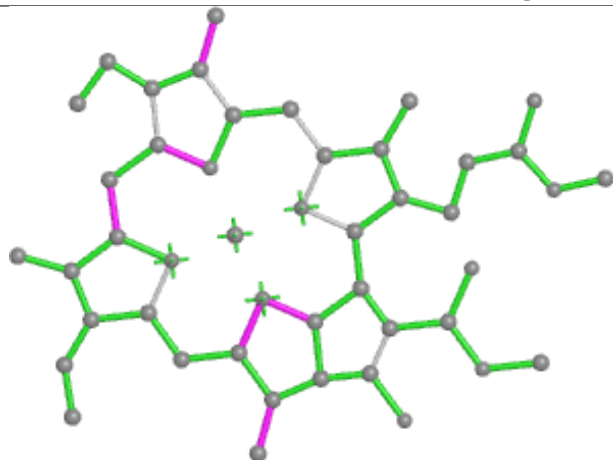
## Ligand CLA 4 306



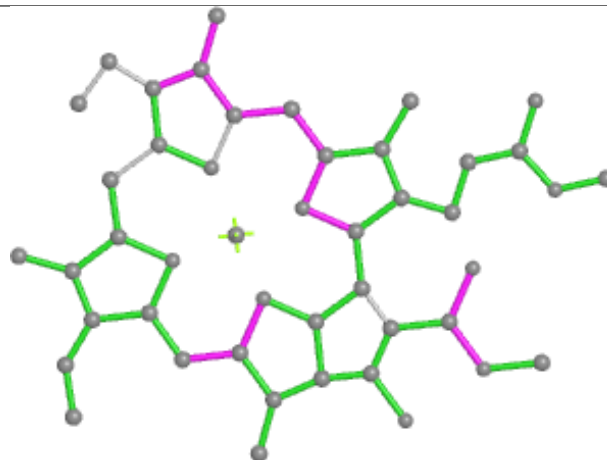
## Ligand XAT 3 303



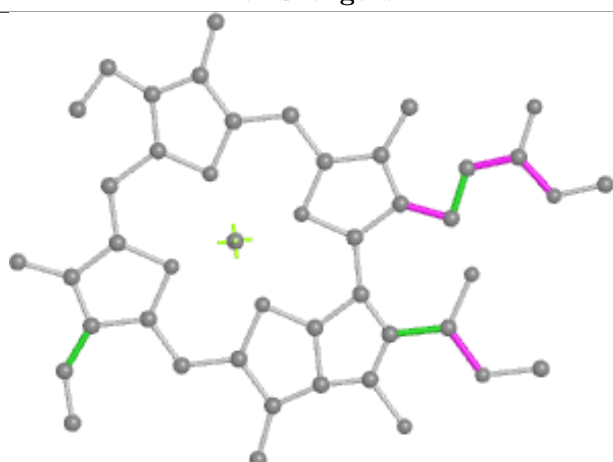
## Ligand CLA 3 315



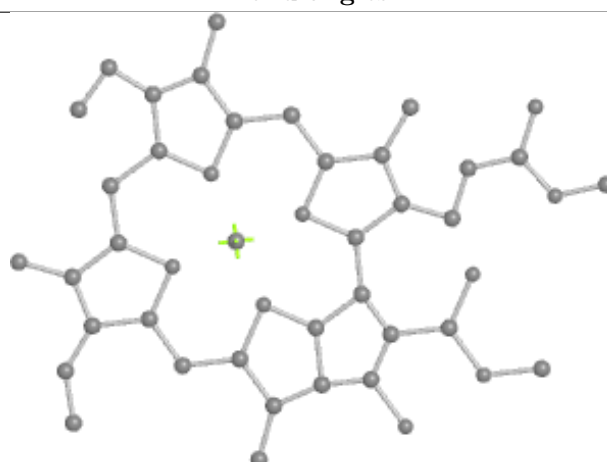
Bond lengths



Bond angles

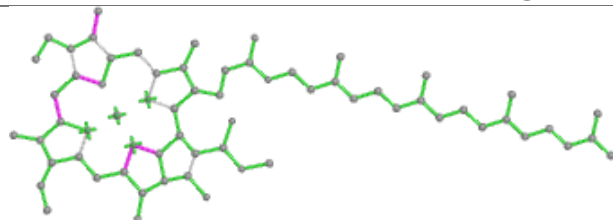


Torsions

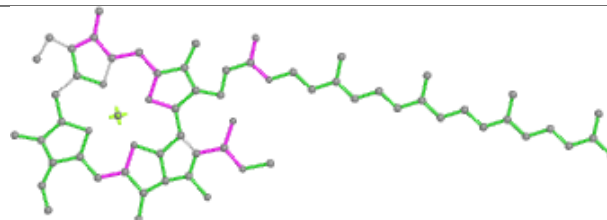


Rings

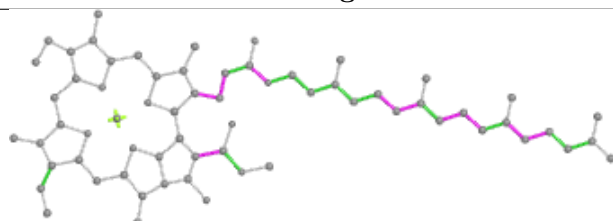
## Ligand CLA a 809



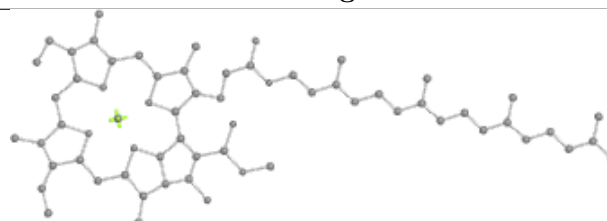
Bond lengths



Bond angles

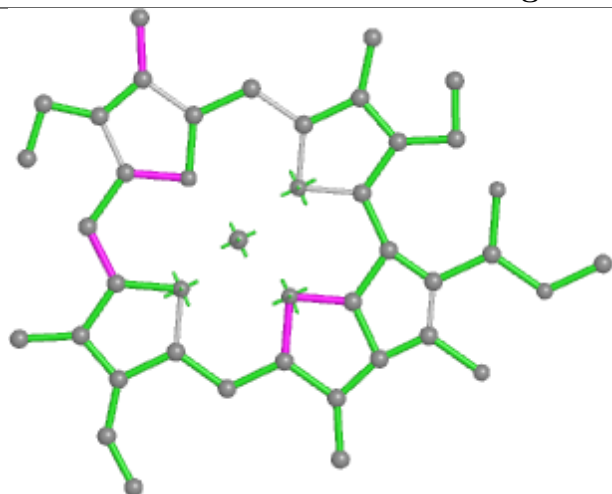


Torsions

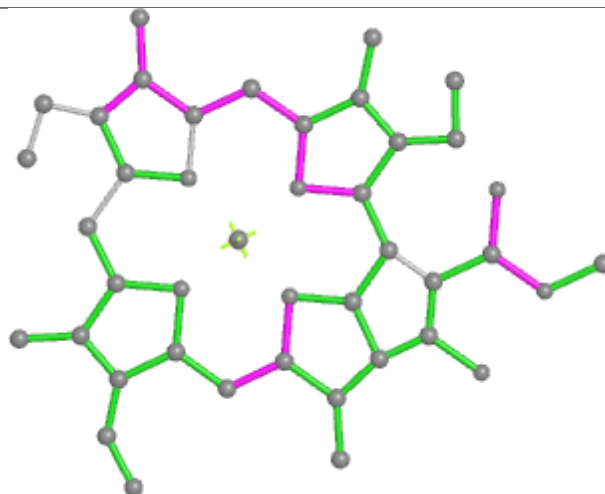


Rings

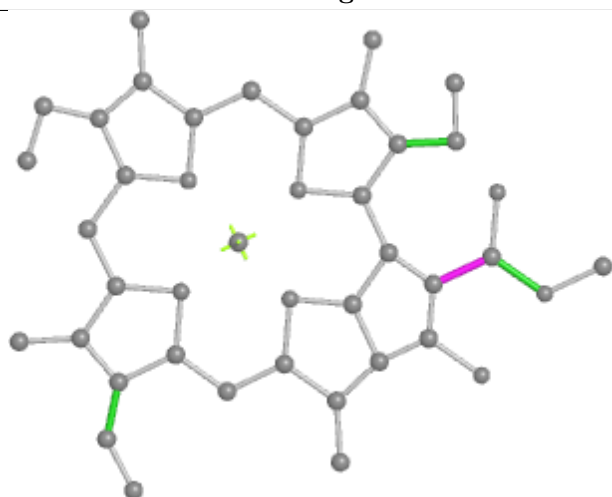
## Ligand CLA 1 202



Bond lengths



Bond angles

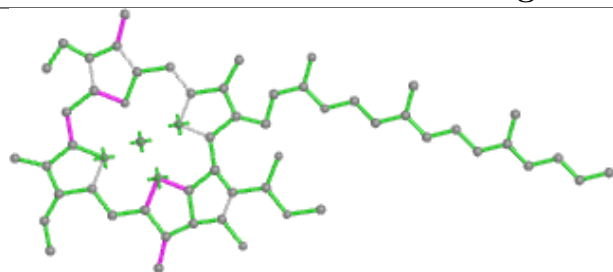


Torsions

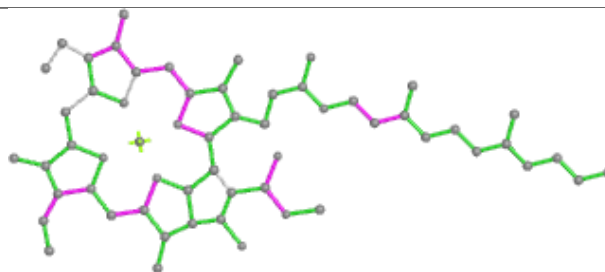


Rings

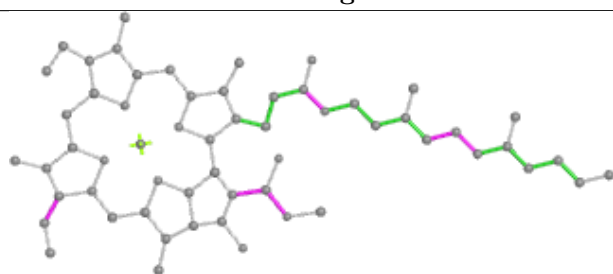
## Ligand CLA b 836



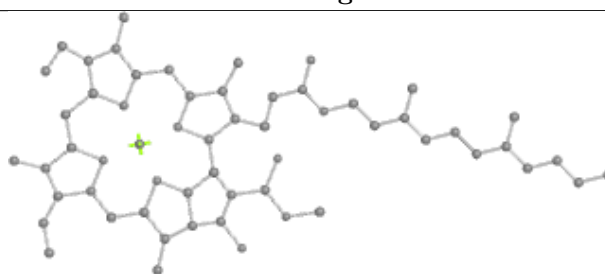
Bond lengths



Bond angles

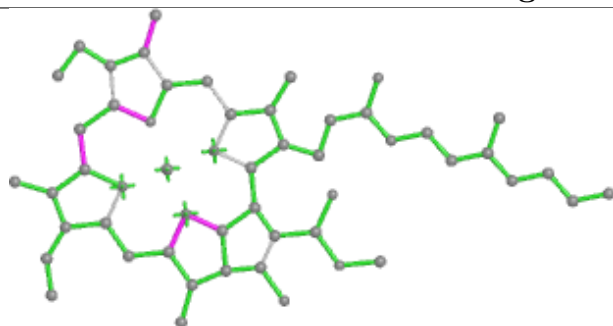


Torsions

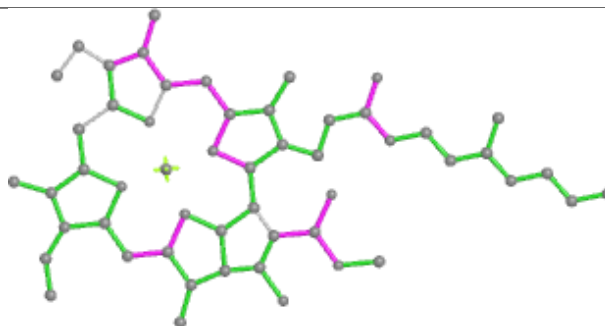


Rings

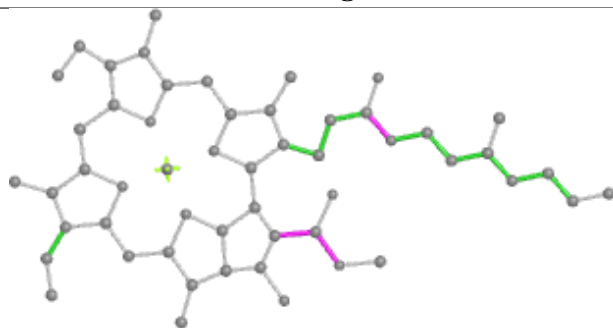
## Ligand CLA 1 311



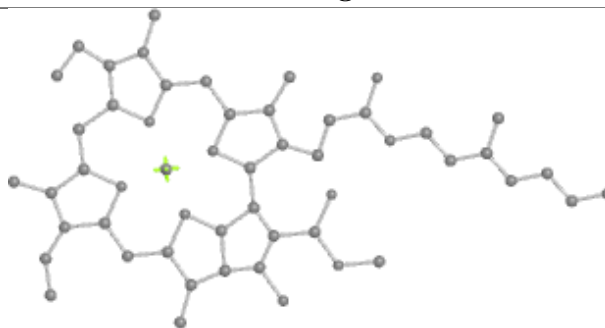
Bond lengths



Bond angles

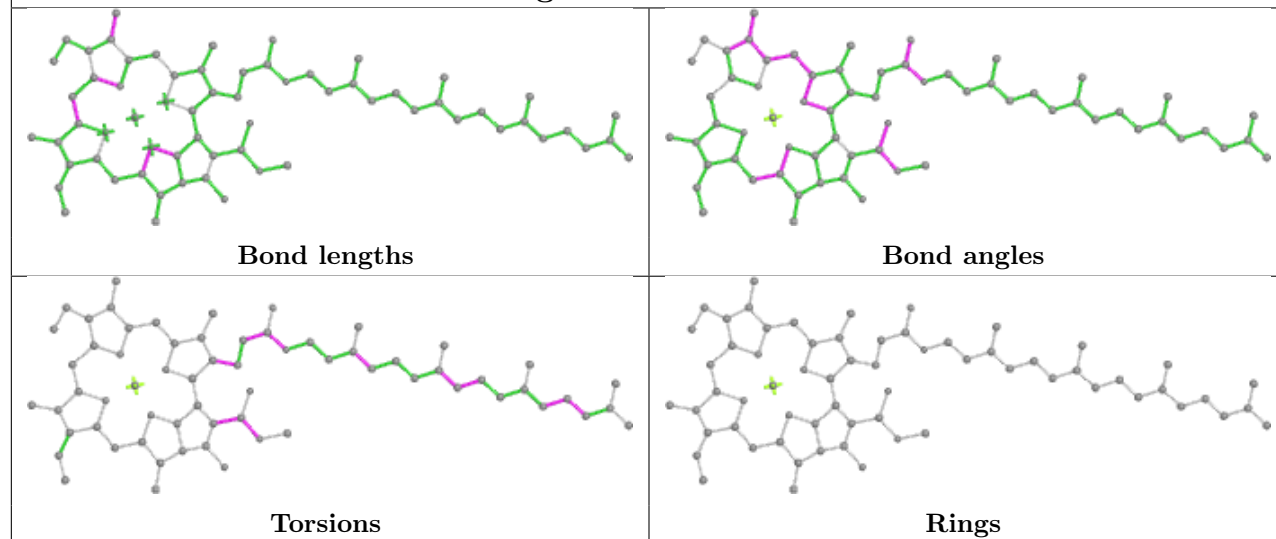


Torsions

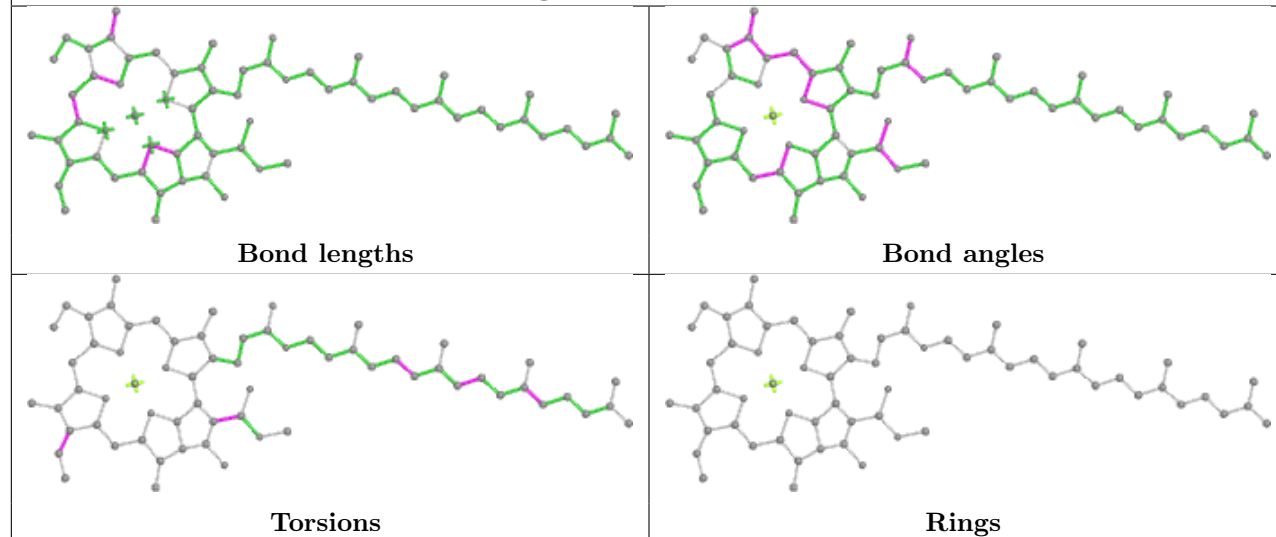


Rings

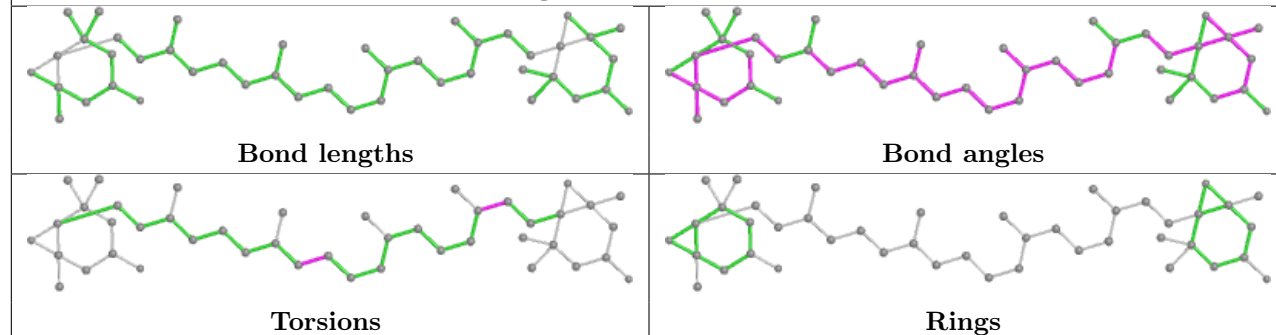
## Ligand CLA 4 310



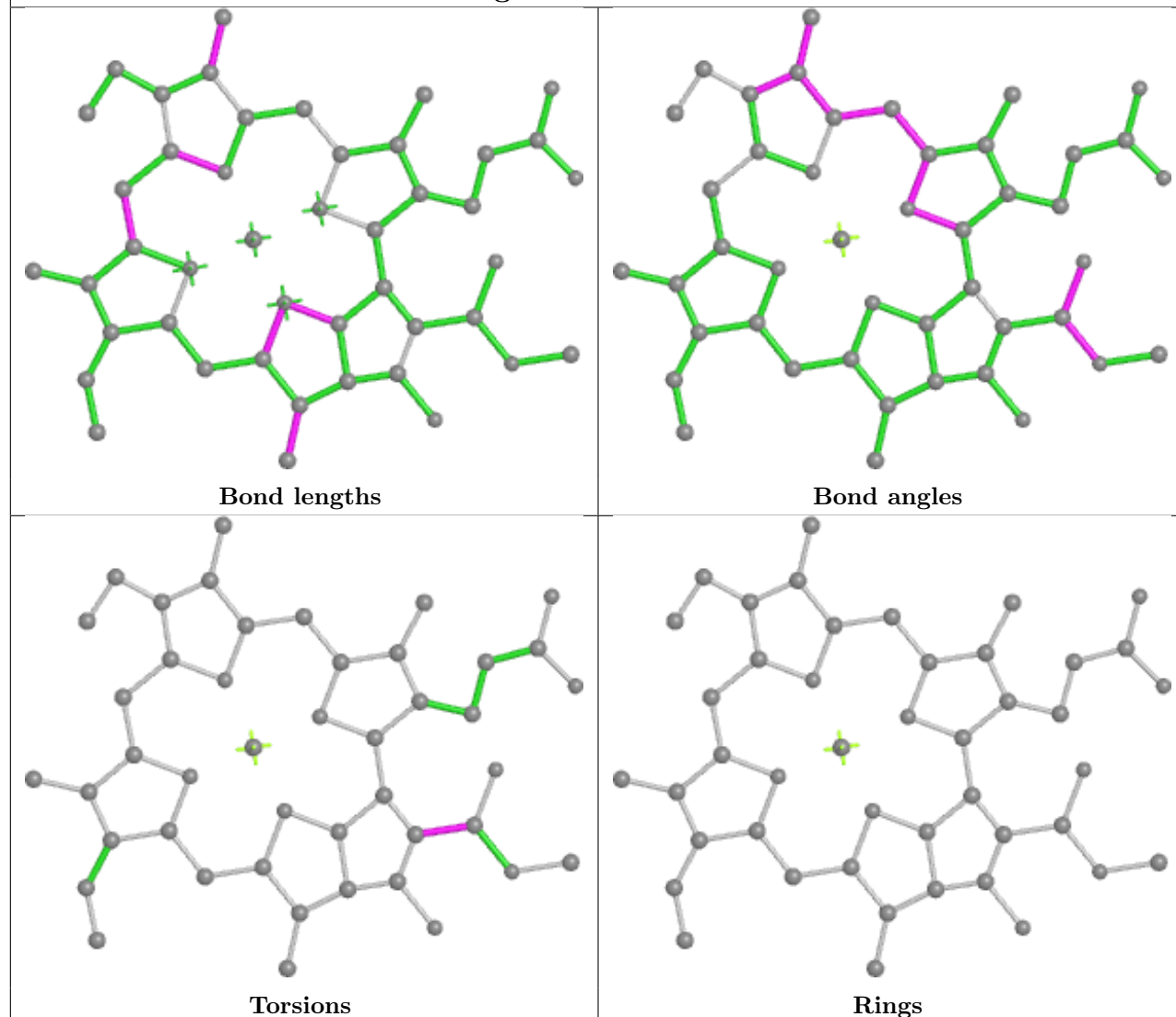
## Ligand CLA b 837



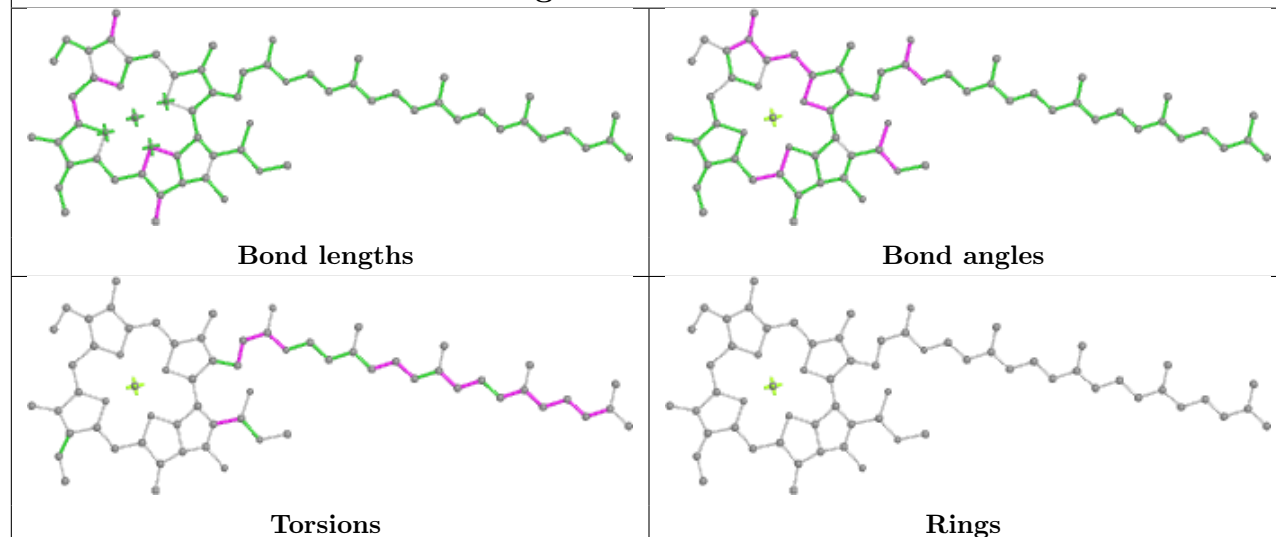
## Ligand XAT 2 304

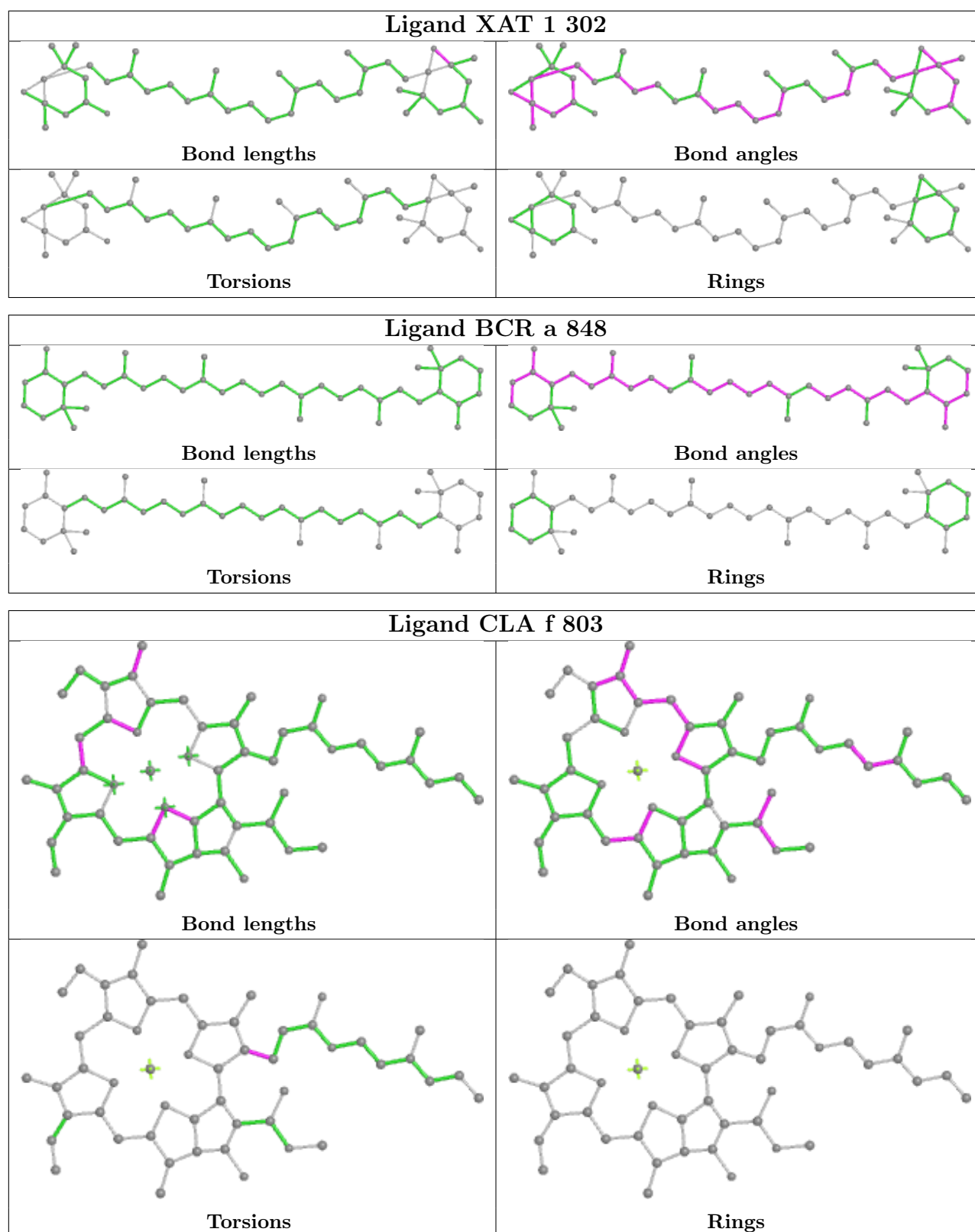


## Ligand CLA 3 307

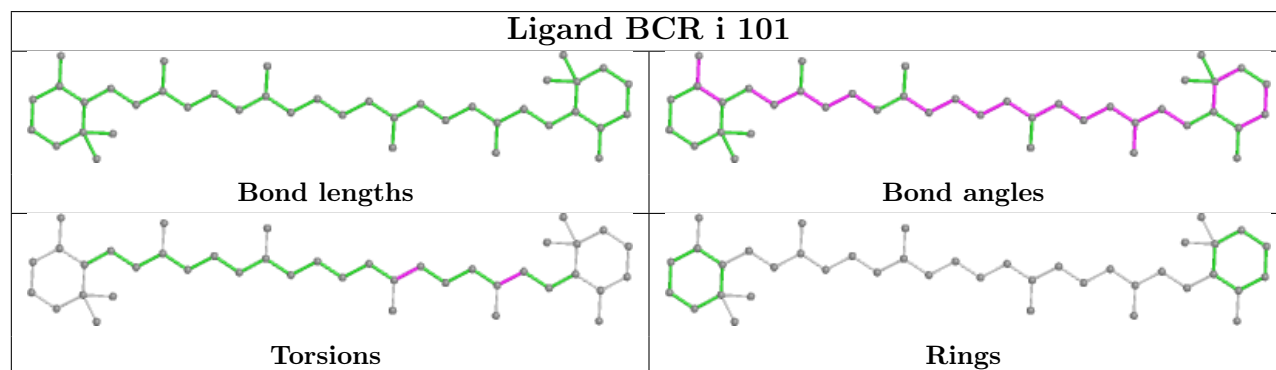
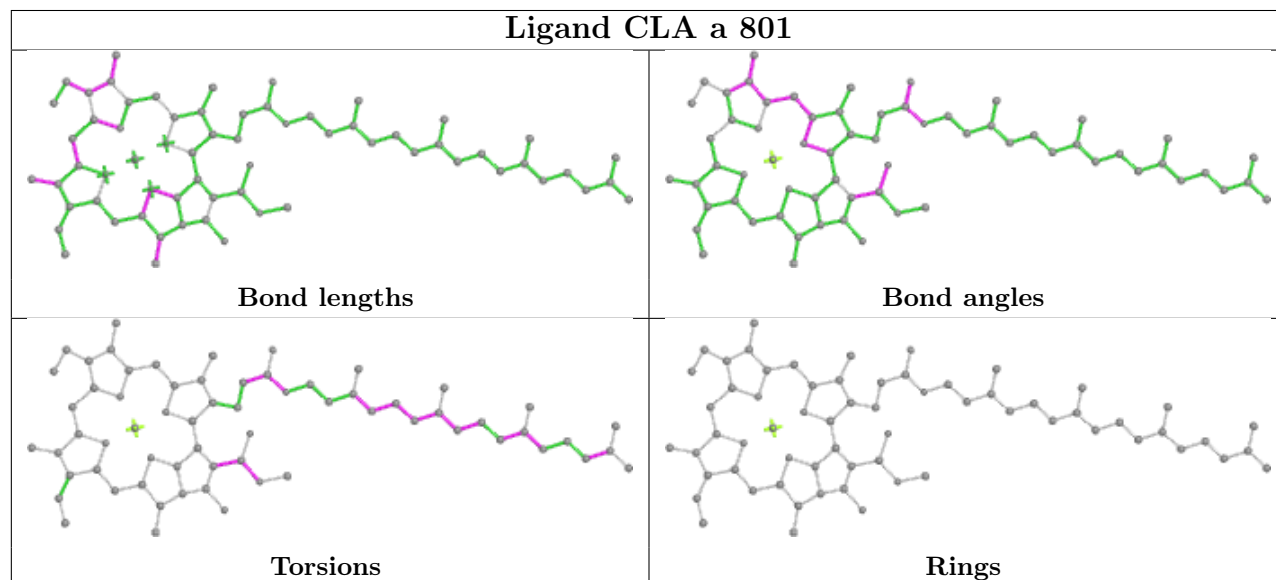
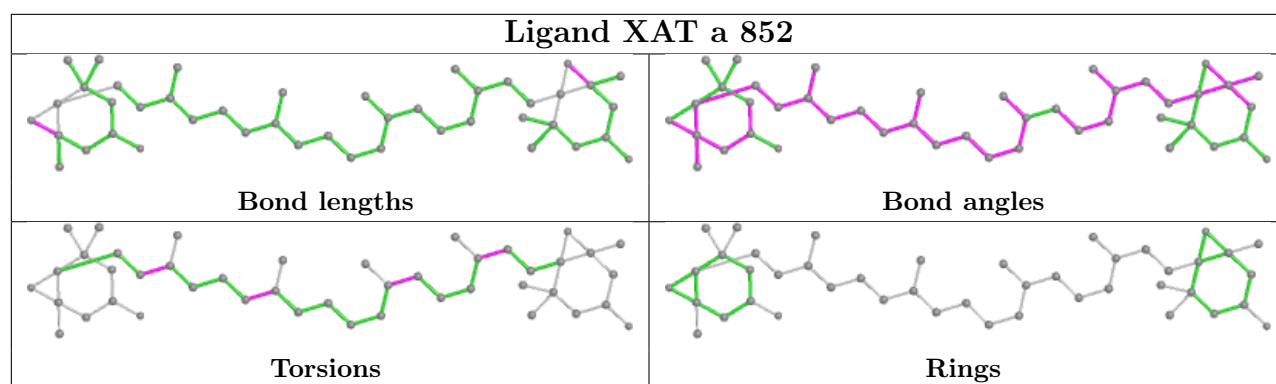


## Ligand CLA b 801

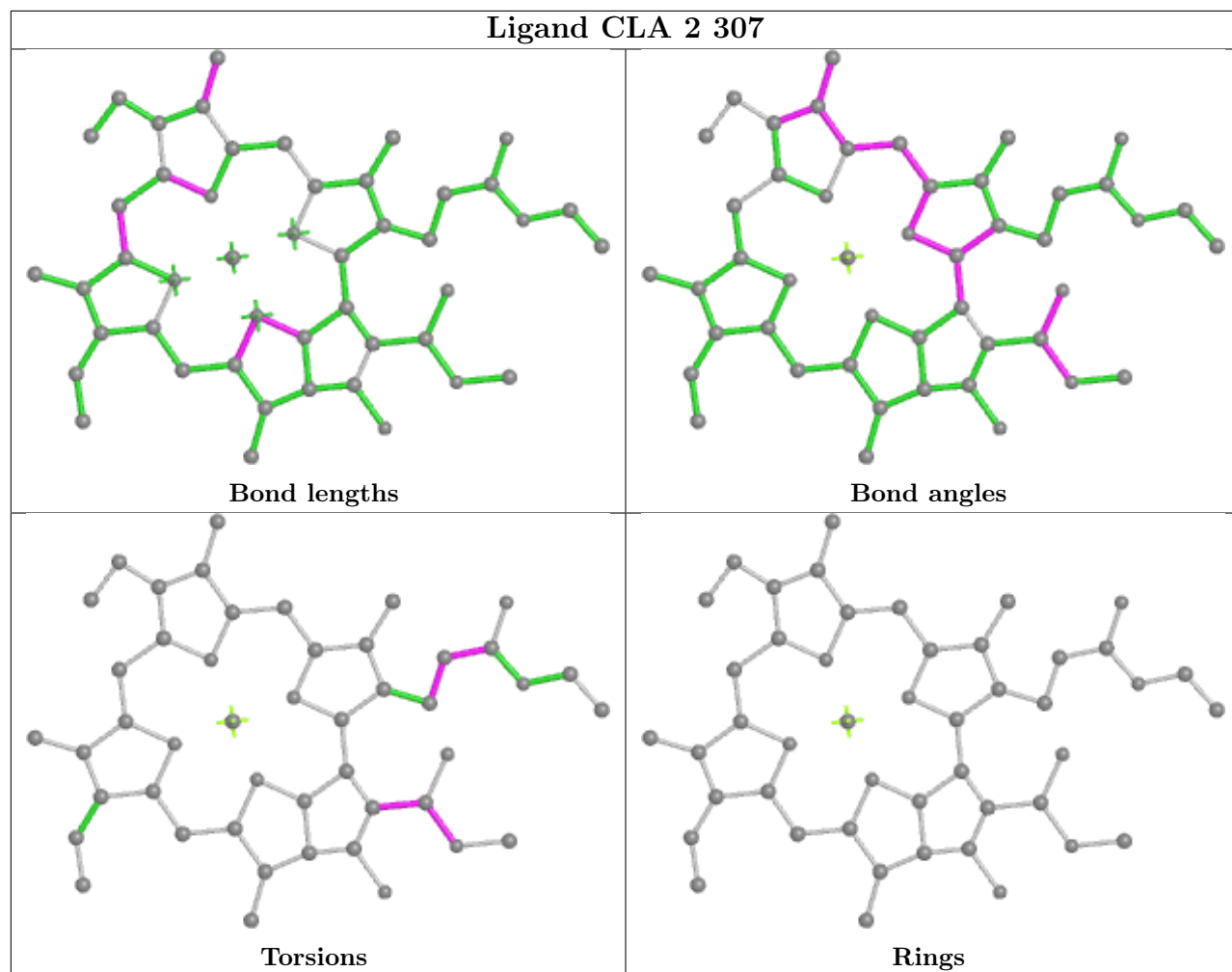




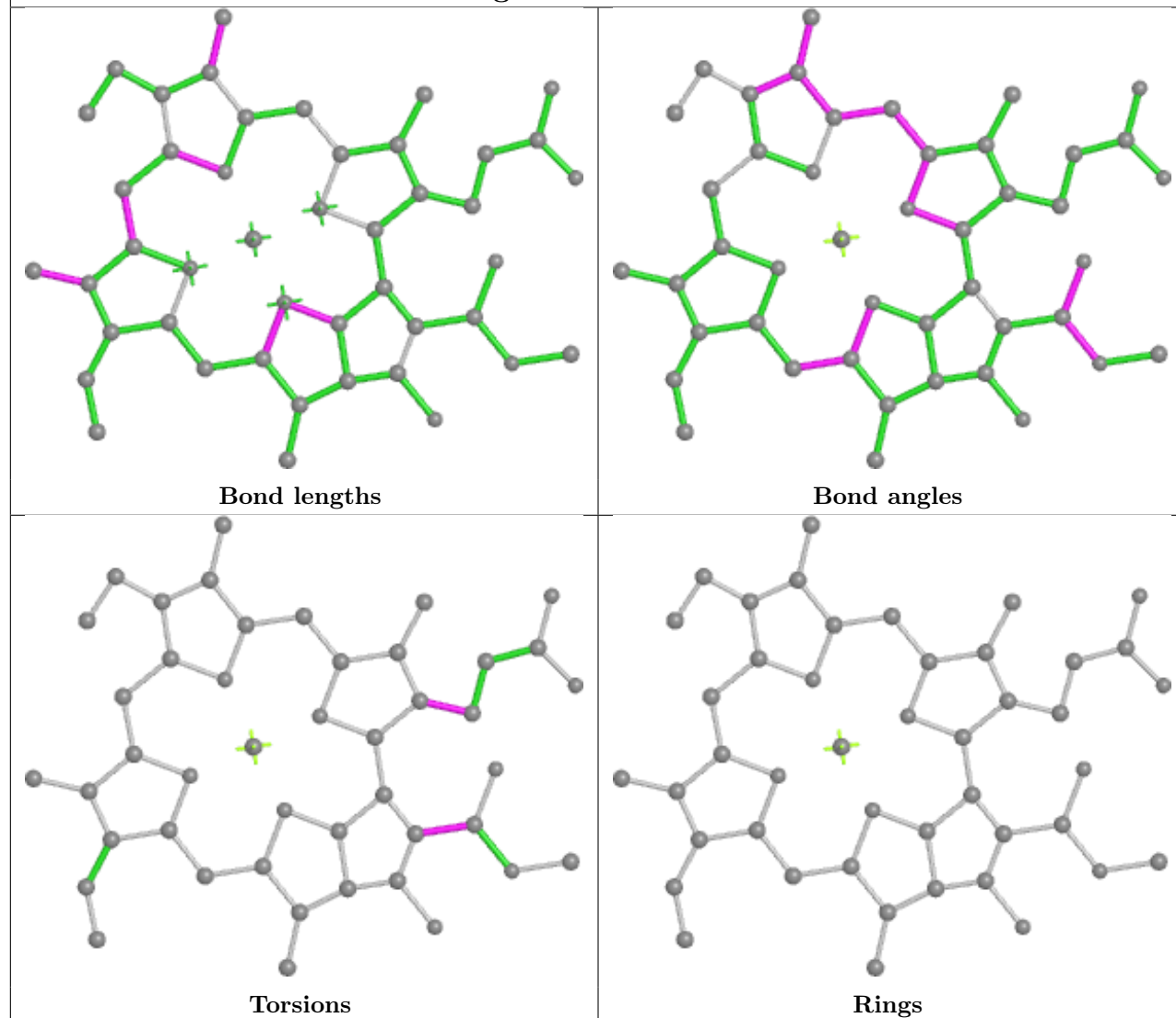




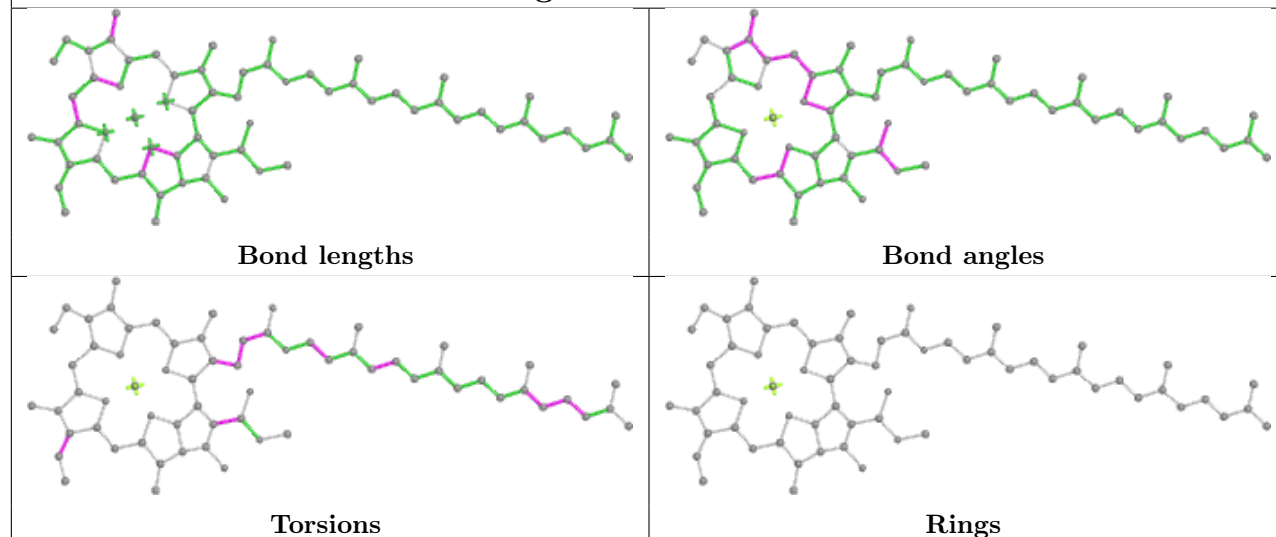
## Ligand CLA 2 307

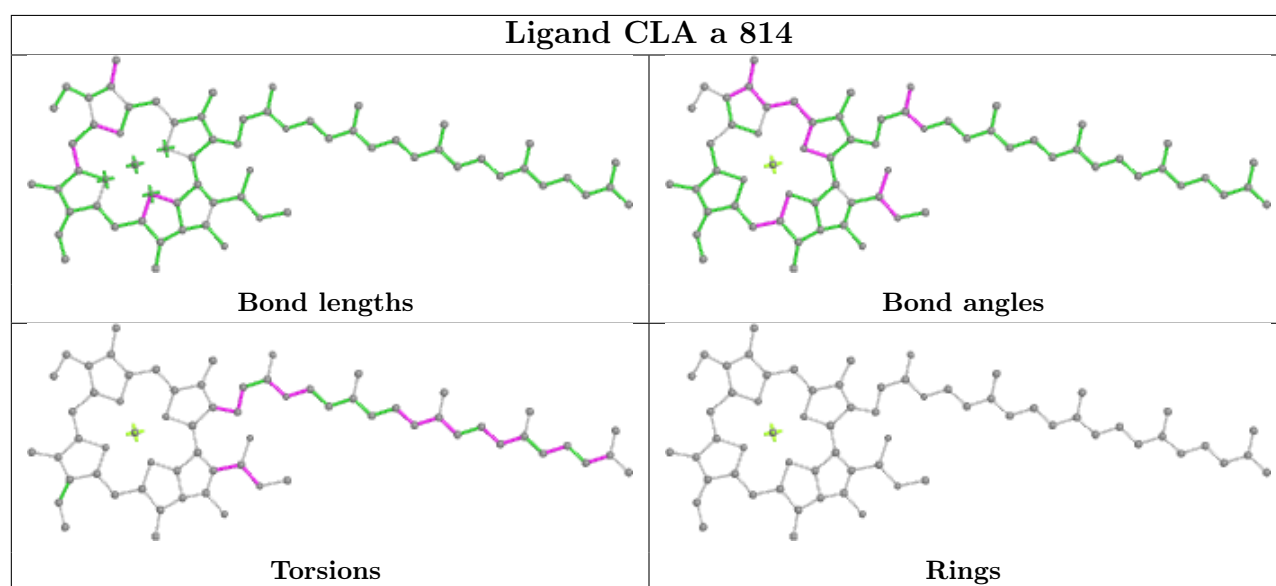
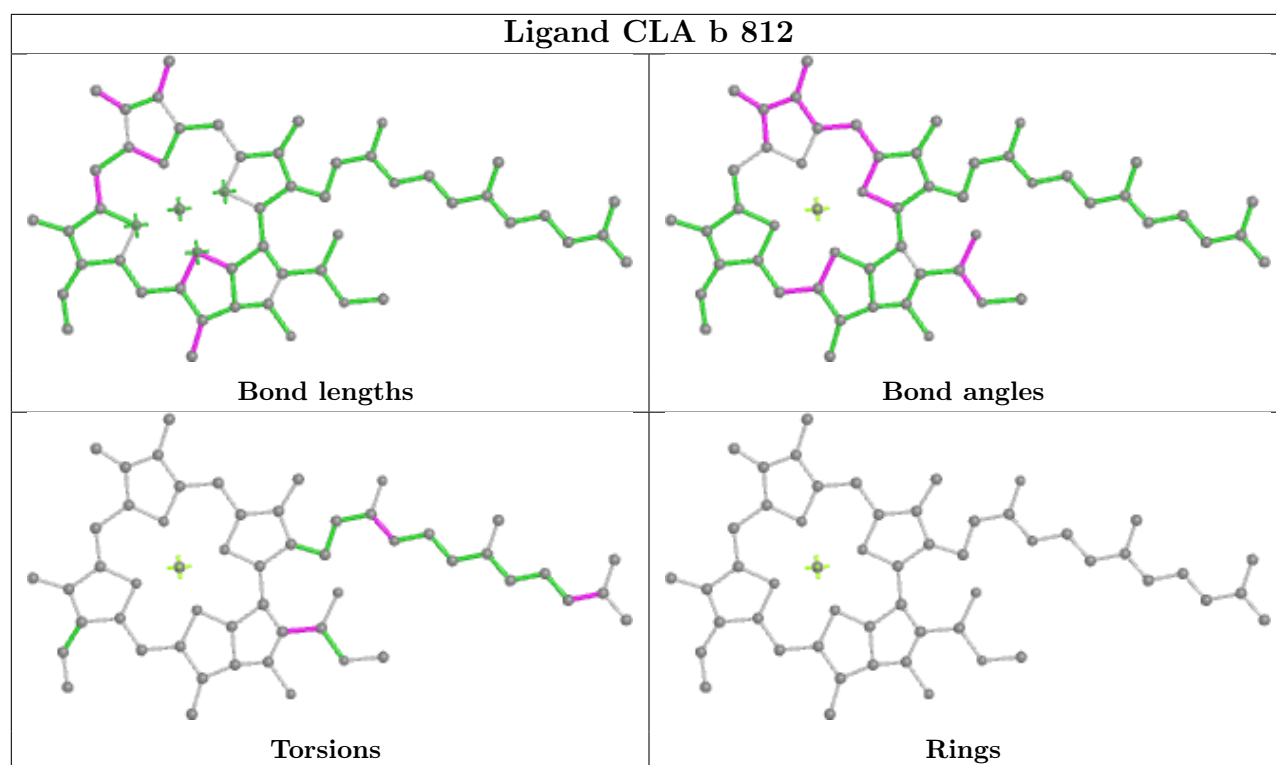


## Ligand CLA b 816

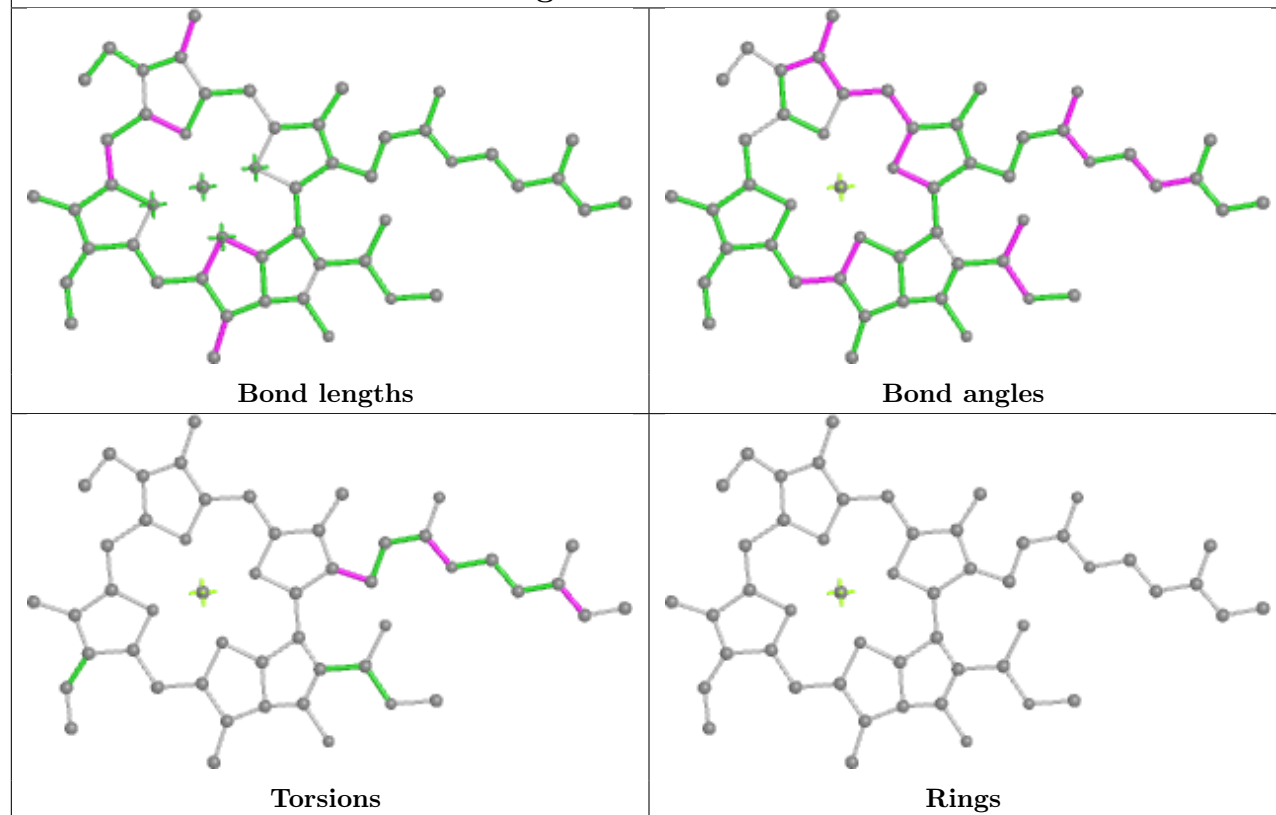


## Ligand CLA b 833

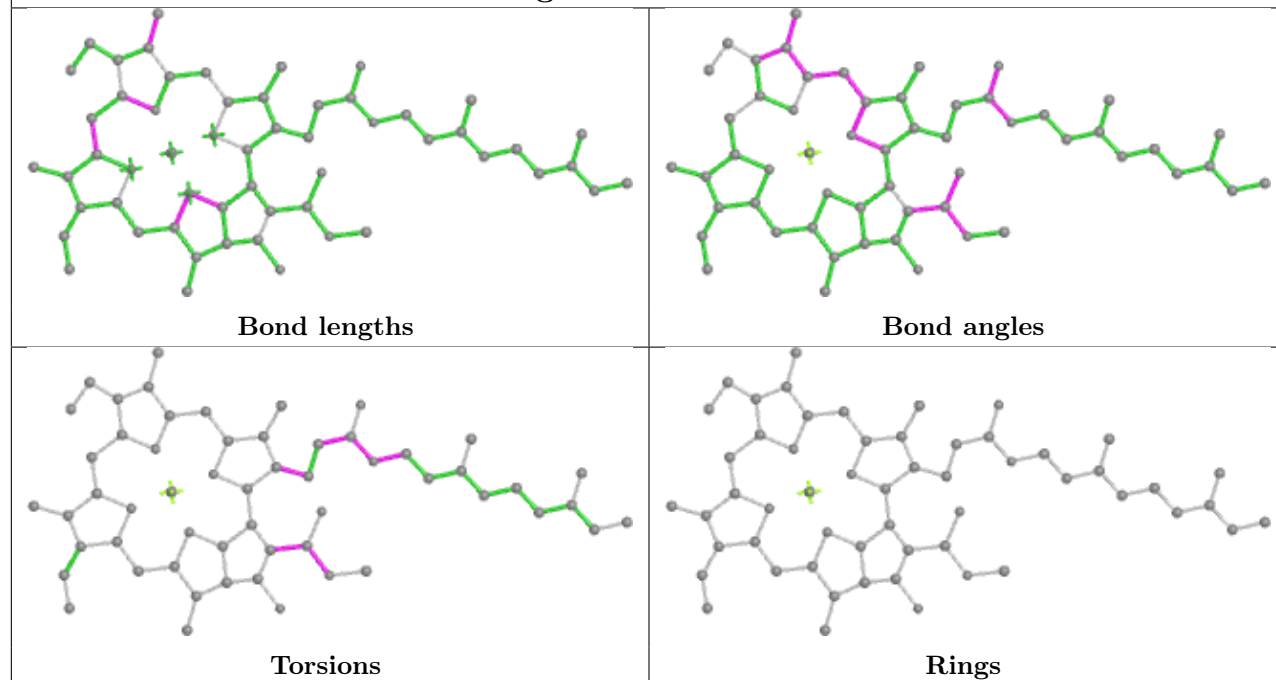




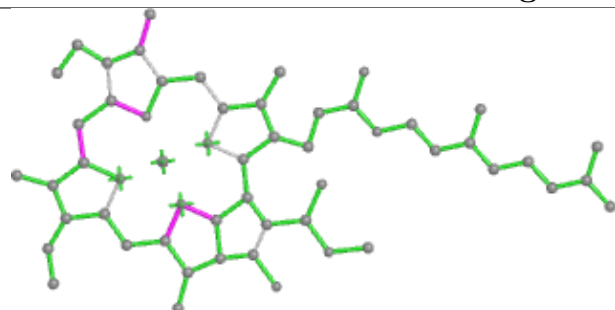
## Ligand CLA a 838



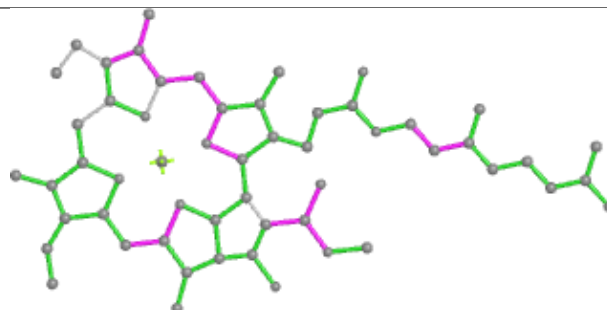
## Ligand CLA a 818



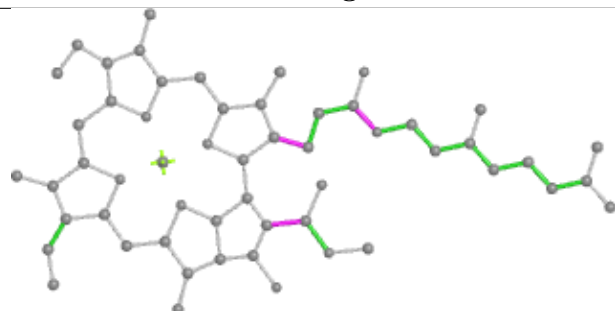
## Ligand CLA b 817



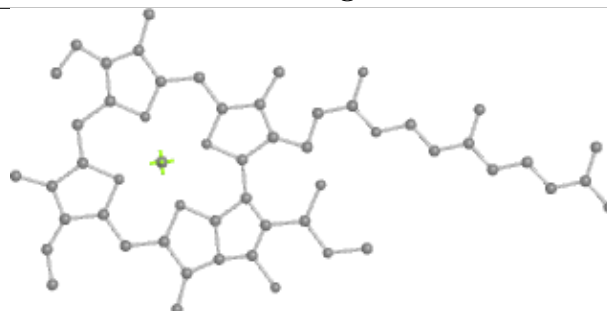
Bond lengths



Bond angles

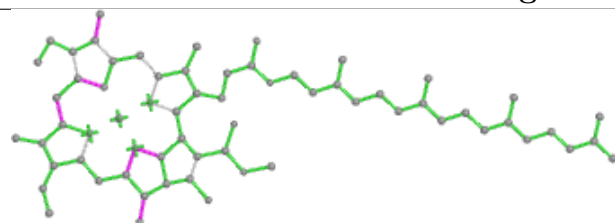


Torsions

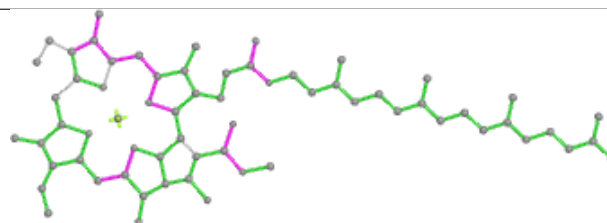


Rings

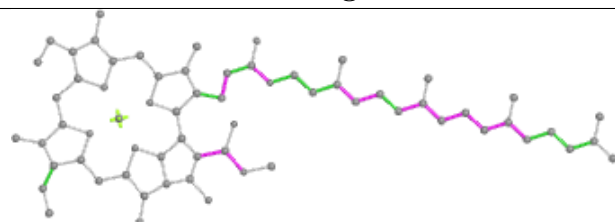
## Ligand CLA b 802



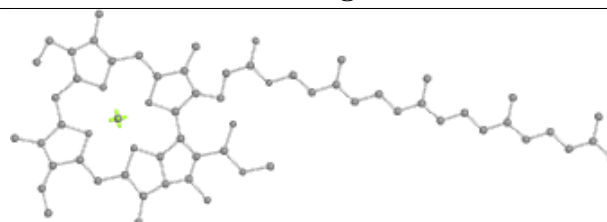
Bond lengths



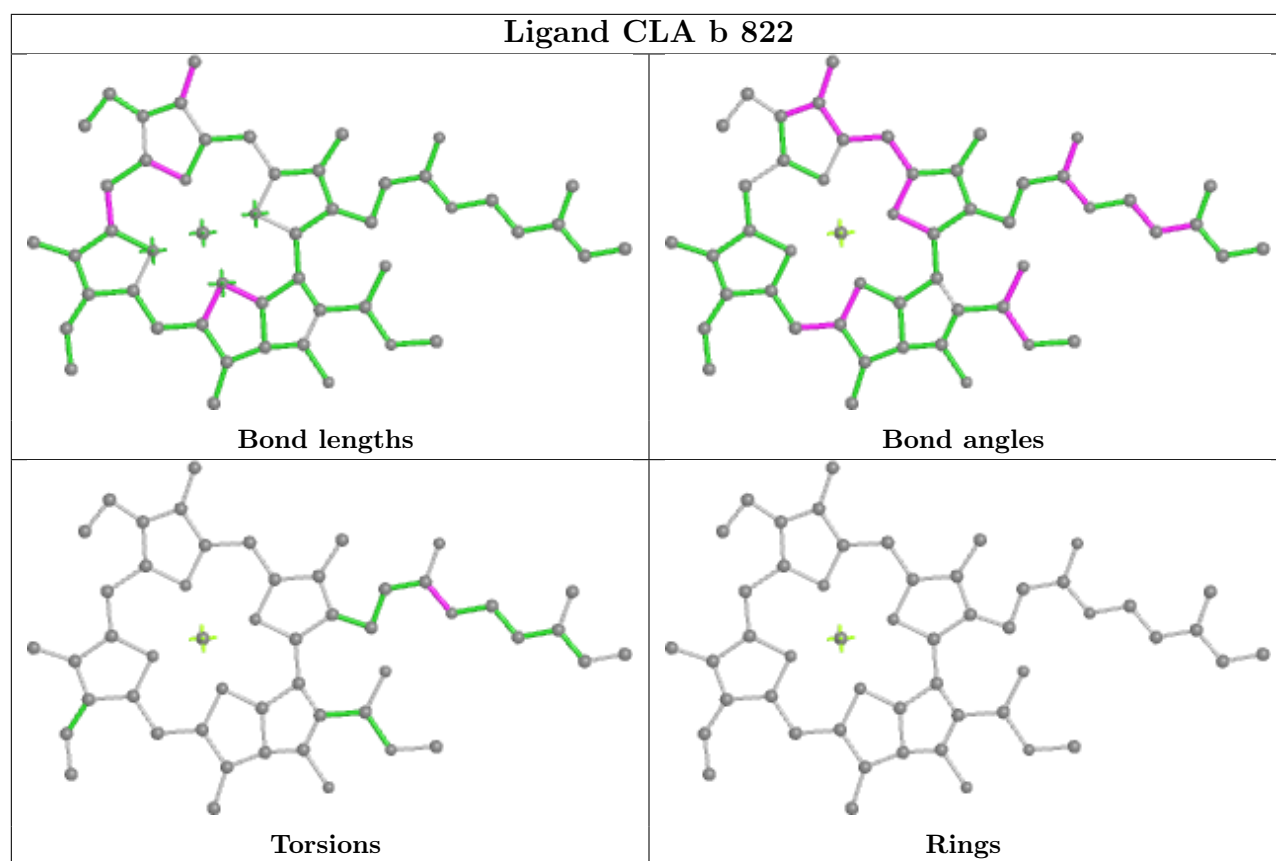
Bond angles



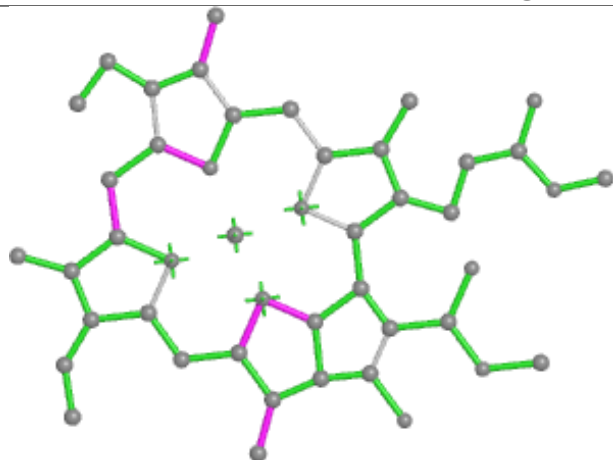
Torsions



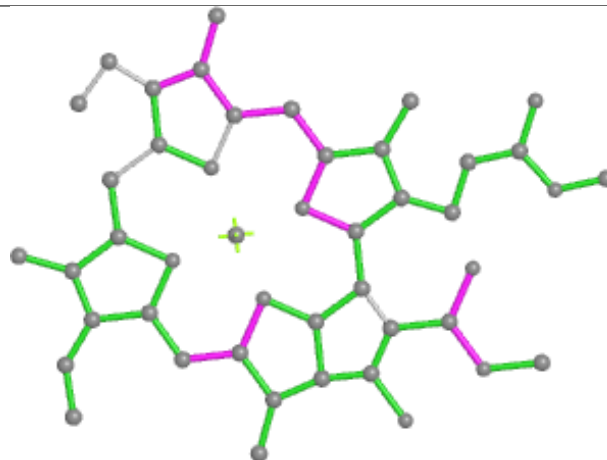
Rings



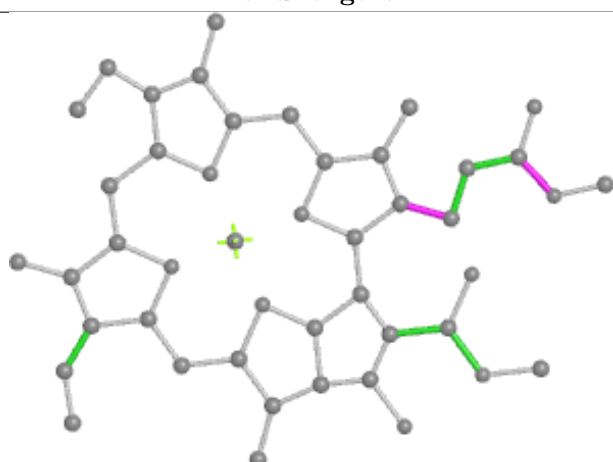
## Ligand CLA 4 312



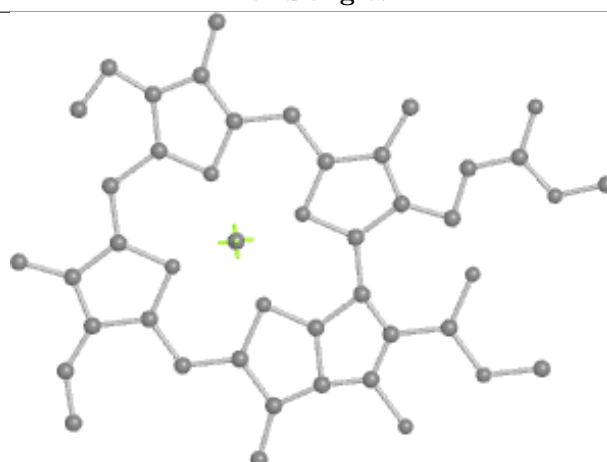
Bond lengths



Bond angles

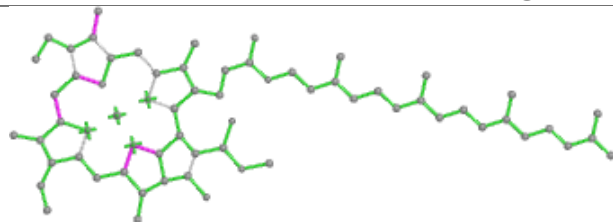


Torsions

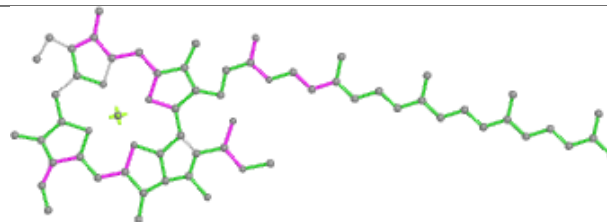


Rings

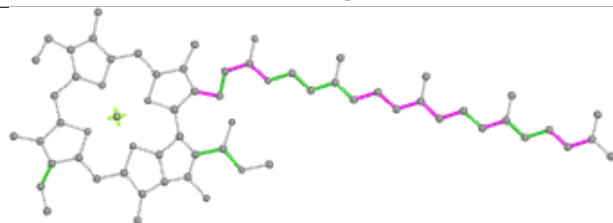
## Ligand CLA 1 306



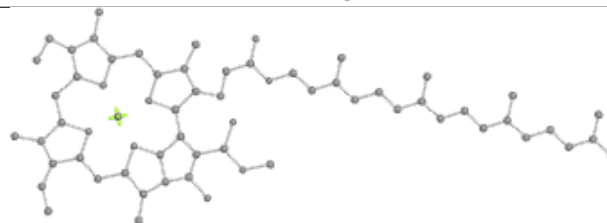
Bond lengths



Bond angles



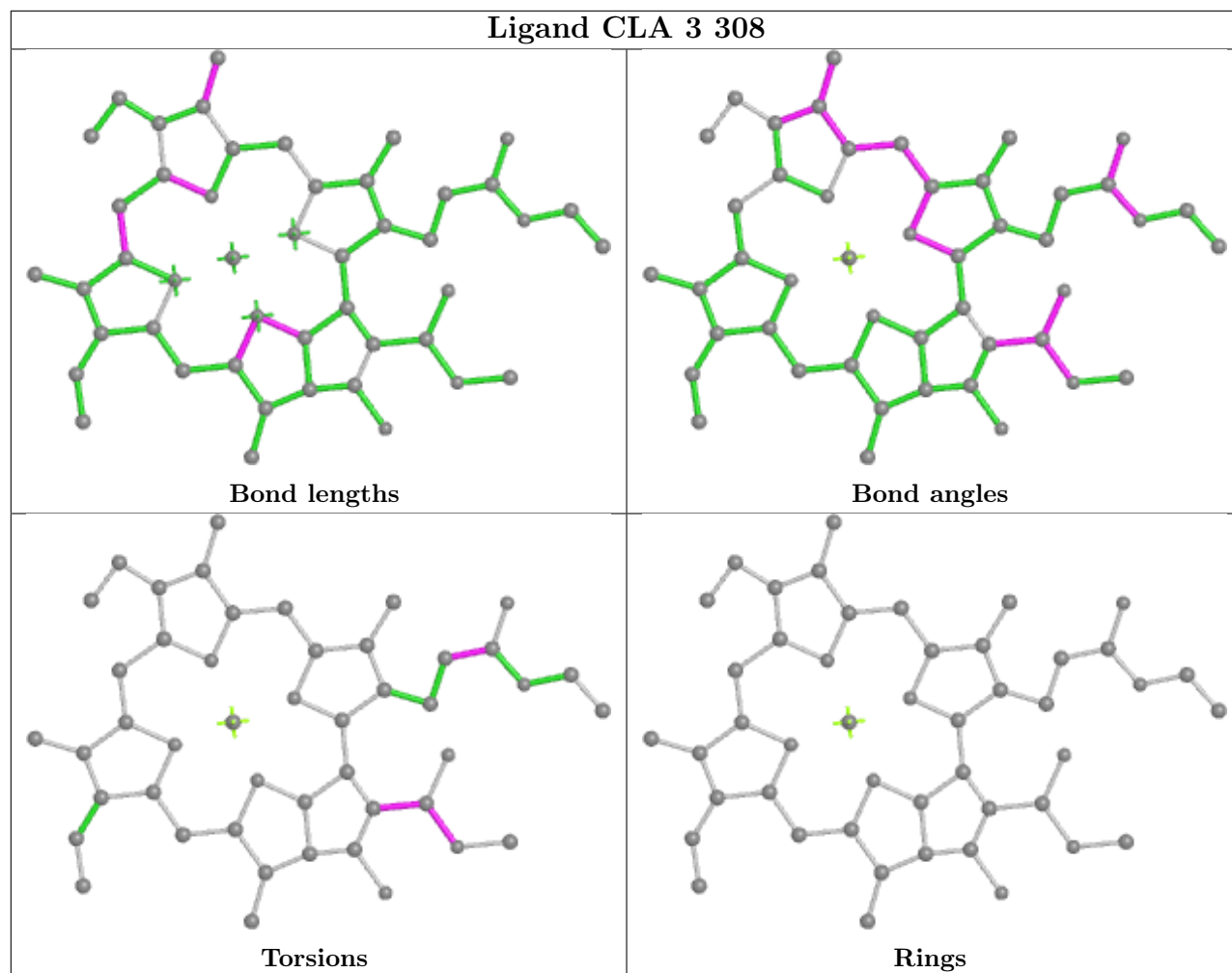
Torsions



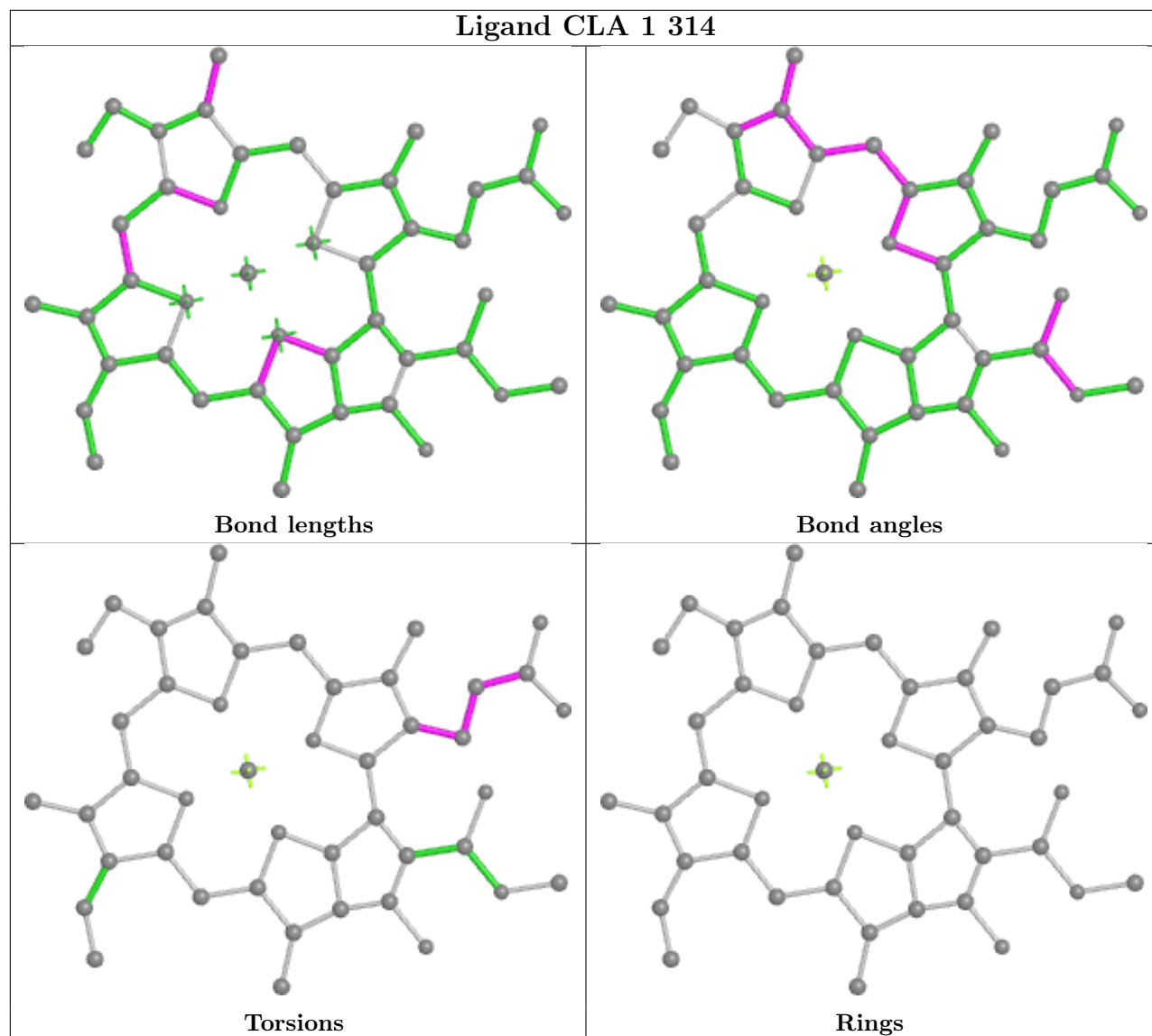
Rings



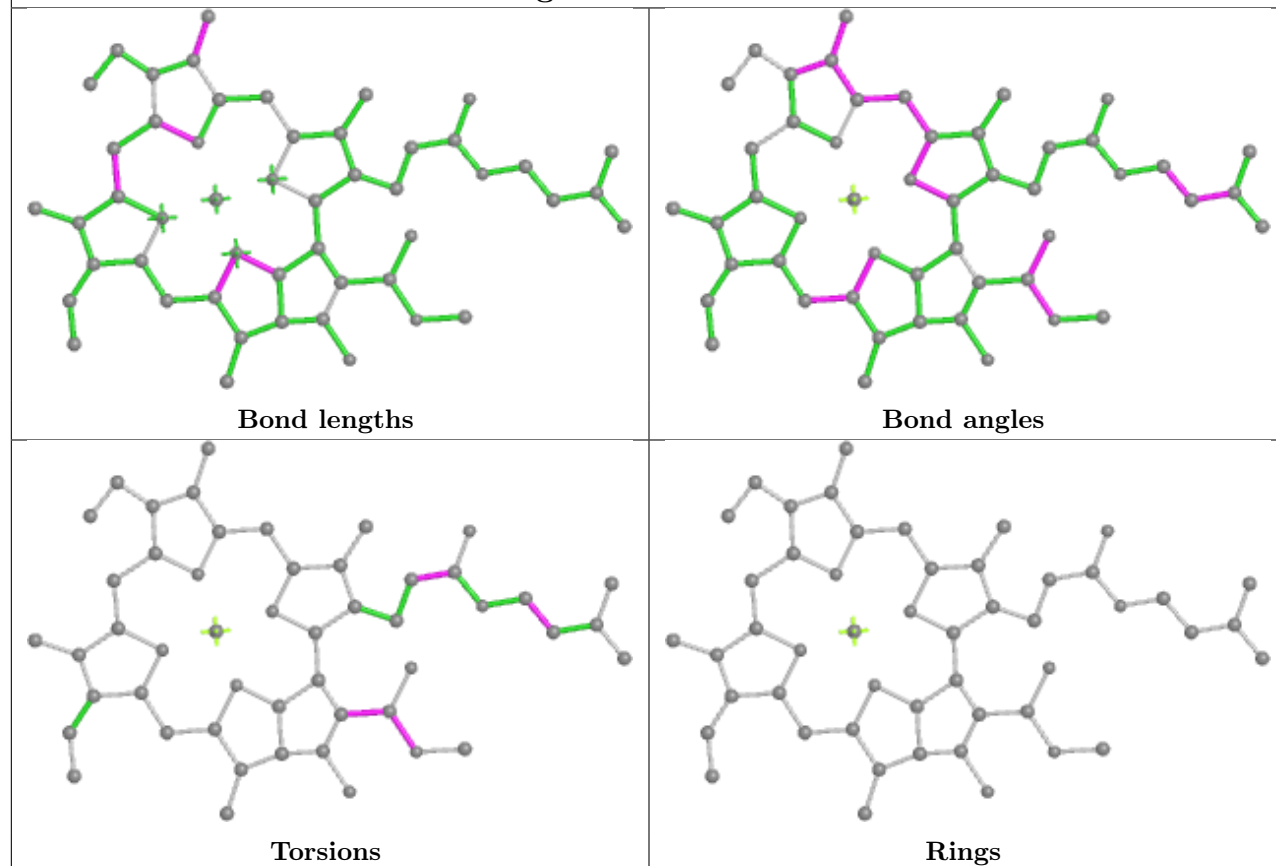
## Ligand CLA 3 308



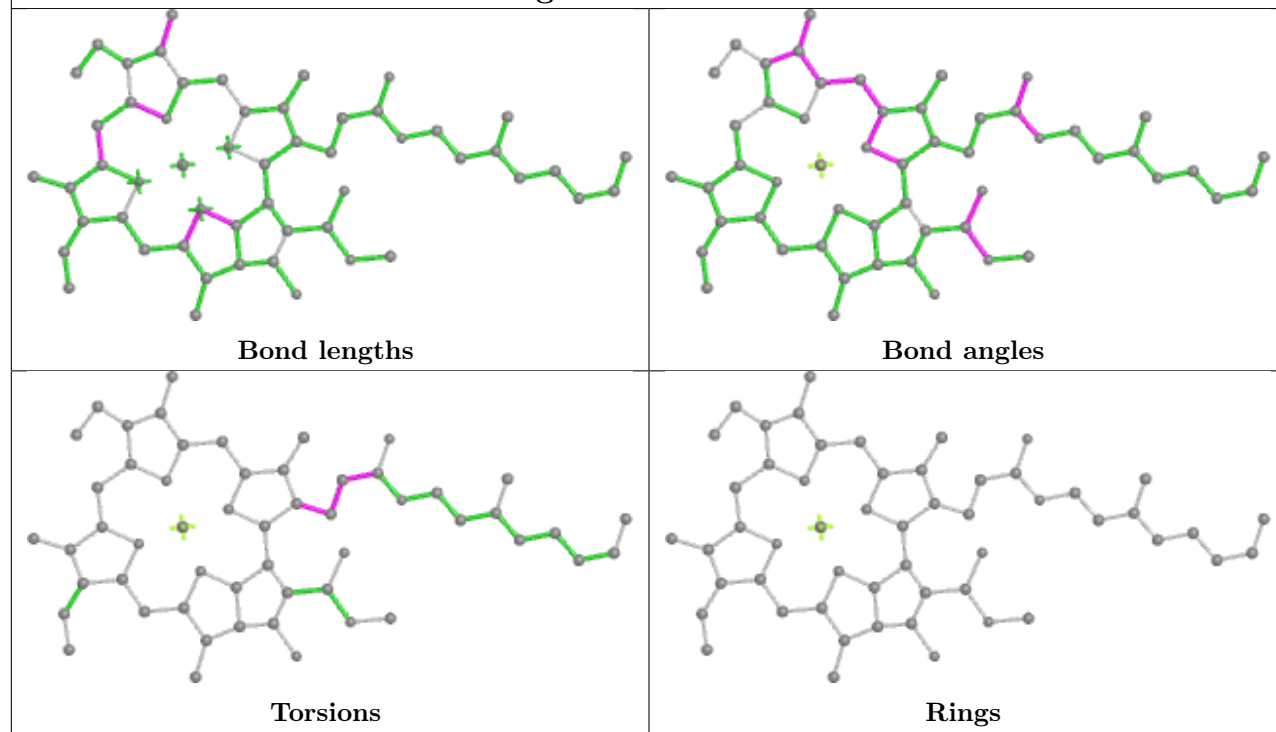
## Ligand CLA 1 314

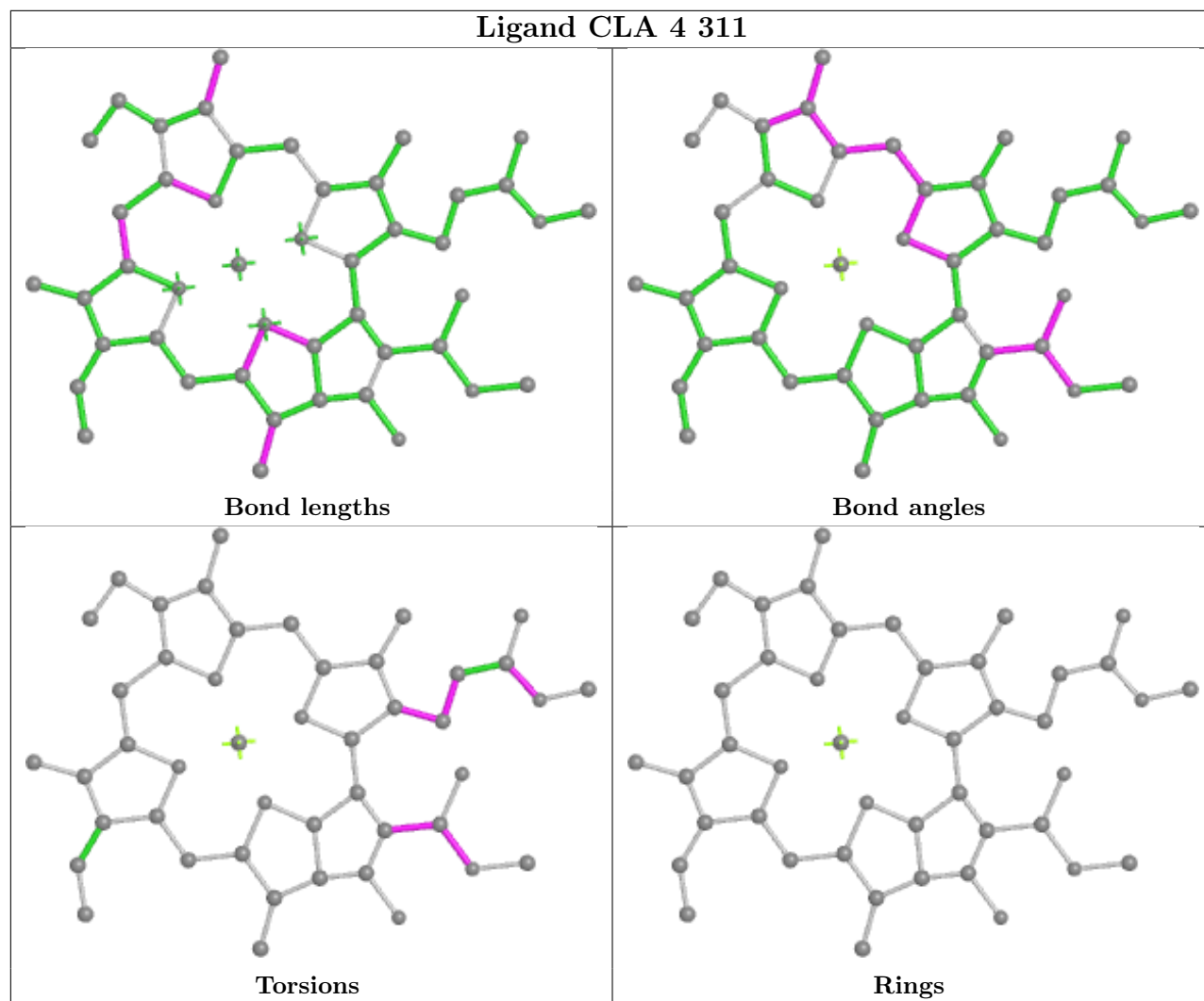
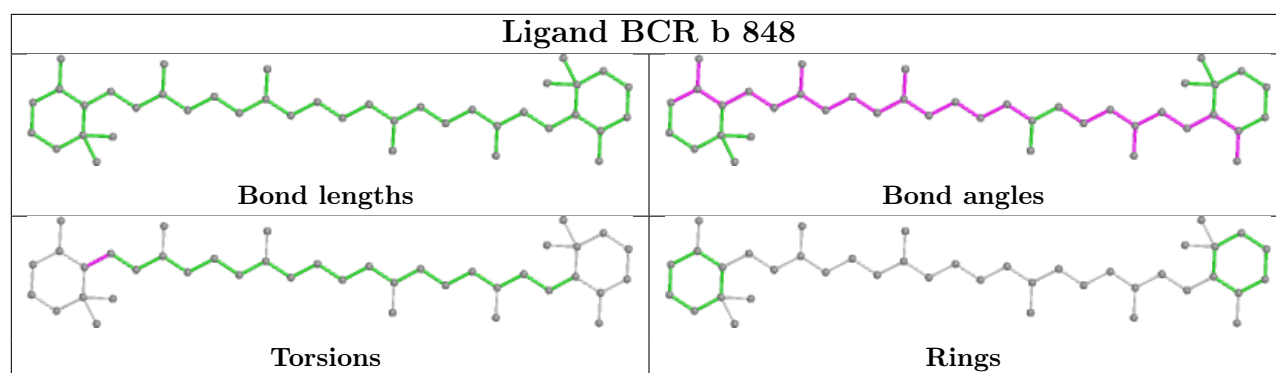


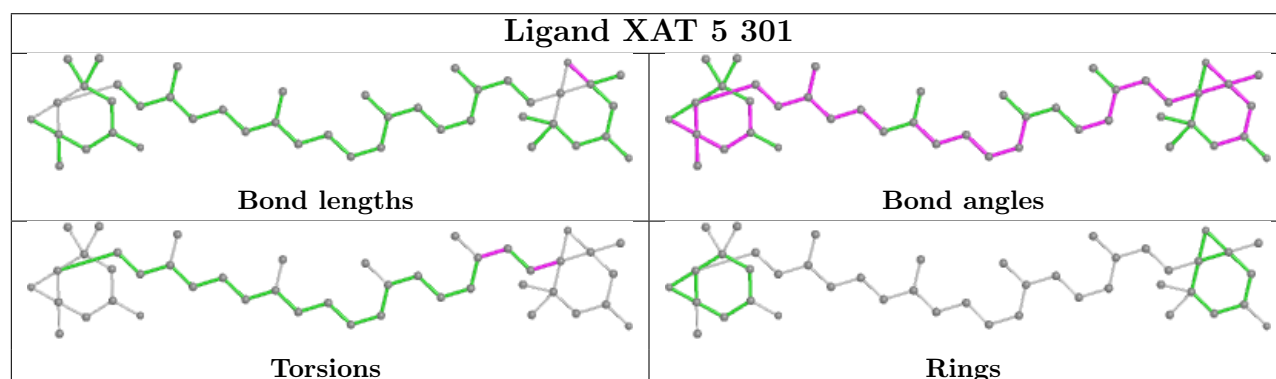
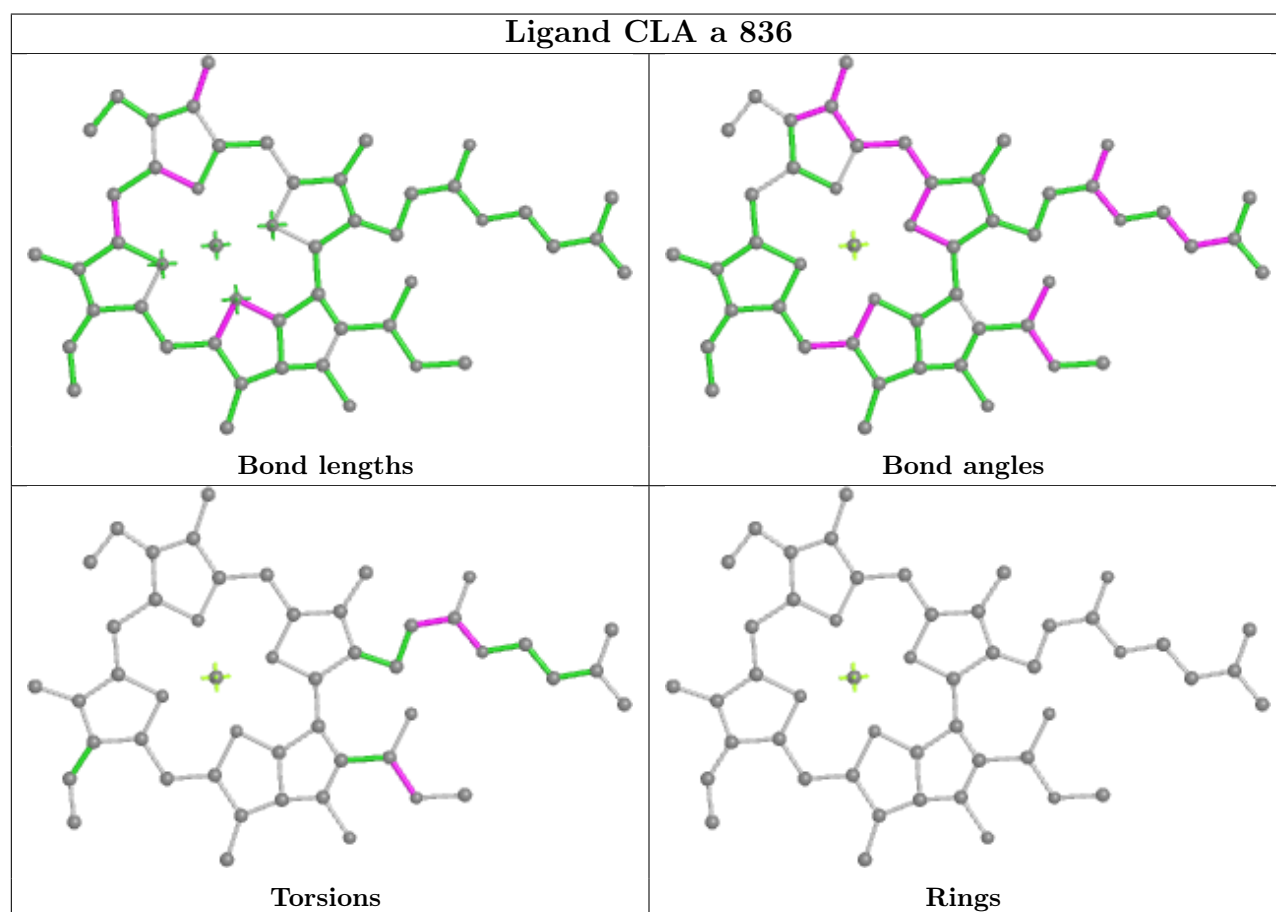
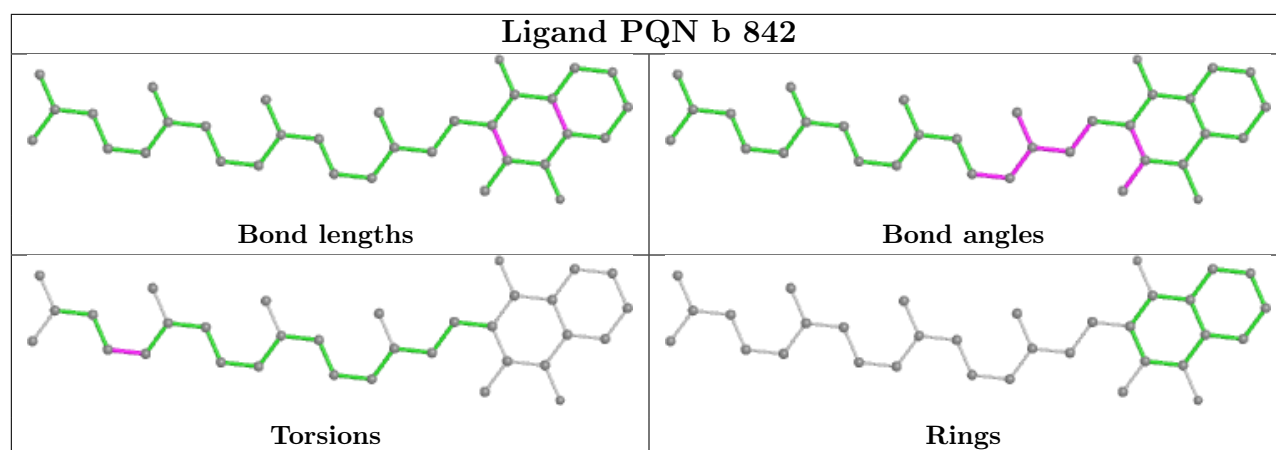
## Ligand CLA 4 309



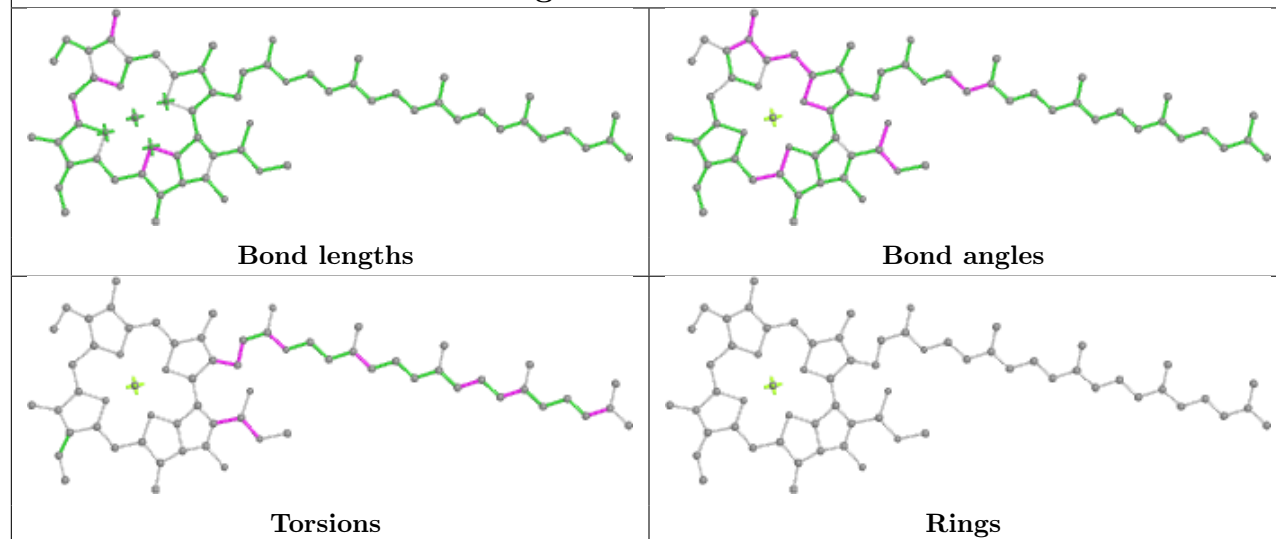
## Ligand CLA a 819



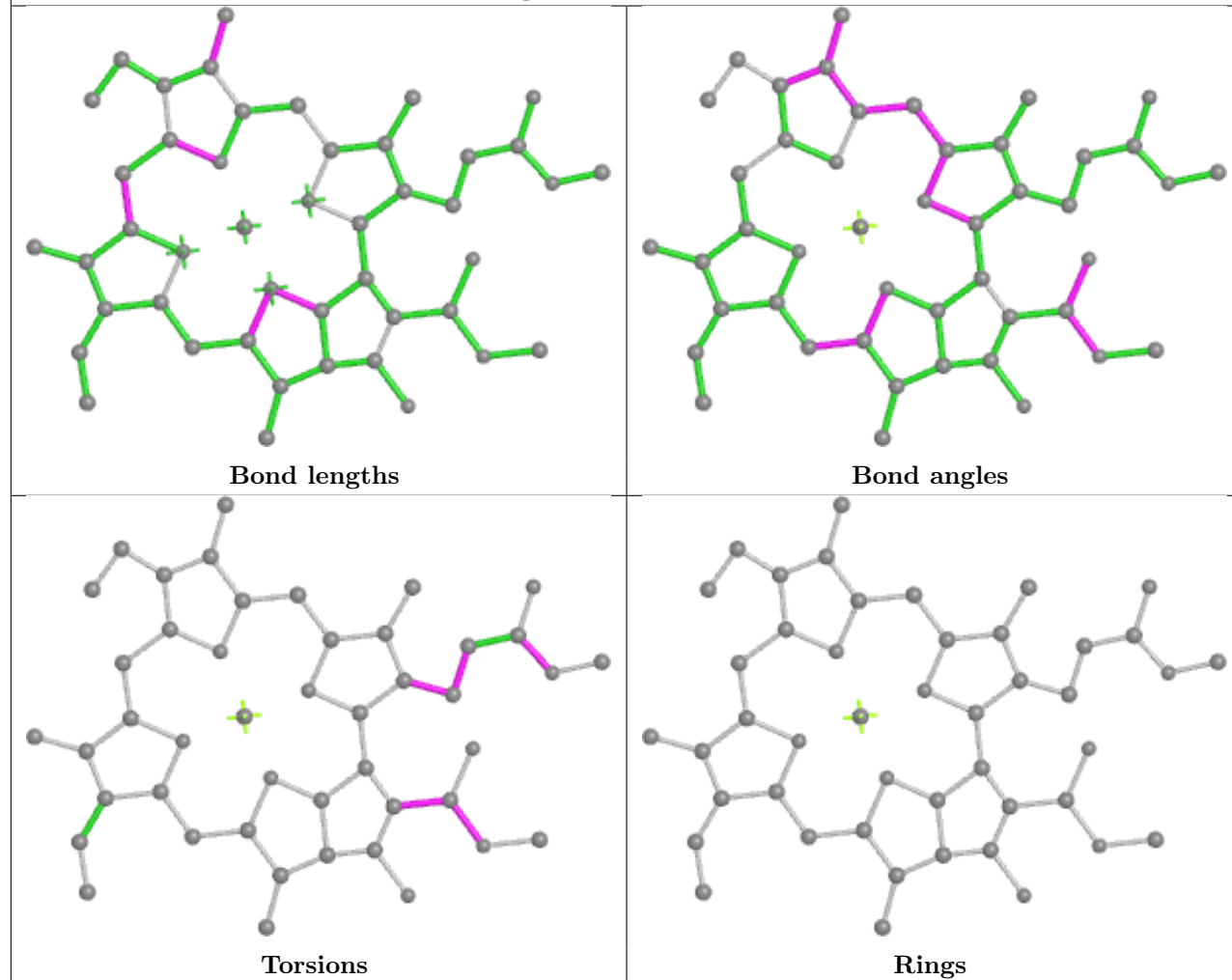




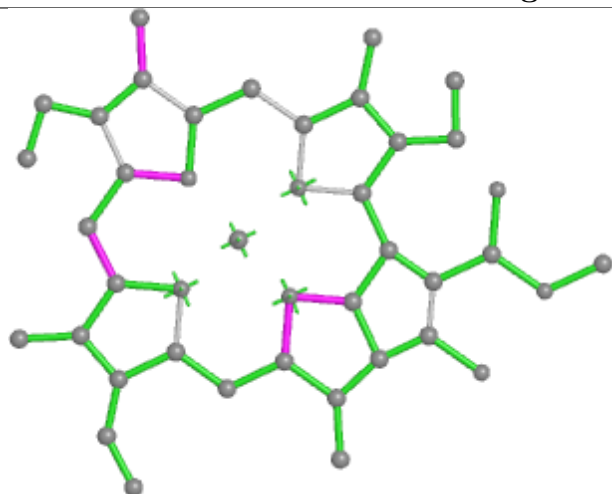
## Ligand CLA b 811



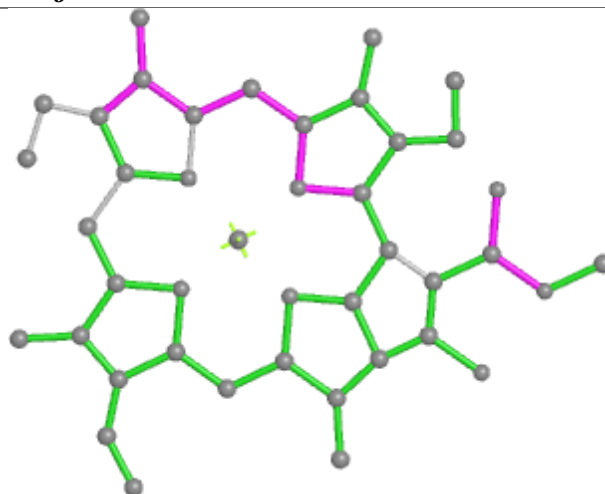
## Ligand CLA 4 316



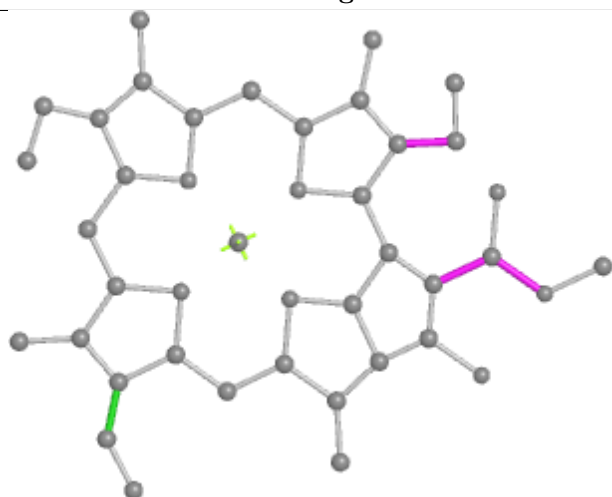
## Ligand CLA j 103



Bond lengths



Bond angles

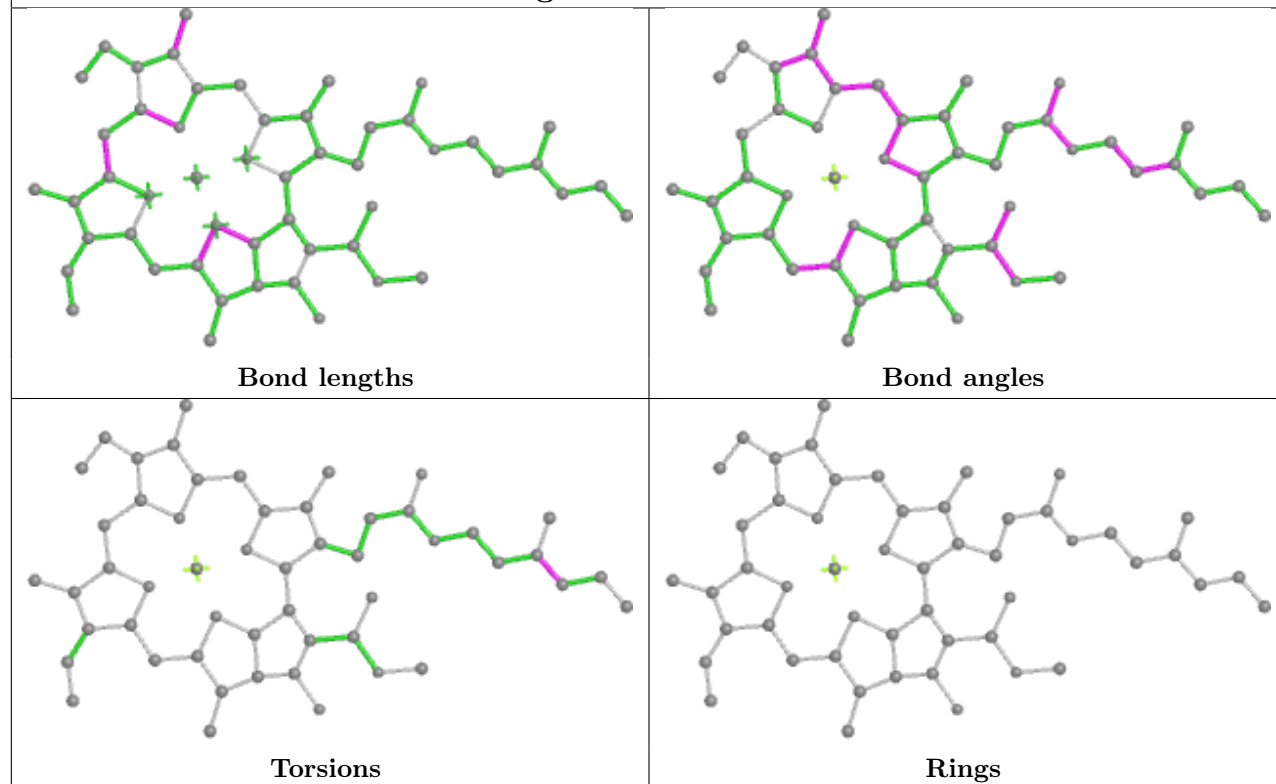


Torsions

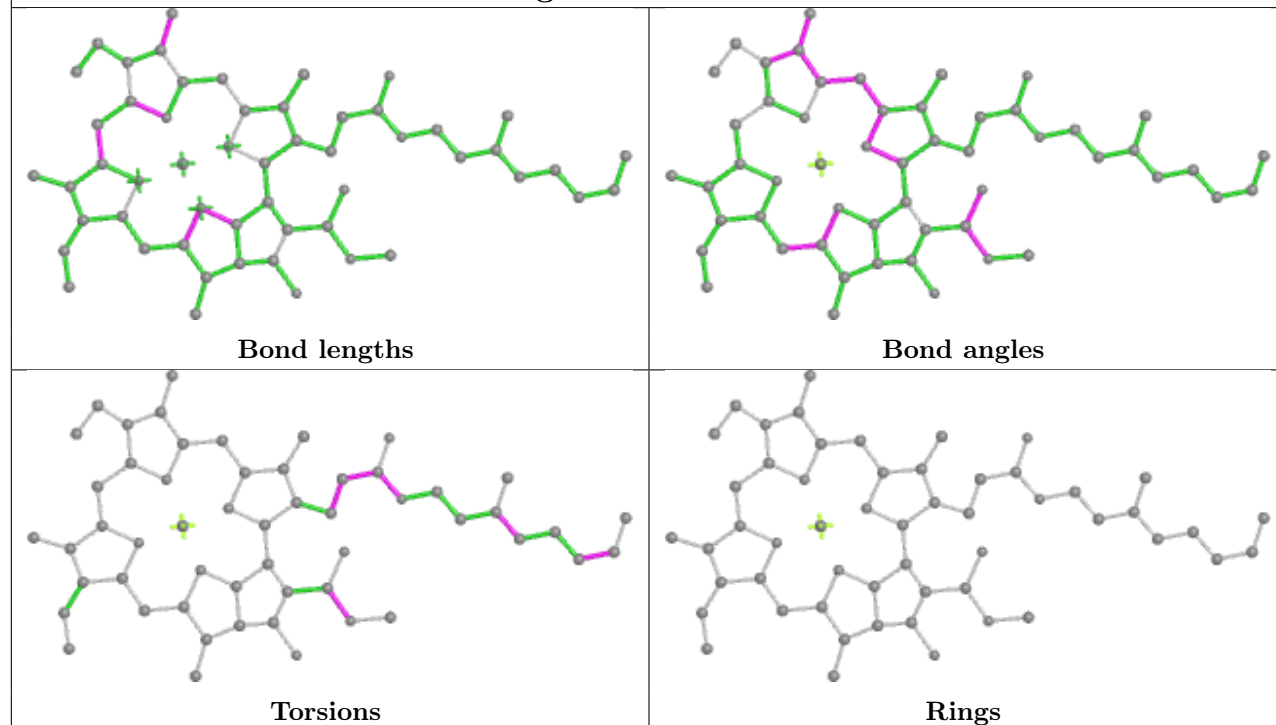


Rings

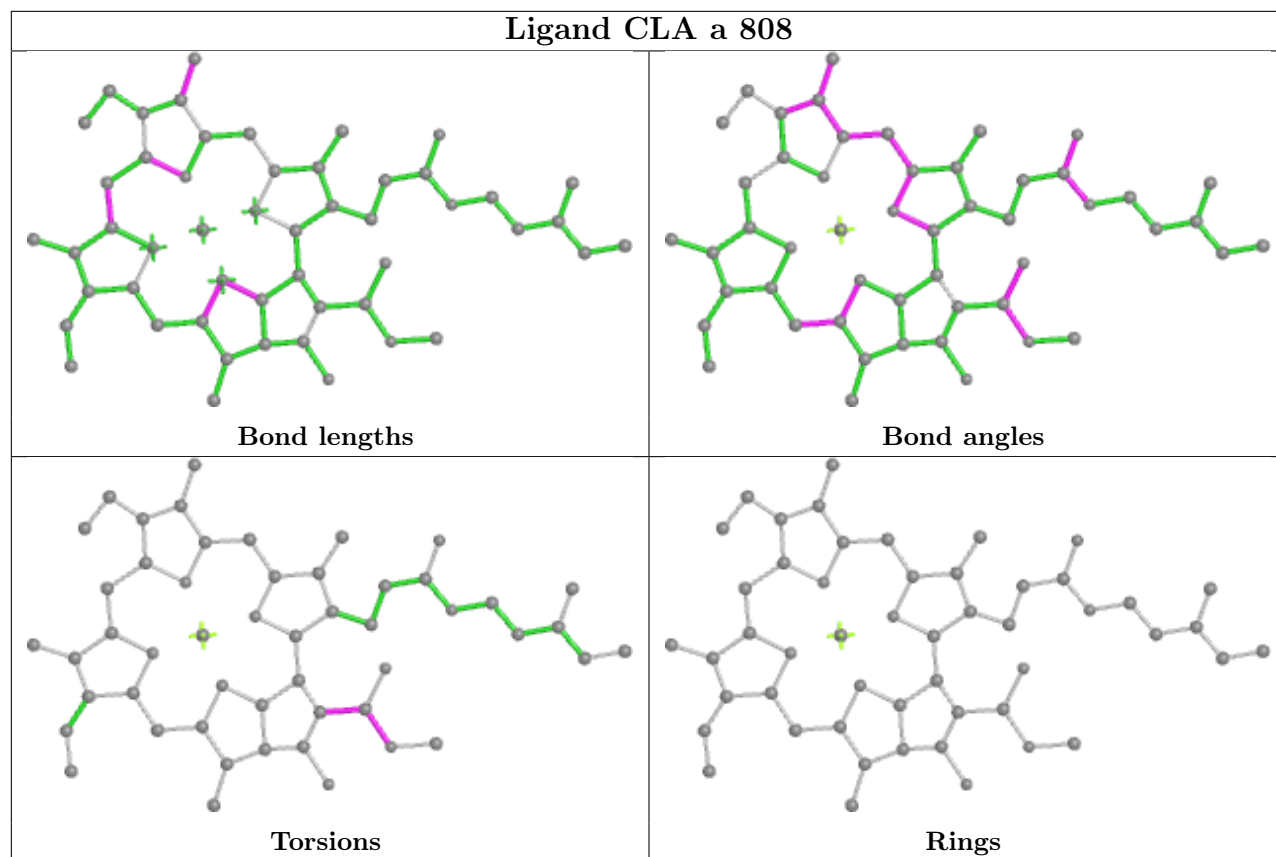
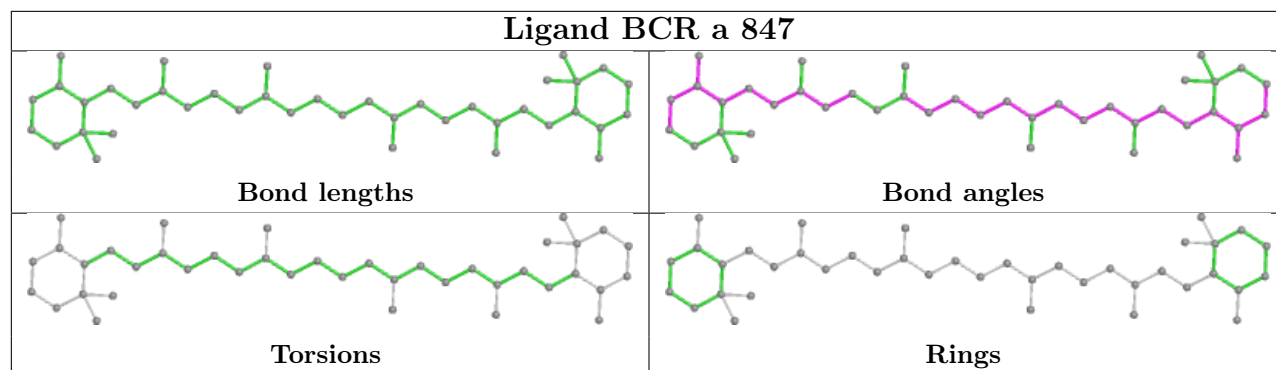
## Ligand CLA 3 313



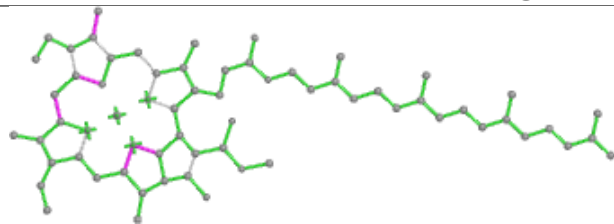
## Ligand CLA a 813



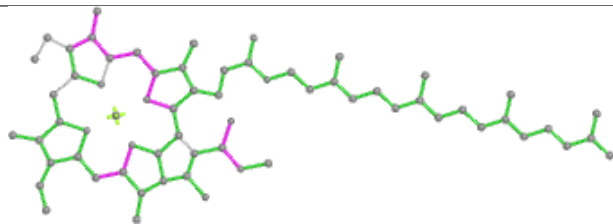




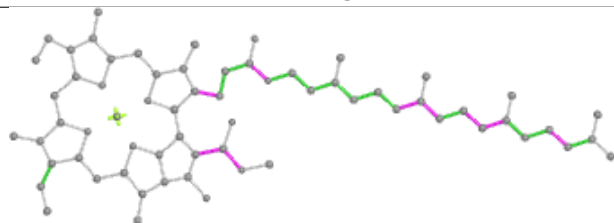
## Ligand CLA b 806



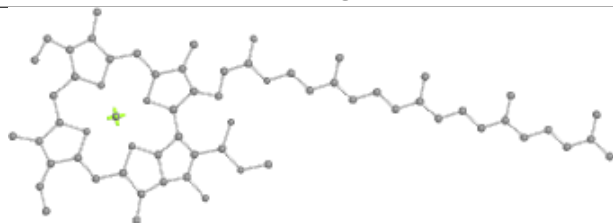
Bond lengths



Bond angles

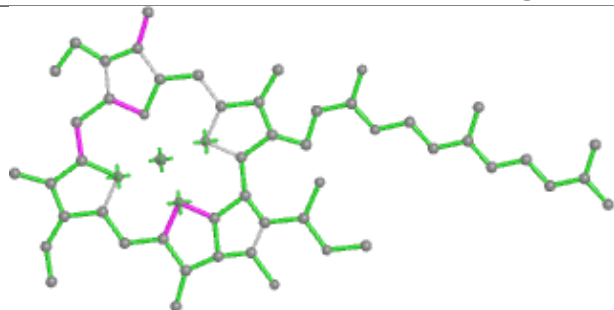


Torsions

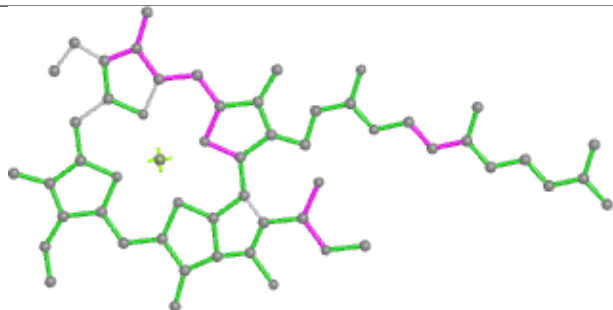


Rings

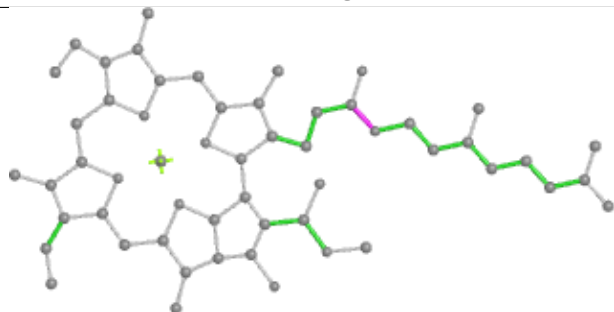
## Ligand CLA a 833



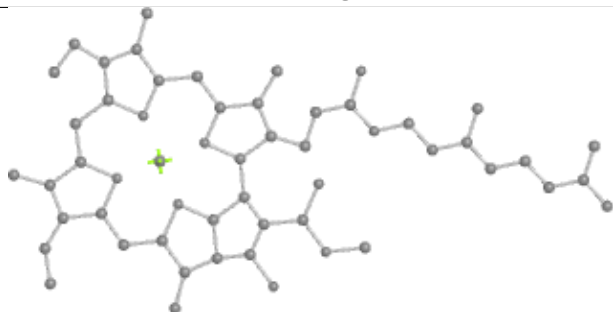
Bond lengths



Bond angles

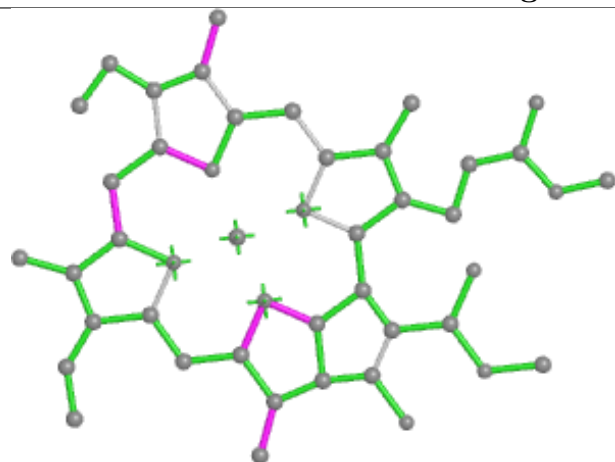


Torsions

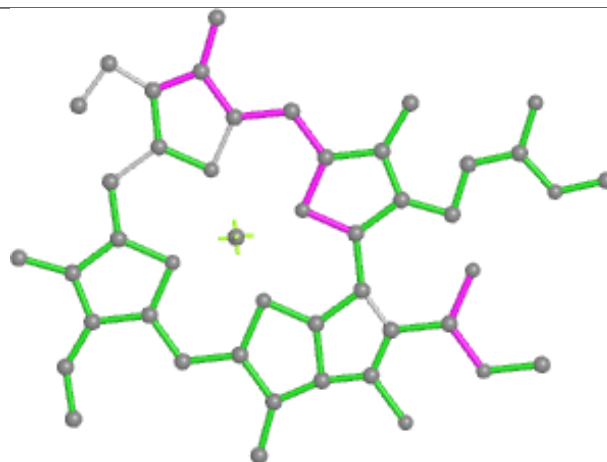


Rings

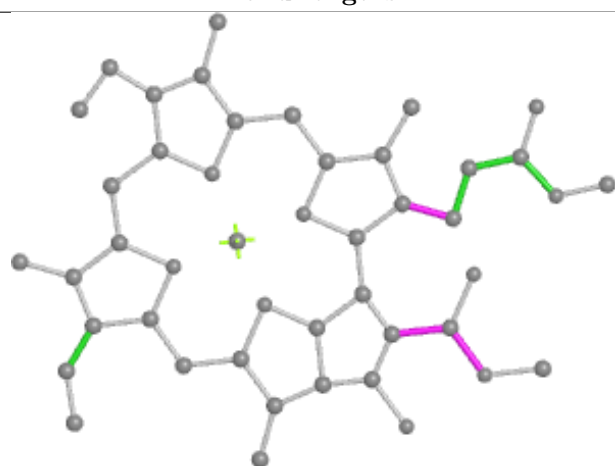
## Ligand CLA 2 316



Bond lengths



Bond angles

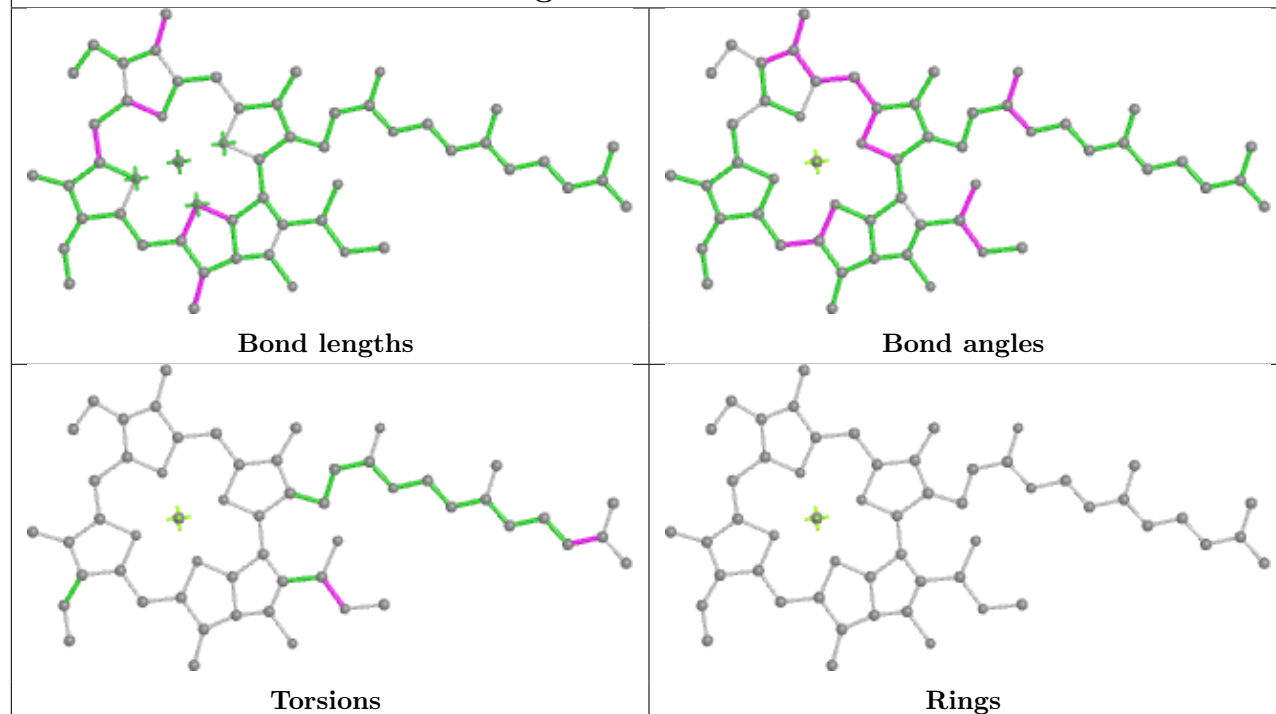


Torsions

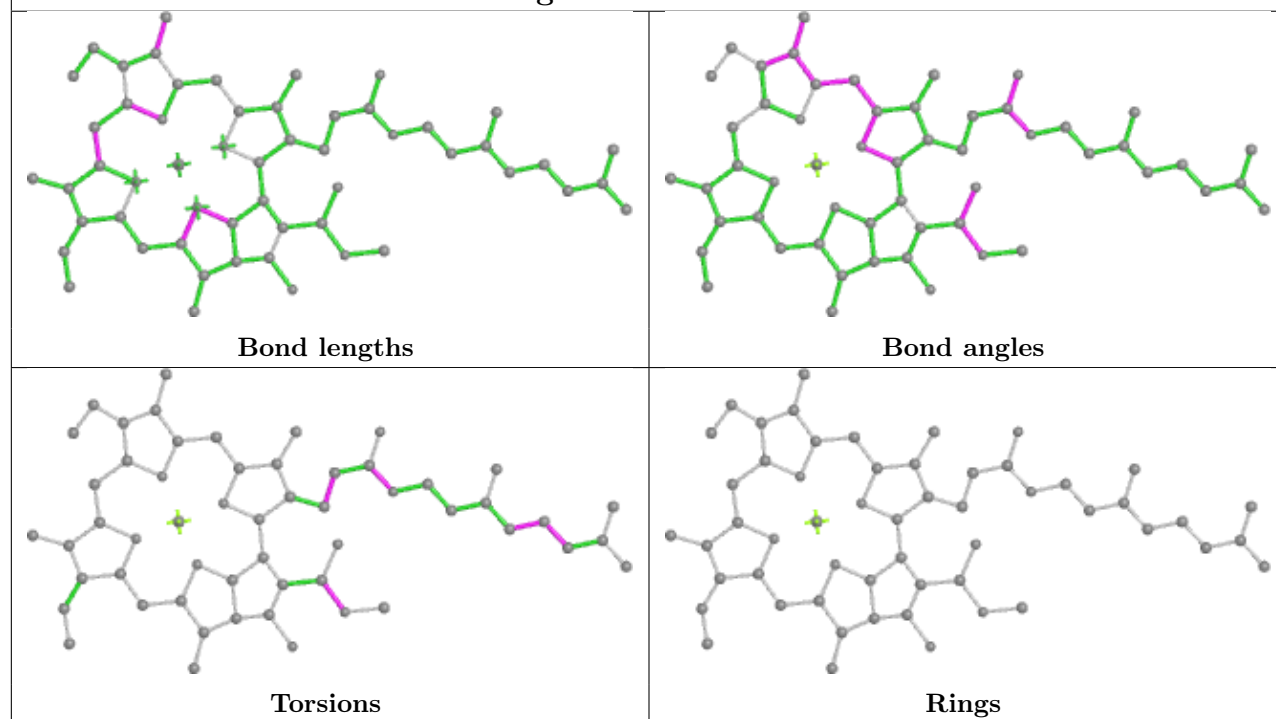


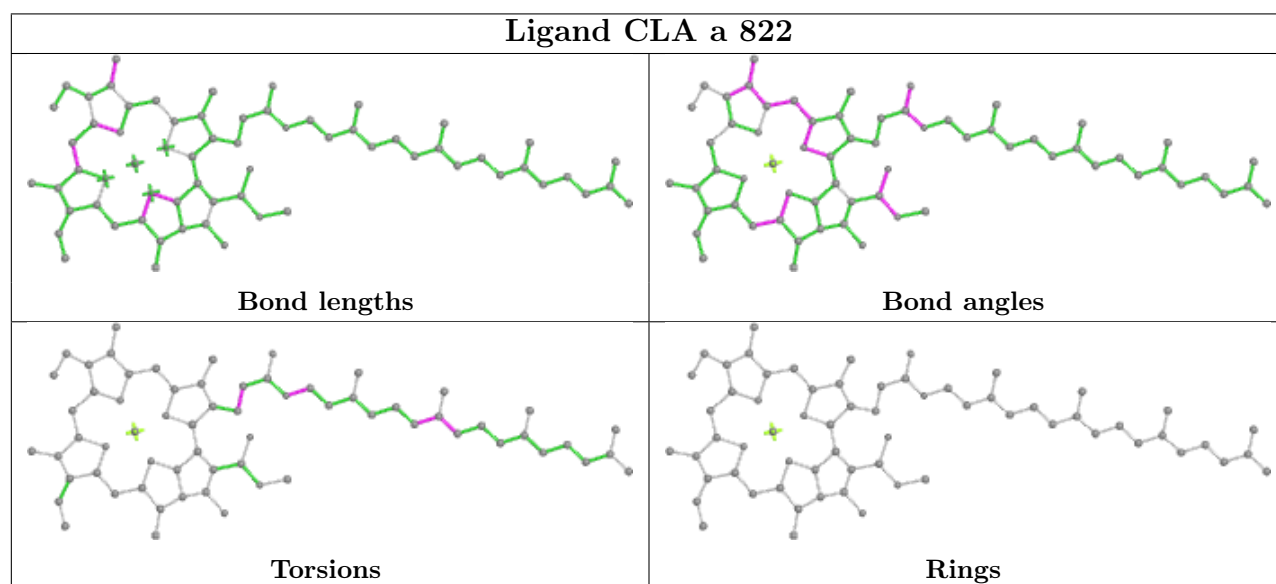
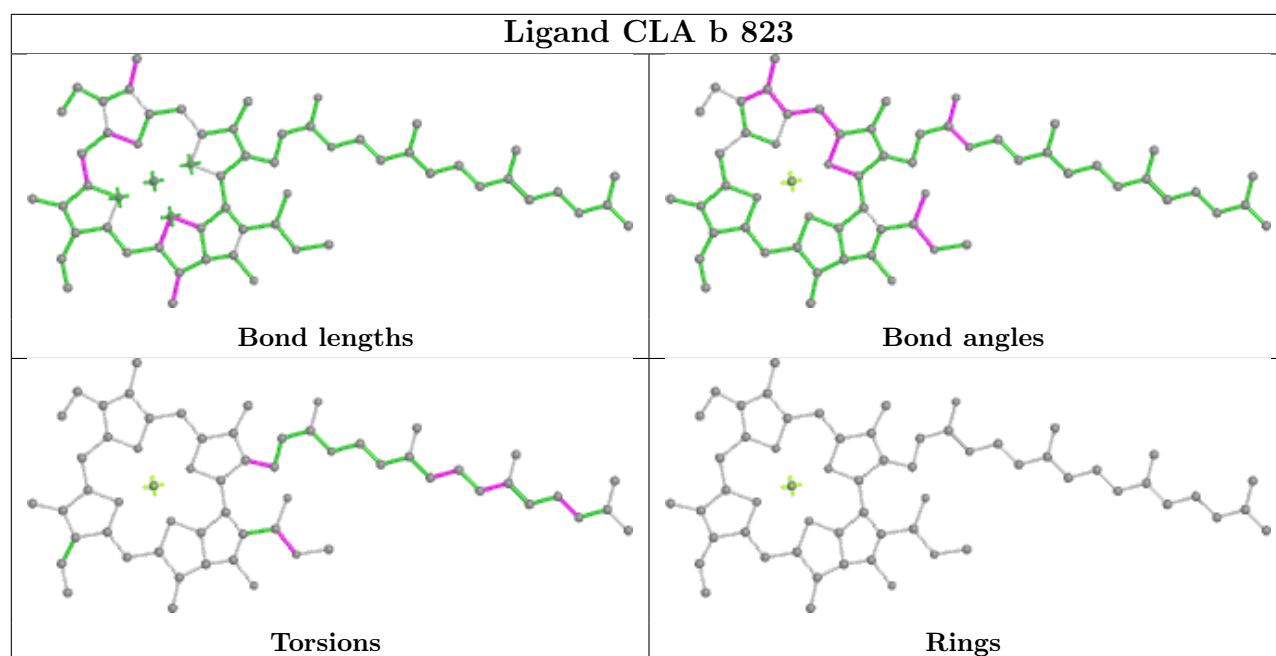
Rings

## Ligand CLA b 820

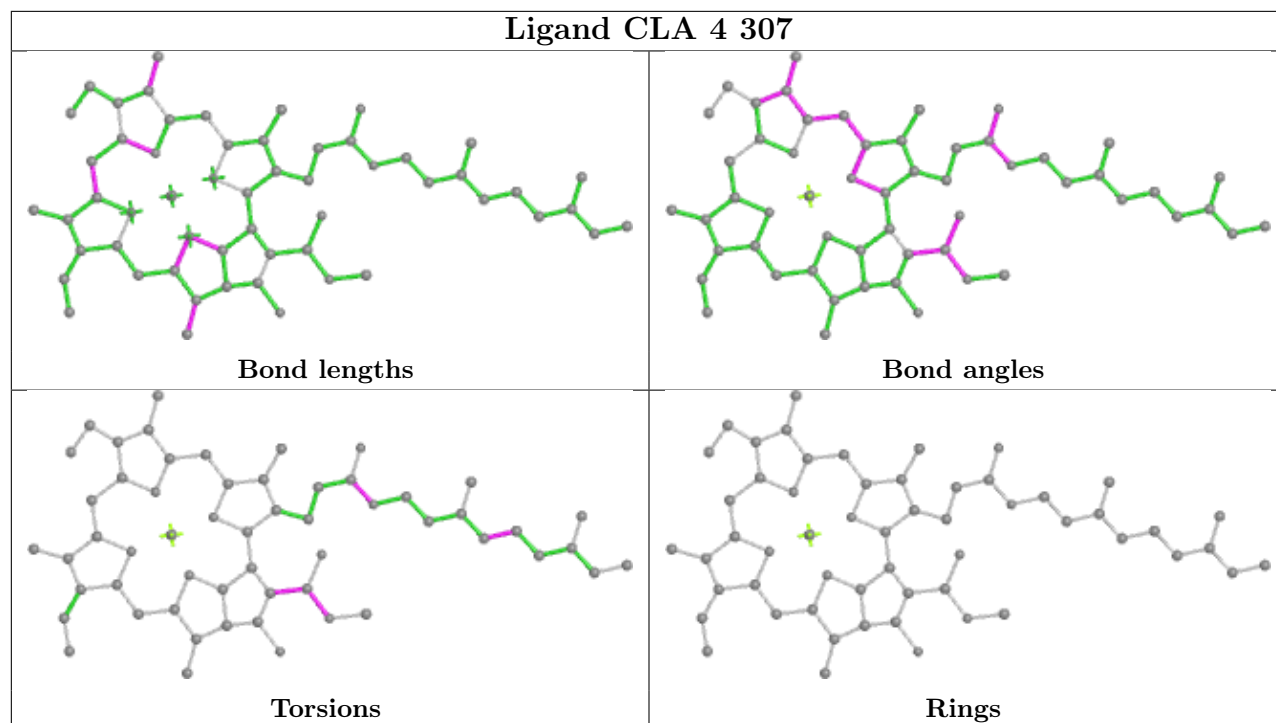


## Ligand CLA 4 317

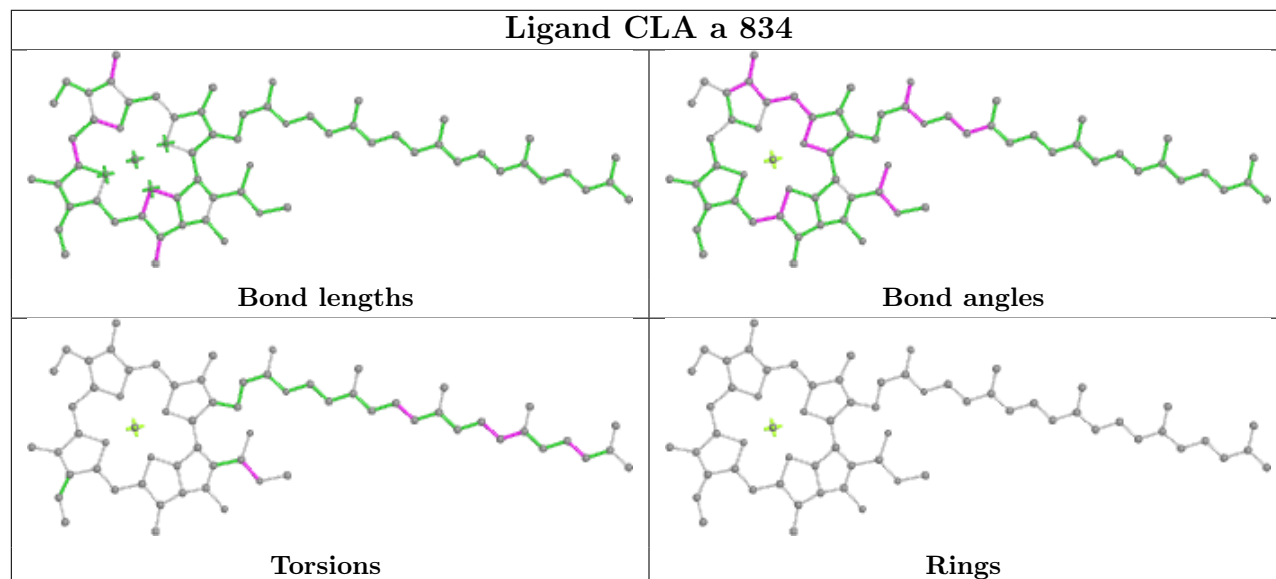


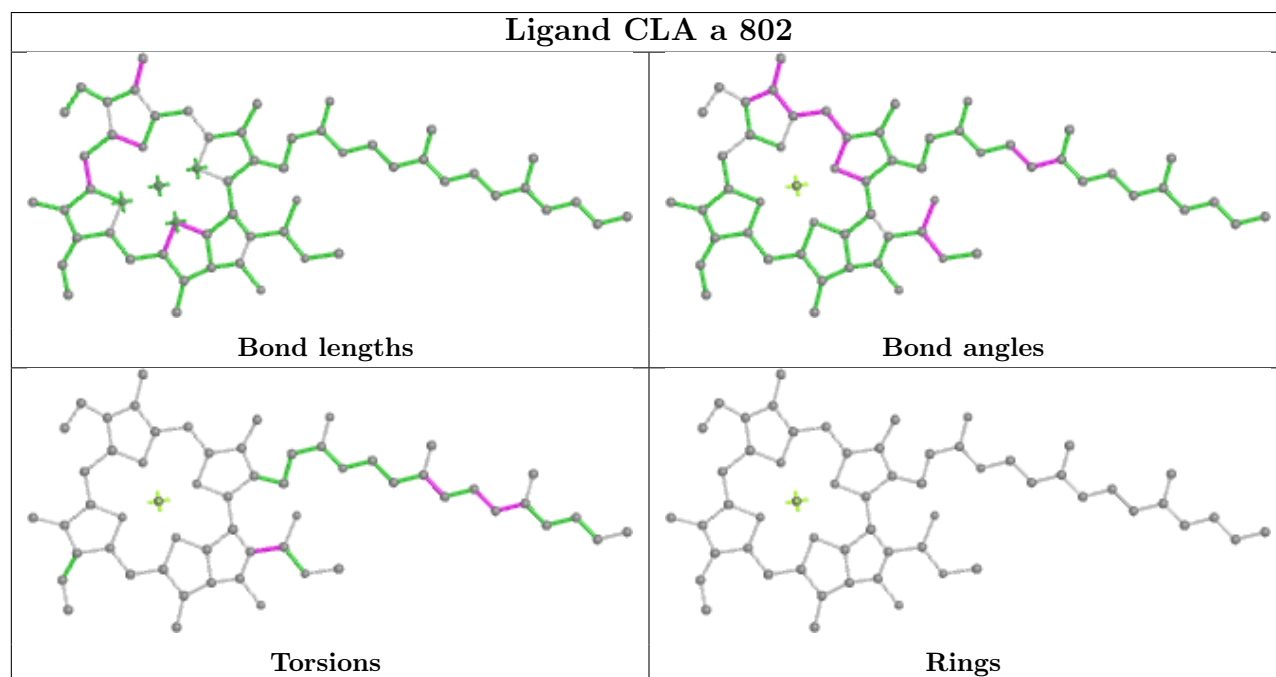
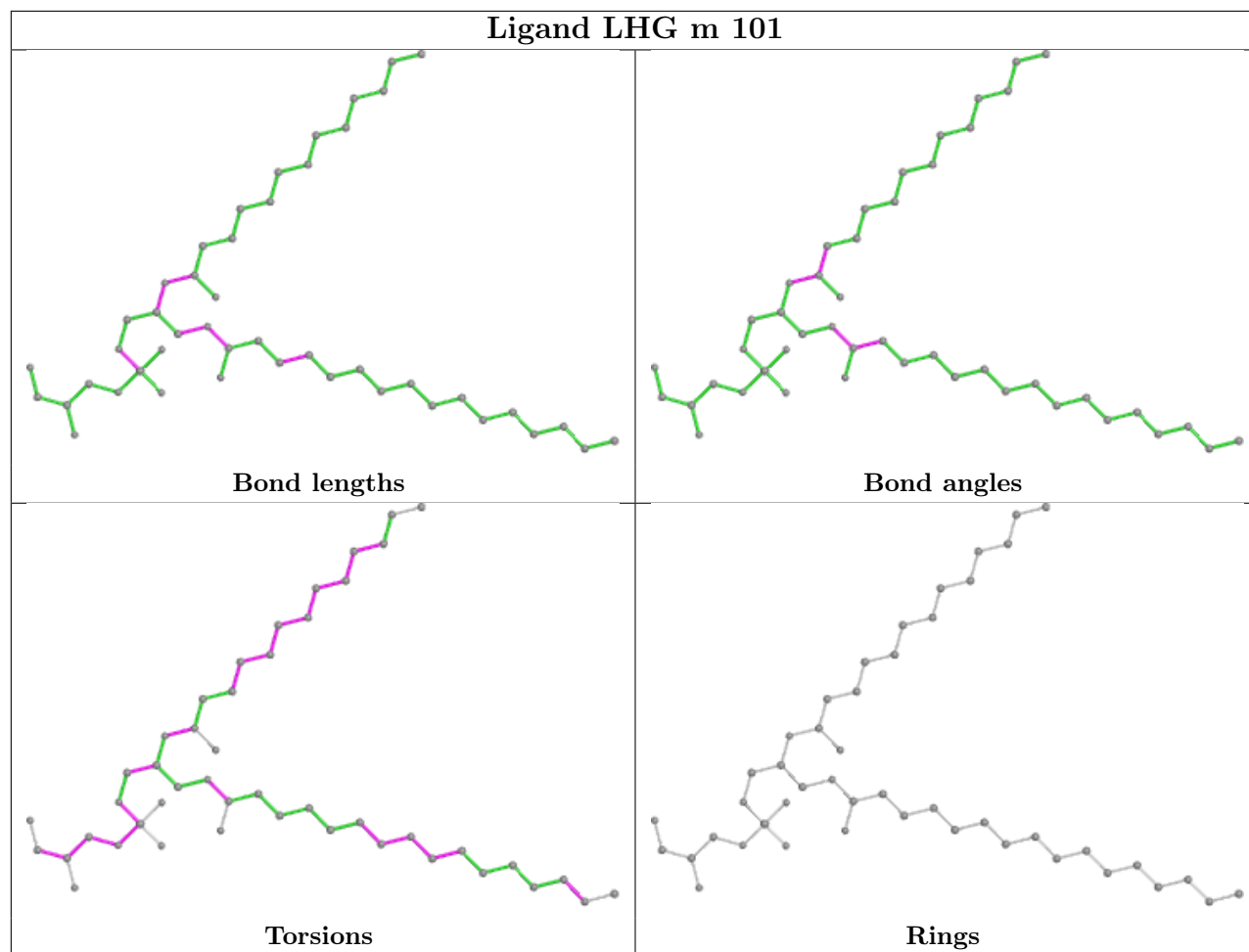


## Ligand CLA 4 307

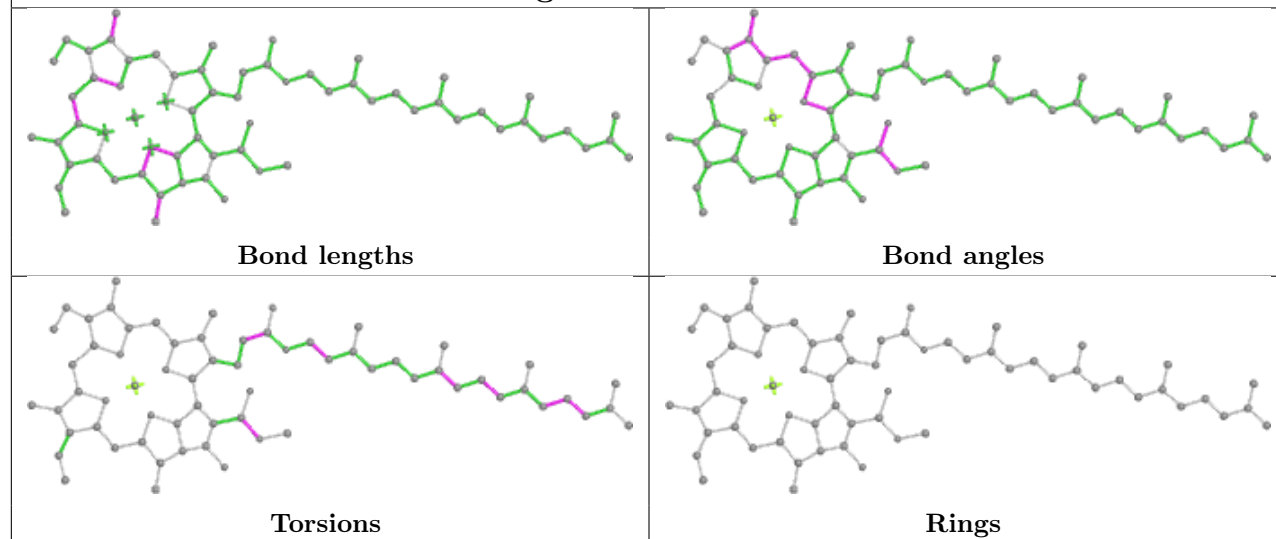


## Ligand CLA a 834

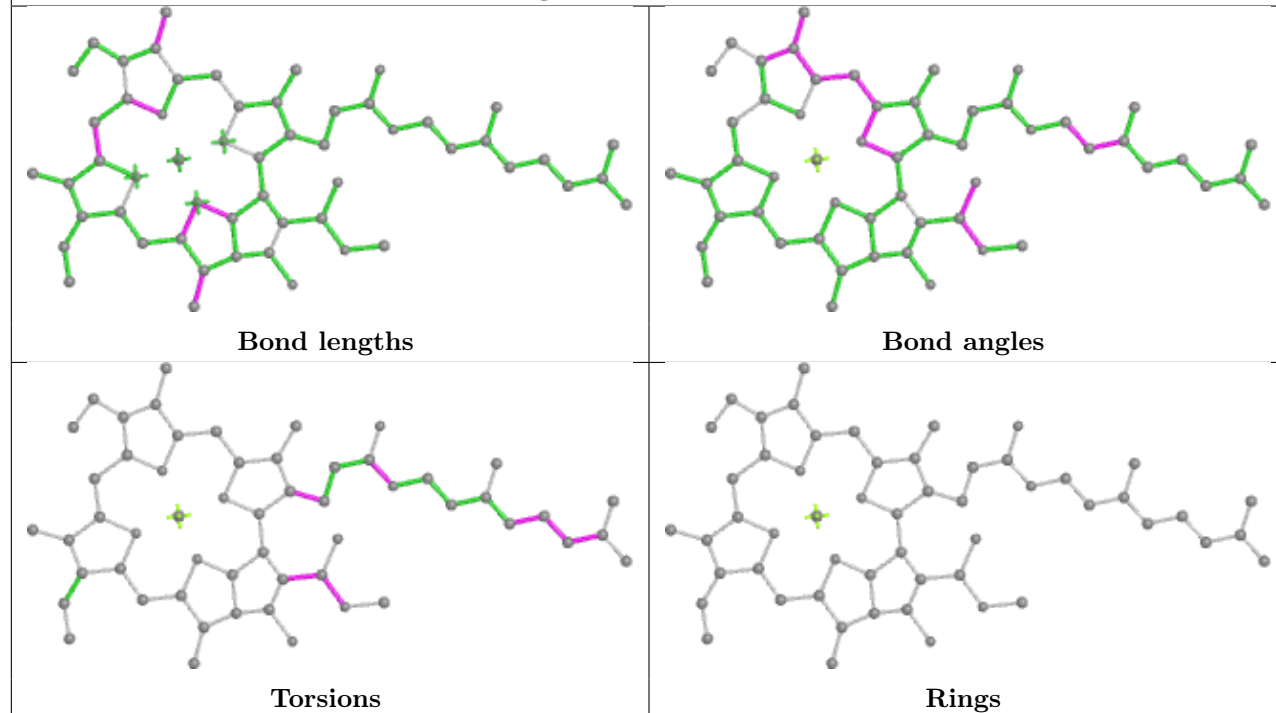




## Ligand CLA a 826

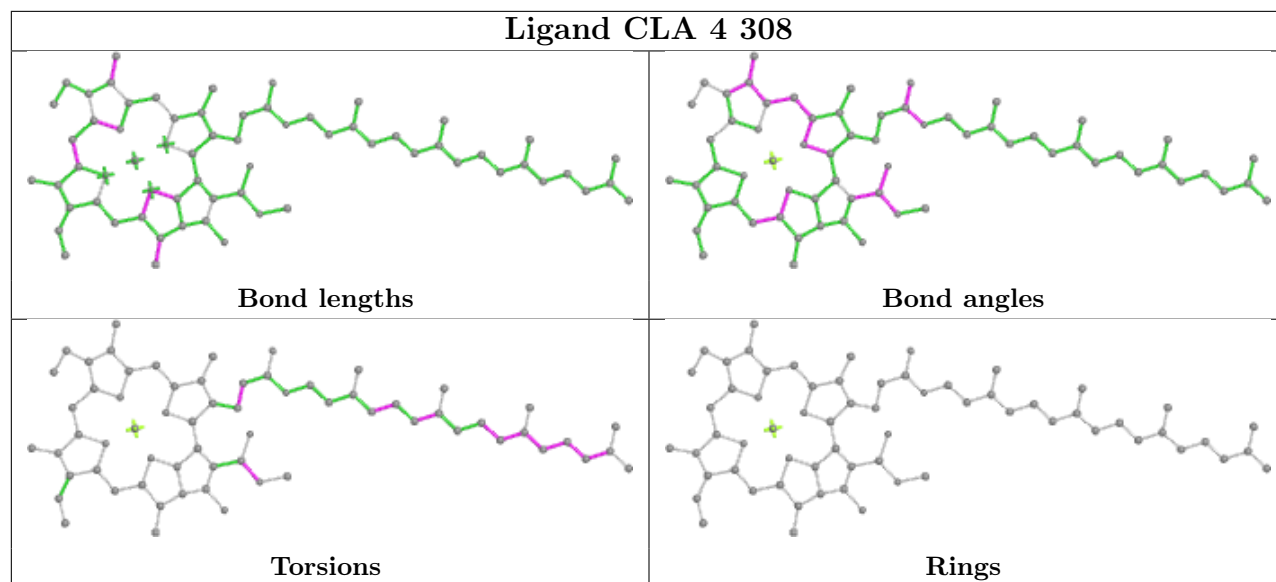


## Ligand CLA b 815

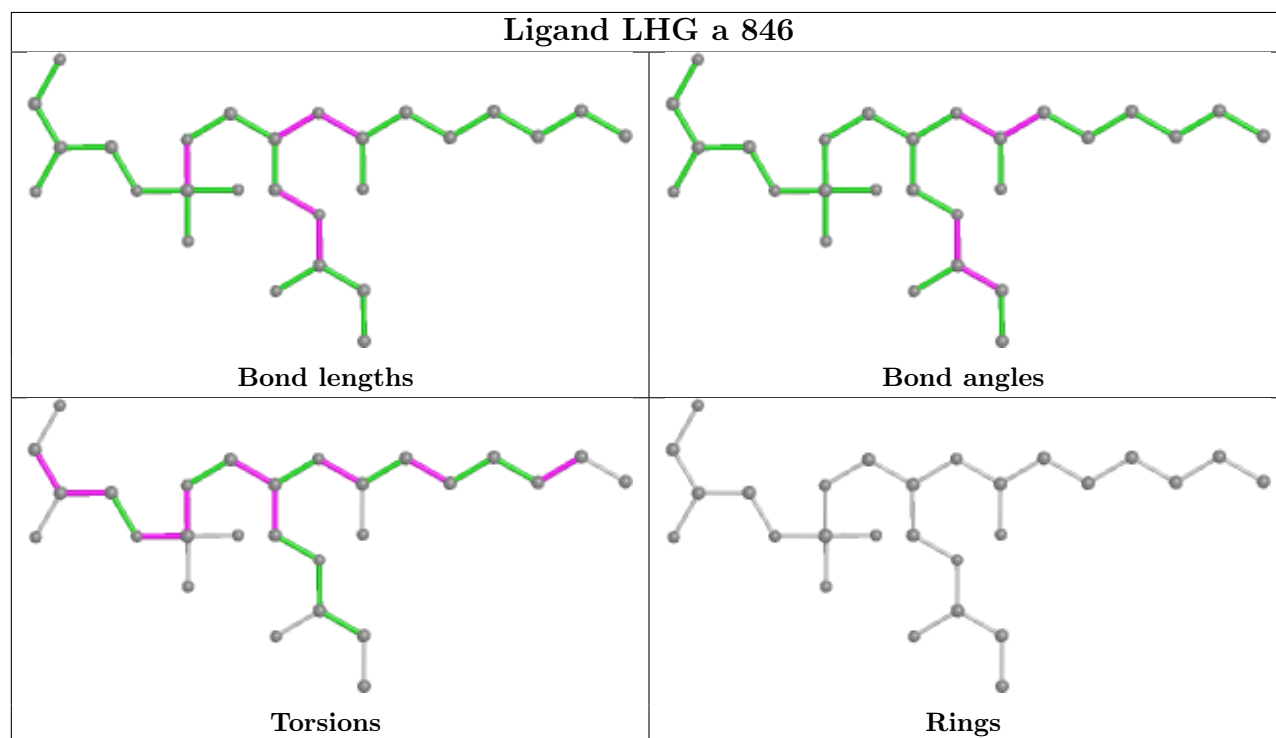




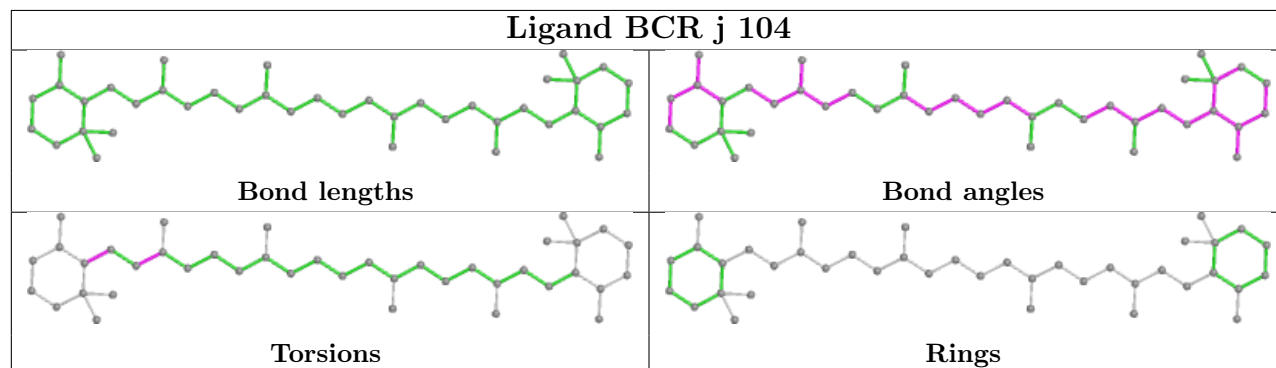
## Ligand CLA 4 308

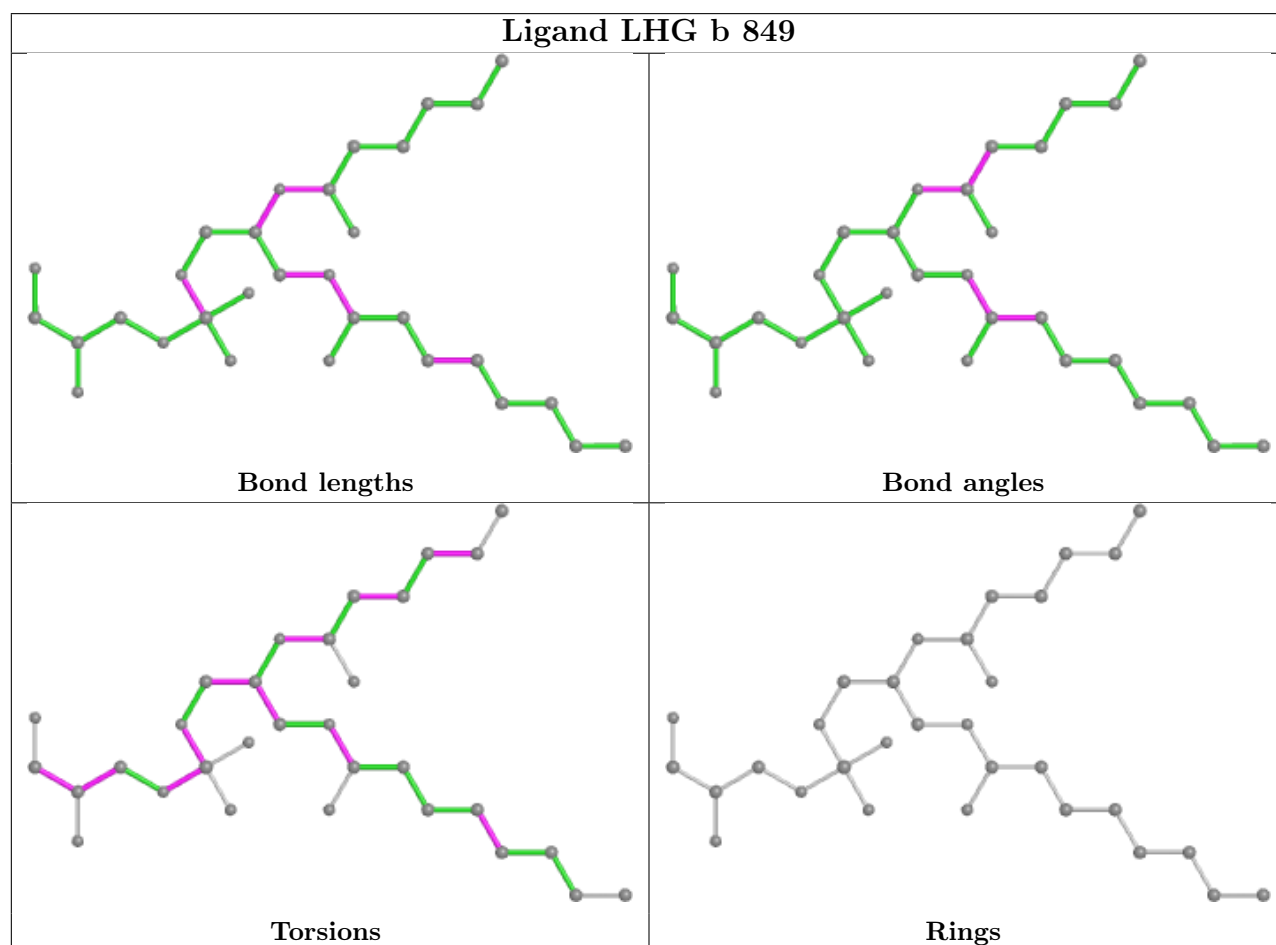
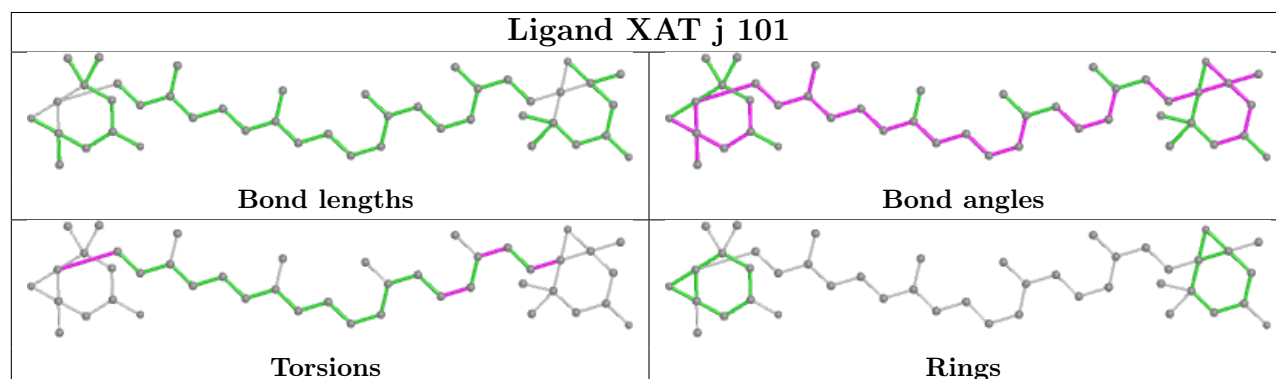
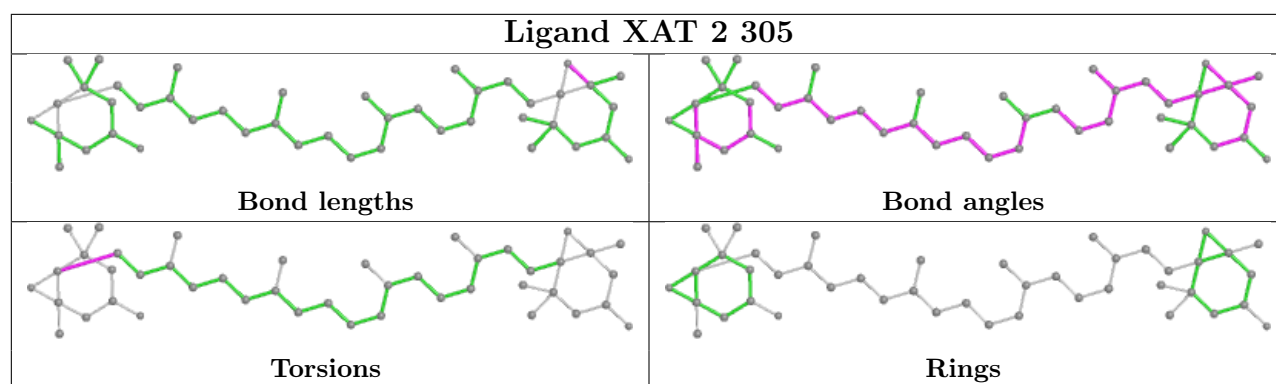


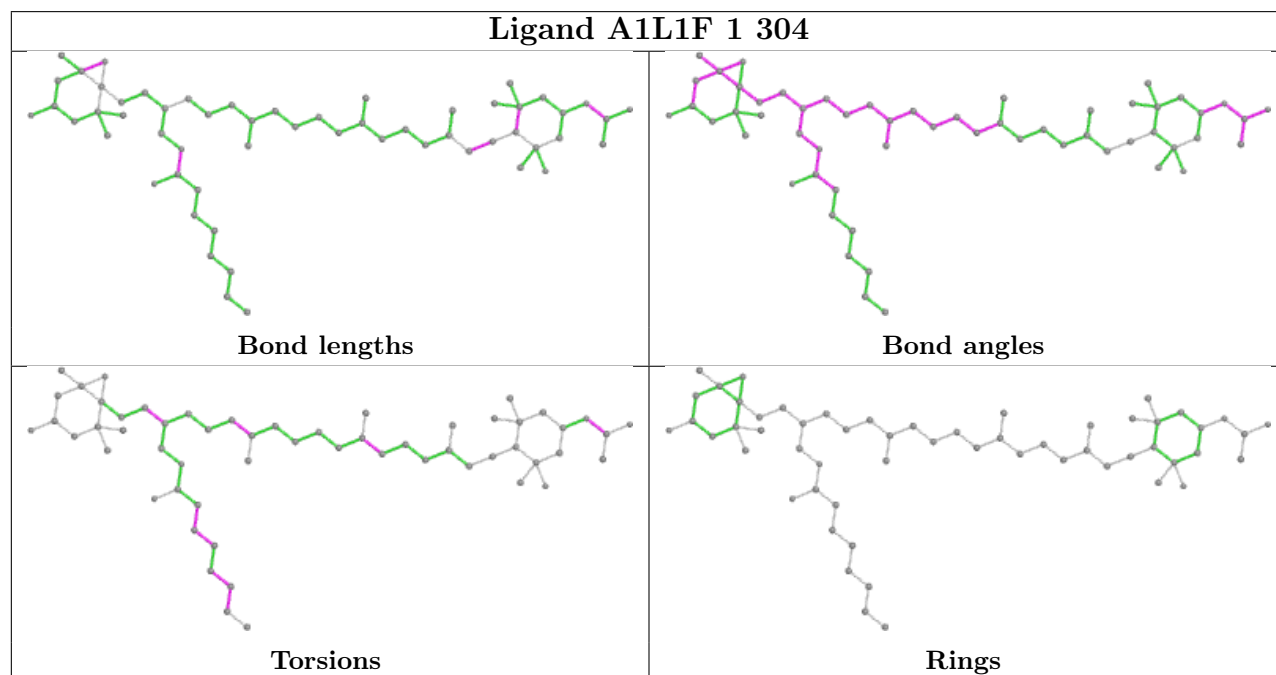
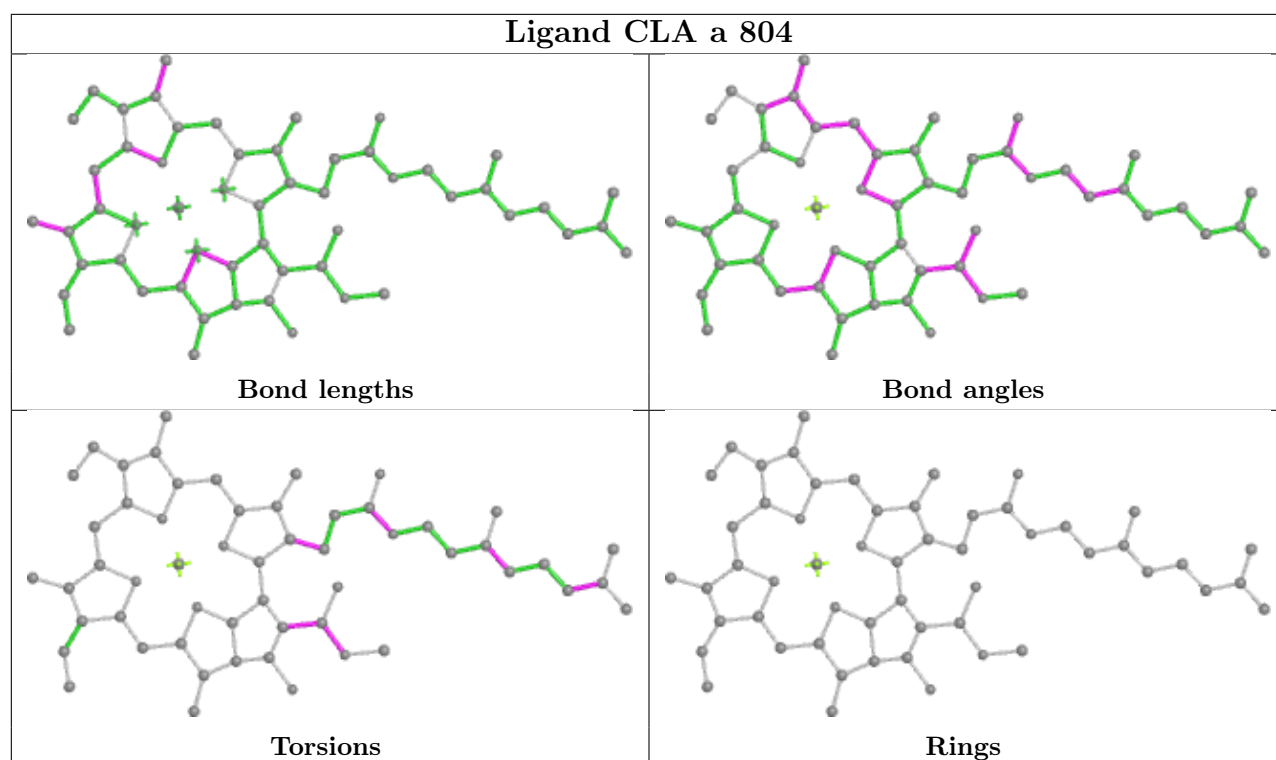
## Ligand LHG a 846

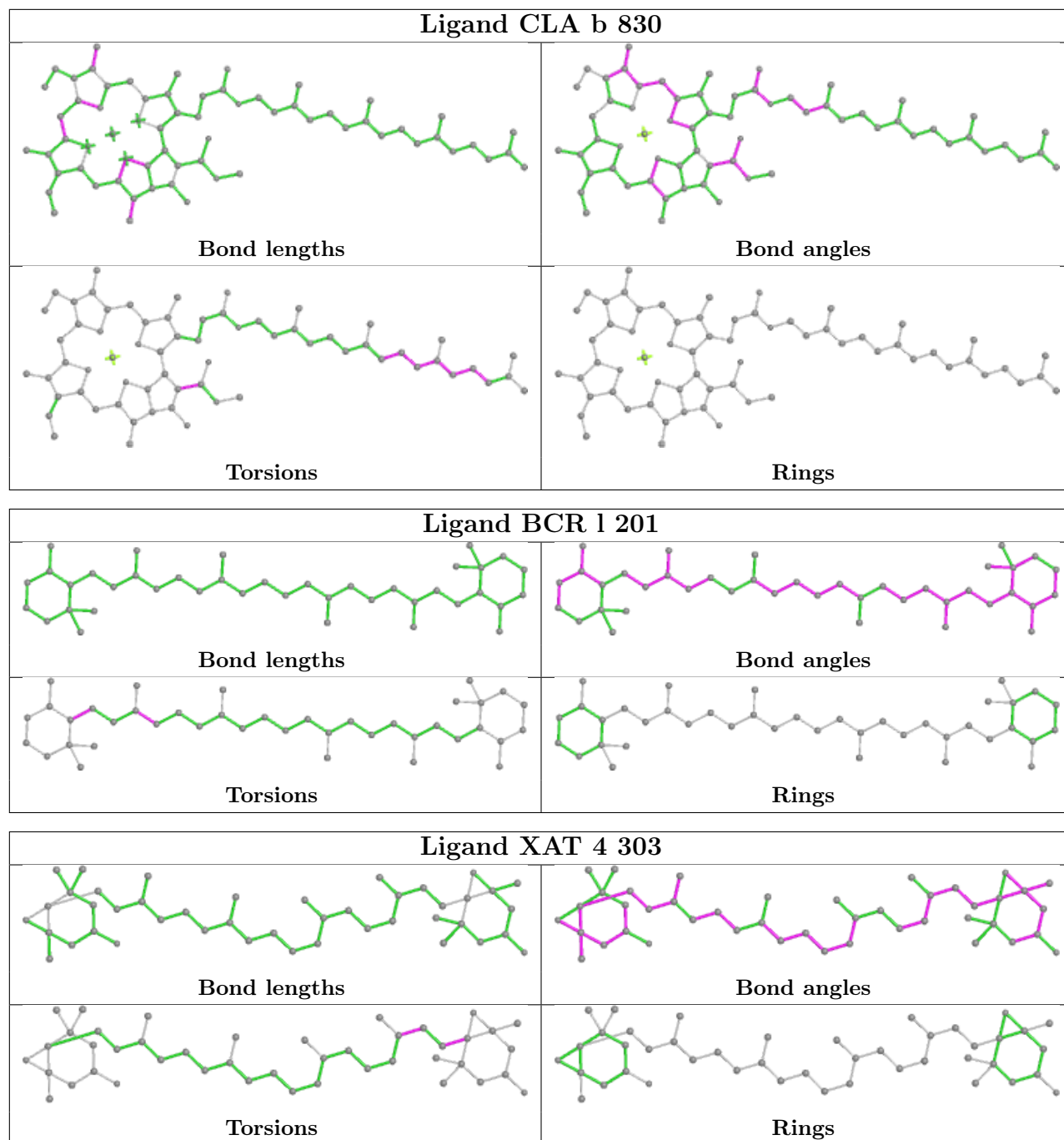


## Ligand BCR j 104

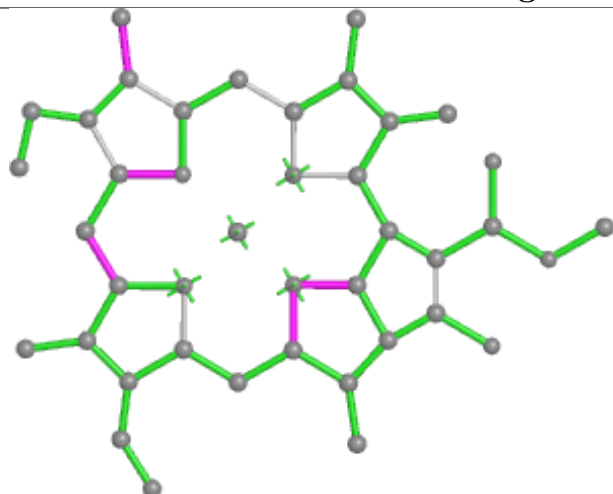




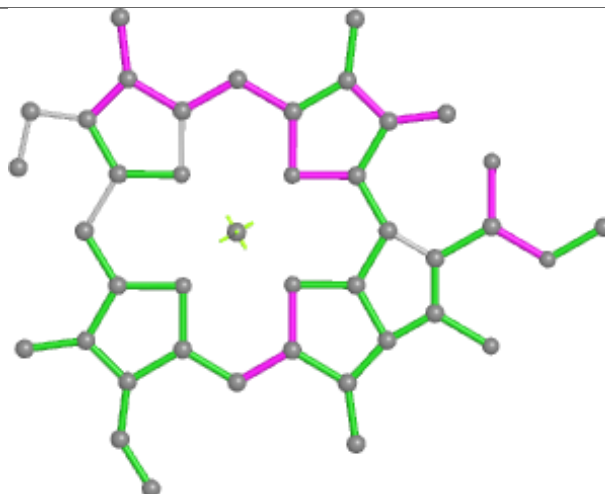




## Ligand CLA 4 315



Bond lengths



Bond angles

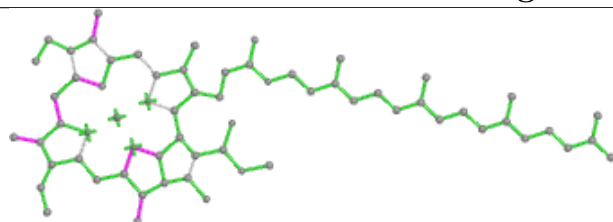


Torsions

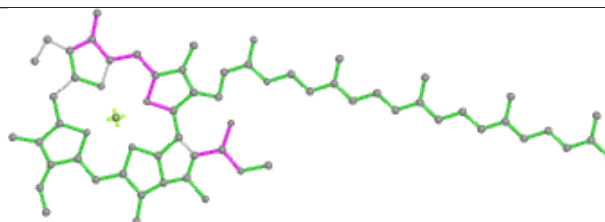


Rings

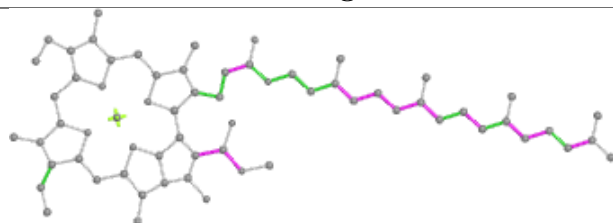
## Ligand CLA b 803



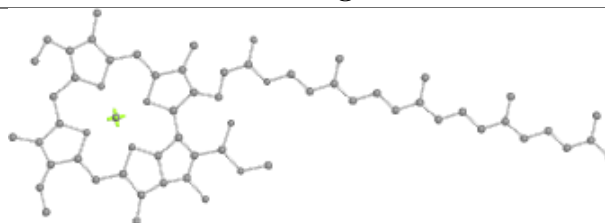
Bond lengths



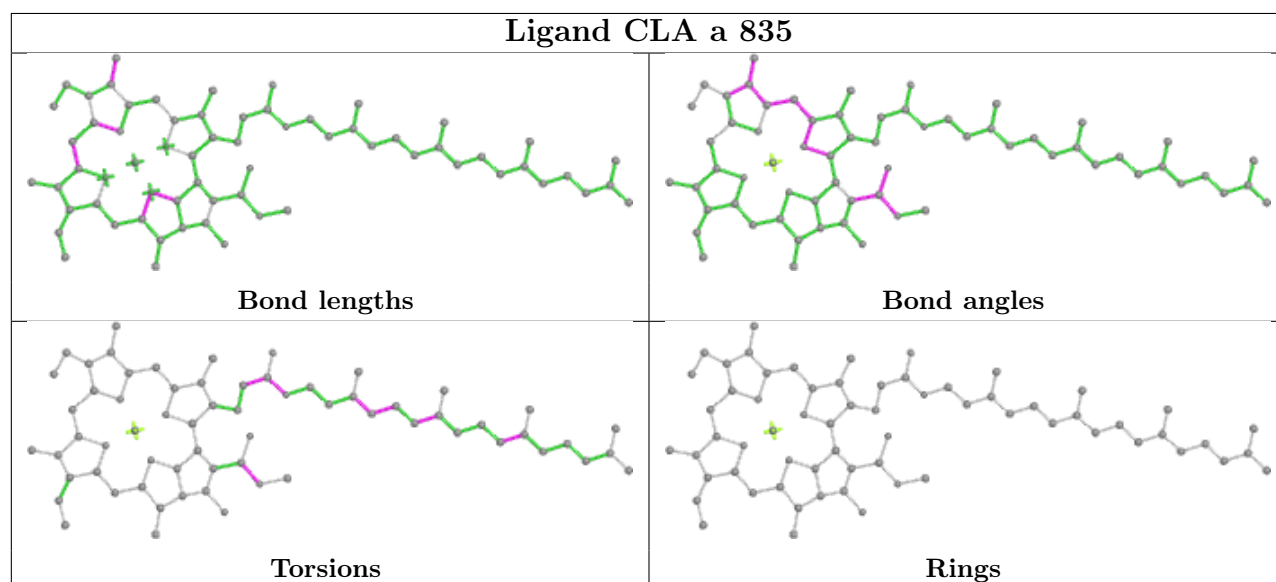
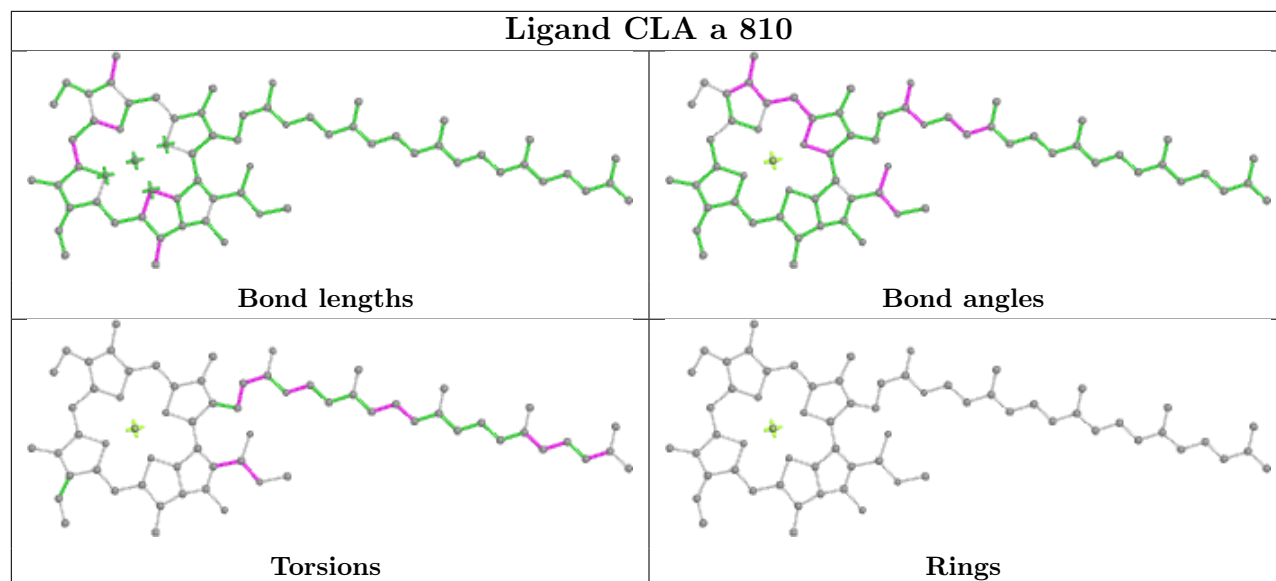
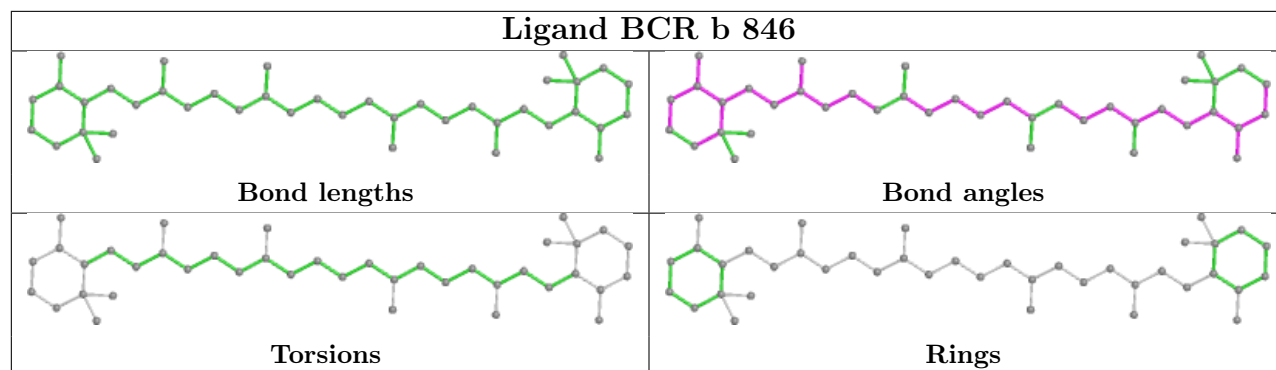
Bond angles



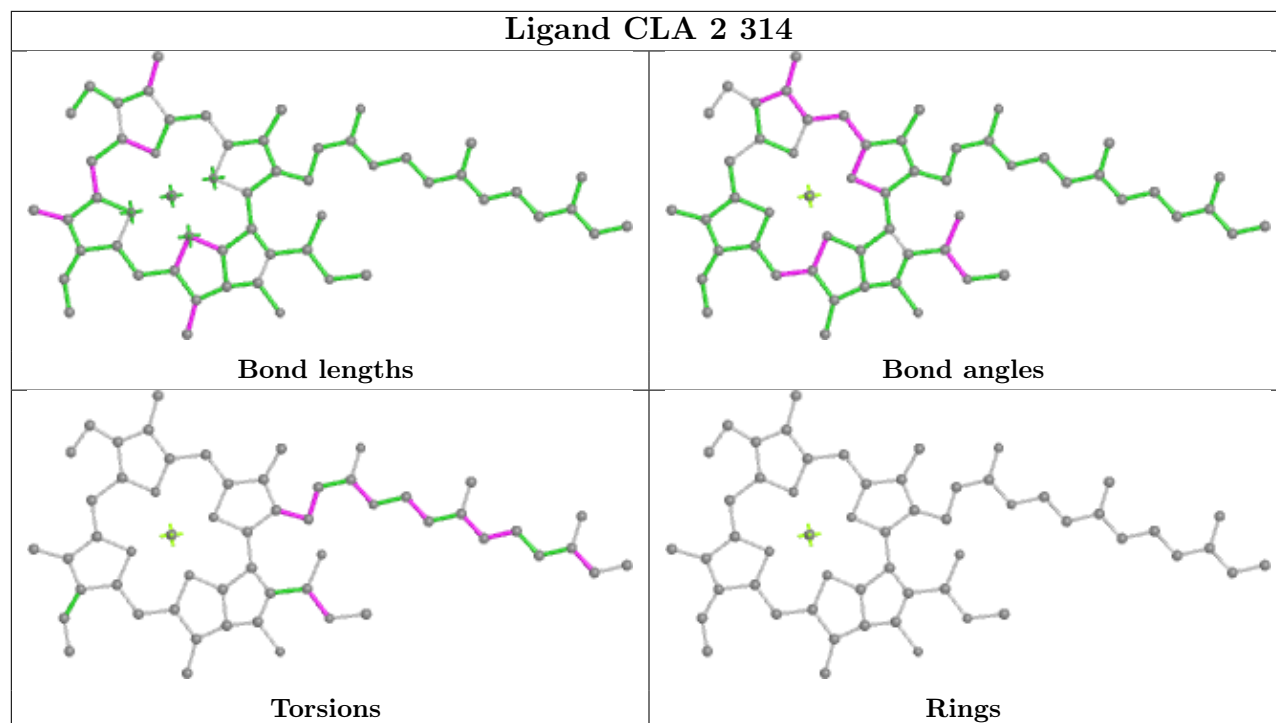
Torsions



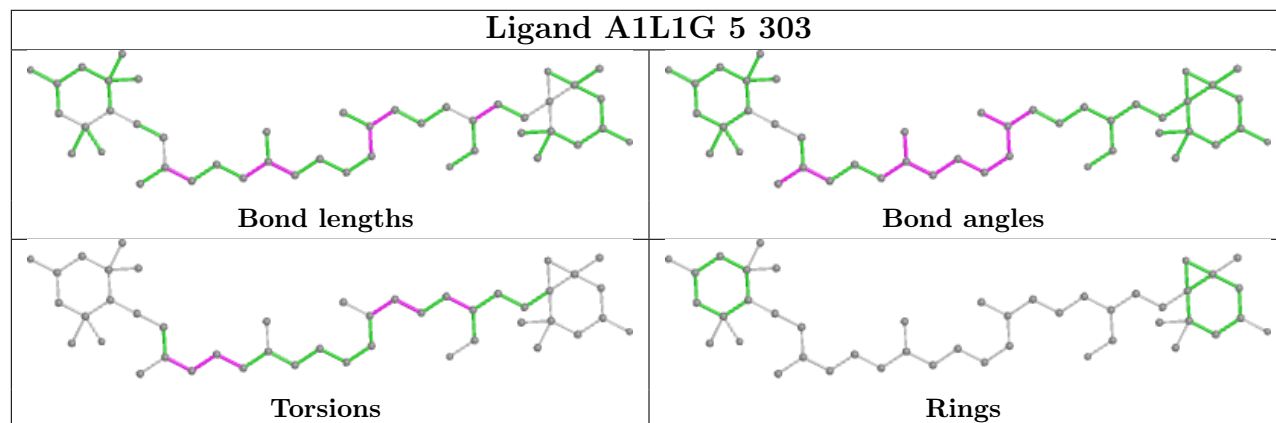
Rings



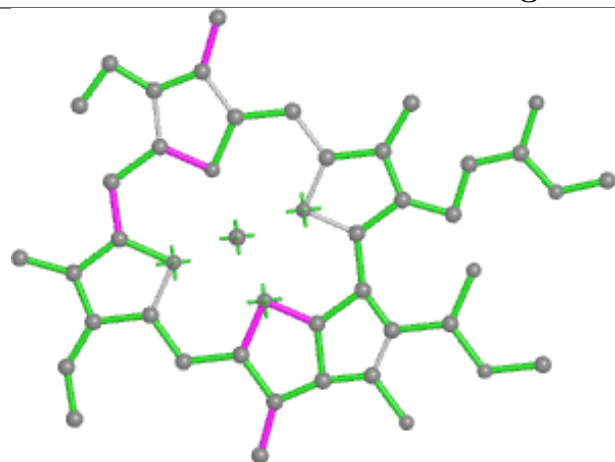
## Ligand CLA 2 314



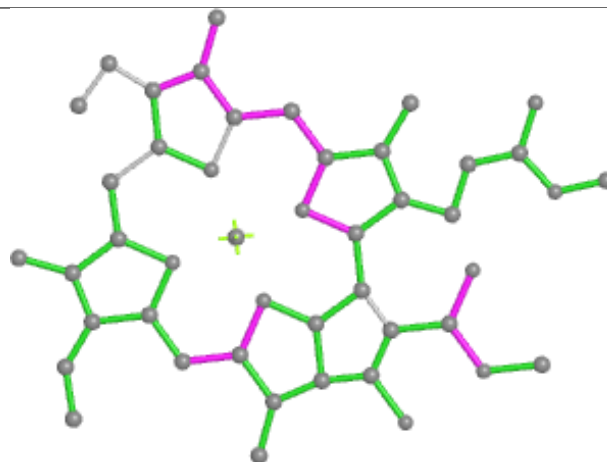
## Ligand A1L1G 5 303



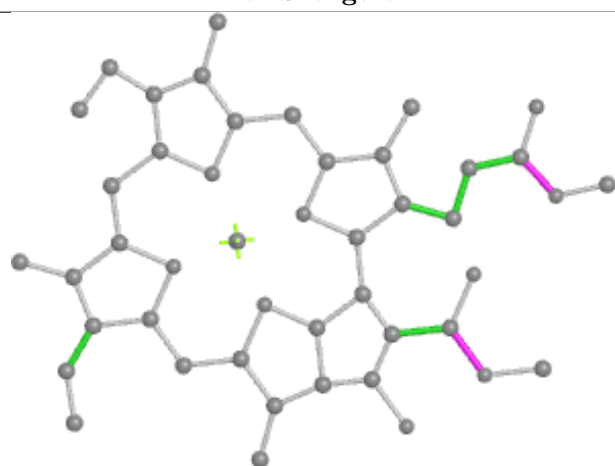
## Ligand CLA 5 305



Bond lengths



Bond angles

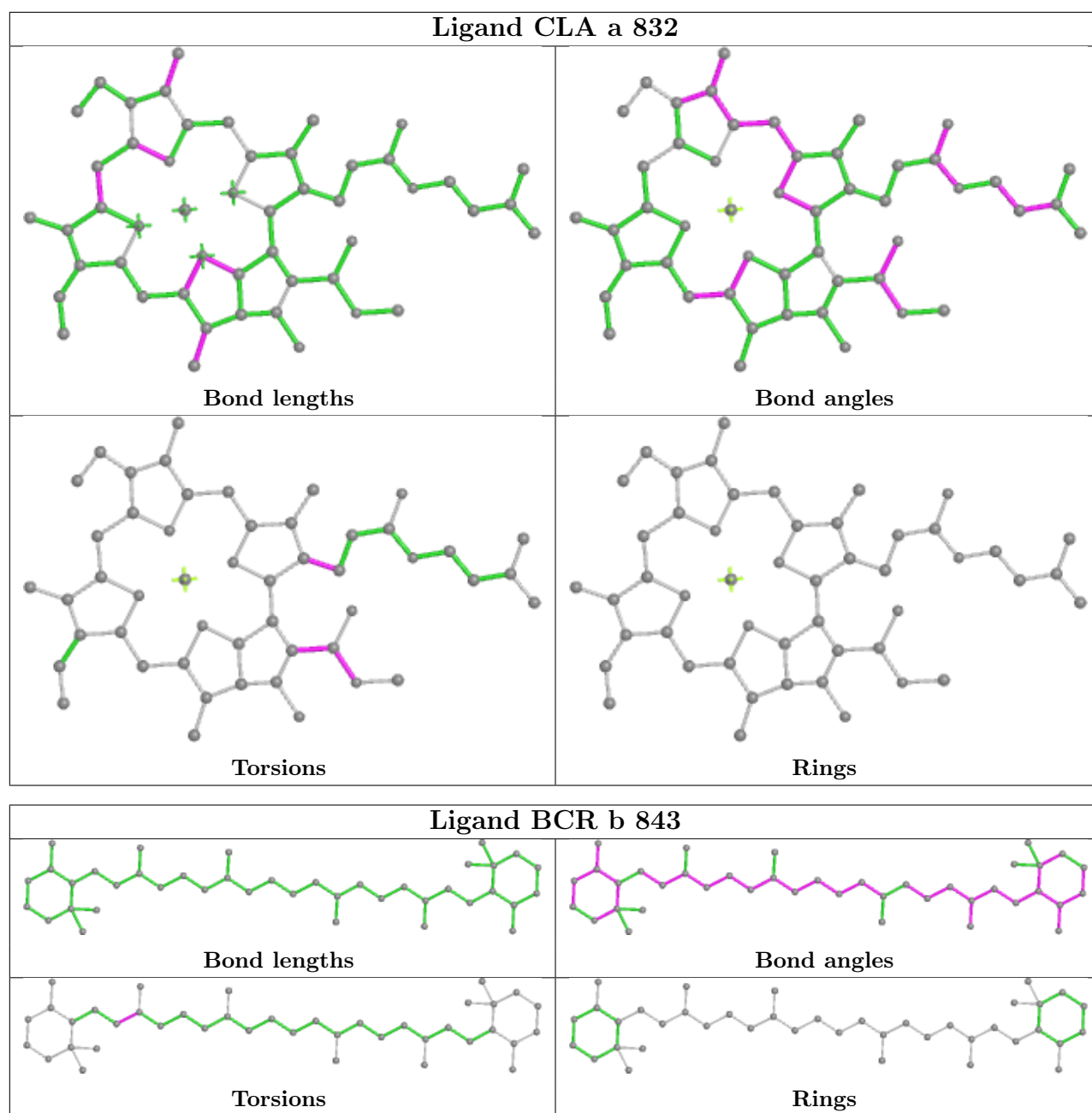


Torsions

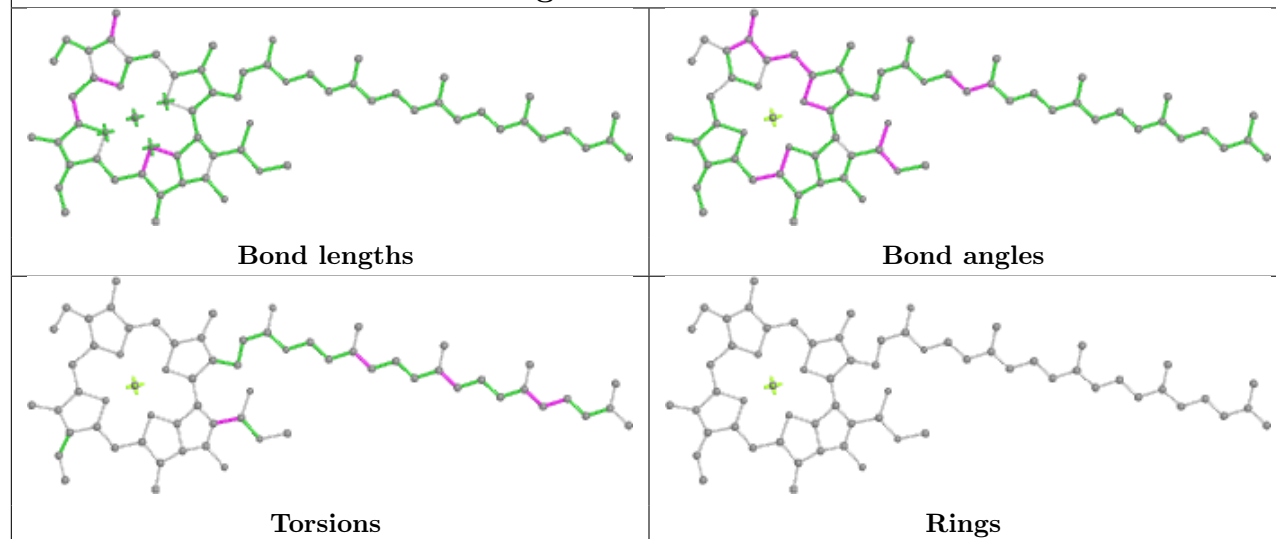


Rings

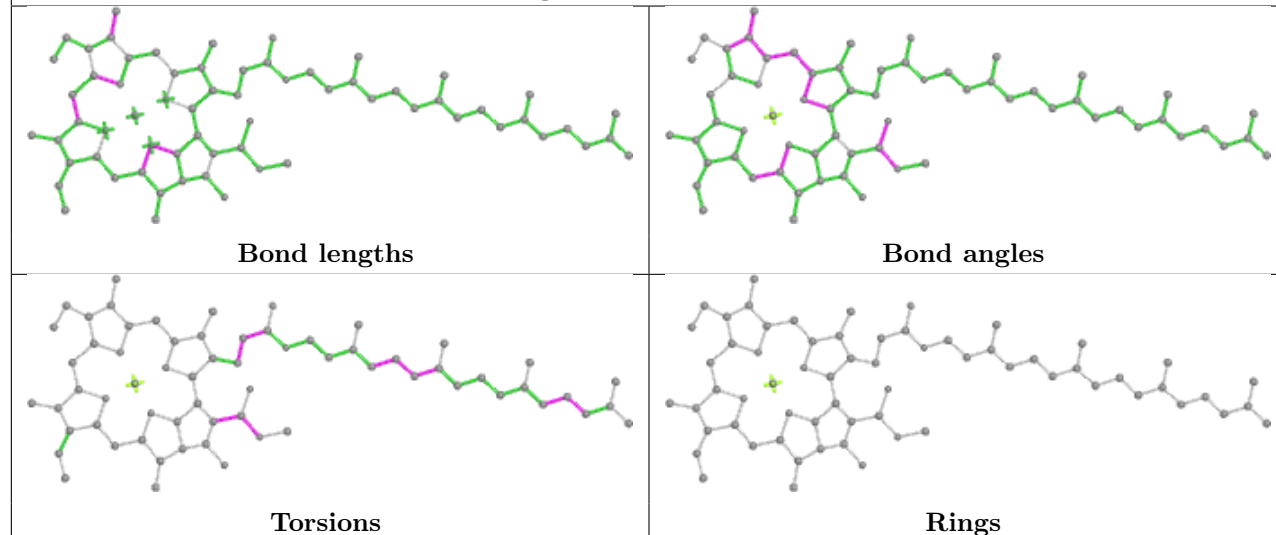




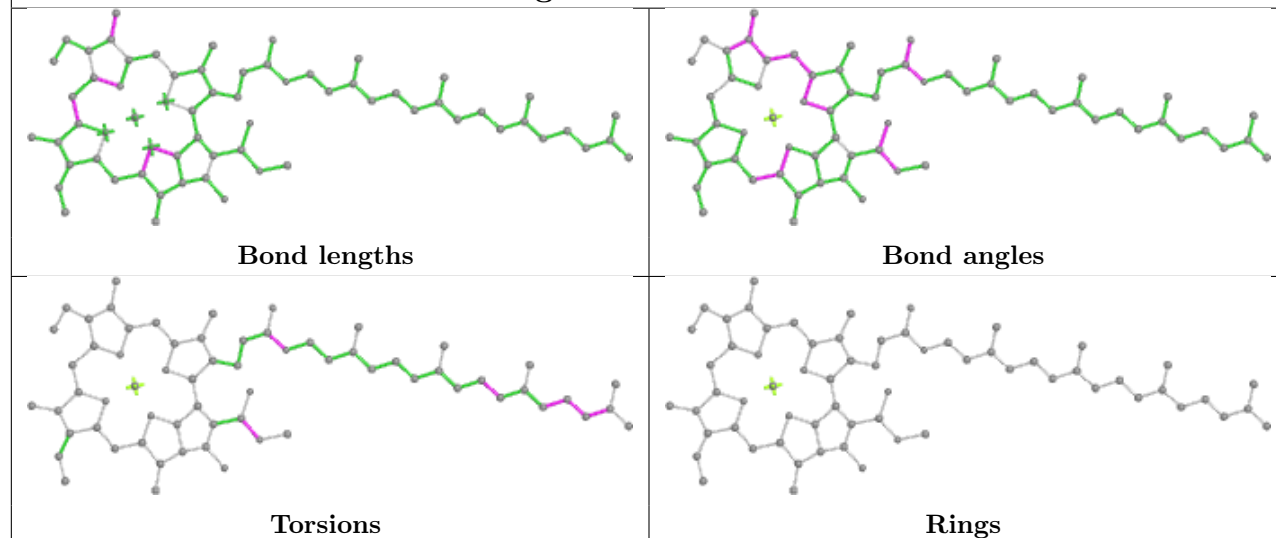
## Ligand CLA a 840



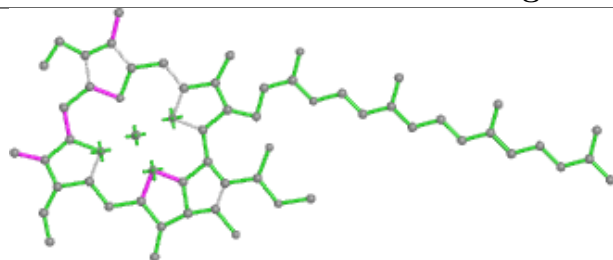
## Ligand CLA 5 309



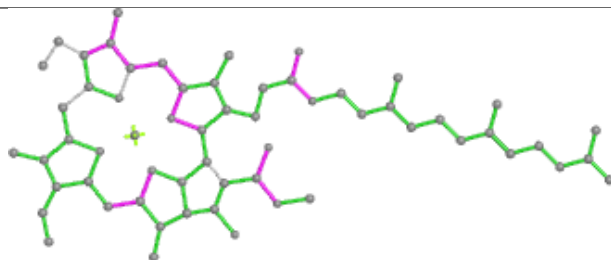
## Ligand CLA b 841



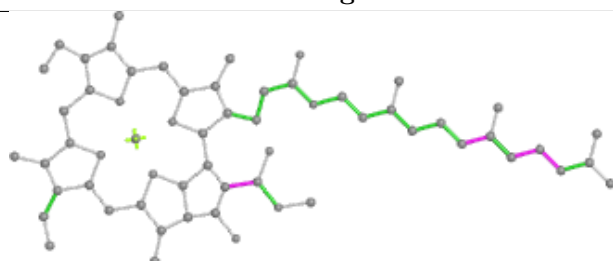
## Ligand CLA l 203



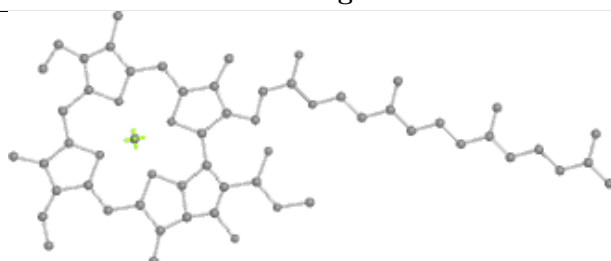
Bond lengths



Bond angles

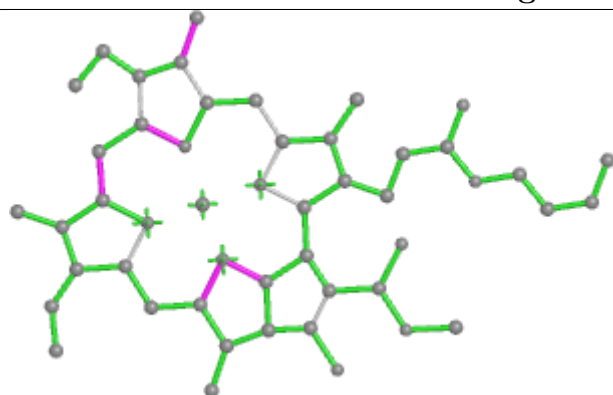


Torsions

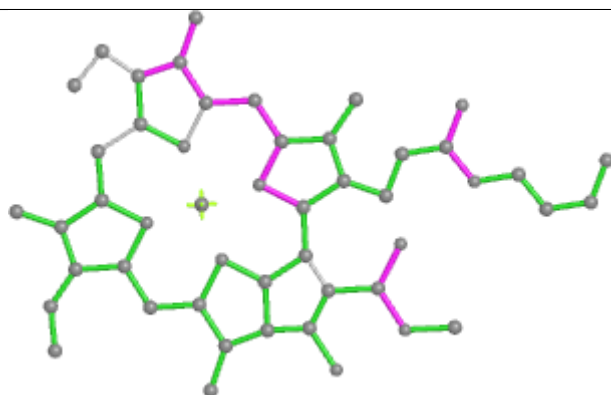


Rings

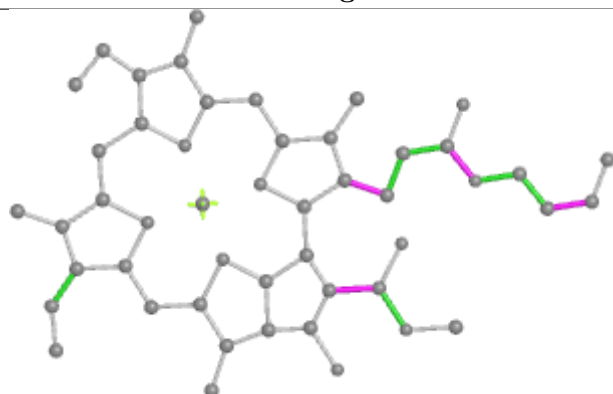
## Ligand CLA a 823



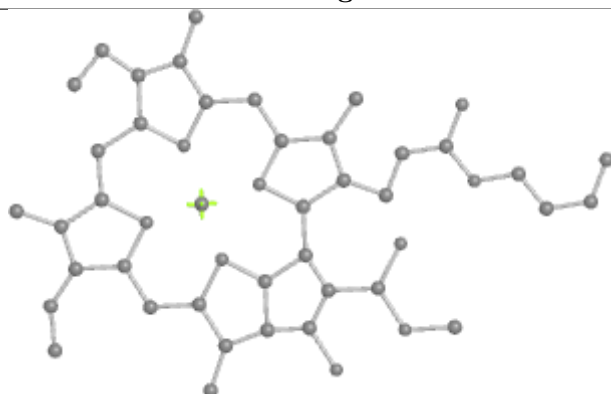
Bond lengths



Bond angles

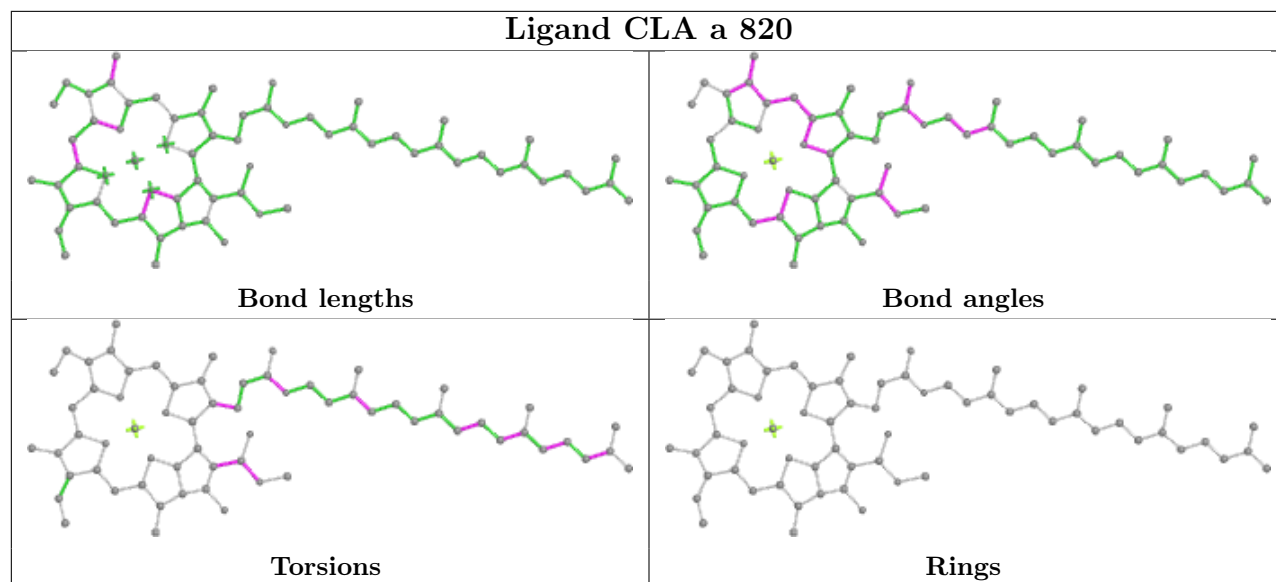


Torsions

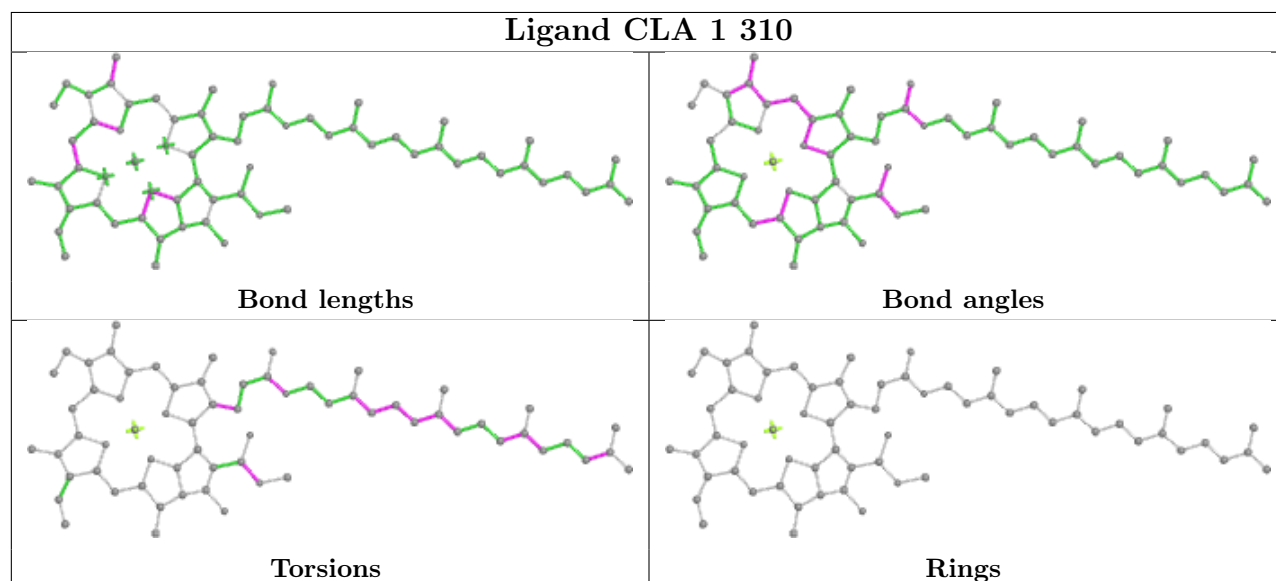


Rings

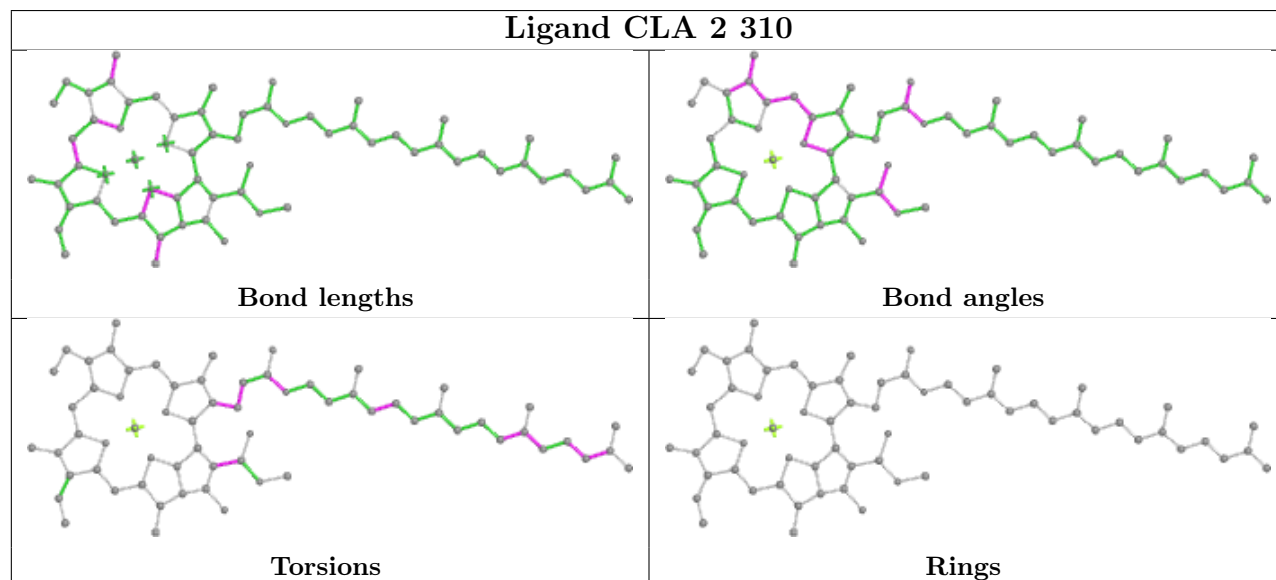
## Ligand CLA a 820



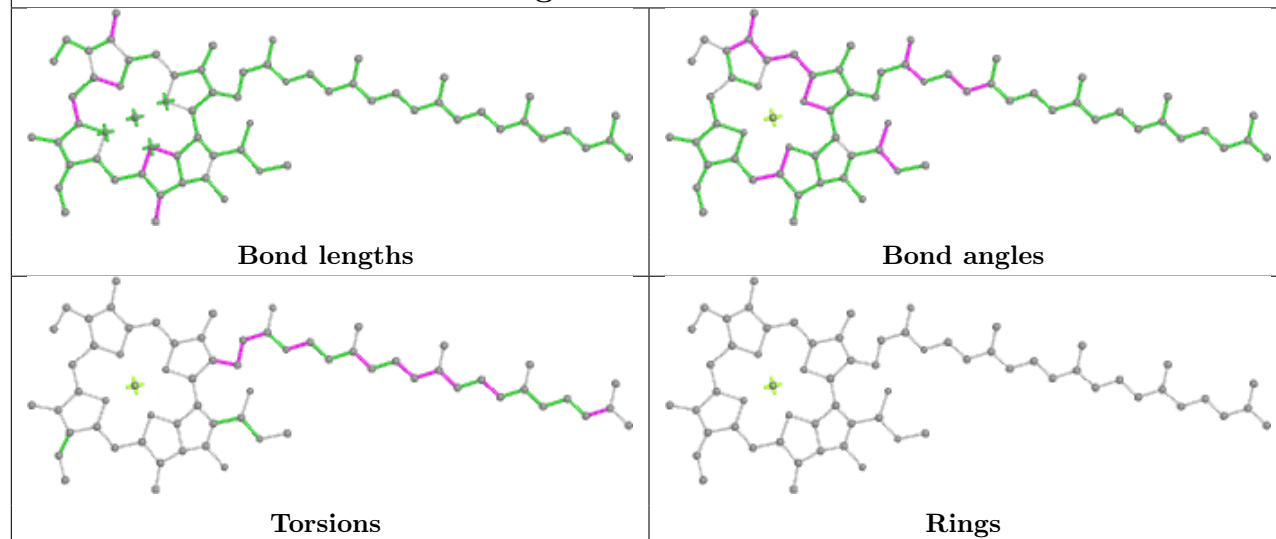
## Ligand CLA 1 310



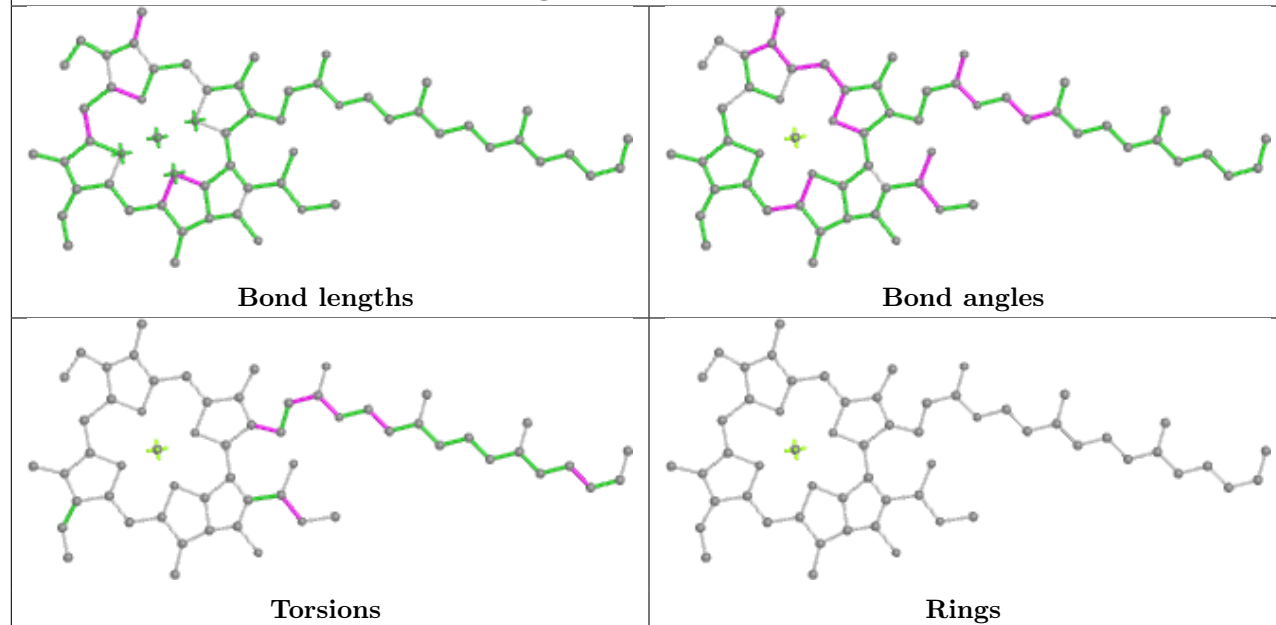
## Ligand CLA 2 310



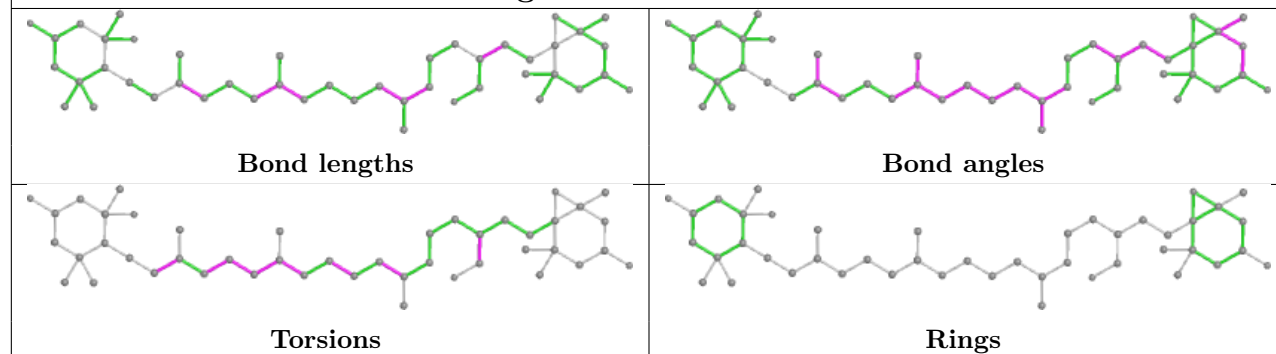
## Ligand CLA b 810



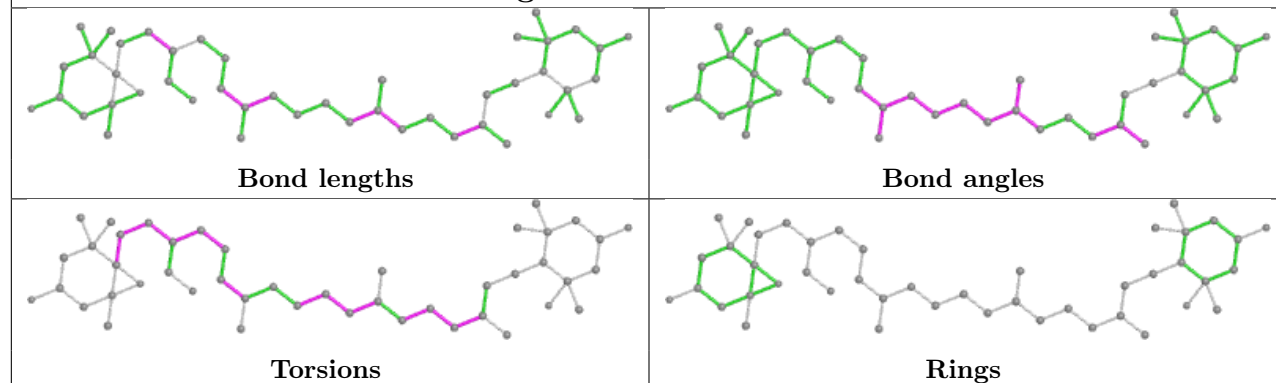
## Ligand CLA b 818



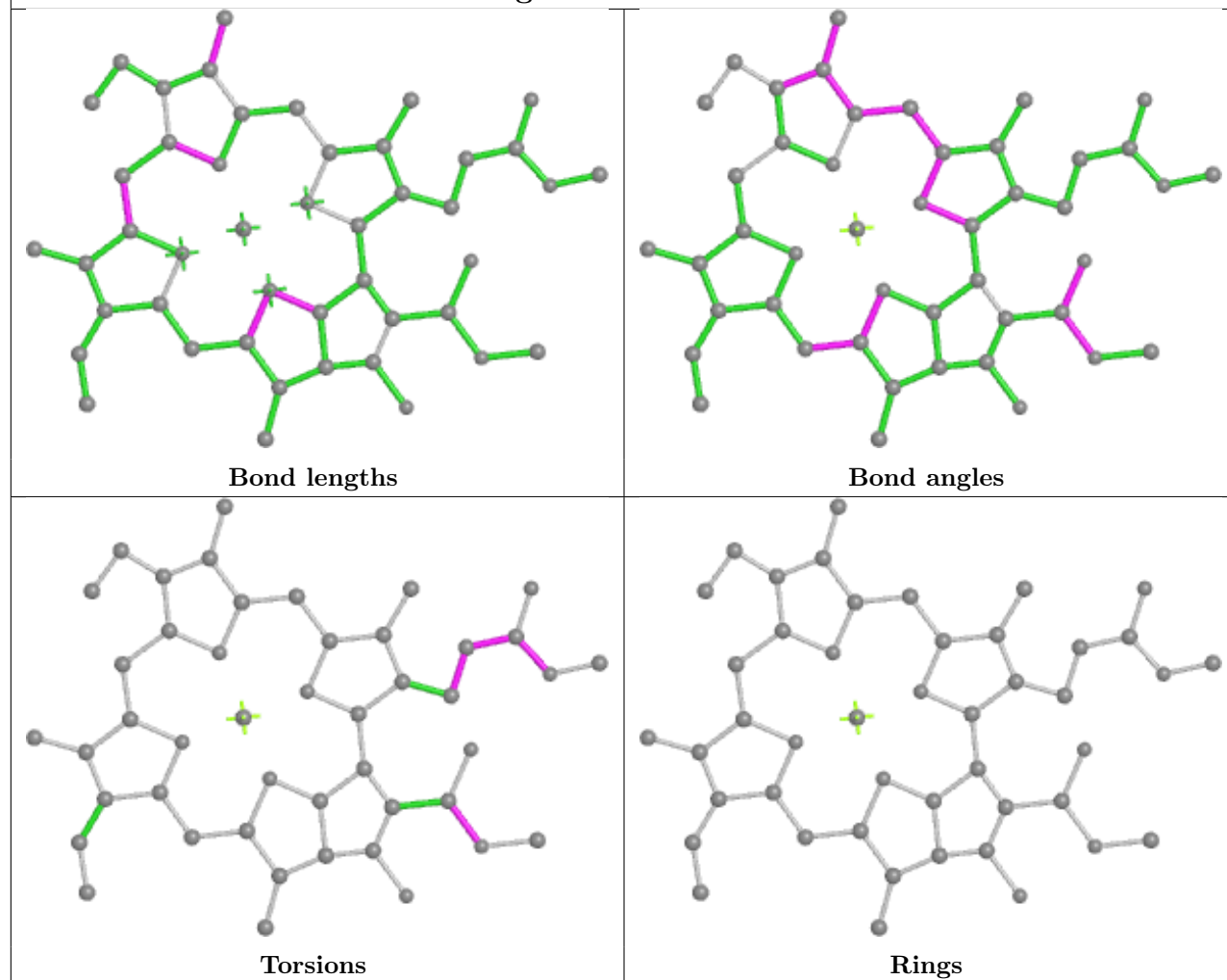
## Ligand A1L1G 1 301

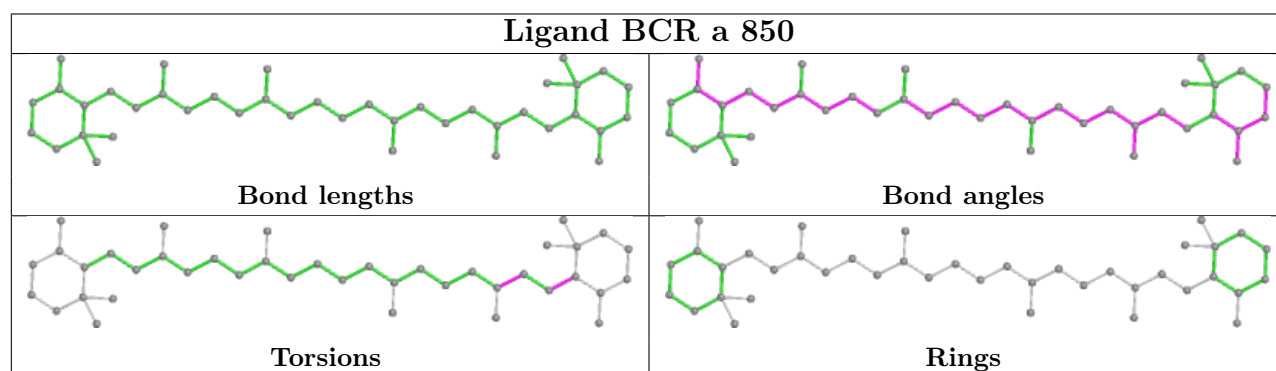
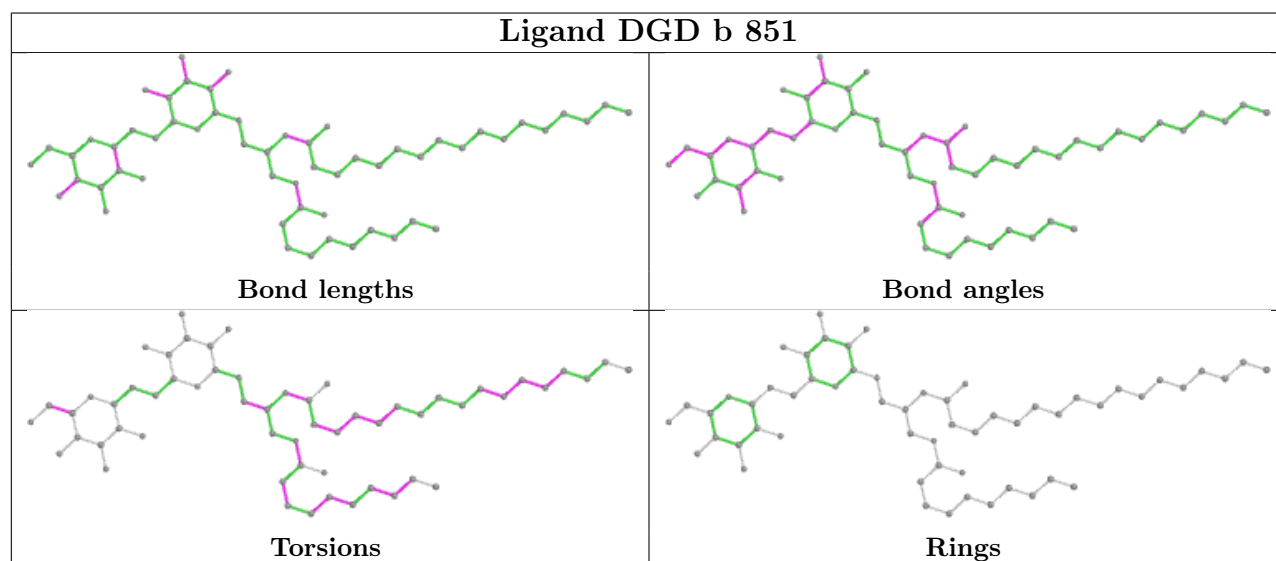
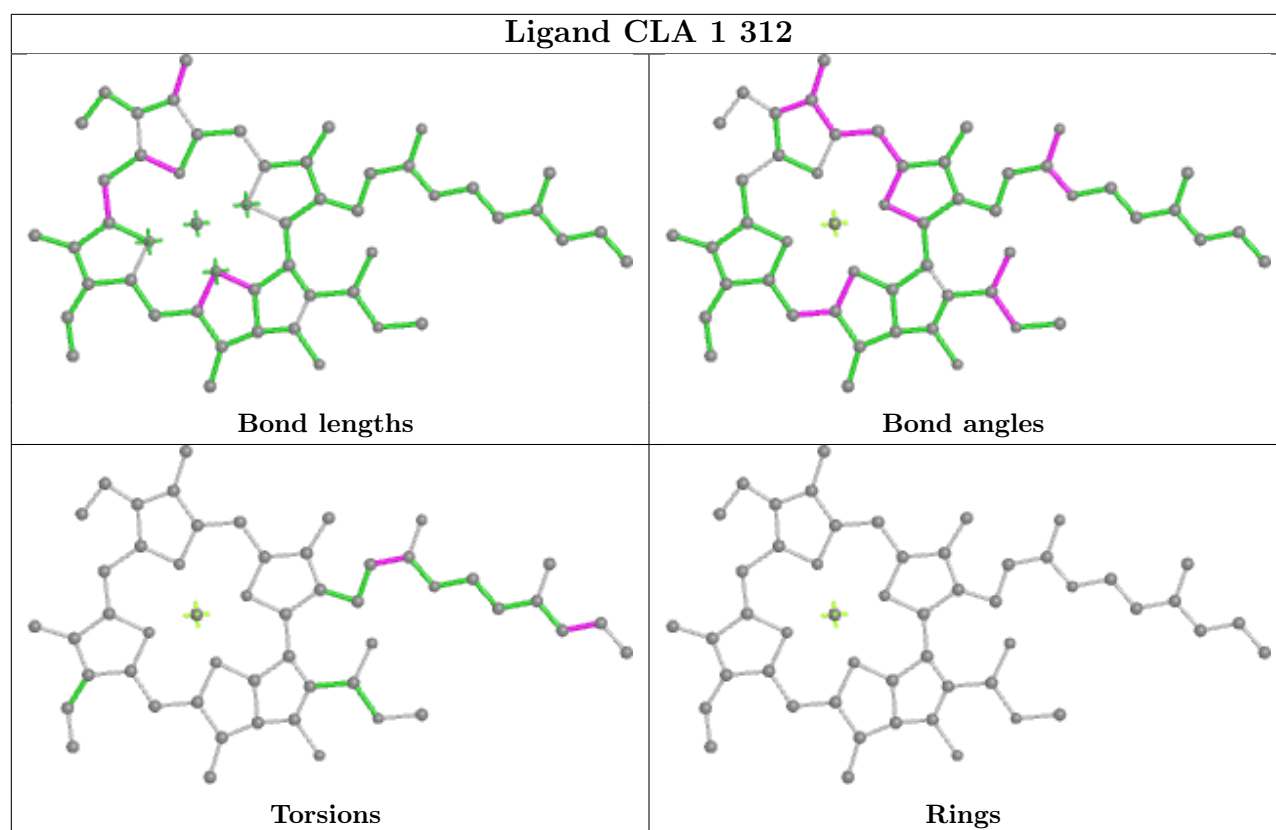


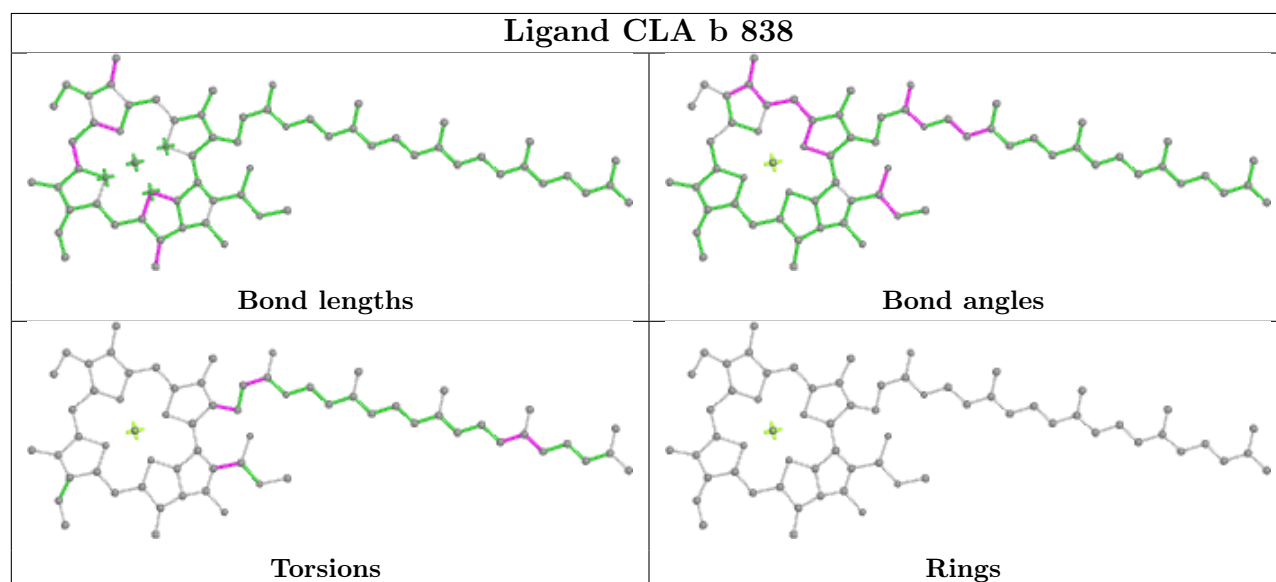
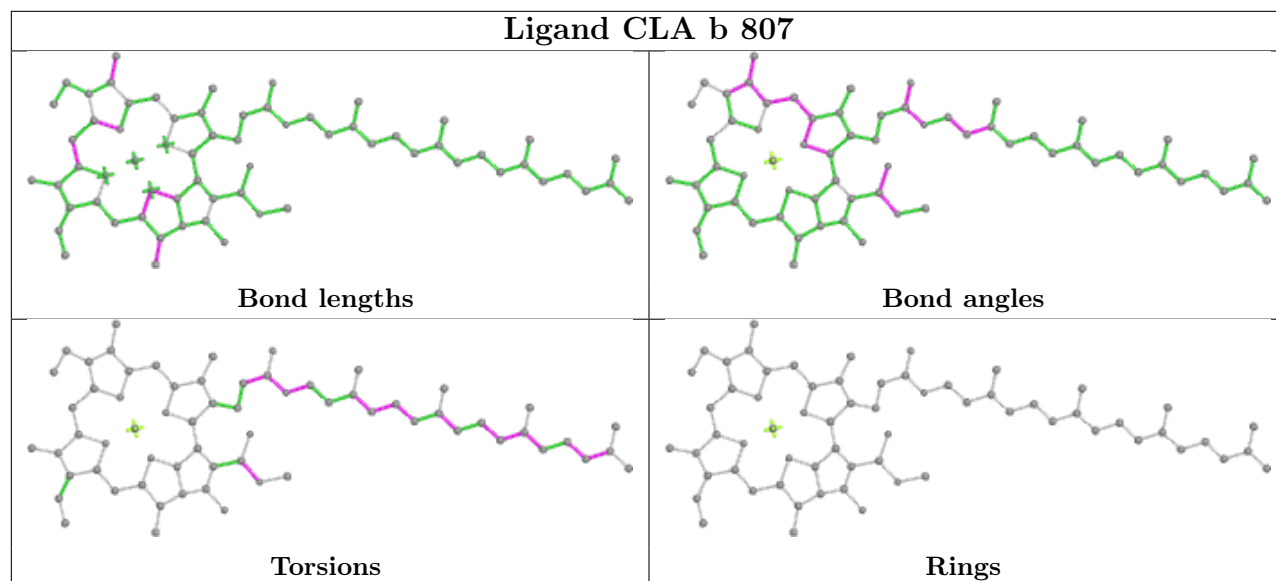
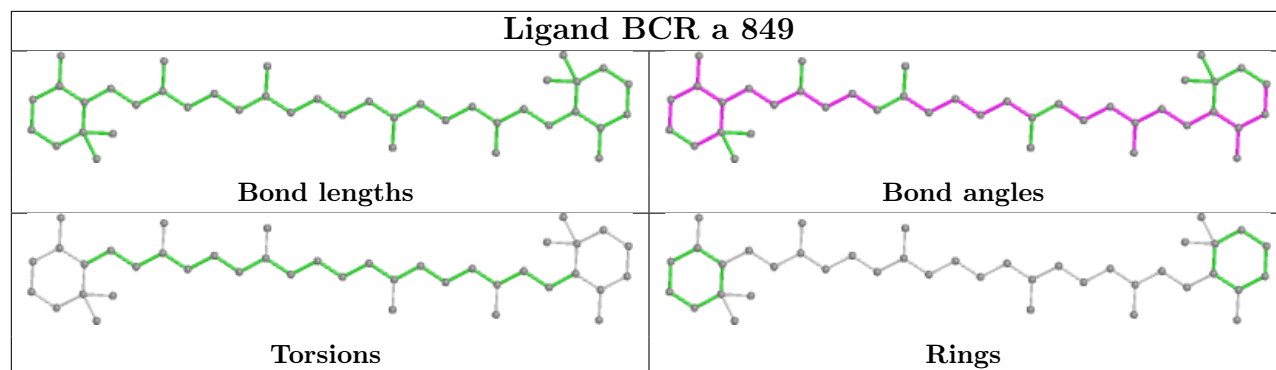
## Ligand A1L1G 3 302



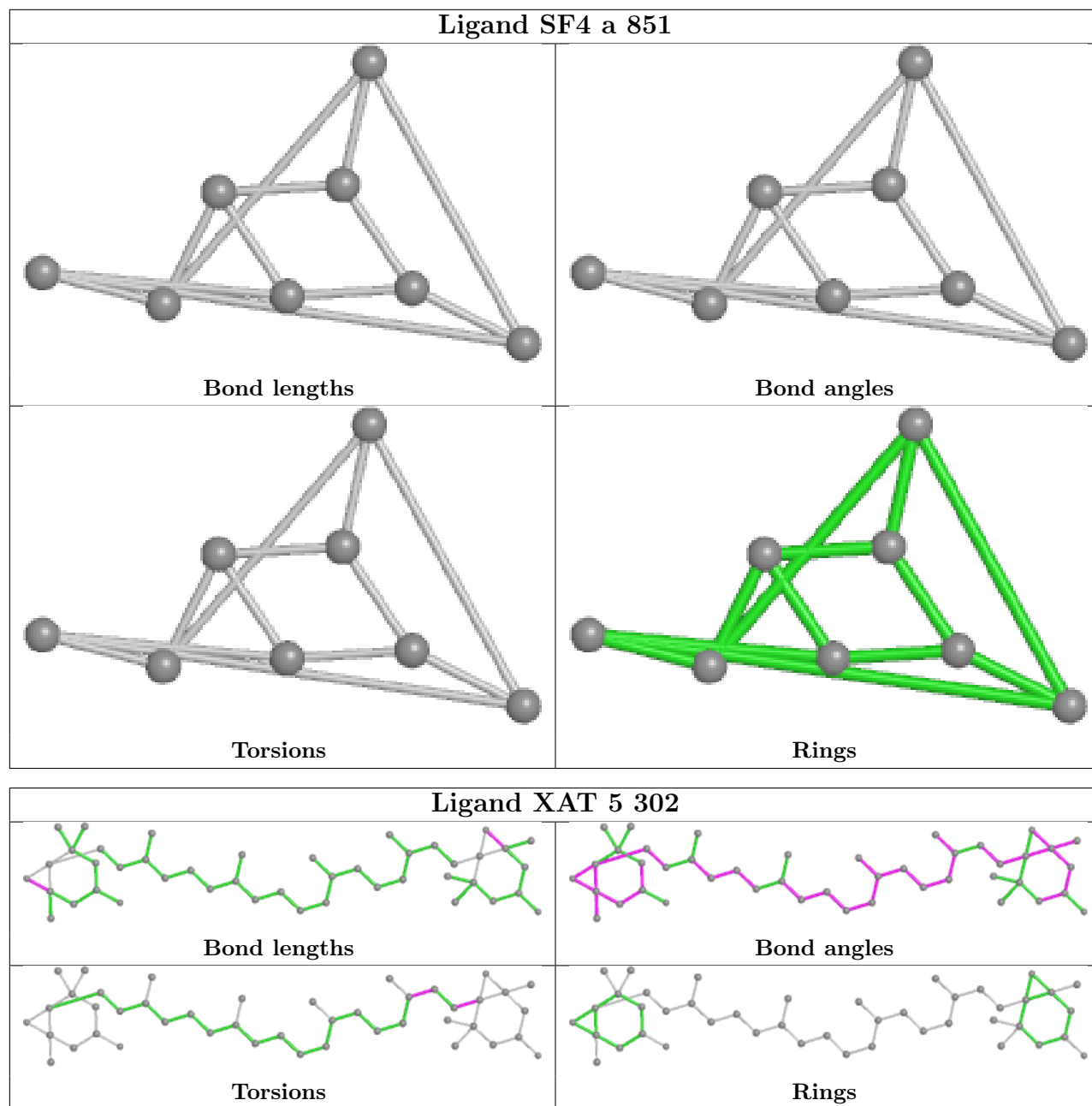
## Ligand CLA 5 310



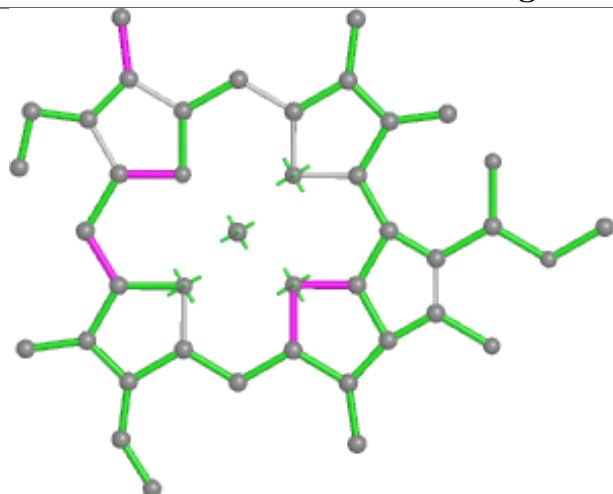




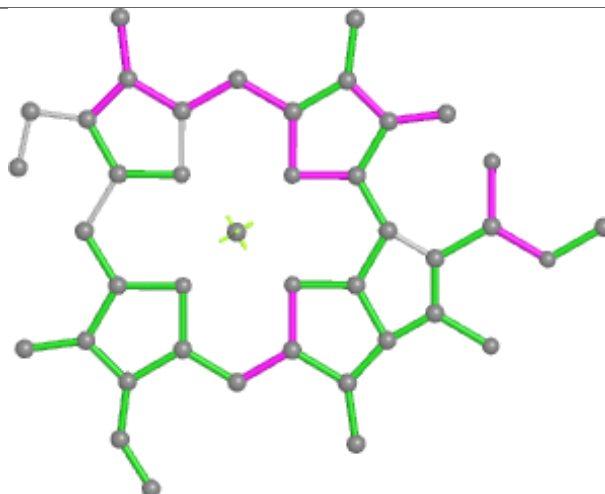




## Ligand CLA 2 313



Bond lengths



Bond angles

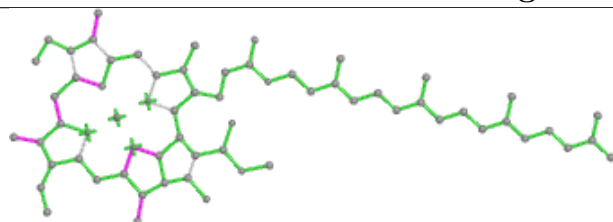


Torsions

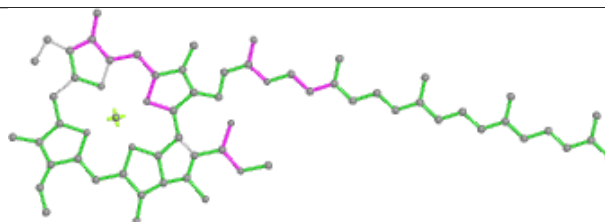


Rings

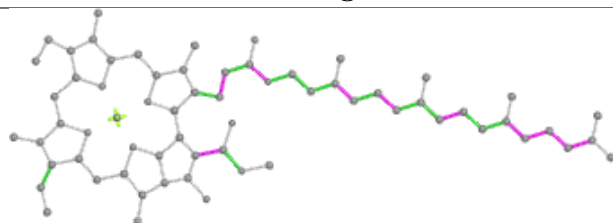
## Ligand CLA a 830



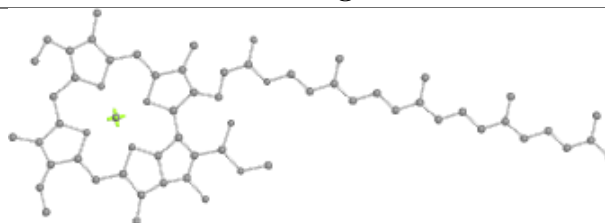
Bond lengths



Bond angles

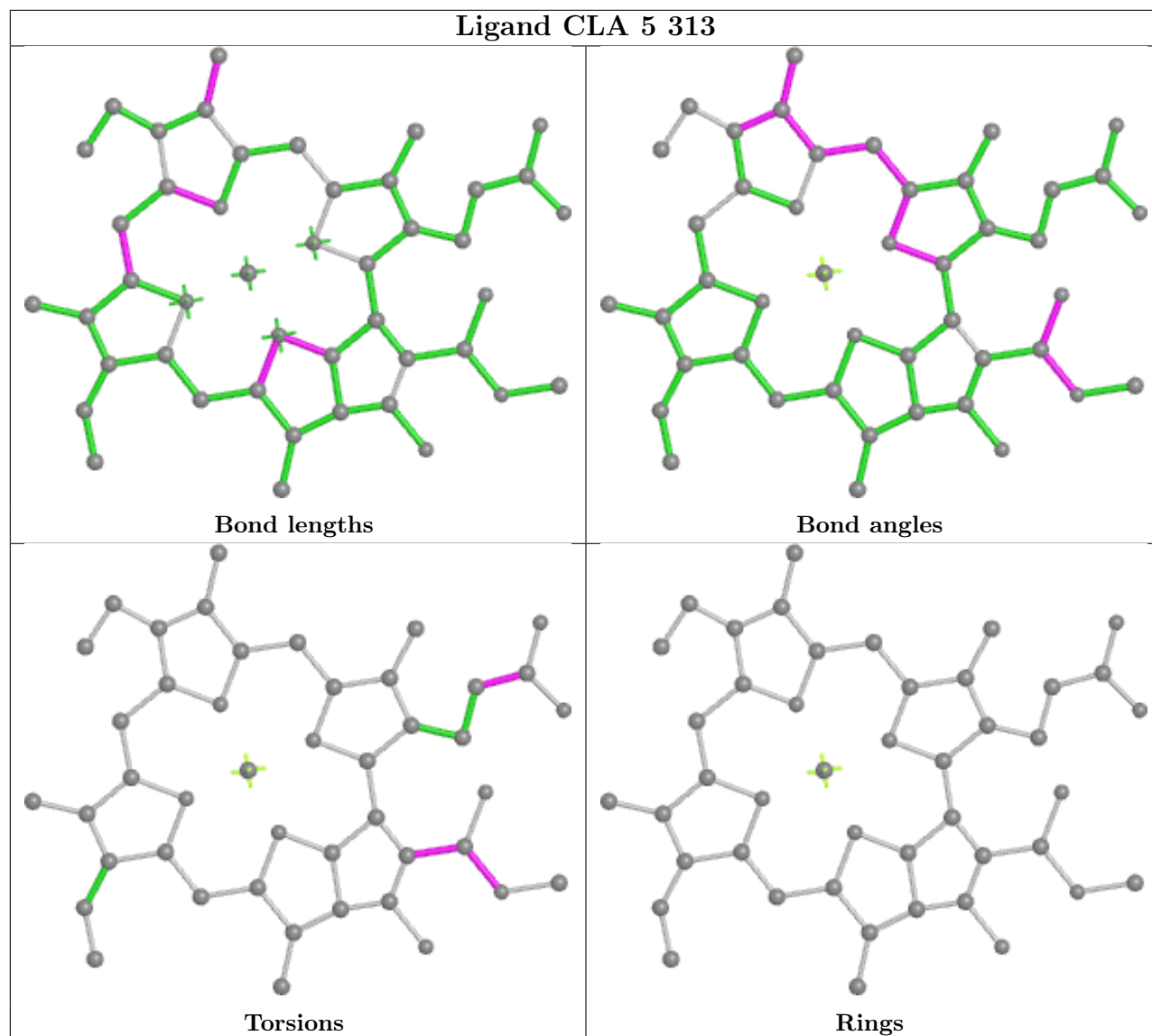


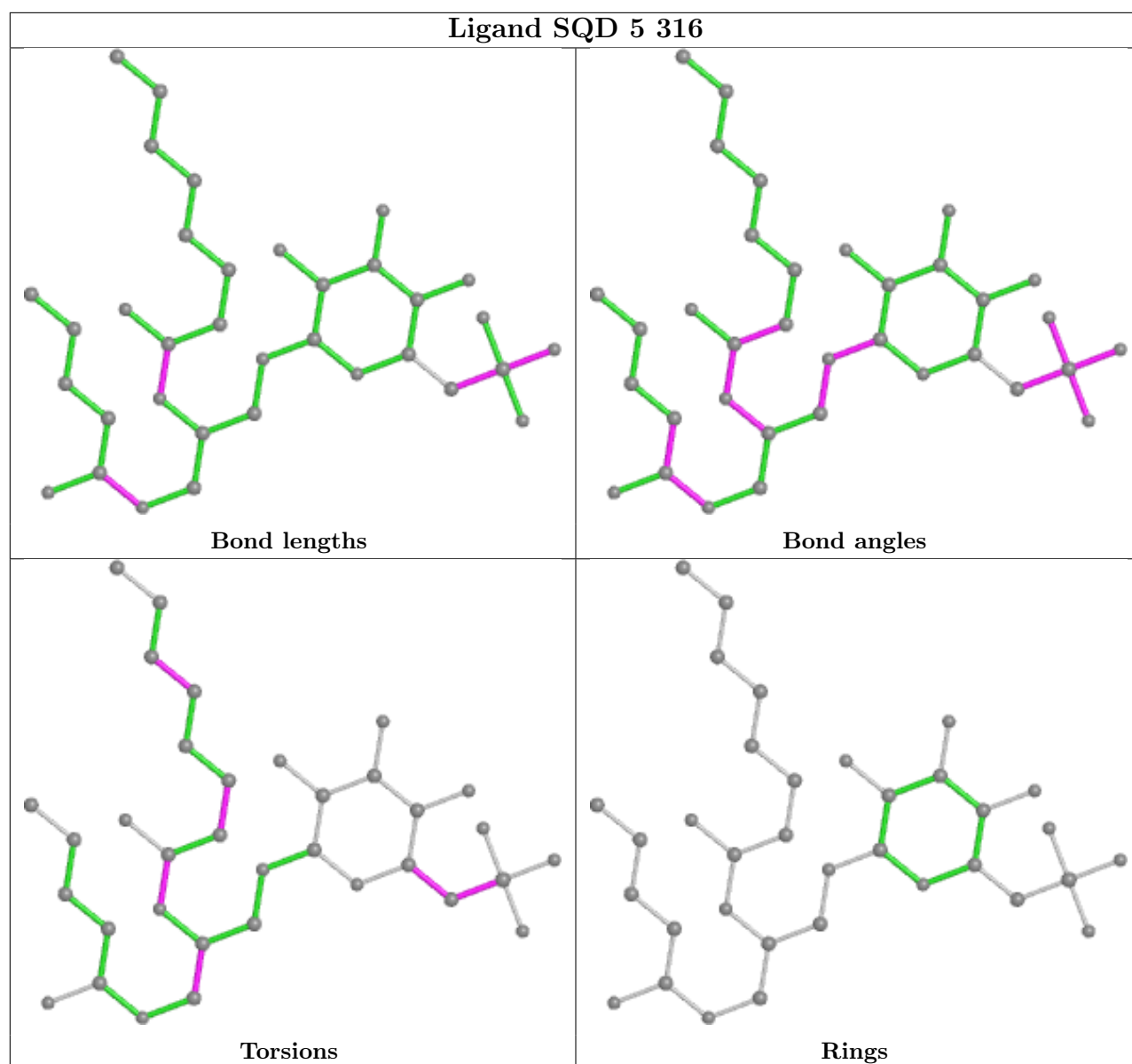
Torsions



Rings

## Ligand CLA 5 313





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

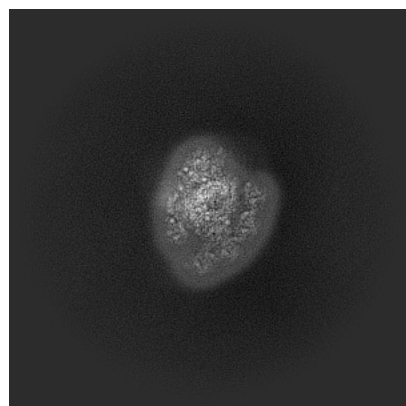
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60289. These allow visual inspection of the internal detail of the map and identification of artifacts.

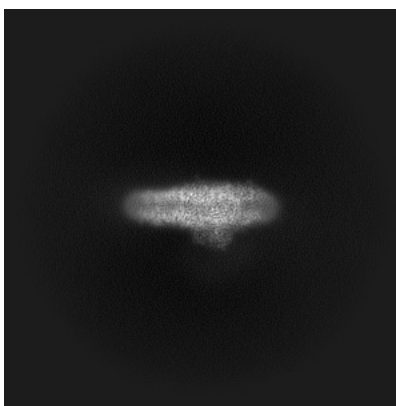
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

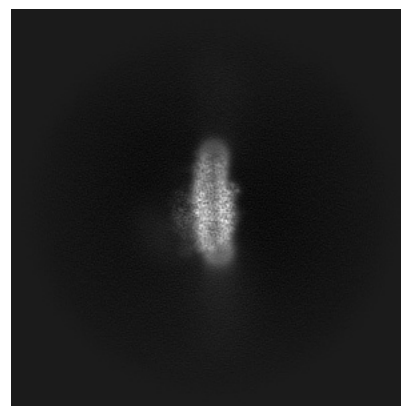
#### 6.1.1 Primary map



X

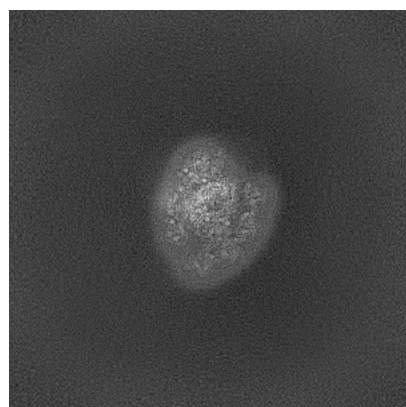


Y

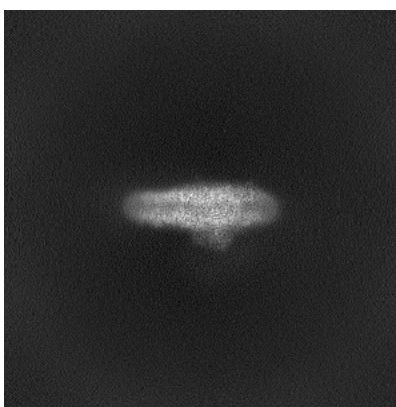


Z

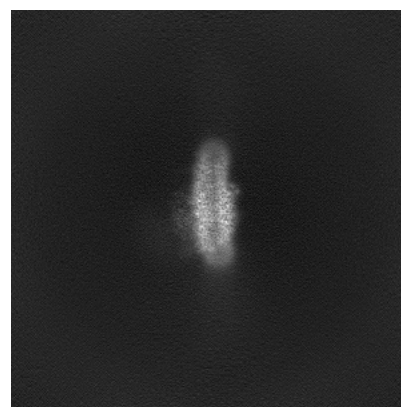
#### 6.1.2 Raw map



X



Y

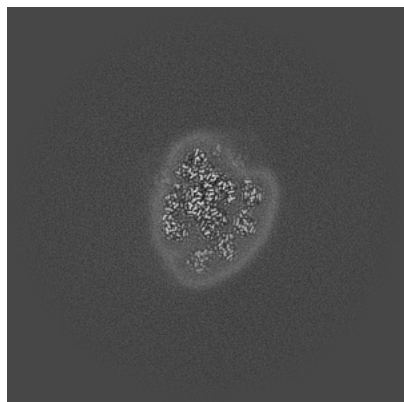


Z

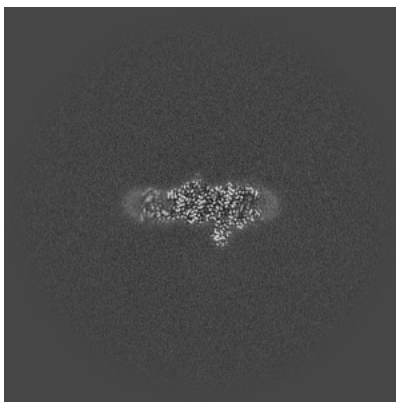
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

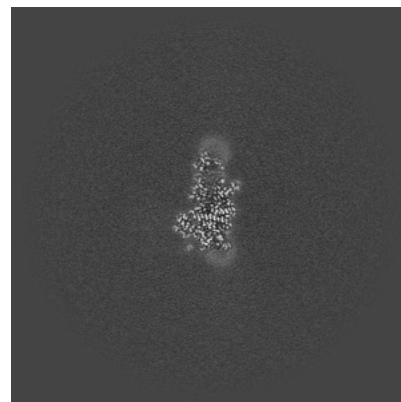
### 6.2.1 Primary map



X Index: 256

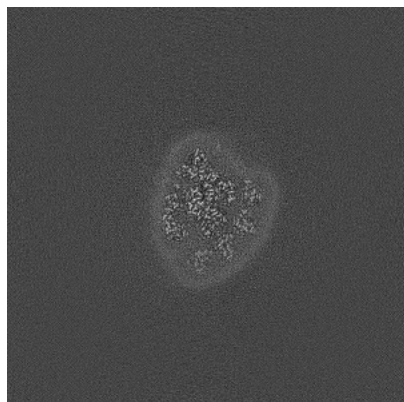


Y Index: 256

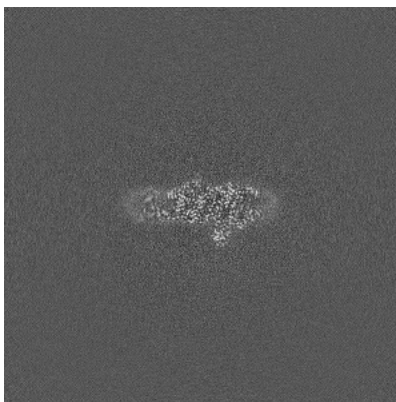


Z Index: 256

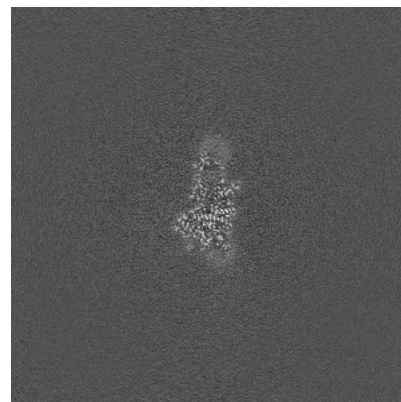
### 6.2.2 Raw map



X Index: 256



Y Index: 256

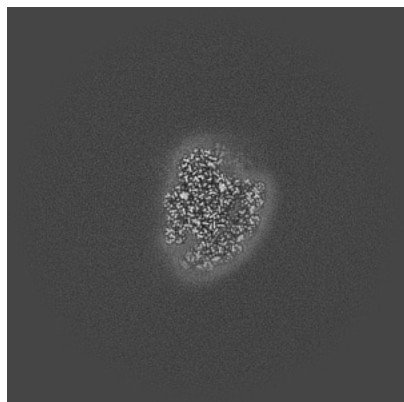


Z Index: 256

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

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

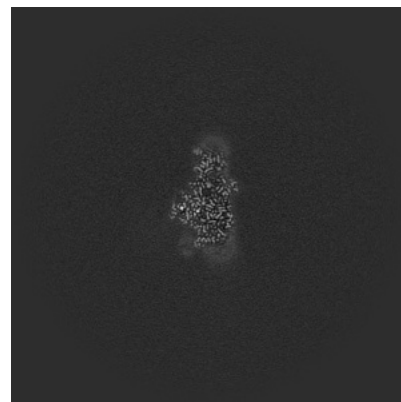
### 6.3.1 Primary map



X Index: 246

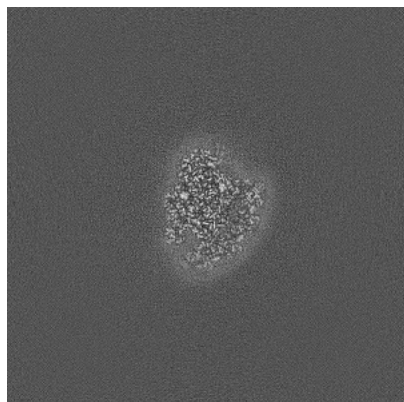


Y Index: 251



Z Index: 273

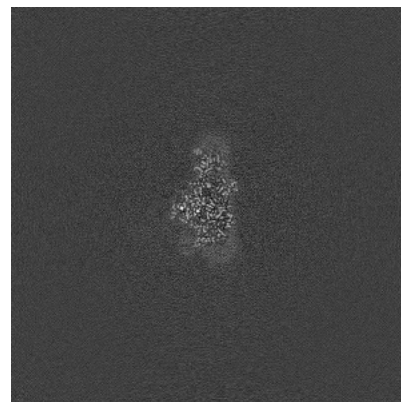
### 6.3.2 Raw map



X Index: 246



Y Index: 251



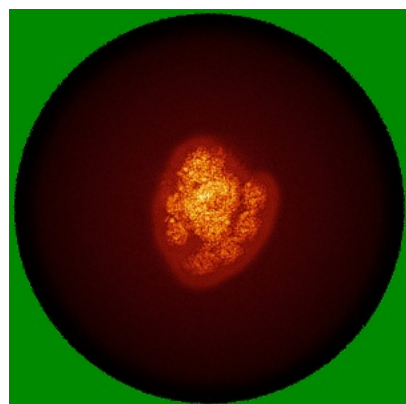
Z Index: 273

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

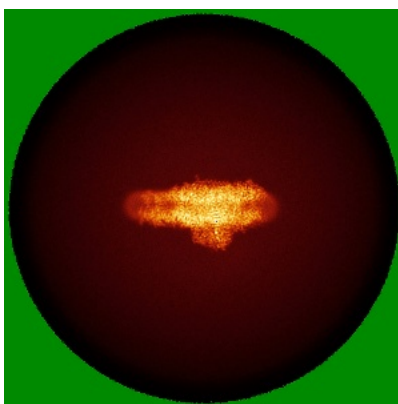


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

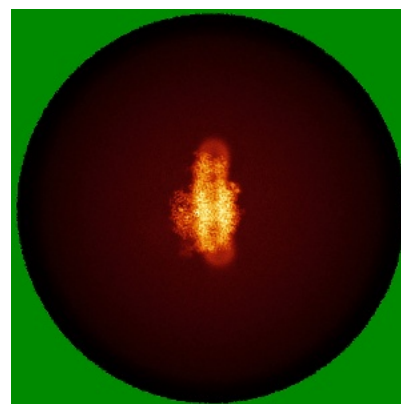
### 6.4.1 Primary map



X

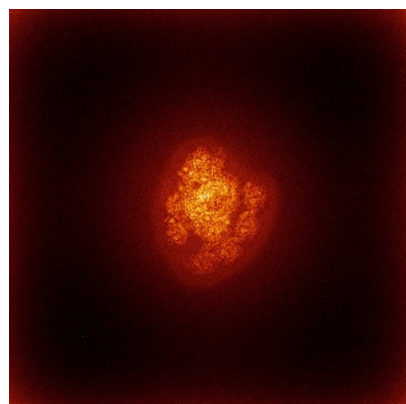


Y

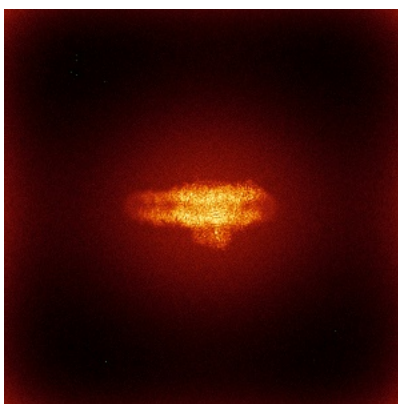


Z

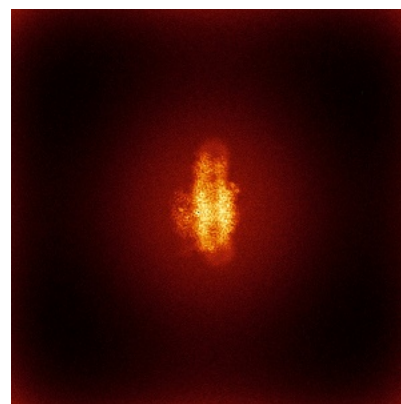
### 6.4.2 Raw map



X



Y



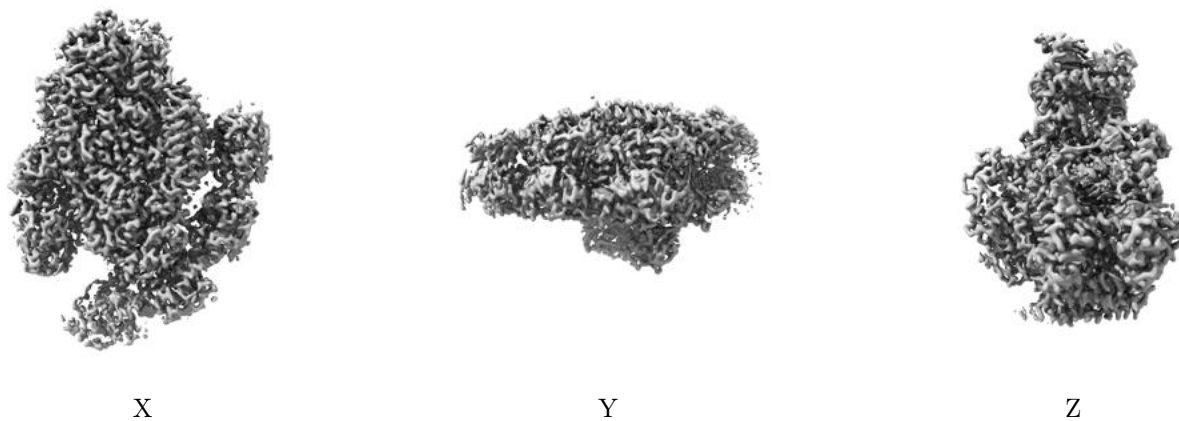
Z

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.



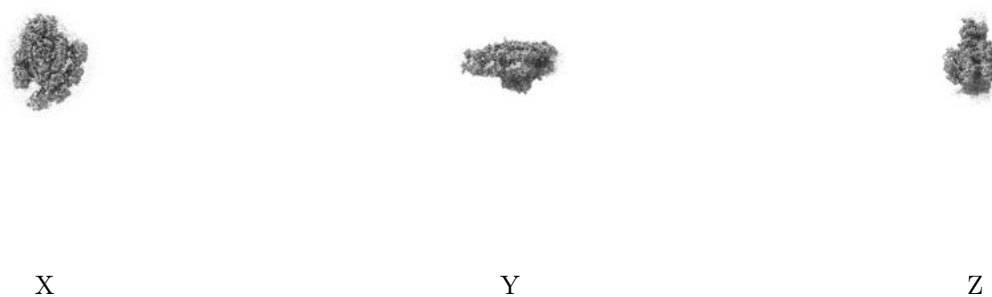
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.333. 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.

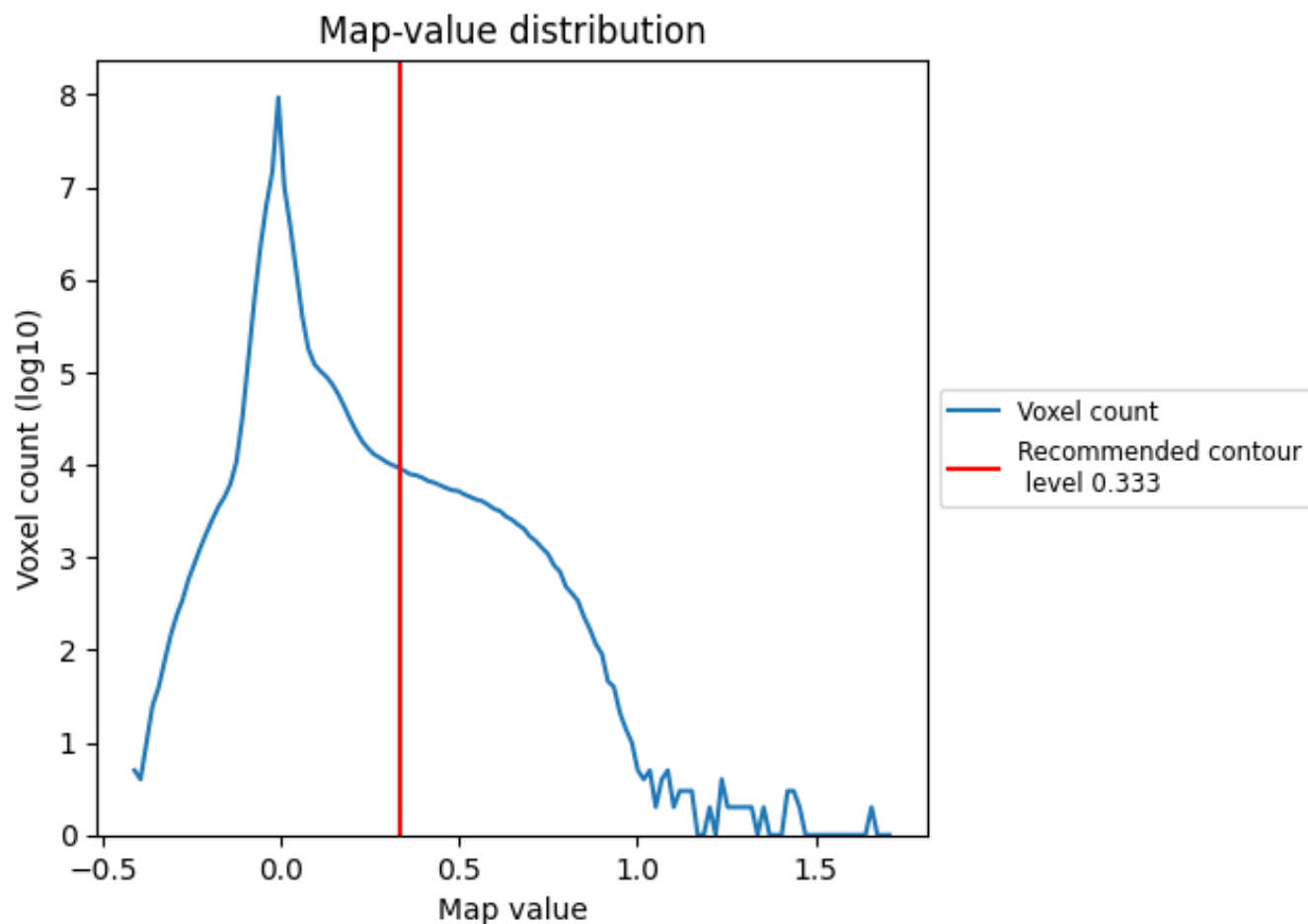
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

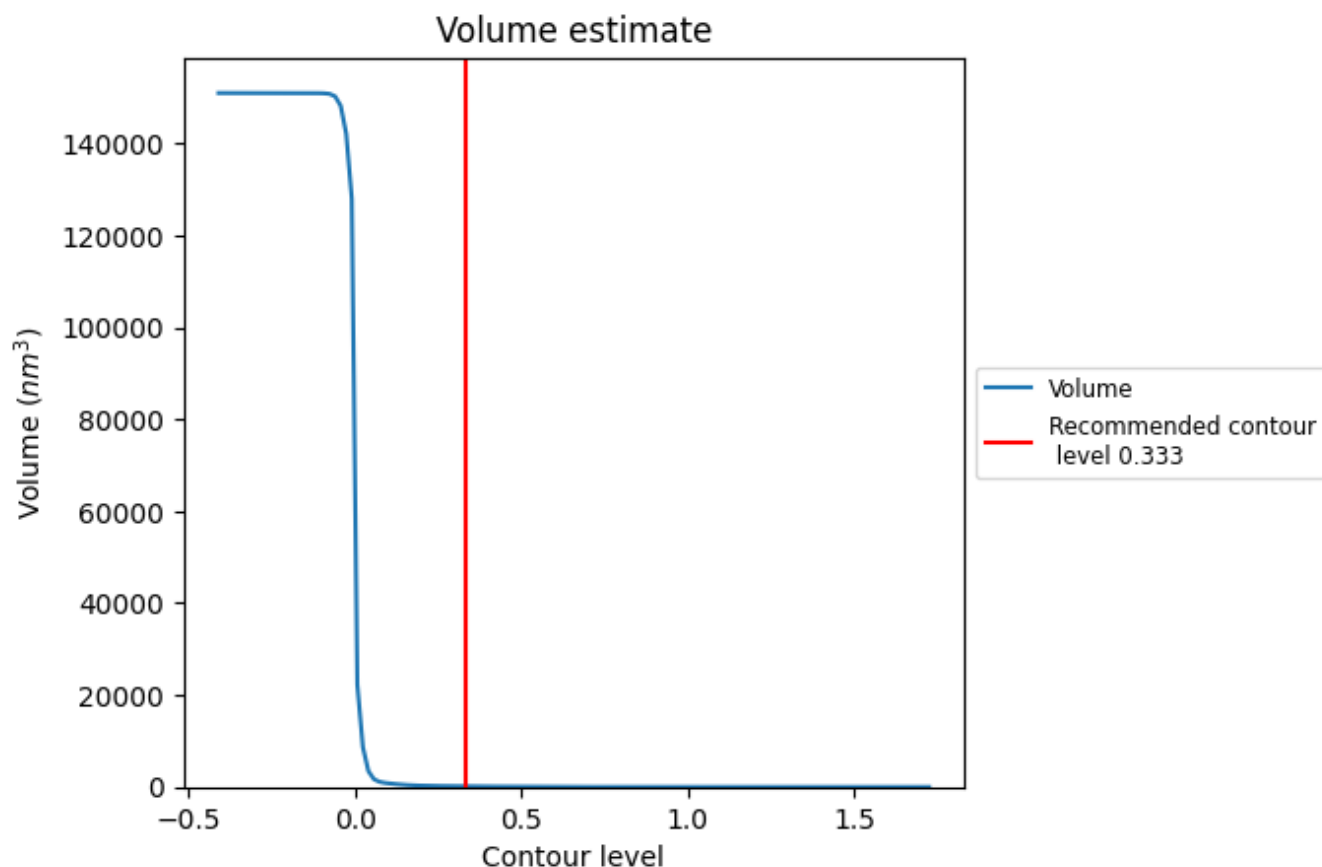
This section contains the results of statistical analysis of the map.

### 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.

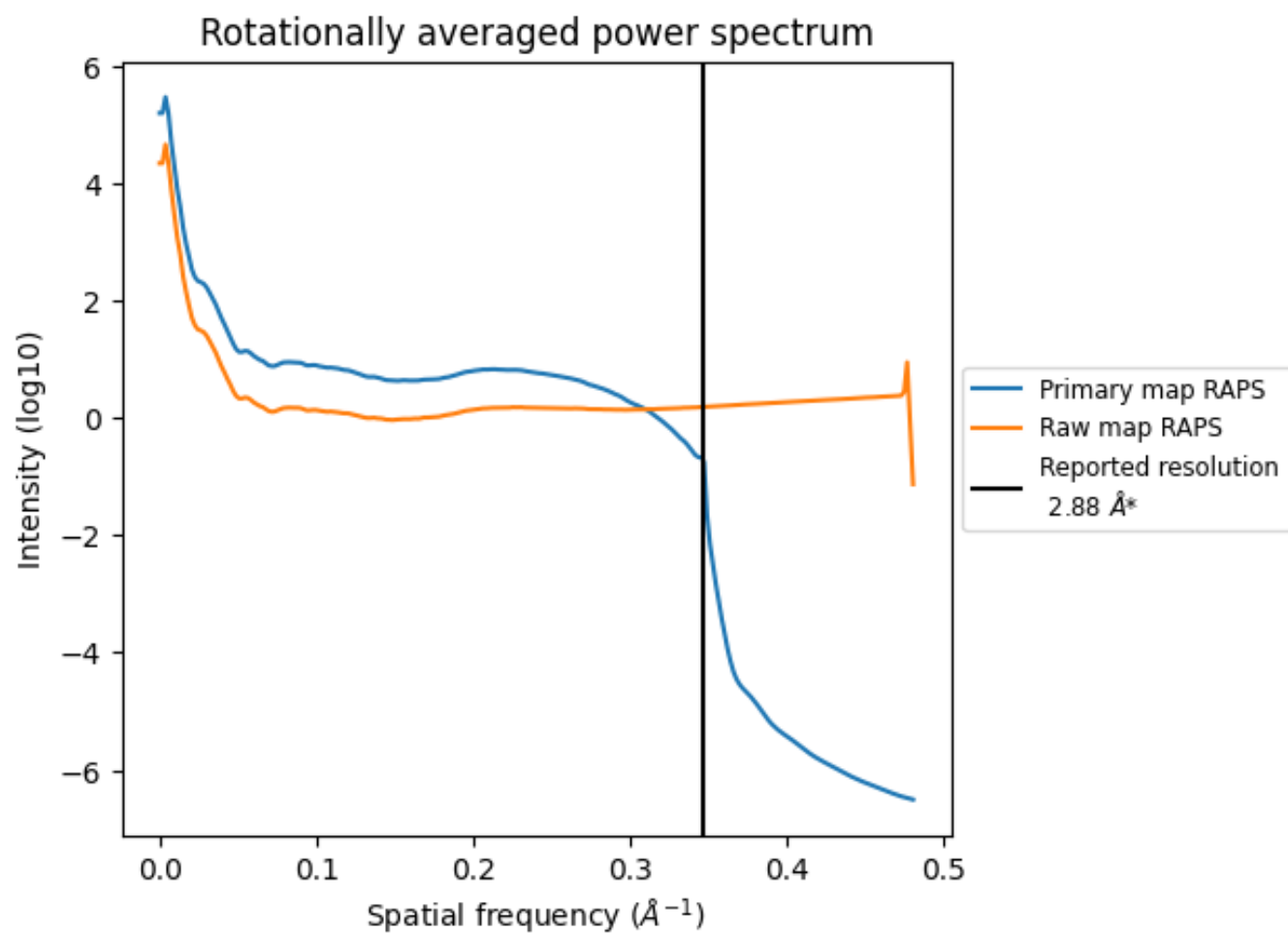
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136  $\text{nm}^3$ ; this corresponds to an approximate mass of 123 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 ⓘ

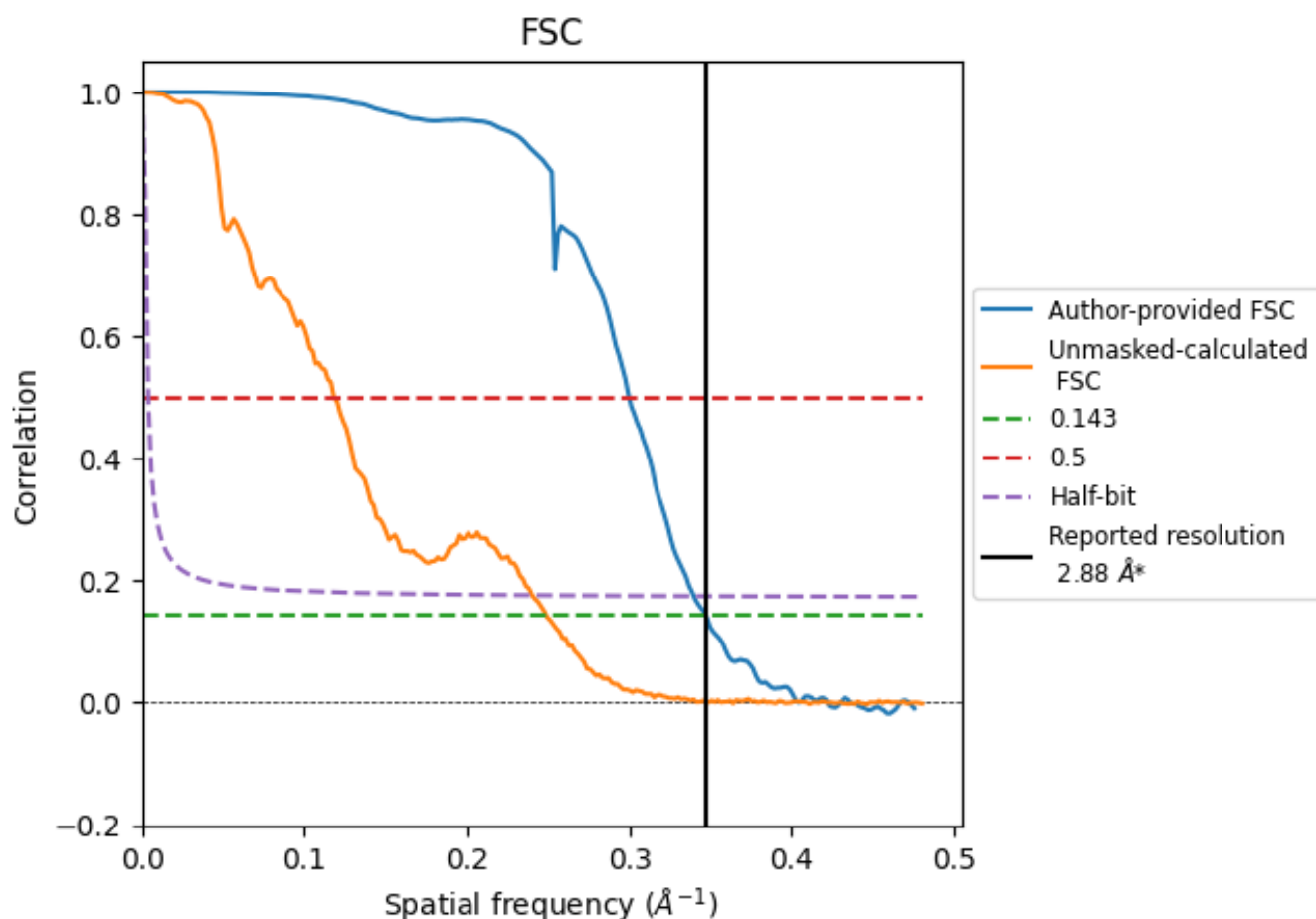


\*Reported resolution corresponds to spatial frequency of 0.347 Å<sup>-1</sup>

## 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 0.347  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

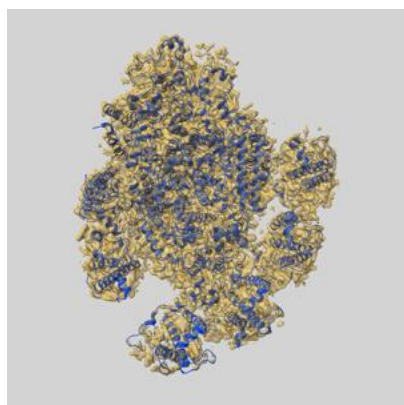
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.33	2.94
Unmasked-calculated*	4.01	8.45	4.16

\*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 4.01 differs from the reported value 2.88 by more than 10 %

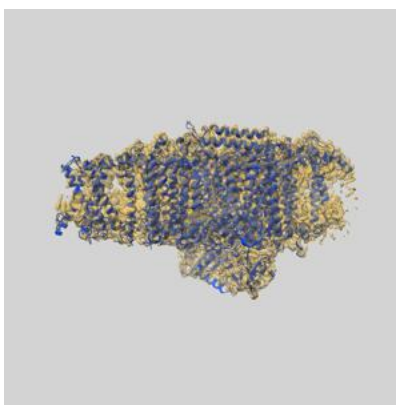
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60289 and PDB model 8ZOD. Per-residue inclusion information can be found in section 3 on page 26.

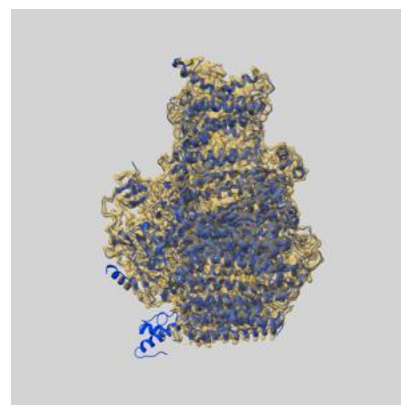
### 9.1 Map-model overlay [i](#)



X



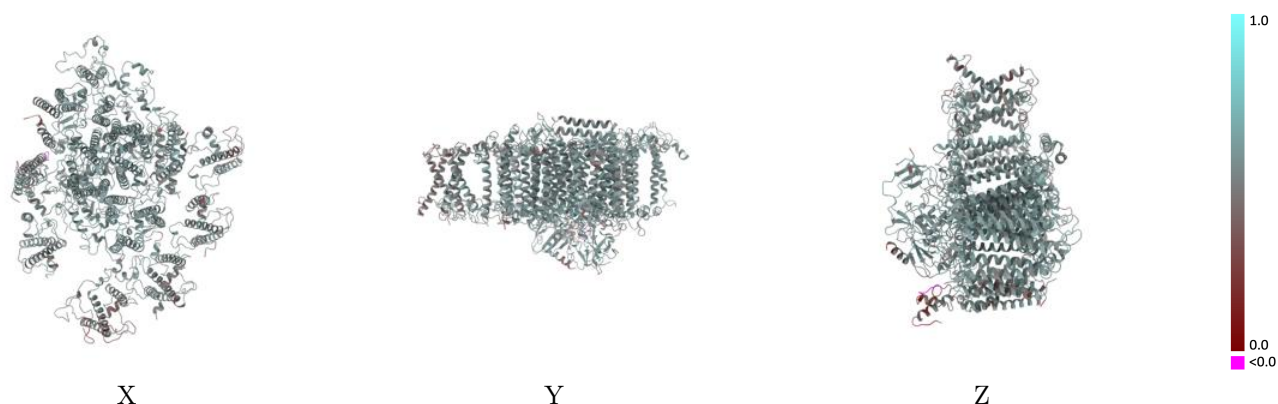
Y



Z

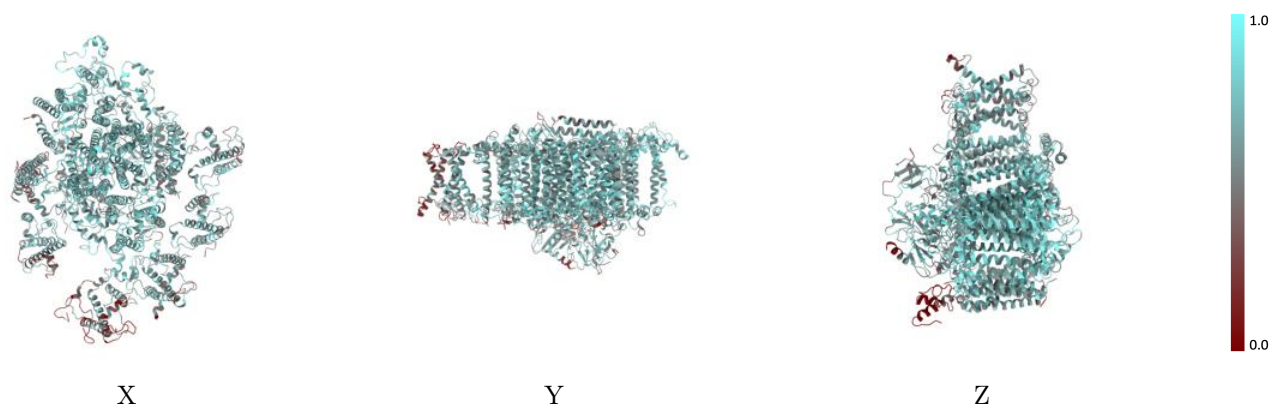
The images above show the 3D surface view of the map at the recommended contour level 0.333 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

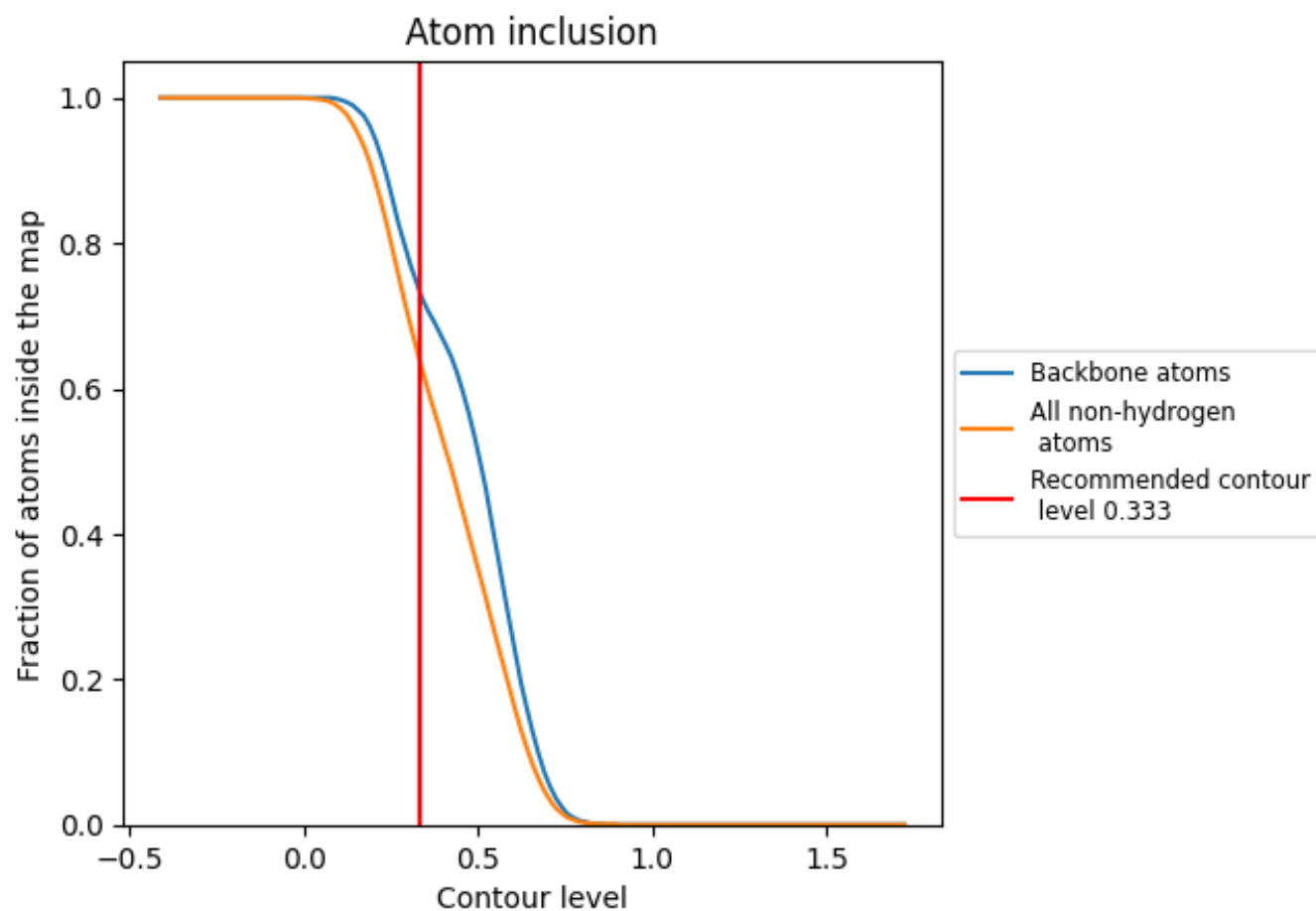
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.333).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.333) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6390	<div></div> 0.5470
1	<div></div> 0.5870	<div></div> 0.5340
2	<div></div> 0.3690	<div></div> 0.4550
3	<div></div> 0.5770	<div></div> 0.5300
4	<div></div> 0.5980	<div></div> 0.5290
5	<div></div> 0.5930	<div></div> 0.5250
a	<div></div> 0.7120	<div></div> 0.5780
b	<div></div> 0.7010	<div></div> 0.5680
c	<div></div> 0.7260	<div></div> 0.5600
d	<div></div> 0.6320	<div></div> 0.5540
e	<div></div> 0.6180	<div></div> 0.5490
f	<div></div> 0.6440	<div></div> 0.5420
g	<div></div> 0.3270	<div></div> 0.4330
i	<div></div> 0.5140	<div></div> 0.4990
j	<div></div> 0.6220	<div></div> 0.5630
l	<div></div> 0.6000	<div></div> 0.5130
m	<div></div> 0.5630	<div></div> 0.4950

