



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 07:08 PM JST

PDB ID : 8ZOB / pdb_00008zob
EMDB ID : EMD-60287
Title : Structure of the wild-type PSI-5VCPI supercomplex in *Nannochloropsis 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

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

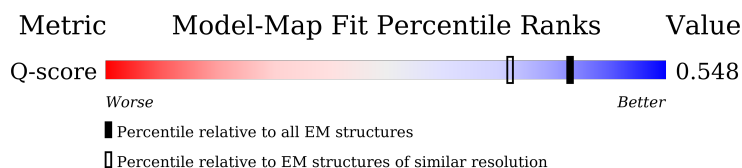
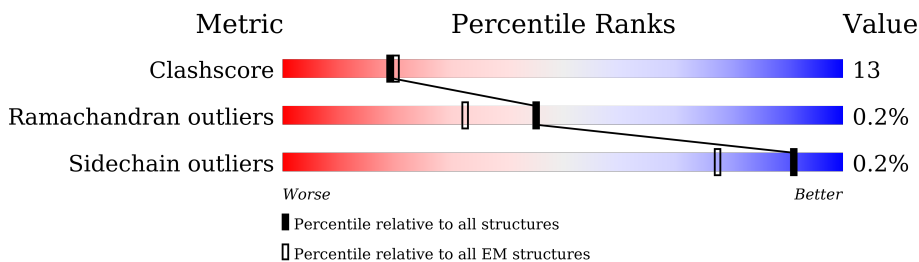
1 Overall quality at a glance

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 ≥ 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>19%</div> <div> <div></div> <div>52%</div> <div>18%</div> <div>31%</div> </div> </div>
2	4	202	<div> <div>18%</div> <div> <div></div> <div>73%</div> <div>10%</div> <div>17%</div> </div> </div>
3	3	220	<div> <div>23%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>20%</div> </div> </div>
4	2	223	<div> <div>66%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>17%</div> </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		

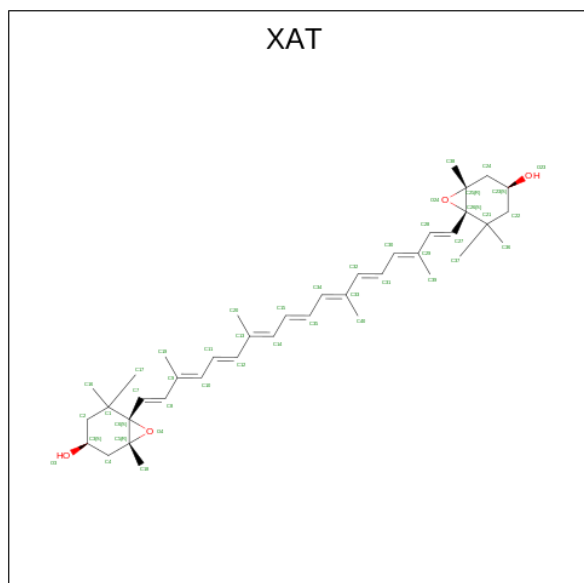
- Molecule 15 is a protein called PsaS.

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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



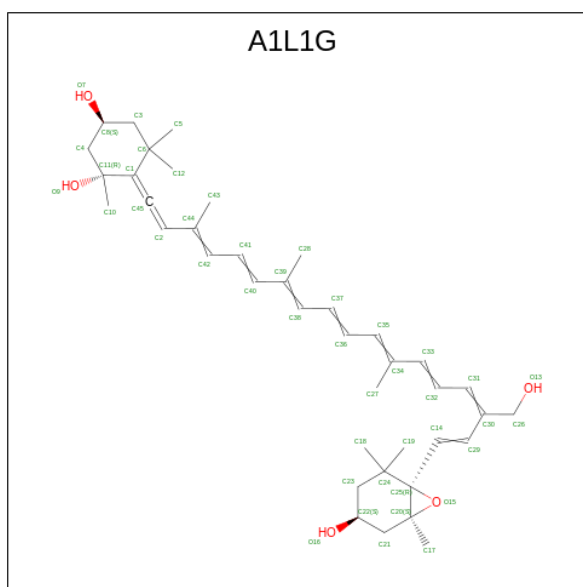
Mol	Chain	Residues	Atoms			AltConf
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

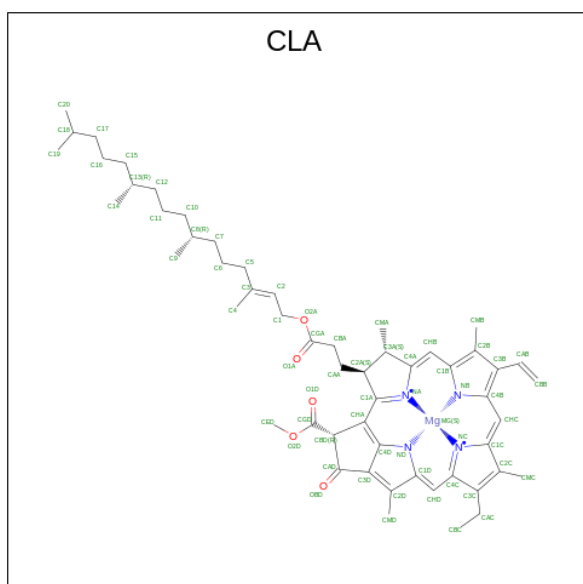
Mol	Chain	Residues	Atoms			AltConf
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			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: C₄₀H₅₆O₅) (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 55	C 45	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	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
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
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

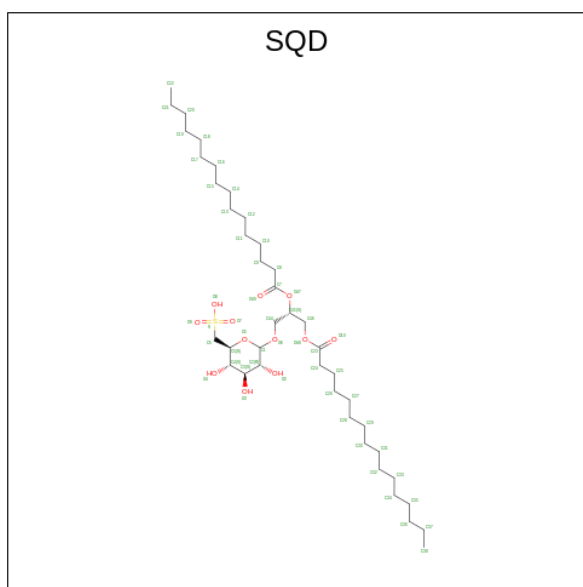
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0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

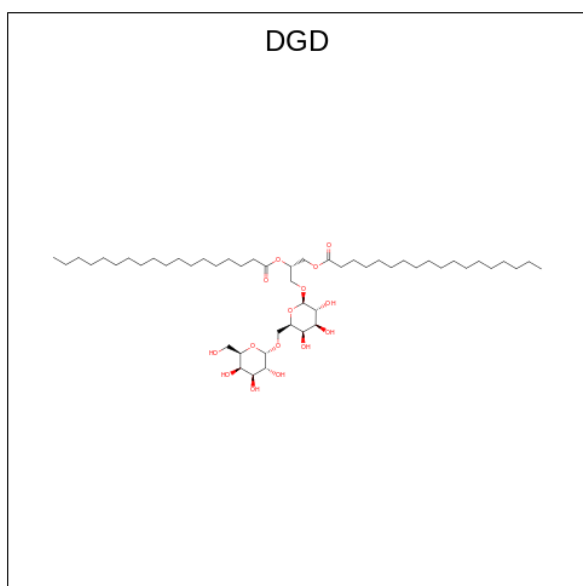
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			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: C₄₁H₇₈O₁₂S) (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).



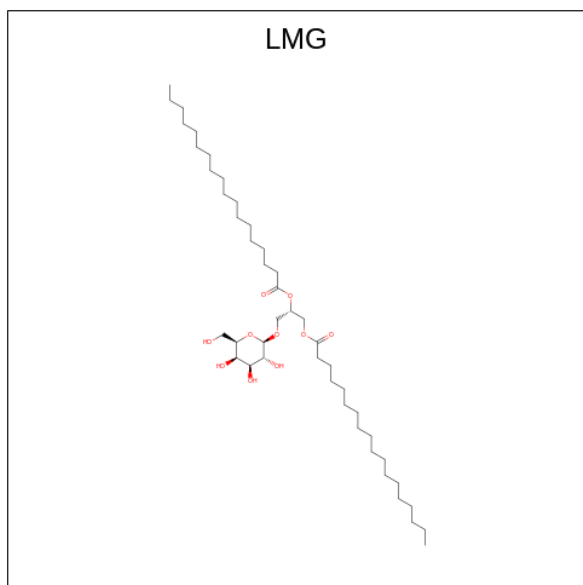
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			40	25	15	

Continued on next page...

Continued from previous page...

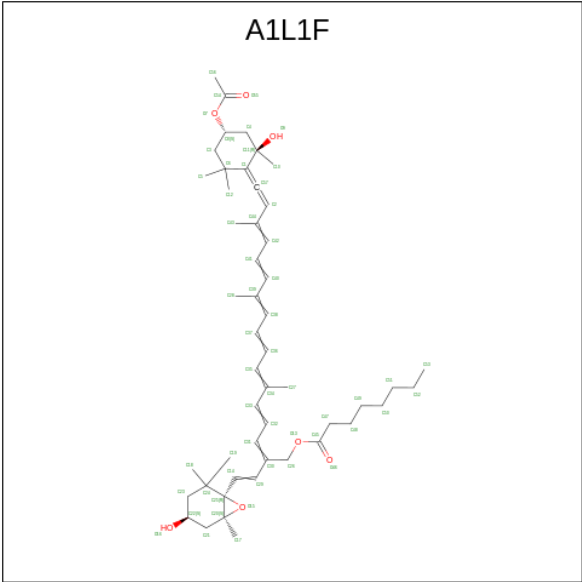
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			57	42	15	

- 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).



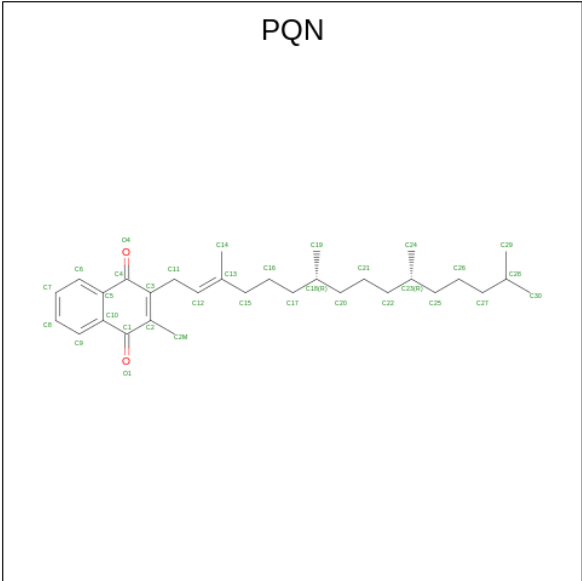
Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	C	O	0
			35	25	10	
22	a	1	Total	C	O	0
			34	24	10	
22	j	1	Total	C	O	0
			32	22	10	

- 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).



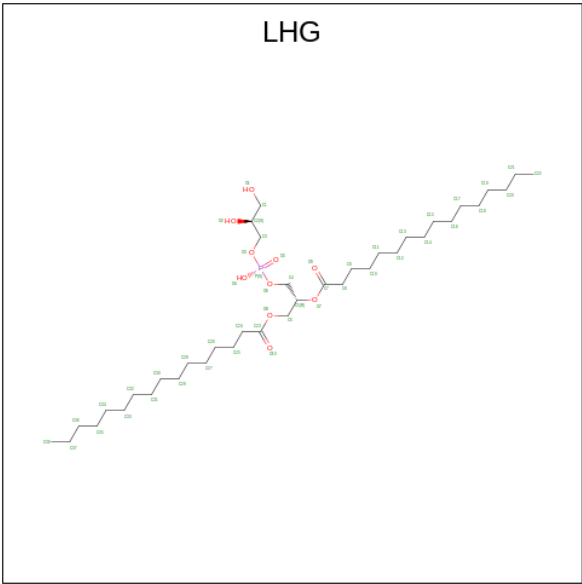
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			57	50	7	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



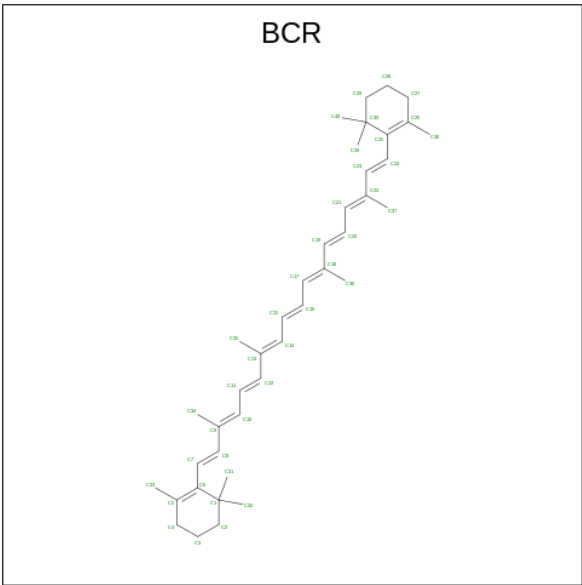
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			33	31	2	
24	b	1	Total	C	O	0
			33	31	2	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (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: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



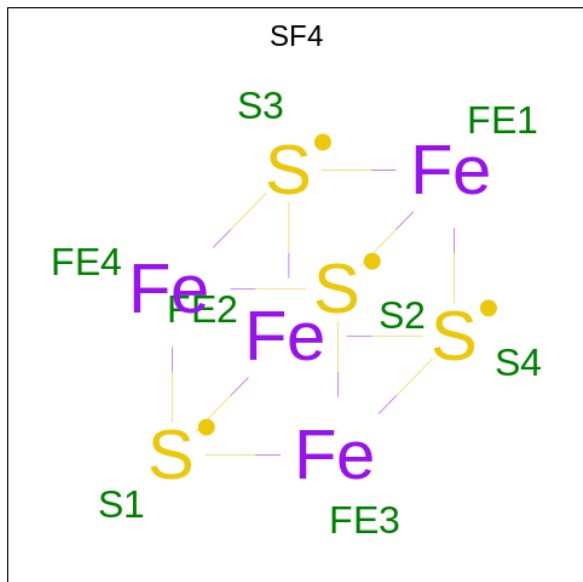
Mol	Chain	Residues	Atoms	AltConf
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C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

Continued on next page...

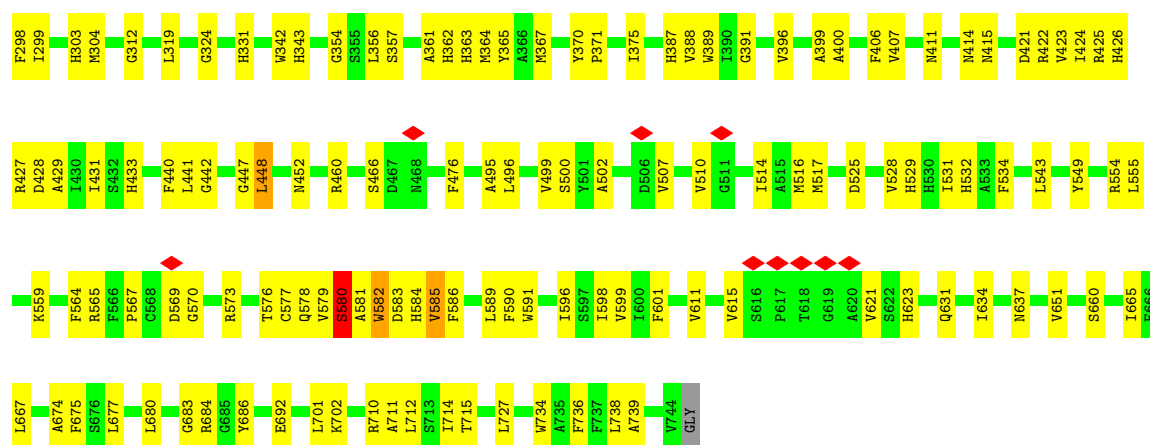
Continued from previous page...

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

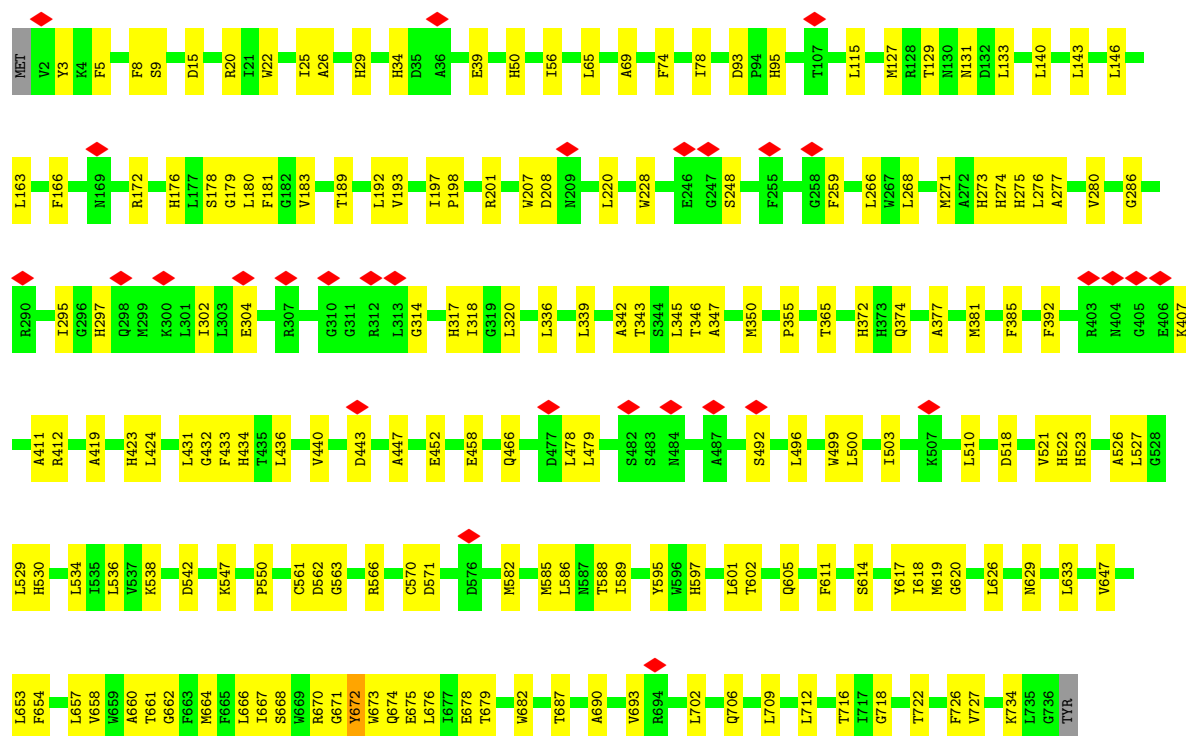
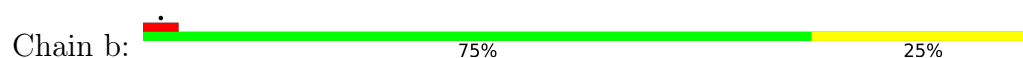
- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



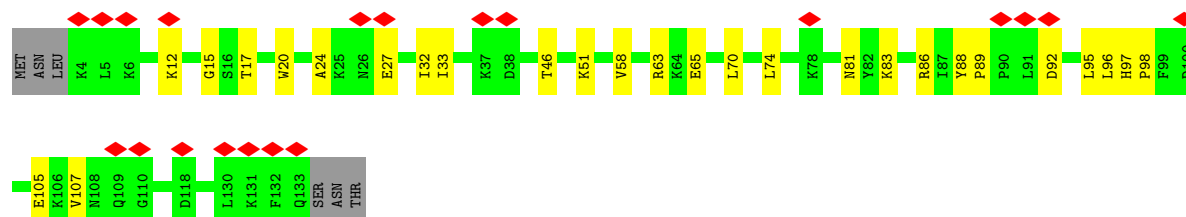
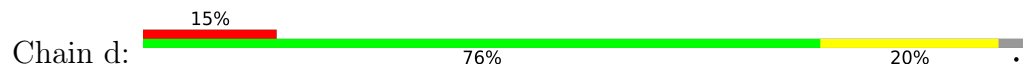
Mol	Chain	Residues	Atoms	AltConf
27	a	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0



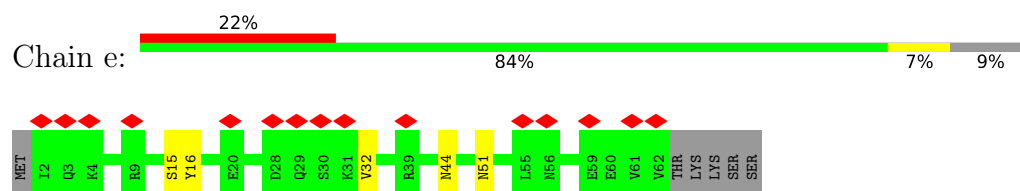
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2



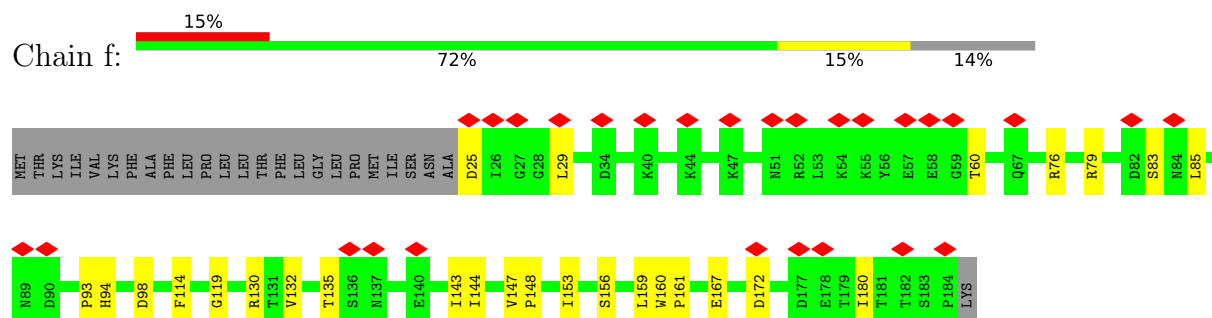
• Molecule 8: Photosystem I reaction center subunit II



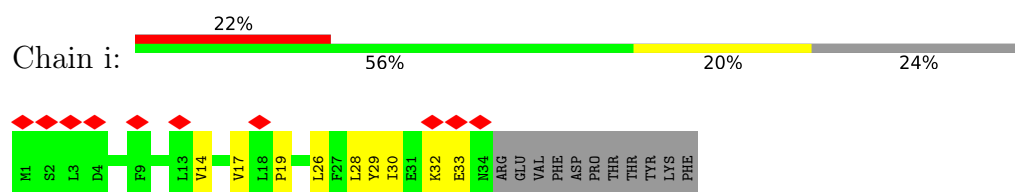
- Molecule 9: Photosystem I reaction center subunit IV



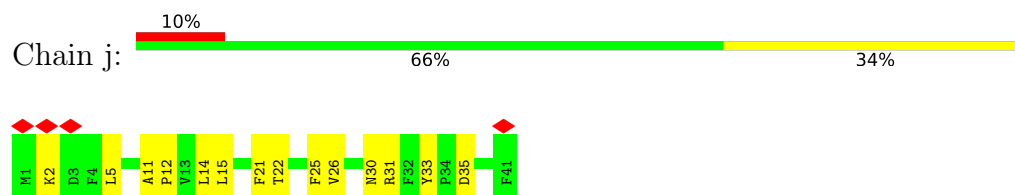
- Molecule 10: Photosystem I reaction center subunit III



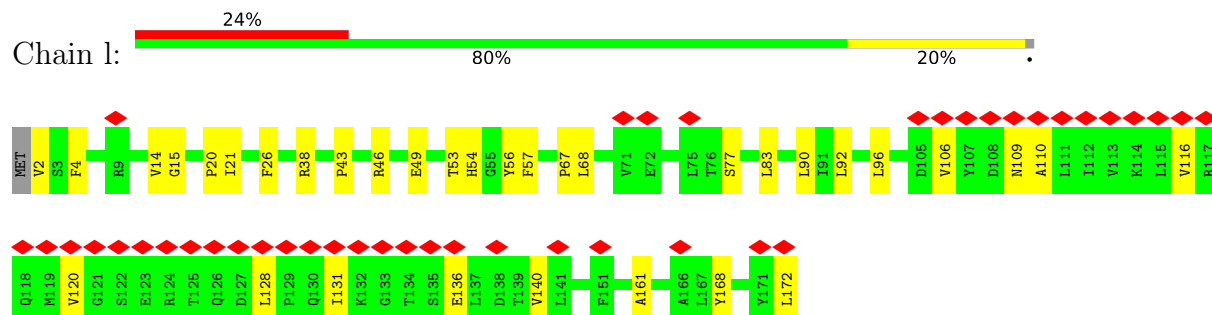
- Molecule 11: Photosystem I reaction center subunit VIII



- Molecule 12: Photosystem I reaction center subunit IX

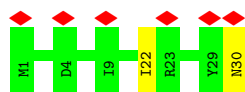


- Molecule 13: PSI subunit V

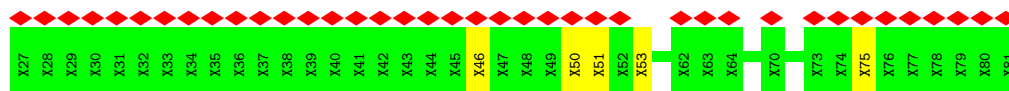
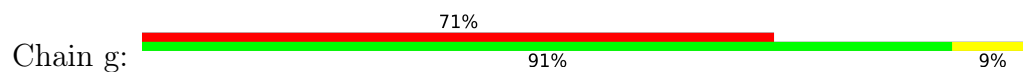


- Molecule 14: Psam

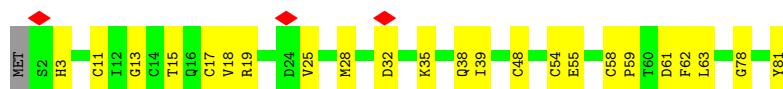




- Molecule 15: PsaS



- 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	66059	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	1.601	Depositor
Minimum map value	-0.390	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.367	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/1761
3	3	0.12	0/1350	0.27	0/1821
4	2	0.14	0/1405	0.36	0/1904
5	1	0.14	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	0.15	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	-7.07	1.43	1.52
6	a	581	ALA	CA-C	-5.43	1.45	1.52
6	a	582	TRP	CA-C	-5.00	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	102.51	113.72
6	a	448	LEU	N-CA-C	-6.10	104.18	111.69
6	a	584	HIS	N-CA-C	-5.83	106.51	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	-5.57	106.32	113.23
6	a	585	VAL	N-CA-C	-5.04	105.49	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	23	0
3	3	1324	0	1340	23	0
4	2	1372	0	1347	23	0
5	1	1262	0	1237	40	0
6	a	5827	0	5697	142	0
7	b	5865	0	5710	147	0
8	d	1014	0	1015	21	0
9	e	494	0	495	5	0
10	f	1266	0	1262	23	0
11	i	271	0	292	11	0
12	j	339	0	342	21	0
13	l	1283	0	1278	24	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	7	0
17	2	220	0	280	20	0
17	3	176	0	224	16	0
17	4	220	0	280	28	0
17	5	132	0	168	17	0
17	a	44	0	56	5	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	14	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	12	0
19	3	458	0	378	9	0
19	4	613	0	522	32	0
19	5	563	0	472	27	0
19	a	2579	0	2562	148	0
19	b	2475	0	2536	127	0
19	f	117	0	115	2	0
19	i	62	0	63	3	0
19	j	100	0	86	10	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	6	0
22	2	35	0	40	3	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	4	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	4	0
26	a	160	0	224	15	0
26	b	320	0	448	29	0
26	f	80	0	112	13	0
26	i	40	0	56	3	0
26	j	40	0	56	9	0
26	l	80	0	112	13	0
26	m	40	0	56	2	0
27	a	8	0	0	0	0
27	c	16	0	0	2	0
All	All	34630	0	34141	860	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (860) 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:C6E	1.85	1.07

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:HE62	1.13	1.07
17:2:303:XAT:H32	19:2:308:CLA:HAB	1.52	0.89
17:5:302:XAT:H12	19:5:307:CLA:HAB	1.53	0.89
21:4:318:DGD:O4E	21:4:318:DGD:O5E	1.61	0.88
6:a:531:ILE:HD12	19:a:801:CLA:H172	1.63	0.80
19:a:806:CLA:O1A	19:a:814:CLA:HBA1	1.81	0.80
19:b:826:CLA:HMA1	26:b:847:BCR:H17C	1.66	0.78
17:4:303:XAT:H12	19:4:308:CLA:HAB	1.67	0.76
19:1:312:CLA:HHC	19:1:312:CLA:HBB1	1.69	0.73
17:2:303:XAT:H181	19:2:314:CLA:HBB1	1.70	0.73
19:b:834:CLA:H72	26:b:847:BCR:H391	1.72	0.70
19:4:317:CLA:H2A	21:4:318:DGD:HE62	1.73	0.70
5:1:43:ILE:O	5:1:70:ARG:NH2	2.25	0.70
10:f:167:GLU:HG3	10:f:172:ASP:HB3	1.73	0.70
26:a:847:BCR:H362	26:a:848:BCR:H21C	1.73	0.69
2:4:193:ALA:CB	21:4:318:DGD:HE62	2.07	0.69
7:b:273:HIS:HD1	19:b:818:CLA:HAB	1.58	0.69
12:j:22:THR:HA	12:j:25:PHE:CE1	2.28	0.69
19:b:807:CLA:H151	19:b:829:CLA:HBB2	1.74	0.68
19:a:804:CLA:HED1	12:j:15:LEU:HD22	1.76	0.67
7:b:295:ILE:HG13	19:b:821:CLA:HED1	1.77	0.67
1:5:179:LEU:HD12	10:f:159:LEU:HD11	1.75	0.67
17:4:302:XAT:H14	19:4:310:CLA:H12	1.76	0.67
5:1:194:GLN:HG3	5:1:199:ASN:HB3	1.77	0.67
6:a:569:ASP:OD2	6:a:573:ARG:NH2	2.27	0.67
6:a:363:HIS:ND1	19:a:819:CLA:OBD	2.26	0.67
19:4:317:CLA:HAA2	21:4:318:DGD:HE5	1.77	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
7:b:336:LEU:HD21	19:b:830:CLA:HAB	1.78	0.66
5:1:146:LEU:HD13	19:a:844:CLA:H91	1.77	0.65
12:j:31:ARG:HD3	17:j:101:XAT:H222	1.77	0.65
19:a:834:CLA:H142	26:b:848:BCR:H15C	1.79	0.65
7:b:304:GLU:HG2	7:b:318:ILE:HG13	1.78	0.65
11:i:29:TYR:HA	11:i:32:LYS:HE2	1.78	0.65
6:a:112:TRP:HB3	17:j:101:XAT:H373	1.77	0.65
19:b:824:CLA:HBB1	19:b:838:CLA:H151	1.79	0.65
10:f:79:ARG:NH1	12:j:35:ASP:O	2.30	0.64
6:a:356:LEU:HD11	19:a:820:CLA:H71	1.79	0.64
17:4:303:XAT:H193	19:4:308:CLA:H142	1.78	0.64
6:a:429:ALA:O	6:a:433:HIS:ND1	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:808:CLA:HMB2	26:j:104:BCR:HC8	1.79	0.64
10:f:25:ASP:N	10:f:29:LEU:O	2.30	0.64
17:3:305:XAT:H32	19:3:313:CLA:HAB	1.79	0.64
7:b:115:LEU:HA	7:b:365:THR:HG22	1.80	0.64
19:b:814:CLA:H121	19:b:819:CLA:H72	1.79	0.64
6:a:197:GLY:O	6:a:201:LEU:HB2	1.97	0.64
7:b:9:SER:HB2	21:b:851:DGD:HE62	1.78	0.64
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
17:4:304:XAT:H32	19:4:313:CLA:HAB	1.80	0.63
6:a:298:PHE:HE1	19:a:822:CLA:HAB	1.64	0.63
6:a:362:HIS:HA	6:a:365:TYR:CE1	2.33	0.63
1:5:130:PHE:CE1	17:5:302:XAT:O24	2.52	0.63
7:b:129:THR:HG22	7:b:131:ASN:H	1.63	0.63
7:b:424:LEU:HD13	7:b:534:LEU:HA	1.81	0.63
17:4:305:XAT:H363	17:3:301:XAT:H10	1.80	0.62
6:a:114:ILE:HB	17:j:101:XAT:H372	1.81	0.62
7:b:29:HIS:ND1	19:b:807:CLA:O1A	2.28	0.62
6:a:298:PHE:CE1	19:a:822:CLA:HAB	2.34	0.62
12:j:21:PHE:HA	19:j:103:CLA:HBB2	1.80	0.62
20:5:316:SQD:H2	17:4:301:XAT:H373	1.82	0.62
6:a:70:HIS:ND1	19:a:814:CLA:OBD	2.31	0.62
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
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
19:b:831:CLA:HAB	19:b:838:CLA:HBB2	1.82	0.61
19:a:818:CLA:C3D	22:a:853:LMG:HC91	2.30	0.61
8:d:12:LYS:HB2	8:d:51:LYS:HB3	1.82	0.61
19:a:833:CLA:HBC2	19:a:840:CLA:HMC2	1.83	0.61
19:b:832:CLA:HBC3	26:f:804:BCR:H362	1.83	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
4:2:76:THR:O	4:2:82:ARG:NH1	2.33	0.61
23:1:304:A1L1F:C2	19:a:844:CLA:H11	2.31	0.61
6:a:121:ASN:HB3	6:a:129:GLN:HB3	1.82	0.61
7:b:561:CYS:SG	7:b:563:GLY:N	2.71	0.61
8:d:86:ARG:HB2	8:d:96:LEU:HD11	1.82	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	0.60
6:a:162:ALA:O	6:a:166:MET:HG2	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:412:ARG:NH2	19:b:831:CLA:O1D	2.35	0.60
5:1:186:ILE:HG13	5:1:187:THR:HG23	1.83	0.60
7:b:660:ALA:HB3	19:b:804:CLA:HBB2	1.83	0.60
1:5:111:TRP:NE1	19:5:308:CLA:O1A	2.33	0.60
7:b:431:LEU:HD11	19:b:837:CLA:HMB2	1.84	0.60
6:a:53:ASP:OD2	6:a:343:HIS:NE2	2.35	0.60
2:4:170:MET:HE1	19:4:313:CLA:H43	1.84	0.60
3:3:83:TYR:OH	3:3:163:ARG:NH1	2.35	0.60
3:3:199:ALA:O	3:3:203:MET:HG3	2.01	0.60
5:1:72:SER:O	5:1:76:HIS:ND1	2.28	0.60
19:a:820:CLA:H92	19:a:830:CLA:H91	1.84	0.59
3:3:92:HIS:HB3	3:3:197:MET:SD	2.42	0.59
13:l:38:ARG:O	13:l:46:ARG:NH2	2.35	0.59
19:a:804:CLA:ND	12:j:12:PRO:HG3	2.17	0.59
18:1:301:A1L1G:C18	19:1:306:CLA:HAC2	2.32	0.59
6:a:507:VAL:HG22	6:a:517:MET:HG3	1.85	0.59
17:2:303:XAT:H363	19:2:308:CLA:H2	1.84	0.59
6:a:167:LEU:HD11	19:a:810:CLA:H193	1.83	0.59
2:4:185:PHE:CZ	17:4:303:XAT:H30	2.37	0.59
4:2:44:PRO:HG3	4:2:58:ASP:HB3	1.83	0.59
26:b:843:BCR:H23C	26:b:850:BCR:H323	1.86	0.58
1:5:112:LEU:HD22	19:5:307:CLA:H12	1.86	0.58
19:a:818:CLA:C1D	22:a:853:LMG:H291	2.34	0.58
6:a:734:TRP:NE1	19:a:829:CLA:O1A	2.36	0.58
19:3:312:CLA:H42	26:a:848:BCR:H272	1.85	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
19:a:826:CLA:HBA1	19:a:830:CLA:H193	1.86	0.58
7:b:74:PHE:O	7:b:78:ILE:HG12	2.04	0.58
6:a:517:MET:HE1	6:a:623:HIS:NE2	2.19	0.57
1:5:155:VAL:HG21	19:5:309:CLA:HAA2	1.86	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.57
6:a:7:SER:H	6:a:12:PHE:HE2	1.53	0.57
19:b:804:CLA:CGA	19:b:804:CLA:H3A	2.34	0.57
26:f:801:BCR:HC32	19:j:102:CLA:H43	1.86	0.57
6:a:107:SER:HB2	6:a:124:VAL:HG11	1.85	0.57
6:a:292:LEU:HD21	19:a:818:CLA:CAB	2.34	0.57
7:b:69:ALA:HB2	7:b:133:LEU:HB2	1.86	0.57
17:2:303:XAT:C36	19:2:308:CLA:H2	2.35	0.57
6:a:598:ILE:HG13	19:a:801:CLA:H192	1.86	0.57
7:b:582:MET:HG3	7:b:712:LEU:HD21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:213:ILE:HG23	6:a:233:PRO:HB3	1.87	0.57
7:b:39:GLU:HB3	7:b:163:LEU:HD11	1.87	0.57
19:b:805:CLA:H18	11:i:14:VAL:HG22	1.86	0.57
6:a:651:VAL:HG22	6:a:739:ALA:HB3	1.87	0.57
8:d:97:HIS:HB3	8:d:98:PRO:HD3	1.86	0.57
17:5:301:XAT:H14	19:5:309:CLA:H12	1.86	0.56
3:3:86:ARG:NH1	3:3:89:GLU:OE1	2.38	0.56
7:b:693:VAL:HG11	19:b:801:CLA:HAB	1.87	0.56
22:a:853:LMG:H112	22:a:853:LMG:C9	2.35	0.56
19:a:802:CLA:CGA	19:a:802:CLA:H3A	2.35	0.56
13:l:54:HIS:HA	13:l:57:PHE:CE2	2.41	0.56
4:2:35:SER:OG	4:2:37:ALA:O	2.22	0.56
19:a:841:CLA:H72	26:f:801:BCR:H17C	1.88	0.56
6:a:324:GLY:HA3	25:a:846:LHG:HC32	1.87	0.56
11:i:26:LEU:HD13	26:l:205:BCR:HC8	1.86	0.56
22:a:853:LMG:H112	22:a:853:LMG:O8	2.05	0.56
6:a:114:ILE:HG13	6:a:115:VAL:HG13	1.86	0.56
19:a:822:CLA:HBC3	19:a:828:CLA:H172	1.87	0.56
6:a:441:LEU:HB3	6:a:534:PHE:HB2	1.88	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.55
6:a:660:SER:HB2	7:b:447:ALA:HB1	1.88	0.55
13:l:92:LEU:HB3	26:l:205:BCR:H401	1.88	0.55
19:a:818:CLA:CHD	22:a:853:LMG:H291	2.36	0.55
19:b:806:CLA:HBA1	19:b:814:CLA:HBA1	1.87	0.55
2:4:136:VAL:HG22	19:4:312:CLA:HMA1	1.87	0.55
6:a:290:HIS:HB2	19:a:819:CLA:C1B	2.36	0.55
19:a:825:CLA:H12	26:a:849:BCR:H14C	1.88	0.55
3:3:48:LEU:HD13	3:3:51:LEU:HD12	1.87	0.55
7:b:178:SER:HB3	7:b:286:GLY:HA3	1.86	0.55
8:d:105:GLU:HG2	16:c:19:ARG:HB3	1.88	0.55
2:4:185:PHE:CE2	17:4:303:XAT:H30	2.42	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
6:a:388:VAL:HG12	6:a:596:ILE:HG23	1.89	0.55
19:a:854:CLA:H112	12:j:14:LEU:HD22	1.88	0.55
7:b:317:HIS:HB3	7:b:320:LEU:HD12	1.89	0.55
5:1:115:ILE:O	5:1:119:GLN:NE2	2.40	0.55
6:a:197:GLY:HA3	19:a:814:CLA:HBB1	1.89	0.55
6:a:651:VAL:HG21	6:a:736:PHE:HA	1.88	0.55
3:3:182:PHE:HZ	19:3:313:CLA:HED3	1.70	0.55
6:a:702:LYS:HB3	10:f:130:ARG:HD3	1.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:210:GLN:HA	6:a:214:ALA:HB3	1.89	0.54
5:1:88:ILE:HG22	5:1:92:PHE:HE1	1.71	0.54
19:b:822:CLA:HBB	19:b:823:CLA:H2	1.88	0.54
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.54
6:a:591:TRP:HE1	19:b:804:CLA:C1D	2.21	0.54
9:e:32:VAL:HG11	16:c:35:LYS:HD3	1.89	0.54
5:1:61:ALA:HB1	5:1:65:THR:HB	1.90	0.54
12:j:14:LEU:HD21	22:j:105:LMG:H141	1.89	0.54
8:d:63:ARG:NH2	8:d:65:GLU:OE1	2.41	0.54
16:c:15:THR:HG22	16:c:28:MET:HG3	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
7:b:140:LEU:HG	26:b:845:BCR:H382	1.90	0.54
19:a:829:CLA:H101	26:j:104:BCR:H341	1.89	0.54
19:a:831:CLA:H42	25:a:845:LHG:H251	1.90	0.54
6:a:219:LYS:HD3	6:a:246:LEU:HB3	1.90	0.54
7:b:661:THR:O	7:b:664:MET:HB3	2.08	0.53
19:b:830:CLA:H42	21:b:851:DGD:HB42	1.91	0.53
3:3:87:GLU:OE2	3:3:163:ARG:NH2	2.31	0.53
18:5:303:A1L1G:C41	19:5:312:CLA:HMC1	2.38	0.53
6:a:667:LEU:HD11	7:b:619:MET:HB2	1.89	0.53
7:b:5:PHE:HB2	11:i:30:ILE:HA	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
7:b:355:PRO:HG3	19:b:819:CLA:HBA1	1.90	0.53
2:4:83:ILE:HD11	17:4:302:XAT:H362	1.90	0.53
19:a:835:CLA:O2D	19:a:835:CLA:H2A	2.09	0.53
7:b:633:LEU:HD22	7:b:726:PHE:HA	1.89	0.53
19:a:809:CLA:CHC	19:a:810:CLA:HMD2	2.39	0.53
7:b:189:THR:HG21	7:b:276:LEU:HB2	1.91	0.53
6:a:396:VAL:HG11	6:a:589:LEU:HG	1.90	0.53
19:a:810:CLA:HAB	19:j:102:CLA:HMD2	1.91	0.53
19:b:837:CLA:HBC3	26:f:804:BCR:H292	1.91	0.53
2:4:193:ALA:O	21:4:318:DGD:O6E	2.28	0.52
5:1:77:GLY:O	5:1:81:MET:HG3	2.09	0.52
17:5:302:XAT:C16	19:5:307:CLA:H2	2.39	0.52
7:b:718:GLY:O	7:b:722:THR:HG22	2.09	0.52
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.92	0.52
4:2:77:LYS:O	4:2:79:ASP:N	2.43	0.52
5:1:85:LEU:HB3	19:1:308:CLA:HMC2	1.92	0.52
6:a:573:ARG:HG3	16:c:78:GLY:HA3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:121:LEU:HD23	2:4:124:ILE:HD12	1.90	0.52
19:a:825:CLA:HMA3	19:a:844:CLA:HAB	1.91	0.52
3:3:79:GLY:O	3:3:158:ARG:NH1	2.43	0.52
19:a:834:CLA:H151	24:b:842:PQN:H202	1.91	0.52
19:b:801:CLA:H101	19:b:801:CLA:HBB1	1.91	0.52
7:b:709:LEU:HD11	21:b:851:DGD:HB41	1.90	0.52
10:f:85:LEU:HD13	10:f:93:PRO:HB3	1.92	0.52
19:a:827:CLA:H93	19:a:840:CLA:H52	1.92	0.52
2:4:81:CYS:HB3	2:4:178:GLY:HA3	1.91	0.52
19:4:317:CLA:O2D	21:4:318:DGD:HE61	2.09	0.51
7:b:662:GLY:O	7:b:666:LEU:HG	2.10	0.51
15:g:51:UNK:O	15:g:53:UNK:N	2.42	0.51
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.51
7:b:208:ASP:OD1	7:b:208:ASP:N	2.43	0.51
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
4:2:121:ALA:O	4:2:122:LYS:HG2	2.10	0.51
6:a:460:ARG:NH2	19:a:835:CLA:O1D	2.44	0.51
7:b:26:ALA:HA	19:b:830:CLA:H43	1.93	0.51
7:b:179:GLY:O	7:b:183:VAL:HB	2.10	0.51
6:a:431:ILE:HG13	6:a:549:TYR:HE1	1.74	0.51
19:b:824:CLA:HAB	19:b:831:CLA:HMD1	1.93	0.51
16:c:58:CYS:SG	16:c:63:LEU:HA	2.51	0.51
1:5:130:PHE:HE1	17:5:302:XAT:O24	1.94	0.51
22:a:853:LMG:C11	22:a:853:LMG:HC92	2.41	0.51
8:d:33:ILE:HG22	8:d:58:VAL:HG22	1.93	0.51
8:d:95:LEU:HD22	15:g:75:UNK:HA	1.92	0.51
10:f:160:TRP:CD1	10:f:161:PRO:HD3	2.46	0.51
16:c:11:CYS:SG	16:c:39:ILE:HG13	2.50	0.51
6:a:577:CYS:O	7:b:671:GLY:HA3	2.11	0.51
7:b:342:ALA:O	7:b:346:THR:HG23	2.11	0.51
7:b:434:HIS:CD2	26:b:852:BCR:H333	2.46	0.51
23:1:304:A1L1F:C56	25:a:846:LHG:H241	2.41	0.51
19:a:818:CLA:HHC	19:a:818:CLA:HBB1	1.93	0.51
7:b:722:THR:HG23	19:b:803:CLA:O1D	2.11	0.50
19:b:837:CLA:HBC3	26:f:804:BCR:H401	1.91	0.50
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
4:2:107:LEU:HB3	19:2:310:CLA:HMC2	1.94	0.50
19:b:807:CLA:H52	21:b:851:DGD:HB72	1.93	0.50
16:c:13:GLY:O	16:c:38:GLN:NE2	2.44	0.50
10:f:143:ILE:HG13	10:f:144:ILE:HG13	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:312:CLA:CGA	19:5:312:CLA:H3A	2.41	0.50
13:l:38:ARG:NH1	13:l:49:GLU:OE1	2.40	0.50
22:a:853:LMG:H131	22:a:853:LMG:H292	1.94	0.50
7:b:274:HIS:HB2	19:b:818:CLA:C1B	2.41	0.50
19:b:812:CLA:H72	19:b:813:CLA:HBC3	1.93	0.50
4:2:183:ASP:O	4:2:186:LYS:N	2.44	0.50
6:a:712:LEU:N	24:a:843:PQN:O4	2.45	0.50
7:b:602:THR:HG21	7:b:611:PHE:HB2	1.92	0.49
6:a:422:ARG:O	6:a:426:HIS:ND1	2.41	0.49
6:a:440:PHE:HE2	19:a:839:CLA:HAB	1.76	0.49
7:b:526:ALA:O	7:b:530:HIS:ND1	2.37	0.49
13:l:106:VAL:H	13:l:140:VAL:HG23	1.77	0.49
16:c:17:CYS:SG	16:c:18:VAL:N	2.85	0.49
5:1:112:VAL:HB	5:1:117:TRP:NE1	2.27	0.49
6:a:423:VAL:HA	6:a:426:HIS:CE1	2.47	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
6:a:425:ARG:NH2	8:d:15:GLY:O	2.44	0.49
7:b:273:HIS:ND1	19:b:818:CLA:HAB	2.25	0.49
13:l:109:ASN:OD1	13:l:110:ALA:N	2.36	0.49
6:a:615:VAL:HG22	6:a:621:VAL:HG22	1.95	0.49
6:a:554:ARG:HB2	7:b:678:GLU:OE1	2.13	0.49
6:a:674:ALA:HB3	19:a:802:CLA:HBB2	1.94	0.49
6:a:686:TYR:OH	19:a:802:CLA:OBD	2.22	0.49
19:a:818:CLA:O1A	22:a:853:LMG:O10	2.30	0.49
17:5:301:XAT:H193	19:5:310:CLA:HBA2	1.94	0.49
19:4:309:CLA:HAC1	19:4:316:CLA:HAB	1.95	0.49
7:b:181:PHE:HE2	19:b:820:CLA:HAB	1.78	0.49
7:b:266:LEU:HD22	19:b:818:CLA:HBA1	1.95	0.49
7:b:492:SER:HA	7:b:496:LEU:HD12	1.94	0.49
19:a:803:CLA:H2	7:b:657:LEU:HD22	1.95	0.49
22:a:853:LMG:C9	22:a:853:LMG:C11	2.91	0.49
26:b:852:BCR:H23C	12:j:33:TYR:CD2	2.47	0.49
13:l:43:PRO:HD3	13:l:136:GLU:CD	2.38	0.49
6:a:565:ARG:HG2	6:a:715:THR:HG21	1.93	0.49
7:b:419:ALA:O	7:b:423:HIS:ND1	2.40	0.49
16:c:17:CYS:HB3	27:c:102:SF4:S4	2.52	0.49
2:4:159:ASN:C	2:4:161:ALA:H	2.20	0.48
19:3:308:CLA:HED2	19:3:308:CLA:H2A	1.94	0.48
19:a:802:CLA:H41	7:b:436:LEU:HD22	1.95	0.48
7:b:3:TYR:HB2	11:i:33:GLU:HA	1.95	0.48
7:b:595:TYR:CZ	19:b:836:CLA:HBC3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:597:HIS:CE1	7:b:601:LEU:HD11	2.49	0.48
11:i:26:LEU:HD22	26:l:205:BCR:H323	1.94	0.48
15:g:46:UNK:O	15:g:50:UNK:N	2.45	0.48
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.48
19:1:306:CLA:H93	19:1:306:CLA:H61	1.70	0.48
19:b:824:CLA:H2A	19:b:824:CLA:HED3	1.95	0.48
3:3:78:VAL:HG12	3:3:78:VAL:O	2.13	0.48
6:a:411:ASN:ND2	6:a:414:ASN:OD1	2.37	0.48
7:b:166:PHE:O	7:b:172:ARG:NH2	2.46	0.48
19:b:833:CLA:HBB2	26:f:801:BCR:HC41	1.94	0.48
3:3:203:MET:HE2	17:3:305:XAT:O4	2.13	0.48
6:a:292:LEU:HD12	19:a:816:CLA:HMC3	1.95	0.48
19:b:840:CLA:H13	26:i:101:BCR:H19C	1.95	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.48
19:2:316:CLA:C2C	22:2:317:LMG:H111	2.44	0.48
5:1:88:ILE:HG22	5:1:92:PHE:CE1	2.49	0.48
6:a:400:ALA:HB2	6:a:585:VAL:HG11	1.96	0.48
19:a:841:CLA:H61	19:b:833:CLA:H42	1.95	0.48
7:b:25:ILE:HG12	26:l:205:BCR:H312	1.94	0.48
12:j:2:LYS:O	22:j:105:LMG:HC61	2.13	0.48
6:a:712:LEU:HD21	24:a:843:PQN:H151	1.95	0.48
19:a:818:CLA:CHD	19:a:819:CLA:HBB2	2.43	0.48
3:3:145:ILE:O	3:3:149:ILE:HG12	2.13	0.48
6:a:287:THR:HG23	19:a:820:CLA:HMA3	1.96	0.48
6:a:290:HIS:HB2	19:a:819:CLA:CHB	2.44	0.48
7:b:93:ASP:OD1	7:b:95:HIS:ND1	2.33	0.48
7:b:271:MET:O	7:b:275:HIS:ND1	2.46	0.48
9:e:51:ASN:CG	16:c:61:ASP:HB2	2.39	0.48
1:5:171:GLU:HG3	19:5:311:CLA:NB	2.28	0.48
17:5:304:XAT:C10	19:5:315:CLA:HBC3	2.43	0.48
17:4:303:XAT:H11	17:4:303:XAT:H191	1.74	0.48
5:1:42:MET:HE1	5:1:66:LEU:HD22	1.95	0.48
7:b:670:ARG:C	7:b:672:TYR:H	2.22	0.48
19:b:831:CLA:HAB	19:b:838:CLA:CBB	2.44	0.48
2:4:184:ALA:HA	19:4:315:CLA:HBB1	1.95	0.48
7:b:176:HIS:O	7:b:180:LEU:HB3	2.14	0.48
7:b:407:LYS:HB3	7:b:411:ALA:HB3	1.95	0.48
7:b:478:LEU:HG	7:b:479:LEU:HG	1.93	0.48
12:j:5:LEU:HB3	22:j:105:LMG:HC72	1.96	0.48
19:3:308:CLA:H2A	19:3:308:CLA:CED	2.44	0.48
6:a:514:ILE:HD11	6:a:621:VAL:HG13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:825:CLA:H71	19:a:840:CLA:H62	1.96	0.48
7:b:412:ARG:HH21	19:b:831:CLA:CGD	2.27	0.48
19:b:825:CLA:H193	19:b:825:CLA:H141	1.95	0.48
11:i:26:LEU:HB3	26:l:205:BCR:H323	1.96	0.48
6:a:637:ASN:HB2	7:b:653:LEU:HD11	1.94	0.47
19:a:820:CLA:H203	19:a:828:CLA:H3A	1.96	0.47
19:b:811:CLA:H202	13:l:90:LEU:HD22	1.96	0.47
19:b:839:CLA:HAB	24:b:842:PQN:H172	1.96	0.47
8:d:95:LEU:HD11	8:d:98:PRO:HD2	1.95	0.47
7:b:432:GLY:HA2	7:b:527:LEU:HD22	1.96	0.47
19:b:809:CLA:H142	19:b:809:CLA:H111	1.70	0.47
26:b:852:BCR:H23C	12:j:33:TYR:HD2	1.78	0.47
19:a:832:CLA:HAB	19:a:840:CLA:HBB2	1.96	0.47
7:b:277:ALA:HA	19:b:817:CLA:HMC2	1.95	0.47
7:b:518:ASP:O	7:b:522:HIS:ND1	2.38	0.47
4:2:92:ARG:NH1	4:2:95:GLU:OE1	2.47	0.47
6:a:68:SER:OG	6:a:174:TYR:HB2	2.14	0.47
5:1:84:VAL:O	5:1:88:ILE:HG12	2.14	0.47
7:b:50:HIS:ND1	19:b:814:CLA:OBD	2.38	0.47
19:b:808:CLA:H93	19:b:808:CLA:H61	1.71	0.47
26:b:845:BCR:H311	26:b:845:BCR:HC8	1.97	0.47
19:j:102:CLA:NB	26:j:104:BCR:H281	2.30	0.47
17:3:304:XAT:H391	17:3:304:XAT:H31	1.78	0.47
6:a:476:PHE:HB3	19:a:838:CLA:H11	1.96	0.47
7:b:127:MET:HE1	26:b:845:BCR:H282	1.97	0.47
7:b:443:ASP:OD1	7:b:618:ILE:N	2.46	0.47
7:b:538:LYS:O	7:b:542:ASP:HB2	2.15	0.47
7:b:687:THR:HG23	7:b:690:ALA:HB3	1.97	0.47
17:2:305:XAT:H391	17:2:305:XAT:H31	1.71	0.47
17:1:302:XAT:H35	17:1:302:XAT:H401	1.72	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	1.95	0.47
6:a:354:GLY:HA2	6:a:391:GLY:HA2	1.97	0.47
19:a:834:CLA:CAD	26:l:201:BCR:H10C	2.45	0.47
7:b:8:PHE:HB2	7:b:34:HIS:CG	2.49	0.47
7:b:372:HIS:HB2	19:b:828:CLA:C1B	2.45	0.47
2:4:185:PHE:CZ	17:4:303:XAT:H28	2.50	0.47
17:4:305:XAT:H15	17:4:305:XAT:H201	1.71	0.47
7:b:65:LEU:HD11	26:b:845:BCR:H281	1.95	0.47
7:b:385:PHE:HB3	7:b:536:LEU:HB3	1.97	0.47
26:b:843:BCR:H15C	26:b:843:BCR:H351	1.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:83:LYS:HG2	8:d:98:PRO:HG2	1.97	0.47
19:4:317:CLA:CGD	21:4:318:DGD:HE61	2.45	0.46
4:2:105:ALA:HB1	17:2:303:XAT:H161	1.97	0.46
7:b:50:HIS:HE1	19:b:806:CLA:H171	1.81	0.46
19:b:812:CLA:H51	19:b:813:CLA:H43	1.97	0.46
5:1:73:GLU:HB2	19:1:306:CLA:C1B	2.45	0.46
6:a:144:GLU:HG2	6:a:206:TRP:HH2	1.80	0.46
19:b:818:CLA:H41	19:b:834:CLA:HAA2	1.98	0.46
19:b:822:CLA:CHB	19:b:823:CLA:H2	2.44	0.46
19:b:828:CLA:H61	19:b:828:CLA:H102	1.85	0.46
1:5:96:VAL:HG12	19:5:307:CLA:OBD	2.15	0.46
17:4:303:XAT:H15	17:4:303:XAT:H201	1.82	0.46
17:3:305:XAT:H35	17:3:305:XAT:H401	1.77	0.46
19:a:827:CLA:H13	19:a:827:CLA:H172	1.77	0.46
19:b:823:CLA:HHC	19:b:841:CLA:HED1	1.98	0.46
19:b:824:CLA:HBA1	26:b:846:BCR:H16C	1.98	0.46
19:b:839:CLA:H12	26:l:205:BCR:H15C	1.98	0.46
3:3:179:PRO:C	3:3:181:LYS:H	2.24	0.46
4:2:191:GLN:O	4:2:195:ILE:HD12	2.15	0.46
6:a:127:ASN:HD21	10:f:60:THR:HG21	1.80	0.46
7:b:143:LEU:HD23	7:b:146:LEU:HD12	1.97	0.46
19:b:811:CLA:H71	13:l:83:LEU:HG	1.97	0.46
17:4:305:XAT:H391	17:4:305:XAT:H31	1.62	0.46
3:3:81:ASP:N	3:3:81:ASP:OD1	2.46	0.46
5:1:40:ASP:HB2	5:1:42:MET:HG3	1.98	0.46
7:b:297:HIS:HB3	7:b:302:ILE:HD11	1.97	0.46
13:l:168:TYR:O	13:l:172:LEU:HB2	2.16	0.46
19:4:310:CLA:H141	19:4:310:CLA:H162	1.69	0.46
4:2:118:LEU:N	19:2:310:CLA:OBD	2.47	0.46
19:2:316:CLA:C1C	22:2:317:LMG:H111	2.46	0.46
6:a:502:ALA:HB2	6:a:516:MET:HE2	1.97	0.46
19:a:803:CLA:H151	19:b:811:CLA:HBC3	1.97	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
7:b:433:PHE:HZ	26:f:801:BCR:H372	1.80	0.46
7:b:586:LEU:HD21	7:b:716:THR:HG23	1.96	0.46
19:b:811:CLA:HBA2	13:l:67:PRO:HG3	1.97	0.46
19:b:834:CLA:HBA2	19:b:834:CLA:H3A	1.52	0.46
8:d:20:TRP:CZ2	13:l:14:VAL:HG12	2.50	0.46
11:i:28:LEU:O	11:i:32:LYS:HG3	2.16	0.46
1:5:232:HIS:HE1	17:5:304:XAT:H14	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:813:CLA:H62	19:b:813:CLA:H41	1.62	0.46
1:5:116:GLU:HB2	19:5:307:CLA:C1B	2.46	0.46
4:2:127:ASN:OD1	4:2:130:GLN:N	2.46	0.46
6:a:375:ILE:HG21	6:a:510:VAL:HB	1.96	0.46
19:a:834:CLA:H201	26:l:205:BCR:H343	1.98	0.46
5:1:105:PRO:C	5:1:107:LYS:H	2.24	0.46
4:2:65:ILE:HG22	4:2:67:PHE:H	1.80	0.45
19:a:829:CLA:HBB1	19:a:829:CLA:HMB1	1.97	0.45
19:a:854:CLA:H143	22:j:105:LMG:H142	1.97	0.45
19:b:826:CLA:HAA2	19:b:827:CLA:OBD	2.16	0.45
26:b:845:BCR:H24C	26:b:845:BCR:H371	1.70	0.45
6:a:114:ILE:O	6:a:117:GLN:HG2	2.16	0.45
19:a:801:CLA:H61	19:a:803:CLA:O1D	2.15	0.45
19:a:818:CLA:NC	22:a:853:LMG:H302	2.31	0.45
19:b:839:CLA:H41	19:b:839:CLA:H62	1.71	0.45
19:3:310:CLA:H61	19:3:310:CLA:H41	1.86	0.45
5:1:89:VAL:O	5:1:93:TRP:N	2.49	0.45
6:a:665:ILE:HG23	19:a:809:CLA:H171	1.99	0.45
19:a:806:CLA:H162	19:a:806:CLA:H141	1.59	0.45
19:a:826:CLA:H202	19:a:826:CLA:H162	1.79	0.45
7:b:228:TRP:HZ3	26:b:850:BCR:H363	1.81	0.45
7:b:678:GLU:HG2	16:c:81:TYR:HE1	1.82	0.45
19:b:840:CLA:H92	19:b:840:CLA:H61	1.73	0.45
19:4:308:CLA:H112	19:4:308:CLA:H143	1.66	0.45
19:a:825:CLA:H62	19:a:825:CLA:H41	1.84	0.45
7:b:339:LEU:O	7:b:343:THR:HG22	2.16	0.45
19:b:833:CLA:H18	26:f:804:BCR:H17C	1.97	0.45
17:1:303:XAT:H183	19:1:308:CLA:C2B	2.47	0.45
6:a:312:GLY:HA2	19:a:823:CLA:HMD2	1.99	0.45
19:a:804:CLA:H41	19:a:841:CLA:HMC1	1.98	0.45
7:b:268:LEU:HD23	7:b:271:MET:HE3	1.98	0.45
10:f:119:GLY:HA3	10:f:160:TRP:CE2	2.51	0.45
26:i:101:BCR:H11C	26:i:101:BCR:H341	1.86	0.45
12:j:26:VAL:CG1	26:j:104:BCR:H403	2.46	0.45
1:5:106:PHE:HB2	10:f:148:PRO:HG3	1.99	0.45
2:4:170:MET:CE	19:4:313:CLA:H12	2.47	0.45
17:4:302:XAT:H30	19:4:310:CLA:H151	1.98	0.45
17:3:304:XAT:H15	17:3:304:XAT:H201	1.78	0.45
6:a:580:SER:HB2	6:a:582:TRP:H	1.82	0.45
7:b:562:ASP:OD2	7:b:566:ARG:NH2	2.38	0.45
10:f:153:ILE:O	10:f:156:SER:OG	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:101:LHG:H291	25:m:101:LHG:H321	1.65	0.45
6:a:367:MET:HG2	6:a:500:SER:HB2	1.99	0.45
6:a:407:VAL:HG11	6:a:564:PHE:N	2.32	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	1.99	0.45
7:b:26:ALA:HB1	21:b:851:DGD:O1B	2.17	0.45
7:b:280:VAL:HG21	19:b:817:CLA:HAB	1.98	0.45
11:i:14:VAL:O	11:i:19:PRO:HD2	2.17	0.45
16:c:3:HIS:HB2	16:c:48:CYS:SG	2.57	0.45
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.45
2:4:37:SER:HB3	2:4:45:ARG:HA	1.98	0.45
17:4:301:XAT:H35	17:4:301:XAT:H401	1.66	0.45
6:a:683:GLY:HA3	7:b:571:ASP:HB2	1.99	0.45
19:b:825:CLA:H92	19:b:825:CLA:H61	1.72	0.45
3:3:121:GLN:HA	3:3:124:VAL:HG12	1.99	0.45
6:a:25:PRO:HB2	6:a:41:TRP:HH2	1.81	0.45
6:a:342:TRP:CD1	19:a:826:CLA:H192	2.51	0.45
19:a:826:CLA:HMB3	19:a:826:CLA:HBB1	1.99	0.45
22:a:853:LMG:H112	22:a:853:LMG:HC92	1.98	0.45
19:b:821:CLA:H3A	19:b:821:CLA:HBA2	1.33	0.45
19:4:310:CLA:H142	19:4:310:CLA:H112	1.78	0.45
19:4:311:CLA:H2A	19:4:311:CLA:O2D	2.17	0.45
3:3:189:GLU:HB2	19:3:313:CLA:C1B	2.47	0.45
17:2:305:XAT:H15	17:2:305:XAT:H201	1.78	0.45
5:1:62:ASP:OD1	5:1:62:ASP:N	2.49	0.45
19:a:835:CLA:H61	26:l:201:BCR:H363	1.99	0.44
7:b:302:ILE:HD13	19:b:823:CLA:HMD2	1.99	0.44
19:b:802:CLA:H93	19:b:802:CLA:H112	1.70	0.44
10:f:143:ILE:O	12:j:11:ALA:N	2.48	0.44
22:j:105:LMG:H292	22:j:105:LMG:H111	1.98	0.44
6:a:71:PHE:HD1	6:a:166:MET:HE3	1.82	0.44
6:a:304:MET:HG3	19:a:823:CLA:C3C	2.47	0.44
6:a:686:TYR:CE1	7:b:538:LYS:HD2	2.52	0.44
7:b:654:PHE:O	7:b:658:VAL:HG23	2.17	0.44
19:b:829:CLA:H61	19:b:829:CLA:H41	1.75	0.44
10:f:160:TRP:CG	10:f:161:PRO:HD3	2.52	0.44
13:l:116:VAL:HG11	13:l:128:LEU:C	2.43	0.44
1:5:124:MET:HE3	19:5:312:CLA:HMC2	1.98	0.44
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.44
5:1:141:ARG:HD3	5:1:149:TRP:HB3	1.99	0.44
5:1:152:VAL:HG11	5:1:159:TRP:CD1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:807:CLA:H192	19:a:807:CLA:H161	1.82	0.44
10:f:79:ARG:O	10:f:83:SER:HB2	2.17	0.44
1:5:164:PHE:HE1	19:f:802:CLA:H121	1.81	0.44
2:4:59:PHE:HE1	19:4:306:CLA:HBC3	1.83	0.44
17:4:305:XAT:H11	17:4:305:XAT:H191	1.81	0.44
19:1:312:CLA:HMA2	20:1:315:SQD:H141	1.99	0.44
6:a:701:LEU:HD12	19:a:841:CLA:HMA2	2.00	0.44
7:b:192:LEU:HD23	7:b:192:LEU:HA	1.83	0.44
26:b:846:BCR:H15C	26:b:846:BCR:H351	1.83	0.44
26:f:804:BCR:H11C	26:f:804:BCR:H341	1.73	0.44
17:5:301:XAT:H35	17:5:301:XAT:H401	1.77	0.44
6:a:84:MET:SD	19:a:829:CLA:HED1	2.58	0.44
6:a:282:LEU:HD21	6:a:367:MET:HB3	1.98	0.44
6:a:442:GLY:HA3	19:b:804:CLA:O1A	2.18	0.44
6:a:570:GLY:O	6:a:576:THR:OG1	2.32	0.44
7:b:172:ARG:HB2	19:b:814:CLA:HBC2	2.00	0.44
7:b:259:PHE:CZ	7:b:510:LEU:HD12	2.52	0.44
17:4:301:XAT:H11	17:4:301:XAT:H191	1.86	0.44
6:a:565:ARG:HD2	25:a:845:LHG:HC61	2.00	0.44
19:a:805:CLA:HBA1	19:a:805:CLA:H3A	1.89	0.44
7:b:172:ARG:HD2	19:b:825:CLA:OBD	2.18	0.44
7:b:201:ARG:HG2	7:b:248:SER:HB2	1.99	0.44
7:b:466:GLN:NE2	19:b:836:CLA:OBD	2.34	0.44
19:b:824:CLA:HHB	19:b:841:CLA:O1D	2.16	0.44
19:b:839:CLA:H162	19:b:839:CLA:H192	1.73	0.44
3:3:133:PRO:HB2	17:3:301:XAT:H23	2.00	0.44
6:a:415:ASN:O	6:a:421:ASP:HB2	2.18	0.44
19:a:801:CLA:CED	19:a:801:CLA:HAA2	2.46	0.44
19:b:836:CLA:H12	19:b:837:CLA:O1A	2.18	0.44
26:b:847:BCR:H15C	26:b:847:BCR:H351	1.85	0.44
16:c:59:PRO:HD2	27:c:102:SF4:S2	2.58	0.44
19:5:309:CLA:H92	19:5:309:CLA:H61	1.77	0.44
2:4:193:ALA:HB1	21:4:318:DGD:O5E	2.16	0.44
17:4:301:XAT:H391	17:4:301:XAT:H31	1.73	0.44
17:4:302:XAT:H401	17:4:302:XAT:H35	1.76	0.44
5:1:156:ASP:OD2	13:l:2:VAL:N	2.51	0.44
6:a:466:SER:HG	6:a:631:GLN:HE22	1.65	0.44
19:a:819:CLA:HBA2	19:a:819:CLA:H3A	1.53	0.44
19:a:829:CLA:H91	19:a:831:CLA:H192	2.00	0.44
7:b:605:GLN:HE21	7:b:734:LYS:HB3	1.82	0.44
19:b:808:CLA:H162	19:b:808:CLA:H122	1.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:840:CLA:HBA1	19:b:840:CLA:H3A	1.59	0.44
2:4:175:LEU:HD23	2:4:175:LEU:HA	1.87	0.43
4:2:131:ALA:HA	4:2:134:VAL:HG12	1.98	0.43
19:a:801:CLA:HBD	19:a:801:CLA:HED2	1.48	0.43
26:a:847:BCR:H20C	26:a:847:BCR:H361	1.80	0.43
19:b:809:CLA:H143	19:b:809:CLA:H161	1.84	0.43
19:b:813:CLA:HBA2	19:b:813:CLA:H3A	1.61	0.43
16:c:54:CYS:SG	16:c:55:GLU:N	2.91	0.43
1:5:143:TYR:OH	19:5:310:CLA:OBD	2.23	0.43
17:4:302:XAT:H11	17:4:302:XAT:H191	1.89	0.43
4:2:118:LEU:HB2	4:2:123:TYR:HD2	1.83	0.43
19:1:306:CLA:H202	19:1:306:CLA:H162	1.69	0.43
6:a:447:GLY:HA3	19:a:835:CLA:HAB	1.99	0.43
6:a:532:HIS:CE1	6:a:599:VAL:HA	2.53	0.43
19:b:814:CLA:H143	19:b:825:CLA:H51	1.99	0.43
19:b:839:CLA:H161	13:l:92:LEU:HD21	1.99	0.43
19:j:103:CLA:O1D	19:j:103:CLA:H2A	2.18	0.43
2:4:85:MET:HE3	2:4:177:ASN:HB3	2.00	0.43
19:4:309:CLA:HED2	19:4:309:CLA:HBD	1.83	0.43
19:a:807:CLA:H161	19:a:807:CLA:H102	2.00	0.43
19:a:807:CLA:H92	19:a:807:CLA:H61	1.69	0.43
19:a:832:CLA:HBA1	19:a:832:CLA:H3A	1.80	0.43
7:b:350:MET:HE2	7:b:350:MET:HB3	1.89	0.43
7:b:647:VAL:HG21	19:b:809:CLA:HAC1	2.00	0.43
8:d:81:ASN:H	8:d:81:ASN:ND2	2.16	0.43
19:4:310:CLA:C1A	19:4:310:CLA:CGA	2.96	0.43
17:3:303:XAT:H15	17:3:303:XAT:H201	1.79	0.43
17:3:304:XAT:H11	17:3:304:XAT:H191	1.88	0.43
7:b:343:THR:HG23	7:b:377:ALA:HB2	1.99	0.43
26:b:844:BCR:H341	26:b:844:BCR:H11C	1.76	0.43
8:d:20:TRP:HB2	8:d:24:ALA:HB3	1.99	0.43
5:1:95:PRO:HD2	19:1:308:CLA:HMD3	2.00	0.43
6:a:215:LEU:HD23	6:a:215:LEU:HA	1.88	0.43
19:a:820:CLA:HBA2	19:a:820:CLA:H3A	1.48	0.43
7:b:207:TRP:HE1	19:b:815:CLA:H11	1.84	0.43
7:b:424:LEU:HG	19:b:838:CLA:CBB	2.48	0.43
19:b:825:CLA:H12	19:b:825:CLA:H52	1.85	0.43
19:5:307:CLA:HBC1	17:4:301:XAT:H383	2.01	0.43
3:3:56:ASN:HB3	3:3:82:LEU:HD22	2.01	0.43
3:3:172:PRO:HD2	17:3:305:XAT:H242	2.00	0.43
6:a:578:GLN:HA	6:a:583:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:850:BCR:H11C	26:a:850:BCR:H341	1.88	0.43
7:b:529:LEU:HD23	7:b:588:THR:HG21	2.00	0.43
19:b:801:CLA:H161	19:b:801:CLA:H141	1.63	0.43
19:b:811:CLA:H141	19:b:811:CLA:H162	1.75	0.43
19:b:811:CLA:HBB1	19:b:811:CLA:HMB3	2.00	0.43
19:b:817:CLA:CHD	19:b:818:CLA:HBB2	2.49	0.43
12:j:14:LEU:CD2	22:j:105:LMG:H141	2.49	0.43
13:l:68:LEU:O	13:l:77:SER:OG	2.24	0.43
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.43
17:5:302:XAT:H383	19:5:309:CLA:C2B	2.48	0.43
17:1:302:XAT:H11	17:1:302:XAT:H191	1.85	0.43
19:a:823:CLA:HBA1	19:a:823:CLA:H3A	1.87	0.43
19:a:833:CLA:H72	19:l:203:CLA:H12	2.00	0.43
19:a:844:CLA:C1C	25:a:846:LHG:HC31	2.48	0.43
19:b:825:CLA:H41	19:b:825:CLA:H62	1.78	0.43
5:1:171:ARG:HA	5:1:174:MET:CE	2.49	0.43
6:a:73:GLN:HG2	19:a:806:CLA:H3A	2.00	0.43
6:a:194:HIS:HE1	19:a:826:CLA:H72	1.83	0.43
19:a:803:CLA:O1A	19:a:803:CLA:H3A	2.19	0.43
19:a:813:CLA:H62	19:a:813:CLA:H41	1.85	0.43
19:b:836:CLA:H51	19:b:836:CLA:H11	1.73	0.43
9:e:16:TYR:CD2	9:e:44:ASN:HA	2.54	0.43
19:4:307:CLA:H41	19:4:307:CLA:H61	1.86	0.43
5:1:171:ARG:HA	5:1:174:MET:HE3	2.00	0.43
6:a:52:PHE:CD2	19:a:806:CLA:HMC2	2.53	0.43
6:a:559:LYS:NZ	7:b:675:GLU:OE2	2.39	0.43
19:a:807:CLA:H43	25:a:845:LHG:H252	2.00	0.43
19:a:829:CLA:H3A	19:a:829:CLA:HBA2	1.83	0.43
26:a:849:BCR:H351	26:a:849:BCR:H15C	1.79	0.43
19:b:811:CLA:H112	19:i:102:CLA:HAB	1.99	0.43
19:b:814:CLA:H141	19:b:814:CLA:H161	1.77	0.43
12:j:12:PRO:HB2	17:j:101:XAT:H21	2.01	0.43
5:1:151:TRP:CH2	13:l:20:PRO:HA	2.54	0.43
19:1:310:CLA:H92	19:1:310:CLA:H61	1.73	0.43
19:b:807:CLA:H102	19:b:807:CLA:H161	2.01	0.43
6:a:357:SER:HB2	19:a:830:CLA:HMC2	2.01	0.42
6:a:555:LEU:HD11	7:b:674:GLN:HB3	2.01	0.42
19:a:823:CLA:CHD	17:a:852:XAT:H183	2.49	0.42
17:a:852:XAT:H173	17:a:852:XAT:H3	1.83	0.42
7:b:626:LEU:HD22	19:b:803:CLA:HMD3	2.01	0.42
11:i:17:VAL:HG21	19:i:102:CLA:HMC2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:25:VAL:HG21	16:c:48:CYS:HA	2.00	0.42
17:5:302:XAT:H11	17:5:302:XAT:H191	1.65	0.42
17:5:302:XAT:H173	17:5:302:XAT:H3	1.86	0.42
4:2:205:PHE:HE1	17:2:303:XAT:H162	1.84	0.42
17:2:304:XAT:H11	17:2:304:XAT:H191	1.89	0.42
5:1:82:LEU:HD11	19:1:311:CLA:HBC1	2.01	0.42
6:a:364:MET:HE1	19:a:830:CLA:CAD	2.49	0.42
19:a:822:CLA:OBD	19:a:824:CLA:HMD3	2.19	0.42
19:a:841:CLA:HED3	19:a:841:CLA:H2A	2.01	0.42
7:b:220:LEU:HD21	26:b:843:BCR:H391	2.01	0.42
7:b:274:HIS:HB2	19:b:818:CLA:CHB	2.49	0.42
19:b:826:CLA:H3A	19:b:826:CLA:HBA2	1.72	0.42
8:d:32:ILE:HG21	8:d:70:LEU:HD23	2.00	0.42
8:d:107:VAL:HG21	16:c:38:GLN:HB3	2.01	0.42
2:4:183:LEU:HD11	19:4:308:CLA:HAC1	2.00	0.42
17:3:304:XAT:H35	17:3:304:XAT:H401	1.68	0.42
17:2:303:XAT:H11	17:2:303:XAT:H191	1.66	0.42
22:2:317:LMG:H292	22:2:317:LMG:H321	1.35	0.42
19:a:834:CLA:H162	19:a:834:CLA:H202	1.79	0.42
19:a:835:CLA:H141	19:a:835:CLA:H161	1.84	0.42
19:a:840:CLA:H72	26:a:850:BCR:H373	2.01	0.42
7:b:458:GLU:OE1	10:f:94:HIS:ND1	2.46	0.42
8:d:70:LEU:O	8:d:74:LEU:HG	2.19	0.42
8:d:88:TYR:HB3	8:d:89:PRO:HD2	2.01	0.42
4:2:205:PHE:CD2	17:2:303:XAT:H12	2.54	0.42
17:2:303:XAT:H373	17:2:303:XAT:H23	1.87	0.42
6:a:517:MET:HE2	6:a:611:VAL:HA	2.00	0.42
19:a:809:CLA:HBA2	19:a:809:CLA:H3A	1.67	0.42
19:a:810:CLA:HBB1	26:j:104:BCR:H23C	2.00	0.42
7:b:345:LEU:CD1	19:b:827:CLA:HAA1	2.49	0.42
7:b:381:MET:HE1	26:b:847:BCR:H352	2.02	0.42
10:f:114:PHE:HB2	26:f:801:BCR:C32	2.49	0.42
26:l:201:BCR:H352	19:l:203:CLA:HAB	2.01	0.42
17:4:303:XAT:H35	17:4:303:XAT:H401	1.84	0.42
6:a:143:ALA:HB2	6:a:371:PRO:HD2	2.00	0.42
19:a:834:CLA:H142	26:b:848:BCR:H17C	2.01	0.42
19:a:839:CLA:H62	19:a:839:CLA:H41	1.54	0.42
26:a:848:BCR:H15C	26:a:848:BCR:H351	1.78	0.42
19:i:102:CLA:H142	19:i:102:CLA:H111	1.61	0.42
1:5:149:VAL:HG22	17:5:304:XAT:H182	2.02	0.42
17:3:304:XAT:H12	19:3:309:CLA:HAB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:290:HIS:O	6:a:294:ILE:HG12	2.20	0.42
6:a:427:ARG:NH2	8:d:46:THR:O	2.53	0.42
6:a:727:LEU:HD22	19:a:842:CLA:HMA3	2.01	0.42
19:a:816:CLA:C4B	17:a:852:XAT:H242	2.50	0.42
19:a:820:CLA:CAD	19:a:830:CLA:H41	2.48	0.42
19:b:815:CLA:CHA	19:b:815:CLA:HBA1	2.49	0.42
25:m:101:LHG:H272	25:m:101:LHG:H302	1.86	0.42
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.42
17:5:304:XAT:H35	17:5:304:XAT:H401	1.80	0.42
5:1:168:ASN:HA	5:1:171:ARG:HD2	2.01	0.42
17:1:302:XAT:H31	17:1:302:XAT:H391	1.88	0.42
6:a:67:PHE:HE2	6:a:173:HIS:CG	2.38	0.42
6:a:342:TRP:HB3	19:a:806:CLA:HAC1	2.02	0.42
19:a:841:CLA:HAA2	19:b:832:CLA:HMB1	2.02	0.42
7:b:526:ALA:HB2	19:b:837:CLA:HMA1	2.00	0.42
19:b:817:CLA:CBB	26:b:850:BCR:H14C	2.50	0.42
11:i:29:TYR:HE1	14:m:30:ASN:HD21	1.67	0.42
13:l:53:THR:HG22	19:l:202:CLA:C1B	2.49	0.42
19:1:311:CLA:H72	13:l:21:ILE:HG12	2.02	0.42
6:a:252:LYS:NZ	6:a:264:GLU:OE1	2.41	0.42
7:b:452:GLU:OE2	10:f:76:ARG:NE	2.42	0.42
26:b:843:BCR:H341	26:b:843:BCR:H11C	1.74	0.42
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.42
19:4:317:CLA:H92	19:4:317:CLA:H62	1.83	0.42
17:2:303:XAT:H15	17:2:303:XAT:H201	1.79	0.42
5:1:71:GLU:HG2	5:1:142:PRO:O	2.20	0.42
6:a:271:PHE:HE2	6:a:495:ALA:HB2	1.84	0.42
6:a:272:LYS:HG2	6:a:496:LEU:HD12	2.02	0.42
6:a:601:PHE:CZ	19:a:801:CLA:HED3	2.55	0.42
19:a:826:CLA:H141	19:a:826:CLA:H161	1.81	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:j:104:BCR:H15C	26:j:104:BCR:H351	1.78	0.42
3:3:103:ILE:HD11	17:3:304:XAT:H363	2.01	0.42
19:a:842:CLA:H12	24:a:843:PQN:H301	2.02	0.42
13:l:96:LEU:HG	26:l:205:BCR:H24C	2.01	0.42
26:l:205:BCR:H11C	26:l:205:BCR:H341	1.84	0.42
19:2:310:CLA:H162	19:2:310:CLA:H192	1.71	0.41
19:1:306:CLA:H3A	19:1:306:CLA:O2A	2.20	0.41
6:a:75:ALA:HB2	6:a:166:MET:HB2	2.01	0.41
7:b:500:LEU:HA	7:b:503:ILE:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:597:HIS:CE1	7:b:727:VAL:HG23	2.54	0.41
19:5:309:CLA:H202	19:5:309:CLA:H161	1.89	0.41
4:2:109:TRP:CE3	17:2:303:XAT:H22	2.54	0.41
6:a:194:HIS:ND1	19:a:826:CLA:OBD	2.48	0.41
6:a:361:ALA:HB2	6:a:387:HIS:HB2	2.01	0.41
6:a:440:PHE:CE2	19:a:839:CLA:HAB	2.55	0.41
6:a:452:ASN:HD22	6:a:634:ILE:HB	1.85	0.41
6:a:567:PRO:HB3	6:a:714:ILE:HB	2.00	0.41
6:a:684:ARG:NH1	6:a:711:ALA:O	2.52	0.41
6:a:692:GLU:CD	7:b:547:LYS:HB2	2.44	0.41
19:a:826:CLA:HMD2	19:a:826:CLA:H143	2.03	0.41
26:a:848:BCR:H24C	26:a:848:BCR:H371	1.86	0.41
7:b:140:LEU:HD23	7:b:143:LEU:HD12	2.01	0.41
7:b:440:VAL:HG12	19:j:102:CLA:HAC1	2.01	0.41
19:b:828:CLA:H13	19:b:830:CLA:H141	2.02	0.41
19:b:840:CLA:H141	19:b:840:CLA:H161	1.91	0.41
25:m:101:LHG:HC81	25:m:101:LHG:HC5	1.97	0.41
19:5:309:CLA:H93	19:5:309:CLA:H111	1.84	0.41
17:4:301:XAT:H15	17:4:301:XAT:H201	1.80	0.41
4:2:97:LYS:NZ	4:2:152:GLU:OE1	2.38	0.41
17:2:301:XAT:H15	17:2:301:XAT:H201	1.77	0.41
5:1:54:PRO:HD2	17:1:303:XAT:H242	2.02	0.41
5:1:128:GLU:HG3	17:1:302:XAT:H372	2.01	0.41
6:a:299:ILE:O	6:a:303:HIS:ND1	2.53	0.41
26:a:847:BCR:H11C	26:a:847:BCR:H341	1.84	0.41
19:b:805:CLA:H2	19:b:805:CLA:H61	1.62	0.41
19:b:819:CLA:H3A	19:b:819:CLA:HBA2	1.37	0.41
17:j:101:XAT:H35	17:j:101:XAT:H401	1.80	0.41
26:j:104:BCR:H341	26:j:104:BCR:H11C	1.72	0.41
1:5:98:PHE:HE1	19:5:305:CLA:HBC3	1.84	0.41
4:2:57:PHE:CZ	17:2:305:XAT:H172	2.56	0.41
4:2:125:GLY:O	4:2:127:ASN:N	2.44	0.41
4:2:203:LEU:HD13	17:2:301:XAT:C10	2.50	0.41
5:1:147:GLY:HA2	5:1:149:TRP:CZ3	2.55	0.41
19:a:804:CLA:C4D	12:j:12:PRO:HG3	2.50	0.41
19:a:820:CLA:H161	19:a:820:CLA:H122	1.83	0.41
19:a:831:CLA:H93	19:a:842:CLA:HED3	2.01	0.41
19:a:839:CLA:H141	19:a:839:CLA:H161	1.68	0.41
7:b:433:PHE:CZ	26:f:801:BCR:H372	2.56	0.41
7:b:585:MET:O	7:b:589:ILE:HG12	2.20	0.41
12:j:30:ASN:ND2	19:j:102:CLA:O1A	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:307:CLA:HBD	19:4:314:CLA:OBD	2.20	0.41
6:a:525:ASP:HA	6:a:528:VAL:HG12	2.01	0.41
7:b:193:VAL:O	7:b:198:PRO:HD3	2.20	0.41
12:j:14:LEU:HD23	12:j:14:LEU:HA	1.84	0.41
16:c:32:ASP:OD1	16:c:32:ASP:N	2.53	0.41
19:1:310:CLA:H62	19:1:310:CLA:H41	1.80	0.41
19:a:806:CLA:H62	19:a:806:CLA:H2	1.67	0.41
24:a:843:PQN:H211	24:a:843:PQN:H252	1.82	0.41
17:a:852:XAT:H15	17:a:852:XAT:H201	1.67	0.41
26:b:847:BCR:H361	26:b:847:BCR:H20C	1.86	0.41
19:5:314:CLA:H62	19:5:314:CLA:H41	1.93	0.41
17:4:304:XAT:H35	17:4:304:XAT:H401	1.80	0.41
17:2:302:XAT:H35	17:2:302:XAT:H401	1.71	0.41
17:1:303:XAT:H31	17:1:303:XAT:H391	1.93	0.41
6:a:399:ALA:HB1	6:a:543:LEU:HB3	2.02	0.41
19:a:818:CLA:H3A	19:a:818:CLA:HBA2	1.57	0.41
7:b:523:HIS:CE1	26:b:852:BCR:H322	2.56	0.41
19:b:801:CLA:H51	19:b:839:CLA:H102	2.02	0.41
19:5:305:CLA:HAB	2:4:153:PHE:O	2.21	0.41
19:a:818:CLA:OBD	19:a:837:CLA:HED2	2.21	0.41
7:b:140:LEU:HD23	7:b:140:LEU:HA	1.86	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
7:b:676:LEU:O	7:b:679:THR:OG1	2.33	0.41
19:b:802:CLA:HMA1	19:b:803:CLA:H161	2.02	0.41
26:m:102:BCR:H15C	26:m:102:BCR:H351	1.98	0.41
17:5:304:XAT:H201	17:5:304:XAT:H15	1.76	0.41
17:4:303:XAT:H383	19:4:310:CLA:C2B	2.51	0.41
5:1:58:ALA:HB1	5:1:66:LEU:HD21	2.01	0.41
5:1:133:LYS:HA	5:1:133:LYS:HD2	1.81	0.41
5:1:134:ILE:HD11	13:l:26:PHE:HA	2.03	0.41
6:a:680:LEU:HB3	7:b:667:ILE:HG12	2.02	0.41
19:a:806:CLA:H72	26:a:848:BCR:C8	2.50	0.41
19:a:828:CLA:H122	19:a:828:CLA:H162	1.66	0.41
19:a:829:CLA:O1D	19:a:830:CLA:HMA1	2.21	0.41
19:a:831:CLA:H92	19:a:831:CLA:H61	1.70	0.41
7:b:56:ILE:HD11	26:m:102:BCR:HC7	2.02	0.41
7:b:547:LYS:NZ	9:e:15:SER:O	2.45	0.41
19:b:805:CLA:HHC	19:b:807:CLA:OBD	2.21	0.41
19:b:834:CLA:H161	19:b:834:CLA:H141	1.85	0.41
19:b:839:CLA:H92	19:b:839:CLA:H61	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e:51:ASN:ND2	16:c:61:ASP:HB2	2.35	0.41
10:f:114:PHE:HB2	26:f:801:BCR:H321	2.02	0.41
26:i:101:BCR:H15C	26:i:101:BCR:H351	1.85	0.41
19:j:102:CLA:H111	19:j:102:CLA:H91	1.83	0.41
14:m:22:ILE:HD12	25:m:101:LHG:H312	2.02	0.41
6:a:165:LEU:HD23	6:a:165:LEU:HA	1.90	0.41
6:a:356:LEU:HB2	19:a:828:CLA:H41	2.02	0.41
6:a:406:PHE:HE2	6:a:424:ILE:HD11	1.86	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
19:a:828:CLA:H152	19:a:840:CLA:H191	2.03	0.41
7:b:702:LEU:HD22	7:b:706:GLN:NE2	2.35	0.41
7:b:709:LEU:CD1	21:b:851:DGD:HB41	2.51	0.41
19:b:841:CLA:H141	19:b:841:CLA:H161	1.74	0.41
8:d:27:GLU:O	8:d:89:PRO:HD3	2.21	0.41
13:l:4:PHE:HB3	13:l:20:PRO:HG3	2.03	0.41
19:5:308:CLA:CBB	19:5:315:CLA:HAB	2.51	0.40
3:3:106:VAL:HG11	19:3:311:CLA:HED1	2.04	0.40
4:2:92:ARG:NH2	19:2:308:CLA:HED3	2.36	0.40
5:1:87:TRP:CG	5:1:180:LEU:HD13	2.56	0.40
5:1:162:TYR:CE2	19:a:844:CLA:HBD	2.56	0.40
6:a:529:HIS:CG	19:a:839:CLA:HED2	2.56	0.40
19:a:806:CLA:H52	26:a:848:BCR:HC8	2.03	0.40
7:b:668:SER:OG	7:b:673:TRP:NE1	2.52	0.40
7:b:682:TRP:NE1	13:l:15:GLY:O	2.43	0.40
19:b:801:CLA:H12	19:b:801:CLA:H52	1.85	0.40
19:b:802:CLA:H122	19:b:802:CLA:H162	1.60	0.40
26:b:850:BCR:H15C	26:b:850:BCR:H351	1.90	0.40
13:l:56:TYR:CD2	13:l:161:ALA:HB2	2.56	0.40
17:4:304:XAT:H30	19:4:313:CLA:H71	2.02	0.40
3:3:97:MET:HG3	3:3:193:GLY:HA2	2.03	0.40
19:2:307:CLA:H3A	19:2:307:CLA:HBA2	1.76	0.40
5:1:131:GLN:O	5:1:135:LYS:HG3	2.21	0.40
5:1:186:ILE:HG13	5:1:187:THR:N	2.37	0.40
6:a:209:HIS:HB2	19:a:815:CLA:C1C	2.52	0.40
6:a:319:LEU:O	6:a:331:HIS:HB2	2.21	0.40
7:b:499:TRP:CD1	19:b:834:CLA:HED2	2.57	0.40
7:b:614:SER:O	7:b:620:GLY:HA3	2.21	0.40
7:b:629:ASN:HA	7:b:734:LYS:HE2	2.02	0.40
19:b:815:CLA:H2	19:b:815:CLA:H61	1.77	0.40
26:b:846:BCR:H24C	26:b:846:BCR:H371	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:f:98:ASP:OD1	10:f:98:ASP:N	2.54	0.40
19:f:802:CLA:H11	19:j:102:CLA:H122	2.03	0.40
26:j:104:BCR:H24C	26:j:104:BCR:H371	1.85	0.40
17:5:301:XAT:H31	17:5:301:XAT:H391	1.88	0.40
17:3:301:XAT:H201	17:3:301:XAT:H15	1.79	0.40
17:3:303:XAT:H35	17:3:303:XAT:H401	1.79	0.40
6:a:226:SER:OG	6:a:229:GLU:HG2	2.21	0.40
6:a:370:TYR:OH	19:a:830:CLA:OBD	2.28	0.40
6:a:426:HIS:HA	8:d:17:THR:OG1	2.21	0.40
17:a:852:XAT:H11	17:a:852:XAT:H191	1.91	0.40
7:b:197:ILE:HB	7:b:198:PRO:HD3	2.02	0.40
7:b:314:GLY:HA3	7:b:412:ARG:HD2	2.02	0.40
19:j:102:CLA:H61	19:j:102:CLA:H41	1.63	0.40
2:4:136:VAL:CG2	19:4:312:CLA:HMA1	2.52	0.40
17:2:302:XAT:H15	17:2:302:XAT:H201	1.82	0.40
19:2:308:CLA:H51	19:2:309:CLA:H3A	2.04	0.40
20:1:315:SQD:H311	20:1:315:SQD:H282	1.84	0.40
6:a:114:ILE:HG22	6:a:117:GLN:NE2	2.37	0.40
6:a:389:TRP:HB3	19:a:829:CLA:HMC3	2.04	0.40
6:a:586:PHE:CE1	6:a:590:PHE:HE2	2.39	0.40
6:a:738:LEU:HD23	6:a:738:LEU:HA	1.80	0.40
19:a:827:CLA:H193	19:a:827:CLA:H161	1.94	0.40
26:a:850:BCR:H361	26:a:850:BCR:H20C	1.80	0.40
7:b:342:ALA:HB2	19:b:825:CLA:H43	2.02	0.40
19:b:807:CLA:H201	19:b:828:CLA:H143	2.03	0.40
1:5:98:PHE:CD2	19:5:305:CLA:HMD2	2.56	0.40
19:4:309:CLA:H3A	19:4:309:CLA:HBA1	1.76	0.40
19:4:317:CLA:HMB3	17:3:301:XAT:H392	2.03	0.40
3:3:205:LEU:HD12	3:3:205:LEU:HA	1.86	0.40
17:2:303:XAT:H31	17:2:303:XAT:H391	1.70	0.40
19:a:827:CLA:HBA2	19:a:827:CLA:H3A	1.79	0.40
26:a:850:BCR:H351	26:a:850:BCR:H15C	1.77	0.40
7:b:550:PRO:HD2	16:c:62:PHE:CE1	2.57	0.40
19:b:805:CLA:H141	19:b:805:CLA:H162	1.67	0.40
19:b:807:CLA:H161	19:b:807:CLA:H192	1.72	0.40
19:b:809:CLA:C4A	19:b:809:CLA:HBA2	2.50	0.40
10:f:132:VAL:O	10:f:135:THR:HG22	2.22	0.40
10:f:147:VAL:HG22	12:j:14:LEU:HD11	2.04	0.40
26:l:201:BCR:H15C	26:l:201:BCR:H351	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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	l	120	VAL
4	2	127	ASN
4	2	213	VAL
6	a	580	SER
13	l	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
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
7	b	80	ASN
7	b	169	ASN
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
17	XAT	4	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.75	19 (35%)
19	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
19	CLA	l	203	-	60,68,73	1.55	5 (8%)	70,107,113	1.46	7 (10%)
26	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
19	CLA	a	801	-	65,73,73	1.49	9 (13%)	76,113,113	1.39	7 (9%)
19	CLA	2	311	-	58,66,73	1.59	5 (8%)	67,104,113	1.42	8 (11%)
19	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
19	CLA	a	819	-	54,62,73	1.64	5 (9%)	62,99,113	1.46	7 (11%)
19	CLA	3	309	3	56,64,73	1.60	6 (10%)	65,102,113	1.46	7 (10%)
19	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.43	8 (12%)
17	XAT	3	301	-	39,47,47	0.92	2 (5%)	54,74,74	2.54	18 (33%)
27	SF4	c	102	-	0,12,12	-	-	-	-	-
26	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	15 (26%)
19	CLA	b	836	-	58,66,73	1.57	5 (8%)	67,104,113	1.53	8 (11%)
19	CLA	a	826	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
19	CLA	a	840	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
19	CLA	3	314	3	47,55,73	1.74	6 (12%)	54,91,113	1.55	6 (11%)
19	CLA	b	805	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
19	CLA	b	813	-	53,61,73	1.64	5 (9%)	61,98,113	1.51	8 (13%)
18	A1L1G	3	302	-	38,47,47	1.46	6 (15%)	49,71,71	1.38	7 (14%)
19	CLA	b	811	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
19	CLA	a	810	6	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
19	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.50	7 (13%)
26	BCR	l	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
26	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
17	XAT	3	305	-	39,47,47	0.88	1 (2%)	54,74,74	2.57	16 (29%)
19	CLA	a	829	-	62,70,73	1.52	6 (9%)	72,109,113	1.40	8 (11%)
19	CLA	b	838	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
25	LHG	a	846	19	26,26,48	1.28	4 (15%)	29,32,54	1.20	2 (6%)
19	CLA	b	839	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
26	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
17	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
26	BCR	b	852	-	41,41,41	0.73	0	56,56,56	2.06	15 (26%)
19	CLA	b	829	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
19	CLA	2	312	-	47,55,73	1.74	5 (10%)	54,91,113	1.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
19	CLA	b	827	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
19	CLA	b	809	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
27	SF4	a	851	-	0,12,12	-	-	-	-	-
19	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
19	CLA	4	314	2	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
19	CLA	a	813	-	54,62,73	1.64	5 (9%)	62,99,113	1.45	7 (11%)
19	CLA	b	826	-	64,72,73	1.49	6 (9%)	74,111,113	1.45	7 (9%)
19	CLA	f	803	10	52,60,73	1.66	5 (9%)	60,97,113	1.49	8 (13%)
19	CLA	5	313	1	45,53,73	1.81	5 (11%)	52,89,113	1.56	6 (11%)
19	CLA	4	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	6 (11%)
19	CLA	a	837	6	45,53,73	1.80	5 (11%)	52,89,113	1.59	7 (13%)
19	CLA	b	803	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
19	CLA	b	821	-	50,58,73	1.70	6 (12%)	58,95,113	1.60	10 (17%)
26	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.05	16 (28%)
19	CLA	4	306	2	45,53,73	1.81	5 (11%)	52,89,113	1.57	7 (13%)
17	XAT	5	302	-	39,47,47	0.92	2 (5%)	54,74,74	2.58	20 (37%)
19	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
25	LHG	b	849	19	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
19	CLA	a	815	-	45,53,73	1.78	5 (11%)	52,89,113	1.59	7 (13%)
19	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
17	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
19	CLA	2	316	4	46,54,73	1.75	6 (13%)	53,90,113	1.53	6 (11%)
19	CLA	2	313	4	41,49,73	1.84	5 (12%)	47,84,113	1.70	8 (17%)
17	XAT	4	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.56	17 (31%)
17	XAT	j	101	-	39,47,47	0.88	0	54,74,74	2.72	18 (33%)
19	CLA	a	821	-	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
19	CLA	4	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
19	CLA	a	802	-	58,66,73	1.55	5 (8%)	67,104,113	1.50	7 (10%)
17	XAT	2	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.71	18 (33%)
26	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.14	14 (25%)
18	A1L1G	5	303	-	38,47,47	1.42	6 (15%)	49,71,71	1.45	7 (14%)
19	CLA	5	310	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
19	CLA	l	204	-	46,54,73	1.75	6 (13%)	53,90,113	1.58	7 (13%)
19	CLA	b	817	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	5	314	-	52,60,73	1.66	6 (11%)	60,97,113	1.55	8 (13%)
19	CLA	a	803	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
19	CLA	a	822	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	4	307	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	9 (13%)
19	CLA	a	823	-	49,57,73	1.68	5 (10%)	55,93,113	1.61	7 (12%)
19	CLA	a	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
19	CLA	4	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
19	CLA	a	830	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
26	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
23	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
19	CLA	4	312	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	7 (13%)
19	CLA	a	844	25	65,73,73	1.46	5 (7%)	76,113,113	1.39	9 (11%)
19	CLA	b	835	-	53,61,73	1.67	6 (11%)	61,98,113	1.51	8 (13%)
19	CLA	a	816	-	50,58,73	1.68	7 (14%)	58,95,113	1.58	8 (13%)
19	CLA	1	305	-	61,69,73	1.54	5 (8%)	71,108,113	1.39	7 (9%)
19	CLA	2	310	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
19	CLA	4	309	-	50,58,73	1.68	5 (10%)	58,95,113	1.57	8 (13%)
19	CLA	1	312	5	52,60,73	1.71	5 (9%)	60,97,113	1.48	8 (13%)
17	XAT	3	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.63	19 (35%)
24	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.21	4 (9%)
17	XAT	1	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.52	20 (37%)
19	CLA	b	818	-	59,67,73	1.56	6 (10%)	68,105,113	1.50	8 (11%)
17	XAT	2	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.50	18 (33%)
19	CLA	3	310	-	56,64,73	1.60	5 (8%)	65,102,113	1.46	7 (10%)
26	BCR	b	844	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
24	PQN	a	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.10	3 (7%)
19	CLA	5	307	1	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
19	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.48	8 (10%)
21	DGD	4	318	-	41,41,67	1.06	2 (4%)	55,55,81	1.82	6 (10%)
19	CLA	4	317	-	55,63,73	1.63	5 (9%)	64,101,113	1.46	7 (10%)
19	CLA	a	806	-	65,73,73	1.48	11 (16%)	76,113,113	1.67	13 (17%)
26	BCR	b	843	-	41,41,41	0.70	0	56,56,56	2.29	20 (35%)
26	BCR	m	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	b	841	25	65,73,73	1.52	5 (7%)	76,113,113	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	l	202	-	42,50,73	1.82	6 (14%)	48,85,113	1.63	7 (14%)
26	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	16 (28%)
19	CLA	2	308	4	54,62,73	1.65	5 (9%)	62,99,113	1.46	8 (12%)
19	CLA	3	307	3	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
19	CLA	i	102	-	62,70,73	1.55	6 (9%)	72,109,113	1.38	8 (11%)
19	CLA	4	315	2	41,49,73	1.87	5 (12%)	47,84,113	1.64	7 (14%)
19	CLA	3	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.56	8 (14%)
19	CLA	a	825	-	55,63,73	1.61	5 (9%)	64,101,113	1.46	8 (12%)
19	CLA	a	833	-	55,63,73	1.59	5 (9%)	64,101,113	1.53	7 (10%)
19	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	7 (9%)
26	BCR	j	104	-	41,41,41	0.74	0	56,56,56	2.08	17 (30%)
19	CLA	3	312	3	59,67,73	1.57	5 (8%)	68,105,113	1.43	7 (10%)
19	CLA	b	810	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)
19	CLA	a	817	-	45,53,73	1.81	5 (11%)	52,89,113	1.58	7 (13%)
19	CLA	4	313	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
19	CLA	b	825	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
19	CLA	5	305	1	46,54,73	1.76	6 (13%)	53,90,113	1.55	7 (13%)
19	CLA	b	814	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	8 (10%)
19	CLA	5	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
19	CLA	1	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.65	7 (14%)
19	CLA	5	311	-	51,59,73	1.66	5 (9%)	59,96,113	1.53	9 (15%)
19	CLA	a	841	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
19	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.55	8 (13%)
26	BCR	b	846	-	41,41,41	0.70	0	56,56,56	1.97	21 (37%)
19	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.44	9 (11%)
19	CLA	1	314	-	45,53,73	1.79	5 (11%)	52,89,113	1.55	6 (11%)
19	CLA	b	802	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
19	CLA	b	815	-	55,63,73	1.60	6 (10%)	64,101,113	1.55	8 (12%)
19	CLA	5	309	1	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
17	XAT	5	304	-	39,47,47	0.88	0	54,74,74	2.86	22 (40%)
19	CLA	b	807	-	65,73,73	1.46	5 (7%)	76,113,113	1.41	9 (11%)
19	CLA	a	812	19	62,70,73	1.51	6 (9%)	72,109,113	1.43	8 (11%)
17	XAT	2	305	-	39,47,47	0.90	0	54,74,74	2.43	18 (33%)
19	CLA	2	306	-	41,50,73	1.85	6 (14%)	46,85,113	1.56	6 (13%)
22	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.16	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	b	831	-	41,49,73	1.83	6 (14%)	47,84,113	1.65	9 (19%)
19	CLA	a	814	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
19	CLA	j	102	-	58,66,73	1.58	5 (8%)	67,104,113	1.42	8 (11%)
19	CLA	3	315	3	46,54,73	1.79	6 (13%)	53,90,113	1.53	7 (13%)
22	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
26	BCR	a	849	-	41,41,41	0.72	0	56,56,56	2.17	20 (35%)
19	CLA	a	805	19	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
19	CLA	a	811	-	56,64,73	1.58	5 (8%)	65,102,113	1.47	8 (12%)
19	CLA	b	822	-	51,59,73	1.65	5 (9%)	59,96,113	1.58	9 (15%)
19	CLA	3	313	-	52,60,73	1.67	6 (11%)	60,97,113	1.52	9 (15%)
19	CLA	b	833	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	7 (9%)
19	CLA	b	804	-	65,73,73	1.45	5 (7%)	76,113,113	1.55	12 (15%)
19	CLA	1	310	5	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
27	SF4	c	101	-	0,12,12	-	-	-	-	-
19	CLA	5	308	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	7 (10%)
19	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	9 (14%)
19	CLA	a	834	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	9 (11%)
19	CLA	j	103	12	42,50,73	1.81	5 (11%)	48,85,113	1.65	6 (12%)
22	LMG	2	317	-	35,35,55	1.09	2 (5%)	43,43,63	1.30	4 (9%)
19	CLA	5	312	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	9 (15%)
18	A1L1G	3	306	-	38,47,47	1.43	6 (15%)	49,71,71	1.49	9 (18%)
19	CLA	4	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	7 (13%)
20	SQD	5	316	19	34,35,54	1.46	4 (11%)	43,46,65	1.34	7 (16%)
19	CLA	2	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	7 (12%)
19	CLA	b	820	-	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
19	CLA	a	809	6	65,73,73	1.44	5 (7%)	76,113,113	1.44	8 (10%)
19	CLA	2	315	-	42,50,73	1.86	6 (14%)	48,85,113	1.57	7 (14%)
19	CLA	b	812	-	54,62,73	1.67	7 (12%)	67,100,113	1.49	9 (13%)
18	A1L1G	1	301	-	38,47,47	1.44	6 (15%)	49,71,71	1.58	11 (22%)
17	XAT	3	303	-	39,47,47	0.90	0	54,74,74	2.59	20 (37%)
19	CLA	1	307	-	54,62,73	1.63	6 (11%)	62,99,113	1.52	8 (12%)
19	CLA	b	832	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	8 (14%)
17	XAT	4	302	-	39,47,47	0.92	0	54,74,74	2.57	20 (37%)
19	CLA	b	828	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
19	CLA	1	308	5	65,73,73	1.48	6 (9%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	7 (13%)
17	XAT	2	304	-	39,47,47	0.89	0	54,74,74	2.54	21 (38%)
19	CLA	b	823	-	60,68,73	1.55	6 (10%)	70,107,113	1.39	7 (10%)
19	CLA	b	830	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
26	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	21 (37%)
17	XAT	a	852	-	39,47,47	0.94	2 (5%)	54,74,74	2.69	20 (37%)
19	CLA	a	808	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	8 (13%)
26	BCR	b	845	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)
19	CLA	5	306	20	45,53,73	1.80	5 (11%)	52,89,113	1.58	7 (13%)
20	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
25	LHG	m	101	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
19	CLA	b	816	-	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
26	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
19	CLA	2	314	-	56,64,73	1.61	6 (10%)	65,102,113	1.45	7 (10%)
25	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
19	CLA	a	832	-	50,58,73	1.69	6 (12%)	58,95,113	1.53	9 (15%)
19	CLA	b	840	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
19	CLA	b	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	a	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
19	CLA	3	311	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
17	XAT	4	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.63	19 (35%)
19	CLA	b	819	-	60,68,73	1.56	5 (8%)	70,107,113	1.42	7 (10%)
19	CLA	1	311	-	53,61,73	1.64	5 (9%)	61,98,113	1.51	9 (14%)
19	CLA	b	824	-	53,61,73	1.64	6 (11%)	61,98,113	1.47	8 (13%)
19	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	7 (9%)
19	CLA	1	306	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	10 (13%)
17	XAT	4	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.57	18 (33%)
19	CLA	a	854	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	8 (10%)
17	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	17 (31%)
19	CLA	b	808	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	9 (11%)
19	CLA	1	309	5	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
19	CLA	a	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)

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	b	801	-	1/1/15/20	20/37/115/115	-
19	CLA	l	203	-	1/1/14/20	6/31/109/115	-
17	XAT	4	305	-	-	4/31/93/93	0/4/4/4
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2
19	CLA	a	801	-	1/1/15/20	22/37/115/115	-
19	CLA	2	311	-	1/1/13/20	5/29/107/115	-
19	CLA	a	827	-	1/1/15/20	8/37/115/115	-
19	CLA	a	819	-	1/1/12/20	4/24/102/115	-
19	CLA	3	309	3	1/1/13/20	5/27/105/115	-
19	CLA	a	818	-	1/1/13/20	11/27/105/115	-
17	XAT	3	301	-	-	3/31/93/93	0/4/4/4
27	SF4	c	102	-	-	-	0/6/5/5
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
19	CLA	b	836	-	1/1/13/20	11/29/107/115	-
19	CLA	a	826	-	1/1/15/20	9/37/115/115	-
19	CLA	a	840	-	1/1/15/20	8/37/115/115	-
19	CLA	3	314	3	1/1/11/20	7/16/94/115	-
19	CLA	b	805	-	1/1/15/20	12/37/115/115	-
19	CLA	b	813	-	1/1/12/20	6/23/101/115	-
18	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
19	CLA	b	811	-	1/1/15/20	17/37/115/115	-
19	CLA	a	810	6	1/1/15/20	13/37/115/115	-
19	CLA	a	824	-	1/1/11/20	4/15/93/115	-
26	BCR	l	205	-	-	8/29/63/63	0/2/2/2
26	BCR	l	201	-	-	4/29/63/63	0/2/2/2
19	CLA	a	829	-	1/1/14/20	15/34/112/115	-
17	XAT	3	305	-	-	0/31/93/93	0/4/4/4
19	CLA	b	838	-	1/1/15/20	8/37/115/115	-
25	LHG	a	846	19	-	16/31/31/53	-
19	CLA	b	839	-	1/1/15/20	14/37/115/115	-
26	BCR	b	848	-	-	2/29/63/63	0/2/2/2
17	XAT	5	301	-	-	3/31/93/93	0/4/4/4
26	BCR	b	852	-	-	5/29/63/63	0/2/2/2
19	CLA	b	829	-	1/1/15/20	11/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	312	-	1/1/11/20	4/16/94/115	-
21	DGD	b	851	-	-	20/46/86/95	0/2/2/2
19	CLA	b	827	-	1/1/15/20	5/37/115/115	-
19	CLA	b	809	-	1/1/15/20	10/37/115/115	-
27	SF4	a	851	-	-	-	0/6/5/5
19	CLA	a	807	-	1/1/15/20	18/37/115/115	-
19	CLA	4	314	2	1/1/11/20	3/13/91/115	-
19	CLA	a	813	-	1/1/12/20	9/24/102/115	-
19	CLA	b	826	-	1/1/14/20	6/36/114/115	-
19	CLA	f	803	10	1/1/12/20	2/22/100/115	-
19	CLA	5	313	1	1/1/11/20	5/13/91/115	-
19	CLA	4	316	-	1/1/11/20	7/15/93/115	-
19	CLA	a	837	6	1/1/11/20	4/13/91/115	-
19	CLA	b	803	-	1/1/15/20	18/37/115/115	-
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	4	306	2	1/1/11/20	7/13/91/115	-
17	XAT	5	302	-	-	3/31/93/93	0/4/4/4
19	CLA	b	837	-	1/1/15/20	8/37/115/115	-
25	LHG	b	849	19	-	20/35/35/53	-
19	CLA	a	815	-	1/1/11/20	2/13/91/115	-
19	CLA	a	835	-	1/1/15/20	12/37/115/115	-
19	CLA	2	316	4	1/1/11/20	5/15/93/115	-
17	XAT	2	303	-	-	6/31/93/93	0/4/4/4
19	CLA	2	313	4	1/1/10/20	4/8/86/115	-
17	XAT	4	304	-	-	0/31/93/93	0/4/4/4
17	XAT	j	101	-	-	5/31/93/93	0/4/4/4
19	CLA	a	821	-	1/1/11/20	2/13/91/115	-
19	CLA	4	310	-	1/1/15/20	16/37/115/115	-
19	CLA	a	802	-	1/1/13/20	7/29/107/115	-
17	XAT	2	301	-	-	3/31/93/93	0/4/4/4
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
19	CLA	5	310	-	1/1/11/20	6/15/93/115	-
19	CLA	l	204	-	1/1/11/20	4/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
19	CLA	b	817	-	1/1/13/20	4/25/103/115	-
19	CLA	5	314	-	1/1/12/20	4/22/100/115	-
19	CLA	a	803	-	1/1/15/20	3/37/115/115	-
19	CLA	f	802	-	1/1/15/20	13/37/115/115	-
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	823	-	1/1/11/20	7/18/96/115	-
19	CLA	a	839	-	1/1/15/20	15/37/115/115	-
19	CLA	4	308	-	1/1/15/20	14/37/115/115	-
19	CLA	a	830	-	1/1/15/20	15/37/115/115	-
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
23	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
19	CLA	4	312	-	1/1/11/20	4/15/93/115	-
19	CLA	a	844	25	1/1/15/20	16/37/115/115	-
19	CLA	b	835	-	1/1/12/20	8/23/101/115	-
19	CLA	a	816	-	1/1/12/20	5/19/97/115	-
19	CLA	1	305	-	1/1/14/20	10/33/111/115	-
19	CLA	2	310	-	1/1/15/20	14/37/115/115	-
19	CLA	4	309	-	1/1/12/20	7/19/97/115	-
19	CLA	1	312	5	1/1/12/20	3/22/100/115	-
17	XAT	3	304	-	-	3/31/93/93	0/4/4/4
24	PQN	b	842	-	-	1/23/43/43	0/2/2/2
17	XAT	1	303	-	-	0/31/93/93	0/4/4/4
19	CLA	b	818	-	1/1/13/20	10/30/108/115	-
19	CLA	3	310	-	1/1/13/20	4/27/105/115	-
17	XAT	2	302	-	-	0/31/93/93	0/4/4/4
26	BCR	b	844	-	-	2/29/63/63	0/2/2/2
24	PQN	a	843	-	-	5/23/43/43	0/2/2/2
19	CLA	5	307	1	1/1/14/20	7/31/109/115	-
19	CLA	a	831	-	1/1/15/20	11/37/115/115	-
21	DGD	4	318	-	-	10/29/69/95	0/2/2/2
19	CLA	4	317	-	1/1/13/20	7/25/103/115	-
19	CLA	a	806	-	1/1/15/20	12/37/115/115	-
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	m	102	-	-	9/29/63/63	0/2/2/2
19	CLA	b	841	25	1/1/15/20	9/37/115/115	-
19	CLA	l	202	-	1/1/10/20	2/10/88/115	-
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2
19	CLA	2	308	4	1/1/12/20	5/24/102/115	-
19	CLA	3	307	3	1/1/11/20	1/13/91/115	-
19	CLA	i	102	-	1/1/14/20	9/34/112/115	-
19	CLA	4	315	2	1/1/10/20	5/8/86/115	-
19	CLA	3	308	-	1/1/11/20	5/16/94/115	-
19	CLA	a	825	-	1/1/13/20	8/25/103/115	-
19	CLA	a	833	-	1/1/13/20	2/25/103/115	-
19	CLA	a	842	-	1/1/15/20	9/37/115/115	-
26	BCR	j	104	-	-	4/29/63/63	0/2/2/2
19	CLA	3	312	3	1/1/13/20	9/30/108/115	-
19	CLA	b	810	-	1/1/15/20	16/37/115/115	-
19	CLA	a	817	-	1/1/11/20	6/13/91/115	-
19	CLA	4	313	-	1/1/12/20	6/23/101/115	-
19	CLA	b	825	-	1/1/15/20	14/37/115/115	-
19	CLA	5	305	1	1/1/11/20	4/15/93/115	-
19	CLA	b	814	-	1/1/15/20	14/37/115/115	-
19	CLA	5	315	-	1/1/11/20	5/15/93/115	-
19	CLA	1	313	-	1/1/10/20	3/8/86/115	-
19	CLA	5	311	-	1/1/12/20	8/21/99/115	-
19	CLA	a	841	-	1/1/15/20	15/37/115/115	-
19	CLA	a	838	-	1/1/12/20	6/21/99/115	-
26	BCR	b	846	-	-	0/29/63/63	0/2/2/2
19	CLA	a	820	-	1/1/15/20	16/37/115/115	-
19	CLA	1	314	-	1/1/11/20	5/13/91/115	-
19	CLA	b	802	-	1/1/15/20	17/37/115/115	-
19	CLA	b	815	-	1/1/13/20	13/25/103/115	-
19	CLA	5	309	1	1/1/15/20	14/37/115/115	-
17	XAT	5	304	-	-	1/31/93/93	0/4/4/4
19	CLA	b	807	-	1/1/15/20	19/37/115/115	-
19	CLA	a	812	19	1/1/14/20	9/34/112/115	-
17	XAT	2	305	-	-	2/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	306	-	1/1/10/20	2/9/87/115	-
22	LMG	a	853	-	-	13/29/49/70	0/1/1/1
19	CLA	b	831	-	1/1/10/20	1/8/86/115	-
19	CLA	a	814	-	1/1/15/20	20/37/115/115	-
19	CLA	j	102	-	1/1/13/20	16/29/107/115	-
19	CLA	3	315	3	1/1/11/20	8/15/93/115	-
22	LMG	j	105	-	-	11/27/47/70	0/1/1/1
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
19	CLA	a	805	19	1/1/13/20	6/25/103/115	-
19	CLA	a	811	-	1/1/13/20	8/27/105/115	-
19	CLA	b	822	-	1/1/12/20	2/21/99/115	-
19	CLA	3	313	-	1/1/12/20	1/22/100/115	-
19	CLA	b	833	-	1/1/15/20	13/37/115/115	-
19	CLA	b	804	-	1/1/15/20	10/37/115/115	-
19	CLA	1	310	5	1/1/15/20	18/37/115/115	-
27	SF4	c	101	-	-	-	0/6/5/5
19	CLA	5	308	-	1/1/13/20	4/25/103/115	-
19	CLA	a	804	-	1/1/13/20	10/25/103/115	-
19	CLA	a	834	-	1/1/15/20	7/37/115/115	-
19	CLA	j	103	12	1/1/10/20	5/10/88/115	-
22	LMG	2	317	-	-	11/30/50/70	0/1/1/1
19	CLA	5	312	-	1/1/12/20	0/22/100/115	-
19	CLA	4	311	-	1/1/11/20	8/15/93/115	-
18	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
20	SQD	5	316	19	-	11/30/50/69	0/1/1/1
19	CLA	2	307	-	1/1/11/20	6/16/94/115	-
19	CLA	b	820	-	1/1/13/20	3/25/103/115	-
19	CLA	a	809	6	1/1/15/20	15/37/115/115	-
19	CLA	2	315	-	1/1/10/20	1/10/88/115	-
19	CLA	b	812	-	1/1/13/20	5/25/101/115	-
18	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
17	XAT	3	303	-	-	3/31/93/93	0/4/4/4
19	CLA	1	307	-	1/1/12/20	6/24/102/115	-
19	CLA	b	832	-	1/1/11/20	6/18/96/115	-
17	XAT	4	302	-	-	0/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	828	-	1/1/15/20	14/37/115/115	-
19	CLA	1	308	5	1/1/15/20	13/37/115/115	-
19	CLA	2	309	-	1/1/11/20	4/15/93/115	-
19	CLA	b	823	-	1/1/14/20	7/31/109/115	-
17	XAT	2	304	-	-	3/31/93/93	0/4/4/4
19	CLA	b	830	-	1/1/15/20	10/37/115/115	-
26	BCR	b	847	-	-	1/29/63/63	0/2/2/2
19	CLA	a	808	-	1/1/12/20	3/21/99/115	-
17	XAT	a	852	-	-	7/31/93/93	0/4/4/4
26	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	CLA	5	306	20	1/1/11/20	7/13/91/115	-
20	SQD	1	315	-	-	19/40/60/69	0/1/1/1
25	LHG	m	101	-	-	28/50/50/53	-
19	CLA	b	816	-	1/1/11/20	3/13/91/115	-
26	BCR	b	850	-	-	2/29/63/63	0/2/2/2
19	CLA	2	314	-	1/1/13/20	13/27/105/115	-
25	LHG	a	845	-	-	27/52/52/53	-
19	CLA	a	832	-	1/1/12/20	5/19/97/115	-
19	CLA	b	840	-	1/1/15/20	17/37/115/115	-
19	CLA	b	834	-	1/1/15/20	14/37/115/115	-
19	CLA	a	828	-	1/1/15/20	9/37/115/115	-
19	CLA	3	311	-	1/1/12/20	4/19/97/115	-
17	XAT	4	301	-	-	4/31/93/93	0/4/4/4
19	CLA	b	819	-	1/1/14/20	14/31/109/115	-
19	CLA	1	311	-	1/1/12/20	6/23/101/115	-
19	CLA	b	824	-	1/1/12/20	8/23/101/115	-
19	CLA	b	806	-	1/1/15/20	16/37/115/115	-
19	CLA	1	306	-	1/1/15/20	15/37/115/115	-
17	XAT	4	303	-	-	3/31/93/93	0/4/4/4
19	CLA	a	854	-	1/1/15/20	13/37/115/115	-
17	XAT	1	302	-	-	0/31/93/93	0/4/4/4
19	CLA	b	808	-	1/1/15/20	12/37/115/115	-
19	CLA	1	309	5	1/1/11/20	6/15/93/115	-
19	CLA	a	836	-	1/1/12/20	6/19/97/115	-

All (910) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	312	CLA	C4B-NB	7.89	1.42	1.35
19	3	315	CLA	C4B-NB	7.74	1.42	1.35
19	1	309	CLA	C4B-NB	7.74	1.42	1.35
19	a	842	CLA	C4B-NB	7.71	1.42	1.35
19	a	818	CLA	C4B-NB	7.71	1.42	1.35
19	a	840	CLA	C4B-NB	7.71	1.42	1.35
19	2	315	CLA	C4B-NB	7.70	1.42	1.35
19	a	817	CLA	C4B-NB	7.67	1.42	1.35
19	b	821	CLA	C4B-NB	7.67	1.42	1.35
19	b	830	CLA	C4B-NB	7.66	1.42	1.35
19	4	311	CLA	C4B-NB	7.66	1.42	1.35
19	4	315	CLA	C4B-NB	7.65	1.42	1.35
19	b	835	CLA	C4B-NB	7.64	1.42	1.35
19	b	838	CLA	C4B-NB	7.64	1.42	1.35
19	4	307	CLA	C4B-NB	7.63	1.42	1.35
19	2	308	CLA	C4B-NB	7.62	1.42	1.35
24	a	843	PQN	C3-C2	7.62	1.49	1.35
19	5	310	CLA	C4B-NB	7.62	1.42	1.35
19	4	306	CLA	C4B-NB	7.62	1.42	1.35
19	4	312	CLA	C4B-NB	7.61	1.42	1.35
19	5	313	CLA	C4B-NB	7.61	1.42	1.35
19	i	102	CLA	C4B-NB	7.58	1.42	1.35
19	4	317	CLA	C4B-NB	7.57	1.42	1.35
19	4	314	CLA	C4B-NB	7.55	1.41	1.35
19	a	831	CLA	C4B-NB	7.55	1.41	1.35
19	b	829	CLA	C4B-NB	7.55	1.41	1.35
19	2	312	CLA	C4B-NB	7.54	1.41	1.35
19	5	306	CLA	C4B-NB	7.54	1.41	1.35
19	2	311	CLA	C4B-NB	7.54	1.41	1.35
19	2	314	CLA	C4B-NB	7.54	1.41	1.35
19	3	311	CLA	C4B-NB	7.54	1.41	1.35
19	b	801	CLA	C4B-NB	7.54	1.41	1.35
19	a	808	CLA	C4B-NB	7.53	1.41	1.35
19	a	824	CLA	C4B-NB	7.53	1.41	1.35
19	b	840	CLA	C4B-NB	7.53	1.41	1.35
19	j	102	CLA	C4B-NB	7.53	1.41	1.35
19	3	312	CLA	C4B-NB	7.53	1.41	1.35
19	2	310	CLA	C4B-NB	7.52	1.41	1.35
19	3	308	CLA	C4B-NB	7.52	1.41	1.35
19	1	305	CLA	C4B-NB	7.52	1.41	1.35
19	a	813	CLA	C4B-NB	7.51	1.41	1.35
19	b	805	CLA	C4B-NB	7.51	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	820	CLA	C4B-NB	7.51	1.41	1.35
19	a	805	CLA	C4B-NB	7.51	1.41	1.35
19	a	804	CLA	C4B-NB	7.50	1.41	1.35
19	5	305	CLA	C4B-NB	7.50	1.41	1.35
19	l	202	CLA	C4B-NB	7.50	1.41	1.35
19	a	825	CLA	C4B-NB	7.50	1.41	1.35
19	f	803	CLA	C4B-NB	7.49	1.41	1.35
19	b	819	CLA	C4B-NB	7.48	1.41	1.35
19	b	832	CLA	C4B-NB	7.48	1.41	1.35
19	3	310	CLA	C4B-NB	7.48	1.41	1.35
19	2	313	CLA	C4B-NB	7.48	1.41	1.35
19	1	314	CLA	C4B-NB	7.47	1.41	1.35
19	b	802	CLA	C4B-NB	7.47	1.41	1.35
19	1	313	CLA	C4B-NB	7.47	1.41	1.35
19	4	316	CLA	C4B-NB	7.47	1.41	1.35
19	1	308	CLA	C4B-NB	7.47	1.41	1.35
19	3	307	CLA	C4B-NB	7.47	1.41	1.35
19	a	837	CLA	C4B-NB	7.47	1.41	1.35
19	5	308	CLA	C4B-NB	7.46	1.41	1.35
19	a	854	CLA	C4B-NB	7.46	1.41	1.35
19	2	309	CLA	C4B-NB	7.46	1.41	1.35
19	4	313	CLA	C4B-NB	7.46	1.41	1.35
19	b	803	CLA	C4B-NB	7.45	1.41	1.35
19	3	313	CLA	C4B-NB	7.45	1.41	1.35
19	4	310	CLA	C4B-NB	7.44	1.41	1.35
19	b	837	CLA	C4B-NB	7.44	1.41	1.35
19	1	307	CLA	C4B-NB	7.44	1.41	1.35
19	b	841	CLA	C4B-NB	7.44	1.41	1.35
19	b	817	CLA	C4B-NB	7.44	1.41	1.35
19	b	833	CLA	C4B-NB	7.44	1.41	1.35
19	l	203	CLA	C4B-NB	7.44	1.41	1.35
19	1	306	CLA	C4B-NB	7.44	1.41	1.35
19	b	809	CLA	C4B-NB	7.44	1.41	1.35
19	b	827	CLA	C4B-NB	7.44	1.41	1.35
19	a	822	CLA	C4B-NB	7.43	1.41	1.35
19	b	828	CLA	C4B-NB	7.43	1.41	1.35
19	2	316	CLA	C4B-NB	7.43	1.41	1.35
19	a	815	CLA	C4B-NB	7.43	1.41	1.35
19	a	829	CLA	C4B-NB	7.43	1.41	1.35
19	1	310	CLA	C4B-NB	7.43	1.41	1.35
19	2	306	CLA	C4B-NB	7.42	1.41	1.35
19	5	315	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	826	CLA	C4B-NB	7.40	1.41	1.35
19	a	841	CLA	C4B-NB	7.40	1.41	1.35
19	b	804	CLA	C4B-NB	7.40	1.41	1.35
19	b	823	CLA	C4B-NB	7.40	1.41	1.35
19	a	812	CLA	C4B-NB	7.40	1.41	1.35
19	5	309	CLA	C4B-NB	7.40	1.41	1.35
19	4	309	CLA	C4B-NB	7.40	1.41	1.35
19	j	103	CLA	C4B-NB	7.39	1.41	1.35
19	a	810	CLA	C4B-NB	7.39	1.41	1.35
19	5	314	CLA	C4B-NB	7.39	1.41	1.35
19	a	830	CLA	C4B-NB	7.38	1.41	1.35
24	b	842	PQN	C3-C2	7.38	1.48	1.35
19	5	307	CLA	C4B-NB	7.38	1.41	1.35
19	a	819	CLA	C4B-NB	7.38	1.41	1.35
19	a	834	CLA	C4B-NB	7.38	1.41	1.35
19	a	836	CLA	C4B-NB	7.38	1.41	1.35
19	a	816	CLA	C4B-NB	7.38	1.41	1.35
19	a	833	CLA	C4B-NB	7.37	1.41	1.35
19	b	812	CLA	C4B-NB	7.37	1.41	1.35
19	b	810	CLA	C4B-NB	7.37	1.41	1.35
19	b	820	CLA	C4B-NB	7.37	1.41	1.35
19	b	839	CLA	C4B-NB	7.37	1.41	1.35
19	f	802	CLA	C4B-NB	7.37	1.41	1.35
19	a	827	CLA	C4B-NB	7.37	1.41	1.35
19	b	808	CLA	C4B-NB	7.37	1.41	1.35
19	b	825	CLA	C4B-NB	7.35	1.41	1.35
19	b	815	CLA	C4B-NB	7.35	1.41	1.35
19	b	834	CLA	C4B-NB	7.34	1.41	1.35
19	b	836	CLA	C4B-NB	7.34	1.41	1.35
19	a	835	CLA	C4B-NB	7.33	1.41	1.35
19	a	823	CLA	C4B-NB	7.33	1.41	1.35
19	a	832	CLA	C4B-NB	7.32	1.41	1.35
19	b	816	CLA	C4B-NB	7.32	1.41	1.35
19	3	314	CLA	C4B-NB	7.31	1.41	1.35
19	a	839	CLA	C4B-NB	7.31	1.41	1.35
19	2	307	CLA	C4B-NB	7.31	1.41	1.35
19	3	309	CLA	C4B-NB	7.31	1.41	1.35
19	a	803	CLA	C4B-NB	7.29	1.41	1.35
19	b	806	CLA	C4B-NB	7.29	1.41	1.35
19	1	311	CLA	C4B-NB	7.29	1.41	1.35
19	b	824	CLA	C4B-NB	7.28	1.41	1.35
19	b	813	CLA	C4B-NB	7.27	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	312	CLA	C4B-NB	7.27	1.41	1.35
19	b	811	CLA	C4B-NB	7.27	1.41	1.35
19	a	821	CLA	C4B-NB	7.26	1.41	1.35
19	a	802	CLA	C4B-NB	7.26	1.41	1.35
19	5	311	CLA	C4B-NB	7.26	1.41	1.35
19	b	826	CLA	C4B-NB	7.26	1.41	1.35
19	l	204	CLA	C4B-NB	7.25	1.41	1.35
19	a	811	CLA	C4B-NB	7.24	1.41	1.35
19	a	838	CLA	C4B-NB	7.24	1.41	1.35
19	b	818	CLA	C4B-NB	7.24	1.41	1.35
19	a	807	CLA	C4B-NB	7.24	1.41	1.35
19	b	814	CLA	C4B-NB	7.23	1.41	1.35
19	a	814	CLA	C4B-NB	7.21	1.41	1.35
19	a	844	CLA	C4B-NB	7.20	1.41	1.35
19	b	807	CLA	C4B-NB	7.19	1.41	1.35
19	b	822	CLA	C4B-NB	7.17	1.41	1.35
19	a	801	CLA	C4B-NB	7.16	1.41	1.35
19	4	308	CLA	C4B-NB	7.15	1.41	1.35
19	b	831	CLA	C4B-NB	7.13	1.41	1.35
19	a	809	CLA	C4B-NB	7.10	1.41	1.35
19	a	828	CLA	C4B-NB	7.02	1.41	1.35
19	a	806	CLA	C4B-NB	6.00	1.40	1.35
24	b	842	PQN	C10-C5	4.86	1.48	1.40
24	a	843	PQN	C10-C5	4.78	1.48	1.40
20	5	316	SQD	O8-S	4.62	1.63	1.47
20	1	315	SQD	O8-S	4.59	1.63	1.47
23	1	304	A1L1F	O7-C54	4.45	1.45	1.35
20	1	315	SQD	O48-C23	4.29	1.45	1.33
22	a	853	LMG	O8-C28	4.23	1.45	1.33
20	5	316	SQD	O48-C23	4.23	1.45	1.33
23	1	304	A1L1F	O13-C45	4.21	1.45	1.33
20	1	315	SQD	O47-C7	4.19	1.46	1.34
22	a	853	LMG	O7-C10	4.13	1.45	1.34
22	j	105	LMG	O8-C28	4.09	1.45	1.33
19	a	806	CLA	C4D-ND	-4.06	1.32	1.37
20	5	316	SQD	O47-C7	4.06	1.45	1.34
22	2	317	LMG	O8-C28	4.05	1.45	1.33
21	4	318	DGD	O1G-C1A	4.05	1.45	1.33
21	b	851	DGD	O2G-C1B	4.00	1.45	1.34
19	3	308	CLA	C1D-ND	3.99	1.42	1.37
21	b	851	DGD	O1G-C1A	3.97	1.45	1.33
19	a	804	CLA	C1D-ND	3.96	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	317	LMG	O7-C10	3.95	1.45	1.34
19	4	314	CLA	C1D-ND	3.94	1.42	1.37
19	3	315	CLA	C1D-ND	3.93	1.42	1.37
19	1	312	CLA	C1D-ND	3.92	1.42	1.37
19	a	837	CLA	C1D-ND	3.92	1.42	1.37
19	1	310	CLA	C1D-ND	3.91	1.42	1.37
19	a	839	CLA	C1D-ND	3.91	1.42	1.37
19	b	827	CLA	C1D-ND	3.91	1.42	1.37
19	2	307	CLA	C1D-ND	3.90	1.42	1.37
19	b	841	CLA	C1D-ND	3.89	1.42	1.37
19	b	819	CLA	C1D-ND	3.89	1.42	1.37
19	j	103	CLA	C1D-ND	3.89	1.42	1.37
19	2	313	CLA	C1D-ND	3.89	1.42	1.37
19	5	310	CLA	C1D-ND	3.89	1.42	1.37
18	1	301	A1L1G	C38-C39	3.89	1.40	1.35
19	2	306	CLA	C1D-ND	3.89	1.42	1.37
19	2	314	CLA	C1D-ND	3.88	1.42	1.37
22	j	105	LMG	O7-C10	3.88	1.45	1.34
19	3	314	CLA	C1D-ND	3.88	1.42	1.37
19	2	311	CLA	C1D-ND	3.88	1.42	1.37
19	a	828	CLA	C1D-ND	3.87	1.42	1.37
19	4	307	CLA	C1D-ND	3.87	1.42	1.37
19	b	825	CLA	C1D-ND	3.87	1.42	1.37
19	5	306	CLA	C1D-ND	3.87	1.42	1.37
19	a	835	CLA	C1D-ND	3.87	1.42	1.37
19	a	840	CLA	C1D-ND	3.87	1.42	1.37
19	b	834	CLA	C1D-ND	3.86	1.42	1.37
19	2	315	CLA	C1D-ND	3.86	1.42	1.37
19	5	305	CLA	C1D-ND	3.86	1.42	1.37
19	1	204	CLA	C1D-ND	3.86	1.42	1.37
19	a	819	CLA	C1D-ND	3.86	1.42	1.37
21	4	318	DGD	O2G-C1B	3.86	1.45	1.34
19	3	313	CLA	C1D-ND	3.86	1.42	1.37
19	4	306	CLA	C1D-ND	3.86	1.42	1.37
19	4	316	CLA	C1D-ND	3.86	1.42	1.37
19	3	311	CLA	C1D-ND	3.85	1.42	1.37
19	b	807	CLA	C1D-ND	3.85	1.42	1.37
19	5	308	CLA	C1D-ND	3.85	1.42	1.37
19	a	838	CLA	C1D-ND	3.85	1.42	1.37
19	5	311	CLA	C1D-ND	3.84	1.42	1.37
19	a	811	CLA	C1D-ND	3.84	1.42	1.37
19	b	805	CLA	C1D-ND	3.84	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	832	CLA	C1D-ND	3.84	1.42	1.37
19	5	314	CLA	C1D-ND	3.84	1.42	1.37
19	b	821	CLA	C1D-ND	3.83	1.42	1.37
19	2	309	CLA	C1D-ND	3.83	1.42	1.37
19	b	817	CLA	C1D-ND	3.83	1.42	1.37
19	f	802	CLA	C1D-ND	3.83	1.42	1.37
19	4	315	CLA	C1D-ND	3.83	1.42	1.37
19	b	840	CLA	C1D-ND	3.83	1.42	1.37
19	a	817	CLA	C1D-ND	3.83	1.42	1.37
19	a	813	CLA	C1D-ND	3.82	1.42	1.37
19	a	816	CLA	C1D-ND	3.82	1.42	1.37
19	b	813	CLA	C1D-ND	3.82	1.42	1.37
19	a	832	CLA	C1D-ND	3.81	1.42	1.37
19	b	815	CLA	C1D-ND	3.81	1.42	1.37
19	b	822	CLA	C1D-ND	3.81	1.42	1.37
19	2	312	CLA	C1D-ND	3.81	1.42	1.37
19	a	829	CLA	C1D-ND	3.80	1.42	1.37
19	5	313	CLA	C1D-ND	3.80	1.42	1.37
19	5	315	CLA	C1D-ND	3.80	1.42	1.37
19	2	308	CLA	C1D-ND	3.80	1.42	1.37
19	4	312	CLA	C1D-ND	3.80	1.42	1.37
19	b	835	CLA	C1D-ND	3.80	1.42	1.37
19	a	814	CLA	C1D-ND	3.79	1.42	1.37
19	a	807	CLA	C1D-ND	3.79	1.42	1.37
19	i	102	CLA	C1D-ND	3.79	1.42	1.37
19	a	823	CLA	C1D-ND	3.79	1.42	1.37
19	a	842	CLA	C1D-ND	3.79	1.42	1.37
19	1	307	CLA	C1D-ND	3.79	1.42	1.37
19	1	202	CLA	C1D-ND	3.79	1.42	1.37
19	a	844	CLA	C1D-ND	3.79	1.42	1.37
19	3	312	CLA	C1D-ND	3.78	1.42	1.37
19	a	822	CLA	C1D-ND	3.78	1.42	1.37
19	a	818	CLA	C1D-ND	3.78	1.42	1.37
19	5	309	CLA	C1D-ND	3.78	1.42	1.37
19	4	310	CLA	C1D-ND	3.78	1.42	1.37
19	1	309	CLA	C1D-ND	3.78	1.42	1.37
19	b	818	CLA	C1D-ND	3.78	1.42	1.37
19	b	836	CLA	C1D-ND	3.78	1.42	1.37
19	b	839	CLA	C1D-ND	3.78	1.42	1.37
19	b	829	CLA	C1D-ND	3.77	1.42	1.37
19	b	838	CLA	C1D-ND	3.77	1.42	1.37
19	1	314	CLA	C1D-ND	3.77	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	310	CLA	C1D-ND	3.77	1.42	1.37
19	a	815	CLA	C1D-ND	3.77	1.42	1.37
19	4	317	CLA	C1D-ND	3.77	1.42	1.37
19	1	313	CLA	C1D-ND	3.77	1.42	1.37
19	a	836	CLA	C1D-ND	3.76	1.42	1.37
19	5	312	CLA	C1D-ND	3.76	1.42	1.37
19	a	841	CLA	C1D-ND	3.76	1.42	1.37
19	1	306	CLA	C1D-ND	3.76	1.42	1.37
19	a	826	CLA	C1D-ND	3.76	1.42	1.37
19	3	309	CLA	C1D-ND	3.75	1.42	1.37
19	a	821	CLA	C1D-ND	3.75	1.42	1.37
19	1	308	CLA	C1D-ND	3.75	1.42	1.37
19	1	311	CLA	C1D-ND	3.75	1.42	1.37
18	1	301	A1L1G	C35-C34	3.74	1.40	1.35
19	a	854	CLA	C1D-ND	3.74	1.42	1.37
19	4	308	CLA	C1D-ND	3.74	1.42	1.37
19	a	809	CLA	C1D-ND	3.74	1.42	1.37
19	a	810	CLA	C1D-ND	3.74	1.42	1.37
19	a	825	CLA	C1D-ND	3.73	1.42	1.37
19	j	102	CLA	C1D-ND	3.73	1.42	1.37
19	a	831	CLA	C1D-ND	3.73	1.42	1.37
19	b	801	CLA	C1D-ND	3.73	1.42	1.37
19	4	313	CLA	C1D-ND	3.73	1.42	1.37
19	a	824	CLA	C1D-ND	3.73	1.42	1.37
19	b	808	CLA	C1D-ND	3.73	1.42	1.37
19	b	830	CLA	C1D-ND	3.73	1.42	1.37
19	l	203	CLA	C1D-ND	3.72	1.42	1.37
19	a	830	CLA	C1D-ND	3.72	1.42	1.37
19	4	309	CLA	C1D-ND	3.72	1.42	1.37
19	3	307	CLA	C1D-ND	3.72	1.42	1.37
19	a	834	CLA	C1D-ND	3.72	1.42	1.37
19	a	805	CLA	C1D-ND	3.72	1.42	1.37
19	b	816	CLA	C1D-ND	3.72	1.42	1.37
19	b	820	CLA	C1D-ND	3.72	1.42	1.37
19	b	811	CLA	C1D-ND	3.72	1.42	1.37
19	1	305	CLA	C1D-ND	3.71	1.42	1.37
19	b	814	CLA	C1D-ND	3.71	1.42	1.37
19	b	828	CLA	C1D-ND	3.71	1.42	1.37
19	a	820	CLA	C1D-ND	3.71	1.42	1.37
19	b	810	CLA	C1D-ND	3.70	1.42	1.37
19	b	823	CLA	C1D-ND	3.70	1.42	1.37
19	a	812	CLA	C1D-ND	3.70	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	803	CLA	C1D-ND	3.69	1.42	1.37
19	f	803	CLA	C1D-ND	3.69	1.42	1.37
19	2	316	CLA	C1D-ND	3.68	1.42	1.37
19	b	826	CLA	C1D-ND	3.68	1.42	1.37
19	b	806	CLA	C1D-ND	3.67	1.42	1.37
19	a	827	CLA	C1D-ND	3.67	1.42	1.37
19	b	802	CLA	C1D-ND	3.66	1.42	1.37
18	3	302	A1L1G	C35-C34	3.66	1.40	1.35
26	m	102	BCR	C1-C6	-3.66	1.48	1.53
19	b	824	CLA	C1D-ND	3.66	1.42	1.37
19	2	310	CLA	C1D-ND	3.66	1.42	1.37
19	a	808	CLA	C1D-ND	3.66	1.42	1.37
19	5	307	CLA	C1D-ND	3.64	1.42	1.37
19	b	809	CLA	C1D-ND	3.64	1.42	1.37
18	3	306	A1L1G	C38-C39	3.64	1.40	1.35
19	b	803	CLA	C1D-ND	3.64	1.42	1.37
19	b	833	CLA	C1D-ND	3.63	1.42	1.37
19	4	311	CLA	C1D-ND	3.63	1.42	1.37
19	b	837	CLA	C1D-ND	3.62	1.42	1.37
19	b	812	CLA	C1D-ND	3.61	1.42	1.37
18	3	302	A1L1G	C38-C39	3.60	1.40	1.35
23	1	304	A1L1F	C57-C2	-3.60	1.26	1.32
19	a	801	CLA	C1D-ND	3.58	1.42	1.37
19	a	802	CLA	C1D-ND	3.56	1.42	1.37
18	5	303	A1L1G	C38-C39	3.53	1.40	1.35
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	3.44	1.42	1.37
18	3	302	A1L1G	C42-C44	3.43	1.40	1.35
18	3	306	A1L1G	C35-C34	3.41	1.40	1.35
19	4	313	CLA	CHC-C1C	3.31	1.43	1.35
19	a	822	CLA	CHC-C1C	3.28	1.43	1.35
19	b	817	CLA	CHC-C1C	3.26	1.43	1.35
19	b	804	CLA	C1D-ND	3.26	1.41	1.37
19	4	312	CLA	CHC-C1C	3.26	1.43	1.35
19	a	802	CLA	CHC-C1C	3.23	1.43	1.35
19	a	818	CLA	CHC-C1C	3.23	1.43	1.35
19	b	815	CLA	CHC-C1C	3.23	1.43	1.35
19	a	819	CLA	CHC-C1C	3.23	1.43	1.35
19	3	315	CLA	CHC-C1C	3.23	1.43	1.35
19	2	308	CLA	CHC-C1C	3.23	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	839	CLA	CHC-C1C	3.23	1.43	1.35
19	b	837	CLA	CHC-C1C	3.22	1.43	1.35
19	b	805	CLA	CHC-C1C	3.22	1.43	1.35
19	i	102	CLA	CHC-C1C	3.22	1.43	1.35
19	a	841	CLA	CHC-C1C	3.22	1.43	1.35
19	5	311	CLA	CHC-C1C	3.22	1.43	1.35
19	2	309	CLA	CHC-C1C	3.22	1.43	1.35
19	b	829	CLA	CHC-C1C	3.22	1.43	1.35
19	a	820	CLA	CHC-C1C	3.21	1.43	1.35
19	b	806	CLA	CHC-C1C	3.21	1.43	1.35
19	a	813	CLA	CHC-C1C	3.21	1.43	1.35
19	a	829	CLA	CHC-C1C	3.21	1.43	1.35
19	b	814	CLA	CHC-C1C	3.21	1.43	1.35
19	a	804	CLA	CHC-C1C	3.21	1.43	1.35
19	5	314	CLA	CHC-C1C	3.20	1.43	1.35
19	a	827	CLA	CHC-C1C	3.20	1.43	1.35
19	b	836	CLA	CHC-C1C	3.20	1.43	1.35
19	a	844	CLA	CHC-C1C	3.20	1.43	1.35
19	1	310	CLA	CHC-C1C	3.20	1.43	1.35
19	b	816	CLA	CHC-C1C	3.20	1.43	1.35
19	1	308	CLA	CHC-C1C	3.19	1.43	1.35
19	b	812	CLA	CHC-C1C	3.19	1.43	1.35
19	a	854	CLA	CHC-C1C	3.19	1.43	1.35
19	1	311	CLA	CHC-C1C	3.19	1.43	1.35
19	3	313	CLA	CHC-C1C	3.19	1.43	1.35
19	b	813	CLA	CHC-C1C	3.19	1.43	1.35
19	5	309	CLA	CHC-C1C	3.19	1.43	1.35
19	4	315	CLA	CHC-C1C	3.19	1.43	1.35
19	a	833	CLA	CHC-C1C	3.19	1.43	1.35
19	a	826	CLA	CHC-C1C	3.19	1.43	1.35
19	a	837	CLA	CHC-C1C	3.19	1.43	1.35
19	5	315	CLA	CHC-C1C	3.19	1.43	1.35
19	b	826	CLA	CHC-C1C	3.19	1.43	1.35
19	2	313	CLA	CHC-C1C	3.18	1.43	1.35
19	a	832	CLA	CHC-C1C	3.18	1.43	1.35
19	f	803	CLA	CHC-C1C	3.18	1.43	1.35
19	2	315	CLA	CHC-C1C	3.18	1.43	1.35
19	2	312	CLA	CHC-C1C	3.18	1.43	1.35
19	3	311	CLA	CHC-C1C	3.18	1.43	1.35
19	a	809	CLA	CHC-C1C	3.18	1.43	1.35
19	a	823	CLA	CHC-C1C	3.18	1.43	1.35
19	2	310	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	a	816	CLA	CHC-C1C	3.17	1.43	1.35
19	b	802	CLA	CHC-C1C	3.17	1.43	1.35
19	2	311	CLA	CHC-C1C	3.17	1.43	1.35
19	a	834	CLA	CHC-C1C	3.17	1.43	1.35
19	4	314	CLA	CHC-C1C	3.17	1.43	1.35
19	a	842	CLA	CHC-C1C	3.17	1.43	1.35
19	a	824	CLA	CHC-C1C	3.17	1.43	1.35
19	1	314	CLA	CHC-C1C	3.17	1.43	1.35
19	b	834	CLA	CHC-C1C	3.17	1.43	1.35
19	a	814	CLA	CHC-C1C	3.16	1.43	1.35
19	b	832	CLA	CHC-C1C	3.16	1.43	1.35
19	b	824	CLA	CHC-C1C	3.16	1.43	1.35
19	a	828	CLA	CHC-C1C	3.16	1.43	1.35
19	b	809	CLA	CHC-C1C	3.16	1.43	1.35
19	b	818	CLA	CHC-C1C	3.16	1.43	1.35
19	5	313	CLA	CHC-C1C	3.16	1.43	1.35
19	a	817	CLA	CHC-C1C	3.16	1.43	1.35
19	5	310	CLA	CHC-C1C	3.16	1.43	1.35
19	1	309	CLA	CHC-C1C	3.16	1.43	1.35
19	5	306	CLA	CHC-C1C	3.16	1.43	1.35
19	2	314	CLA	CHC-C1C	3.16	1.43	1.35
19	1	307	CLA	CHC-C1C	3.16	1.43	1.35
19	b	807	CLA	CHC-C1C	3.16	1.43	1.35
19	a	808	CLA	CHC-C1C	3.16	1.43	1.35
19	4	308	CLA	CHC-C1C	3.16	1.43	1.35
19	1	312	CLA	CHC-C1C	3.16	1.43	1.35
19	l	203	CLA	CHC-C1C	3.16	1.43	1.35
19	4	310	CLA	CHC-C1C	3.15	1.43	1.35
26	m	102	BCR	C30-C25	-3.15	1.49	1.53
19	j	102	CLA	CHC-C1C	3.15	1.43	1.35
19	b	823	CLA	CHC-C1C	3.15	1.43	1.35
19	a	839	CLA	CHC-C1C	3.15	1.43	1.35
19	b	833	CLA	CHC-C1C	3.15	1.43	1.35
19	a	828	CLA	C4D-ND	-3.15	1.33	1.37
19	b	835	CLA	CHC-C1C	3.15	1.43	1.35
19	b	828	CLA	CHC-C1C	3.15	1.43	1.35
19	b	841	CLA	CHC-C1C	3.15	1.43	1.35
19	3	312	CLA	CHC-C1C	3.14	1.43	1.35
19	a	803	CLA	CHC-C1C	3.14	1.43	1.35
19	3	309	CLA	C4D-ND	-3.14	1.33	1.37
19	a	830	CLA	CHC-C1C	3.14	1.43	1.35
19	5	312	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	4	309	CLA	CHC-C1C	3.14	1.43	1.35
19	f	802	CLA	CHC-C1C	3.14	1.43	1.35
19	4	317	CLA	CHC-C1C	3.14	1.43	1.35
19	3	309	CLA	CHC-C1C	3.14	1.43	1.35
19	l	202	CLA	CHC-C1C	3.14	1.43	1.35
19	3	310	CLA	CHC-C1C	3.14	1.43	1.35
19	a	810	CLA	CHC-C1C	3.14	1.43	1.35
19	a	815	CLA	CHC-C1C	3.14	1.43	1.35
19	l	204	CLA	CHC-C1C	3.13	1.43	1.35
19	a	805	CLA	CHC-C1C	3.13	1.43	1.35
19	b	838	CLA	CHC-C1C	3.13	1.43	1.35
19	5	308	CLA	CHC-C1C	3.13	1.43	1.35
19	a	811	CLA	CHC-C1C	3.13	1.43	1.35
19	2	316	CLA	CHC-C1C	3.13	1.43	1.35
19	4	308	CLA	C4D-ND	-3.13	1.33	1.37
19	a	803	CLA	C4D-ND	-3.13	1.33	1.37
19	5	307	CLA	CHC-C1C	3.13	1.43	1.35
19	3	314	CLA	CHC-C1C	3.13	1.43	1.35
19	a	812	CLA	CHC-C1C	3.12	1.43	1.35
19	b	825	CLA	CHC-C1C	3.12	1.43	1.35
19	b	818	CLA	C4D-ND	-3.12	1.33	1.37
19	3	307	CLA	CHC-C1C	3.12	1.43	1.35
19	5	312	CLA	C4D-ND	-3.12	1.33	1.37
19	5	305	CLA	CHC-C1C	3.12	1.43	1.35
19	4	307	CLA	CHC-C1C	3.12	1.43	1.35
19	b	822	CLA	CHC-C1C	3.11	1.42	1.35
19	b	831	CLA	CHC-C1C	3.11	1.42	1.35
19	a	835	CLA	CHC-C1C	3.11	1.42	1.35
19	a	821	CLA	CHC-C1C	3.11	1.42	1.35
19	1	305	CLA	CHC-C1C	3.11	1.42	1.35
19	1	313	CLA	CHC-C1C	3.10	1.42	1.35
19	4	311	CLA	CHC-C1C	3.10	1.42	1.35
19	a	836	CLA	CHC-C1C	3.10	1.42	1.35
19	3	308	CLA	CHC-C1C	3.10	1.42	1.35
19	2	306	CLA	CHC-C1C	3.10	1.42	1.35
19	5	307	CLA	C4D-ND	-3.10	1.33	1.37
19	b	831	CLA	C4D-ND	-3.10	1.33	1.37
19	4	306	CLA	CHC-C1C	3.10	1.42	1.35
19	a	825	CLA	CHC-C1C	3.10	1.42	1.35
19	b	803	CLA	CHC-C1C	3.10	1.42	1.35
19	4	316	CLA	CHC-C1C	3.09	1.42	1.35
19	a	830	CLA	C4D-ND	-3.09	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	823	CLA	C4D-ND	-3.09	1.33	1.37
19	b	821	CLA	CHC-C1C	3.09	1.42	1.35
19	1	306	CLA	CHC-C1C	3.09	1.42	1.35
19	b	811	CLA	CHC-C1C	3.09	1.42	1.35
19	a	827	CLA	C4D-ND	-3.08	1.33	1.37
19	b	804	CLA	CHC-C1C	3.08	1.42	1.35
19	a	801	CLA	CHC-C1C	3.08	1.42	1.35
19	b	808	CLA	CHC-C1C	3.08	1.42	1.35
19	b	820	CLA	CHC-C1C	3.08	1.42	1.35
19	b	811	CLA	C4D-ND	-3.08	1.33	1.37
19	b	829	CLA	C4D-ND	-3.08	1.33	1.37
19	2	307	CLA	CHC-C1C	3.07	1.42	1.35
19	a	838	CLA	CHC-C1C	3.07	1.42	1.35
19	j	103	CLA	CHC-C1C	3.07	1.42	1.35
19	b	801	CLA	CHC-C1C	3.07	1.42	1.35
19	a	840	CLA	CHC-C1C	3.07	1.42	1.35
19	b	827	CLA	CHC-C1C	3.07	1.42	1.35
19	a	807	CLA	CHC-C1C	3.06	1.42	1.35
19	a	854	CLA	C4D-ND	-3.05	1.33	1.37
19	a	831	CLA	C4D-ND	-3.05	1.33	1.37
19	b	833	CLA	C4D-ND	-3.04	1.33	1.37
19	a	829	CLA	C4D-ND	-3.04	1.33	1.37
19	b	820	CLA	C4D-ND	-3.04	1.33	1.37
19	b	841	CLA	C4D-ND	-3.04	1.33	1.37
19	b	836	CLA	C4D-ND	-3.03	1.33	1.37
19	a	807	CLA	C4D-ND	-3.03	1.33	1.37
19	l	203	CLA	C4D-ND	-3.03	1.33	1.37
19	b	819	CLA	CHC-C1C	3.03	1.42	1.35
19	b	826	CLA	C4D-ND	-3.02	1.33	1.37
19	4	309	CLA	C4D-ND	-3.02	1.33	1.37
19	b	814	CLA	C4D-ND	-3.02	1.33	1.37
19	1	311	CLA	C4D-ND	-3.02	1.33	1.37
19	i	102	CLA	C4D-ND	-3.02	1.33	1.37
19	b	830	CLA	CMB-C2B	-3.02	1.45	1.51
19	b	817	CLA	C4D-ND	-3.01	1.33	1.37
19	a	808	CLA	C4D-ND	-3.01	1.33	1.37
19	b	827	CLA	C4D-ND	-3.01	1.33	1.37
19	3	313	CLA	C4D-ND	-3.01	1.33	1.37
19	2	308	CLA	C4D-ND	-3.01	1.33	1.37
19	a	814	CLA	C4D-ND	-3.00	1.33	1.37
19	a	816	CLA	C4D-ND	-3.00	1.33	1.37
19	a	819	CLA	C4D-ND	-2.99	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	810	CLA	CHC-C1C	2.99	1.42	1.35
19	b	802	CLA	C4D-ND	-2.99	1.33	1.37
19	b	839	CLA	C4D-ND	-2.99	1.33	1.37
19	a	831	CLA	CHC-C1C	2.99	1.42	1.35
19	b	808	CLA	C4D-ND	-2.98	1.33	1.37
19	a	831	CLA	CMB-C2B	-2.98	1.45	1.51
19	a	812	CLA	C4D-ND	-2.98	1.33	1.37
19	a	842	CLA	C4D-ND	-2.98	1.33	1.37
19	a	844	CLA	C4D-ND	-2.97	1.33	1.37
19	3	311	CLA	C4D-ND	-2.97	1.33	1.37
19	a	832	CLA	C4D-ND	-2.97	1.33	1.37
19	b	824	CLA	C4D-ND	-2.97	1.33	1.37
19	l	204	CLA	C4D-ND	-2.97	1.33	1.37
19	5	311	CLA	C4D-ND	-2.97	1.33	1.37
19	b	821	CLA	C4D-ND	-2.97	1.33	1.37
19	j	102	CLA	C4D-ND	-2.97	1.33	1.37
19	b	816	CLA	C4D-ND	-2.96	1.33	1.37
19	5	315	CLA	C4D-ND	-2.96	1.33	1.37
19	b	830	CLA	CHC-C1C	2.96	1.42	1.35
19	a	838	CLA	C4D-ND	-2.96	1.33	1.37
19	5	313	CLA	C4D-ND	-2.96	1.33	1.37
19	5	308	CLA	C4D-ND	-2.96	1.33	1.37
19	a	815	CLA	C4D-ND	-2.95	1.33	1.37
19	a	824	CLA	C4D-ND	-2.95	1.33	1.37
19	b	837	CLA	C4D-ND	-2.95	1.33	1.37
19	a	804	CLA	C4D-ND	-2.95	1.33	1.37
19	b	806	CLA	C4D-ND	-2.95	1.33	1.37
19	3	314	CLA	C4D-ND	-2.94	1.33	1.37
19	4	316	CLA	C4D-ND	-2.94	1.33	1.37
19	1	310	CLA	C4D-ND	-2.94	1.33	1.37
19	a	811	CLA	C4D-ND	-2.94	1.33	1.37
19	a	834	CLA	C4D-ND	-2.94	1.33	1.37
19	a	817	CLA	C4D-ND	-2.94	1.33	1.37
19	1	305	CLA	C4D-ND	-2.94	1.33	1.37
19	1	308	CLA	C4D-ND	-2.93	1.33	1.37
19	4	313	CLA	C4D-ND	-2.93	1.33	1.37
20	5	316	SQD	C6-S	-2.93	1.66	1.77
19	1	306	CLA	C4D-ND	-2.92	1.33	1.37
19	a	837	CLA	C4D-ND	-2.92	1.33	1.37
19	b	812	CLA	C4D-ND	-2.92	1.33	1.37
19	5	306	CLA	C4D-ND	-2.92	1.33	1.37
19	b	840	CLA	CHC-C1C	2.92	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	802	CLA	C4D-ND	-2.92	1.33	1.37
19	4	310	CLA	C4D-ND	-2.92	1.33	1.37
19	l	202	CLA	C4D-ND	-2.92	1.33	1.37
19	4	312	CLA	C4D-ND	-2.92	1.33	1.37
19	a	825	CLA	C4D-ND	-2.92	1.33	1.37
19	b	807	CLA	C4D-ND	-2.92	1.33	1.37
19	2	309	CLA	C4D-ND	-2.91	1.33	1.37
19	b	803	CLA	C4D-ND	-2.91	1.33	1.37
19	5	309	CLA	C4D-ND	-2.91	1.33	1.37
19	a	806	CLA	CHC-C1C	2.91	1.42	1.35
19	b	838	CLA	C4D-ND	-2.91	1.33	1.37
19	a	822	CLA	C4D-ND	-2.91	1.33	1.37
19	1	312	CLA	C4D-ND	-2.90	1.33	1.37
19	b	835	CLA	C4D-ND	-2.90	1.33	1.37
19	2	310	CLA	C4D-ND	-2.90	1.33	1.37
19	a	810	CLA	C4D-ND	-2.90	1.33	1.37
19	b	819	CLA	C4D-ND	-2.90	1.33	1.37
19	a	801	CLA	C4D-ND	-2.90	1.33	1.37
19	b	813	CLA	C4D-ND	-2.90	1.33	1.37
19	a	833	CLA	C4D-ND	-2.90	1.33	1.37
19	2	315	CLA	C4D-ND	-2.89	1.33	1.37
19	3	310	CLA	C4D-ND	-2.89	1.33	1.37
19	a	805	CLA	C4D-ND	-2.89	1.33	1.37
19	a	813	CLA	C4D-ND	-2.89	1.33	1.37
19	b	805	CLA	C4D-ND	-2.89	1.33	1.37
19	4	317	CLA	C4D-ND	-2.89	1.33	1.37
19	4	306	CLA	C4D-ND	-2.89	1.33	1.37
19	f	803	CLA	C4D-ND	-2.88	1.33	1.37
19	b	822	CLA	C4D-ND	-2.88	1.33	1.37
19	1	313	CLA	C4D-ND	-2.88	1.33	1.37
19	a	840	CLA	C4D-ND	-2.88	1.33	1.37
19	b	825	CLA	C4D-ND	-2.88	1.33	1.37
19	b	834	CLA	C4D-ND	-2.87	1.33	1.37
19	1	309	CLA	C4D-ND	-2.87	1.33	1.37
19	a	839	CLA	C4D-ND	-2.87	1.33	1.37
19	4	314	CLA	C4D-ND	-2.87	1.33	1.37
20	1	315	SQD	C6-S	-2.87	1.66	1.77
19	b	832	CLA	C4D-ND	-2.87	1.33	1.37
19	a	823	CLA	C4D-ND	-2.87	1.33	1.37
19	b	840	CLA	C4D-ND	-2.86	1.33	1.37
25	a	845	LHG	C26-C25	-2.86	1.35	1.51
18	1	301	A1L1G	C42-C44	2.85	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	316	CLA	C4D-ND	-2.85	1.33	1.37
19	j	103	CLA	C4D-ND	-2.85	1.33	1.37
19	a	836	CLA	C4D-ND	-2.85	1.33	1.37
19	5	310	CLA	C4D-ND	-2.85	1.33	1.37
19	a	809	CLA	C4D-ND	-2.85	1.33	1.37
19	b	810	CLA	C4D-ND	-2.85	1.33	1.37
19	a	841	CLA	C4D-ND	-2.85	1.33	1.37
19	2	313	CLA	C4D-ND	-2.85	1.33	1.37
19	1	307	CLA	C4D-ND	-2.84	1.33	1.37
19	3	312	CLA	C4D-ND	-2.83	1.33	1.37
19	b	828	CLA	C4D-ND	-2.83	1.33	1.37
25	m	101	LHG	C26-C25	-2.83	1.35	1.51
19	b	809	CLA	C4D-ND	-2.83	1.33	1.37
19	a	818	CLA	C4D-ND	-2.83	1.33	1.37
19	a	821	CLA	C4D-ND	-2.83	1.33	1.37
19	a	826	CLA	C4D-ND	-2.82	1.33	1.37
19	b	801	CLA	C4D-ND	-2.82	1.33	1.37
25	b	849	LHG	C26-C25	-2.82	1.35	1.51
19	a	820	CLA	C4D-ND	-2.82	1.33	1.37
19	3	308	CLA	C4D-ND	-2.81	1.33	1.37
19	a	802	CLA	C4D-ND	-2.81	1.33	1.37
19	4	315	CLA	C4D-ND	-2.81	1.33	1.37
19	2	306	CLA	C4D-ND	-2.81	1.33	1.37
19	a	806	CLA	CMB-C2B	-2.81	1.45	1.51
19	2	311	CLA	C4D-ND	-2.80	1.33	1.37
19	2	314	CLA	C4D-ND	-2.80	1.33	1.37
19	4	307	CLA	C4D-ND	-2.79	1.33	1.37
19	3	315	CLA	C4D-ND	-2.79	1.33	1.37
19	2	312	CLA	C4D-ND	-2.79	1.33	1.37
19	3	307	CLA	C4D-ND	-2.79	1.33	1.37
19	5	314	CLA	C4D-ND	-2.79	1.33	1.37
19	2	307	CLA	C4D-ND	-2.79	1.33	1.37
19	b	815	CLA	C4D-ND	-2.78	1.33	1.37
19	b	830	CLA	C4D-ND	-2.78	1.33	1.37
19	a	835	CLA	C4D-ND	-2.78	1.33	1.37
19	1	314	CLA	C4D-ND	-2.73	1.33	1.37
19	4	311	CLA	C4D-ND	-2.72	1.34	1.37
19	5	305	CLA	C4D-ND	-2.72	1.34	1.37
19	a	801	CLA	CMB-C2B	-2.71	1.46	1.51
19	b	820	CLA	CMB-C2B	-2.70	1.46	1.51
19	b	810	CLA	CMB-C2B	-2.66	1.46	1.51
18	5	303	A1L1G	C33-C34	-2.64	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	303	A1L1G	C42-C44	2.63	1.39	1.35
19	4	311	CLA	CMB-C2B	-2.62	1.46	1.51
19	2	307	CLA	CMB-C2B	-2.62	1.46	1.51
19	b	801	CLA	CMB-C2B	-2.62	1.46	1.51
19	b	831	CLA	CMB-C2B	-2.62	1.46	1.51
18	3	306	A1L1G	C40-C39	-2.62	1.40	1.45
19	b	840	CLA	CMB-C2B	-2.61	1.46	1.51
18	3	306	A1L1G	C33-C34	-2.60	1.40	1.45
19	b	804	CLA	C4D-ND	-2.60	1.34	1.37
18	3	306	A1L1G	C42-C44	2.60	1.39	1.35
19	a	832	CLA	CMB-C2B	-2.60	1.46	1.51
19	a	836	CLA	CMB-C2B	-2.58	1.46	1.51
19	a	820	CLA	CMB-C2B	-2.55	1.46	1.51
19	2	310	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	803	CLA	CMB-C2B	-2.54	1.46	1.51
19	b	818	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	824	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	835	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	829	CLA	CMB-C2B	-2.52	1.46	1.51
18	3	302	A1L1G	C33-C34	-2.52	1.40	1.45
19	a	837	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	819	CLA	CMB-C2B	-2.51	1.46	1.51
18	5	303	A1L1G	C40-C39	-2.51	1.40	1.45
19	a	806	CLA	C1D-ND	2.50	1.40	1.37
19	a	802	CLA	CMB-C2B	-2.50	1.46	1.51
19	3	307	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	822	CLA	CMB-C2B	-2.48	1.46	1.51
19	4	317	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	808	CLA	CMB-C2B	-2.48	1.46	1.51
19	l	203	CLA	CMB-C2B	-2.48	1.46	1.51
19	b	812	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	854	CLA	CMB-C2B	-2.47	1.46	1.51
19	4	313	CLA	CMB-C2B	-2.47	1.46	1.51
19	l	204	CLA	CMB-C2B	-2.47	1.46	1.51
19	a	806	CLA	CMD-C2D	-2.46	1.45	1.50
19	l	202	CLA	CMB-C2B	-2.46	1.46	1.51
19	1	307	CLA	CMB-C2B	-2.46	1.46	1.51
19	b	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	5	312	CLA	CMB-C2B	-2.45	1.46	1.51
19	a	818	CLA	CMB-C2B	-2.45	1.46	1.51
19	a	827	CLA	CMB-C2B	-2.44	1.46	1.51
19	1	311	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)
18	3	302	A1L1G	C40-C39	-2.44	1.40	1.45
19	1	309	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	819	CLA	CMB-C2B	-2.43	1.46	1.51
18	1	301	A1L1G	C33-C34	-2.43	1.40	1.45
19	a	810	CLA	CMB-C2B	-2.43	1.46	1.51
19	1	313	CLA	CMB-C2B	-2.43	1.46	1.51
19	a	817	CLA	CMB-C2B	-2.43	1.46	1.51
19	4	312	CLA	CMB-C2B	-2.43	1.46	1.51
19	a	838	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	825	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	830	CLA	CMD-C2D	-2.43	1.45	1.50
19	b	826	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	839	CLA	CMB-C2B	-2.42	1.46	1.51
19	3	315	CLA	CMB-C2B	-2.42	1.46	1.51
19	b	813	CLA	CMB-C2B	-2.42	1.46	1.51
19	j	102	CLA	CMB-C2B	-2.42	1.46	1.51
19	a	841	CLA	CMB-C2B	-2.41	1.46	1.51
19	3	311	CLA	CMB-C2B	-2.41	1.46	1.51
19	4	315	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	841	CLA	CMB-C2B	-2.41	1.46	1.51
19	a	842	CLA	CMB-C2B	-2.41	1.46	1.51
19	1	310	CLA	CMB-C2B	-2.41	1.46	1.51
19	2	315	CLA	CMB-C2B	-2.41	1.46	1.51
19	a	835	CLA	CMB-C2B	-2.41	1.46	1.51
19	3	312	CLA	CMB-C2B	-2.41	1.46	1.51
18	3	302	A1L1G	C29-C30	-2.41	1.40	1.45
19	j	103	CLA	CMB-C2B	-2.41	1.46	1.51
19	2	311	CLA	CMB-C2B	-2.41	1.46	1.51
19	2	306	CLA	CMB-C2B	-2.40	1.46	1.51
19	b	838	CLA	CMB-C2B	-2.40	1.46	1.51
19	3	314	CLA	CMB-C2B	-2.40	1.46	1.51
19	b	814	CLA	CMB-C2B	-2.40	1.46	1.51
19	f	803	CLA	CMB-C2B	-2.40	1.46	1.51
19	5	310	CLA	CMB-C2B	-2.40	1.46	1.51
19	a	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	1	314	CLA	CMB-C2B	-2.39	1.46	1.51
19	4	314	CLA	CMB-C2B	-2.39	1.46	1.51
19	a	830	CLA	CMC-C2C	-2.39	1.45	1.50
19	5	308	CLA	CMB-C2B	-2.39	1.46	1.51
19	1	305	CLA	CMB-C2B	-2.39	1.46	1.51
19	a	840	CLA	CMB-C2B	-2.39	1.46	1.51
19	3	313	CLA	CMB-C2B	-2.39	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	834	CLA	CMB-C2B	-2.39	1.46	1.51
19	f	802	CLA	CMB-C2B	-2.39	1.46	1.51
19	2	316	CLA	CMB-C2B	-2.38	1.46	1.51
19	4	310	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	814	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	833	CLA	CMB-C2B	-2.38	1.46	1.51
19	a	811	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	808	CLA	CMB-C2B	-2.38	1.46	1.51
19	2	309	CLA	CMB-C2B	-2.38	1.46	1.51
19	i	102	CLA	CMB-C2B	-2.38	1.46	1.51
19	1	312	CLA	CMB-C2B	-2.38	1.46	1.51
19	4	307	CLA	CMB-C2B	-2.38	1.46	1.51
19	3	308	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	816	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	823	CLA	CMB-C2B	-2.38	1.46	1.51
19	b	837	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	806	CLA	CMC-C2C	-2.37	1.45	1.50
19	5	314	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	849	LHG	O8-C6	-2.37	1.39	1.45
19	5	306	CLA	CMB-C2B	-2.37	1.46	1.51
19	5	315	CLA	CMB-C2B	-2.37	1.46	1.51
19	a	801	CLA	CMD-C2D	-2.37	1.45	1.50
19	2	308	CLA	CMB-C2B	-2.37	1.46	1.51
19	5	313	CLA	CMB-C2B	-2.37	1.46	1.51
19	2	314	CLA	CMB-C2B	-2.37	1.46	1.51
19	b	828	CLA	CMB-C2B	-2.37	1.46	1.51
19	1	306	CLA	CMB-C2B	-2.36	1.46	1.51
19	b	827	CLA	CMB-C2B	-2.36	1.46	1.51
19	5	307	CLA	CMB-C2B	-2.36	1.46	1.51
25	a	846	LHG	O8-C6	-2.36	1.39	1.45
19	b	811	CLA	CMB-C2B	-2.36	1.46	1.51
19	4	316	CLA	CMB-C2B	-2.36	1.46	1.51
19	a	807	CLA	CMB-C2B	-2.36	1.46	1.51
19	b	822	CLA	CMB-C2B	-2.36	1.46	1.51
19	5	309	CLA	CMB-C2B	-2.36	1.46	1.51
19	a	806	CLA	C3B-C2B	-2.36	1.37	1.40
19	4	309	CLA	CMB-C2B	-2.36	1.46	1.51
19	4	306	CLA	CMB-C2B	-2.35	1.46	1.51
19	1	308	CLA	CMB-C2B	-2.35	1.46	1.51
19	b	821	CLA	CMB-C2B	-2.35	1.46	1.51
25	m	101	LHG	O8-C23	2.35	1.40	1.33
19	a	825	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	a	806	CLA	C3B-CAB	-2.35	1.43	1.47
19	3	310	CLA	CMB-C2B	-2.35	1.46	1.51
19	2	312	CLA	CMB-C2B	-2.35	1.46	1.51
19	4	308	CLA	CMB-C2B	-2.35	1.46	1.51
19	a	826	CLA	CMB-C2B	-2.35	1.46	1.51
19	3	309	CLA	CMB-C2B	-2.35	1.46	1.51
19	b	824	CLA	CMB-C2B	-2.35	1.46	1.51
19	5	305	CLA	CMB-C2B	-2.35	1.46	1.51
19	a	813	CLA	CMB-C2B	-2.34	1.46	1.51
25	m	101	LHG	O8-C6	-2.34	1.39	1.45
19	a	839	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	828	CLA	CMB-C2B	-2.34	1.46	1.51
19	b	803	CLA	CMB-C2B	-2.34	1.46	1.51
19	a	804	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	802	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	821	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	830	CLA	CMB-C2B	-2.33	1.46	1.51
19	2	313	CLA	CMB-C2B	-2.33	1.46	1.51
25	a	845	LHG	O8-C6	-2.33	1.39	1.45
19	b	832	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	829	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	834	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	805	CLA	CMB-C2B	-2.33	1.46	1.51
19	b	817	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	823	CLA	CMB-C2B	-2.33	1.46	1.51
25	b	849	LHG	O8-C23	2.33	1.40	1.33
19	b	836	CLA	CMB-C2B	-2.33	1.46	1.51
19	a	812	CLA	CMB-C2B	-2.32	1.46	1.51
19	b	815	CLA	CMB-C2B	-2.32	1.46	1.51
19	a	816	CLA	CMB-C2B	-2.32	1.46	1.51
25	a	845	LHG	O8-C23	2.32	1.40	1.33
19	b	807	CLA	CMB-C2B	-2.32	1.46	1.51
18	1	301	A1L1G	C40-C39	-2.31	1.41	1.45
19	a	844	CLA	CMB-C2B	-2.31	1.46	1.51
19	4	311	CLA	CMD-C2D	-2.31	1.45	1.50
19	a	805	CLA	CMB-C2B	-2.31	1.46	1.51
19	b	833	CLA	CMB-C2B	-2.31	1.46	1.51
19	a	809	CLA	CMB-C2B	-2.31	1.46	1.51
19	b	806	CLA	CMB-C2B	-2.30	1.46	1.51
19	5	311	CLA	CMB-C2B	-2.30	1.46	1.51
25	a	846	LHG	O8-C23	2.29	1.40	1.33
25	a	845	LHG	O7-C7	2.29	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	301	A1L1G	C29-C30	-2.29	1.40	1.45
19	b	809	CLA	CMD-C2D	-2.29	1.46	1.50
25	m	101	LHG	O7-C7	2.29	1.40	1.34
25	a	846	LHG	O7-C5	-2.26	1.40	1.46
18	3	306	A1L1G	C29-C30	-2.25	1.40	1.45
23	1	304	A1L1F	C6-C1	-2.25	1.50	1.54
25	a	846	LHG	O7-C7	2.25	1.40	1.34
18	5	303	A1L1G	C29-C30	-2.23	1.40	1.45
19	b	823	CLA	CMD-C2D	-2.22	1.46	1.50
25	b	849	LHG	O7-C5	-2.22	1.41	1.46
23	1	304	A1L1F	O15-C20	-2.22	1.43	1.46
19	b	831	CLA	CMD-C2D	-2.21	1.46	1.50
17	3	305	XAT	O4-C5	-2.20	1.43	1.46
19	b	824	CLA	CMD-C2D	-2.20	1.46	1.50
25	b	849	LHG	O7-C7	2.20	1.40	1.34
25	a	845	LHG	O7-C5	-2.20	1.41	1.46
19	a	824	CLA	CMD-C2D	-2.19	1.46	1.50
17	4	301	XAT	O24-C25	-2.19	1.43	1.46
25	m	101	LHG	O7-C5	-2.18	1.41	1.46
19	a	828	CLA	CMC-C2C	-2.18	1.46	1.50
19	a	830	CLA	CMD-C2D	-2.17	1.46	1.50
19	3	307	CLA	CMD-C2D	-2.17	1.46	1.50
19	a	804	CLA	CMC-C2C	-2.16	1.46	1.50
19	a	810	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	801	CLA	CMC-C2C	-2.16	1.46	1.50
19	b	804	CLA	CMB-C2B	-2.16	1.47	1.51
19	b	803	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	801	CLA	C3B-CAB	-2.15	1.43	1.47
17	1	302	XAT	O4-C5	-2.15	1.43	1.46
19	5	305	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	806	CLA	CAA-C2A	-2.14	1.50	1.54
17	4	304	XAT	O24-C25	-2.13	1.43	1.46
19	b	815	CLA	CMD-C2D	-2.13	1.46	1.50
21	b	851	DGD	O3D-C3D	-2.12	1.38	1.43
19	b	812	CLA	CMD-C2D	-2.12	1.46	1.50
19	2	310	CLA	CMD-C2D	-2.12	1.46	1.50
21	b	851	DGD	O4D-C4D	-2.11	1.38	1.43
17	5	302	XAT	O4-C5	-2.10	1.43	1.46
19	2	316	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
19	a	821	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	801	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)
17	3	301	XAT	O24-C25	-2.09	1.43	1.46
19	a	806	CLA	MG-ND	-2.08	2.01	2.05
21	b	851	DGD	C1E-C2E	2.08	1.58	1.52
19	b	839	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	803	CLA	C3B-CAB	-2.08	1.43	1.47
19	b	829	CLA	CMD-C2D	-2.08	1.46	1.50
17	2	302	XAT	O4-C5	-2.08	1.43	1.46
19	i	102	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	838	CLA	CMD-C2D	-2.07	1.46	1.50
17	3	301	XAT	O4-C5	-2.07	1.43	1.46
19	4	308	CLA	CMD-C2D	-2.07	1.46	1.50
17	2	301	XAT	O4-C5	-2.07	1.43	1.46
25	b	849	LHG	P-O6	2.07	1.67	1.59
17	3	304	XAT	O4-C5	-2.07	1.43	1.46
25	a	845	LHG	P-O6	2.07	1.67	1.59
19	b	826	CLA	CMD-C2D	-2.07	1.46	1.50
17	4	305	XAT	O4-C5	-2.06	1.43	1.46
25	m	101	LHG	P-O6	2.06	1.67	1.59
17	5	302	XAT	O24-C25	-2.06	1.43	1.46
19	a	812	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	826	CLA	CMD-C2D	-2.05	1.46	1.50
17	1	303	XAT	O4-C5	-2.05	1.43	1.46
19	a	842	CLA	CMD-C2D	-2.05	1.46	1.50
17	5	301	XAT	O4-C5	-2.05	1.43	1.46
17	2	303	XAT	O4-C5	-2.05	1.43	1.46
19	1	313	CLA	CMD-C2D	-2.05	1.46	1.50
17	4	303	XAT	O4-C5	-2.05	1.43	1.46
21	b	851	DGD	O4E-C4E	-2.05	1.38	1.43
19	3	309	CLA	CMD-C2D	-2.05	1.46	1.50
19	l	204	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	834	CLA	CMD-C2D	-2.04	1.46	1.50
19	1	309	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	829	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	835	CLA	CMD-C2D	-2.04	1.46	1.50
19	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	816	CLA	CMD-C2D	-2.03	1.46	1.50
19	b	802	CLA	CMD-C2D	-2.03	1.46	1.50
21	b	851	DGD	O2D-C2D	-2.03	1.38	1.43
19	a	807	CLA	CMD-C2D	-2.03	1.46	1.50
19	5	310	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	832	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	852	XAT	O4-C5	-2.03	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	814	CLA	CMD-C2D	-2.02	1.46	1.50
19	5	308	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	818	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	820	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	839	CLA	CMD-C2D	-2.02	1.46	1.50
19	3	315	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	816	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	801	CLA	C3B-C2B	-2.01	1.37	1.40
17	a	852	XAT	O24-C25	-2.01	1.43	1.46
19	3	314	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	304	XAT	O4-C5	-2.01	1.43	1.46
19	a	827	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	202	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	822	CLA	CMD-C2D	-2.01	1.46	1.50
19	3	313	CLA	CMD-C2D	-2.01	1.46	1.50
19	2	314	CLA	CMC-C2C	-2.01	1.46	1.50
19	1	307	CLA	CMD-C2D	-2.01	1.46	1.50
19	5	314	CLA	CMD-C2D	-2.01	1.46	1.50
19	2	315	CLA	CMD-C2D	-2.01	1.46	1.50
19	2	307	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	814	CLA	CMD-C2D	-2.00	1.46	1.50
19	b	811	CLA	CMD-C2D	-2.00	1.46	1.50
19	b	814	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	821	CLA	CMD-C2D	-2.00	1.46	1.50
19	2	309	CLA	CMD-C2D	-2.00	1.46	1.50
19	1	308	CLA	CMD-C2D	-2.00	1.46	1.50
19	4	310	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	816	CLA	CMC-C2C	-2.00	1.46	1.50

All (1941) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	318	DGD	C6E-C5E-C4E	-9.38	91.03	113.00
23	1	304	A1L1F	C17-C20-C25	-8.09	108.70	122.26
19	b	840	CLA	C4A-NA-C1A	7.38	110.02	106.71
23	1	304	A1L1F	O15-C20-C21	7.26	118.83	113.38
17	4	305	XAT	C38-C25-C24	7.21	122.40	114.28
19	b	803	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	a	806	CLA	C4A-NA-C1A	7.20	109.94	106.71
17	1	303	XAT	C38-C25-C24	7.19	122.37	114.28
17	5	304	XAT	C38-C25-C24	7.18	122.36	114.28
17	3	305	XAT	C38-C25-C24	7.18	122.35	114.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	821	CLA	C4A-NA-C1A	7.17	109.93	106.71
19	4	310	CLA	C4A-NA-C1A	7.12	109.91	106.71
19	b	821	CLA	C4A-NA-C1A	7.12	109.91	106.71
19	a	835	CLA	C4A-NA-C1A	7.10	109.90	106.71
17	a	852	XAT	C15-C14-C13	-7.07	117.23	127.31
17	j	101	XAT	C38-C25-C24	7.05	122.21	114.28
19	a	823	CLA	C4A-NA-C1A	7.04	109.87	106.71
19	j	103	CLA	C4A-NA-C1A	7.04	109.87	106.71
19	b	809	CLA	C4A-NA-C1A	7.03	109.87	106.71
19	l	203	CLA	C4A-NA-C1A	7.03	109.87	106.71
17	3	304	XAT	C38-C25-C24	7.00	122.16	114.28
19	a	833	CLA	C4A-NA-C1A	7.00	109.85	106.71
17	4	304	XAT	C38-C25-C24	6.99	122.15	114.28
26	f	801	BCR	C24-C23-C22	-6.98	115.69	126.23
17	5	304	XAT	C18-C5-C4	6.97	122.13	114.28
19	a	826	CLA	C4A-NA-C1A	6.97	109.84	106.71
19	b	822	CLA	C4A-NA-C1A	6.96	109.83	106.71
19	a	801	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	b	828	CLA	C4A-NA-C1A	6.89	109.80	106.71
17	1	302	XAT	C38-C25-C24	6.89	122.03	114.28
19	4	316	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	b	813	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	a	810	CLA	C4A-NA-C1A	6.87	109.80	106.71
19	4	317	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	5	301	XAT	C38-C25-C26	-6.86	110.76	122.26
19	a	807	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	2	301	XAT	C18-C5-C6	-6.85	110.78	122.26
19	b	805	CLA	C4A-NA-C1A	6.84	109.78	106.71
17	4	305	XAT	C38-C25-C26	-6.84	110.80	122.26
19	5	306	CLA	C4A-NA-C1A	6.82	109.77	106.71
17	5	304	XAT	C6-C7-C8	-6.82	111.58	125.99
17	4	303	XAT	C38-C25-C24	6.81	121.94	114.28
19	a	828	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	f	802	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	b	815	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	5	310	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	b	810	CLA	C4A-NA-C1A	6.80	109.76	106.71
17	a	852	XAT	C38-C25-C24	6.79	121.92	114.28
19	5	314	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	b	837	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	b	801	CLA	C4A-NA-C1A	6.78	109.76	106.71
17	3	304	XAT	C38-C25-C26	-6.78	110.89	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	304	XAT	C38-C25-C24	6.78	121.91	114.28
19	4	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	a	809	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	1	204	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	3	308	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	a	831	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	1	308	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	a	825	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	1	306	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	3	313	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	2	311	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	1	305	CLA	C4A-NA-C1A	6.72	109.72	106.71
19	a	839	CLA	C4A-NA-C1A	6.72	109.72	106.71
19	b	811	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	3	303	XAT	C38-C25-C24	6.71	121.83	114.28
19	b	807	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	3	312	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	4	302	XAT	C38-C25-C24	6.68	121.80	114.28
19	b	806	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	a	805	CLA	C4A-NA-C1A	6.68	109.71	106.71
17	5	304	XAT	C18-C5-C6	-6.68	111.07	122.26
19	2	312	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	a	834	CLA	C4A-NA-C1A	6.68	109.71	106.71
17	2	304	XAT	C18-C5-C4	6.67	121.78	114.28
19	a	841	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	4	307	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	a	840	CLA	C4A-NA-C1A	6.66	109.70	106.71
17	3	304	XAT	C18-C5-C6	-6.66	111.09	122.26
17	2	301	XAT	C18-C5-C4	6.66	121.77	114.28
19	b	819	CLA	C4A-NA-C1A	6.65	109.70	106.71
26	i	101	BCR	C24-C23-C22	-6.65	116.19	126.23
19	a	817	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	a	838	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	1	307	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	a	837	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	833	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	a	842	CLA	C4A-NA-C1A	6.63	109.69	106.71
17	j	101	XAT	C38-C25-C26	-6.63	111.16	122.26
17	3	301	XAT	C18-C5-C4	6.62	121.73	114.28
19	5	308	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	a	804	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	3	311	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	b	808	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	l	202	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	5	311	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	4	314	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	2	316	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	a	830	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	a	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	3	314	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	b	825	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	5	302	XAT	C18-C5-C6	-6.58	111.22	122.26
17	5	301	XAT	C38-C25-C24	6.58	121.69	114.28
19	a	854	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	2	313	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	j	102	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	4	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	3	309	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	3	315	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	b	816	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	f	803	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	5	312	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	b	836	CLA	C4A-NA-C1A	6.55	109.65	106.71
17	4	301	XAT	C18-C5-C4	6.55	121.65	114.28
19	b	823	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	i	102	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	4	301	XAT	C31-C30-C29	-6.54	117.98	127.31
19	a	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	a	811	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	4	303	XAT	C18-C5-C6	-6.52	111.33	122.26
19	5	313	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	2	303	XAT	C18-C5-C6	-6.52	111.33	122.26
19	4	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	b	839	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	2	315	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	a	827	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	4	301	XAT	C18-C5-C6	-6.51	111.34	122.26
19	2	314	CLA	C4A-NA-C1A	6.51	109.63	106.71
19	b	827	CLA	C4A-NA-C1A	6.51	109.63	106.71
17	5	304	XAT	C38-C25-C26	-6.50	111.37	122.26
19	1	313	CLA	C4A-NA-C1A	6.49	109.63	106.71
26	a	850	BCR	C24-C23-C22	-6.49	116.42	126.23
19	4	306	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	a	829	CLA	C4A-NA-C1A	6.48	109.62	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	305	XAT	C38-C25-C26	-6.48	111.40	122.26
19	1	311	CLA	C4A-NA-C1A	6.47	109.62	106.71
19	a	844	CLA	C4A-NA-C1A	6.47	109.62	106.71
17	2	305	XAT	C18-C5-C6	-6.47	111.42	122.26
19	b	814	CLA	C4A-NA-C1A	6.47	109.61	106.71
17	4	303	XAT	C38-C25-C26	-6.46	111.43	122.26
19	a	816	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	4	302	XAT	C18-C5-C4	6.46	121.55	114.28
19	3	310	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	b	832	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	a	836	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	2	307	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	2	303	XAT	C38-C25-C26	-6.46	111.44	122.26
19	5	315	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	a	832	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	1	312	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	2	304	XAT	C18-C5-C6	-6.45	111.45	122.26
19	a	819	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	a	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	b	834	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	4	308	CLA	C4A-NA-C1A	6.43	109.59	106.71
19	2	309	CLA	C4A-NA-C1A	6.43	109.59	106.71
19	b	824	CLA	C4A-NA-C1A	6.43	109.59	106.71
19	b	835	CLA	C4A-NA-C1A	6.43	109.59	106.71
17	2	304	XAT	C38-C25-C26	-6.43	111.49	122.26
17	3	303	XAT	C18-C5-C6	-6.41	111.51	122.26
19	a	814	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	5	302	XAT	C26-C27-C28	-6.40	112.46	125.99
19	5	305	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	5	309	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	a	818	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	a	822	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	3	303	XAT	C38-C25-C26	-6.40	111.54	122.26
17	2	302	XAT	C38-C25-C24	6.39	121.47	114.28
19	a	824	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	1	302	XAT	C38-C25-C26	-6.37	111.58	122.26
17	3	301	XAT	C18-C5-C6	-6.37	111.59	122.26
17	j	101	XAT	C18-C5-C6	-6.37	111.59	122.26
19	2	306	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	b	820	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	3	307	CLA	C4A-NA-C1A	6.34	109.56	106.71
17	4	304	XAT	C18-C5-C6	-6.34	111.64	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	2	303	XAT	C38-C25-C24	6.33	121.40	114.28
19	2	310	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	4	302	XAT	C18-C5-C6	-6.33	111.65	122.26
17	j	101	XAT	C18-C5-C4	6.33	121.40	114.28
19	a	813	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	b	826	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	3	303	XAT	C18-C5-C4	6.32	121.39	114.28
19	5	307	CLA	C4A-NA-C1A	6.31	109.54	106.71
17	4	305	XAT	C31-C30-C29	-6.31	118.30	127.31
17	3	304	XAT	C18-C5-C4	6.29	121.36	114.28
17	1	302	XAT	C18-C5-C4	6.29	121.36	114.28
19	4	312	CLA	C4A-NA-C1A	6.29	109.53	106.71
26	i	101	BCR	C20-C21-C22	-6.29	118.34	127.31
17	4	302	XAT	C38-C25-C26	-6.28	111.73	122.26
17	1	302	XAT	C18-C5-C6	-6.28	111.73	122.26
17	3	305	XAT	C18-C5-C4	6.27	121.33	114.28
17	3	301	XAT	C38-C25-C26	-6.27	111.75	122.26
17	4	305	XAT	C18-C5-C6	-6.27	111.76	122.26
19	a	802	CLA	C4A-NA-C1A	6.26	109.52	106.71
17	2	302	XAT	C18-C5-C6	-6.26	111.77	122.26
17	4	304	XAT	C38-C25-C26	-6.26	111.77	122.26
17	2	301	XAT	C38-C25-C24	6.26	121.32	114.28
19	b	841	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	3	305	XAT	C18-C5-C6	-6.25	111.78	122.26
19	1	309	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	4	303	XAT	C18-C5-C4	6.24	121.30	114.28
17	1	303	XAT	C18-C5-C6	-6.24	111.80	122.26
17	a	852	XAT	C38-C25-C26	-6.23	111.81	122.26
19	1	310	CLA	C4A-NA-C1A	6.23	109.50	106.71
19	b	830	CLA	C4A-NA-C1A	6.23	109.50	106.71
17	4	304	XAT	C18-C5-C4	6.23	121.28	114.28
17	1	303	XAT	C38-C25-C26	-6.22	111.83	122.26
17	5	301	XAT	C18-C5-C6	-6.22	111.84	122.26
17	2	302	XAT	C38-C25-C26	-6.19	111.88	122.26
19	a	820	CLA	C4A-NA-C1A	6.19	109.49	106.71
19	b	812	CLA	C4A-NA-C1A	6.18	109.48	106.71
17	3	301	XAT	C38-C25-C24	6.18	121.23	114.28
17	5	302	XAT	C38-C25-C24	6.17	121.23	114.28
19	b	838	CLA	C4A-NA-C1A	6.13	109.46	106.71
17	1	303	XAT	C18-C5-C4	6.12	121.16	114.28
19	b	829	CLA	C4A-NA-C1A	6.12	109.46	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	804	CLA	C4A-NA-C1A	6.10	109.45	106.71
17	2	301	XAT	C38-C25-C26	-6.10	112.04	122.26
17	a	852	XAT	C26-C27-C28	-6.08	113.13	125.99
19	2	308	CLA	C4A-NA-C1A	6.08	109.44	106.71
19	b	817	CLA	C4A-NA-C1A	6.07	109.44	106.71
17	2	305	XAT	C18-C5-C4	6.07	121.11	114.28
17	2	301	XAT	C31-C30-C29	-6.02	118.71	127.31
17	2	302	XAT	C18-C5-C4	6.00	121.03	114.28
17	4	305	XAT	C18-C5-C4	5.98	121.01	114.28
26	b	843	BCR	C7-C8-C9	-5.97	117.22	126.23
17	5	304	XAT	C26-C27-C28	-5.96	113.39	125.99
19	b	831	CLA	C4A-NA-C1A	5.96	109.39	106.71
17	5	302	XAT	C18-C5-C4	5.95	120.97	114.28
19	b	818	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	4	313	CLA	C4A-NA-C1A	5.89	109.36	106.71
19	b	802	CLA	C4A-NA-C1A	5.88	109.35	106.71
17	j	101	XAT	C6-C7-C8	-5.86	113.60	125.99
17	5	301	XAT	C18-C5-C4	5.84	120.85	114.28
26	b	852	BCR	C16-C17-C18	-5.83	118.99	127.31
17	2	303	XAT	C18-C5-C4	5.80	120.80	114.28
17	5	302	XAT	C38-C25-C26	-5.78	112.56	122.26
26	a	850	BCR	C20-C21-C22	-5.74	119.11	127.31
17	4	301	XAT	C35-C34-C33	-5.68	119.20	127.31
17	5	302	XAT	C11-C10-C9	-5.67	119.21	127.31
26	b	845	BCR	C24-C23-C22	-5.65	117.70	126.23
26	b	843	BCR	C11-C10-C9	-5.63	119.28	127.31
17	4	301	XAT	C38-C25-C24	5.62	120.60	114.28
26	f	801	BCR	C16-C17-C18	-5.62	119.29	127.31
23	1	304	A1L1F	O15-C20-C17	5.62	121.79	115.06
19	a	803	CLA	C4A-NA-C1A	5.49	109.17	106.71
26	b	845	BCR	C7-C8-C9	-5.48	117.95	126.23
26	j	104	BCR	C28-C27-C26	-5.47	104.31	114.08
26	b	847	BCR	C16-C17-C18	-5.47	119.50	127.31
17	3	301	XAT	C6-C7-C8	-5.44	114.50	125.99
26	f	801	BCR	C20-C21-C22	-5.41	119.59	127.31
17	3	304	XAT	C35-C34-C33	-5.40	119.61	127.31
26	f	804	BCR	C15-C14-C13	-5.38	119.62	127.31
17	2	303	XAT	C35-C34-C33	-5.38	119.63	127.31
17	2	303	XAT	C31-C30-C29	-5.35	119.67	127.31
26	b	845	BCR	C33-C5-C6	-5.33	118.54	124.53
26	b	843	BCR	C3-C4-C5	-5.33	104.56	114.08
17	a	852	XAT	C18-C5-C6	-5.33	113.33	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	301	XAT	C38-C25-C26	-5.33	113.33	122.26
17	4	303	XAT	C26-C27-C28	-5.31	114.77	125.99
17	4	305	XAT	C15-C14-C13	-5.30	119.75	127.31
26	a	849	BCR	C3-C4-C5	-5.29	104.63	114.08
21	b	851	DGD	O2G-C1B-C2B	5.29	122.91	111.50
26	b	843	BCR	C15-C14-C13	-5.28	119.78	127.31
17	2	305	XAT	C31-C30-C29	-5.28	119.78	127.31
17	4	304	XAT	C26-C27-C28	-5.27	114.84	125.99
26	l	201	BCR	C7-C8-C9	-5.25	118.31	126.23
17	a	852	XAT	C18-C5-C4	5.24	120.18	114.28
17	a	852	XAT	C6-C7-C8	-5.24	114.91	125.99
17	2	303	XAT	C11-C10-C9	-5.23	119.84	127.31
17	2	302	XAT	C35-C34-C33	-5.23	119.84	127.31
17	2	301	XAT	C35-C34-C33	-5.19	119.90	127.31
17	2	304	XAT	C6-C7-C8	-5.19	115.02	125.99
17	j	101	XAT	C26-C27-C28	-5.17	115.07	125.99
26	l	205	BCR	C24-C23-C22	-5.11	118.51	126.23
26	b	846	BCR	C3-C4-C5	-5.11	104.96	114.08
17	2	305	XAT	C35-C34-C33	-5.08	120.05	127.31
17	3	305	XAT	C26-C27-C28	-5.04	115.35	125.99
17	1	302	XAT	C35-C34-C33	-5.03	120.12	127.31
17	5	301	XAT	C26-C27-C28	-5.00	115.42	125.99
17	1	302	XAT	C26-C27-C28	-4.99	115.44	125.99
26	a	847	BCR	C16-C17-C18	-4.98	120.20	127.31
26	b	852	BCR	C20-C21-C22	-4.98	120.20	127.31
17	4	304	XAT	C6-C7-C8	-4.97	115.49	125.99
17	3	305	XAT	C6-C7-C8	-4.96	115.50	125.99
26	f	804	BCR	C11-C10-C9	-4.95	120.25	127.31
26	b	852	BCR	C11-C10-C9	-4.94	120.25	127.31
26	a	850	BCR	C16-C17-C18	-4.92	120.29	127.31
17	1	303	XAT	C6-C7-C8	-4.89	115.65	125.99
17	2	305	XAT	C6-C7-C8	-4.88	115.67	125.99
17	2	301	XAT	C15-C14-C13	-4.87	120.35	127.31
26	a	849	BCR	C16-C17-C18	-4.87	120.35	127.31
17	2	301	XAT	C6-C7-C8	-4.85	115.74	125.99
26	b	852	BCR	C38-C26-C25	-4.84	119.09	124.53
26	j	104	BCR	C11-C10-C9	-4.83	120.42	127.31
17	4	303	XAT	C11-C10-C9	-4.83	120.42	127.31
17	1	302	XAT	C6-C7-C8	-4.81	115.83	125.99
17	j	101	XAT	C11-C10-C9	-4.81	120.45	127.31
17	5	302	XAT	C15-C14-C13	-4.80	120.46	127.31
26	i	101	BCR	C16-C17-C18	-4.79	120.47	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	850	BCR	C16-C17-C18	-4.78	120.48	127.31
19	a	831	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
26	l	205	BCR	C15-C14-C13	-4.77	120.50	127.31
17	5	304	XAT	C15-C14-C13	-4.75	120.53	127.31
17	4	302	XAT	C26-C27-C28	-4.75	115.96	125.99
19	b	830	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
19	b	818	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
26	b	852	BCR	C7-C8-C9	-4.68	119.16	126.23
17	3	303	XAT	C26-C27-C28	-4.67	116.11	125.99
17	4	302	XAT	C6-C7-C8	-4.66	116.13	125.99
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
17	5	301	XAT	C35-C34-C33	-4.57	120.79	127.31
26	b	844	BCR	C11-C10-C9	-4.57	120.79	127.31
26	b	848	BCR	C16-C17-C18	-4.57	120.79	127.31
17	2	305	XAT	C15-C14-C13	-4.56	120.80	127.31
17	4	305	XAT	C26-C27-C28	-4.54	116.39	125.99
26	b	844	BCR	C7-C8-C9	-4.53	119.38	126.23
17	2	302	XAT	C6-C7-C8	-4.51	116.46	125.99
19	a	802	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
17	3	303	XAT	C6-C7-C8	-4.49	116.49	125.99
17	2	304	XAT	C26-C27-C28	-4.47	116.55	125.99
26	a	848	BCR	C16-C17-C18	-4.45	120.96	127.31
17	3	305	XAT	C35-C34-C33	-4.43	120.98	127.31
21	b	851	DGD	O5D-C6D-C5D	-4.42	100.86	109.05
26	a	848	BCR	C15-C14-C13	-4.41	121.01	127.31
26	a	850	BCR	C15-C14-C13	-4.41	121.02	127.31
26	j	104	BCR	C15-C14-C13	-4.39	121.05	127.31
26	a	849	BCR	C15-C14-C13	-4.38	121.06	127.31
22	2	317	LMG	O7-C10-C11	4.38	120.93	111.50
26	b	843	BCR	C16-C17-C18	-4.38	121.07	127.31
26	b	845	BCR	C16-C17-C18	-4.37	121.07	127.31
17	3	303	XAT	C35-C34-C33	-4.37	121.08	127.31
21	4	318	DGD	O6E-C5E-C6E	4.35	117.25	106.44
19	b	836	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
17	3	303	XAT	C15-C14-C13	-4.34	121.11	127.31
26	b	848	BCR	C33-C5-C6	-4.31	119.68	124.53
19	2	307	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
17	j	101	XAT	C35-C34-C33	-4.31	121.16	127.31
26	j	104	BCR	C16-C17-C18	-4.31	121.16	127.31
17	5	304	XAT	C35-C34-C33	-4.30	121.18	127.31
17	4	301	XAT	C6-C7-C8	-4.29	116.91	125.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	833	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
19	a	844	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
17	3	304	XAT	C31-C30-C29	-4.25	121.24	127.31
26	b	844	BCR	C15-C14-C13	-4.24	121.25	127.31
19	a	826	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
19	4	313	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
19	b	826	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
24	b	842	PQN	C11-C12-C13	-4.24	119.74	126.79
21	4	318	DGD	O2G-C1B-C2B	4.24	120.63	111.50
17	2	305	XAT	C38-C25-C24	4.23	119.04	114.28
26	b	845	BCR	C15-C14-C13	-4.21	121.30	127.31
19	a	820	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
26	f	804	BCR	C24-C23-C22	-4.21	119.87	126.23
19	a	809	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
17	4	304	XAT	C35-C34-C33	-4.20	121.32	127.31
19	a	829	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
26	b	847	BCR	C24-C23-C22	-4.20	119.90	126.23
19	a	823	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	l	205	BCR	C20-C21-C22	-4.19	121.33	127.31
17	3	301	XAT	C15-C14-C13	-4.19	121.33	127.31
25	a	845	LHG	O7-C7-C8	4.19	120.53	111.50
26	b	846	BCR	C16-C17-C18	-4.19	121.33	127.31
23	1	304	A1L1F	O7-C54-C56	4.19	118.79	111.09
26	l	201	BCR	C15-C14-C13	-4.18	121.34	127.31
23	1	304	A1L1F	C37-C38-C39	-4.18	121.34	127.31
19	a	806	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
26	b	850	BCR	C33-C5-C6	-4.18	119.83	124.53
26	j	104	BCR	C7-C8-C9	-4.18	119.92	126.23
19	3	310	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
17	4	305	XAT	C35-C34-C33	-4.17	121.36	127.31
19	b	815	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
26	a	850	BCR	C38-C26-C25	-4.16	119.85	124.53
23	1	304	A1L1F	C17-C20-C21	4.16	118.96	114.28
26	b	847	BCR	C20-C21-C22	-4.15	121.39	127.31
26	l	201	BCR	C33-C5-C6	-4.14	119.88	124.53
17	3	304	XAT	C15-C14-C13	-4.12	121.42	127.31
19	a	816	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
26	f	804	BCR	C7-C8-C9	-4.11	120.03	126.23
19	1	307	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
25	b	849	LHG	O7-C7-C8	4.10	120.34	111.50
22	a	853	LMG	O7-C10-C11	4.10	120.34	111.50
19	b	833	CLA	CMB-C2B-C1B	-4.09	122.17	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	801	BCR	C3-C4-C5	-4.09	106.78	114.08
17	5	301	XAT	C11-C10-C9	-4.09	121.48	127.31
17	4	301	XAT	C15-C14-C13	-4.08	121.48	127.31
19	a	803	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
26	l	205	BCR	C38-C26-C25	-4.06	119.96	124.53
19	b	811	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
19	2	308	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
19	a	805	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
19	a	804	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	b	847	BCR	C7-C8-C9	-4.05	120.12	126.23
26	a	847	BCR	C38-C26-C25	-4.05	119.98	124.53
19	5	311	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
26	b	847	BCR	C16-C15-C14	-4.04	115.20	123.47
26	a	848	BCR	C11-C10-C9	-4.03	121.55	127.31
26	b	843	BCR	C28-C27-C26	-4.03	106.88	114.08
19	b	822	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
19	5	307	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
19	b	806	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
19	a	839	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
19	b	810	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
17	4	305	XAT	C6-C7-C8	-4.00	117.54	125.99
25	m	101	LHG	O7-C7-C8	3.98	120.09	111.50
26	f	804	BCR	C33-C5-C6	-3.98	120.06	124.53
19	4	308	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
19	b	827	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
19	b	807	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
17	4	305	XAT	C11-C10-C9	-3.97	121.64	127.31
26	b	847	BCR	C28-C27-C26	-3.97	106.99	114.08
17	a	852	XAT	C31-C30-C29	-3.96	121.65	127.31
19	1	308	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
25	a	846	LHG	O7-C7-C8	3.96	120.03	111.50
26	l	201	BCR	C11-C10-C9	-3.95	121.67	127.31
26	b	847	BCR	C15-C14-C13	-3.95	121.67	127.31
19	3	309	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
22	j	105	LMG	O7-C10-C11	3.94	120.00	111.50
17	1	303	XAT	C26-C27-C28	-3.94	117.66	125.99
19	b	832	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
19	a	838	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
17	3	301	XAT	C35-C34-C33	-3.94	121.69	127.31
19	4	309	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
26	i	101	BCR	C7-C8-C9	-3.93	120.30	126.23
19	b	817	CLA	CMB-C2B-C1B	-3.92	122.44	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	303	XAT	C15-C14-C13	-3.91	121.72	127.31
19	b	802	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
17	2	302	XAT	C31-C30-C29	-3.91	121.73	127.31
17	2	303	XAT	C15-C14-C13	-3.91	121.73	127.31
19	b	804	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
19	a	822	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
26	a	847	BCR	C20-C21-C22	-3.91	121.74	127.31
19	2	310	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
17	j	101	XAT	C15-C14-C13	-3.89	121.76	127.31
19	b	814	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
19	f	802	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
26	f	804	BCR	C38-C26-C25	-3.88	120.17	124.53
17	2	302	XAT	C15-C14-C13	-3.88	121.77	127.31
19	b	816	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	5	312	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	b	818	CLA	CMB-C2B-C3B	3.87	131.92	124.68
19	a	815	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
26	f	804	BCR	C20-C21-C22	-3.86	121.79	127.31
17	2	305	XAT	C27-C28-C29	-3.86	119.54	125.53
18	1	301	A1L1G	C37-C36-C35	3.86	131.38	123.47
26	l	205	BCR	C33-C5-C6	-3.86	120.20	124.53
19	l	202	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
26	l	205	BCR	C16-C17-C18	-3.85	121.81	127.31
19	1	306	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
18	3	306	A1L1G	C36-C37-C38	3.84	131.35	123.47
26	l	201	BCR	C16-C17-C18	-3.84	121.83	127.31
19	a	827	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
19	b	825	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
19	2	312	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
26	f	804	BCR	C16-C17-C18	-3.82	121.85	127.31
17	2	302	XAT	C26-C27-C28	-3.82	117.91	125.99
19	a	811	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
19	5	314	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
19	l	203	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
17	5	301	XAT	C15-C14-C13	-3.81	121.88	127.31
19	a	814	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
19	b	828	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
19	b	805	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
19	2	313	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	a	849	BCR	C28-C27-C26	-3.79	107.32	114.08
17	1	303	XAT	C35-C34-C33	-3.78	121.91	127.31
19	a	806	CLA	O2D-CGD-O1D	-3.78	116.45	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	846	BCR	C15-C14-C13	-3.76	121.94	127.31
19	5	315	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
19	2	309	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
26	b	848	BCR	C15-C14-C13	-3.75	121.95	127.31
20	1	315	SQD	O47-C7-C8	3.75	119.59	111.50
19	a	812	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	1	310	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
18	5	303	A1L1G	C36-C37-C38	3.73	131.12	123.47
19	b	831	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	f	801	BCR	C16-C15-C14	-3.72	115.85	123.47
17	2	303	XAT	C26-C27-C28	-3.72	118.13	125.99
19	b	804	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
26	j	104	BCR	C20-C21-C22	-3.71	122.01	127.31
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	3	311	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
19	a	803	CLA	CMB-C2B-C3B	3.70	131.60	124.68
17	3	301	XAT	C31-C30-C29	-3.70	122.03	127.31
26	b	844	BCR	C3-C4-C5	-3.69	107.48	114.08
26	a	850	BCR	C33-C5-C6	-3.69	120.39	124.53
19	a	830	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	a	828	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
19	1	311	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
17	3	301	XAT	C26-C27-C28	-3.68	118.21	125.99
19	a	837	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
19	a	802	CLA	CMB-C2B-C3B	3.68	131.56	124.68
17	2	303	XAT	C6-C7-C8	-3.68	118.22	125.99
19	a	826	CLA	CMB-C2B-C3B	3.67	131.54	124.68
19	b	835	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
19	5	309	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
19	a	821	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
19	b	829	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
19	b	836	CLA	CMB-C2B-C3B	3.64	131.50	124.68
26	a	849	BCR	C20-C21-C22	-3.64	122.11	127.31
19	b	837	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
17	4	302	XAT	C35-C15-C14	-3.63	116.03	123.47
19	b	821	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
19	b	813	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
17	2	301	XAT	C27-C28-C29	-3.62	119.91	125.53
19	b	839	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
26	b	850	BCR	C7-C8-C9	-3.62	120.77	126.23
26	b	847	BCR	C3-C4-C5	-3.62	107.62	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	849	BCR	C11-C10-C9	-3.61	122.16	127.31
19	a	829	CLA	CMB-C2B-C3B	3.60	131.42	124.68
19	2	307	CLA	CMB-C2B-C3B	3.60	131.42	124.68
17	1	302	XAT	C11-C10-C9	-3.60	122.17	127.31
19	b	823	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
26	b	844	BCR	C33-C5-C6	-3.58	120.50	124.53
26	a	847	BCR	C33-C5-C6	-3.58	120.50	124.53
19	b	834	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
19	b	812	CLA	CAB-C3B-C4B	-3.58	122.96	128.46
19	a	833	CLA	CMB-C2B-C3B	3.57	131.36	124.68
19	4	310	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	l	205	BCR	C11-C10-C9	-3.56	122.23	127.31
19	a	809	CLA	CMB-C2B-C3B	3.55	131.33	124.68
26	a	847	BCR	C15-C14-C13	-3.55	122.24	127.31
19	a	808	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	l	204	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
17	1	303	XAT	C15-C14-C13	-3.55	122.25	127.31
19	b	808	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	1	312	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	a	844	CLA	CMB-C2B-C3B	3.54	131.31	124.68
26	l	205	BCR	C3-C4-C5	-3.54	107.76	114.08
19	b	811	CLA	CMB-C2B-C3B	3.54	131.30	124.68
17	4	303	XAT	C35-C34-C33	-3.53	122.27	127.31
26	i	101	BCR	C33-C5-C6	-3.53	120.56	124.53
19	b	815	CLA	CMB-C2B-C3B	3.53	131.28	124.68
19	b	812	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
19	b	819	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
19	a	832	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
19	b	804	CLA	CHB-C4A-NA	3.53	129.39	124.51
19	a	813	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
19	a	835	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
19	b	833	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	a	847	BCR	C7-C8-C9	-3.52	120.92	126.23
17	4	302	XAT	C11-C10-C9	-3.52	122.29	127.31
19	a	823	CLA	CMB-C2B-C3B	3.52	131.26	124.68
19	4	313	CLA	CMB-C2B-C3B	3.52	131.25	124.68
19	b	826	CLA	CMB-C2B-C3B	3.51	131.25	124.68
19	a	806	CLA	CAA-CBA-CGA	-3.51	102.99	113.25
19	a	842	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	3	310	CLA	CMB-C2B-C3B	3.51	131.24	124.68
19	4	314	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
26	b	850	BCR	C38-C26-C25	-3.50	120.60	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	313	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
19	5	305	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
20	5	316	SQD	O47-C7-C8	3.49	119.01	111.50
19	3	314	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	i	101	BCR	C28-C27-C26	-3.48	107.86	114.08
19	b	824	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
19	4	317	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	b	846	BCR	C24-C23-C22	-3.47	120.99	126.23
19	3	307	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
26	a	849	BCR	C4-C5-C6	-3.47	117.69	122.73
19	b	809	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
19	5	306	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
19	a	841	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
19	a	805	CLA	CMB-C2B-C3B	3.47	131.16	124.68
19	2	308	CLA	CMB-C2B-C3B	3.46	131.16	124.68
19	a	806	CLA	CMB-C2B-C3B	3.46	131.16	124.68
19	b	802	CLA	CMB-C2B-C3B	3.46	131.15	124.68
19	4	315	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
17	3	305	XAT	C15-C14-C13	-3.46	122.37	127.31
26	a	848	BCR	C24-C23-C22	-3.46	121.01	126.23
17	2	304	XAT	C31-C30-C29	-3.45	122.38	127.31
19	1	305	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	4	306	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	b	820	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
18	3	302	A1L1G	C36-C37-C38	3.45	130.54	123.47
17	2	304	XAT	C11-C10-C9	-3.45	122.39	127.31
19	a	807	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
19	b	827	CLA	CMB-C2B-C3B	3.45	131.13	124.68
18	5	303	A1L1G	C28-C39-C38	-3.45	118.09	122.92
17	2	305	XAT	C24-C23-C22	-3.45	104.12	110.77
26	a	849	BCR	C7-C8-C9	-3.44	121.03	126.23
17	3	303	XAT	C11-C10-C9	-3.44	122.39	127.31
19	5	308	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
19	a	831	CLA	CMB-C2B-C3B	3.44	131.12	124.68
19	1	309	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
26	a	847	BCR	C24-C23-C22	-3.44	121.04	126.23
19	i	102	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	1	313	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	a	820	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	a	846	LHG	O8-C23-C24	3.44	120.39	111.38
26	a	847	BCR	C11-C10-C9	-3.43	122.41	127.31
19	2	314	CLA	CMB-C2B-C1B	-3.43	123.19	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	302	A1L1G	C28-C39-C38	-3.43	118.12	122.92
18	1	301	A1L1G	C28-C39-C38	-3.43	118.12	122.92
18	3	302	A1L1G	C37-C36-C35	3.43	130.49	123.47
19	a	818	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
19	a	819	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
18	1	301	A1L1G	C27-C34-C35	-3.42	118.13	122.92
19	a	816	CLA	CMB-C2B-C3B	3.42	131.08	124.68
19	3	315	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	a	825	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	3	308	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	5	302	XAT	C6-C7-C8	-3.41	118.78	125.99
19	j	102	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
19	2	306	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
19	4	316	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
19	5	311	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	a	817	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	4	307	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
19	4	312	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
18	3	306	A1L1G	C27-C34-C35	-3.39	118.17	122.92
19	2	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	a	848	BCR	C20-C21-C22	-3.39	122.47	127.31
19	a	840	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
19	b	822	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	1	307	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	b	806	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	b	838	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
19	a	854	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	f	803	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	a	810	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	1	314	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	b	807	CLA	CMB-C2B-C3B	3.37	130.99	124.68
18	3	306	A1L1G	C28-C39-C38	-3.37	118.20	122.92
18	3	302	A1L1G	C27-C34-C35	-3.37	118.20	122.92
23	1	304	A1L1F	C8-O7-C54	-3.37	111.62	117.90
19	5	310	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
19	a	804	CLA	CMB-C2B-C3B	3.36	130.97	124.68
17	5	301	XAT	C7-C8-C9	-3.36	120.31	125.53
19	4	308	CLA	CMB-C2B-C3B	3.36	130.97	124.68
26	a	849	BCR	C24-C23-C22	-3.36	121.16	126.23
19	b	832	CLA	CMB-C2B-C3B	3.36	130.96	124.68
19	b	804	CLA	CMB-C2B-C3B	3.35	130.95	124.68
19	2	315	CLA	CMB-C2B-C1B	-3.35	123.32	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	847	BCR	C10-C11-C12	-3.35	112.77	123.22
19	j	103	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
19	2	316	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
26	b	850	BCR	C11-C10-C9	-3.35	122.53	127.31
24	a	843	PQN	C14-C13-C15	3.34	120.90	115.27
26	a	847	BCR	C3-C4-C5	-3.34	108.11	114.08
19	3	309	CLA	CMB-C2B-C3B	3.34	130.93	124.68
18	5	303	A1L1G	C37-C36-C35	3.34	130.32	123.47
17	j	101	XAT	C10-C11-C12	-3.34	112.80	123.22
19	5	307	CLA	CMB-C2B-C3B	3.34	130.92	124.68
17	5	301	XAT	C6-C7-C8	-3.33	118.94	125.99
19	a	834	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	1	303	XAT	C31-C30-C29	-3.33	122.56	127.31
18	5	303	A1L1G	C27-C34-C35	-3.33	118.26	122.92
19	b	830	CLA	CMB-C2B-C3B	3.33	130.91	124.68
19	b	814	CLA	CMB-C2B-C3B	3.33	130.90	124.68
19	a	838	CLA	CMB-C2B-C3B	3.32	130.90	124.68
18	1	301	A1L1G	C36-C37-C38	3.32	130.28	123.47
19	a	839	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	i	101	BCR	C15-C14-C13	-3.31	122.58	127.31
19	b	801	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
17	1	303	XAT	C24-C23-C22	-3.31	104.39	110.77
19	a	827	CLA	CMB-C2B-C3B	3.31	130.87	124.68
21	b	851	DGD	C2G-O2G-C1B	-3.31	109.65	117.79
19	1	308	CLA	CMB-C2B-C3B	3.31	130.86	124.68
19	a	824	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
17	4	301	XAT	C11-C10-C9	-3.30	122.60	127.31
19	f	802	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	4	309	CLA	CMB-C2B-C3B	3.30	130.84	124.68
19	b	817	CLA	CMB-C2B-C3B	3.29	130.83	124.68
17	4	303	XAT	C6-C7-C8	-3.28	119.05	125.99
19	5	312	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
19	4	311	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
17	5	301	XAT	C24-C23-C22	-3.27	104.47	110.77
19	3	312	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
17	3	304	XAT	C26-C27-C28	-3.25	119.11	125.99
26	j	104	BCR	C24-C23-C22	-3.25	121.32	126.23
19	5	314	CLA	CMB-C2B-C3B	3.25	130.76	124.68
19	j	103	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	5	304	XAT	C4-C3-C2	-3.24	104.51	110.77
17	5	304	XAT	C24-C23-C22	-3.24	104.51	110.77
19	b	841	CLA	CMB-C2B-C1B	-3.24	123.49	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	815	CLA	CMB-C2B-C3B	3.24	130.73	124.68
26	i	101	BCR	C11-C10-C9	-3.23	122.70	127.31
19	b	816	CLA	CMB-C2B-C3B	3.23	130.72	124.68
18	1	301	A1L1G	C43-C44-C42	-3.23	118.40	122.92
19	b	821	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
26	a	848	BCR	C33-C5-C6	-3.22	120.91	124.53
26	l	201	BCR	C38-C26-C25	-3.22	120.91	124.53
19	b	809	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
19	b	825	CLA	CMB-C2B-C3B	3.22	130.69	124.68
19	2	312	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	a	814	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	1	304	A1L1F	C14-C29-C30	-3.21	119.81	125.47
19	a	822	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	a	836	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
19	1	306	CLA	CMB-C2B-C3B	3.21	130.68	124.68
26	a	850	BCR	C7-C8-C9	-3.20	121.39	126.23
18	1	301	A1L1G	C33-C34-C35	3.20	123.86	118.94
19	b	805	CLA	CMB-C2B-C3B	3.20	130.66	124.68
17	4	304	XAT	C15-C14-C13	-3.20	122.74	127.31
17	a	852	XAT	C10-C11-C12	-3.20	113.23	123.22
19	a	828	CLA	CMB-C2B-C3B	3.19	130.65	124.68
26	b	852	BCR	C24-C23-C22	-3.19	121.42	126.23
19	a	835	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
19	2	313	CLA	CMB-C2B-C3B	3.18	130.63	124.68
19	b	828	CLA	CMB-C2B-C3B	3.18	130.63	124.68
26	b	846	BCR	C20-C21-C22	-3.18	122.77	127.31
19	a	804	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
19	5	315	CLA	CMB-C2B-C3B	3.18	130.62	124.68
19	b	840	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
26	b	844	BCR	C16-C17-C18	-3.17	122.78	127.31
19	l	202	CLA	CMB-C2B-C3B	3.17	130.61	124.68
19	5	312	CLA	CMB-C2B-C3B	3.17	130.60	124.68
19	a	811	CLA	CMB-C2B-C3B	3.17	130.60	124.68
18	5	303	A1L1G	C40-C39-C38	3.17	123.80	118.94
17	3	304	XAT	C11-C10-C9	-3.17	122.79	127.31
17	1	302	XAT	C15-C14-C13	-3.16	122.79	127.31
26	a	848	BCR	C3-C4-C5	-3.16	108.43	114.08
26	l	201	BCR	C24-C23-C22	-3.16	121.46	126.23
18	3	306	A1L1G	C37-C36-C35	3.16	129.94	123.47
17	4	304	XAT	C24-C23-C22	-3.16	104.67	110.77
17	a	852	XAT	C11-C10-C9	-3.16	122.81	127.31
19	1	311	CLA	CMB-C2B-C3B	3.15	130.58	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	850	BCR	C11-C10-C9	-3.15	122.81	127.31
17	2	301	XAT	C11-C10-C9	-3.15	122.81	127.31
26	a	848	BCR	C38-C26-C25	-3.15	120.99	124.53
19	1	310	CLA	CMB-C2B-C3B	3.15	130.57	124.68
19	b	810	CLA	CMB-C2B-C3B	3.15	130.56	124.68
17	3	303	XAT	C24-C23-C22	-3.14	104.70	110.77
17	4	303	XAT	C24-C23-C22	-3.14	104.71	110.77
19	1	313	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
18	1	301	A1L1G	C40-C39-C38	3.14	123.76	118.94
19	2	309	CLA	CMB-C2B-C3B	3.14	130.55	124.68
19	a	803	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
19	a	812	CLA	CMB-C2B-C3B	3.13	130.53	124.68
26	b	848	BCR	C10-C11-C12	-3.12	113.47	123.22
26	b	852	BCR	C33-C5-C6	-3.12	121.02	124.53
19	b	833	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
19	a	818	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
19	a	830	CLA	CMB-C2B-C3B	3.12	130.51	124.68
26	b	846	BCR	C33-C5-C4	3.11	119.58	113.62
21	4	318	DGD	O1G-C1A-C2A	3.11	121.66	111.91
26	a	849	BCR	C33-C5-C4	3.11	119.58	113.62
17	2	301	XAT	C26-C27-C28	-3.10	119.43	125.99
19	5	309	CLA	CMB-C2B-C3B	3.10	130.49	124.68
19	b	831	CLA	CMB-C2B-C3B	3.10	130.47	124.68
18	3	302	A1L1G	C33-C34-C35	3.10	123.69	118.94
26	b	846	BCR	C38-C26-C25	-3.09	121.05	124.53
26	a	849	BCR	C38-C26-C25	-3.09	121.06	124.53
19	3	313	CLA	CMB-C2B-C3B	3.09	130.46	124.68
19	4	311	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
19	a	837	CLA	CMB-C2B-C3B	3.09	130.45	124.68
19	2	310	CLA	CMB-C2B-C3B	3.09	130.45	124.68
19	1	203	CLA	CMB-C2B-C3B	3.09	130.45	124.68
17	4	304	XAT	C35-C15-C14	-3.07	117.18	123.47
17	1	302	XAT	C31-C30-C29	-3.07	122.92	127.31
17	2	303	XAT	C19-C9-C10	-3.07	118.62	122.92
18	3	306	A1L1G	C40-C39-C38	3.07	123.65	118.94
19	3	311	CLA	CMB-C2B-C3B	3.07	130.42	124.68
17	a	852	XAT	C35-C15-C14	-3.07	117.19	123.47
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
19	a	809	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
26	b	843	BCR	C20-C21-C22	-3.06	122.94	127.31
26	1	205	BCR	C8-C7-C6	-3.06	118.61	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	821	CLA	CMB-C2B-C3B	3.06	130.40	124.68
19	b	809	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
19	a	801	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
26	b	847	BCR	C11-C10-C9	-3.06	122.95	127.31
19	a	821	CLA	CMB-C2B-C3B	3.05	130.39	124.68
17	5	301	XAT	C31-C30-C29	-3.05	122.96	127.31
19	4	307	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	b	802	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
26	a	848	BCR	C8-C7-C6	-3.04	118.65	127.20
17	3	304	XAT	C4-C3-C2	-3.04	104.90	110.77
19	b	837	CLA	CMB-C2B-C3B	3.04	130.36	124.68
18	3	306	A1L1G	C43-C44-C42	-3.04	118.67	122.92
19	3	308	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
17	a	852	XAT	C31-C32-C33	-3.03	117.89	126.42
26	f	801	BCR	C8-C7-C6	-3.03	118.69	127.20
19	b	823	CLA	CMB-C2B-C3B	3.03	130.34	124.68
19	b	808	CLA	CMB-C2B-C3B	3.02	130.32	124.68
17	4	305	XAT	C24-C23-C22	-3.01	104.96	110.77
18	3	302	A1L1G	C40-C39-C38	3.01	123.56	118.94
19	b	834	CLA	CMB-C2B-C3B	3.01	130.30	124.68
26	b	850	BCR	C15-C14-C13	-3.01	123.02	127.31
17	3	305	XAT	C31-C30-C29	-3.00	123.02	127.31
19	a	835	CLA	CMB-C2B-C3B	3.00	130.29	124.68
19	l	204	CLA	CMB-C2B-C3B	3.00	130.29	124.68
26	b	850	BCR	C16-C15-C14	-3.00	117.33	123.47
19	b	817	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	a	807	CLA	CMB-C2B-C3B	3.00	130.29	124.68
19	b	803	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
19	b	812	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	a	831	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
19	b	835	CLA	CMB-C2B-C3B	2.99	130.28	124.68
21	b	851	DGD	O3E-C3E-C2E	-2.98	103.45	110.35
19	b	808	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	b	839	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	a	830	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
19	a	839	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
19	5	308	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	3	305	XAT	C4-C3-C2	-2.97	105.04	110.77
19	2	313	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	b	815	CLA	CHB-C4A-NA	2.96	128.61	124.51
19	1	314	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
18	3	306	A1L1G	C33-C34-C35	2.96	123.49	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	848	BCR	C8-C7-C6	-2.96	118.89	127.20
18	5	303	A1L1G	C33-C34-C35	2.96	123.48	118.94
19	b	815	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	b	844	BCR	C38-C26-C25	-2.95	121.21	124.53
17	4	301	XAT	C31-C32-C33	-2.95	118.12	126.42
19	b	835	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	b	837	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	3	314	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	4	310	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	1	311	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	b	852	BCR	C16-C15-C14	-2.94	117.44	123.47
19	2	309	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	4	309	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	b	845	BCR	C38-C26-C25	-2.94	121.23	124.53
26	b	846	BCR	C8-C7-C6	-2.94	118.95	127.20
26	a	850	BCR	C28-C27-C26	-2.94	108.84	114.08
18	5	303	A1L1G	C43-C44-C42	-2.93	118.82	122.92
19	b	819	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	3	307	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	b	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	b	830	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	1	302	XAT	C4-C3-C2	-2.93	105.12	110.77
19	3	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	1	302	XAT	C35-C15-C14	-2.93	117.47	123.47
19	b	819	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	4	304	XAT	C4-C3-C2	-2.92	105.13	110.77
19	j	102	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	3	305	XAT	C24-C23-C22	-2.92	105.14	110.77
17	3	301	XAT	C4-C3-C2	-2.91	105.14	110.77
19	a	808	CLA	CMB-C2B-C3B	2.91	130.13	124.68
19	a	812	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	b	825	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
17	5	304	XAT	C5-C4-C3	-2.91	106.98	112.75
19	b	824	CLA	CMB-C2B-C3B	2.91	130.13	124.68
19	a	817	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	4	308	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	4	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	2	303	XAT	C4-C3-C2	-2.91	105.16	110.77
17	4	303	XAT	C30-C31-C32	-2.91	114.15	123.22
19	b	818	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	1	202	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	5	315	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	5	307	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	2	316	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	a	832	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	b	805	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	b	829	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	4	314	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	a	841	CLA	CMB-C2B-C3B	2.90	130.09	124.68
19	1	313	CLA	CMB-C2B-C3B	2.89	130.09	124.68
17	2	305	XAT	C11-C10-C9	-2.89	123.18	127.31
17	4	302	XAT	C24-C23-C22	-2.89	105.19	110.77
17	5	302	XAT	C24-C23-C22	-2.89	105.20	110.77
17	2	304	XAT	C24-C23-C22	-2.89	105.20	110.77
26	a	848	BCR	C7-C8-C9	-2.88	121.88	126.23
19	a	840	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	f	801	BCR	C20-C19-C18	-2.88	118.32	126.42
19	a	813	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	b	841	CLA	CMB-C2B-C3B	2.88	130.07	124.68
19	b	827	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	2	310	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
19	a	837	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
17	1	302	XAT	C24-C23-C22	-2.88	105.22	110.77
19	a	810	CLA	CMB-C2B-C3B	2.87	130.06	124.68
19	b	806	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	b	850	BCR	C23-C24-C25	-2.87	119.13	127.20
19	4	317	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	b	846	BCR	C4-C5-C6	-2.87	118.56	122.73
19	b	809	CLA	CMB-C2B-C3B	2.87	130.05	124.68
19	a	816	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	5	316	SQD	C44-O6-C1	-2.87	108.14	113.74
17	5	302	XAT	C35-C34-C33	-2.87	123.22	127.31
19	a	820	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	2	307	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	4	302	XAT	C4-C3-C2	-2.86	105.24	110.77
19	b	838	CLA	CMB-C2B-C3B	2.86	130.03	124.68
26	f	801	BCR	C33-C5-C6	-2.86	121.31	124.53
19	1	307	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	b	804	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
19	a	826	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	2	314	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	1	312	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	3	302	A1L1G	C43-C44-C42	-2.85	118.93	122.92
17	a	852	XAT	C24-C23-C22	-2.85	105.27	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	309	CLA	CMB-C2B-C3B	2.85	130.01	124.68
19	a	819	CLA	CMB-C2B-C3B	2.85	130.01	124.68
19	a	823	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	a	825	CLA	CMB-C2B-C3B	2.85	130.00	124.68
19	3	307	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	3	308	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	4	315	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	a	813	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	5	304	XAT	C19-C9-C8	2.84	122.55	118.08
26	b	847	BCR	C33-C5-C6	-2.84	121.34	124.53
17	3	303	XAT	C4-C3-C2	-2.84	105.29	110.77
19	a	833	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	3	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	2	304	XAT	C4-C3-C2	-2.84	105.29	110.77
19	b	839	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	a	825	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	5	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	4	318	DGD	O5E-C6E-C5E	-2.83	101.57	111.29
26	b	848	BCR	C15-C16-C17	-2.83	117.67	123.47
19	5	312	CLA	O2D-CGD-CBD	2.83	116.30	111.27
19	b	838	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	2	307	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	a	811	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	5	310	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	b	843	BCR	C38-C26-C25	-2.83	121.35	124.53
17	j	101	XAT	C4-C3-C2	-2.83	105.31	110.77
17	4	301	XAT	C4-C3-C2	-2.83	105.32	110.77
19	b	822	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	j	102	CLA	CMB-C2B-C3B	2.83	129.96	124.68
19	1	305	CLA	CMB-C2B-C3B	2.82	129.96	124.68
19	b	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	a	842	CLA	CMB-C2B-C3B	2.82	129.96	124.68
19	5	305	CLA	CMB-C2B-C3B	2.82	129.95	124.68
26	b	848	BCR	C21-C20-C19	-2.82	114.43	123.22
26	b	845	BCR	C34-C9-C10	-2.81	118.98	122.92
19	a	802	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	1	314	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	j	103	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	i	102	CLA	CMB-C2B-C3B	2.81	129.94	124.68
17	1	303	XAT	C4-C3-C2	-2.81	105.35	110.77
19	1	306	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	a	827	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	306	CLA	CMB-C2B-C3B	2.81	129.93	124.68
19	5	313	CLA	CMB-C2B-C3B	2.80	129.93	124.68
19	b	829	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
19	a	841	CLA	CHB-C4A-NA	2.80	128.39	124.51
17	4	304	XAT	C11-C10-C9	-2.80	123.31	127.31
19	a	836	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	4	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	a	821	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	b	843	BCR	C33-C5-C4	2.80	119.00	113.62
19	3	312	CLA	CHB-C4A-NA	2.80	128.38	124.51
19	a	817	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	2	311	CLA	CMB-C2B-C3B	2.79	129.91	124.68
17	3	304	XAT	C24-C23-C22	-2.79	105.38	110.77
19	f	803	CLA	CMB-C2B-C3B	2.79	129.91	124.68
19	3	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	5	306	CLA	CMB-C2B-C3B	2.79	129.91	124.68
19	a	840	CLA	CMB-C2B-C3B	2.79	129.91	124.68
19	5	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	b	801	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
24	b	842	PQN	C16-C15-C13	-2.79	106.13	113.45
19	3	314	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	2	301	XAT	C4-C3-C2	-2.79	105.38	110.77
26	j	104	BCR	C38-C26-C27	2.79	118.97	113.62
19	1	310	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
19	a	834	CLA	CMB-C2B-C3B	2.78	129.89	124.68
19	3	315	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	a	805	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	l	203	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	2	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	1	301	A1L1G	C20-C21-C22	-2.78	107.25	112.75
19	a	832	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	4	305	XAT	C4-C3-C2	-2.78	105.41	110.77
19	a	844	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
19	4	312	CLA	CMB-C2B-C3B	2.78	129.87	124.68
21	b	851	DGD	O1G-C1A-C2A	2.78	120.62	111.91
19	2	306	CLA	CMB-C2B-C3B	2.78	129.87	124.68
19	5	313	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
19	b	820	CLA	CMB-C2B-C3B	2.77	129.87	124.68
19	a	828	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	831	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	1	308	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	3	312	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	1	304	A1L1F	C20-C21-C22	-2.77	107.27	112.75
21	b	851	DGD	C6D-O5D-C1E	2.77	119.15	113.74
26	b	845	BCR	C20-C21-C22	-2.77	123.36	127.31
19	a	815	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	1	305	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	2	316	CLA	CMB-C2B-C3B	2.77	129.85	124.68
19	b	841	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	a	854	CLA	CMB-C2B-C3B	2.76	129.85	124.68
19	a	841	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	b	816	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	1	304	A1L1F	C36-C35-C34	-2.76	123.37	127.31
23	1	304	A1L1F	C26-O13-C45	2.76	121.82	115.68
19	b	832	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	2	317	LMG	O8-C28-C29	2.76	120.56	111.91
26	b	844	BCR	C21-C20-C19	-2.76	114.61	123.22
19	b	820	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	3	315	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	a	803	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	b	826	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
17	4	302	XAT	C31-C30-C29	-2.75	123.38	127.31
19	5	310	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	4	316	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	2	315	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	b	843	BCR	C4-C5-C6	-2.75	118.73	122.73
17	4	301	XAT	C26-C27-C28	-2.75	120.17	125.99
17	2	301	XAT	C24-C23-C22	-2.75	105.46	110.77
19	f	802	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	a	819	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	b	811	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	b	812	CLA	CMB-C2B-C3B	2.75	130.07	124.69
26	a	850	BCR	C38-C26-C27	2.75	118.89	113.62
19	2	314	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	2	315	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	4	307	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	b	824	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	5	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	b	845	BCR	C37-C22-C21	-2.74	119.09	122.92
17	3	301	XAT	C10-C11-C12	-2.73	114.69	123.22
19	b	823	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
19	l	204	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	a	849	BCR	C2-C1-C6	2.73	114.69	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	305	XAT	C38-C25-C26	-2.73	117.68	122.26
19	b	813	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	a	820	CLA	C1-C2-C3	-2.73	121.32	126.04
22	a	853	LMG	O8-C28-C29	2.73	120.48	111.91
19	a	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	i	101	BCR	C20-C19-C18	-2.73	118.75	126.42
17	3	305	XAT	C35-C15-C14	-2.73	117.89	123.47
17	2	305	XAT	C4-C3-C2	-2.73	105.51	110.77
19	5	305	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	b	836	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	a	838	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	a	821	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	4	313	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
19	4	314	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
17	2	301	XAT	C31-C32-C33	-2.71	118.79	126.42
19	b	810	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
19	f	803	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
20	1	315	SQD	O48-C23-C24	2.71	120.42	111.91
19	5	314	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	a	808	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	a	824	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	2	312	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
17	j	101	XAT	C24-C23-C22	-2.71	105.55	110.77
26	j	104	BCR	C23-C24-C25	-2.71	119.60	127.20
17	j	101	XAT	C15-C35-C34	-2.70	117.93	123.47
24	b	842	PQN	C2M-C2-C3	-2.70	119.99	124.40
26	b	852	BCR	C20-C19-C18	-2.70	118.83	126.42
17	4	301	XAT	C39-C29-C30	-2.70	119.14	122.92
17	j	101	XAT	C31-C30-C29	-2.70	123.45	127.31
26	b	843	BCR	C24-C23-C22	-2.70	122.16	126.23
17	1	303	XAT	C10-C11-C12	-2.70	114.79	123.22
17	4	302	XAT	C15-C14-C13	-2.70	123.46	127.31
17	3	303	XAT	C31-C30-C29	-2.70	123.46	127.31
17	2	302	XAT	C35-C15-C14	-2.69	117.95	123.47
26	b	843	BCR	C23-C24-C25	-2.69	119.64	127.20
19	a	835	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	2	302	XAT	C24-C23-C22	-2.69	105.58	110.77
17	3	301	XAT	C19-C9-C8	2.69	122.31	118.08
26	b	846	BCR	C7-C8-C9	-2.69	122.17	126.23
19	a	805	CLA	CHB-C4A-NA	2.69	128.22	124.51
26	b	850	BCR	C24-C23-C22	-2.68	122.18	126.23
25	m	101	LHG	O8-C23-C24	2.68	120.33	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	315	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	a	826	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	4	315	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
19	3	312	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
19	a	829	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	5	302	XAT	C4-C3-C2	-2.68	105.60	110.77
19	b	801	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	i	101	BCR	C29-C30-C25	2.68	114.60	110.48
19	b	812	CLA	CAB-C3B-C2B	2.68	129.93	124.69
26	m	102	BCR	C33-C5-C6	-2.67	121.53	124.53
19	a	804	CLA	C1-C2-C3	-2.67	121.42	126.04
19	2	313	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
19	a	822	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	b	847	BCR	C35-C13-C12	2.67	122.28	118.08
26	b	850	BCR	C20-C21-C22	-2.67	123.50	127.31
19	b	819	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
17	4	305	XAT	C39-C29-C30	-2.66	119.19	122.92
17	4	305	XAT	C31-C32-C33	-2.66	118.94	126.42
17	j	101	XAT	C31-C32-C33	-2.66	118.94	126.42
19	4	310	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	b	845	BCR	C11-C10-C9	-2.66	123.52	127.31
26	b	846	BCR	C10-C11-C12	-2.66	114.93	123.22
19	a	814	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
17	4	303	XAT	C39-C29-C28	2.65	122.26	118.08
17	4	301	XAT	C27-C28-C29	-2.65	121.41	125.53
17	5	304	XAT	C31-C30-C29	-2.65	123.53	127.31
17	5	304	XAT	C10-C11-C12	-2.65	114.95	123.22
19	b	827	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
19	a	814	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	4	303	XAT	C4-C3-C2	-2.65	105.66	110.77
19	b	807	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	a	834	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
17	3	301	XAT	C27-C28-C29	-2.64	121.43	125.53
20	5	316	SQD	O48-C23-C24	2.64	120.20	111.91
17	5	301	XAT	C35-C15-C14	-2.64	118.06	123.47
26	a	847	BCR	C16-C15-C14	-2.64	118.06	123.47
19	a	810	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	1	312	CLA	CMB-C2B-C3B	2.64	129.62	124.68
17	2	304	XAT	C15-C14-C13	-2.64	123.54	127.31
26	f	801	BCR	C33-C5-C4	2.64	118.68	113.62
19	4	308	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
17	4	305	XAT	C7-C8-C9	-2.64	121.44	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	l	203	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	3	301	XAT	C24-C23-C22	-2.63	105.69	110.77
19	a	829	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	b	843	BCR	C2-C1-C6	2.63	114.53	110.48
19	5	306	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	a	807	CLA	CHB-C4A-NA	2.63	128.14	124.51
19	b	806	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	f	801	BCR	C10-C11-C12	-2.62	115.03	123.22
26	b	850	BCR	C21-C20-C19	-2.62	115.03	123.22
19	a	809	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	a	842	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
17	2	305	XAT	C31-C32-C33	-2.62	119.06	126.42
19	b	820	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
19	4	310	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	b	850	BCR	C28-C27-C26	-2.62	109.41	114.08
19	b	809	CLA	CHB-C4A-NA	2.61	128.13	124.51
19	5	311	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	2	311	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
19	3	310	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	4	317	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	a	819	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	b	825	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	2	304	XAT	C35-C15-C14	-2.61	118.13	123.47
19	4	317	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	4	304	XAT	C31-C30-C29	-2.61	123.59	127.31
19	1	314	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	1	304	A1L1F	C26-C30-C31	-2.61	121.52	124.93
19	j	103	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	b	802	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	b	846	BCR	C2-C1-C6	2.60	114.49	110.48
19	b	831	CLA	CAA-C2A-C3A	-2.60	110.03	116.10
25	b	849	LHG	O8-C23-C24	2.60	120.06	111.91
19	a	824	CLA	CMB-C2B-C3B	2.60	129.54	124.68
26	m	102	BCR	C15-C16-C17	-2.60	118.15	123.47
21	b	851	DGD	C1E-O6E-C5E	2.60	118.79	113.69
19	1	309	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
19	b	809	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
26	m	102	BCR	C27-C26-C25	2.60	126.50	122.73
19	a	802	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
26	b	848	BCR	C24-C23-C22	-2.59	122.31	126.23
19	b	841	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
26	l	205	BCR	C28-C27-C26	-2.59	109.45	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	854	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
19	b	811	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	4	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	a	818	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	b	830	CLA	C2D-C1D-ND	-2.59	108.20	110.10
19	b	821	CLA	C1-C2-C3	-2.59	122.57	126.75
19	b	814	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	2	311	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	1	306	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	j	105	LMG	O8-C28-C29	2.59	120.02	111.91
19	b	834	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
19	i	102	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
26	a	849	BCR	C16-C15-C14	-2.58	118.18	123.47
26	j	104	BCR	C33-C5-C6	-2.58	121.63	124.53
19	3	315	CLA	CHB-C4A-NA	2.58	128.09	124.51
19	a	832	CLA	CHB-C4A-NA	2.58	128.09	124.51
19	2	308	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
19	b	817	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
19	4	315	CLA	CAA-C2A-C3A	-2.58	110.07	116.10
17	5	304	XAT	C8-C9-C10	-2.58	114.98	118.94
23	1	304	AI1F	O13-C45-C47	2.58	120.01	111.91
19	1	204	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	2	306	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
19	5	306	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	1	201	BCR	C20-C21-C22	-2.57	123.64	127.31
19	b	818	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
19	b	836	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	b	814	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	5	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	4	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	b	813	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	a	833	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	4	306	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	b	826	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	1	308	CLA	C1-C2-C3	-2.56	121.61	126.04
19	2	307	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	a	806	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	1	303	XAT	C35-C15-C14	-2.56	118.24	123.47
19	a	836	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	b	847	BCR	C8-C7-C6	-2.56	120.03	127.20
19	a	804	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	b	818	CLA	CHB-C4A-NA	2.55	128.04	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	837	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	832	CLA	C1-C2-C3	-2.55	122.62	126.75
19	a	827	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
19	2	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	816	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	b	832	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	b	847	BCR	C38-C26-C25	-2.55	121.66	124.53
19	5	311	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
25	a	845	LHG	O8-C23-C24	2.55	119.90	111.91
26	a	849	BCR	C23-C24-C25	-2.55	120.05	127.20
19	3	308	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	b	801	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	a	806	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	b	821	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	5	305	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	5	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	b	835	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	1	312	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	b	822	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	b	847	BCR	C33-C5-C4	2.54	118.49	113.62
17	2	302	XAT	C4-C3-C2	-2.54	105.87	110.77
19	a	827	CLA	CHB-C4A-NA	2.54	128.02	124.51
17	a	852	XAT	O4-C5-C4	2.54	115.29	113.38
19	5	310	CLA	CHB-C4A-NA	2.53	128.02	124.51
20	5	316	SQD	O7-S-C6	2.53	109.95	106.94
19	b	838	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
19	5	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	802	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	f	802	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	b	803	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
19	4	314	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	b	803	CLA	CMB-C2B-C3B	2.53	129.41	124.68
26	b	844	BCR	C24-C23-C22	-2.53	122.41	126.23
19	a	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	840	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	822	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
19	b	830	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
19	b	805	CLA	CHB-C4A-NA	2.53	128.00	124.51
26	b	848	BCR	C34-C9-C8	2.52	122.06	118.08
17	5	304	XAT	C15-C35-C34	-2.52	118.30	123.47
19	3	312	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
22	a	853	LMG	C8-O7-C10	-2.52	111.58	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	804	CLA	CHD-C1D-ND	-2.52	122.14	124.45
19	f	803	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	a	820	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
19	3	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	b	852	BCR	C15-C14-C13	-2.52	123.71	127.31
19	3	309	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
19	b	807	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	l	205	BCR	C38-C26-C27	2.52	118.45	113.62
19	a	825	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	a	838	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	a	836	CLA	CMB-C2B-C3B	2.52	129.39	124.68
19	a	831	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
19	2	314	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	b	834	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	1	315	SQD	O8-S-C6	2.51	109.74	105.74
19	3	314	CLA	CHB-C4A-NA	2.51	127.99	124.51
26	l	205	BCR	C15-C16-C17	-2.51	118.33	123.47
19	2	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	5	302	XAT	C19-C9-C10	-2.51	119.41	122.92
26	l	201	BCR	C28-C27-C26	-2.51	109.60	114.08
19	5	312	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
19	1	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	a	811	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	b	840	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	a	801	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
26	b	848	BCR	C20-C21-C22	-2.50	123.74	127.31
26	f	804	BCR	C15-C16-C17	-2.50	118.35	123.47
26	l	201	BCR	C34-C9-C10	-2.50	119.42	122.92
19	b	834	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
19	4	311	CLA	CMB-C2B-C3B	2.50	129.36	124.68
19	1	308	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	l	205	BCR	C33-C5-C4	2.50	118.41	113.62
19	a	808	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	a	815	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	a	817	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	l	202	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	1	309	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
17	5	304	XAT	C39-C29-C28	2.49	122.01	118.08
19	l	203	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	b	823	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	5	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	1	310	CLA	C1B-CHB-C4A	-2.49	125.19	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	801	BCR	C2-C1-C6	2.49	114.31	110.48
19	1	310	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	3	307	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	a	841	CLA	C1-C2-C3	-2.49	121.74	126.04
19	b	816	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	a	841	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	a	839	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	820	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	a	837	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	2	302	XAT	C11-C10-C9	-2.48	123.77	127.31
26	j	104	BCR	C15-C16-C17	-2.48	118.39	123.47
19	a	810	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	b	821	CLA	O2D-CGD-CBD	2.48	115.67	111.27
19	a	809	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
19	4	316	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	5	304	XAT	C30-C31-C32	-2.48	115.49	123.22
19	b	835	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	j	104	BCR	C27-C26-C25	-2.47	119.14	122.73
19	a	814	CLA	CHD-C1D-ND	-2.47	122.18	124.45
17	4	301	XAT	C35-C15-C14	-2.47	118.41	123.47
19	a	835	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
19	2	306	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	a	820	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	2	315	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
17	5	301	XAT	C4-C3-C2	-2.47	106.01	110.77
26	b	844	BCR	C15-C16-C17	-2.46	118.43	123.47
19	a	823	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	2	316	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	3	311	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	a	812	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	a	802	CLA	C1-C2-C3	-2.46	121.79	126.04
21	b	851	DGD	O2G-C1B-O1B	-2.46	117.76	123.70
19	a	818	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	b	839	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	3	306	A1L1G	C17-C20-C21	2.46	117.04	114.28
24	b	842	PQN	C14-C13-C15	2.46	119.40	115.27
19	b	829	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
19	2	311	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	a	812	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
19	4	309	CLA	CHB-C4A-NA	2.45	127.91	124.51
19	a	806	CLA	O1D-CGD-CBD	2.45	129.50	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	837	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	b	832	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	5	308	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
19	l	204	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
26	b	846	BCR	C21-C20-C19	-2.44	115.59	123.22
19	l	203	CLA	CHD-C1D-ND	-2.44	122.21	124.45
19	4	309	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
26	b	843	BCR	C15-C16-C17	-2.44	118.47	123.47
26	b	850	BCR	C33-C5-C4	2.44	118.31	113.62
19	2	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	5	311	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	b	811	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	a	805	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	a	832	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	b	808	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
19	a	836	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	a	814	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	3	310	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	1	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	1	311	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	b	808	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	b	847	BCR	C39-C30-C25	-2.43	106.36	110.30
26	l	201	BCR	C21-C20-C19	-2.43	115.64	123.22
26	b	848	BCR	C38-C26-C25	-2.43	121.80	124.53
19	4	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	a	830	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
19	a	854	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
19	b	814	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
19	a	804	CLA	O2D-CGD-CBD	2.42	115.58	111.27
19	b	803	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
19	b	819	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	b	828	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	2	303	XAT	C8-C9-C10	2.42	122.65	118.94
19	5	314	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	a	840	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	4	312	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	a	854	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	1	304	AI1F	C27-C34-C33	2.41	121.88	118.08
19	a	810	CLA	C1-C2-C3	-2.41	121.87	126.04
19	5	309	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	5	302	XAT	C31-C30-C29	-2.41	123.86	127.31
19	b	806	CLA	C1B-CHB-C4A	-2.41	125.34	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	315	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	4	308	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	f	804	BCR	C28-C27-C26	-2.41	109.77	114.08
19	3	309	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	a	818	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	a	816	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	b	831	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	b	834	CLA	CHD-C1D-ND	-2.40	122.24	124.45
19	1	305	CLA	CHB-C4A-NA	2.40	127.84	124.51
19	j	102	CLA	CHB-C4A-NA	2.40	127.84	124.51
19	4	312	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	b	828	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
17	4	302	XAT	C10-C11-C12	-2.40	115.72	123.22
19	a	835	CLA	O2D-CGD-CBD	2.40	115.54	111.27
19	b	826	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	a	834	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	i	102	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	a	848	BCR	C33-C5-C4	2.40	118.22	113.62
19	b	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	a	850	BCR	C8-C7-C6	-2.40	120.47	127.20
19	b	823	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	a	807	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	2	315	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	b	843	BCR	C29-C30-C25	2.40	114.17	110.48
26	a	850	BCR	C16-C15-C14	-2.39	118.57	123.47
19	a	813	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	b	816	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	b	846	BCR	C33-C5-C6	-2.39	121.84	124.53
26	b	846	BCR	C16-C15-C14	-2.39	118.57	123.47
26	j	104	BCR	C38-C26-C25	-2.39	121.84	124.53
19	i	102	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	b	843	BCR	C21-C20-C19	-2.39	115.76	123.22
19	j	102	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	b	810	CLA	CHB-C4A-NA	2.39	127.81	124.51
17	3	304	XAT	C31-C32-C33	-2.39	119.71	126.42
17	2	303	XAT	C24-C23-C22	-2.39	106.16	110.77
19	b	817	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	a	804	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
26	b	845	BCR	C28-C27-C26	-2.39	109.82	114.08
19	3	311	CLA	C1-C2-C3	-2.39	122.89	126.75
19	b	837	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
19	a	808	CLA	C1B-CHB-C4A	-2.38	125.39	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	301	XAT	C40-C33-C34	-2.38	119.58	122.92
26	a	850	BCR	C10-C11-C12	-2.38	115.78	123.22
26	b	844	BCR	C28-C27-C26	-2.38	109.82	114.08
19	1	313	CLA	CAA-C2A-C3A	-2.38	110.54	116.10
19	1	311	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	3	313	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	b	812	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	3	310	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	5	307	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
17	3	305	XAT	C10-C11-C12	-2.38	115.80	123.22
19	a	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	1	313	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	b	817	CLA	CHD-C1D-ND	-2.37	122.28	124.45
19	1	308	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	b	850	BCR	C8-C7-C6	-2.37	120.55	127.20
19	a	825	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	a	806	CLA	C5-C3-C2	-2.37	116.32	121.12
19	b	813	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	a	801	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	j	105	LMG	C8-O7-C10	-2.37	111.96	117.79
19	a	842	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	3	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	a	801	CLA	CMB-C2B-C3B	2.37	129.10	124.68
19	2	314	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
17	4	302	XAT	C30-C31-C32	-2.36	115.84	123.22
26	b	843	BCR	C38-C26-C27	2.36	118.16	113.62
19	a	824	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	b	833	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	b	839	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	a	848	BCR	C15-C16-C17	-2.36	118.63	123.47
26	b	844	BCR	C33-C5-C4	2.36	118.15	113.62
19	a	834	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	a	839	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	b	852	BCR	C36-C18-C17	-2.36	119.62	122.92
19	b	810	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	b	833	CLA	CHD-C1D-ND	-2.36	122.29	124.45
19	b	824	CLA	CHB-C4A-NA	2.36	127.77	124.51
19	a	833	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
19	l	202	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
26	b	850	BCR	C10-C11-C12	-2.35	115.87	123.22
19	a	803	CLA	CHD-C1D-ND	-2.35	122.29	124.45
17	5	304	XAT	C25-C24-C23	-2.35	108.09	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	828	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
26	a	847	BCR	C23-C24-C25	-2.35	120.60	127.20
19	b	825	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	f	802	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
17	3	303	XAT	C30-C31-C32	-2.35	115.89	123.22
19	a	819	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	a	812	CLA	CHD-C1D-ND	-2.35	122.30	124.45
19	4	311	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	a	811	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	a	826	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	4	315	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	5	309	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	b	836	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	b	844	BCR	C23-C24-C25	-2.34	120.63	127.20
19	4	313	CLA	CHD-C1D-ND	-2.34	122.30	124.45
19	b	805	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	a	844	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	l	201	BCR	C15-C16-C17	-2.34	118.68	123.47
19	b	801	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	b	831	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	b	841	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	b	821	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	4	317	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	f	803	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	a	806	CLA	C6-C5-C3	-2.33	107.34	113.45
19	b	837	CLA	CHD-C1D-ND	-2.33	122.31	124.45
19	a	815	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	b	804	CLA	C3C-C4C-NC	-2.33	107.96	110.57
19	1	309	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	i	101	BCR	C37-C22-C21	-2.32	119.67	122.92
17	5	301	XAT	O4-C5-C4	2.32	115.13	113.38
26	f	804	BCR	C11-C12-C13	-2.32	119.89	126.42
19	a	827	CLA	CHD-C1D-ND	-2.32	122.32	124.45
24	a	843	PQN	C11-C12-C13	-2.32	122.93	126.79
26	f	804	BCR	C3-C4-C5	-2.32	109.94	114.08
23	1	304	A1L1F	C31-C32-C33	-2.32	115.98	123.22
19	4	312	CLA	CHD-C1D-ND	-2.32	122.32	124.45
19	a	841	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
19	5	310	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	b	843	BCR	C11-C12-C13	-2.32	119.91	126.42
26	a	847	BCR	C33-C5-C4	2.31	118.06	113.62
19	3	314	CLA	C1B-CHB-C4A	-2.31	125.53	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	305	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	m	102	BCR	C8-C7-C6	-2.31	120.70	127.20
19	b	807	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
19	j	103	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	b	826	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	a	848	BCR	C10-C11-C12	-2.31	116.01	123.22
17	2	301	XAT	C10-C11-C12	-2.31	116.01	123.22
19	5	310	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	a	810	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	3	315	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	a	828	CLA	C1-C2-C3	-2.31	122.05	126.04
19	1	309	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	i	101	BCR	C16-C15-C14	-2.31	118.75	123.47
17	j	101	XAT	C39-C29-C28	2.31	121.71	118.08
19	3	311	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	a	816	CLA	C1-C2-C3	-2.31	123.02	126.75
19	4	310	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
19	a	810	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	b	815	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
19	a	821	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	2	312	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	a	844	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	1	303	XAT	C27-C28-C29	-2.30	121.96	125.53
19	2	310	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	1	311	CLA	CHD-C1D-ND	-2.30	122.34	124.45
17	3	304	XAT	C27-C28-C29	-2.30	121.97	125.53
19	5	307	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	4	314	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	b	852	BCR	C23-C24-C25	-2.29	120.76	127.20
19	2	310	CLA	CHB-C4A-NA	2.29	127.68	124.51
17	2	304	XAT	C35-C34-C33	-2.29	124.04	127.31
19	b	806	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	a	841	CLA	CHD-C1D-ND	-2.29	122.35	124.45
17	5	302	XAT	C15-C35-C34	-2.29	118.79	123.47
19	b	807	CLA	C1-C2-C3	-2.29	122.09	126.04
19	a	820	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	a	830	CLA	C1-C2-C3	-2.29	122.09	126.04
19	b	840	CLA	CMB-C2B-C3B	2.28	128.95	124.68
19	3	307	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	2	313	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	2	306	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	a	823	CLA	C1B-CHB-C4A	-2.28	125.60	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	303	XAT	O4-C5-C4	2.28	115.09	113.38
26	j	104	BCR	C34-C9-C10	-2.28	119.73	122.92
19	a	805	CLA	CHD-C1D-ND	-2.28	122.36	124.45
19	a	842	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	1	312	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	a	817	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
17	2	302	XAT	C10-C11-C12	-2.28	116.12	123.22
18	1	301	A1L1G	C17-C20-C21	2.27	116.84	114.28
19	4	306	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
19	a	836	CLA	C1-C2-C3	-2.27	123.07	126.75
19	5	314	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
19	1	314	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	a	824	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	b	852	BCR	C38-C26-C27	2.27	117.98	113.62
19	b	838	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	a	852	XAT	C19-C9-C8	2.27	121.66	118.08
23	1	304	A1L1F	C37-C36-C35	-2.27	118.82	123.47
19	1	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	b	847	BCR	C21-C20-C19	-2.27	116.13	123.22
19	a	836	CLA	CHD-C1D-ND	-2.27	122.37	124.45
26	a	848	BCR	C16-C15-C14	-2.27	118.82	123.47
19	4	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	1	306	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	5	305	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	a	805	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
19	5	306	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	l	201	BCR	C23-C24-C25	-2.27	120.84	127.20
26	a	849	BCR	C38-C26-C27	2.26	117.97	113.62
19	a	838	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
19	b	824	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	1	315	SQD	O9-S-C6	2.26	109.62	106.94
19	5	313	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
19	b	803	CLA	CHB-C4A-NA	2.26	127.63	124.51
19	b	809	CLA	O2D-CGD-CBD	2.26	115.28	111.27
19	b	833	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	a	825	CLA	CHD-C1D-ND	-2.25	122.38	124.45
19	b	804	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	1	304	A1L1F	O7-C54-O55	-2.25	118.49	122.96
17	3	304	XAT	C40-C33-C34	-2.25	119.77	122.92
17	3	301	XAT	C15-C35-C34	-2.25	118.86	123.47
17	5	302	XAT	O4-C5-C4	2.25	115.07	113.38
19	b	822	CLA	O2A-CGA-O1A	-2.25	117.92	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	847	BCR	C38-C26-C27	2.25	117.94	113.62
19	2	316	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	a	827	CLA	CAA-C2A-C1A	-2.25	104.61	111.97
19	a	813	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
26	f	801	BCR	C28-C27-C26	-2.24	110.07	114.08
19	4	310	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
19	b	832	CLA	CHD-C1D-ND	-2.24	122.39	124.45
19	2	309	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
17	5	301	XAT	O24-C25-C38	2.24	117.74	115.06
19	b	841	CLA	CHD-C1D-ND	-2.24	122.40	124.45
19	b	822	CLA	C1-C2-C3	-2.24	122.17	126.04
17	5	302	XAT	C11-C12-C13	-2.24	120.13	126.42
26	m	102	BCR	C24-C23-C22	-2.24	122.85	126.23
17	4	305	XAT	C15-C35-C34	-2.23	118.90	123.47
19	b	827	CLA	CHB-C4A-NA	2.23	127.60	124.51
18	1	301	A1L1G	C14-C29-C30	-2.23	121.54	125.47
19	a	813	CLA	CHD-C1D-ND	-2.23	122.41	124.45
19	b	830	CLA	CHB-C4A-NA	2.23	127.59	124.51
17	2	302	XAT	O4-C5-C4	2.23	115.06	113.38
17	2	303	XAT	O4-C5-C4	2.23	115.05	113.38
19	b	819	CLA	CHD-C1D-ND	-2.23	122.41	124.45
26	b	848	BCR	C35-C13-C12	2.23	121.58	118.08
20	5	316	SQD	C45-O47-C7	-2.22	112.31	117.79
26	a	850	BCR	C20-C19-C18	-2.22	120.17	126.42
26	a	848	BCR	C21-C20-C19	-2.22	116.28	123.22
26	b	847	BCR	C34-C9-C8	2.22	121.58	118.08
17	2	304	XAT	C20-C13-C12	2.22	121.58	118.08
19	b	810	CLA	C1-C2-C3	-2.22	122.20	126.04
19	5	312	CLA	CHD-C1D-ND	-2.22	122.41	124.45
17	3	303	XAT	C15-C35-C34	-2.22	118.92	123.47
26	b	847	BCR	C23-C24-C25	-2.22	120.97	127.20
26	b	850	BCR	C37-C22-C23	2.22	121.57	118.08
19	4	309	CLA	CHD-C1D-ND	-2.22	122.42	124.45
17	2	305	XAT	C19-C9-C8	2.22	121.57	118.08
19	5	307	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
19	a	806	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
19	3	312	CLA	CHD-C1D-ND	-2.21	122.42	124.45
19	b	829	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	3	313	CLA	CHD-C1D-ND	-2.21	122.42	124.45
19	a	819	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
17	3	305	XAT	C19-C9-C8	2.21	121.56	118.08
26	f	801	BCR	C34-C9-C8	2.21	121.55	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	305	XAT	O4-C5-C4	2.20	115.04	113.38
26	b	845	BCR	C33-C5-C4	2.20	117.85	113.62
17	1	303	XAT	O4-C5-C4	2.20	115.04	113.38
19	a	822	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	l	201	BCR	C29-C30-C25	2.20	113.87	110.48
17	2	305	XAT	C15-C35-C34	-2.20	118.97	123.47
19	a	818	CLA	O2D-CGD-CBD	2.20	115.18	111.27
26	b	846	BCR	C11-C10-C9	-2.20	124.17	127.31
19	a	829	CLA	CHB-C4A-NA	2.20	127.55	124.51
26	a	849	BCR	C21-C20-C19	-2.20	116.35	123.22
19	b	836	CLA	CAC-C3C-C4C	2.20	127.66	124.81
19	1	305	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	2	308	CLA	CHB-C4A-NA	2.20	127.55	124.51
19	4	316	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
26	f	801	BCR	C35-C13-C12	2.20	121.54	118.08
19	b	835	CLA	CHD-C1D-ND	-2.20	122.44	124.45
19	1	312	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
19	b	837	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
19	4	308	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	l	202	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	2	311	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
19	b	822	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
17	5	301	XAT	C30-C31-C32	-2.19	116.37	123.22
19	2	309	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	a	820	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
19	b	814	CLA	C1-C2-C3	-2.19	122.26	126.04
19	a	806	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	a	801	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	2	304	XAT	O24-C25-C38	2.19	117.68	115.06
26	f	801	BCR	C15-C14-C13	-2.19	124.19	127.31
19	b	805	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	a	843	PQN	C2M-C2-C3	-2.18	120.84	124.40
19	b	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	f	803	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	3	303	XAT	O24-C25-C38	2.18	117.67	115.06
19	a	811	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	1	303	XAT	C19-C9-C8	2.18	121.51	118.08
17	3	301	XAT	C8-C9-C10	-2.18	115.60	118.94
26	b	845	BCR	C7-C6-C5	-2.18	116.19	121.46
19	a	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	b	846	BCR	C34-C9-C8	2.18	121.51	118.08
19	b	804	CLA	O1D-CGD-CBD	2.18	128.94	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	808	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	2	303	XAT	C39-C29-C30	-2.17	119.88	122.92
17	5	302	XAT	C20-C13-C14	-2.17	119.88	122.92
26	m	102	BCR	C15-C14-C13	-2.17	124.21	127.31
18	3	306	A1L1G	C20-C21-C22	-2.17	108.45	112.75
19	a	833	CLA	C1-C2-C3	-2.17	122.29	126.04
17	2	303	XAT	C40-C33-C34	-2.17	119.89	122.92
26	b	844	BCR	C37-C22-C23	2.17	121.49	118.08
19	j	102	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	3	303	XAT	C35-C15-C14	-2.17	119.04	123.47
17	a	852	XAT	C40-C33-C32	2.16	121.49	118.08
19	1	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	b	851	DGD	O3D-C3D-C4D	-2.16	105.35	110.35
17	4	301	XAT	C28-C29-C30	2.16	122.26	118.94
19	b	802	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	b	840	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
17	5	304	XAT	O24-C25-C38	2.16	117.65	115.06
17	j	101	XAT	O4-C5-C4	2.16	115.00	113.38
17	2	303	XAT	C31-C32-C33	-2.16	120.35	126.42
19	a	804	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	a	848	BCR	C23-C24-C25	-2.16	121.14	127.20
17	4	303	XAT	O24-C25-C38	2.16	117.64	115.06
18	1	301	A1L1G	C29-C30-C31	2.16	122.20	118.93
17	4	302	XAT	C39-C29-C28	2.16	121.47	118.08
17	2	301	XAT	O4-C5-C4	2.16	115.00	113.38
19	a	830	CLA	CHB-C4A-NA	2.16	127.49	124.51
26	a	849	BCR	C8-C7-C6	-2.15	121.15	127.20
26	l	201	BCR	C39-C30-C25	-2.15	106.80	110.30
19	5	311	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	4	301	XAT	O4-C5-C4	2.15	115.00	113.38
19	5	309	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	a	829	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	i	101	BCR	C23-C22-C21	2.15	122.24	118.94
19	a	831	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	b	846	BCR	C15-C16-C17	-2.15	119.07	123.47
20	5	316	SQD	O9-S-C6	2.15	109.49	106.94
19	3	311	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
19	b	840	CLA	C1-C2-C3	-2.15	122.33	126.04
17	3	304	XAT	O4-C5-C18	2.14	117.63	115.06
19	1	308	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
19	b	813	CLA	CHD-C1D-ND	-2.14	122.48	124.45
19	a	816	CLA	CHD-C1D-ND	-2.14	122.48	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	XAT	O4-C5-C18	2.14	117.62	115.06
17	3	303	XAT	C39-C29-C28	2.14	121.45	118.08
17	4	305	XAT	O24-C25-C38	2.14	117.62	115.06
26	j	104	BCR	C16-C15-C14	-2.14	119.09	123.47
17	2	301	XAT	C39-C29-C30	-2.14	119.93	122.92
26	b	850	BCR	C35-C13-C12	2.14	121.44	118.08
26	b	847	BCR	C29-C30-C25	2.14	113.77	110.48
26	i	101	BCR	C10-C11-C12	-2.13	116.56	123.22
17	2	305	XAT	O4-C5-C18	2.13	117.61	115.06
17	j	101	XAT	O24-C25-C38	2.13	117.61	115.06
19	a	854	CLA	CHD-C1D-ND	-2.13	122.49	124.45
26	a	849	BCR	C10-C11-C12	-2.13	116.56	123.22
17	a	852	XAT	O24-C25-C38	2.13	117.61	115.06
26	b	844	BCR	C36-C18-C19	2.13	121.44	118.08
19	3	313	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	b	844	BCR	C11-C12-C13	-2.13	120.43	126.42
19	b	838	CLA	C1-C2-C3	-2.13	122.36	126.04
19	a	834	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
17	3	303	XAT	O4-C5-C4	2.13	114.98	113.38
19	a	812	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	a	806	CLA	C6-C7-C8	-2.13	109.04	115.92
19	5	312	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
26	l	201	BCR	C3-C4-C5	-2.13	110.28	114.08
26	b	846	BCR	C23-C24-C25	-2.13	121.23	127.20
19	b	836	CLA	C1-C2-C3	-2.13	122.36	126.04
26	b	848	BCR	C37-C22-C23	2.13	121.43	118.08
26	a	847	BCR	C38-C26-C27	2.12	117.70	113.62
19	a	831	CLA	O2D-CGD-CBD	2.12	115.04	111.27
19	3	315	CLA	CHD-C1D-ND	-2.12	122.50	124.45
19	i	102	CLA	CHD-C1D-ND	-2.12	122.50	124.45
17	4	303	XAT	C7-C8-C9	-2.12	122.24	125.53
19	a	834	CLA	C1-C2-C3	-2.12	122.37	126.04
19	b	823	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
19	4	307	CLA	O2D-CGD-CBD	2.12	115.03	111.27
17	2	304	XAT	C10-C11-C12	-2.12	116.60	123.22
19	b	812	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	a	839	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	a	809	CLA	CHD-C1D-ND	-2.12	122.51	124.45
26	a	847	BCR	C8-C7-C6	-2.12	121.25	127.20
19	1	306	CLA	C1-C2-C3	-2.12	122.38	126.04
19	a	838	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	a	815	CLA	CHD-C1D-ND	-2.11	122.51	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	317	LMG	C8-O7-C10	-2.11	112.59	117.79
19	4	313	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	2	308	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	4	308	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	b	821	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	b	830	CLA	C1-C2-C3	-2.11	122.39	126.04
26	f	804	BCR	C35-C13-C14	-2.11	119.97	122.92
17	3	305	XAT	O24-C25-C38	2.11	117.58	115.06
17	3	303	XAT	C10-C11-C12	-2.11	116.64	123.22
19	1	312	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	f	802	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	i	102	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
19	2	308	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
26	j	104	BCR	C3-C4-C5	-2.10	110.32	114.08
19	4	311	CLA	O2D-CGD-CBD	2.10	115.00	111.27
19	5	305	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	b	816	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	l	204	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	4	303	XAT	C35-C15-C14	-2.10	119.17	123.47
26	l	201	BCR	C37-C22-C23	2.10	121.39	118.08
26	b	848	BCR	C23-C24-C25	-2.10	121.31	127.20
26	a	848	BCR	C34-C9-C8	2.10	121.39	118.08
17	4	302	XAT	C20-C13-C12	2.10	121.38	118.08
17	5	304	XAT	C35-C15-C14	-2.10	119.18	123.47
17	3	304	XAT	C35-C15-C14	-2.10	119.18	123.47
19	5	307	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	4	310	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	b	824	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	a	807	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	a	825	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	b	839	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	4	308	CLA	O2D-CGD-CBD	2.09	114.99	111.27
19	a	836	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	a	827	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	5	302	XAT	O4-C5-C18	2.09	117.56	115.06
19	b	818	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	b	821	CLA	CHD-C1D-ND	-2.09	122.53	124.45
26	b	845	BCR	C8-C9-C10	2.09	122.15	118.94
26	a	847	BCR	C28-C27-C26	-2.09	110.35	114.08
26	b	852	BCR	C32-C1-C6	-2.09	106.91	110.30
19	a	844	CLA	C1-C2-C3	-2.09	122.43	126.04
17	a	852	XAT	C20-C13-C14	-2.09	120.00	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	802	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	b	807	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
17	5	304	XAT	O4-C5-C18	2.09	117.56	115.06
19	b	811	CLA	CHD-C1D-ND	-2.09	122.54	124.45
19	b	824	CLA	C1-C2-C3	-2.09	122.43	126.04
19	3	309	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	4	309	CLA	C1-C2-C3	-2.09	123.38	126.75
26	j	104	BCR	C29-C30-C25	2.09	113.69	110.48
17	1	302	XAT	O24-C25-C38	2.09	117.56	115.06
26	a	849	BCR	C15-C16-C17	-2.09	119.20	123.47
19	a	844	CLA	CHD-C1D-ND	-2.08	122.54	124.45
17	3	301	XAT	O4-C5-C18	2.08	117.55	115.06
19	4	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	b	817	CLA	C1-C2-C3	-2.08	122.44	126.04
19	b	808	CLA	CHD-C1D-ND	-2.08	122.54	124.45
17	4	304	XAT	O4-C5-C18	2.08	117.55	115.06
17	4	302	XAT	O4-C5-C18	2.08	117.55	115.06
17	2	301	XAT	O24-C25-C38	2.08	117.55	115.06
26	b	843	BCR	C37-C22-C23	2.08	121.35	118.08
19	4	306	CLA	CHD-C1D-ND	-2.08	122.55	124.45
19	b	808	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	b	838	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
17	3	305	XAT	O4-C5-C18	2.07	117.54	115.06
19	b	813	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
19	b	830	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	2	317	LMG	C4-C3-C2	-2.07	107.21	110.82
17	a	852	XAT	C39-C29-C28	2.07	121.34	118.08
17	5	302	XAT	O24-C25-C26	-2.07	57.24	58.96
19	5	315	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	b	801	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
19	5	311	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	1	306	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	5	302	XAT	C30-C31-C32	-2.07	116.76	123.22
19	1	310	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
19	a	829	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
19	2	315	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	a	837	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	b	820	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
26	b	852	BCR	C34-C9-C10	-2.07	120.03	122.92
19	a	809	CLA	O2D-CGD-CBD	2.06	114.93	111.27
19	a	824	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	a	808	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	854	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
17	1	302	XAT	O4-C5-C18	2.06	117.53	115.06
19	4	317	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	b	805	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	b	822	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	1	306	CLA	CAC-C3C-C4C	2.06	127.48	124.81
17	3	303	XAT	O4-C5-C18	2.06	117.52	115.06
17	5	301	XAT	C39-C29-C28	2.06	121.32	118.08
19	b	814	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	3	301	XAT	O24-C25-C38	2.06	117.52	115.06
17	2	305	XAT	O4-C5-C4	2.06	114.93	113.38
19	a	834	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	2	303	XAT	O24-C25-C38	2.06	117.52	115.06
19	a	844	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	b	828	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
19	1	311	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
19	3	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	b	820	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	2	307	CLA	C2A-C1A-CHA	2.05	127.45	123.86
26	b	845	BCR	C16-C15-C14	-2.05	119.27	123.47
17	2	304	XAT	C15-C35-C34	-2.05	119.27	123.47
19	b	832	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	a	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	830	CLA	O2D-CGD-CBD	2.05	114.91	111.27
17	4	305	XAT	O4-C5-C18	2.05	117.51	115.06
17	1	303	XAT	C11-C10-C9	-2.05	124.38	127.31
19	b	831	CLA	CMA-C3A-C2A	-2.05	111.31	116.10
19	2	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	5	308	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	803	CLA	O2D-CGD-CBD	2.05	114.91	111.27
19	1	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	f	801	BCR	C36-C18-C17	-2.05	120.06	122.92
19	a	832	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	2	302	XAT	C19-C9-C8	2.04	121.30	118.08
17	4	302	XAT	O4-C5-C4	2.04	114.92	113.38
17	3	304	XAT	O24-C25-C38	2.04	117.50	115.06
19	a	803	CLA	CHB-C4A-NA	2.04	127.34	124.51
21	b	851	DGD	O5E-C6E-C5E	-2.04	104.28	111.29
19	a	832	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	b	841	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	b	804	CLA	CAC-C3C-C4C	2.04	127.46	124.81
17	3	304	XAT	O4-C5-C4	2.04	114.92	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	302	XAT	O4-C5-C4	2.04	114.92	113.38
19	j	102	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	f	802	CLA	C1-C2-C3	-2.04	122.52	126.04
17	2	304	XAT	O4-C5-C18	2.04	117.50	115.06
26	f	804	BCR	C33-C5-C4	2.04	117.53	113.62
19	a	811	CLA	C1-C2-C3	-2.04	122.52	126.04
19	b	810	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	2	312	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	1	306	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	3	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	l	201	BCR	C33-C5-C4	2.04	117.53	113.62
17	1	303	XAT	C20-C13-C12	2.04	121.28	118.08
26	f	804	BCR	C8-C7-C6	-2.03	121.49	127.20
19	f	803	CLA	C1-C2-C3	-2.03	122.52	126.04
19	1	311	CLA	O2D-CGD-CBD	2.03	114.88	111.27
19	a	822	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	2	302	XAT	C27-C28-C29	-2.03	122.38	125.53
19	b	807	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	b	843	BCR	C33-C5-C6	-2.03	122.25	124.53
19	b	835	CLA	C1-C2-C3	-2.03	122.53	126.04
17	4	303	XAT	O4-C5-C18	2.03	117.49	115.06
20	5	316	SQD	O8-S-C6	2.03	108.97	105.74
26	b	848	BCR	C33-C5-C4	2.03	117.51	113.62
19	b	815	CLA	C1-C2-C3	-2.03	122.53	126.04
19	a	801	CLA	O1D-CGD-CBD	2.03	128.63	124.48
17	1	303	XAT	O24-C25-C38	2.03	117.49	115.06
26	a	847	BCR	C20-C19-C18	-2.03	120.72	126.42
19	b	817	CLA	O2D-CGD-CBD	2.03	114.87	111.27
26	a	849	BCR	C37-C22-C23	2.03	121.27	118.08
21	4	318	DGD	C4D-C3D-C2D	-2.03	107.28	110.82
17	4	304	XAT	O4-C5-C4	2.03	114.90	113.38
19	b	804	CLA	O2D-CGD-CBD	2.03	114.87	111.27
26	b	846	BCR	C28-C27-C26	-2.03	110.46	114.08
19	5	306	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	4	301	XAT	O4-C5-C18	2.02	117.48	115.06
19	a	817	CLA	CHD-C1D-ND	-2.02	122.59	124.45
17	2	304	XAT	C30-C31-C32	-2.02	116.90	123.22
19	b	840	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
17	2	305	XAT	C10-C11-C12	-2.02	116.90	123.22
19	5	314	CLA	CHD-C1D-ND	-2.02	122.59	124.45
26	f	804	BCR	C21-C20-C19	-2.02	116.91	123.22
19	a	842	CLA	CHD-C1D-ND	-2.02	122.60	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	304	XAT	O24-C25-C38	2.02	117.48	115.06
19	a	823	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	b	846	BCR	C35-C13-C12	2.02	121.26	118.08
19	b	811	CLA	C1-C2-C3	-2.02	122.55	126.04
19	2	310	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
20	1	315	SQD	O7-S-C6	2.02	109.34	106.94
17	2	302	XAT	O24-C25-C38	2.02	117.47	115.06
19	b	810	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	2	314	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	a	848	BCR	C28-C27-C26	-2.02	110.47	114.08
17	5	301	XAT	O4-C5-C18	2.02	117.47	115.06
19	1	307	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	a	838	CLA	C1-C2-C3	-2.02	122.56	126.04
19	a	840	CLA	C1-C2-C3	-2.02	122.56	126.04
26	a	850	BCR	C37-C22-C21	-2.02	120.10	122.92
19	a	814	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
17	2	304	XAT	C40-C33-C32	2.02	121.25	118.08
19	b	829	CLA	CHD-C1D-ND	-2.01	122.60	124.45
19	b	818	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
17	1	303	XAT	O4-C5-C18	2.01	117.47	115.06
19	b	808	CLA	O2D-CGD-CBD	2.01	114.84	111.27
19	4	307	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	4	302	XAT	O24-C25-C38	2.01	117.47	115.06
19	5	311	CLA	C1-C2-C3	-2.01	122.57	126.04
19	a	803	CLA	C2D-C1D-ND	-2.01	108.62	110.10
26	b	845	BCR	C1-C6-C7	2.01	121.46	115.78
19	3	308	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
19	2	313	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	1	302	XAT	C30-C31-C32	-2.01	116.95	123.22
19	3	313	CLA	C1-C2-C3	-2.01	122.57	126.04
23	1	304	A1L1F	C25-C14-C29	-2.00	121.75	125.99
19	3	308	CLA	O2D-CGD-CBD	2.00	114.83	111.27
19	b	825	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	2	304	XAT	O4-C5-C4	2.00	114.89	113.38
19	b	831	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	b	828	CLA	C1-C2-C3	-2.00	122.58	126.04
19	b	815	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
17	4	304	XAT	C39-C29-C28	2.00	121.23	118.08
19	a	835	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	4	307	CLA	CHD-C1D-ND	-2.00	122.62	124.45
19	a	821	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

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 (1616) 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	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
19	a	839	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
19	b	829	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
22	j	105	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
19	2	313	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	4	310	CLA	O1A-CGA-O2A-C1
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	2	310	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	l	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
19	b	811	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	817	CLA	C2A-CAA-CBA-CGA
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	807	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	C1-C2-C3-O3
19	b	836	CLA	O1D-CGD-O2D-CED
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	821	CLA	CBA-CGA-O2A-C1
19	b	827	CLA	CBA-CGA-O2A-C1
19	b	834	CLA	CBA-CGA-O2A-C1
19	4	315	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	a	814	CLA	O1D-CGD-O2D-CED
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
23	1	304	A1L1F	C49-C50-C51-C52
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	b	801	CLA	C15-C16-C17-C18
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	a	834	CLA	C15-C16-C17-C18
19	b	807	CLA	C15-C16-C17-C18
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	809	CLA	C8-C10-C11-C12
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
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	b	837	CLA	C5-C6-C7-C8
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	b	828	CLA	CBA-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	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	4	307	CLA	O1D-CGD-O2D-CED
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	b	841	CLA	C10-C11-C12-C13
19	f	802	CLA	C13-C15-C16-C17
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	2	312	CLA	O1A-CGA-O2A-C1
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
21	b	851	DGD	C4E-C5E-C6E-O5E
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
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	825	CLA	C5-C6-C7-C8
21	4	318	DGD	C3B-C4B-C5B-C6B
19	3	309	CLA	O1D-CGD-O2D-CED
19	a	836	CLA	CBD-CGD-O2D-CED
20	1	315	SQD	C8-C7-O47-C45
19	a	824	CLA	CBA-CGA-O2A-C1
19	b	830	CLA	C10-C11-C12-C13
19	b	840	CLA	C5-C6-C7-C8
18	3	302	A1L1G	C37-C38-C39-C28
18	3	306	A1L1G	C27-C34-C35-C36
21	b	851	DGD	C9B-CAB-CBB-CCB
25	a	845	LHG	C11-C10-C9-C8
19	a	841	CLA	O1D-CGD-O2D-CED
19	b	824	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	C24-C23-O48-C46
25	a	845	LHG	C27-C28-C29-C30
20	1	315	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	a	854	CLA	C5-C6-C7-C8
19	b	828	CLA	O1D-CGD-O2D-CED
19	b	839	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C13-C14-C15-C16
19	a	835	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
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	4	308	CLA	C16-C17-C18-C20
19	4	310	CLA	C4-C3-C5-C6
19	b	840	CLA	C4-C3-C5-C6
19	5	315	CLA	C2C-C3C-CAC-CBC
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
21	4	318	DGD	C2B-C3B-C4B-C5B
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	a	814	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	O1A-CGA-O2A-C1
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	C4A-C5A-C6A-C7A
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	841	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	C8-C10-C11-C12
24	a	843	PQN	C25-C26-C27-C28
25	m	101	LHG	C28-C29-C30-C31
22	2	317	LMG	C28-C29-C30-C31
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	814	CLA	C5-C6-C7-C8
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
23	1	304	A1L1F	C47-C48-C49-C50
19	b	809	CLA	C10-C11-C12-C13
25	m	101	LHG	C14-C15-C16-C17
19	4	308	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	a	807	CLA	O1D-CGD-O2D-CED
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
19	j	102	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	O1-C1-C2-O2
25	a	846	LHG	O1-C1-C2-O2
25	b	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	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
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	b	817	CLA	O1A-CGA-O2A-C1
19	a	811	CLA	C11-C10-C8-C7
20	1	315	SQD	C7-C8-C9-C10
22	2	317	LMG	C10-C11-C12-C13
19	a	806	CLA	C13-C15-C16-C17
21	b	851	DGD	C6A-C7A-C8A-C9A
19	4	307	CLA	C3-C5-C6-C7
21	4	318	DGD	O6D-C1D-O3G-C3G
19	5	311	CLA	O1D-CGD-O2D-CED
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	4	308	CLA	C13-C15-C16-C17
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	308	CLA	C11-C10-C8-C9
19	1	310	CLA	C11-C10-C8-C9
19	a	801	CLA	C11-C12-C13-C14
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	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	b	810	CLA	C10-C11-C12-C13
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	b	801	CLA	C16-C17-C18-C19
25	m	101	LHG	C29-C30-C31-C32
19	b	807	CLA	O1D-CGD-O2D-CED
19	5	305	CLA	O1A-CGA-O2A-C1
19	1	305	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	m	101	LHG	C3-O3-P-O6
19	b	823	CLA	O1D-CGD-O2D-CED
19	b	836	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	C10-C11-C12-C13
19	a	844	CLA	C10-C11-C12-C13
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	806	CLA	C16-C17-C18-C19
25	m	101	LHG	C12-C13-C14-C15
19	b	814	CLA	C3-C5-C6-C7
19	4	315	CLA	O1D-CGD-O2D-CED
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
19	b	836	CLA	C2C-C3C-CAC-CBC
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
23	1	304	A1L1F	C50-C51-C52-C53
19	a	820	CLA	C8-C10-C11-C12
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	854	CLA	C10-C11-C12-C13
24	a	843	PQN	C23-C25-C26-C27
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	a	844	CLA	C16-C17-C18-C19
19	1	311	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C13-C15-C16-C17
19	b	840	CLA	C13-C15-C16-C17
22	a	853	LMG	C14-C15-C16-C17
19	a	825	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	802	CLA	O1D-CGD-O2D-CED
19	f	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	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	b	839	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	839	CLA	C6-C7-C8-C10
19	f	802	CLA	C11-C12-C13-C15
19	j	102	CLA	C6-C7-C8-C10
19	4	317	CLA	C3-C5-C6-C7
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-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
19	a	826	CLA	O1D-CGD-O2D-CED
17	4	305	XAT	C27-C28-C29-C30
25	b	849	LHG	C9-C10-C11-C12
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
19	b	807	CLA	C10-C11-C12-C13
25	b	849	LHG	O6-C4-C5-C6
19	b	834	CLA	C3-C5-C6-C7
19	a	836	CLA	O1D-CGD-O2D-CED
19	a	844	CLA	C15-C16-C17-C18
19	j	102	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	802	CLA	C4-C3-C5-C6
19	a	801	CLA	C2-C3-C5-C6
19	a	807	CLA	C2-C3-C5-C6
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	a	809	CLA	C2A-CAA-CBA-CGA
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	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
19	b	801	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
21	b	851	DGD	C7A-C8A-C9A-CAA
19	b	836	CLA	C3-C5-C6-C7
19	a	840	CLA	C4-C3-C5-C6
19	b	819	CLA	C11-C12-C13-C15
19	a	806	CLA	CBD-CGD-O2D-CED
19	3	314	CLA	O1D-CGD-O2D-CED
19	a	827	CLA	C3-C5-C6-C7
19	4	317	CLA	C5-C6-C7-C8
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	a	803	CLA	C15-C16-C17-C18
19	4	307	CLA	O1A-CGA-O2A-C1
19	b	803	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	806	CLA	C10-C11-C12-C13
19	4	308	CLA	C16-C17-C18-C19
19	a	806	CLA	C16-C17-C18-C20
19	b	823	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	a	844	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
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	b	828	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
20	1	315	SQD	C9-C10-C11-C12
18	3	306	A1L1G	C40-C41-C42-C44
19	1	306	CLA	C16-C17-C18-C20
19	b	805	CLA	C16-C17-C18-C19
19	a	808	CLA	O1D-CGD-O2D-CED
19	a	842	CLA	C8-C10-C11-C12
19	a	827	CLA	C5-C6-C7-C8
18	1	301	A1L1G	C37-C38-C39-C28
22	2	317	LMG	C31-C32-C33-C34
19	a	841	CLA	O1A-CGA-O2A-C1
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	a	824	CLA	CAD-CBD-CGD-O2D
19	a	832	CLA	CAD-CBD-CGD-O2D
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	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	823	CLA	CHA-CBD-CGD-O2D
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	815	CLA	CHA-CBD-CGD-O1D
19	b	830	CLA	CHA-CBD-CGD-O1D
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	j	102	CLA	O1D-CGD-O2D-CED
19	1	306	CLA	O1A-CGA-O2A-C1
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	829	CLA	O1A-CGA-O2A-C1
19	b	818	CLA	C10-C11-C12-C13
19	1	310	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	C2-C3-C5-C6
22	a	853	LMG	C31-C32-C33-C34
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
19	1	308	CLA	CBD-CGD-O2D-CED
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	2	314	CLA	C4-C3-C5-C6
19	b	835	CLA	C2-C3-C5-C6
19	1	307	CLA	C5-C6-C7-C8
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	2	310	CLA	C16-C17-C18-C20
19	b	808	CLA	C16-C17-C18-C20
19	a	830	CLA	C8-C10-C11-C12
20	1	315	SQD	C13-C14-C15-C16
19	b	841	CLA	C15-C16-C17-C18
19	3	311	CLA	C2A-CAA-CBA-CGA
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	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	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	a	834	CLA	C5-C6-C7-C8
19	b	819	CLA	C8-C10-C11-C12
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	i	102	CLA	O1A-CGA-O2A-C1
19	1	311	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	C10-C11-C12-C13
19	3	315	CLA	O1A-CGA-O2A-C1
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	a	842	CLA	C14-C13-C15-C16
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	b	840	CLA	C2C-C3C-CAC-CBC
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	805	CLA	CBA-CGA-O2A-C1
19	b	828	CLA	C10-C11-C12-C13
19	1	311	CLA	O1D-CGD-O2D-CED
25	m	101	LHG	C13-C14-C15-C16
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	a	801	CLA	CAA-CBA-CGA-O2A
20	1	315	SQD	C46-C45-O47-C7
19	a	854	CLA	CBD-CGD-O2D-CED
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	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	b	833	CLA	C2C-C3C-CAC-CBC
25	b	849	LHG	C25-C26-C27-C28
19	1	311	CLA	O1A-CGA-O2A-C1
19	b	805	CLA	O1A-CGA-O2A-C1
19	1	308	CLA	O1D-CGD-O2D-CED
26	b	848	BCR	C1-C6-C7-C8
26	f	804	BCR	C23-C24-C25-C30
19	b	839	CLA	C2-C3-C5-C6
19	b	818	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	C16-C17-C18-C19
19	b	808	CLA	C16-C17-C18-C19
19	b	823	CLA	C3-C5-C6-C7
19	b	818	CLA	O1A-CGA-O2A-C1
19	a	839	CLA	C15-C16-C17-C18
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	a	854	CLA	C15-C16-C17-C18
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	b	826	CLA	C11-C10-C8-C7
19	a	801	CLA	C14-C13-C15-C16
19	a	812	CLA	C6-C7-C8-C9
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	b	803	CLA	C16-C17-C18-C20
19	5	307	CLA	C8-C10-C11-C12
19	a	830	CLA	C15-C16-C17-C18
19	b	801	CLA	O1A-CGA-O2A-C1
19	b	801	CLA	CBA-CGA-O2A-C1
19	5	315	CLA	CAA-CBA-CGA-O2A
18	3	306	A1L1G	C32-C33-C34-C35
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	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	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	812	CLA	C3-C5-C6-C7
19	a	854	CLA	O1D-CGD-O2D-CED
19	a	820	CLA	C13-C15-C16-C17
19	b	840	CLA	C16-C17-C18-C20
19	b	814	CLA	C10-C11-C12-C13
25	a	845	LHG	C25-C26-C27-C28
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	3	312	CLA	CBA-CGA-O2A-C1
19	2	310	CLA	C3A-C2A-CAA-CBA
19	b	814	CLA	C3A-C2A-CAA-CBA
19	b	832	CLA	C3A-C2A-CAA-CBA
19	a	832	CLA	O1D-CGD-O2D-CED
19	a	839	CLA	C16-C17-C18-C20
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	b	841	CLA	CBA-CGA-O2A-C1
26	b	845	BCR	C11-C10-C9-C34
26	b	845	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	f	804	BCR	C35-C13-C14-C15
26	l	201	BCR	C11-C10-C9-C34
19	5	306	CLA	CAA-CBA-CGA-O1A
19	3	315	CLA	CAA-CBA-CGA-O1A
19	1	308	CLA	C16-C17-C18-C20
19	a	801	CLA	CBA-CGA-O2A-C1
25	a	845	LHG	C14-C15-C16-C17
19	3	312	CLA	O1A-CGA-O2A-C1
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
25	m	101	LHG	C15-C16-C17-C18
19	b	818	CLA	CBD-CGD-O2D-CED
19	a	807	CLA	C11-C10-C8-C7
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
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
22	a	853	LMG	C11-C12-C13-C14
19	4	310	CLA	O1D-CGD-O2D-CED
19	5	307	CLA	C2A-CAA-CBA-CGA
19	4	306	CLA	C2A-CAA-CBA-CGA
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	1	307	CLA	C6-C7-C8-C9
19	4	310	CLA	C13-C15-C16-C17
19	a	841	CLA	C2-C3-C5-C6
19	1	305	CLA	C3-C5-C6-C7
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	1	301	A1L1G	C40-C41-C42-C44
22	2	317	LMG	C11-C10-O7-C8
19	5	313	CLA	CAA-CBA-CGA-O1A
19	5	310	CLA	CBA-CGA-O2A-C1
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
20	1	315	SQD	C15-C16-C17-C18
19	5	311	CLA	C4-C3-C5-C6
19	a	839	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	O1A-CGA-O2A-C1
26	b	850	BCR	C23-C24-C25-C30
26	j	104	BCR	C1-C6-C7-C8
26	m	102	BCR	C23-C24-C25-C30
19	b	836	CLA	C4C-C3C-CAC-CBC
19	b	818	CLA	O1D-CGD-O2D-CED
19	a	819	CLA	CAA-CBA-CGA-O2A
25	m	101	LHG	O1-C1-C2-C3
19	a	804	CLA	O1A-CGA-O2A-C1
19	a	813	CLA	C6-C7-C8-C9
17	2	304	XAT	C7-C8-C9-C10
17	a	852	XAT	C31-C32-C33-C34
19	b	802	CLA	C10-C11-C12-C13
19	5	313	CLA	CAA-CBA-CGA-O2A
19	2	314	CLA	O1A-CGA-O2A-C1
19	a	830	CLA	O1A-CGA-O2A-C1
19	5	307	CLA	C11-C12-C13-C14
19	b	814	CLA	C16-C17-C18-C19
19	1	314	CLA	CAA-CBA-CGA-O2A
19	a	826	CLA	C13-C15-C16-C17
19	a	830	CLA	CBA-CGA-O2A-C1
19	a	842	CLA	CBA-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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	j	105	LMG	C11-C12-C13-C14
19	a	804	CLA	CBA-CGA-O2A-C1
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	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	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	803	CLA	C10-C11-C12-C13
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
24	a	843	PQN	C18-C20-C21-C22
20	1	315	SQD	O47-C7-C8-C9
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	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
19	b	801	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	2	314	CLA	CBA-CGA-O2A-C1
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	4	312	CLA	O1A-CGA-O2A-C1
19	b	803	CLA	CAA-CBA-CGA-O2A
19	1	306	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	CAA-CBA-CGA-O2A
19	1	310	CLA	C12-C13-C15-C16
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	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	b	825	CLA	C10-C11-C12-C13
19	1	312	CLA	CAA-CBA-CGA-O2A
25	a	845	LHG	O8-C23-C24-C25
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
19	4	309	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	CAA-CBA-CGA-O2A
19	j	102	CLA	C10-C11-C12-C13
19	a	818	CLA	CAA-CBA-CGA-O1A
19	b	801	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	b	820	CLA	C6-C7-C8-C9
19	b	818	CLA	CAA-CBA-CGA-O1A
19	4	306	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	b	803	CLA	C5-C6-C7-C8
25	m	101	LHG	C30-C31-C32-C33
25	m	101	LHG	C27-C28-C29-C30
19	a	826	CLA	C10-C11-C12-C13
19	b	833	CLA	CAA-CBA-CGA-O1A
25	a	846	LHG	C3-O3-P-O5
19	a	814	CLA	C16-C17-C18-C19
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	a	836	CLA	CAA-CBA-CGA-O1A
19	b	807	CLA	CAA-CBA-CGA-O1A
19	b	809	CLA	CAA-CBA-CGA-O1A
19	a	813	CLA	CBD-CGD-O2D-CED
19	b	804	CLA	CAA-CBA-CGA-O2A
19	b	810	CLA	C16-C17-C18-C20
19	1	312	CLA	CAA-CBA-CGA-O1A
19	4	310	CLA	CAD-CBD-CGD-O1D
19	4	316	CLA	CAD-CBD-CGD-O1D
19	3	307	CLA	CAD-CBD-CGD-O1D
19	2	309	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	b	814	CLA	CBD-CGD-O2D-CED
19	a	834	CLA	C10-C11-C12-C13
19	b	805	CLA	C11-C12-C13-C14
19	b	806	CLA	C11-C10-C8-C9
19	j	102	CLA	C11-C10-C8-C9
20	5	316	SQD	C10-C11-C12-C13
19	j	102	CLA	C3-C5-C6-C7
19	a	810	CLA	C16-C17-C18-C20
19	a	813	CLA	CAA-CBA-CGA-O2A
19	4	310	CLA	C8-C10-C11-C12
19	a	801	CLA	C5-C6-C7-C8
19	a	810	CLA	CAA-CBA-CGA-O1A
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	a	835	CLA	CAA-CBA-CGA-O2A
19	5	309	CLA	C15-C16-C17-C18
19	3	313	CLA	C4-C3-C5-C6
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	a	834	CLA	C11-C12-C13-C15
19	b	805	CLA	C11-C12-C13-C15
19	b	819	CLA	C11-C10-C8-C7
19	1	203	CLA	C6-C7-C8-C10
19	3	312	CLA	CAA-CBA-CGA-O1A
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	a	854	CLA	CAA-CBA-CGA-O2A
26	b	847	BCR	C7-C8-C9-C10
20	1	315	SQD	C12-C13-C14-C15
19	2	307	CLA	CAA-CBA-CGA-O2A
19	a	835	CLA	CAA-CBA-CGA-O1A
19	5	309	CLA	CAA-CBA-CGA-O1A
25	a	845	LHG	O10-C23-C24-C25
19	b	839	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	a	820	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

177 monomers are involved in 539 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	305	XAT	4	0
19	b	801	CLA	5	0
19	l	203	CLA	2	0
26	a	848	BCR	7	0
19	a	801	CLA	6	0
19	a	827	CLA	4	0
19	a	819	CLA	6	0
19	3	309	CLA	1	0
19	a	818	CLA	10	0
17	3	301	XAT	4	0
27	c	102	SF4	2	0
26	a	850	BCR	4	0
19	b	836	CLA	4	0
19	a	826	CLA	8	0
19	a	840	CLA	6	0
19	b	805	CLA	4	0
19	b	813	CLA	4	0
19	b	811	CLA	7	0
19	a	810	CLA	4	0
19	a	824	CLA	1	0
26	l	205	BCR	9	0
26	l	201	BCR	4	0
17	3	305	XAT	4	0
19	a	829	CLA	8	0
19	b	838	CLA	4	0
25	a	846	LHG	3	0
19	b	839	CLA	7	0
26	b	848	BCR	2	0
17	5	301	XAT	4	0
26	b	852	BCR	4	0
19	b	829	CLA	2	0
21	b	851	DGD	6	0
19	b	827	CLA	3	0
19	b	809	CLA	4	0
19	a	807	CLA	4	0
19	4	314	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	813	CLA	1	0
19	b	826	CLA	3	0
19	4	316	CLA	1	0
19	a	837	CLA	1	0
19	b	803	CLA	3	0
19	b	821	CLA	2	0
26	f	804	BCR	5	0
19	4	306	CLA	1	0
17	5	302	XAT	8	0
19	b	837	CLA	5	0
19	a	815	CLA	1	0
19	a	835	CLA	5	0
17	2	303	XAT	12	0
19	2	316	CLA	2	0
17	4	304	XAT	3	0
17	j	101	XAT	5	0
19	4	310	CLA	6	0
19	a	802	CLA	5	0
17	2	301	XAT	2	0
26	i	101	BCR	3	0
18	5	303	A1L1G	1	0
19	5	310	CLA	2	0
19	b	817	CLA	4	0
19	5	314	CLA	2	0
19	a	803	CLA	4	0
19	f	802	CLA	2	0
19	a	822	CLA	5	0
19	4	307	CLA	2	0
19	a	823	CLA	4	0
19	a	839	CLA	5	0
19	4	308	CLA	5	0
19	a	830	CLA	7	0
26	a	847	BCR	3	0
23	1	304	A1L1F	2	0
19	4	312	CLA	2	0
19	a	844	CLA	5	0
19	a	816	CLA	2	0
19	2	310	CLA	3	0
19	4	309	CLA	3	0
19	1	312	CLA	2	0
17	3	304	XAT	6	0
24	b	842	PQN	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	303	XAT	3	0
19	b	818	CLA	7	0
17	2	302	XAT	2	0
19	3	310	CLA	1	0
26	b	844	BCR	1	0
24	a	843	PQN	4	0
19	5	307	CLA	7	0
19	a	831	CLA	5	0
21	4	318	DGD	11	0
19	4	317	CLA	7	0
19	a	806	CLA	9	0
26	b	843	BCR	4	0
26	m	102	BCR	2	0
19	b	841	CLA	4	0
19	l	202	CLA	1	0
26	f	801	BCR	8	0
19	2	308	CLA	5	0
19	i	102	CLA	3	0
19	4	315	CLA	1	0
19	3	308	CLA	2	0
19	a	825	CLA	5	0
19	a	833	CLA	2	0
19	a	842	CLA	4	0
26	j	104	BCR	9	0
19	3	312	CLA	1	0
19	4	313	CLA	4	0
19	b	825	CLA	7	0
19	5	305	CLA	3	0
19	b	814	CLA	6	0
19	5	315	CLA	2	0
19	5	311	CLA	1	0
19	a	841	CLA	7	0
19	a	838	CLA	1	0
26	b	846	BCR	3	0
19	a	820	CLA	8	0
19	b	802	CLA	3	0
19	b	815	CLA	3	0
19	5	309	CLA	6	0
17	5	304	XAT	5	0
19	b	807	CLA	7	0
17	2	305	XAT	3	0
22	a	853	LMG	11	0

Continued on next page...

Continued from previous page...

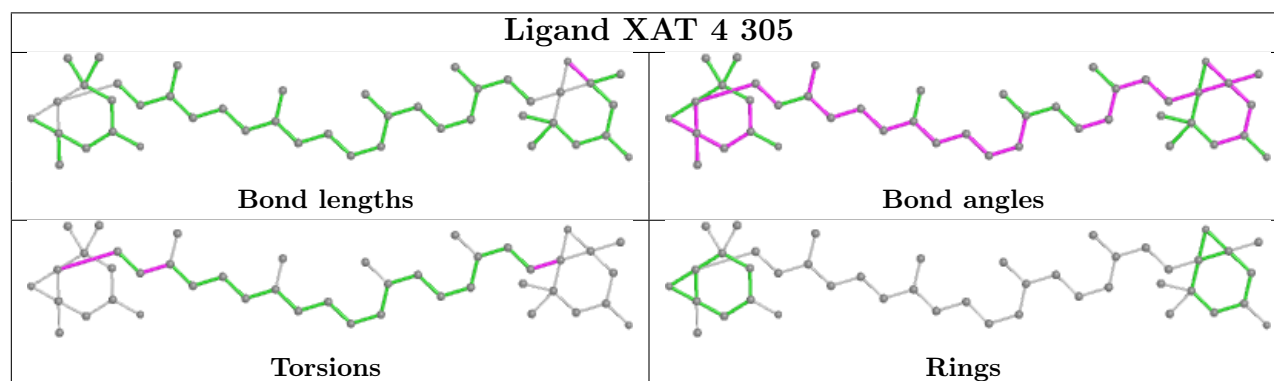
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	831	CLA	5	0
19	a	814	CLA	3	0
19	j	102	CLA	8	0
22	j	105	LMG	6	0
26	a	849	BCR	2	0
19	a	805	CLA	1	0
19	b	822	CLA	2	0
19	3	313	CLA	3	0
19	b	833	CLA	3	0
19	b	804	CLA	4	0
19	1	310	CLA	2	0
19	5	308	CLA	2	0
19	a	804	CLA	4	0
19	a	834	CLA	6	0
19	j	103	CLA	2	0
22	2	317	LMG	3	0
19	5	312	CLA	3	0
19	4	311	CLA	1	0
20	5	316	SQD	1	0
19	2	307	CLA	1	0
19	b	820	CLA	1	0
19	a	809	CLA	3	0
19	b	812	CLA	2	0
18	1	301	A1L1G	1	0
17	3	303	XAT	2	0
19	b	832	CLA	2	0
17	4	302	XAT	5	0
19	b	828	CLA	4	0
19	1	308	CLA	3	0
19	2	309	CLA	1	0
17	2	304	XAT	1	0
19	b	823	CLA	4	0
19	b	830	CLA	4	0
26	b	847	BCR	7	0
17	a	852	XAT	5	0
19	a	808	CLA	1	0
26	b	845	BCR	5	0
20	1	315	SQD	2	0
25	m	101	LHG	4	0
26	b	850	BCR	4	0
19	2	314	CLA	1	0
25	a	845	LHG	3	0

Continued on next page...

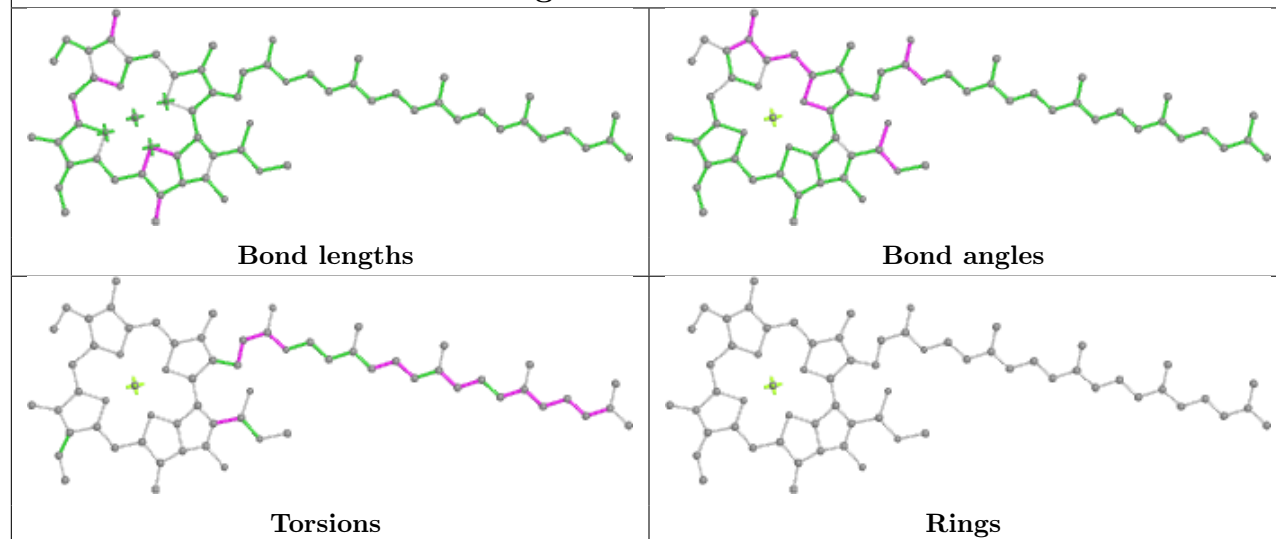
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	832	CLA	2	0
19	b	840	CLA	4	0
19	b	834	CLA	5	0
19	a	828	CLA	5	0
19	3	311	CLA	1	0
17	4	301	XAT	6	0
19	b	819	CLA	3	0
19	1	311	CLA	2	0
19	b	824	CLA	6	0
19	b	806	CLA	2	0
19	1	306	CLA	5	0
17	4	303	XAT	10	0
19	a	854	CLA	2	0
17	1	302	XAT	4	0
19	b	808	CLA	2	0

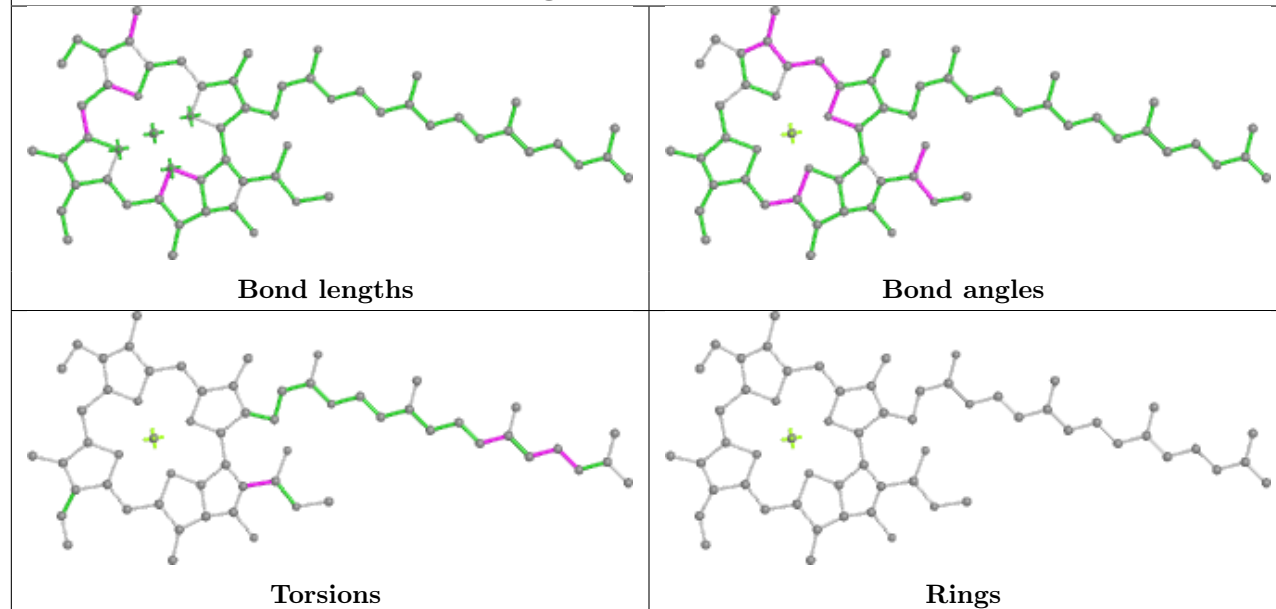
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



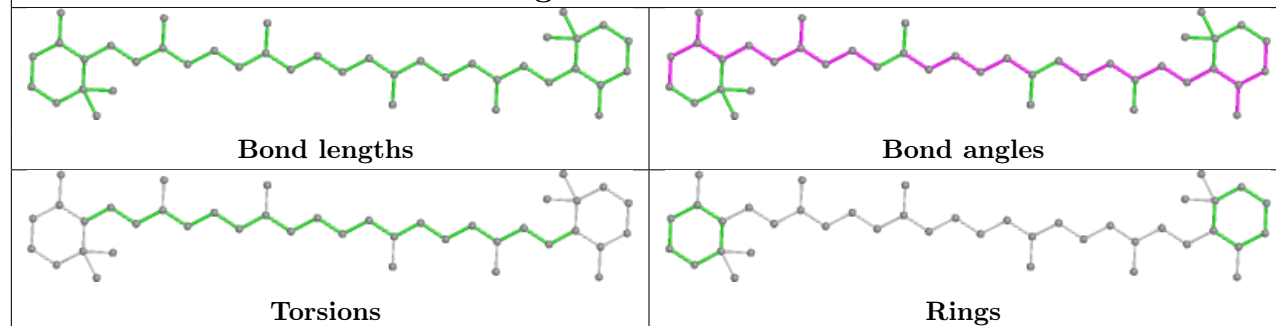
Ligand CLA b 801



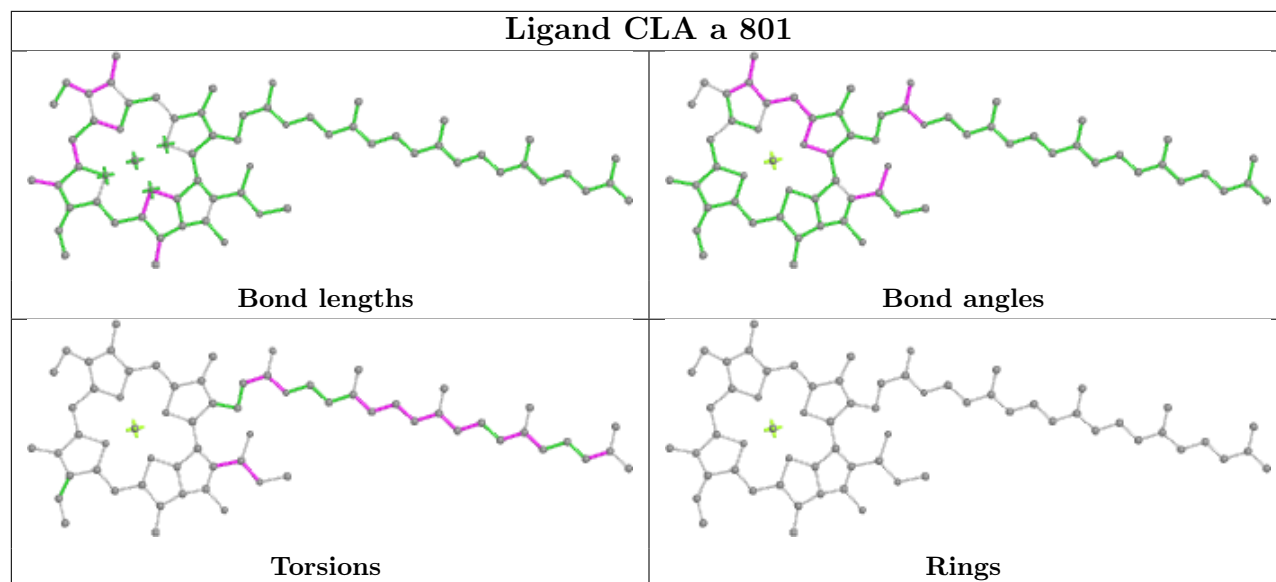
Ligand CLA l 203



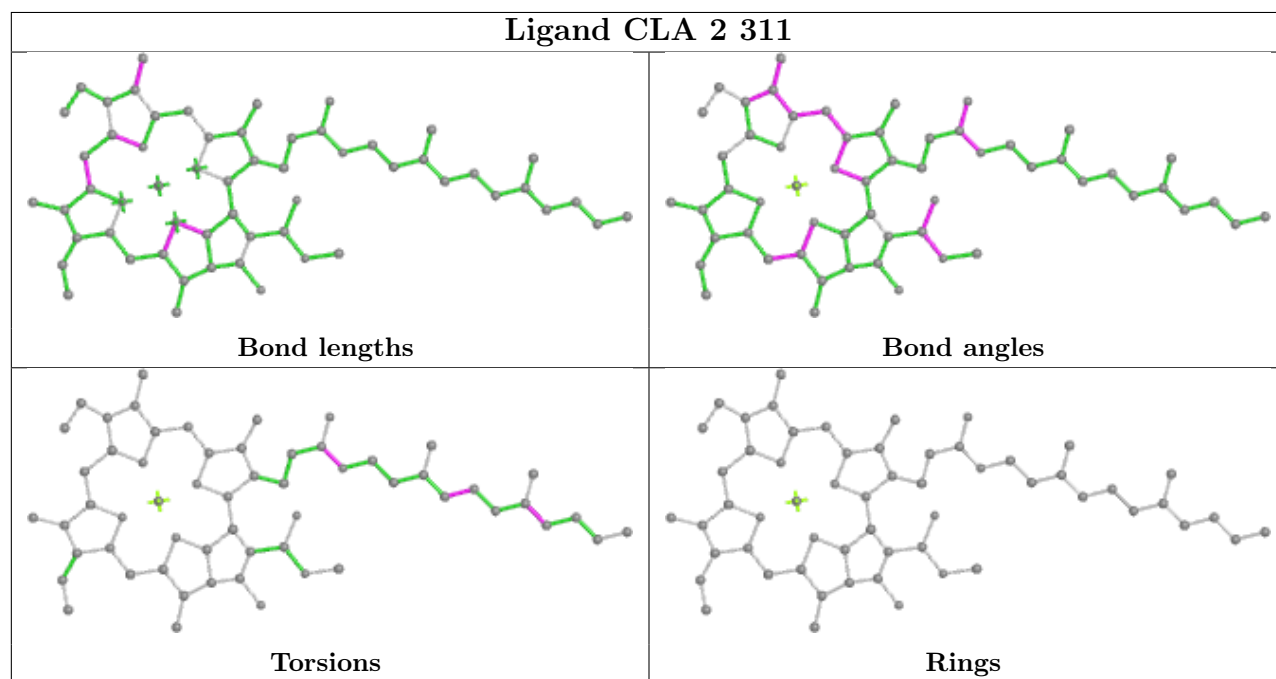
Ligand BCR a 848



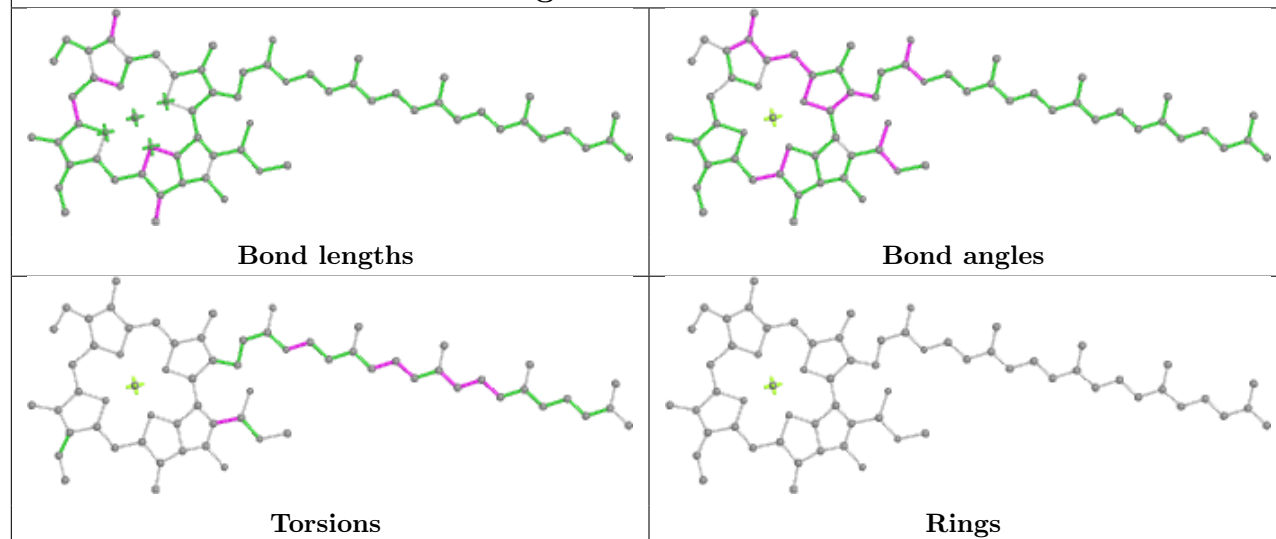
Ligand CLA a 801



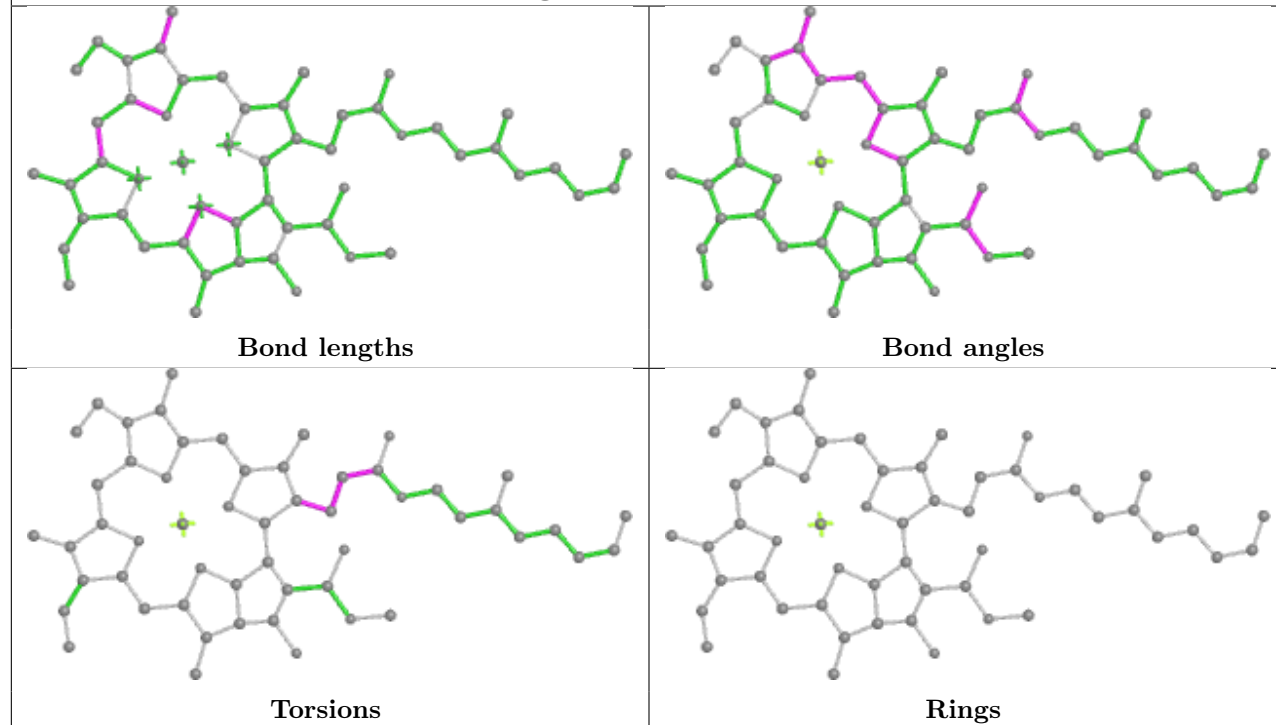
Ligand CLA 2 311



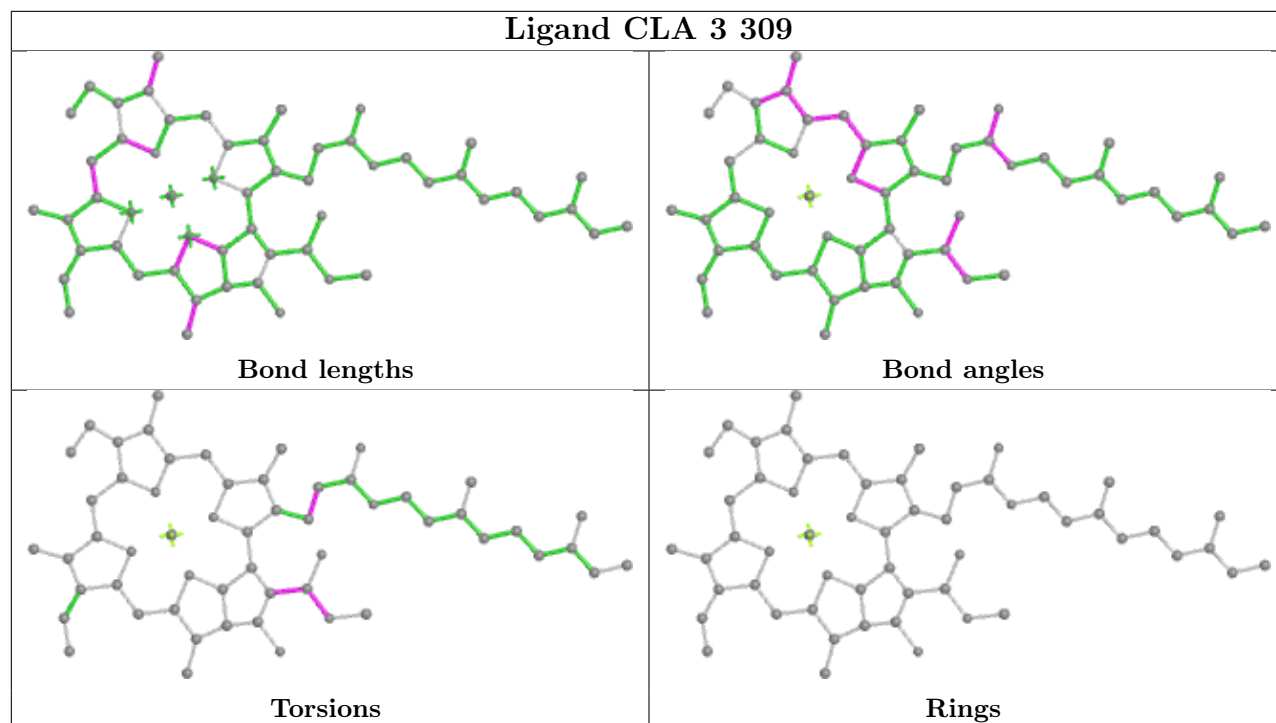
Ligand CLA a 827



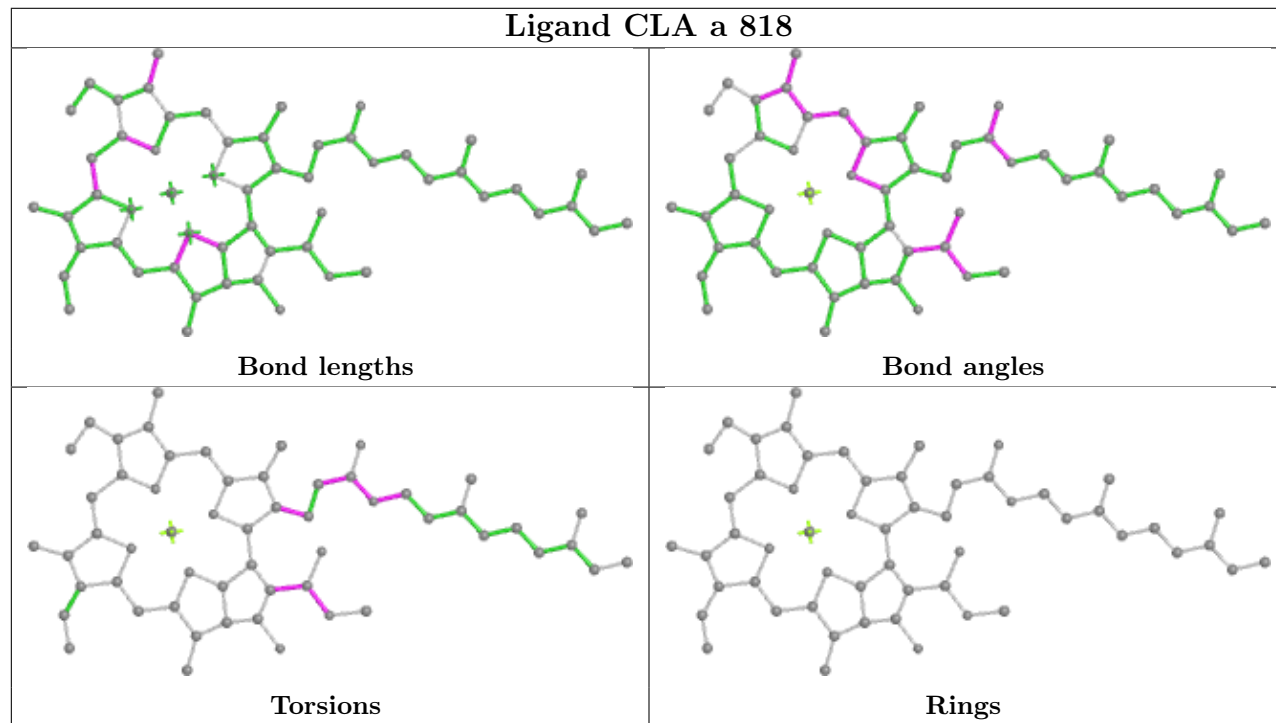
Ligand CLA a 819

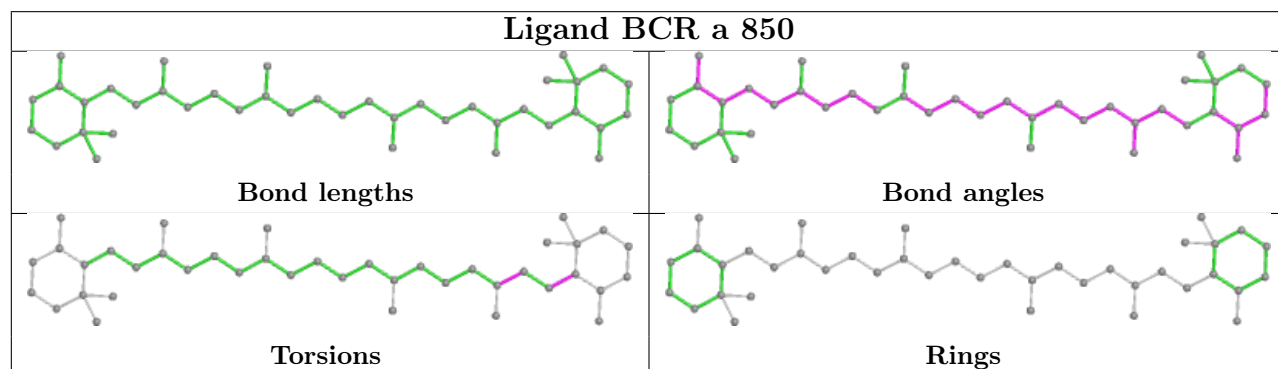
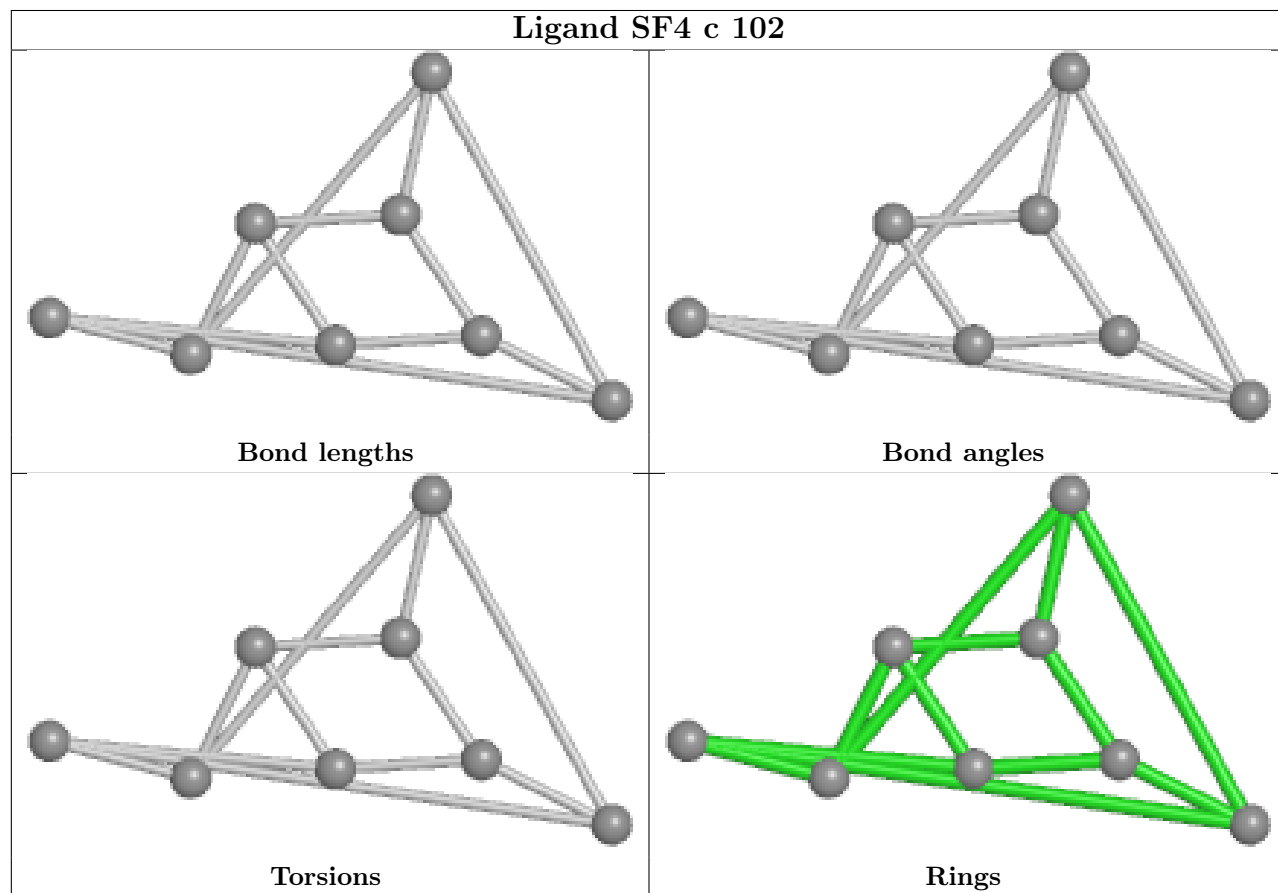
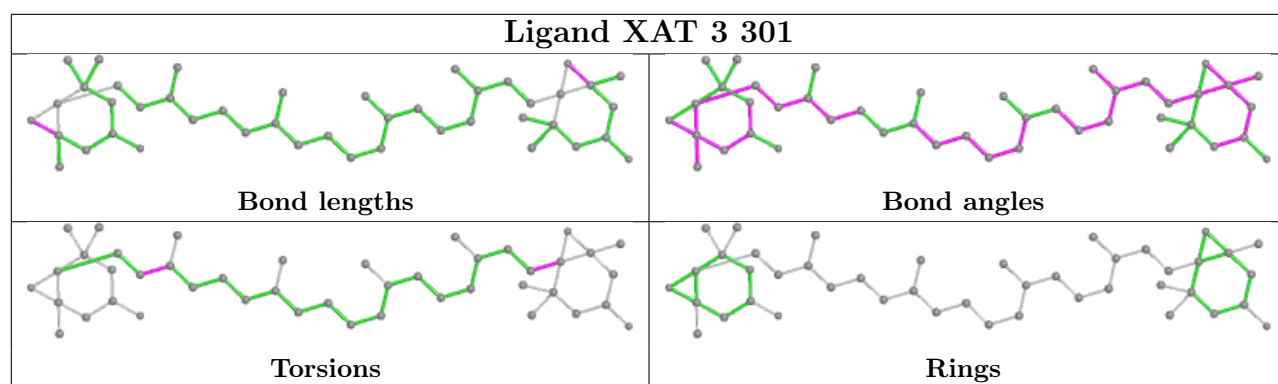


Ligand CLA 3 309

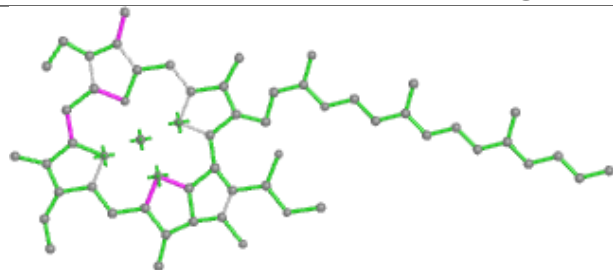


Ligand CLA a 818

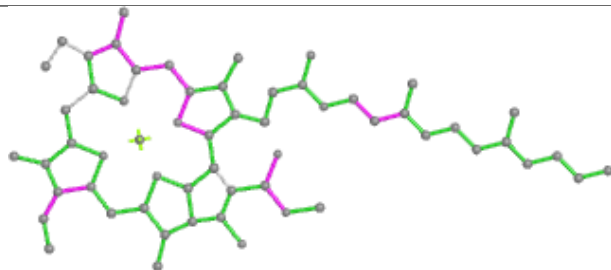




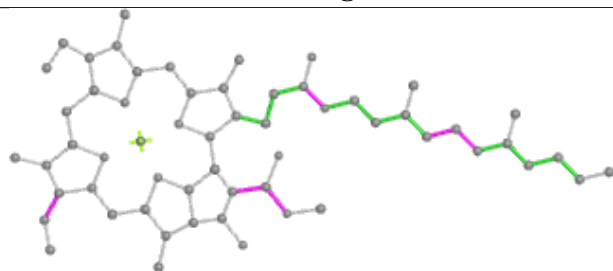
Ligand CLA b 836



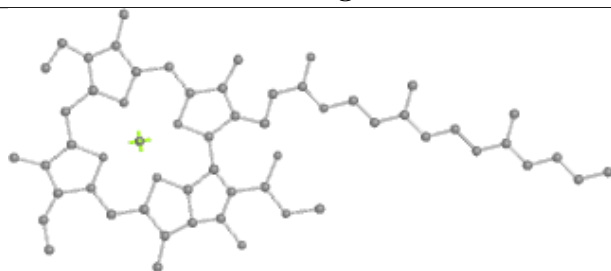
Bond lengths



Bond angles

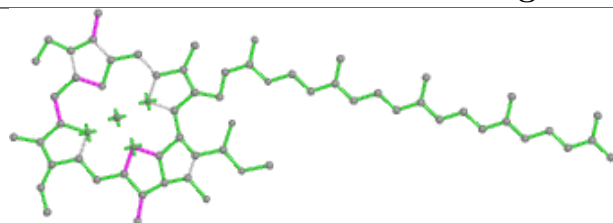


Torsions

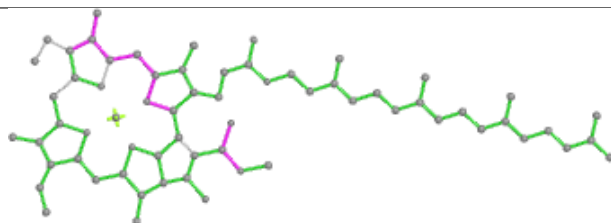


Rings

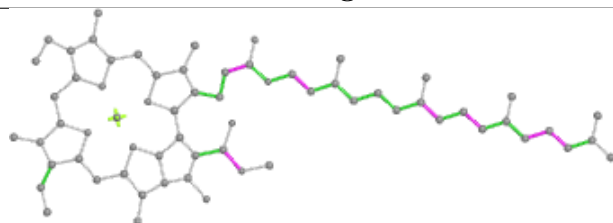
Ligand CLA a 826



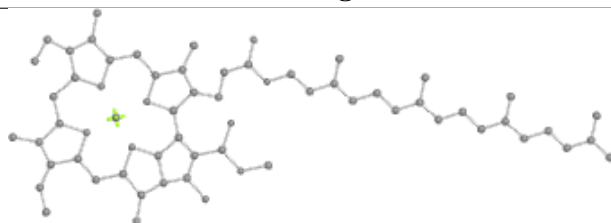
Bond lengths



Bond angles

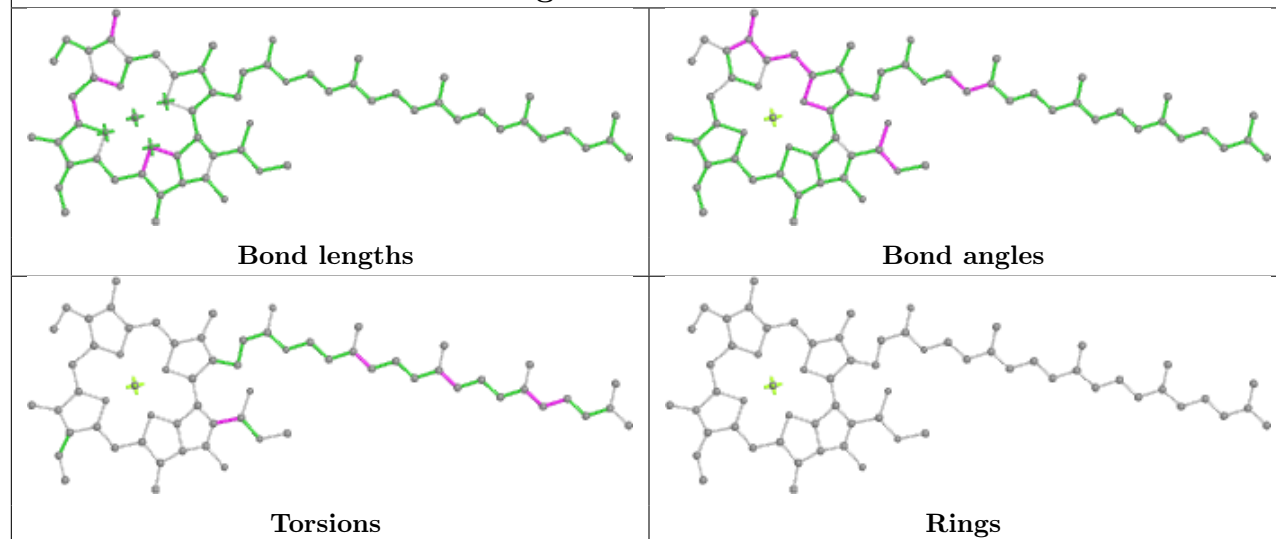


Torsions

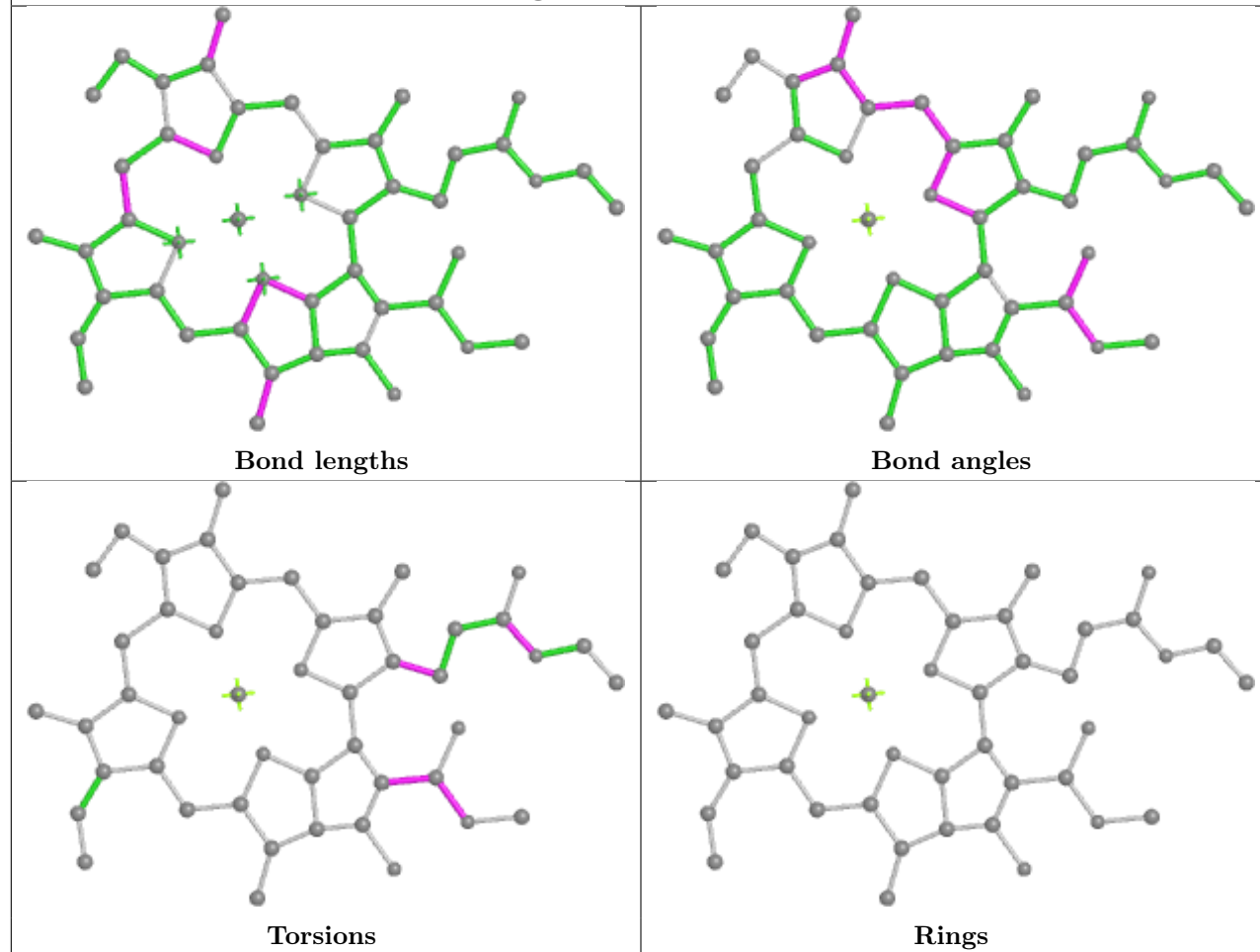


Rings

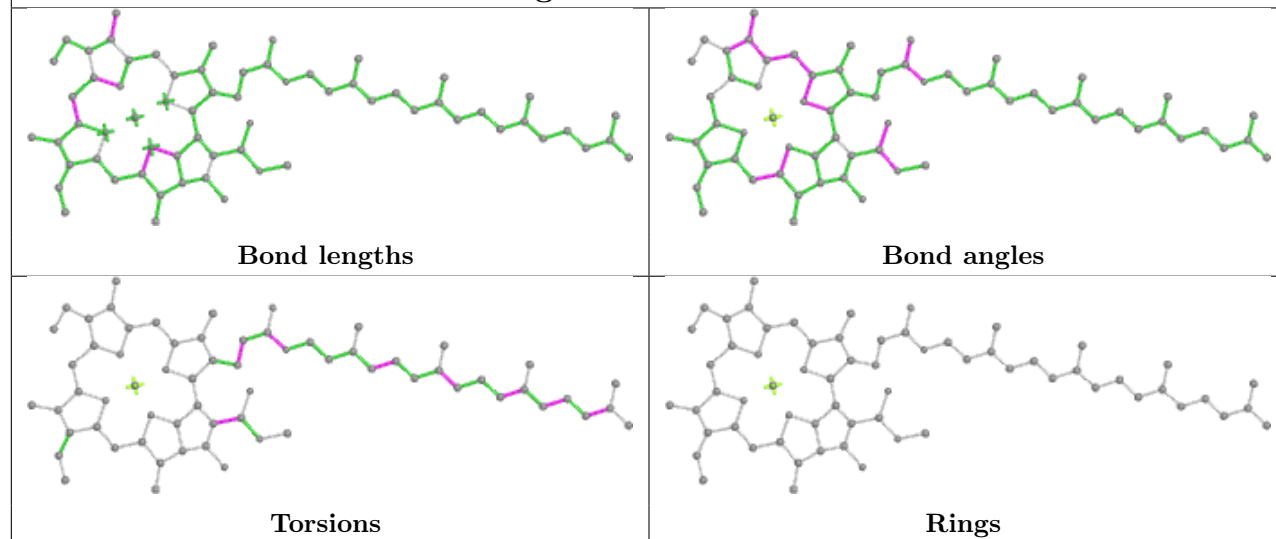
Ligand CLA a 840



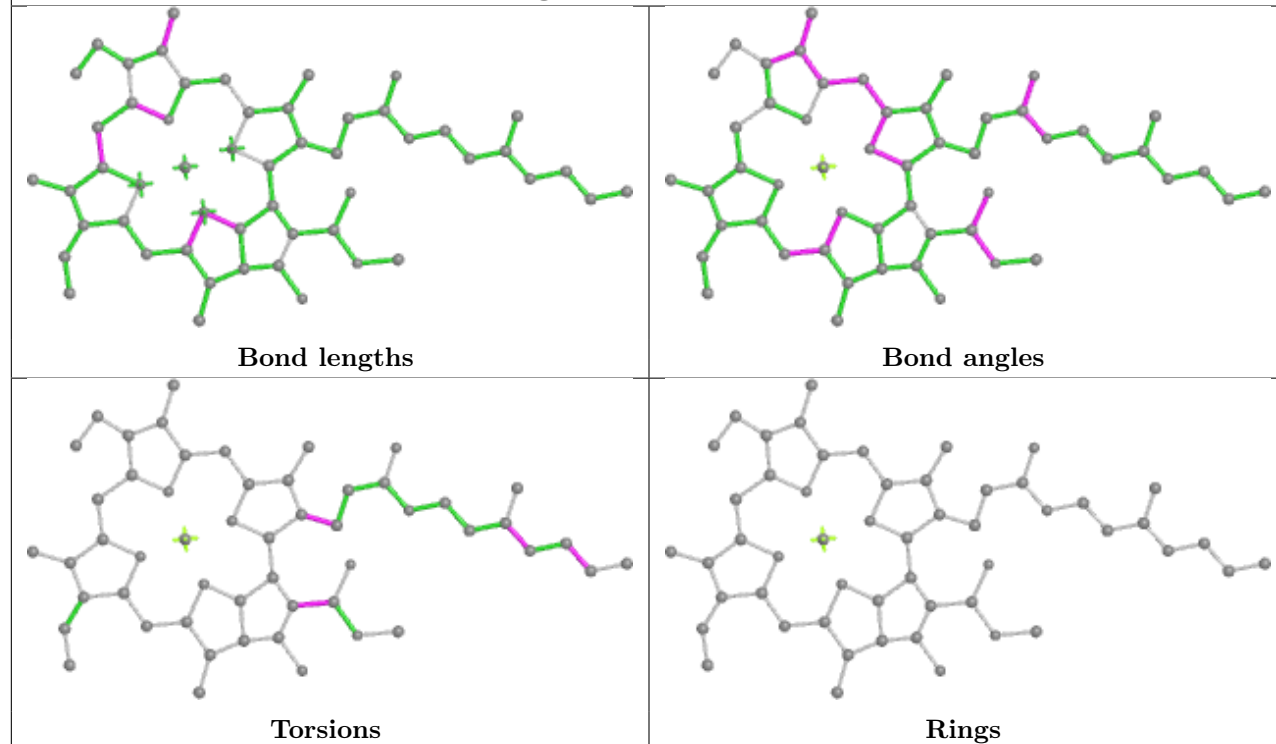
Ligand CLA 3 314

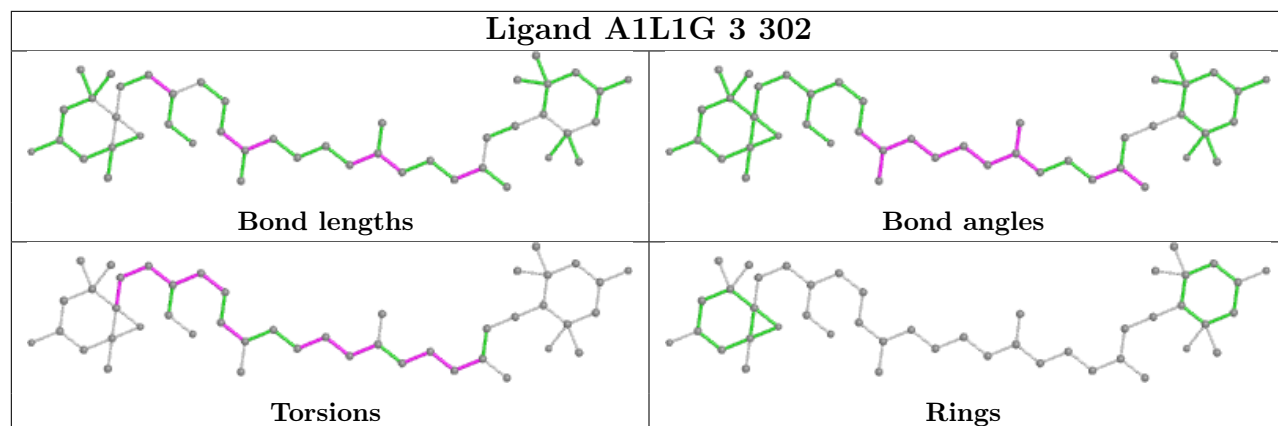
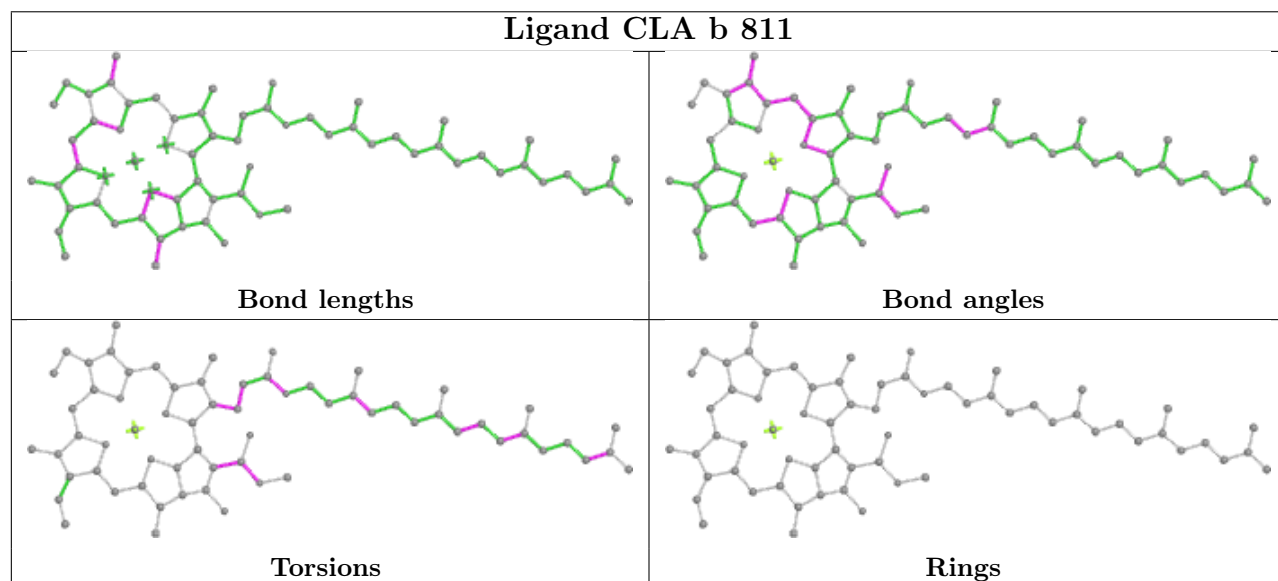
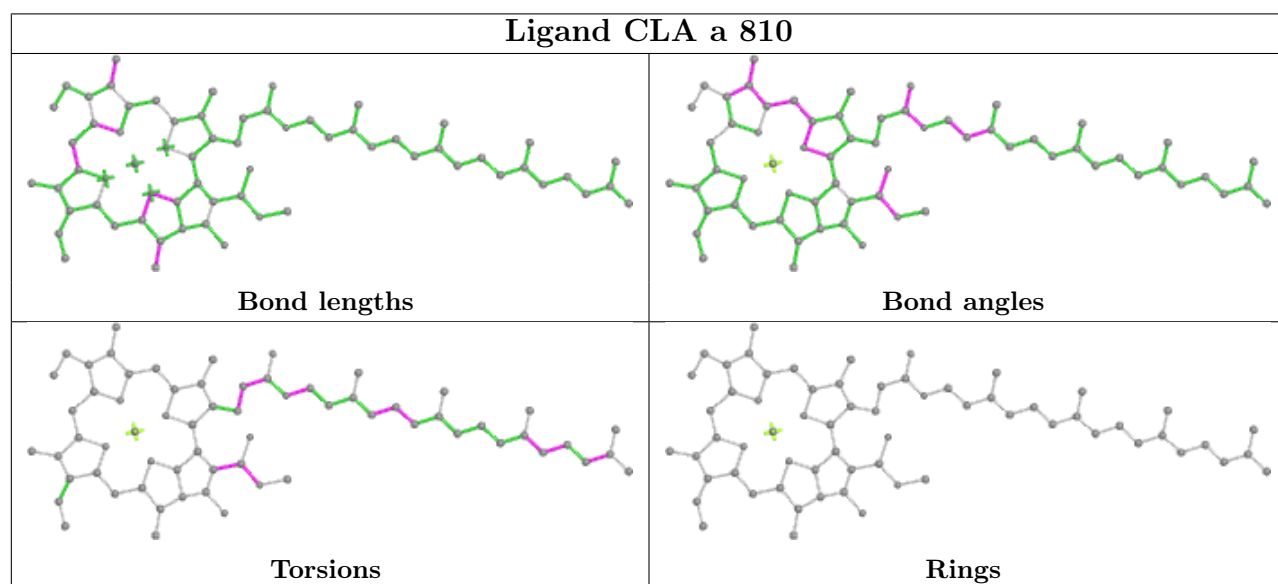


Ligand CLA b 805

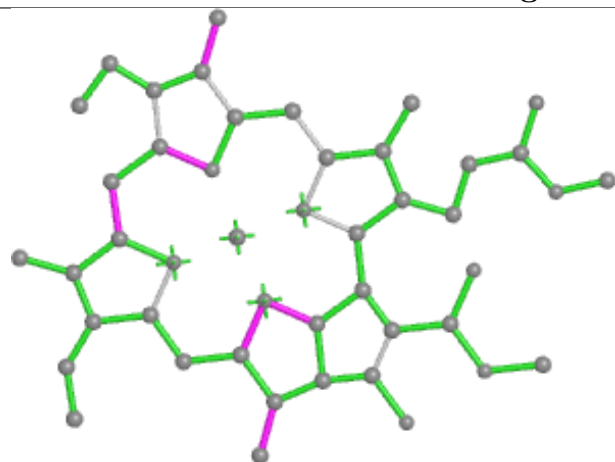


Ligand CLA b 813

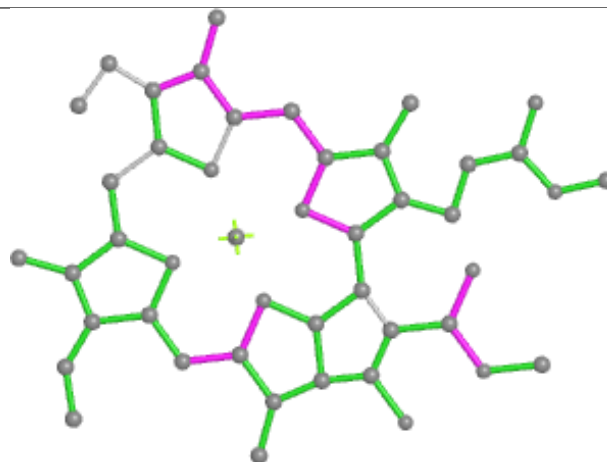


Ligand A1L1G 3 302**Ligand CLA b 811****Ligand CLA a 810**

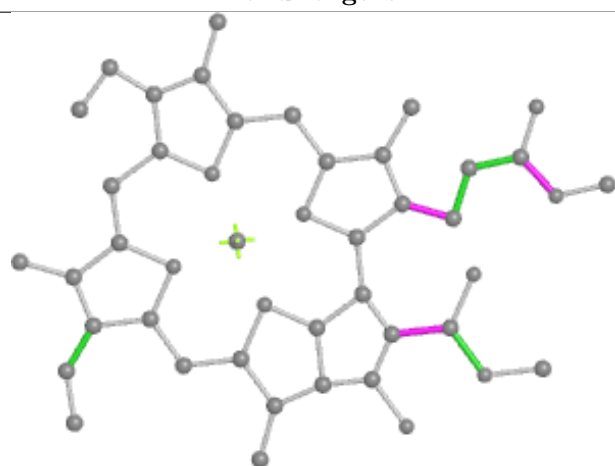
Ligand CLA a 824



Bond lengths



Bond angles

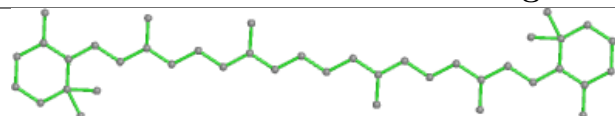


Torsions

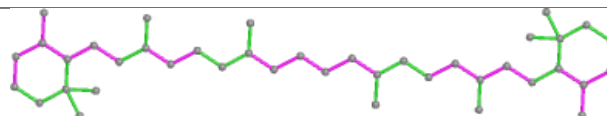


Rings

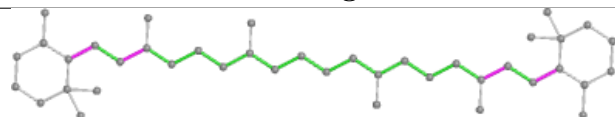
Ligand BCR 1 205



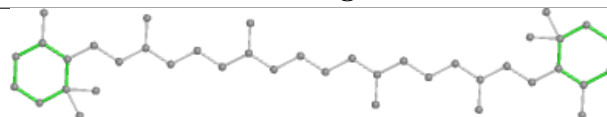
Bond lengths



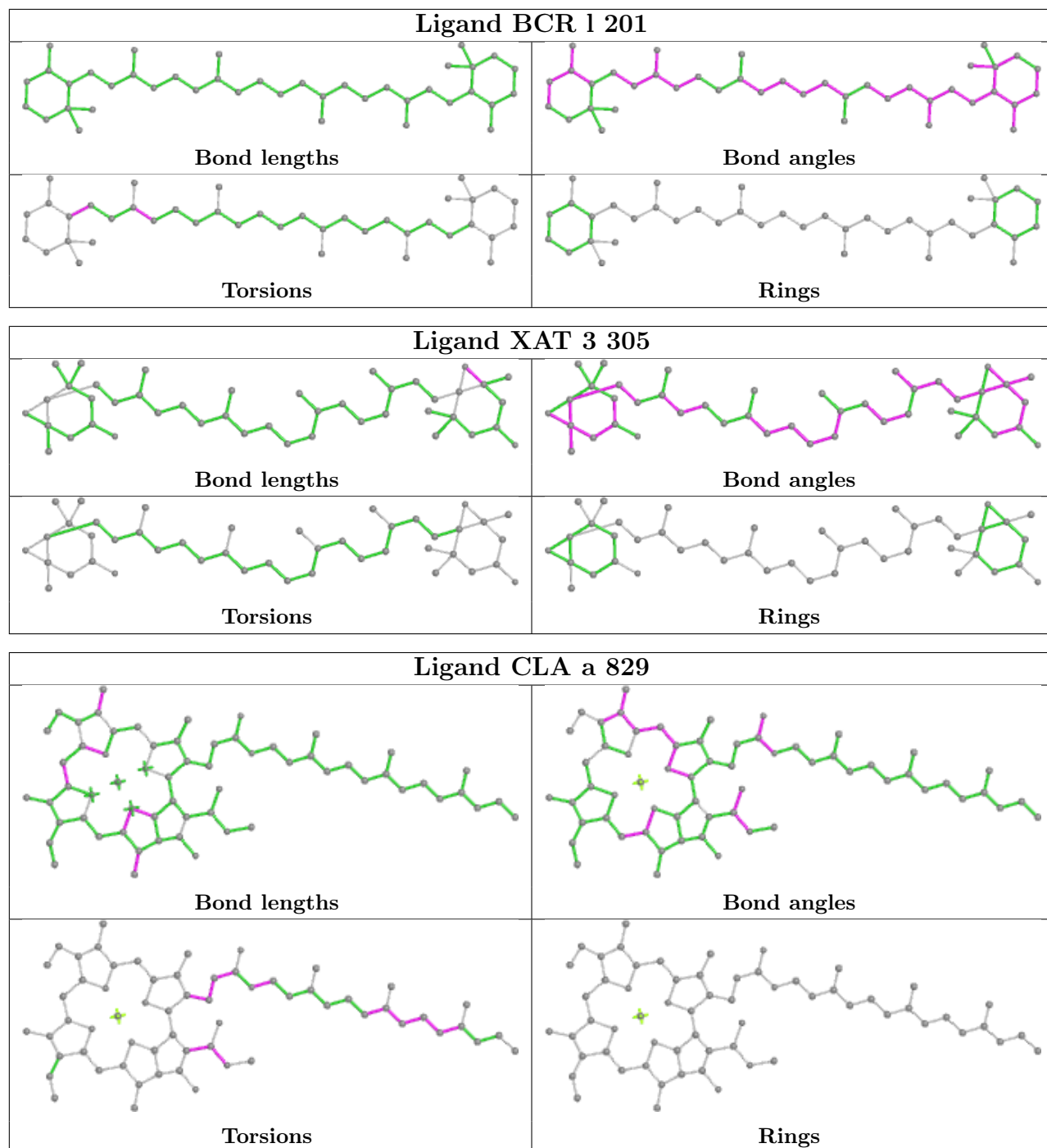
Bond angles



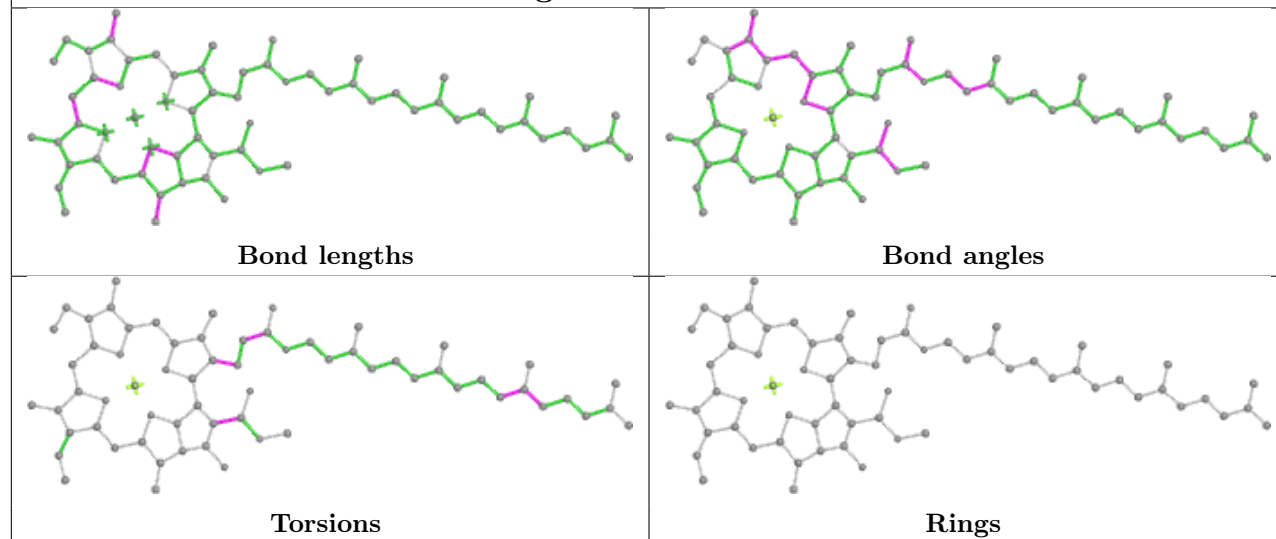
Torsions



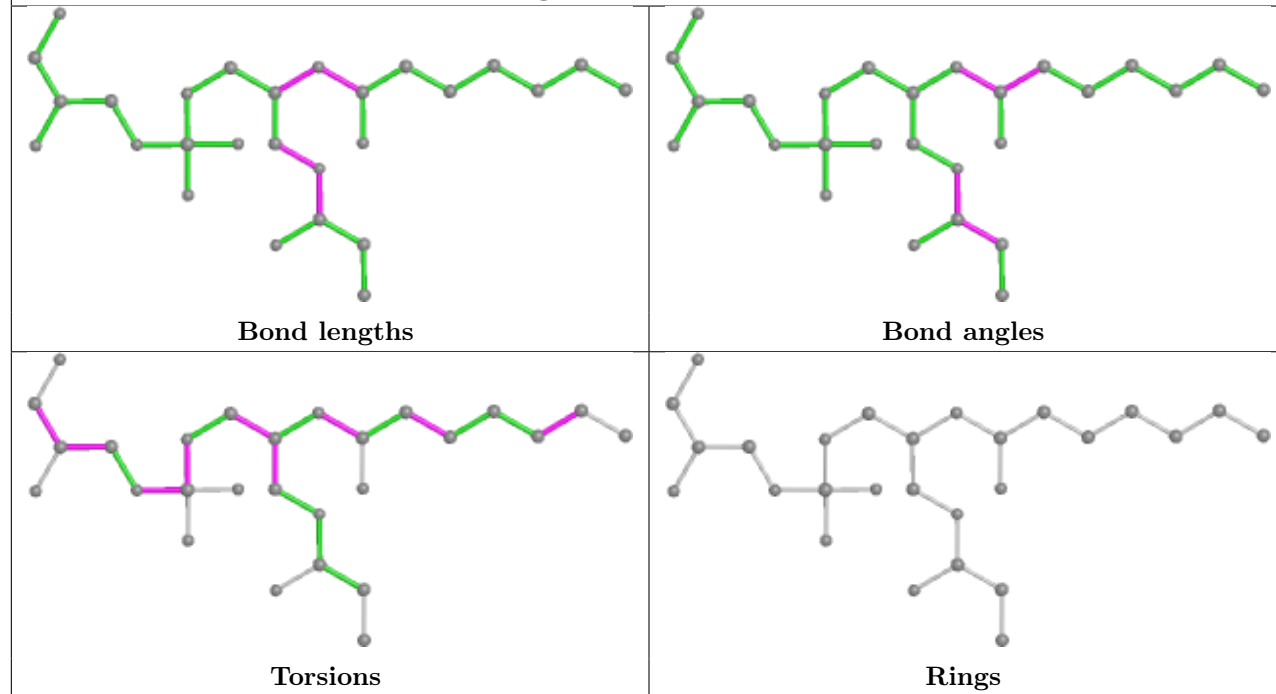
Rings



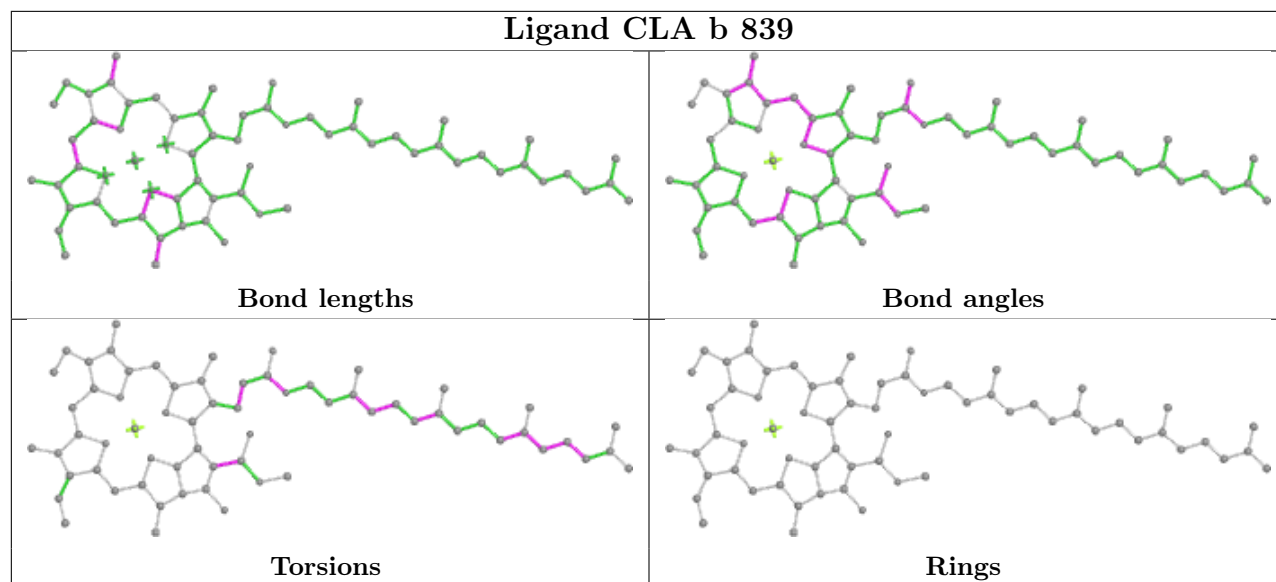
Ligand CLA b 838



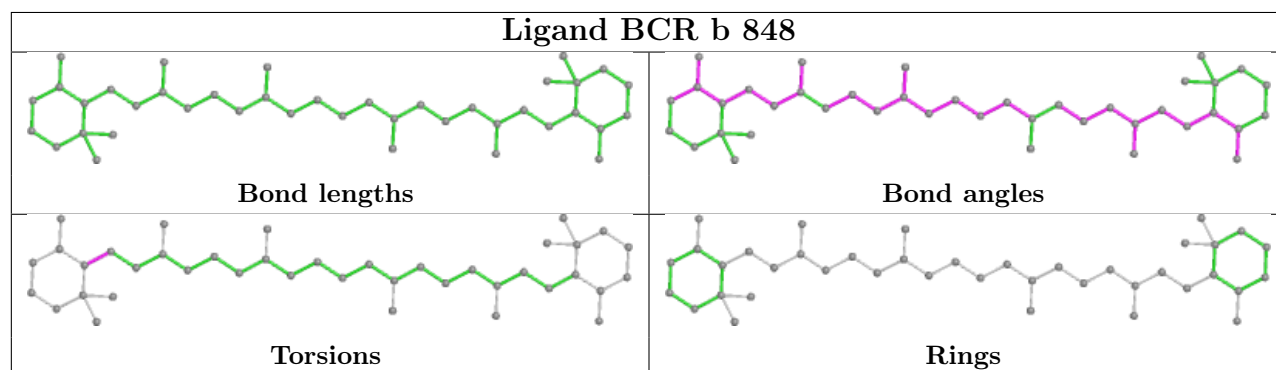
Ligand LHG a 846



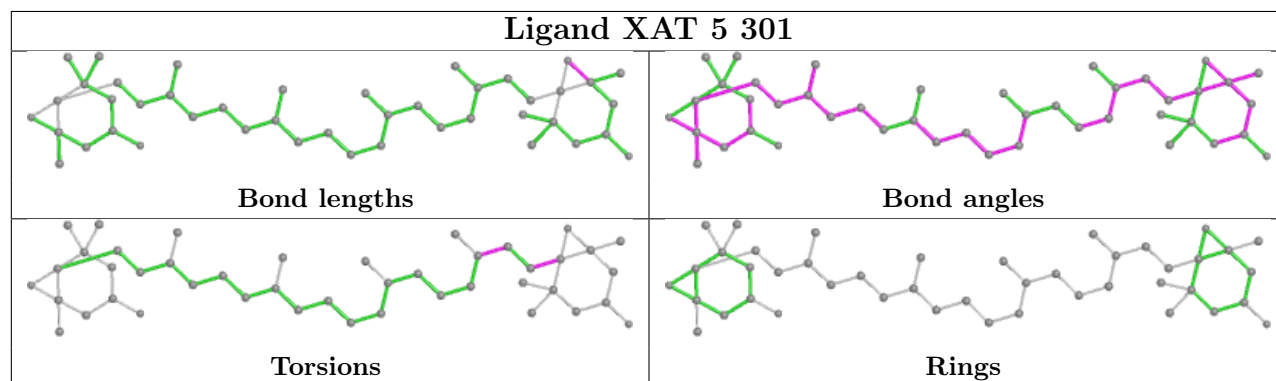
Ligand CLA b 839



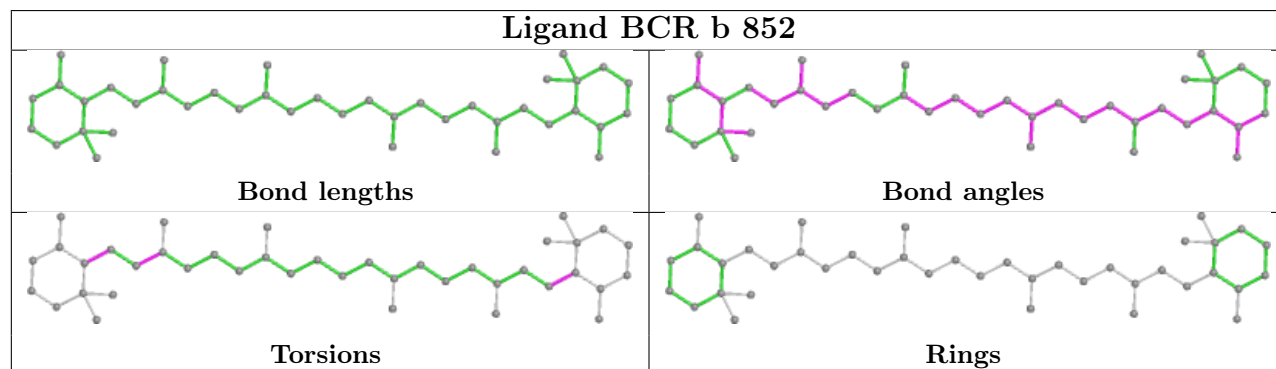
Ligand BCR b 848



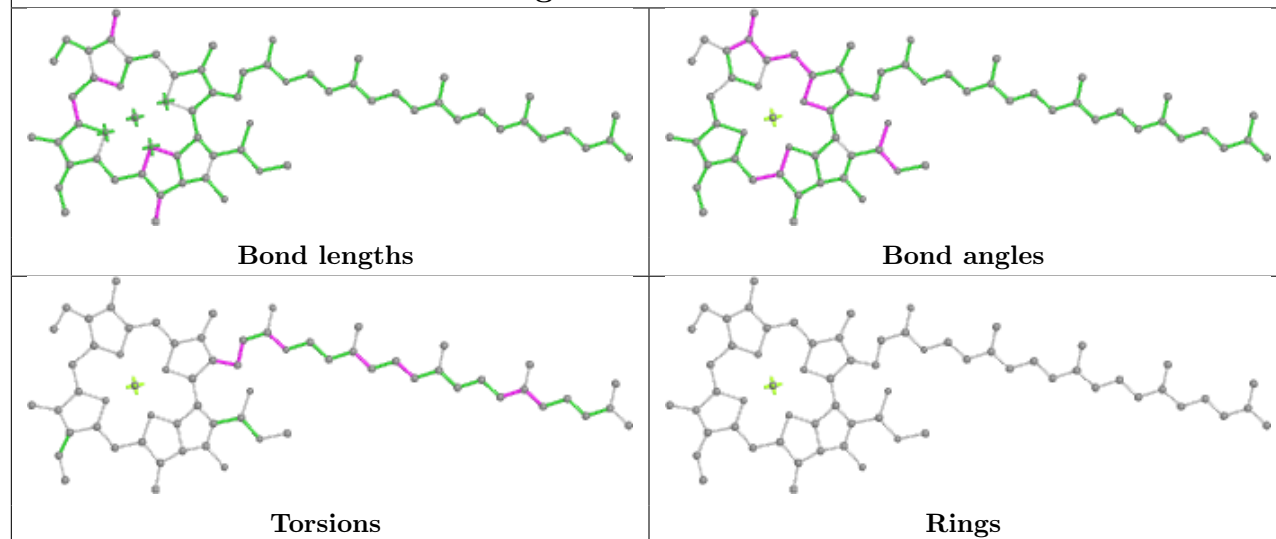
Ligand XAT 5 301



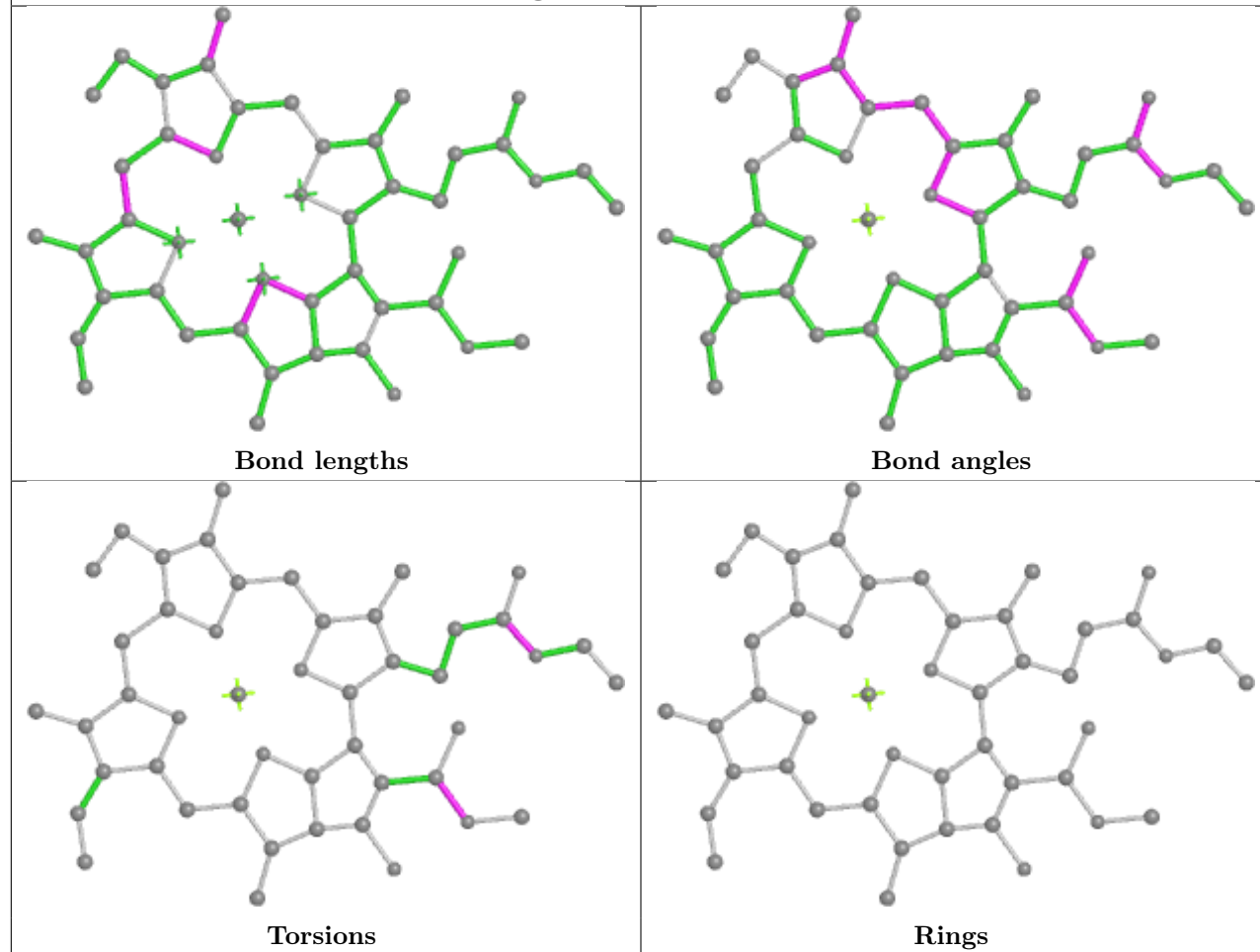
Ligand BCR b 852

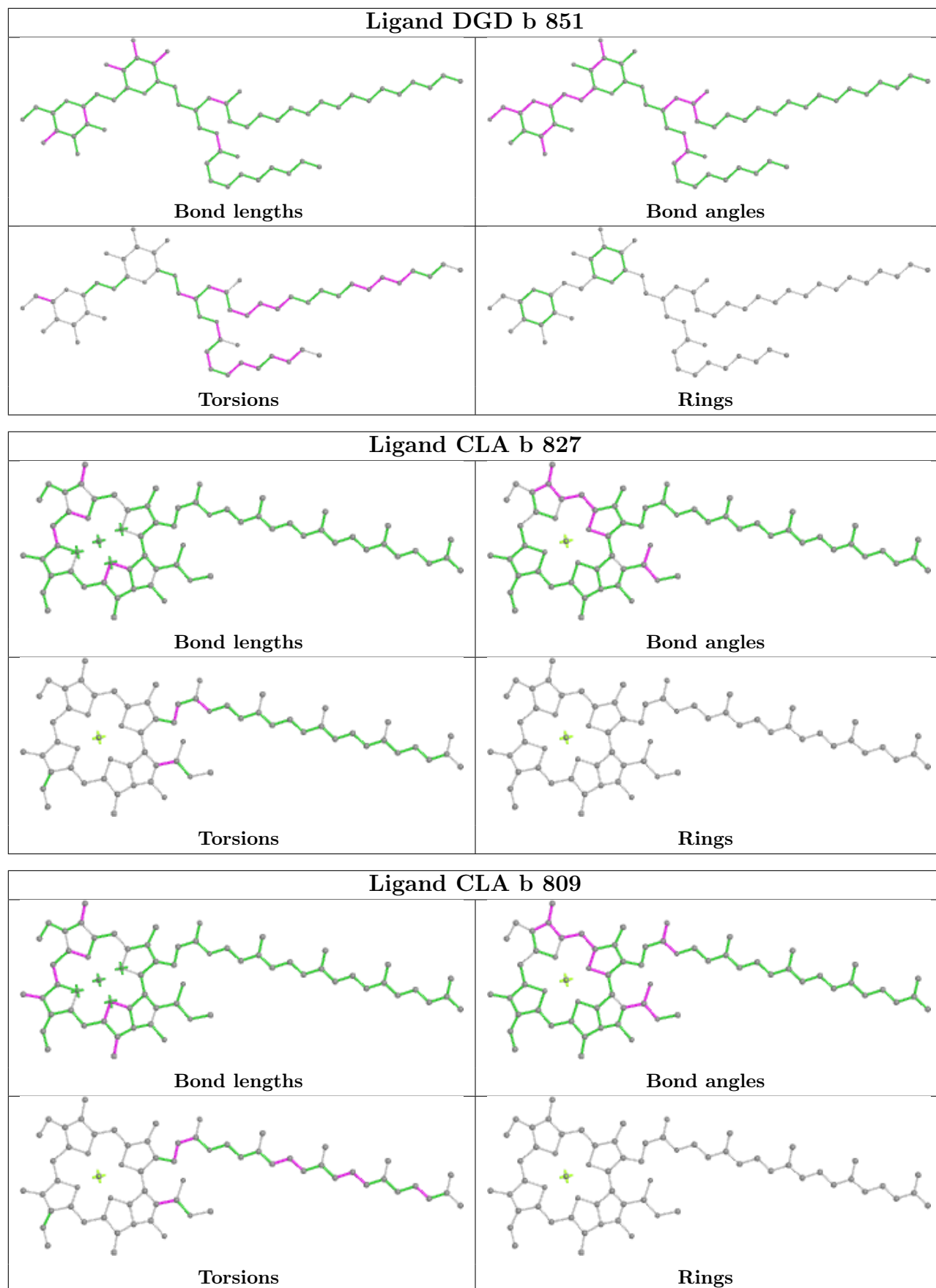


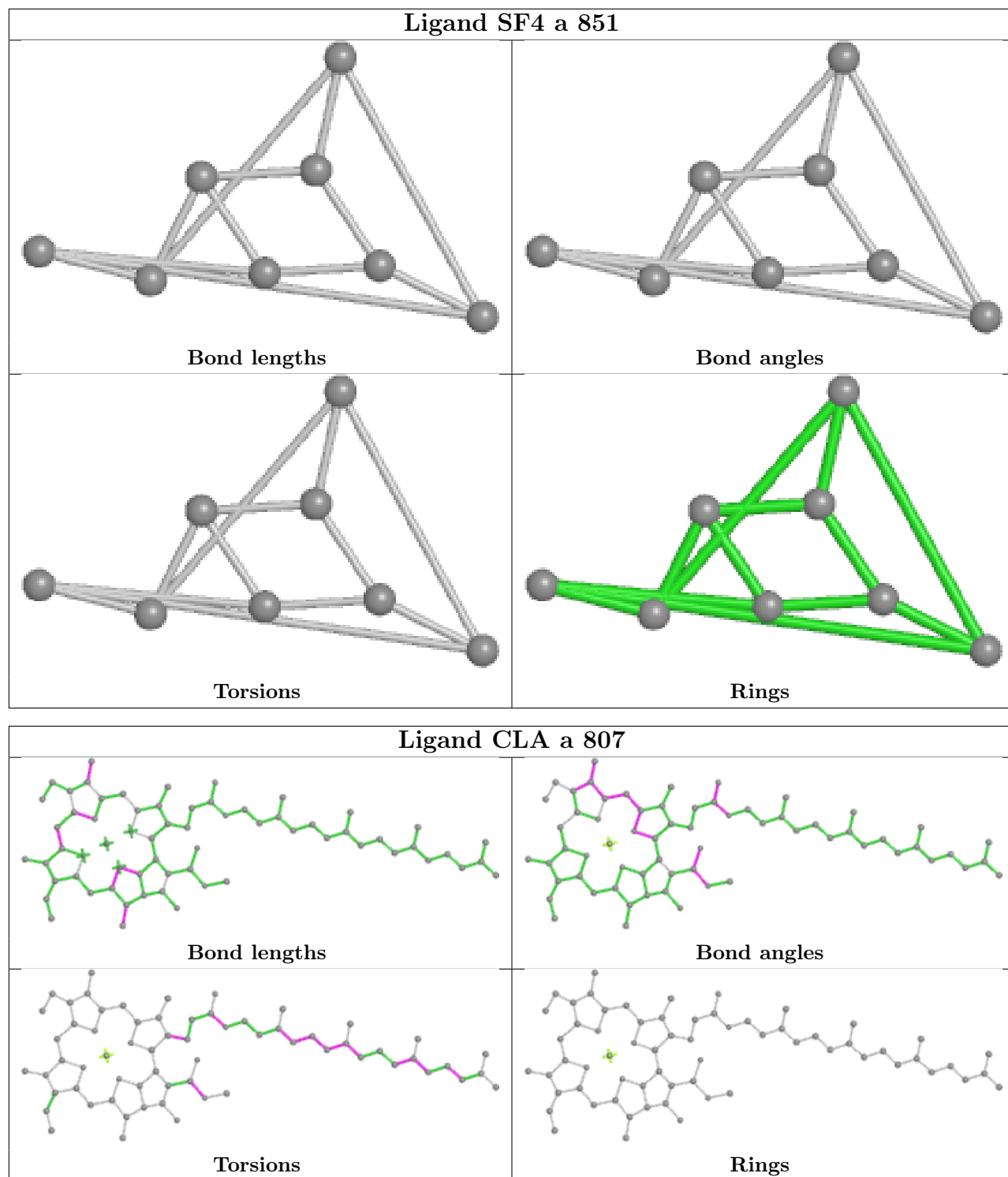
Ligand CLA b 829



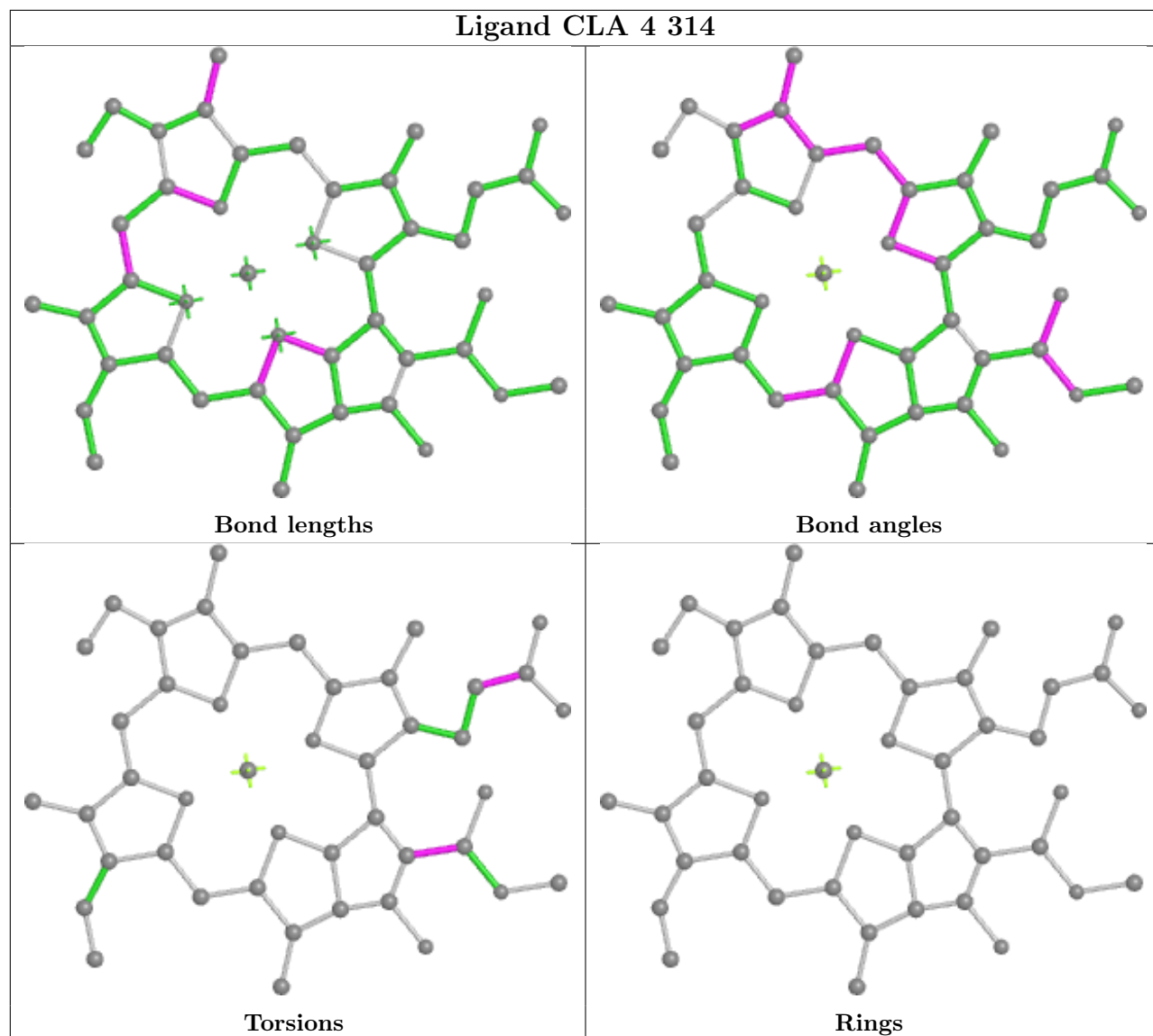
Ligand CLA 2 312



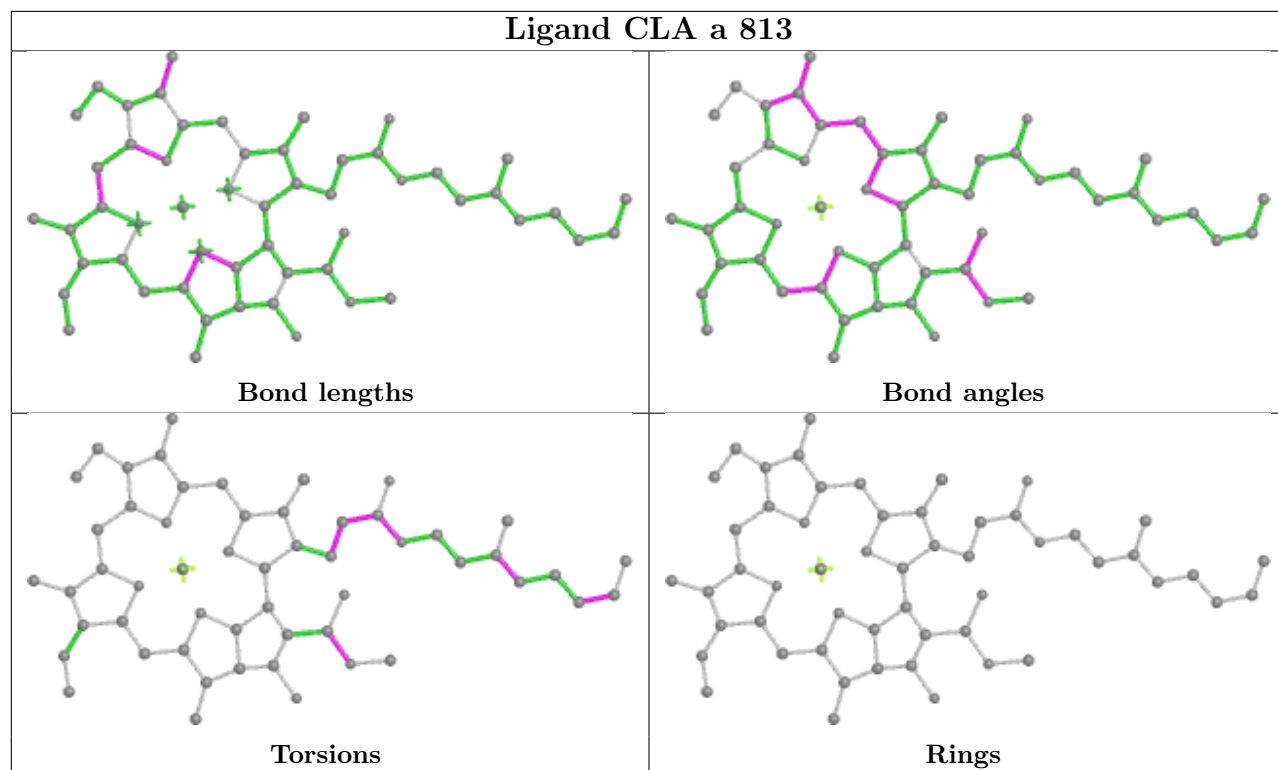




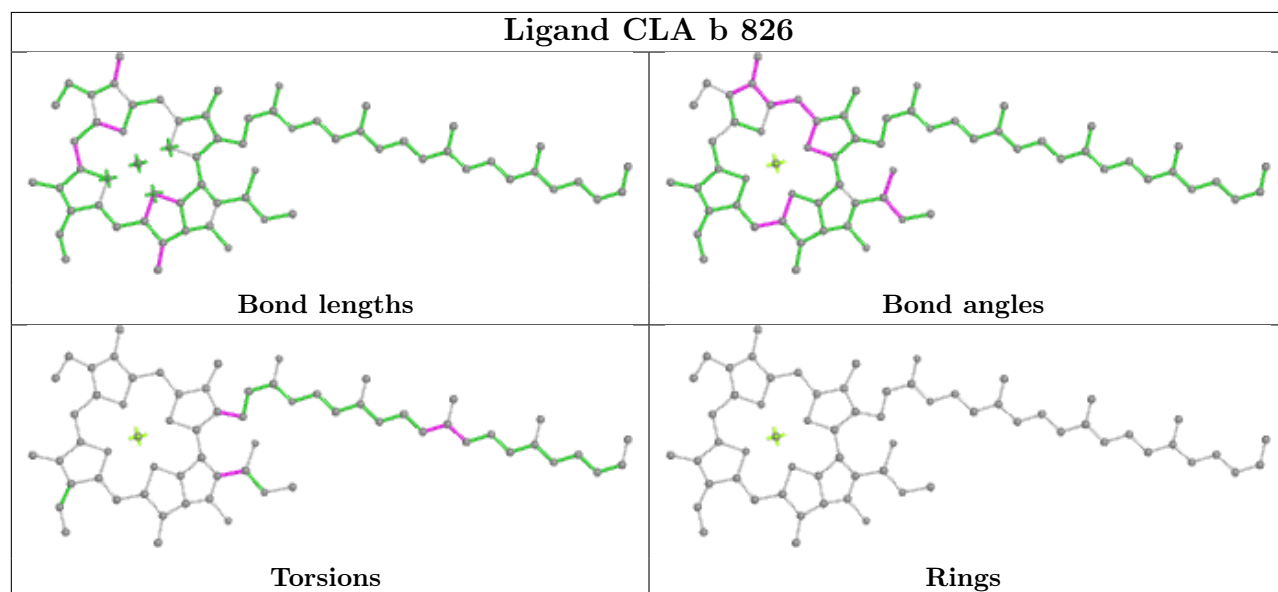
Ligand CLA 4 314

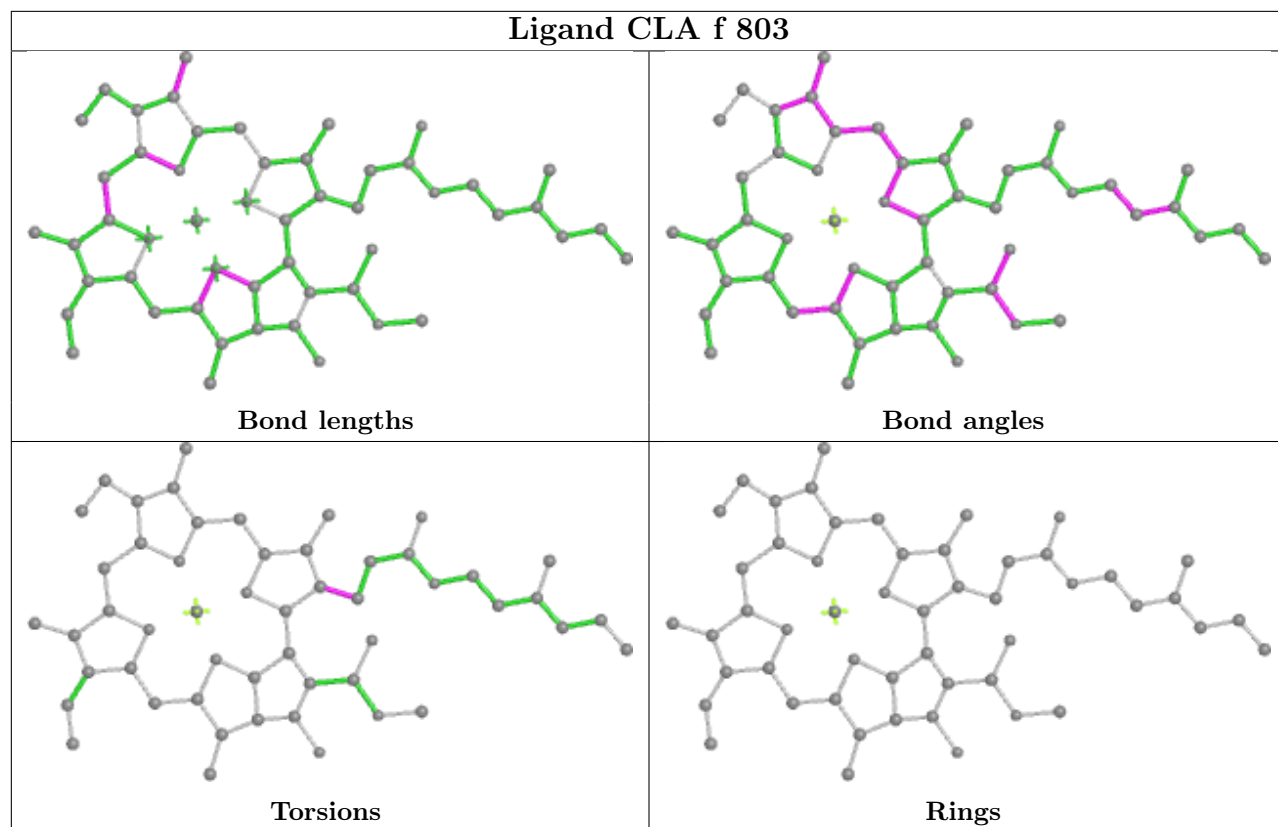


Ligand CLA a 813

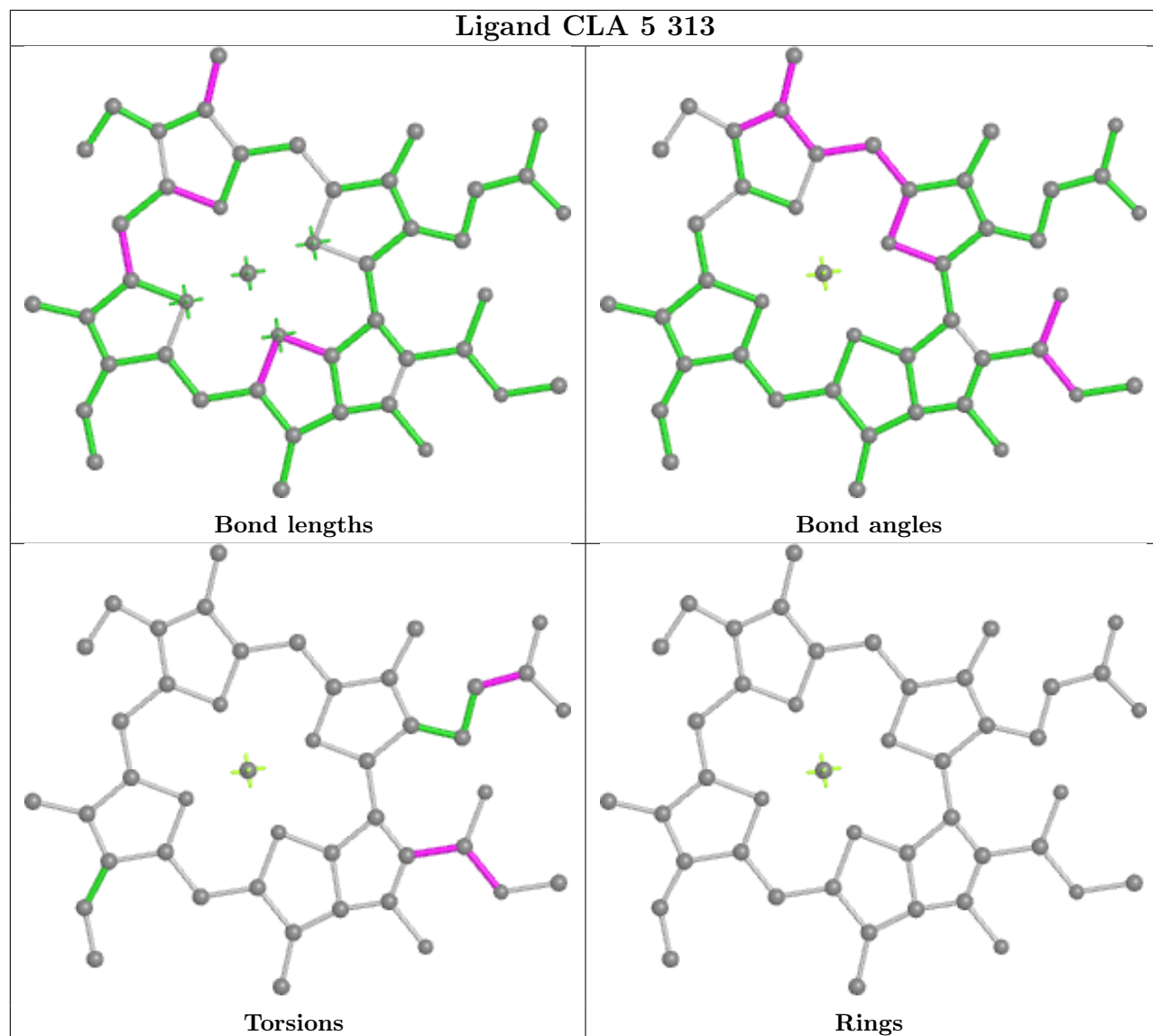


Ligand CLA b 826

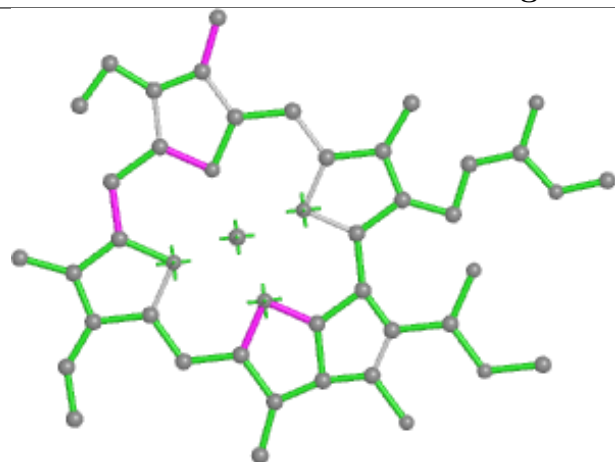




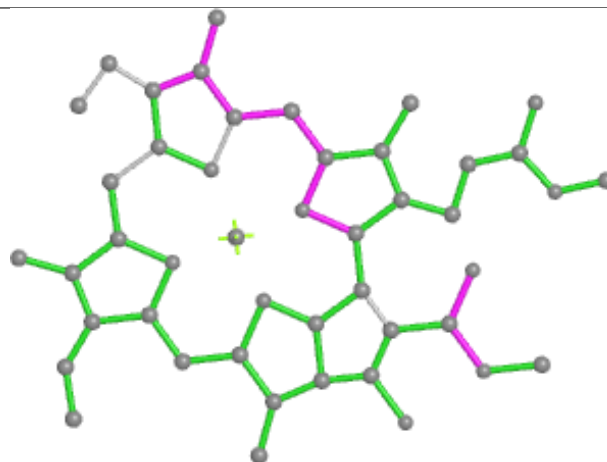
Ligand CLA 5 313



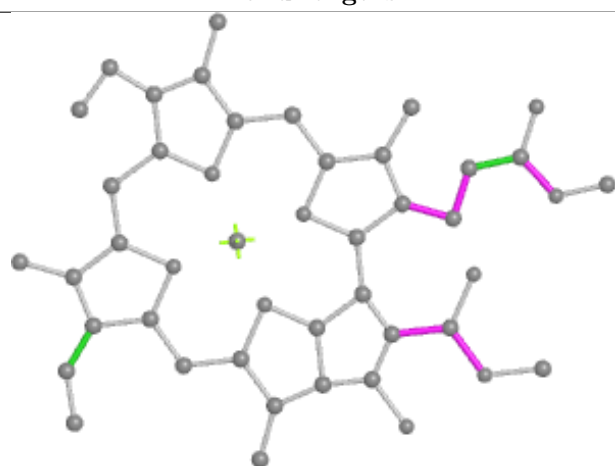
Ligand CLA 4 316



Bond lengths



Bond angles

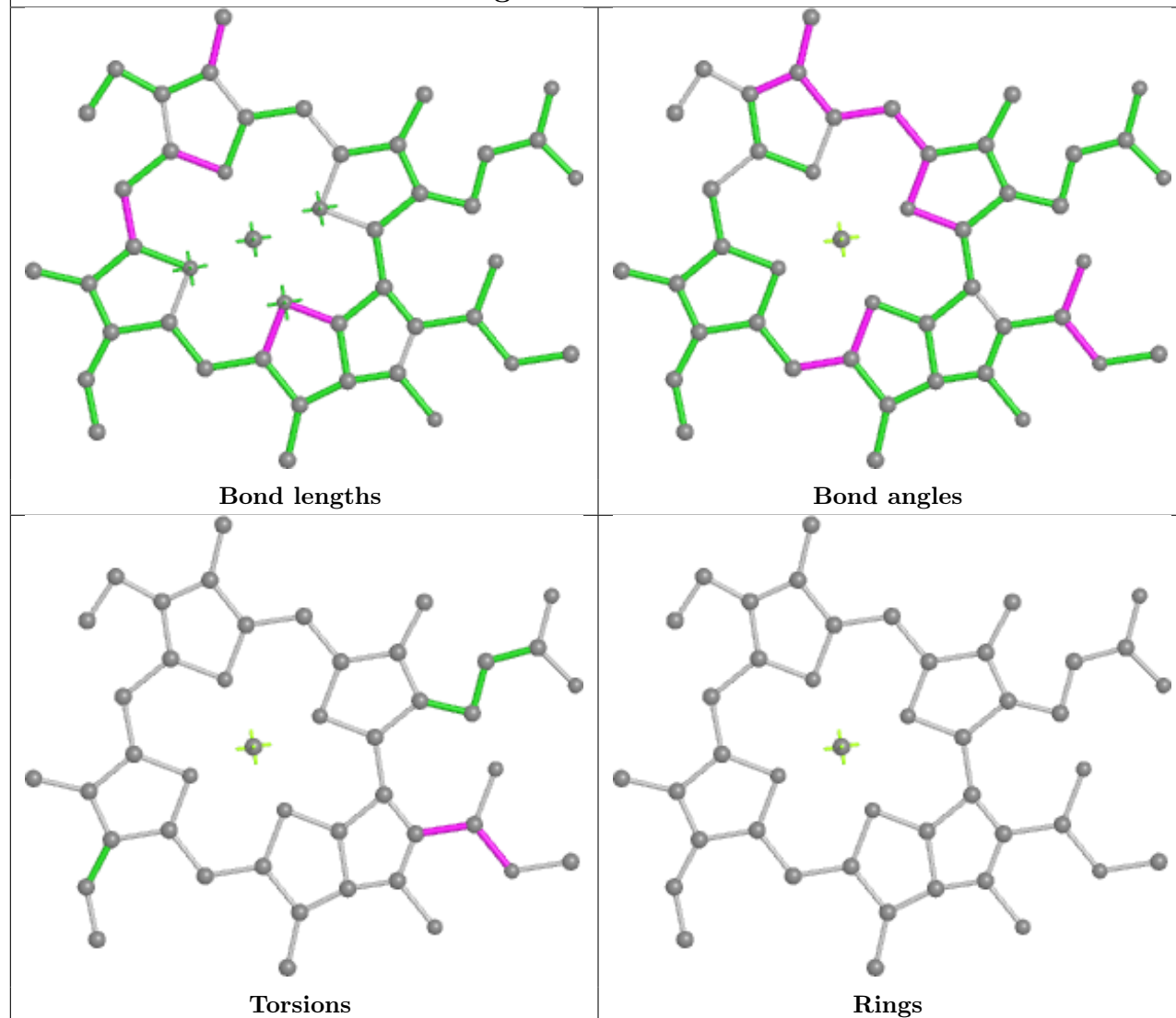


Torsions

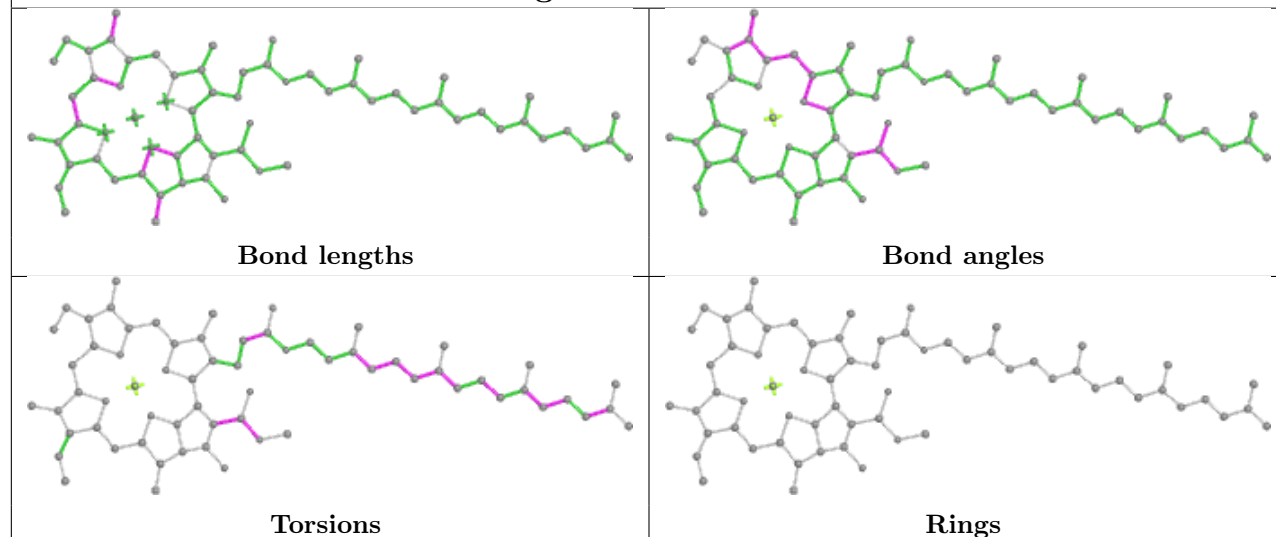


Rings

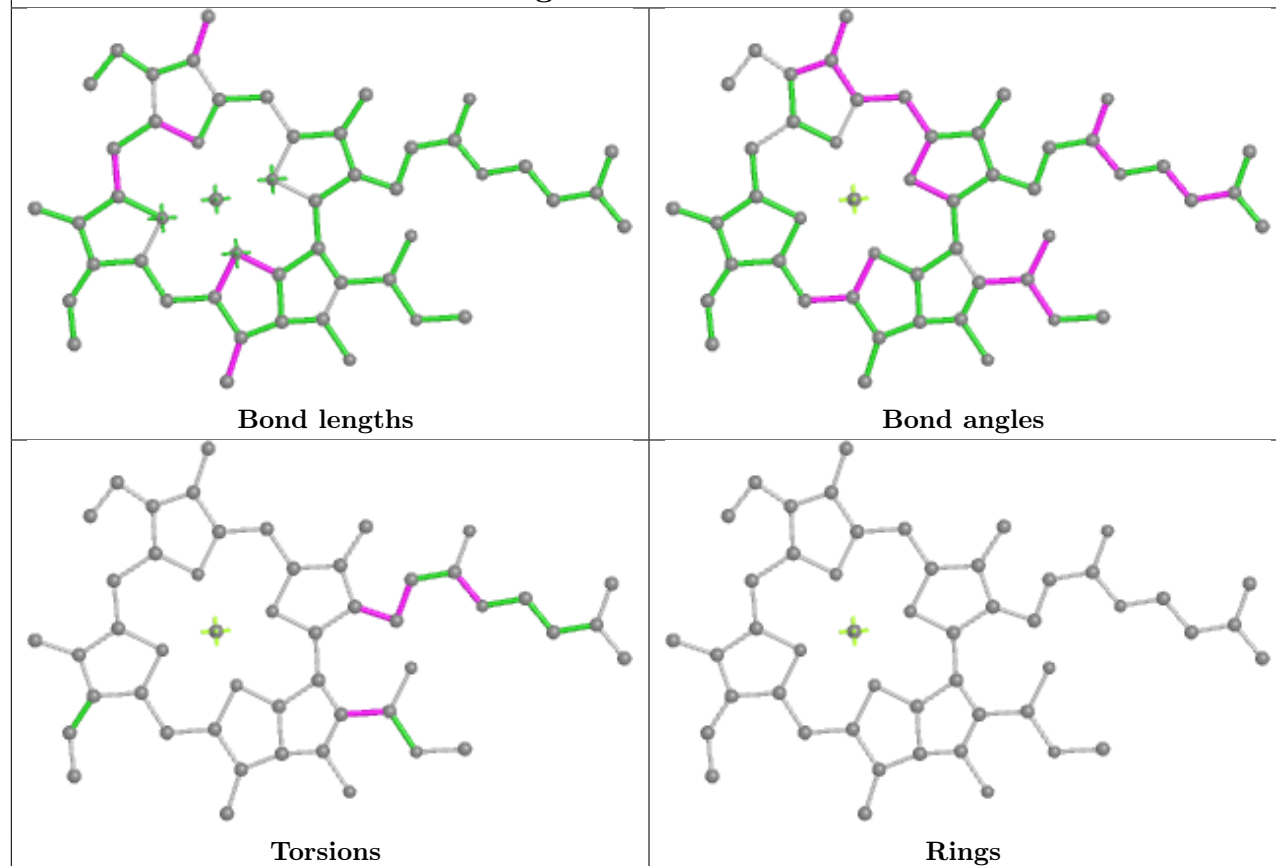
Ligand CLA a 837



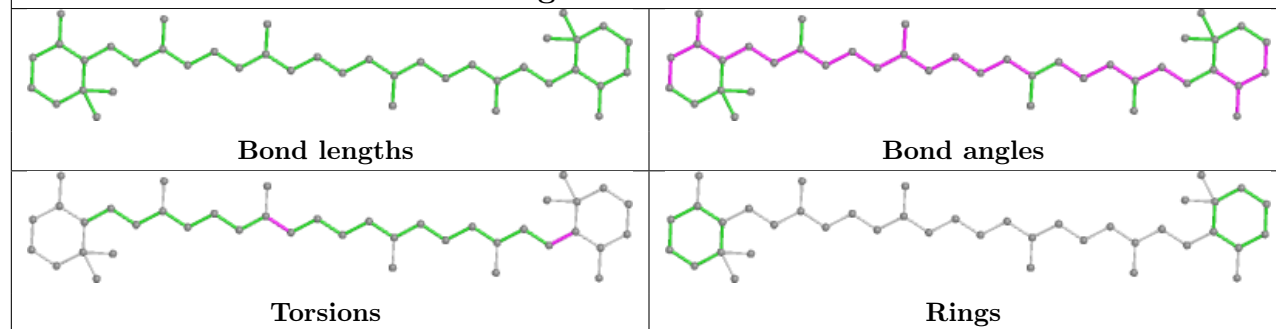
Ligand CLA b 803



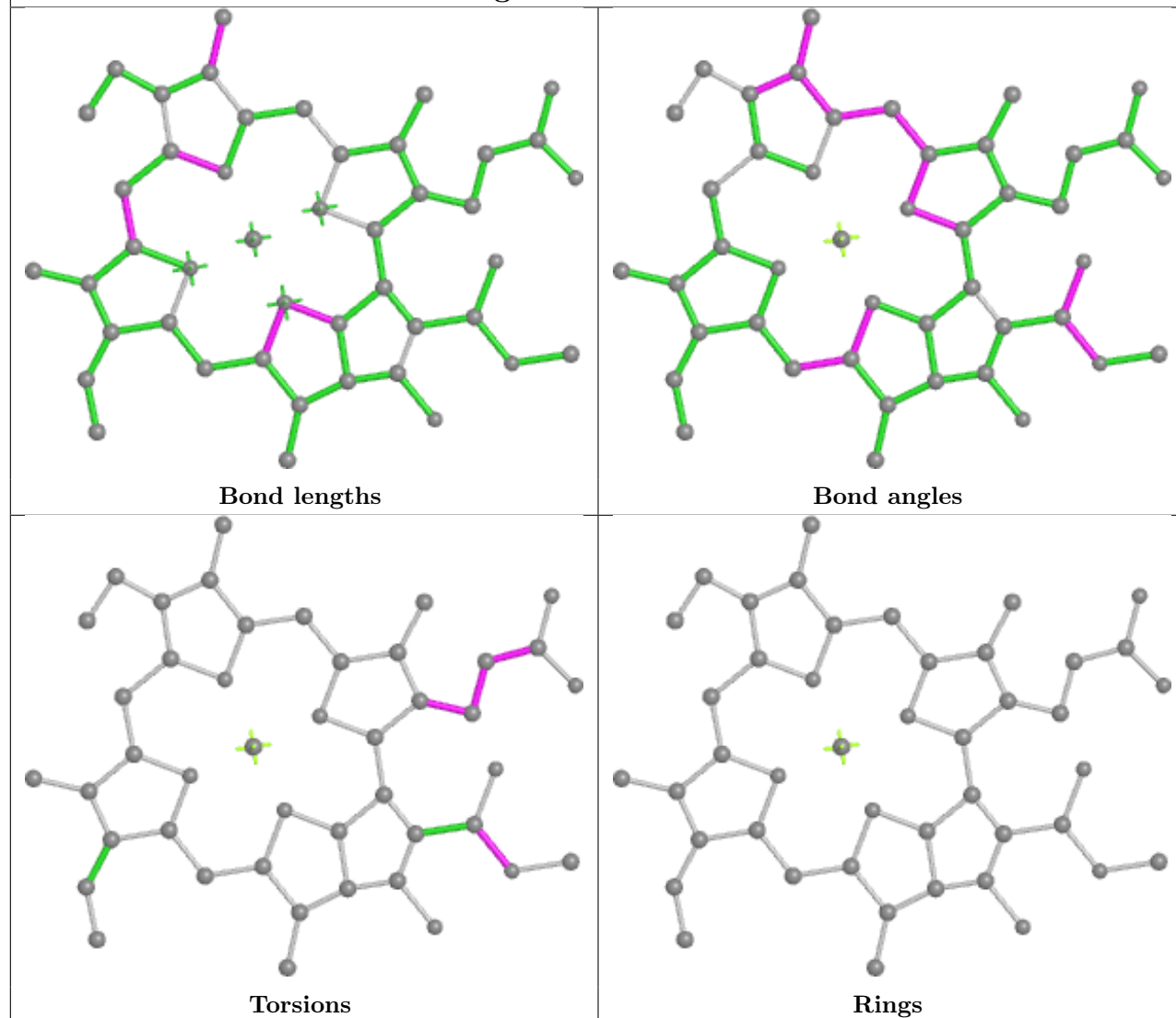
Ligand CLA b 821



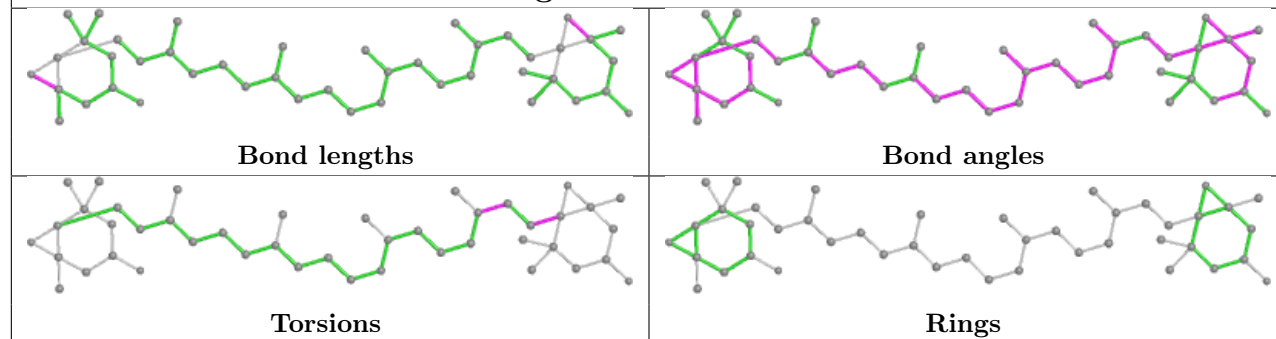
Ligand BCR f 804

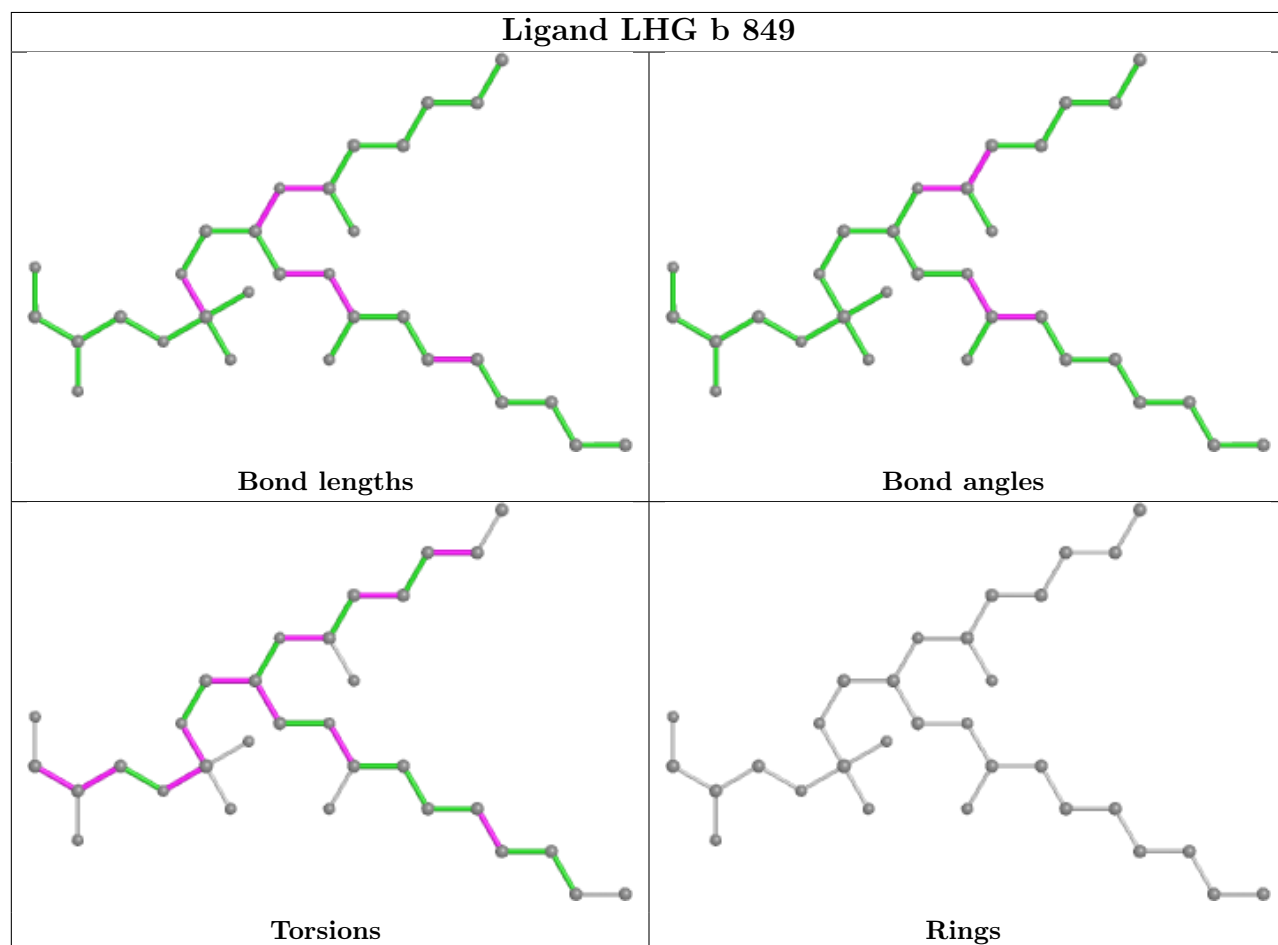
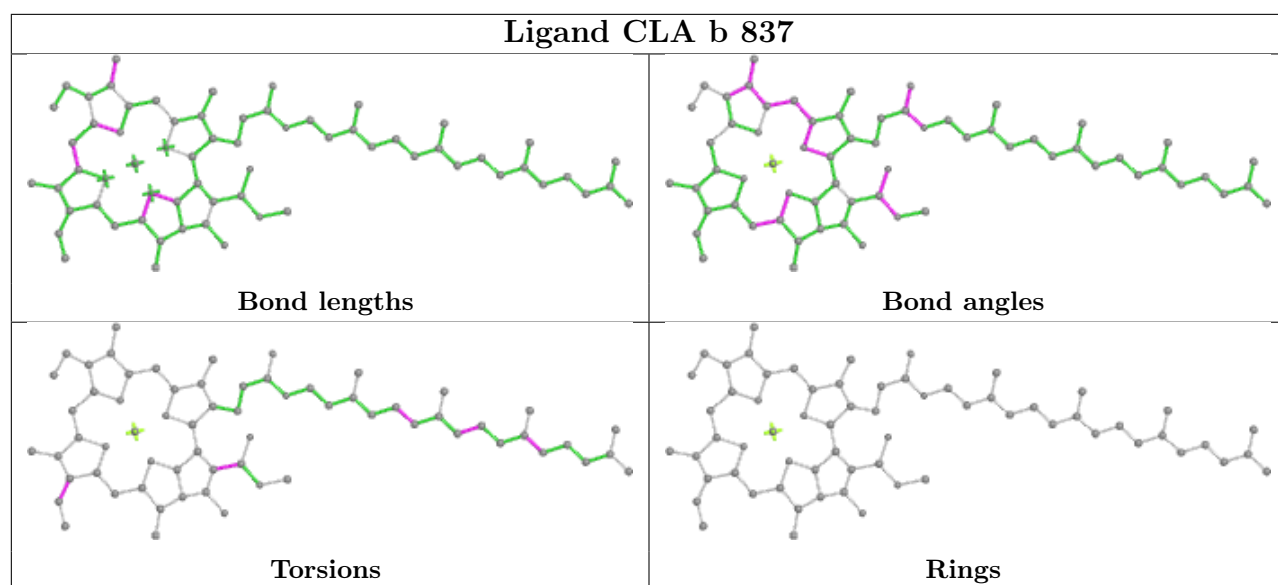


Ligand CLA 4 306

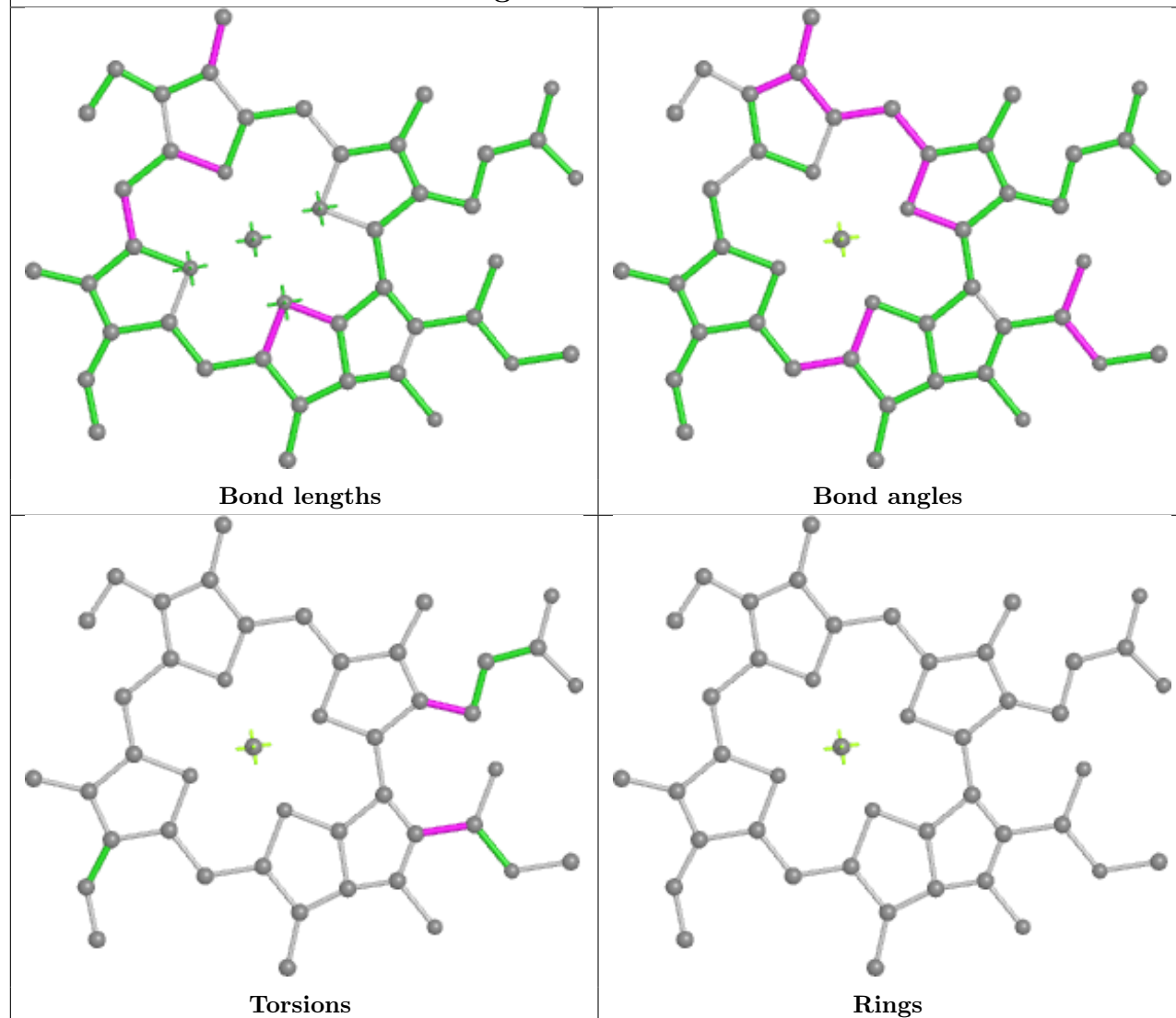


Ligand XAT 5 302

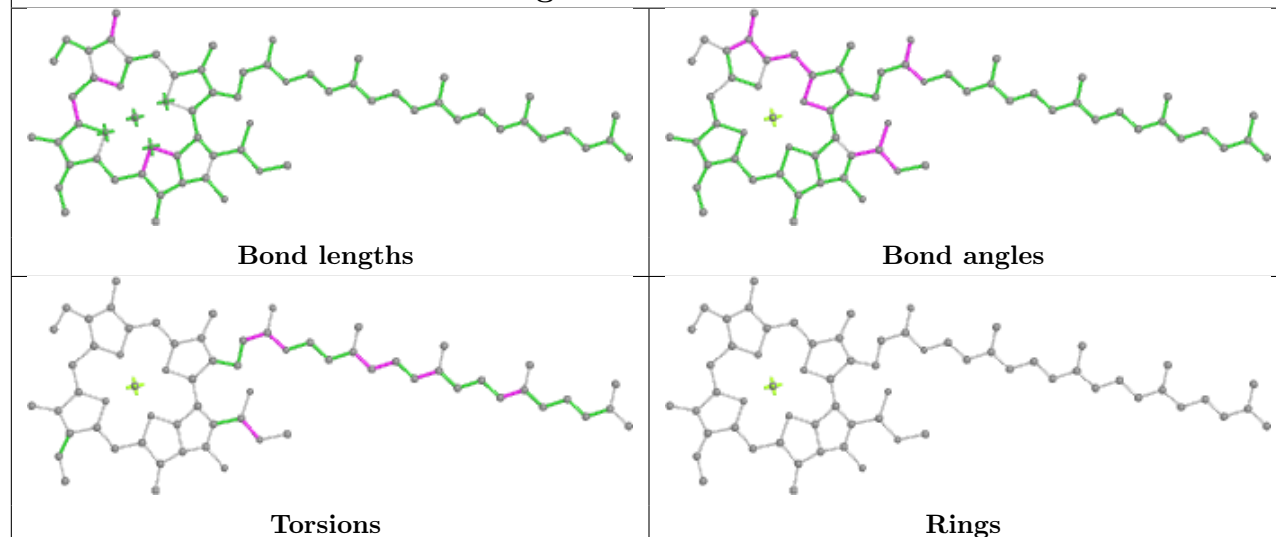




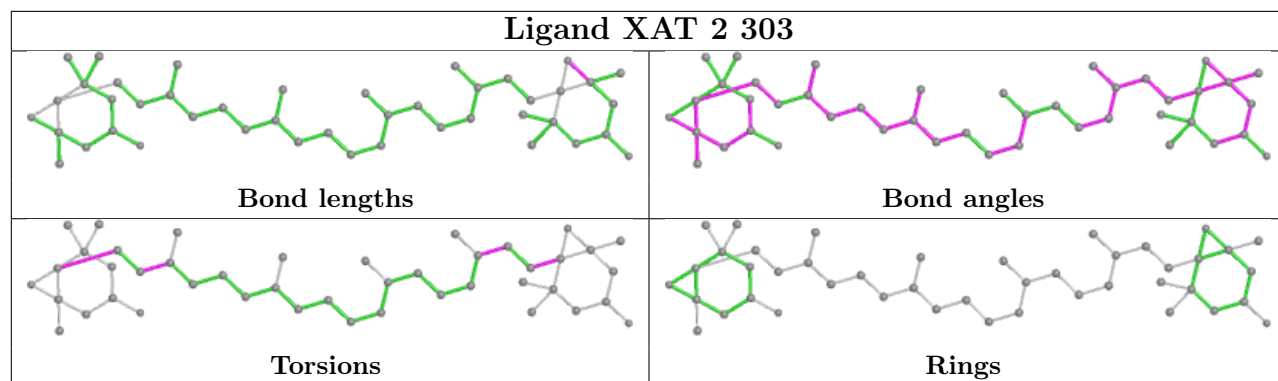
Ligand CLA a 815



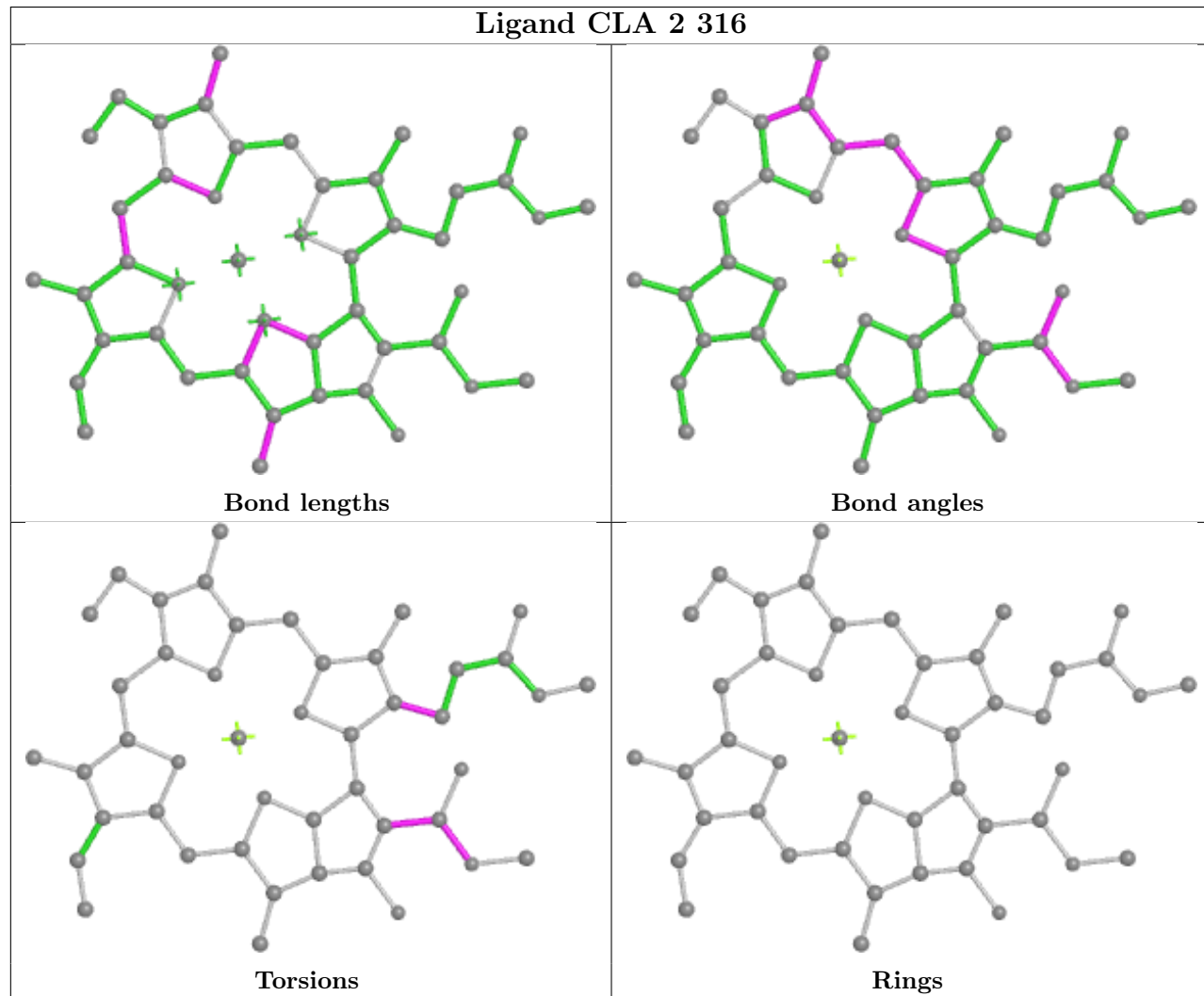
Ligand CLA a 835



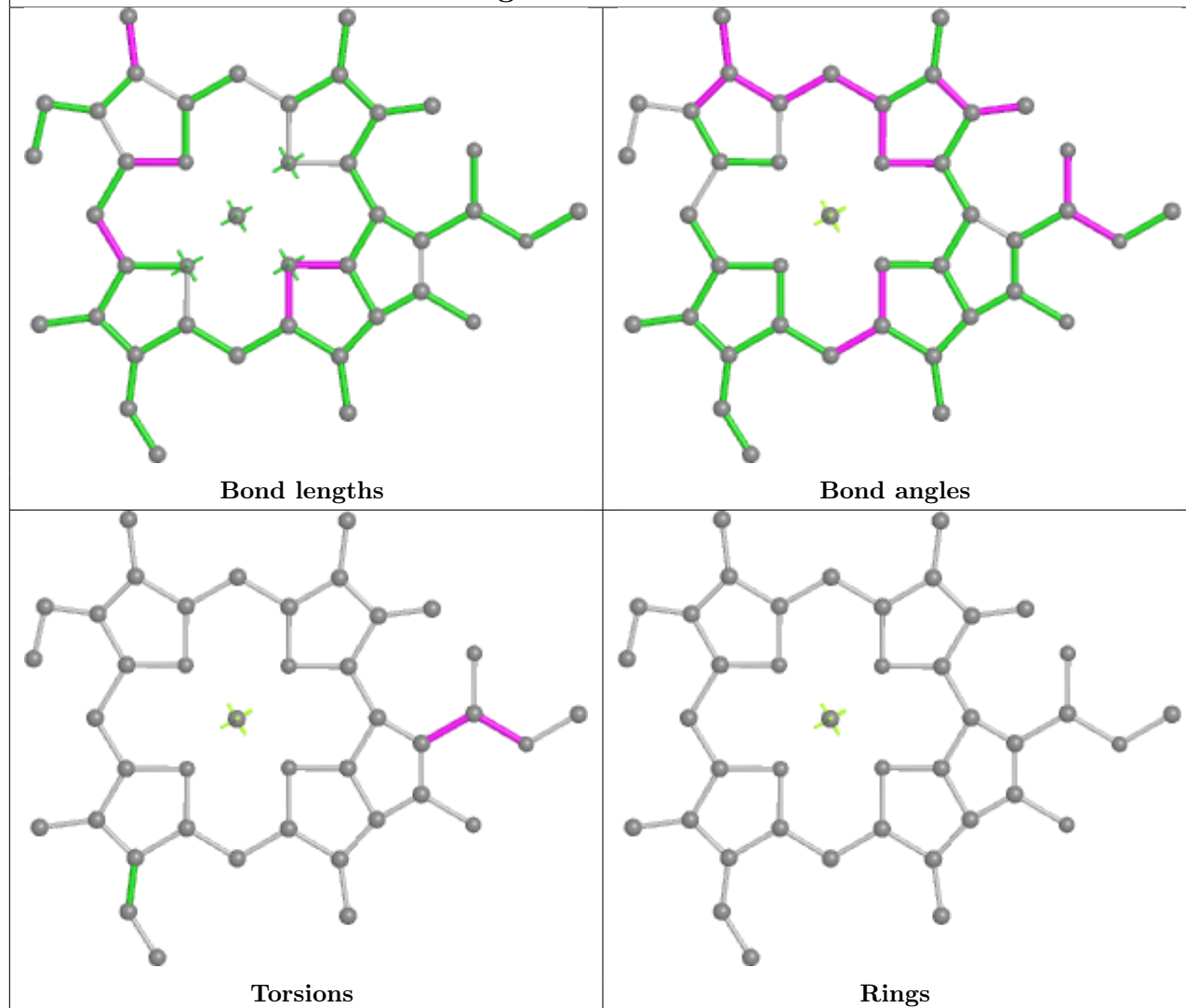
Ligand XAT 2 303



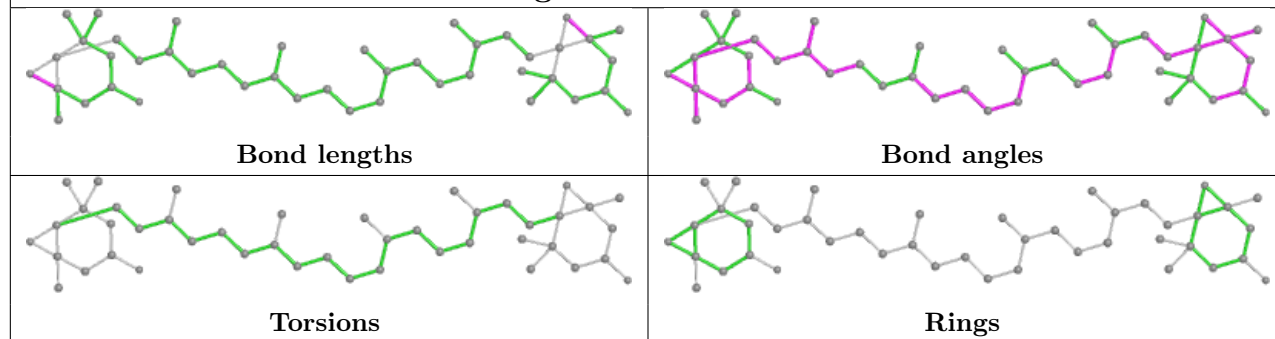
Ligand CLA 2 316



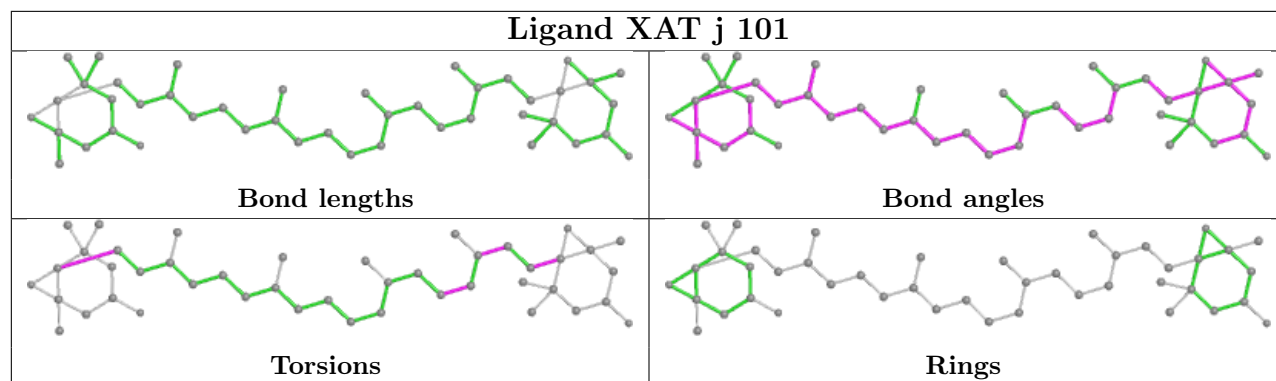
Ligand CLA 2 313



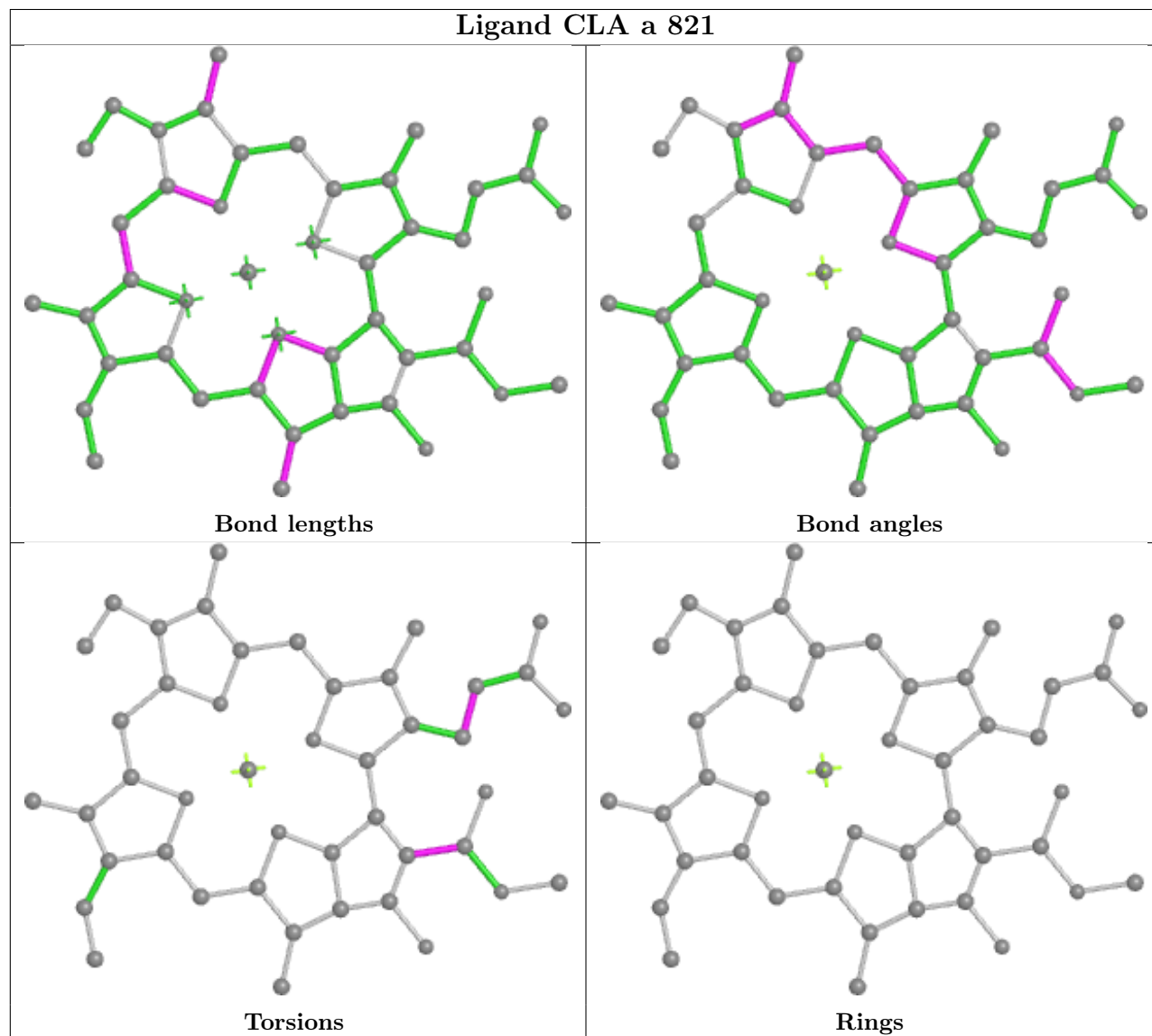
Ligand XAT 4 304



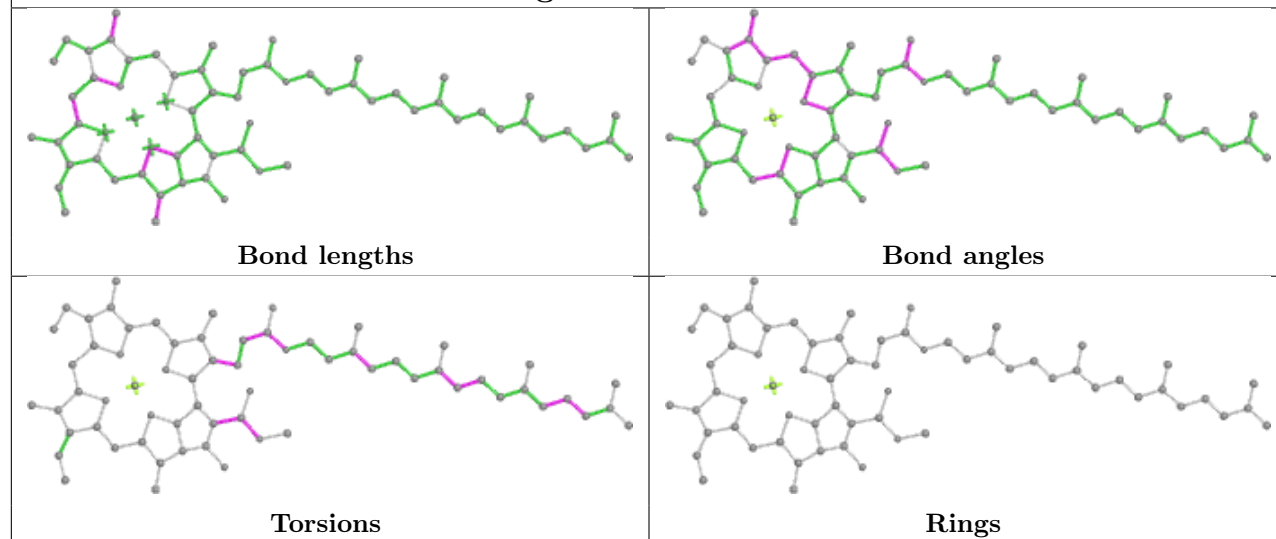
Ligand XAT j 101



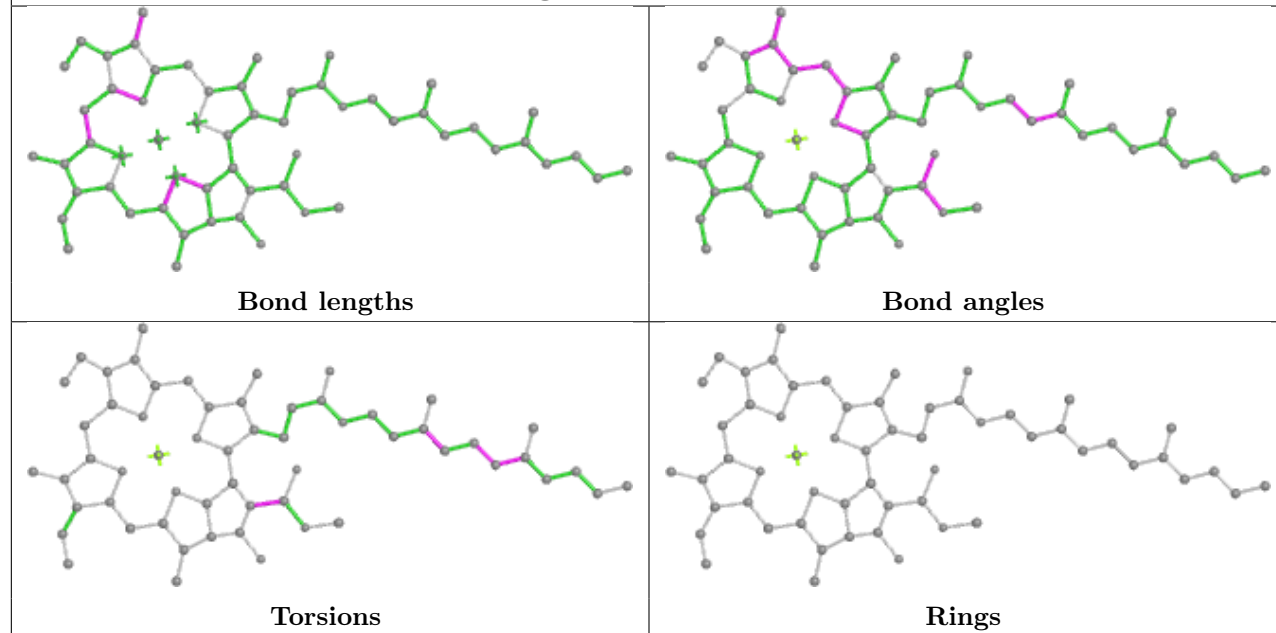
Ligand CLA a 821



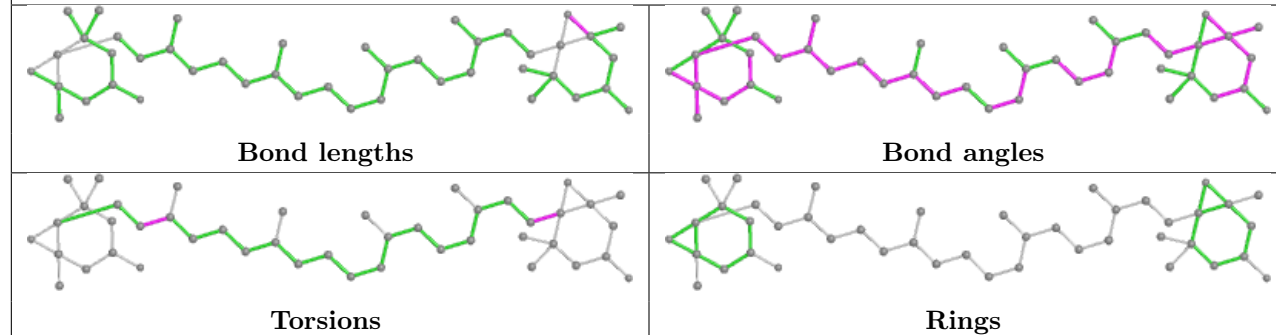
Ligand CLA 4 310

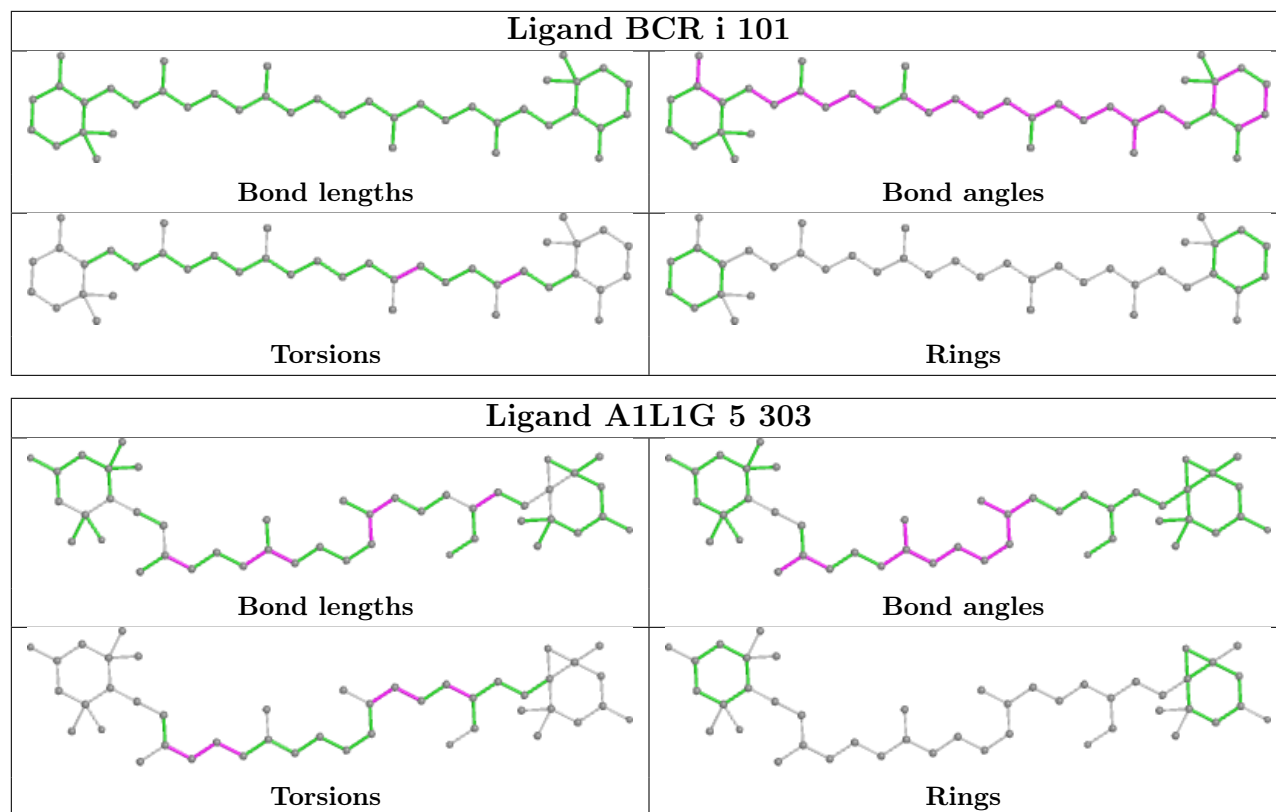


Ligand CLA a 802

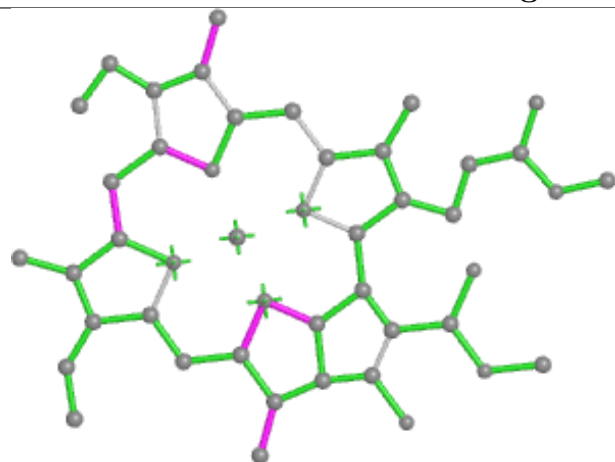


Ligand XAT 2 301

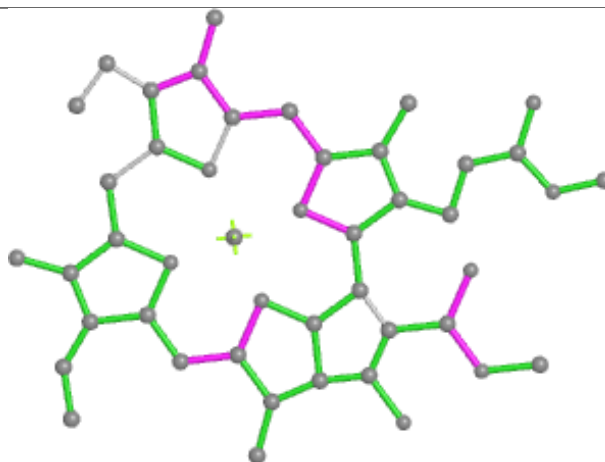




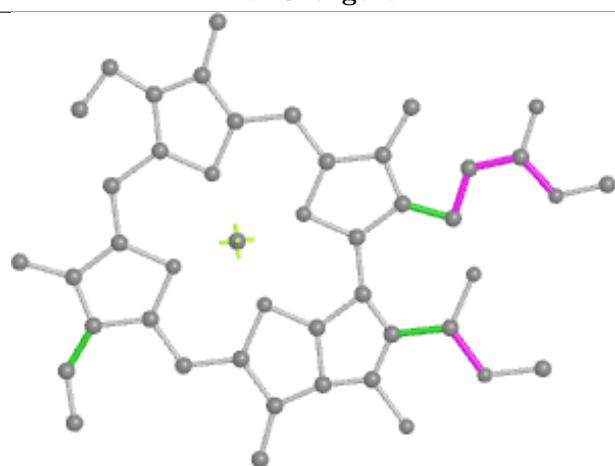
Ligand CLA 5 310



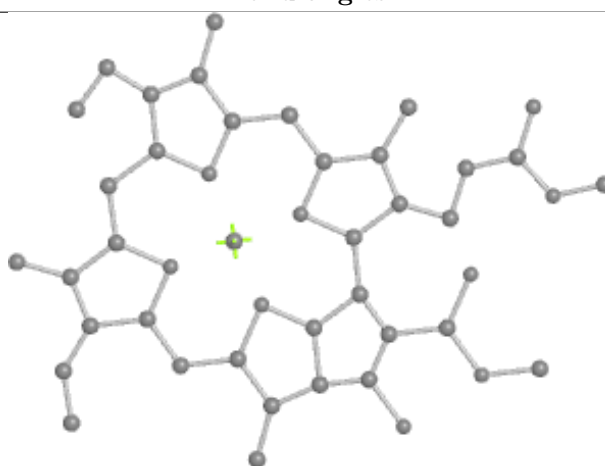
Bond lengths



Bond angles

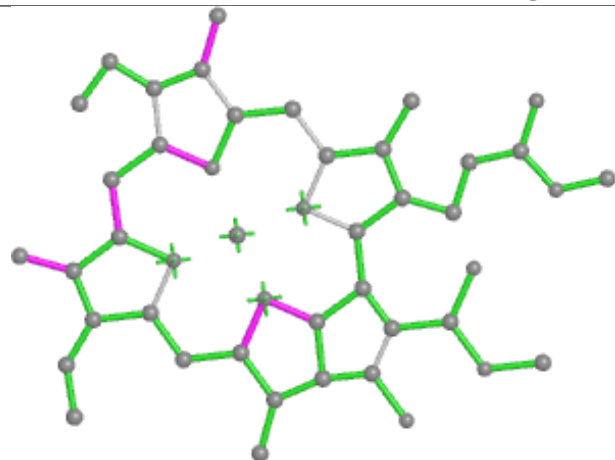


Torsions

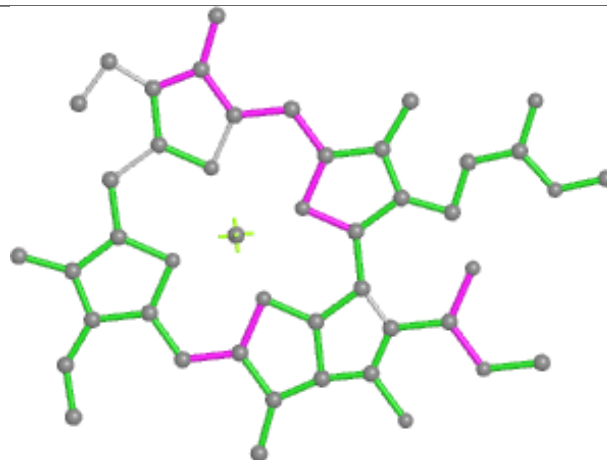


Rings

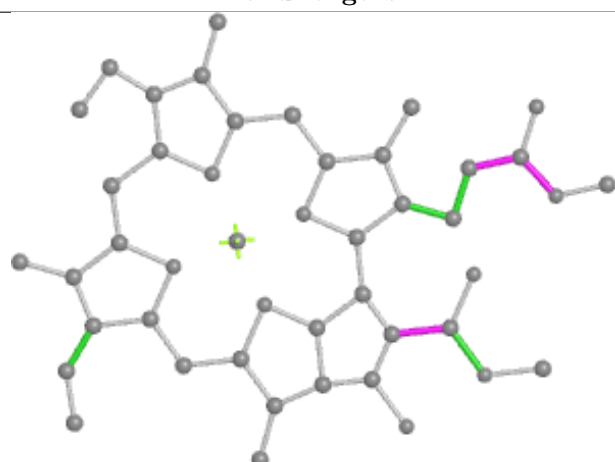
Ligand CLA 1 204



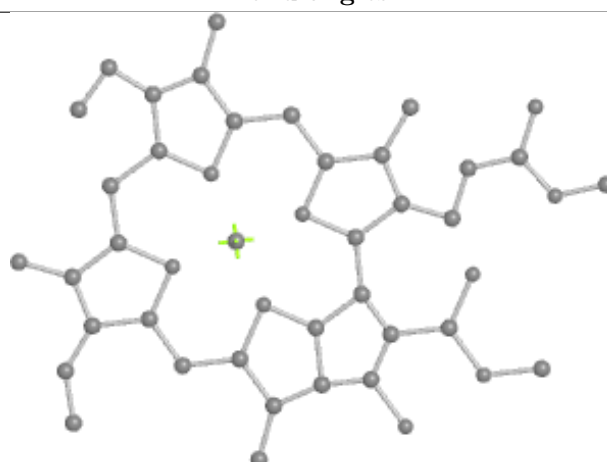
Bond lengths



Bond angles

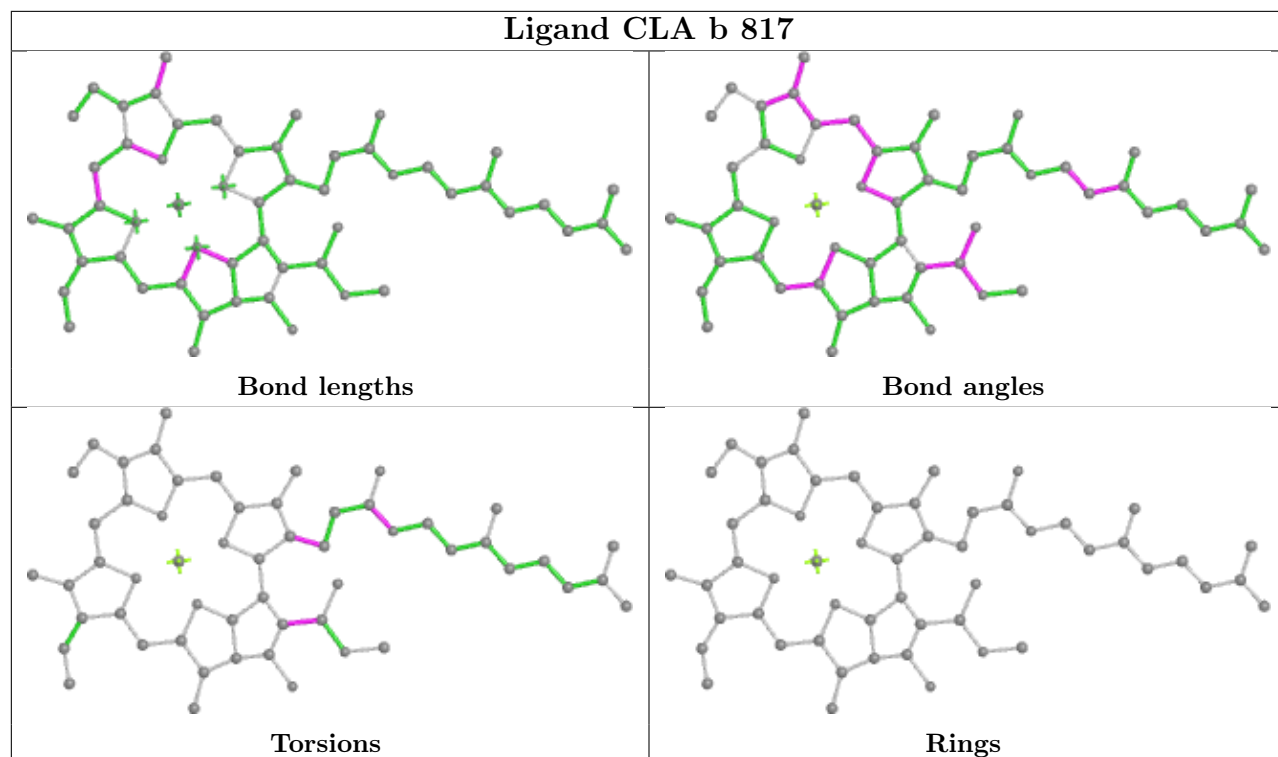


Torsions

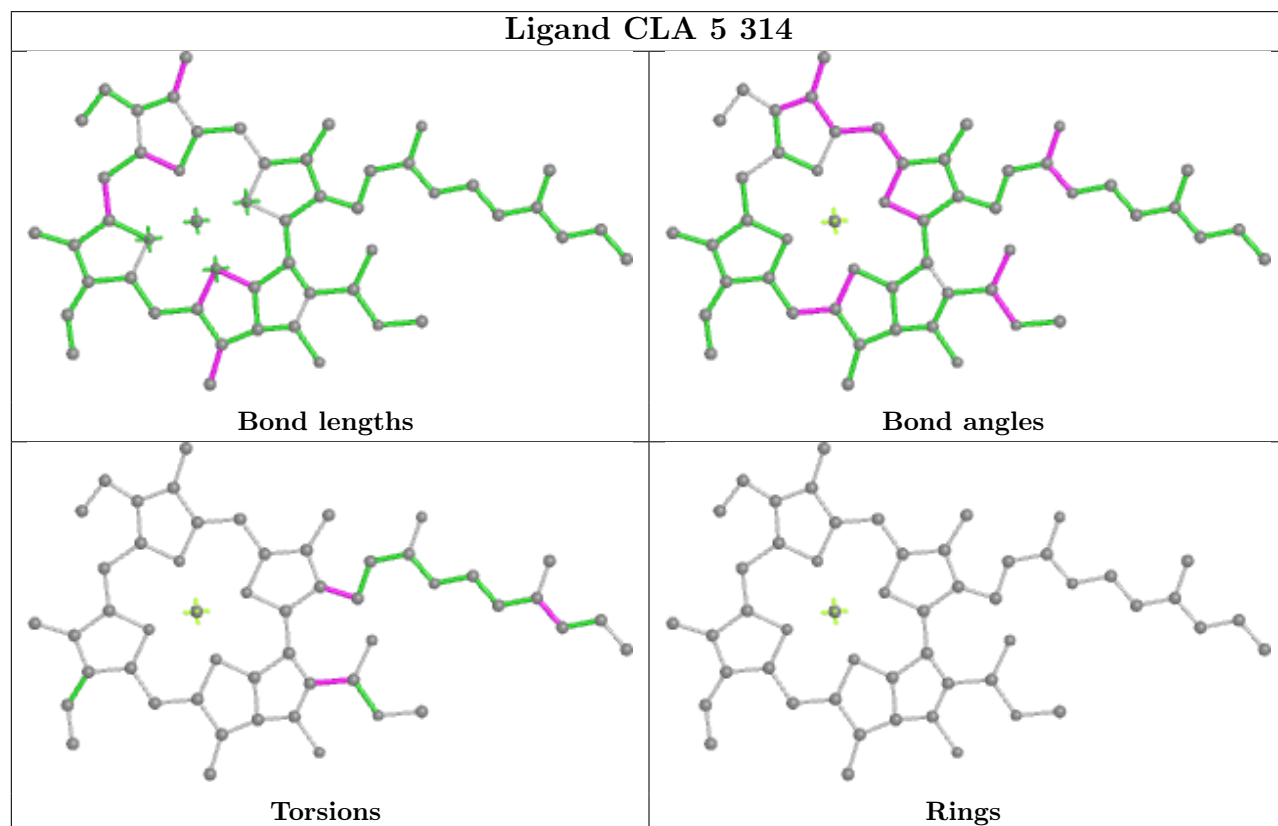


Rings

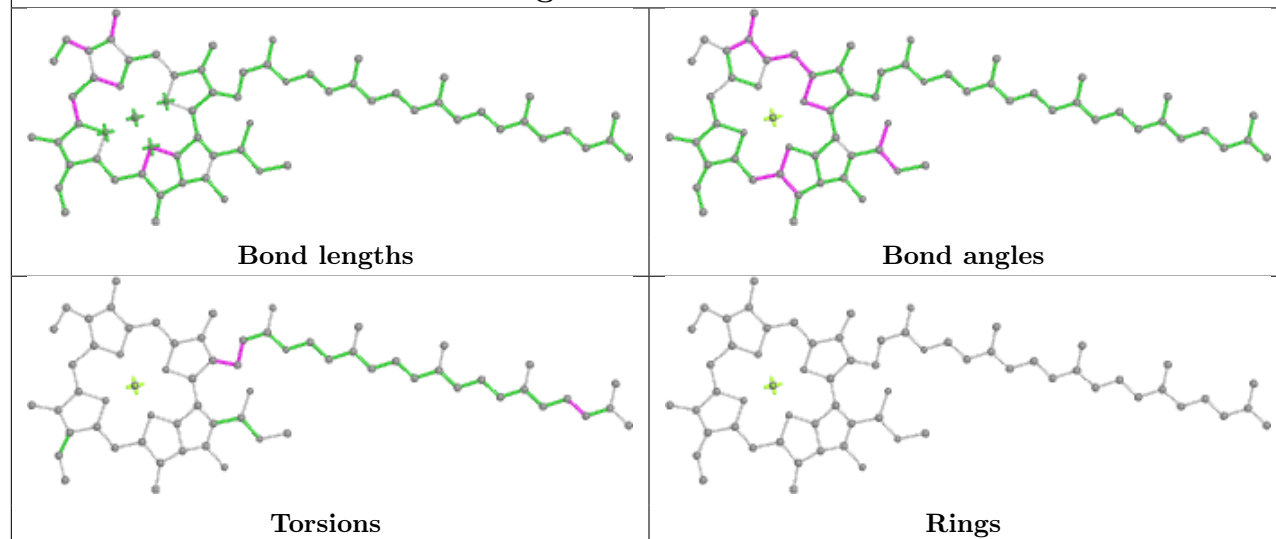
Ligand CLA b 817



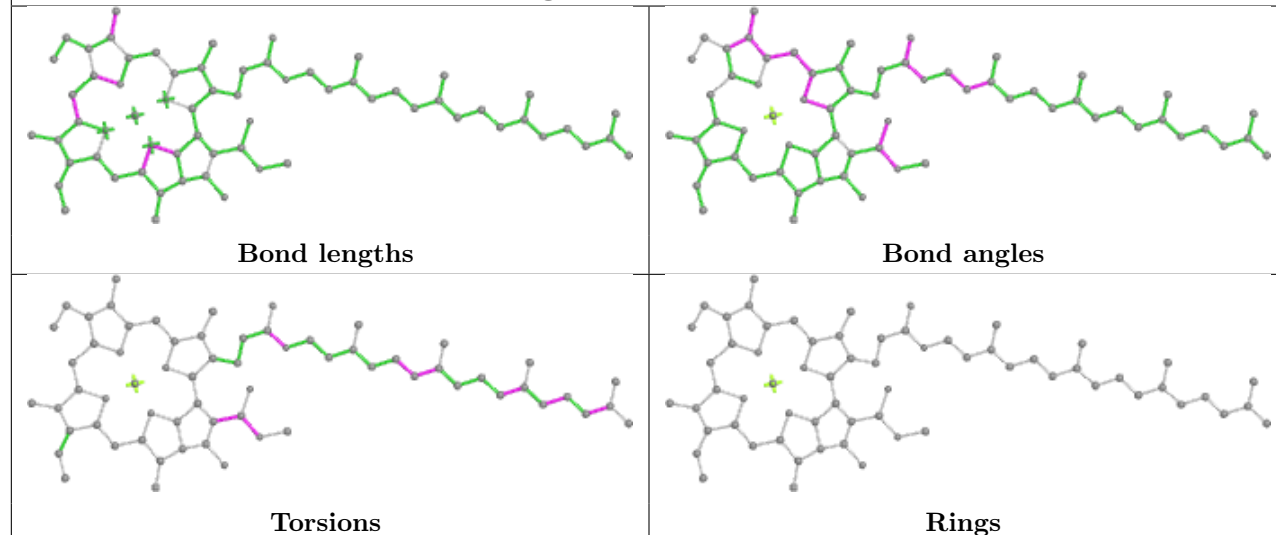
Ligand CLA 5 314



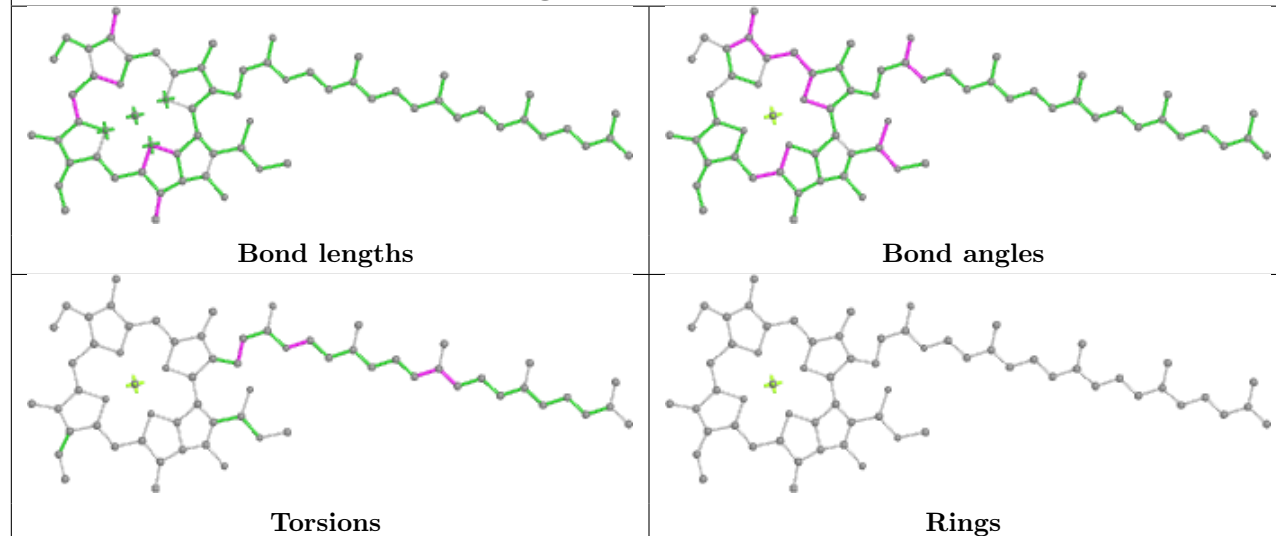
Ligand CLA a 803



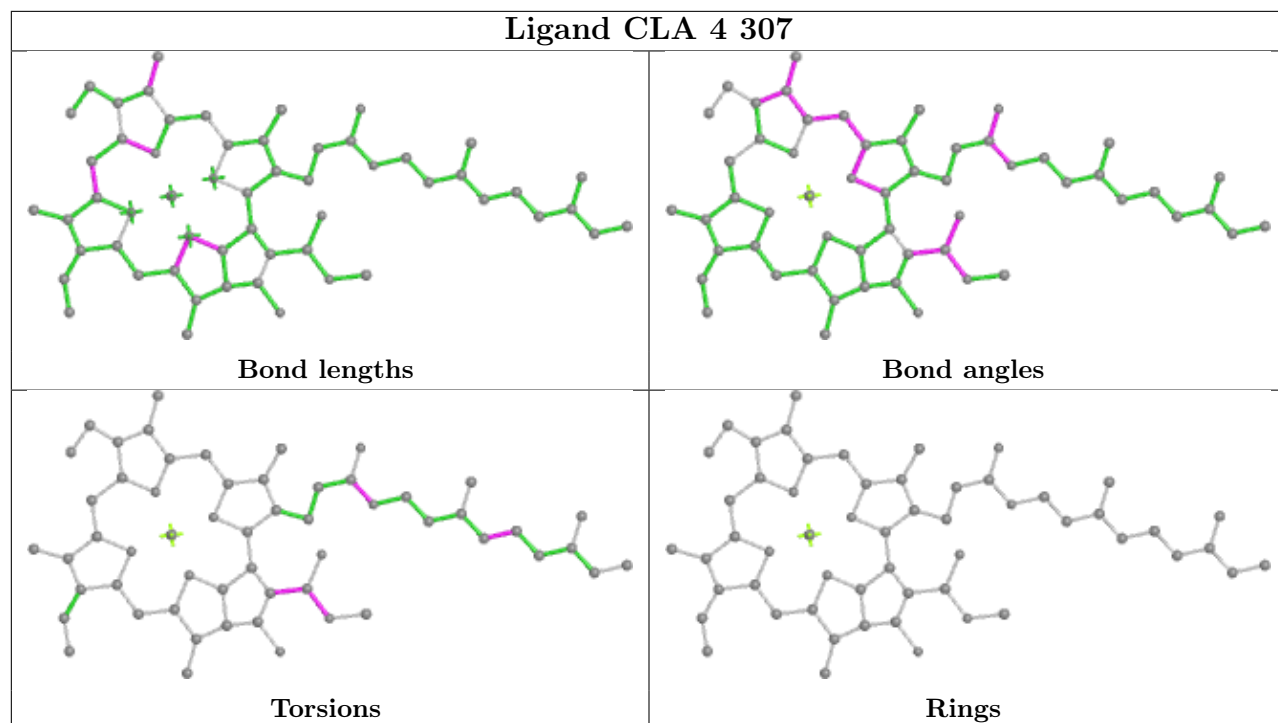
Ligand CLA f 802



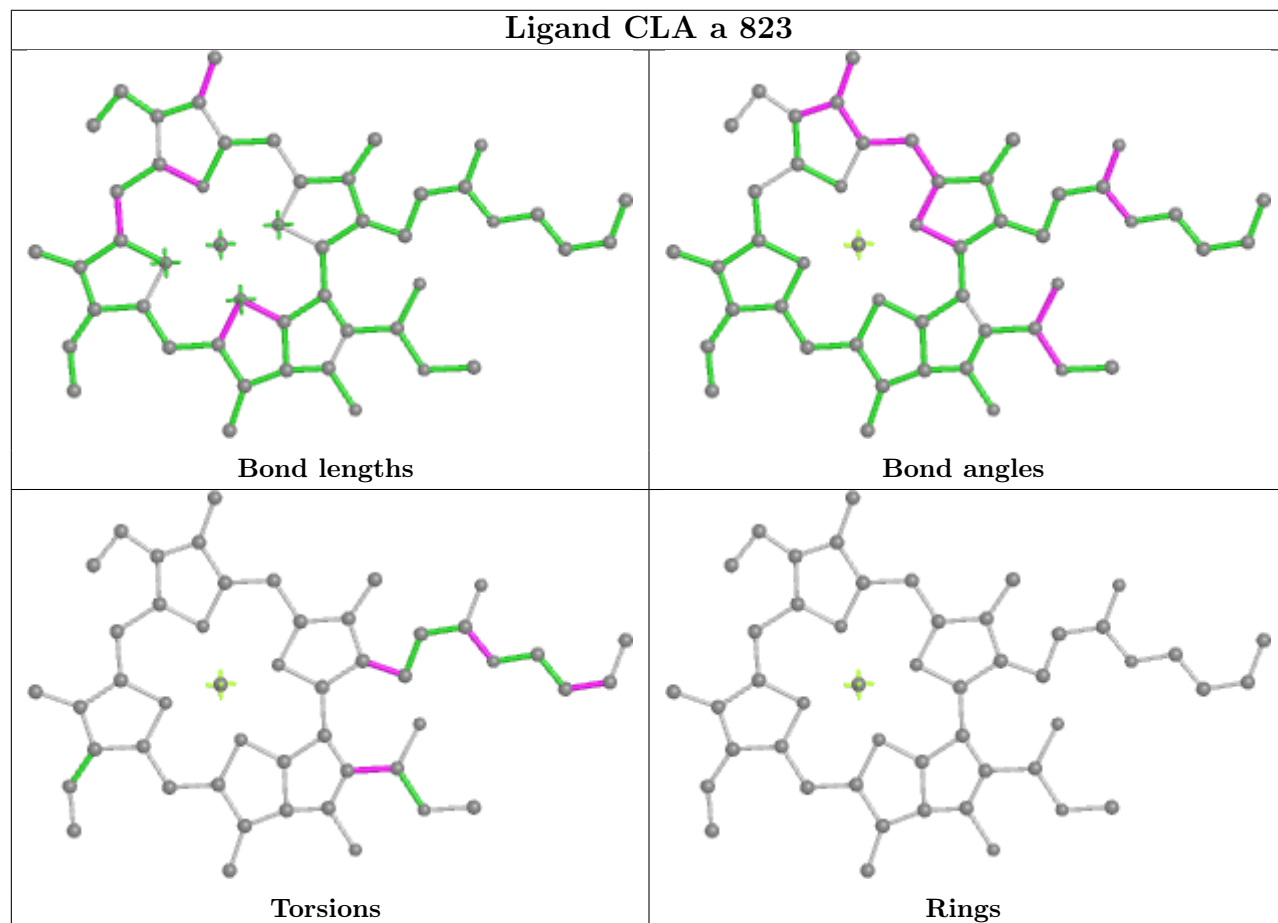
Ligand CLA a 822



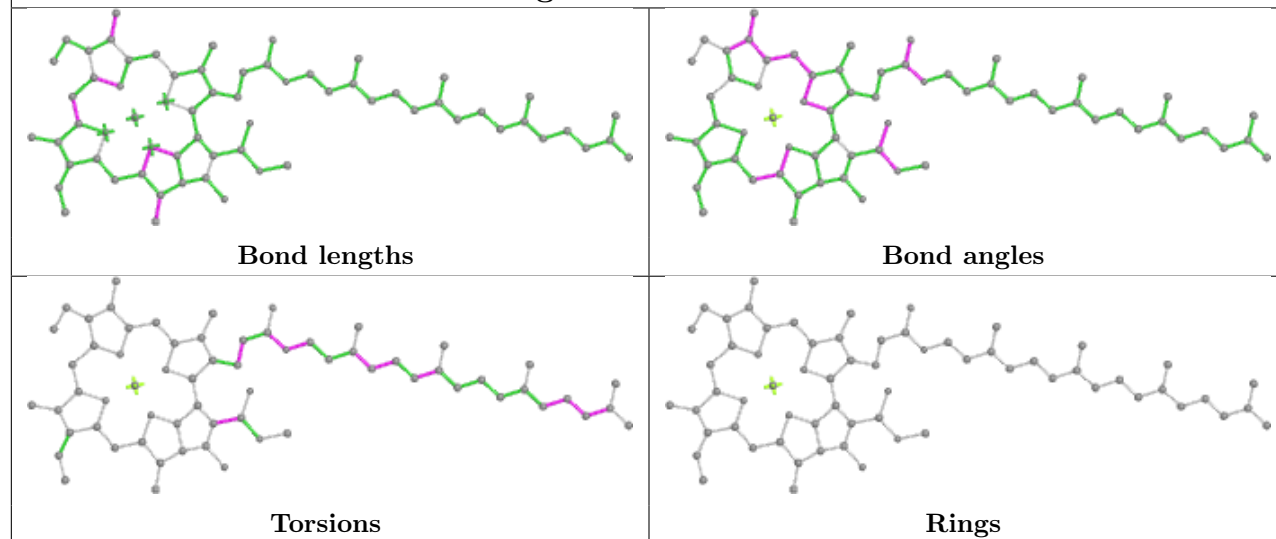
Ligand CLA 4 307



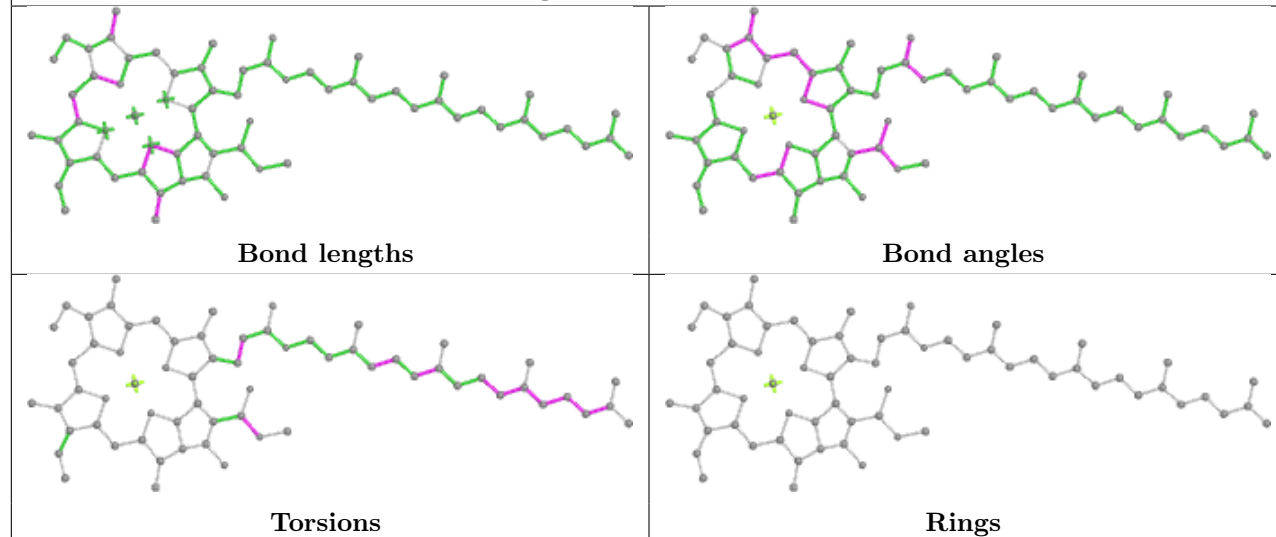
Ligand CLA a 823



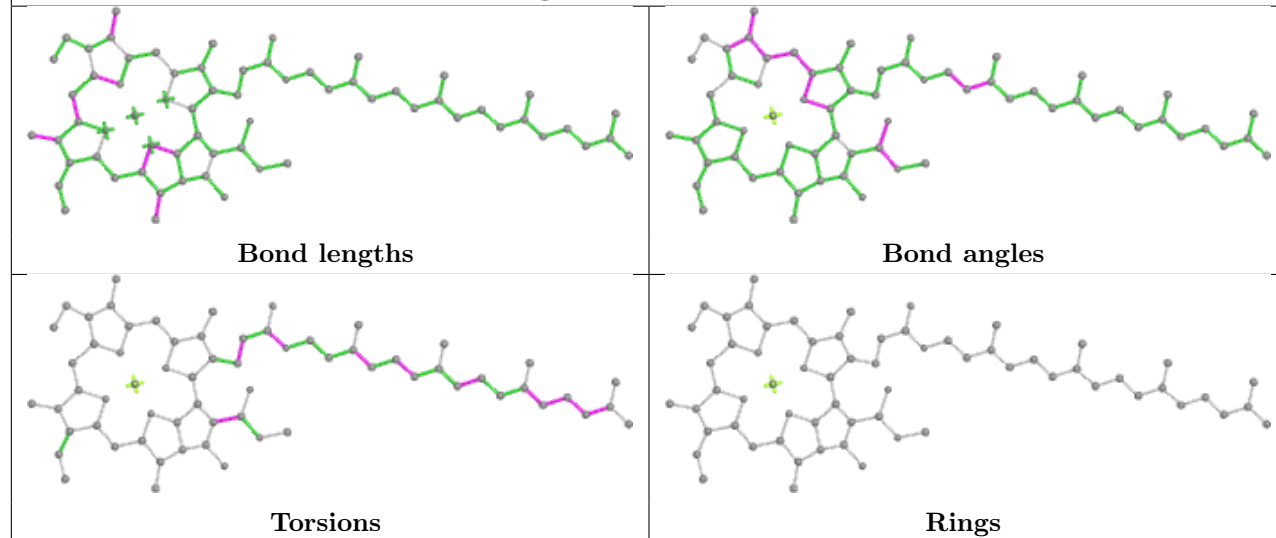
Ligand CLA a 839

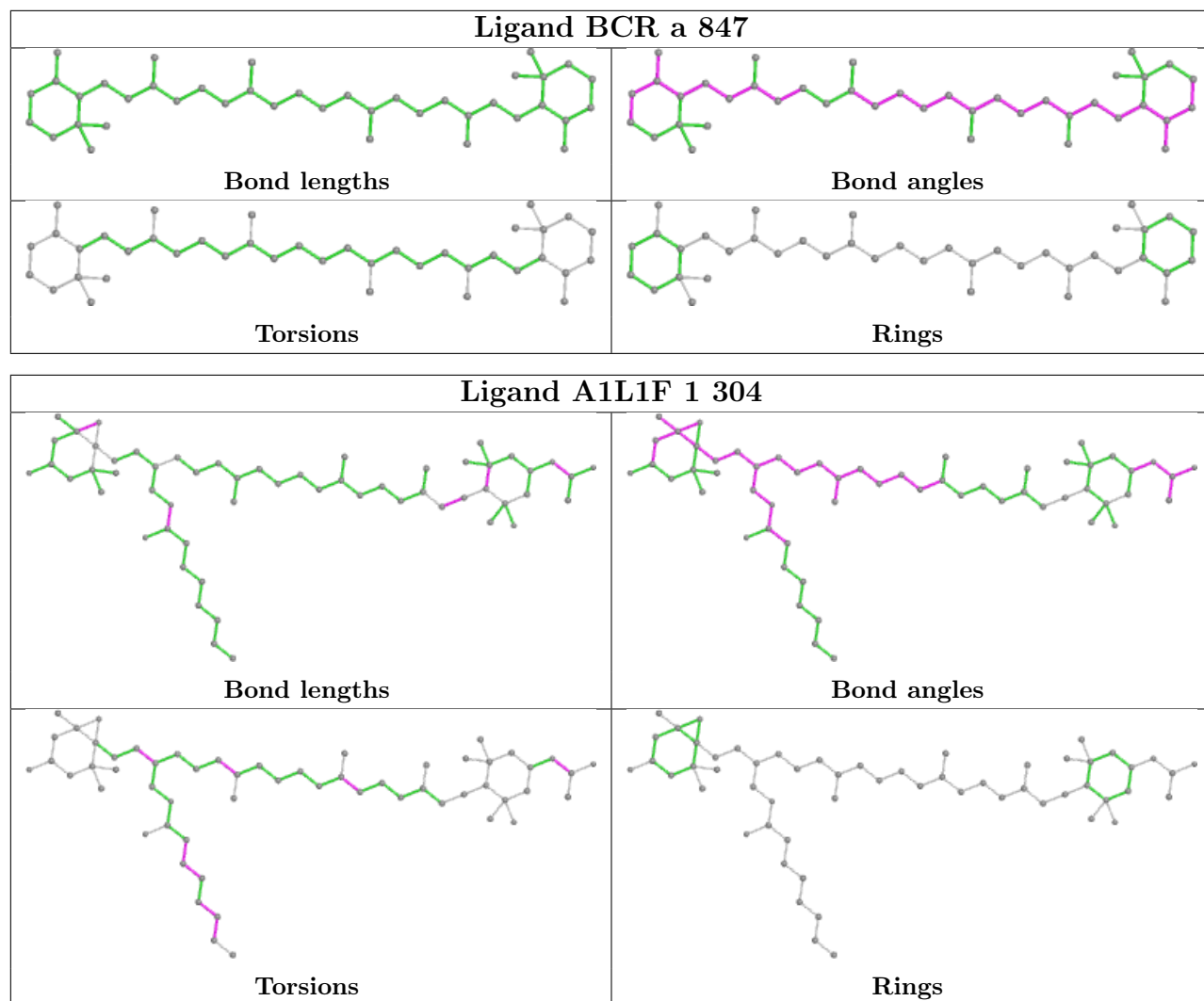


Ligand CLA 4 308

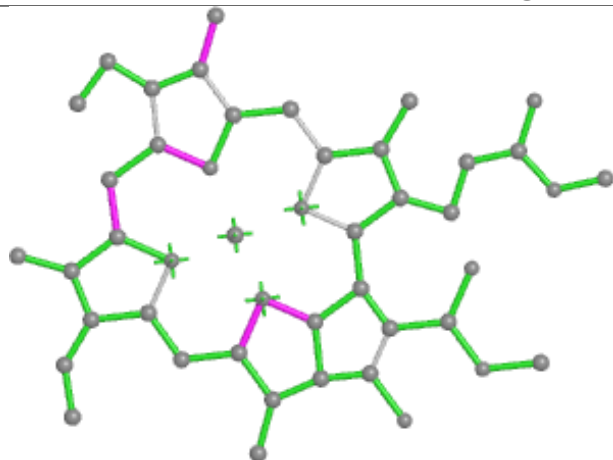


Ligand CLA a 830

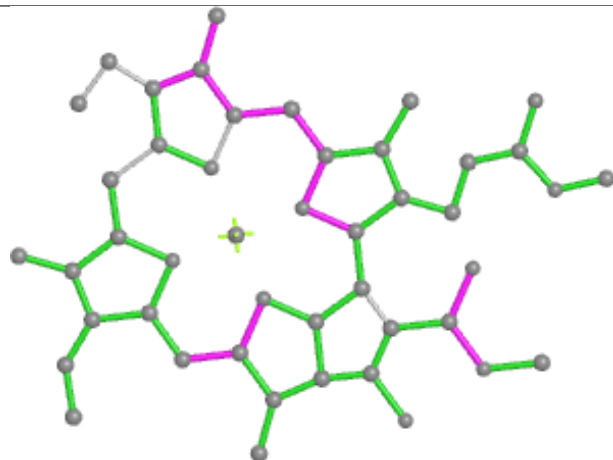




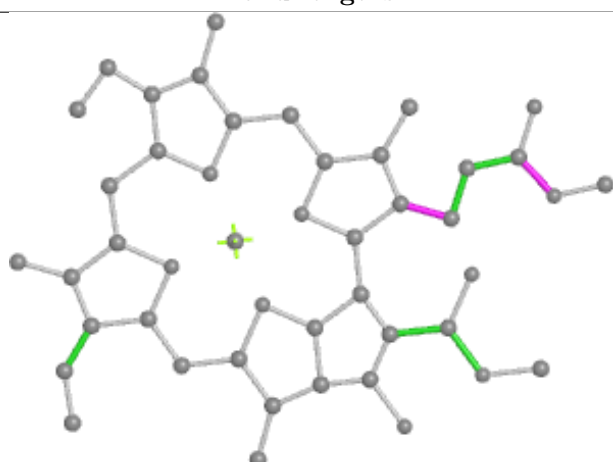
Ligand CLA 4 312



Bond lengths



Bond angles

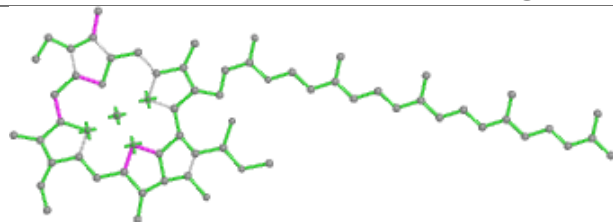


Torsions

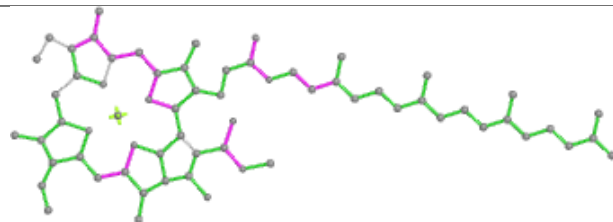


Rings

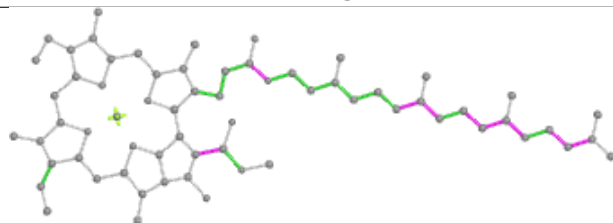
Ligand CLA a 844



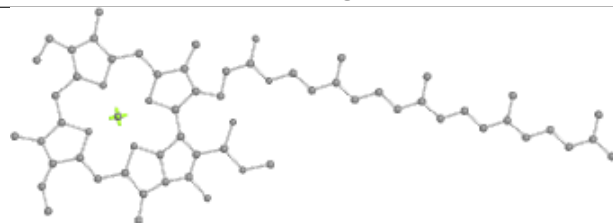
Bond lengths



Bond angles

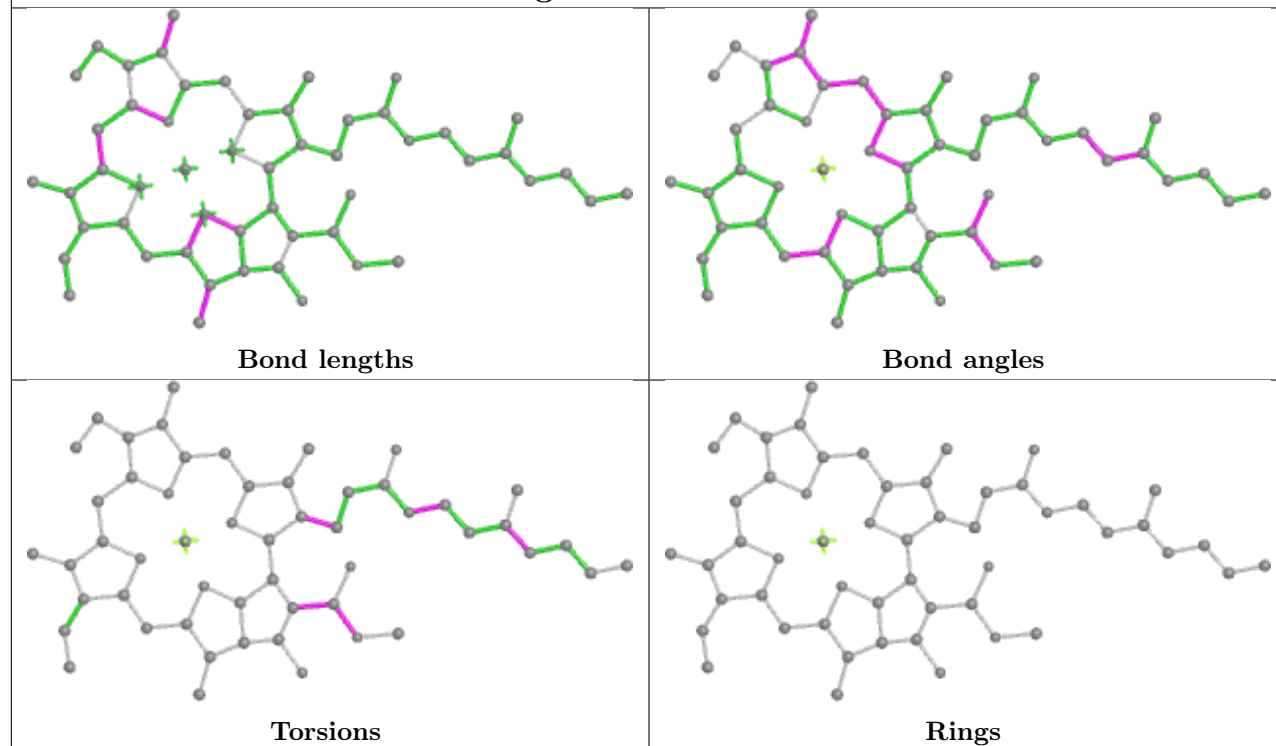


Torsions

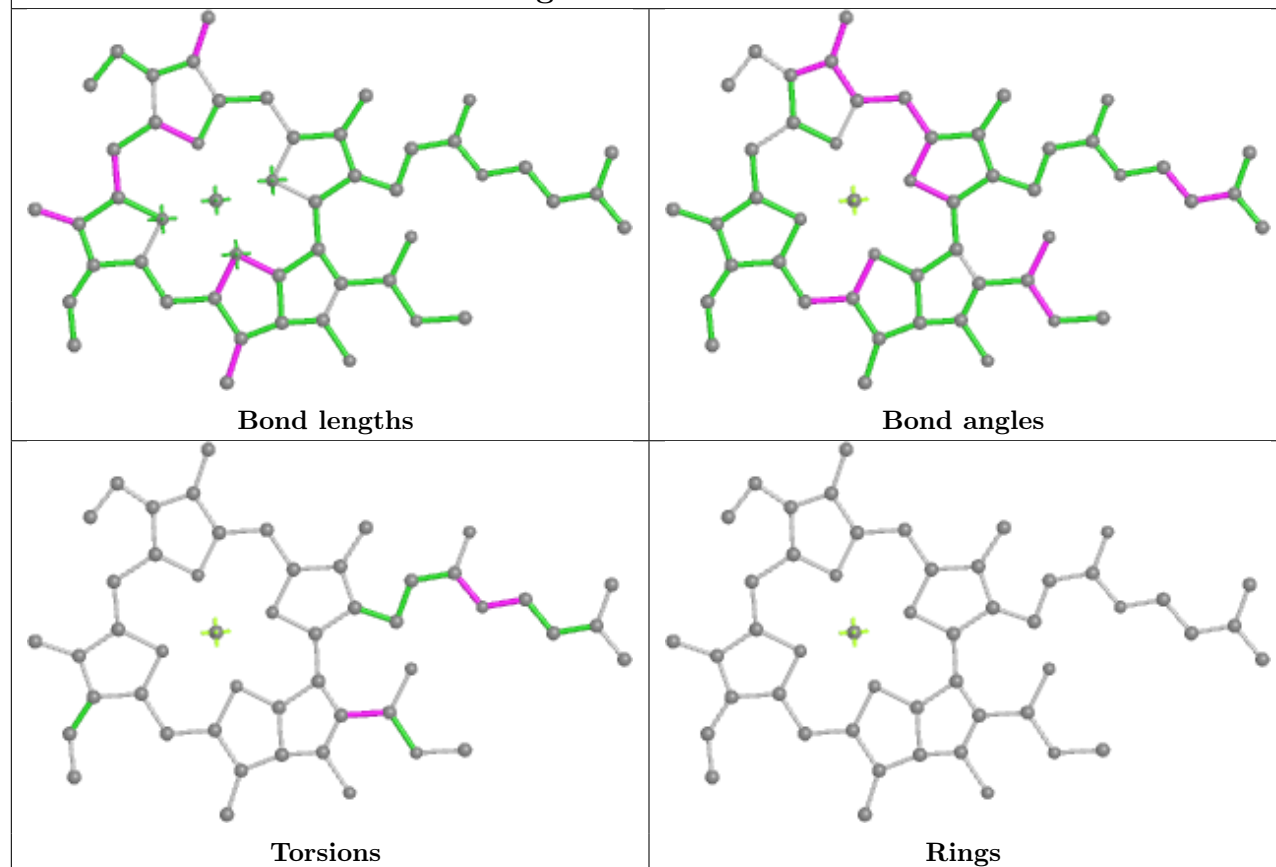


Rings

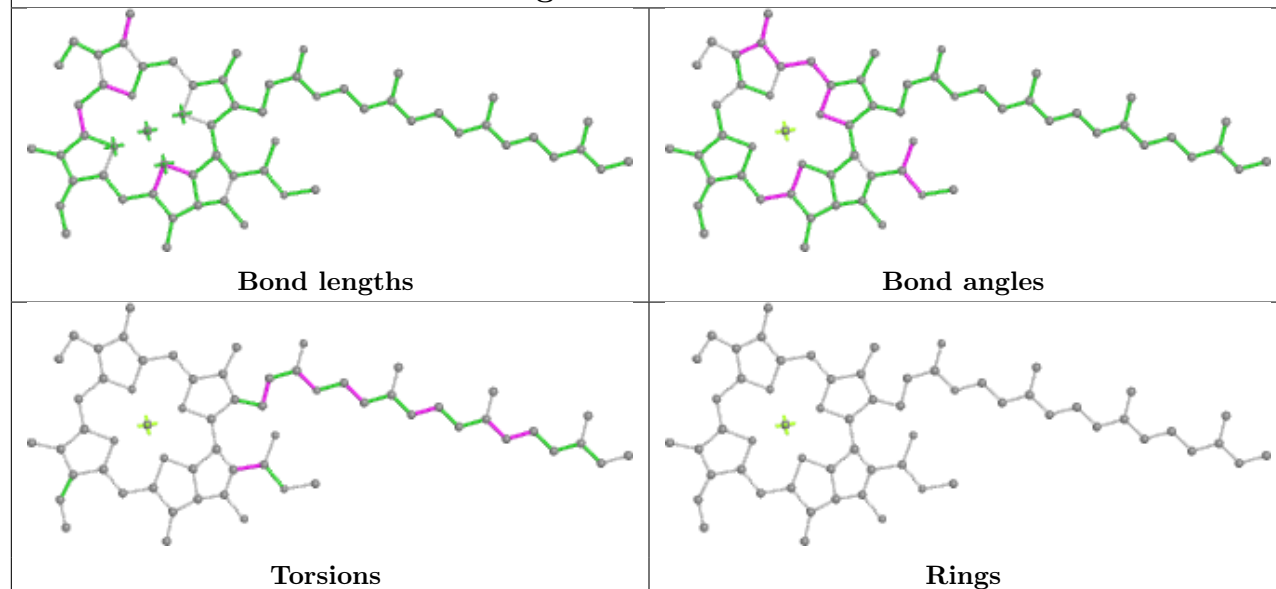
Ligand CLA b 835



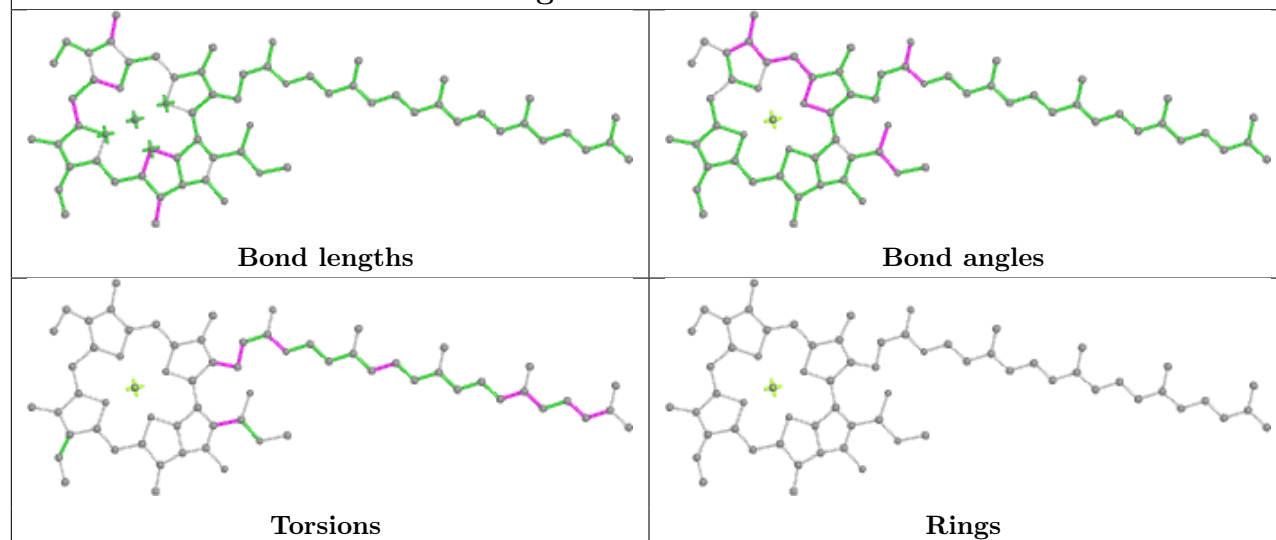
Ligand CLA a 816



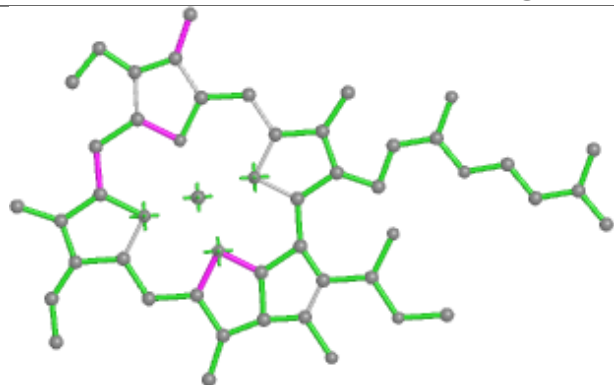
Ligand CLA 1 305



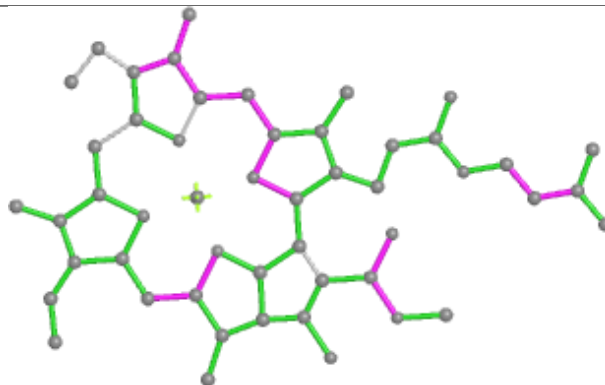
Ligand CLA 2 310



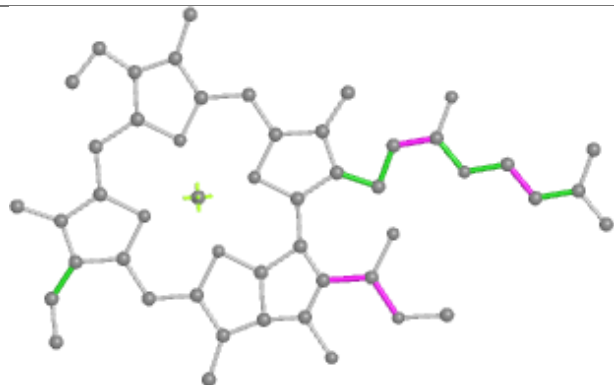
Ligand CLA 4 309



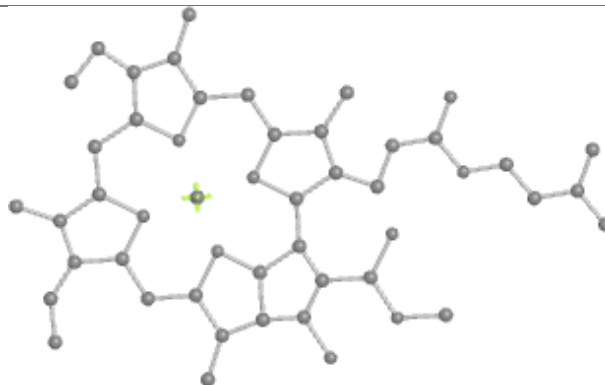
Bond lengths



Bond angles

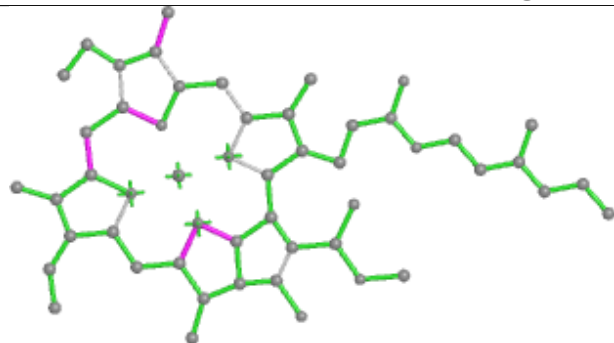


Torsions

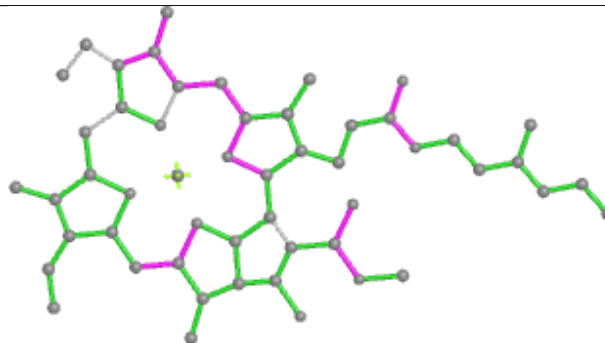


Rings

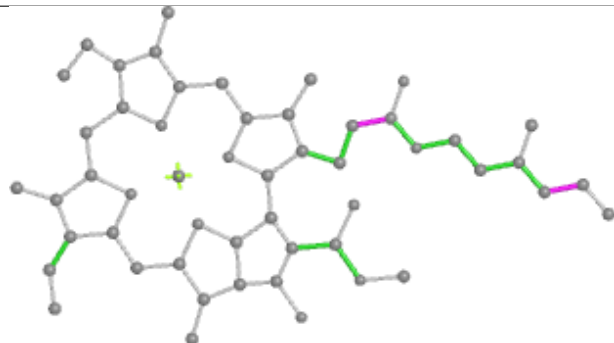
Ligand CLA 1 312



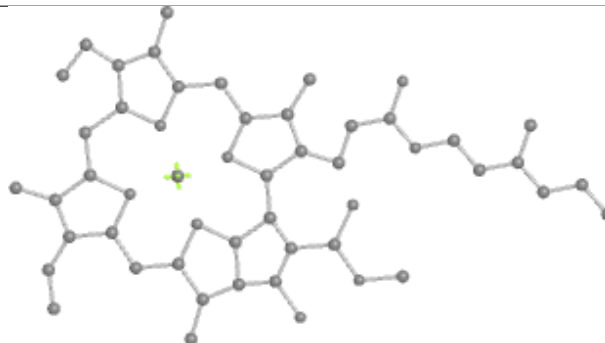
Bond lengths



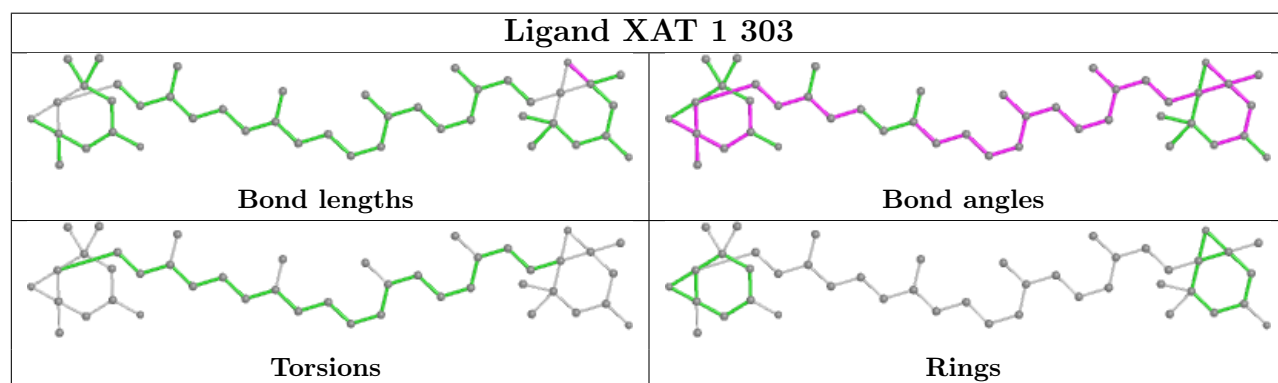
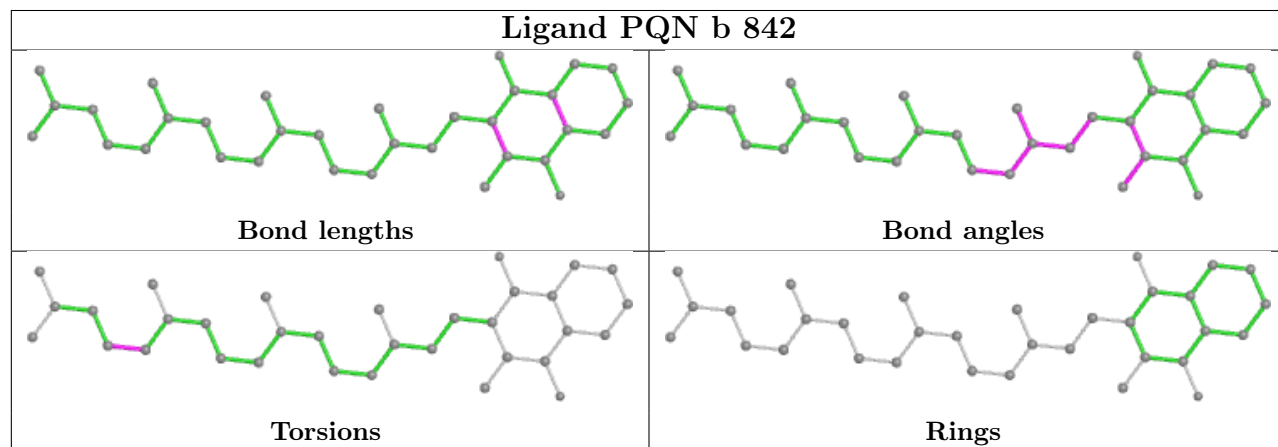
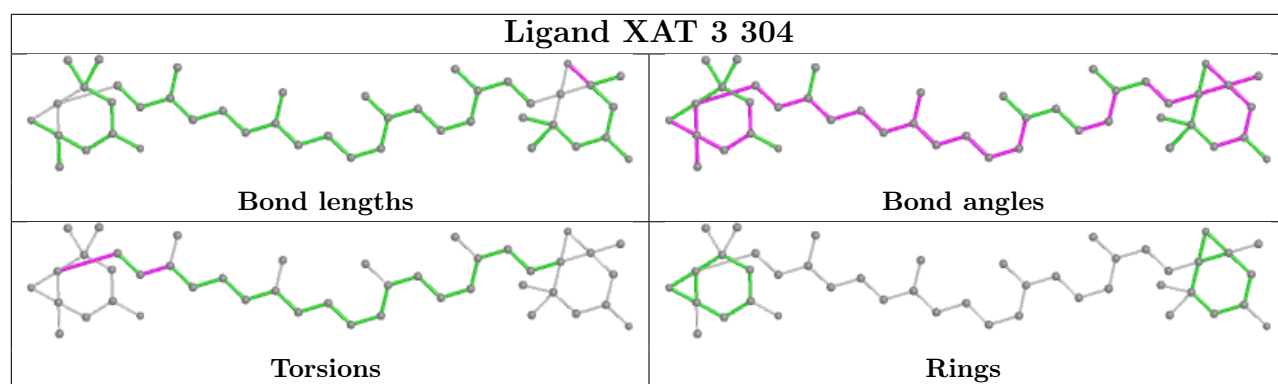
Bond angles



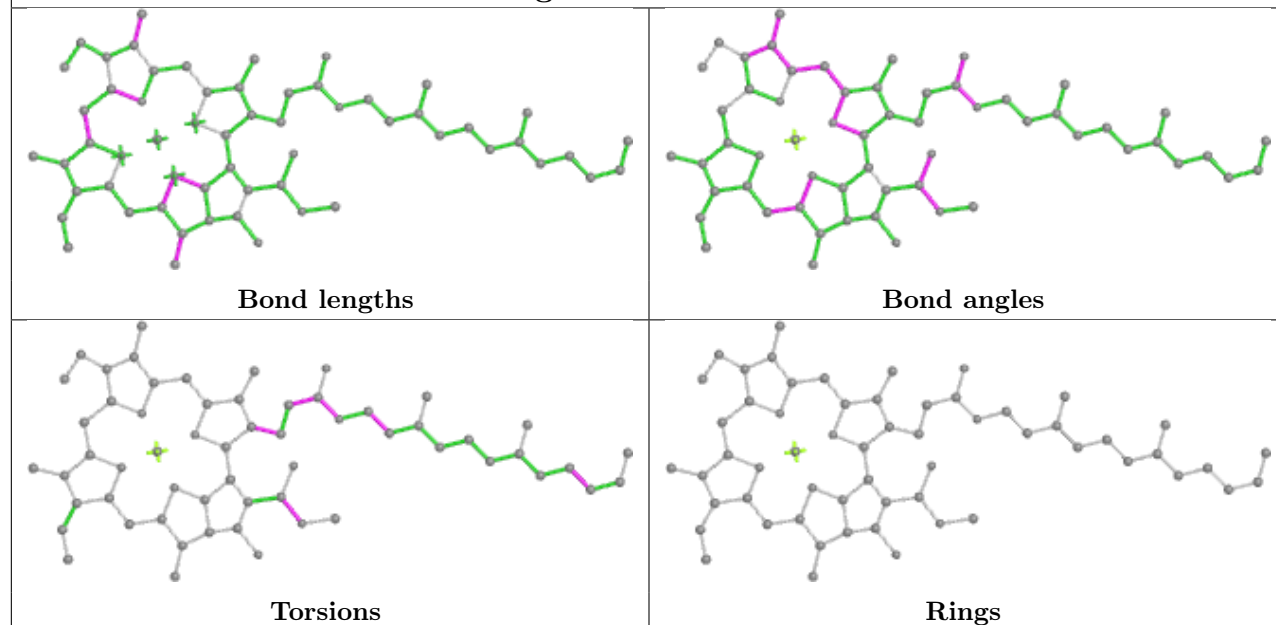
Torsions



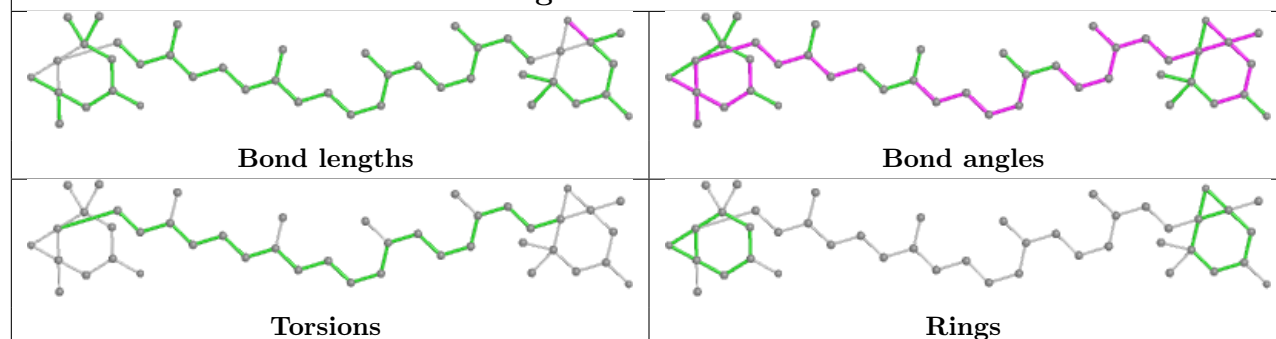
Rings



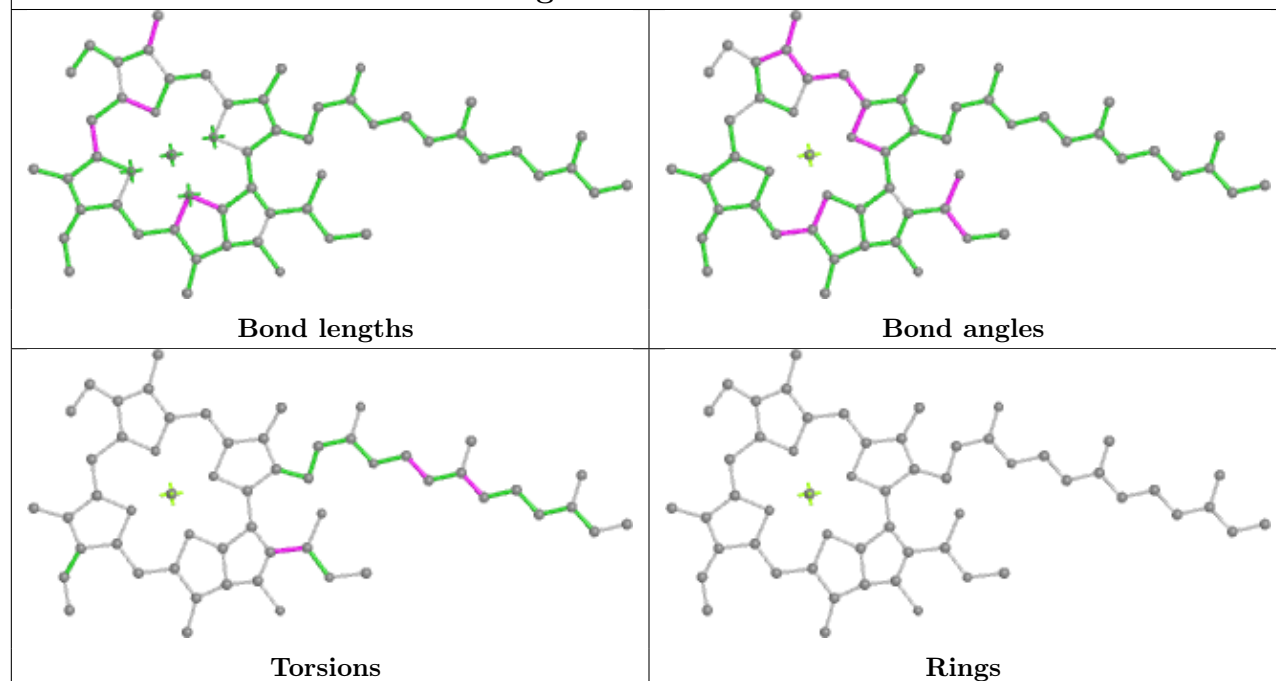
Ligand CLA b 818

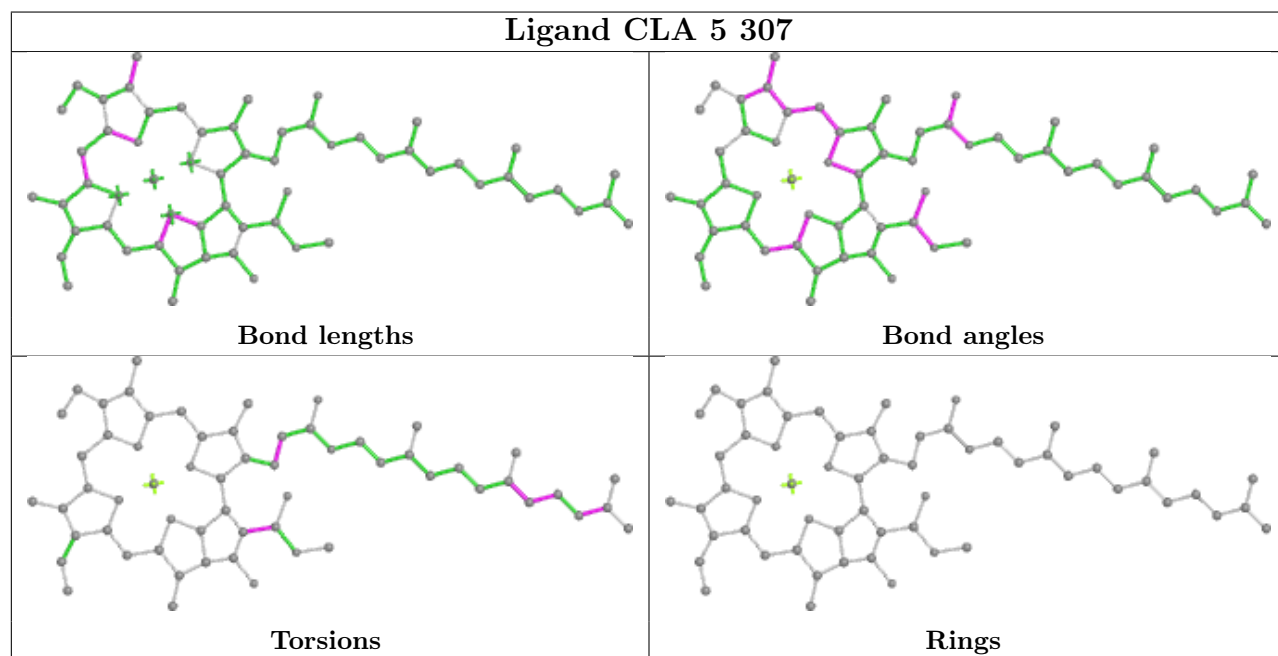
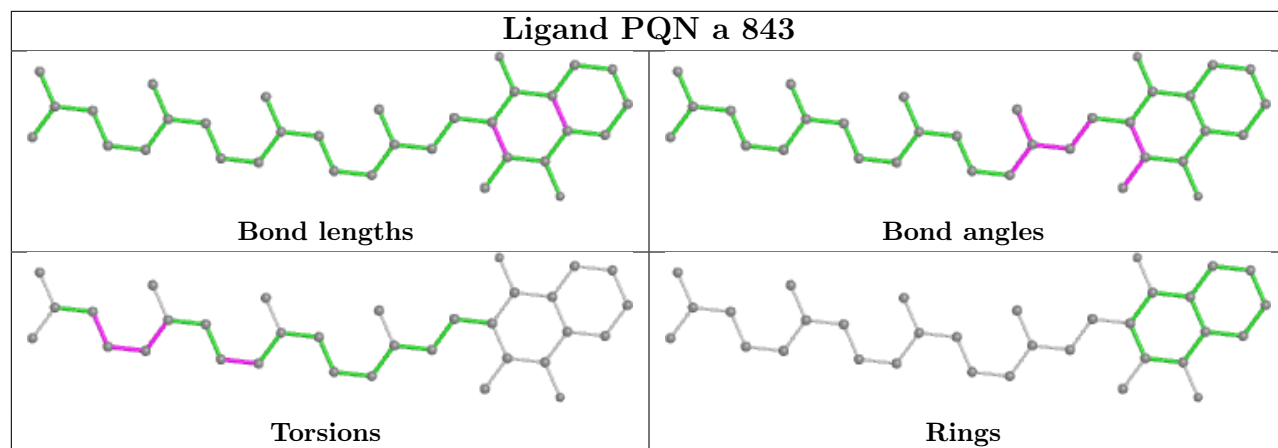
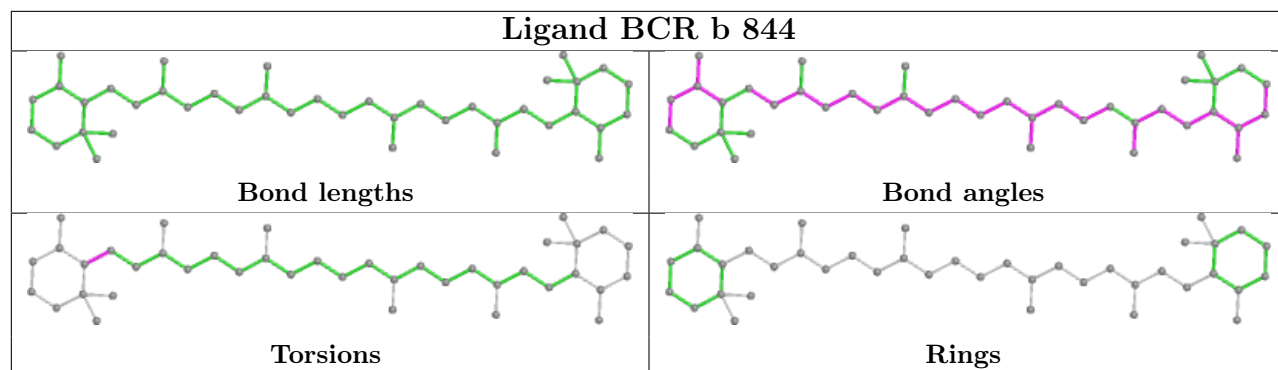


Ligand XAT 2 302

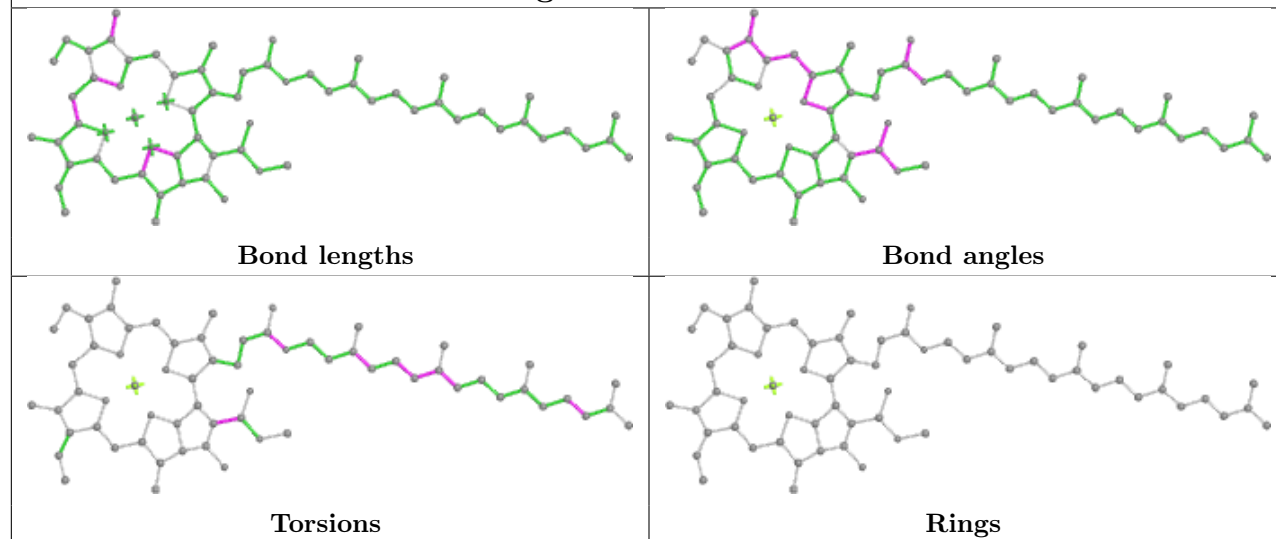


Ligand CLA 3 310

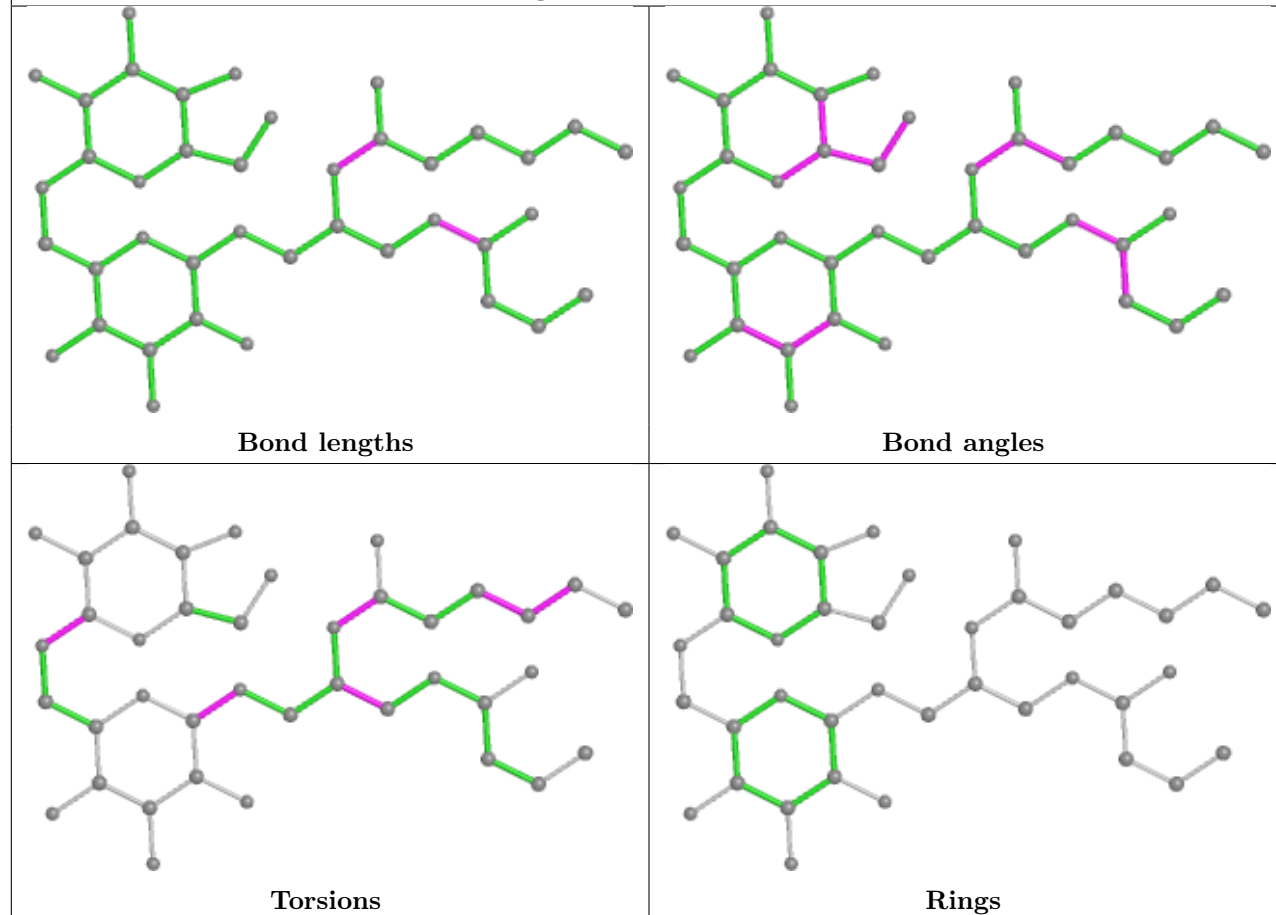




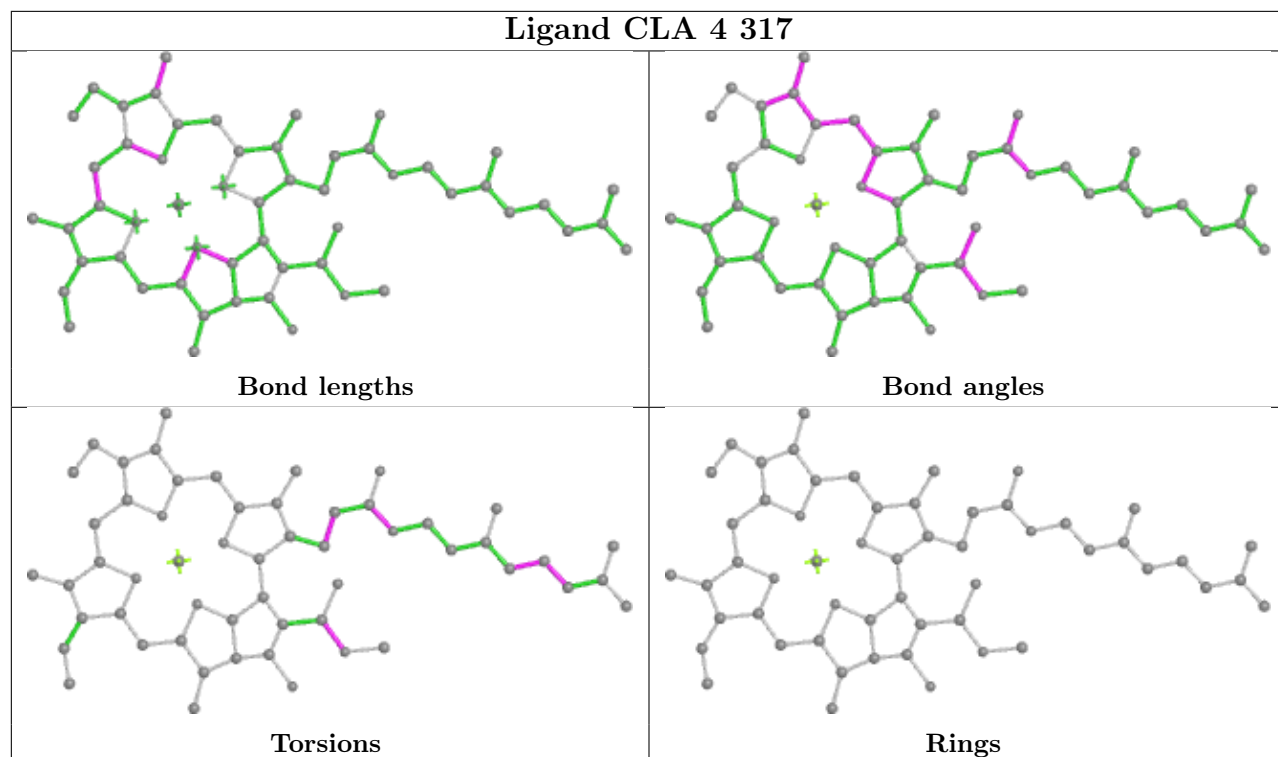
Ligand CLA a 831



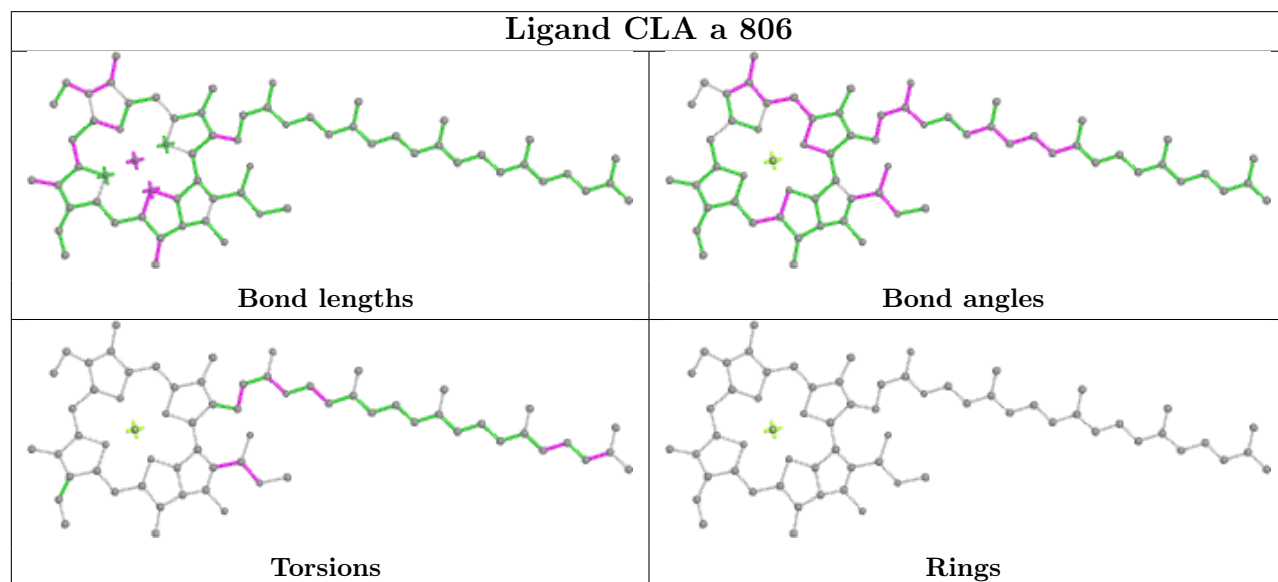
Ligand DGD 4 318



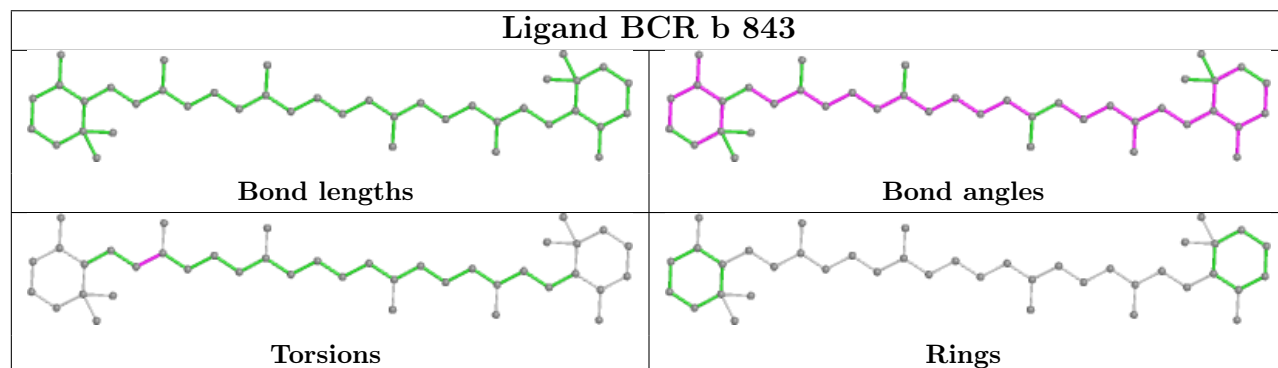
Ligand CLA 4 317

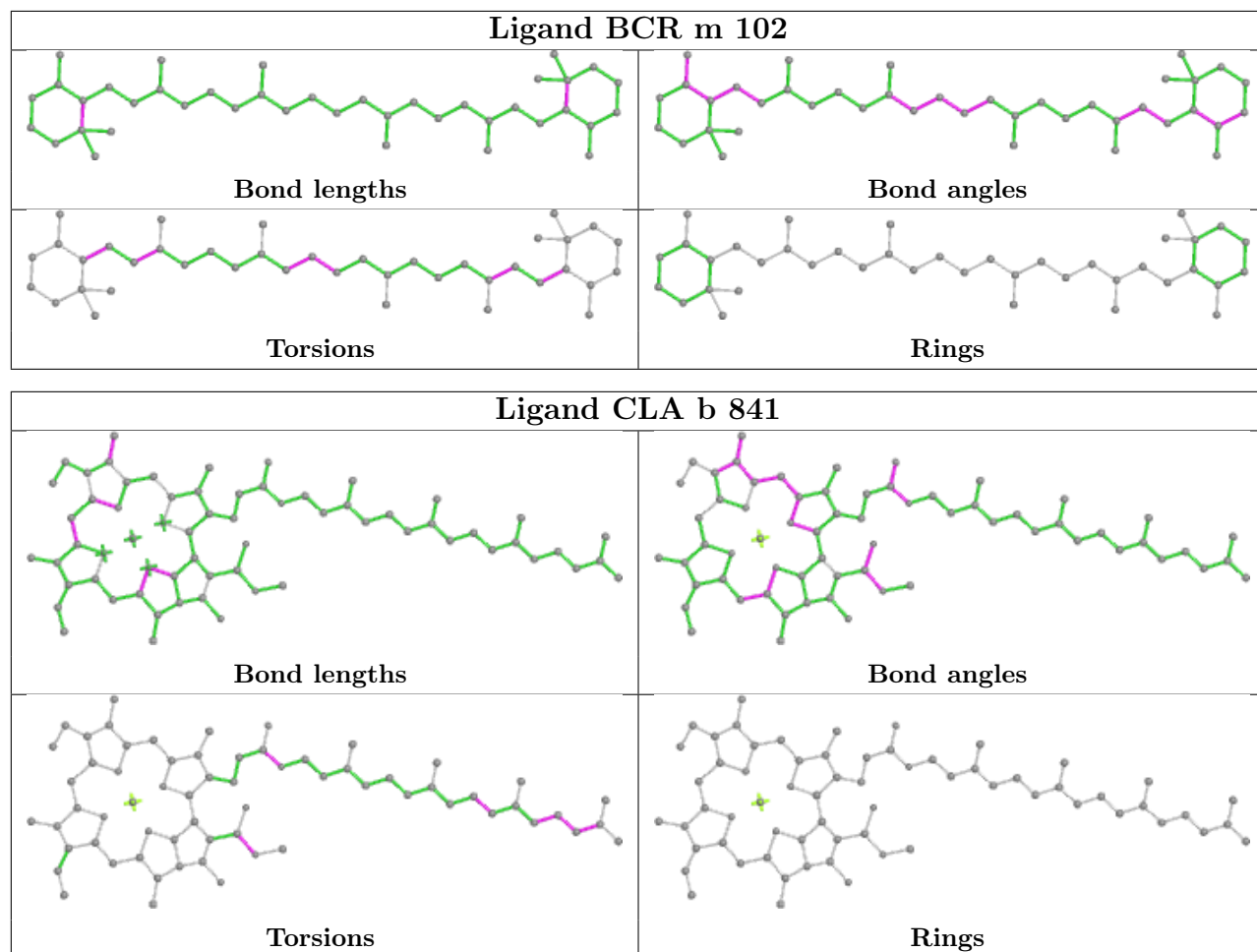


Ligand CLA a 806

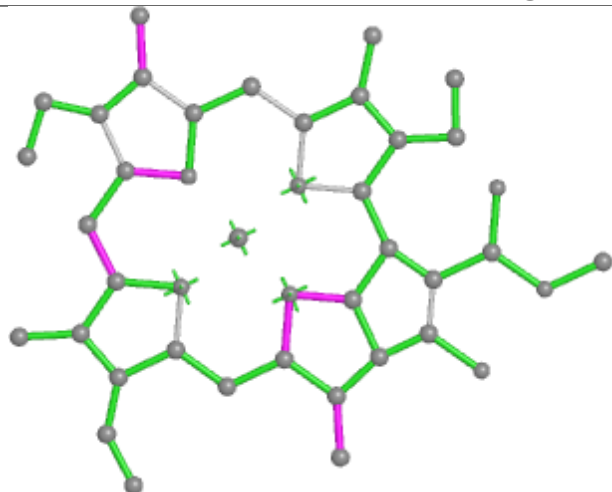


Ligand BCR b 843

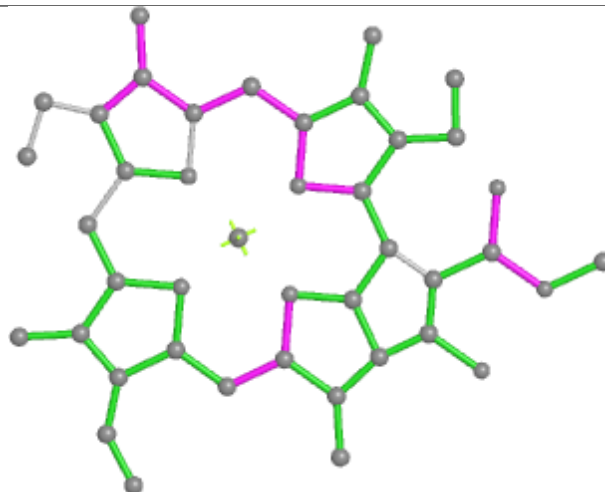




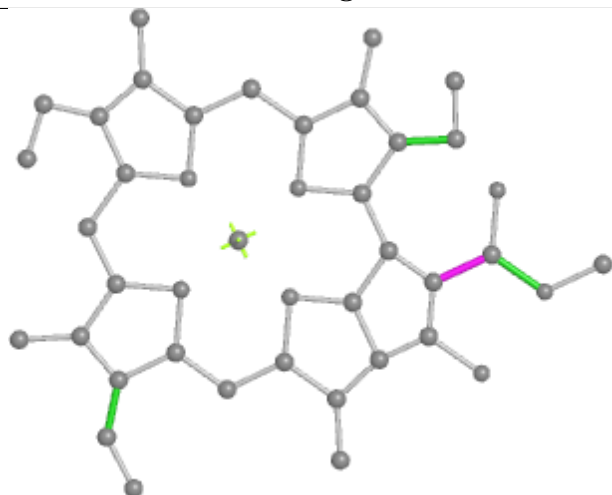
Ligand CLA 1 202



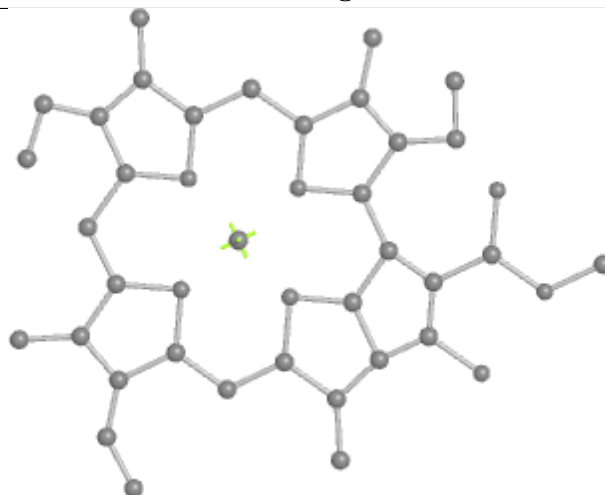
Bond lengths



Bond angles

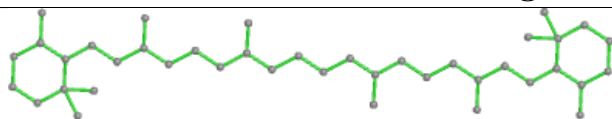


Torsions

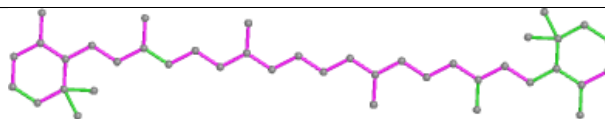


Rings

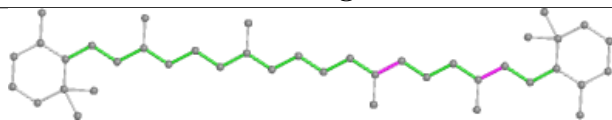
Ligand BCR f 801



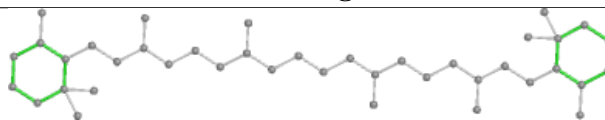
Bond lengths



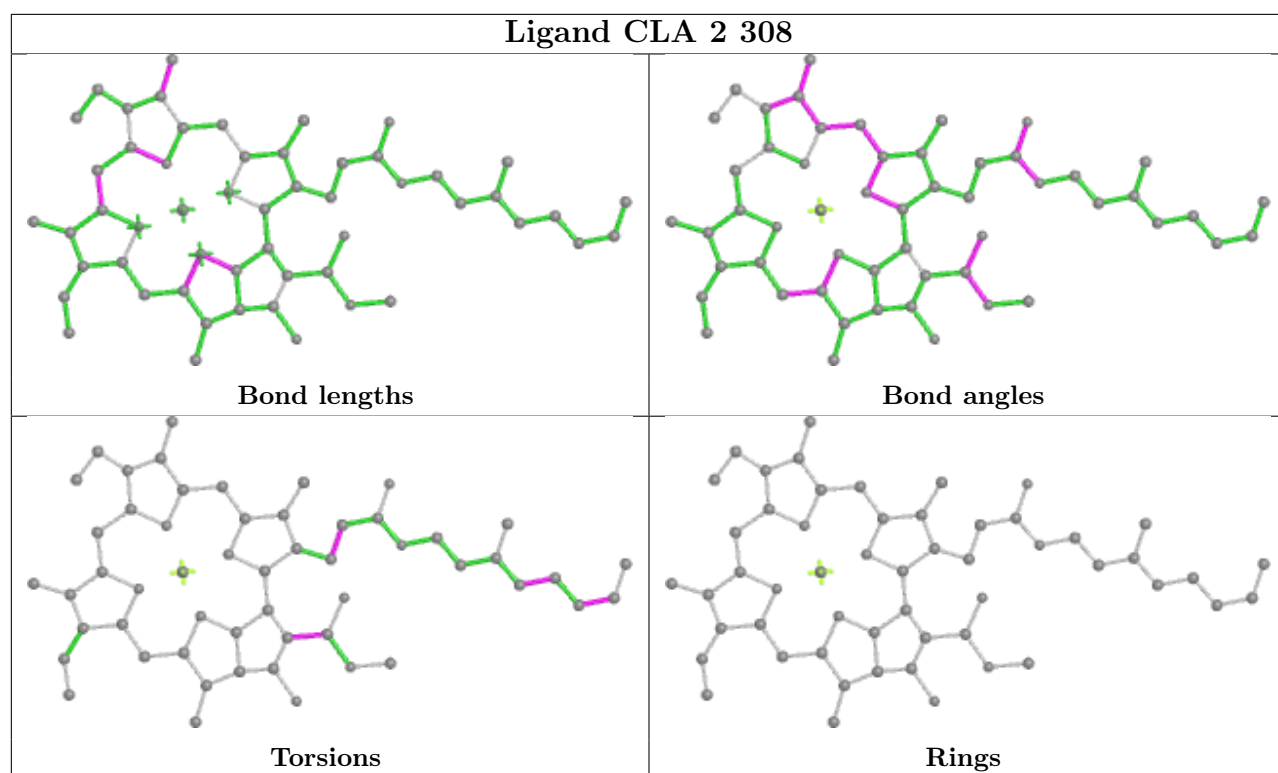
Bond angles



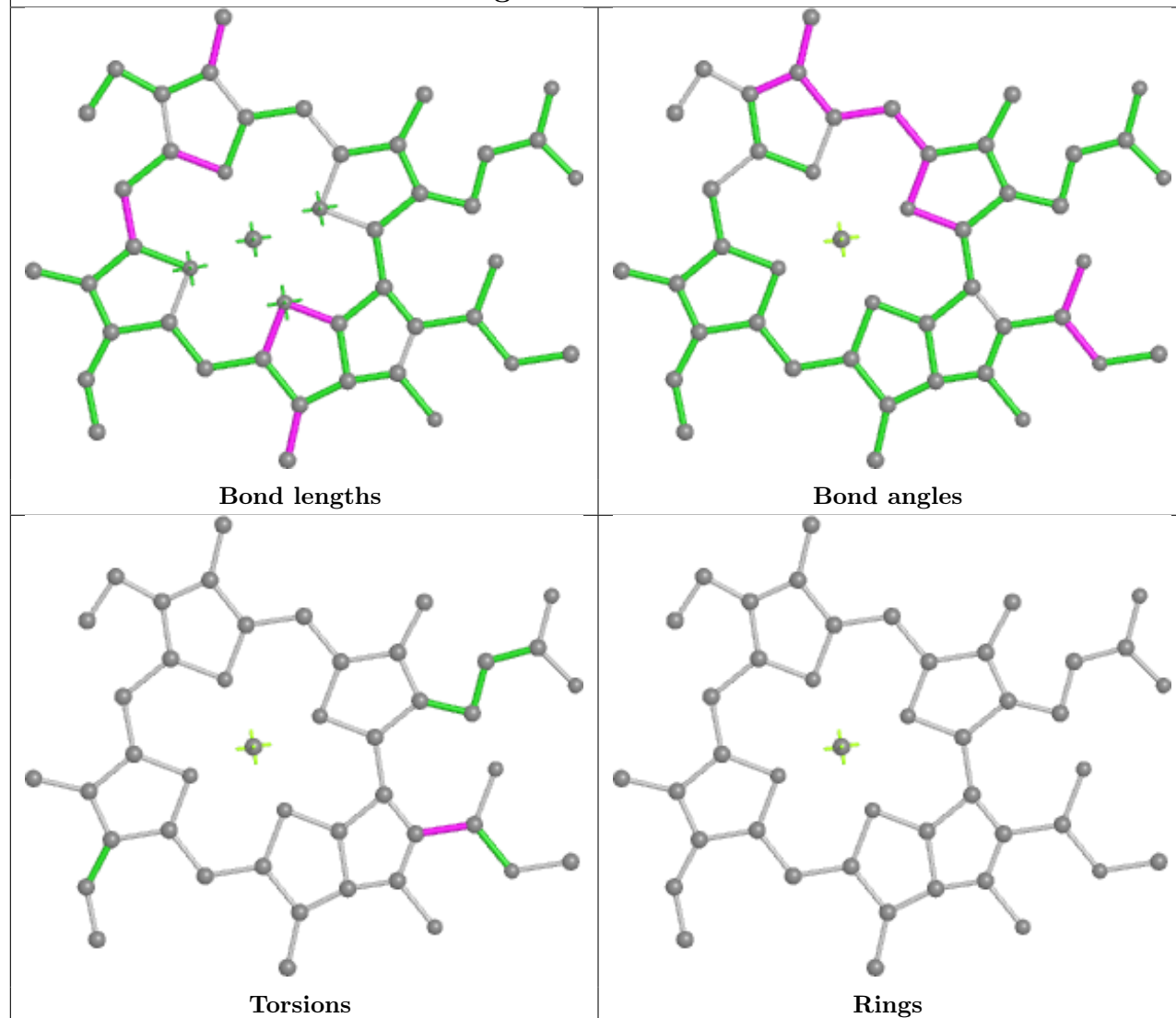
Torsions



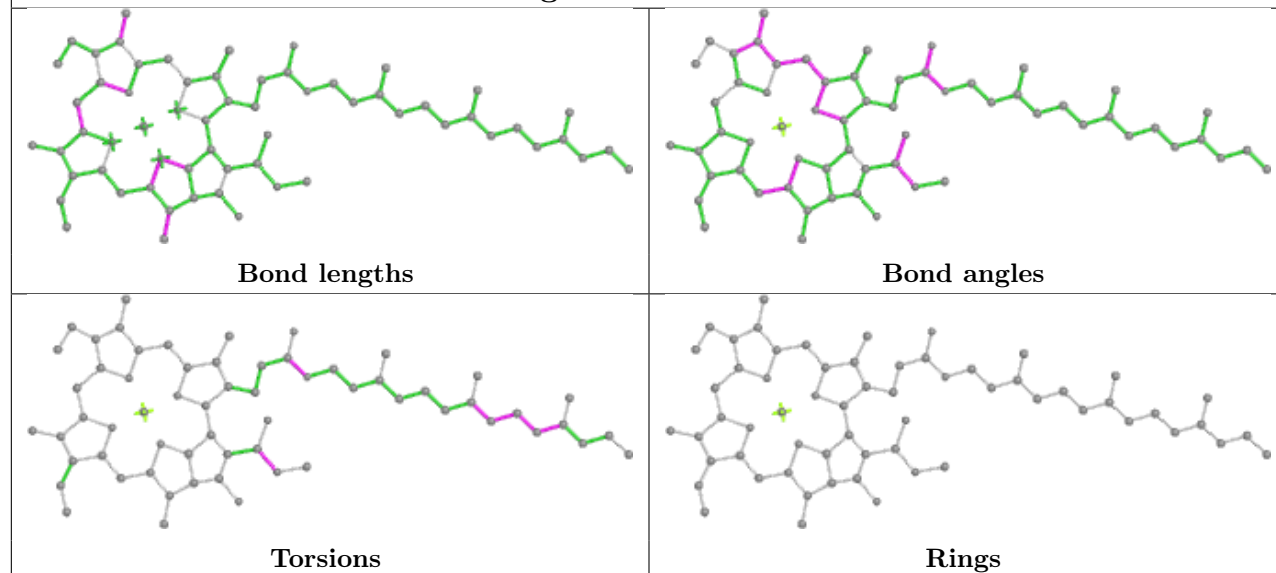
Rings



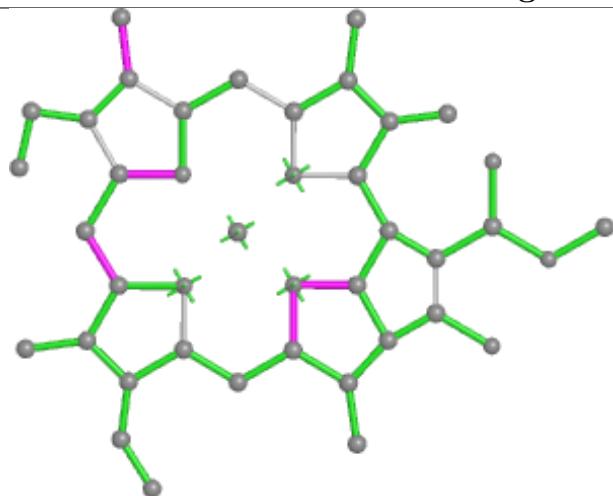
Ligand CLA 3 307



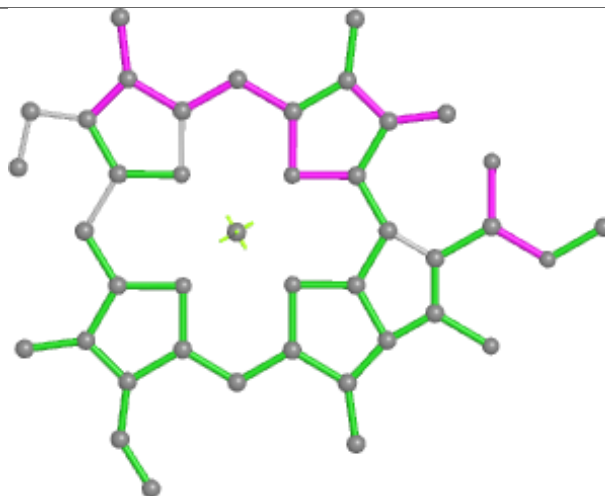
Ligand CLA i 102



Ligand CLA 4 315



Bond lengths



Bond angles

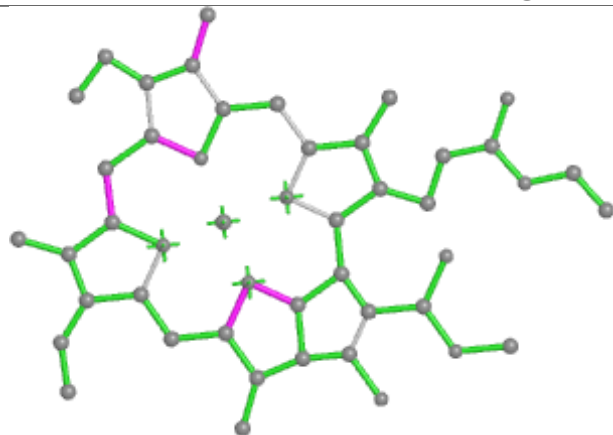


Torsions

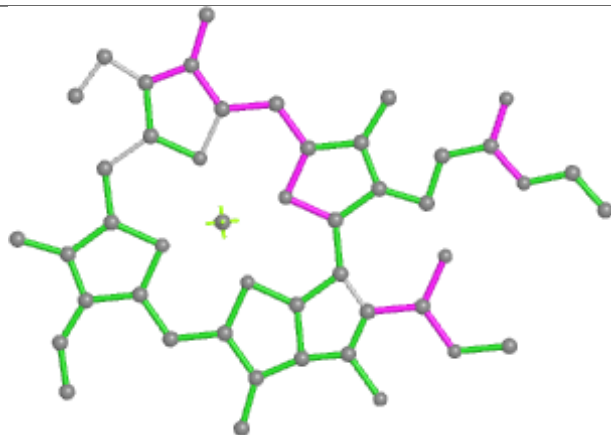


Rings

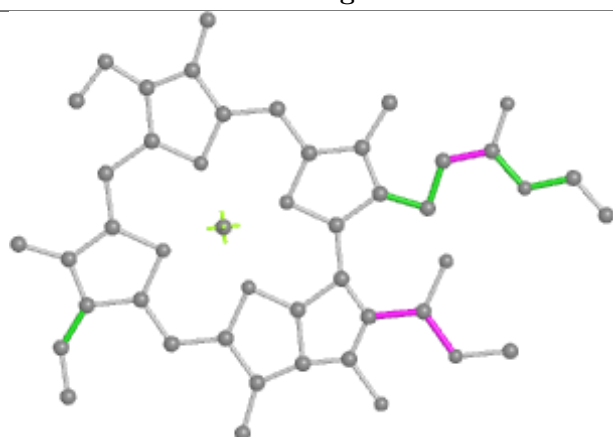
Ligand CLA 3 308



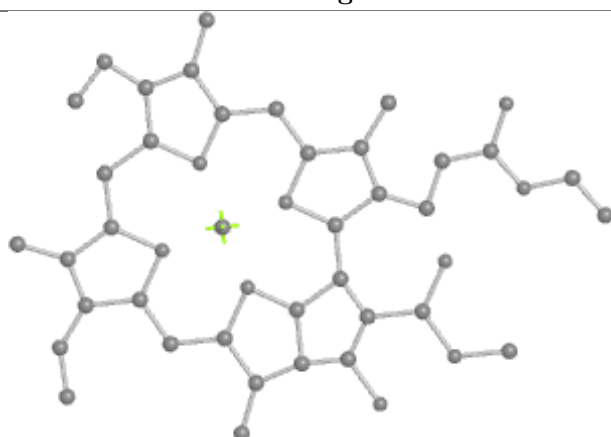
Bond lengths



Bond angles

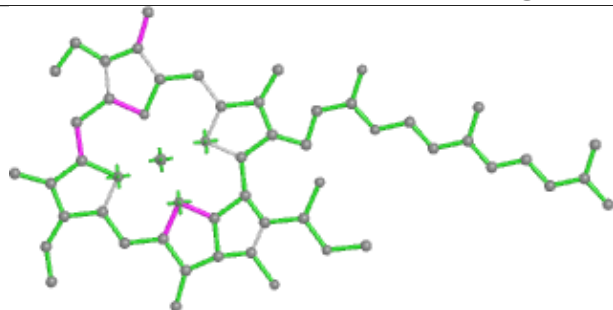


Torsions

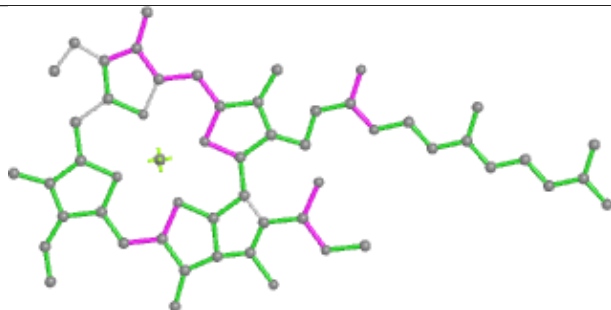


Rings

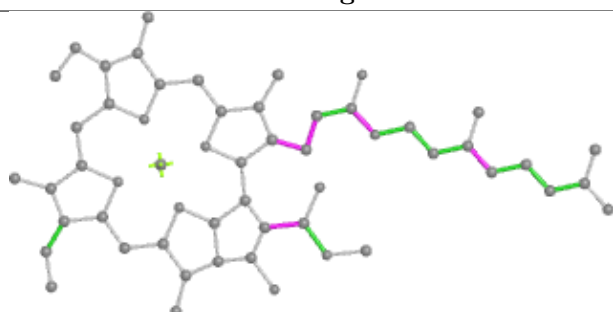
Ligand CLA a 825



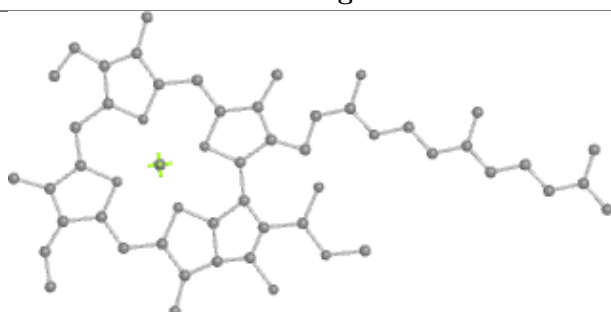
Bond lengths



Bond angles

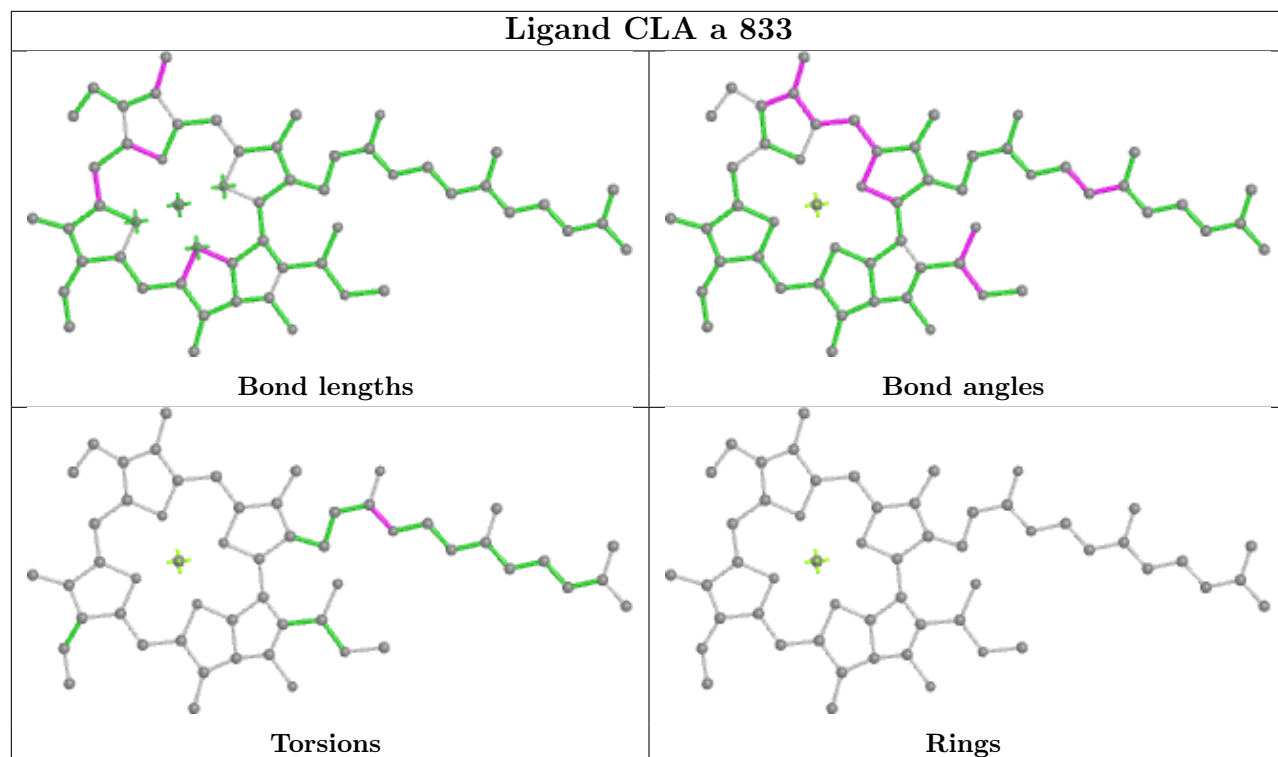


Torsions

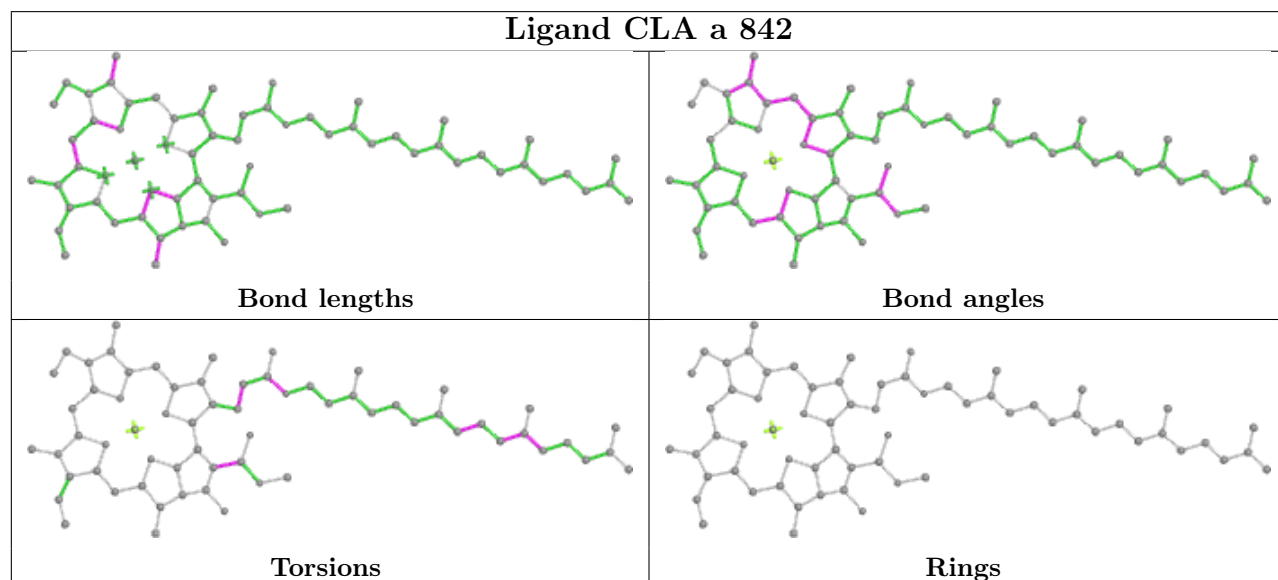


Rings

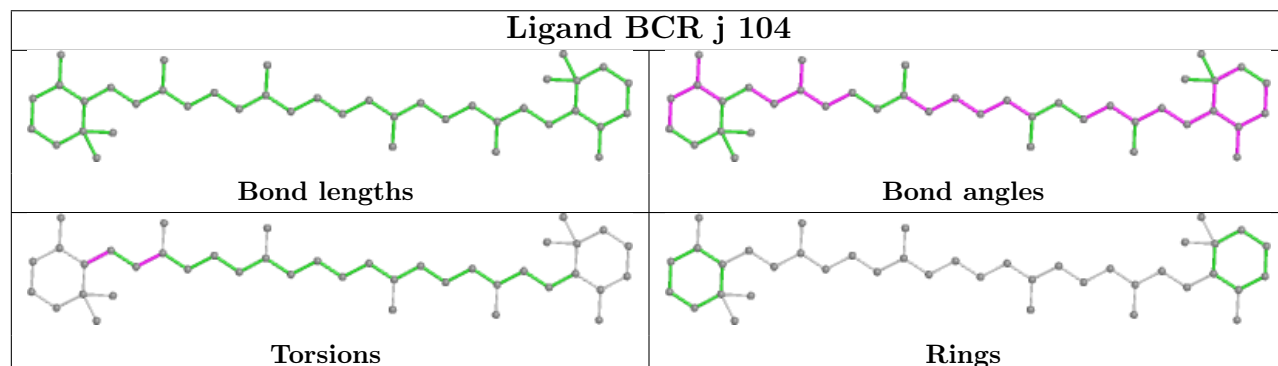
Ligand CLA a 833

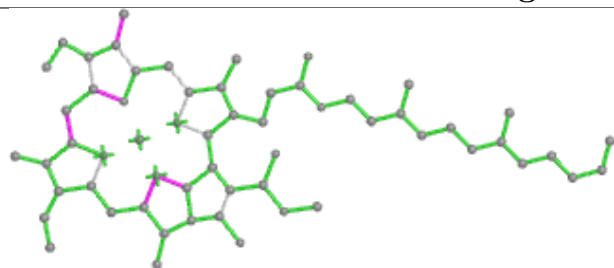


Ligand CLA a 842

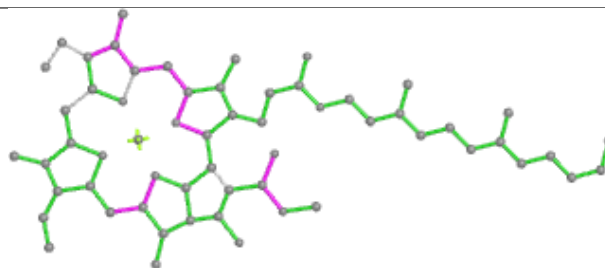


Ligand BCR j 104

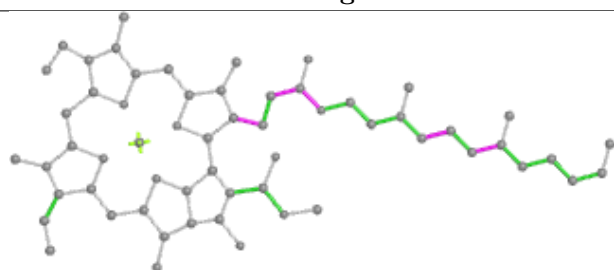


Ligand CLA 3 312

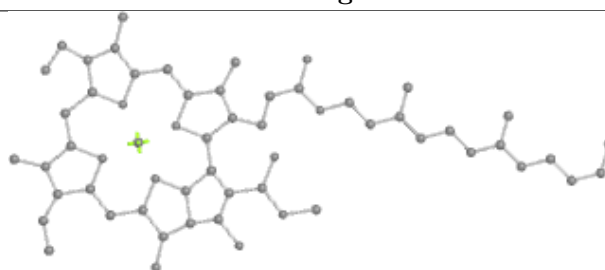
Bond lengths



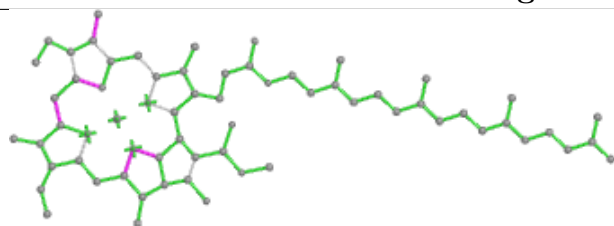
Bond angles



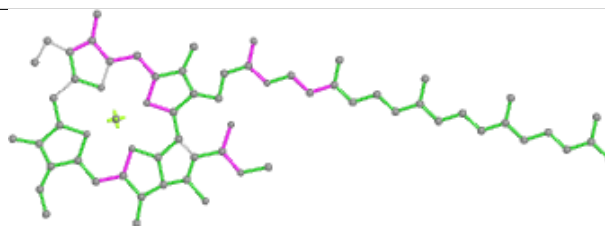
Torsions



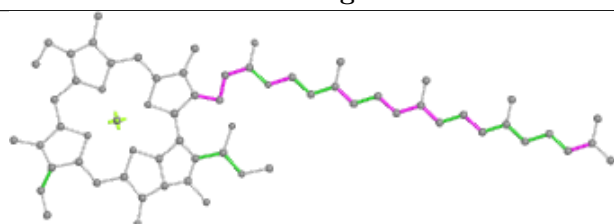
Rings

Ligand CLA b 810

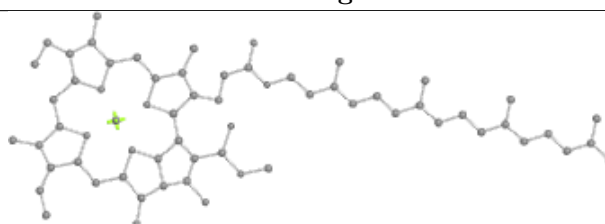
Bond lengths



Bond angles

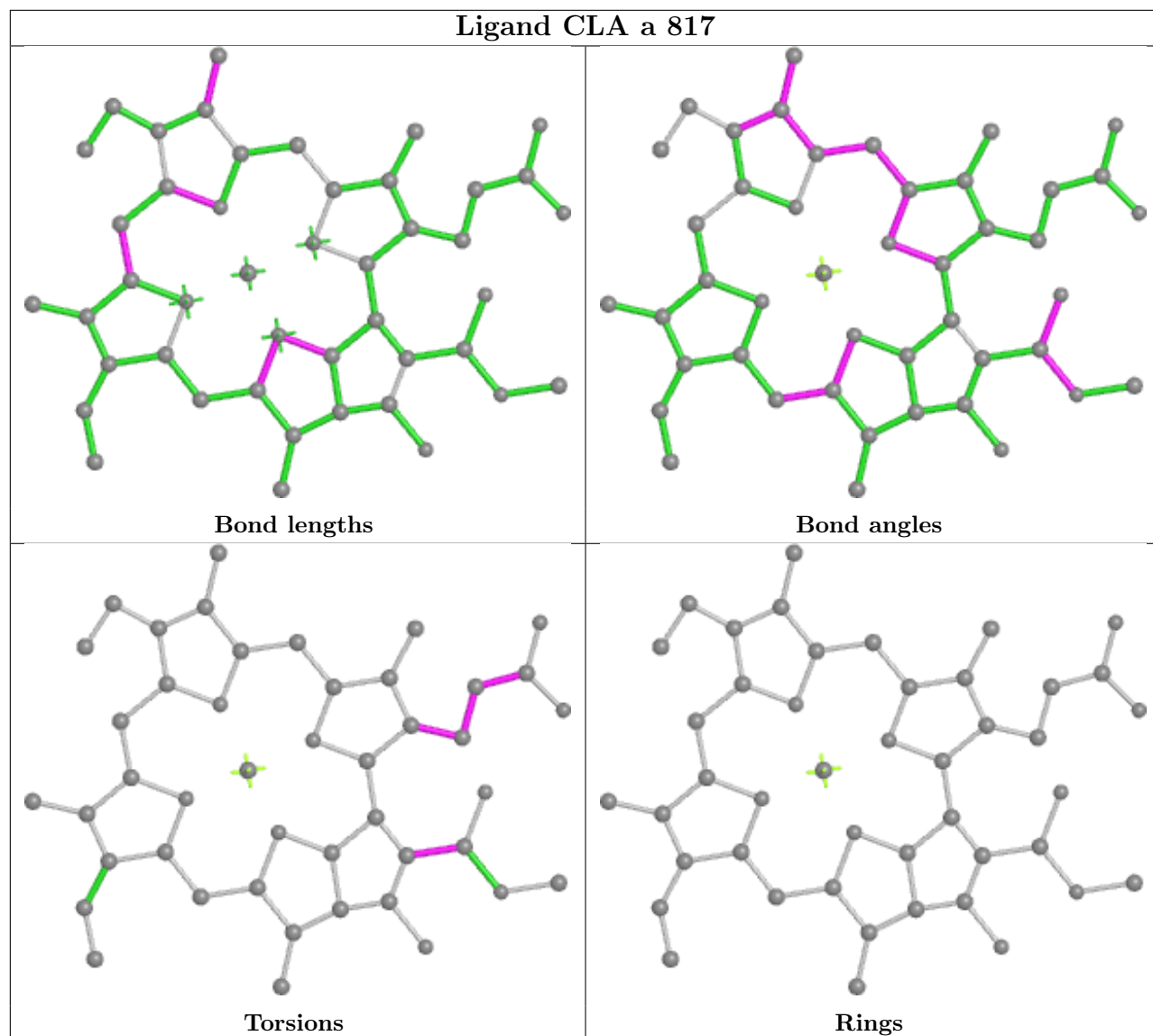


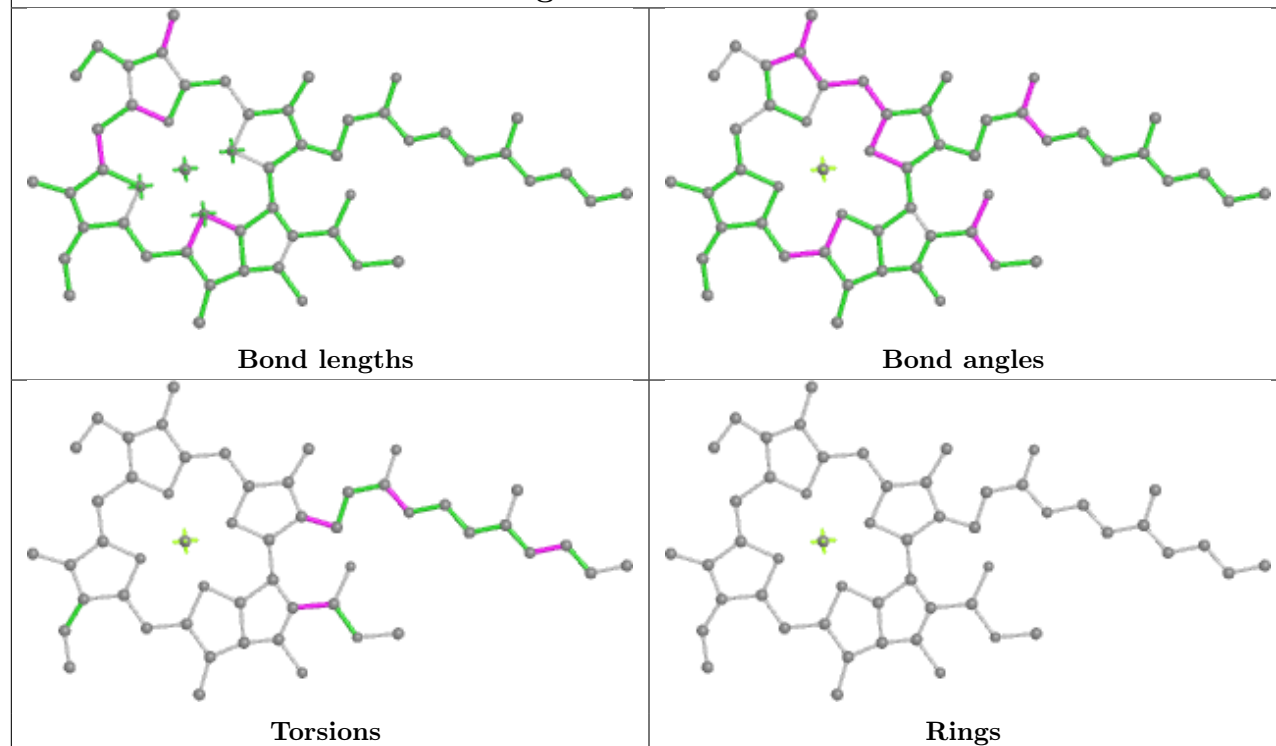
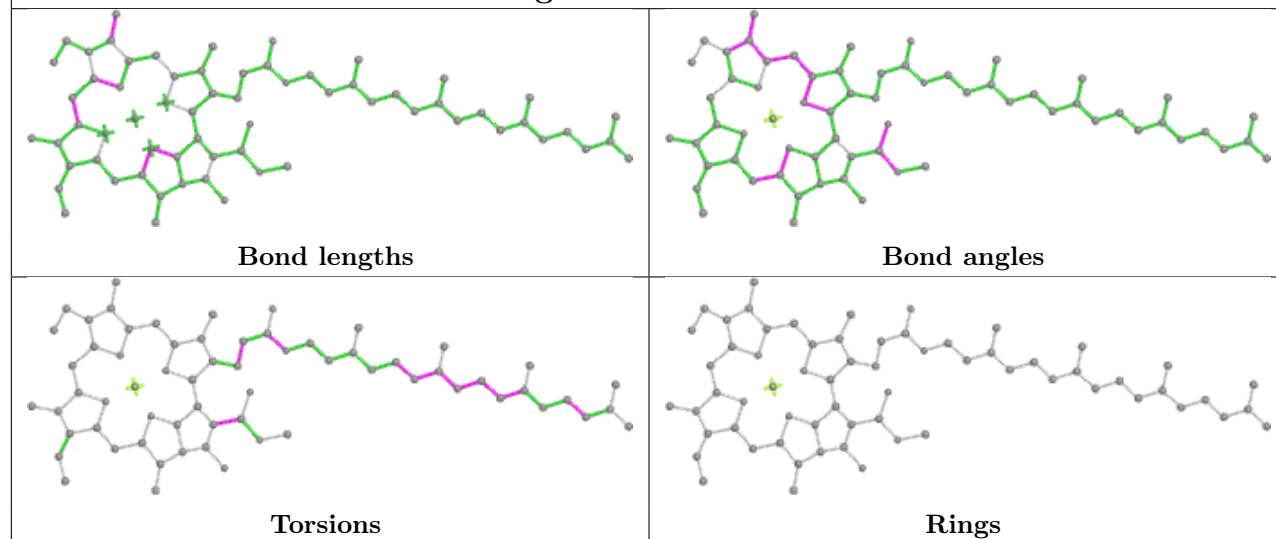
Torsions



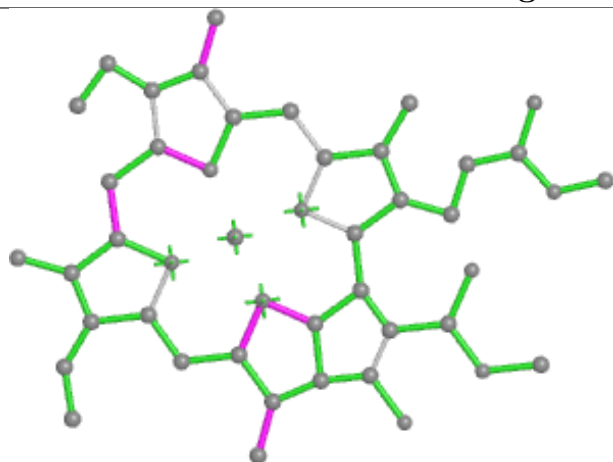
Rings

Ligand CLA a 817

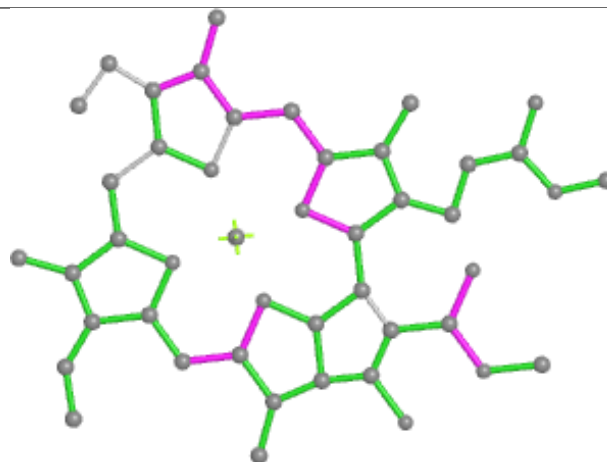


Ligand CLA 4 313**Ligand CLA b 825**

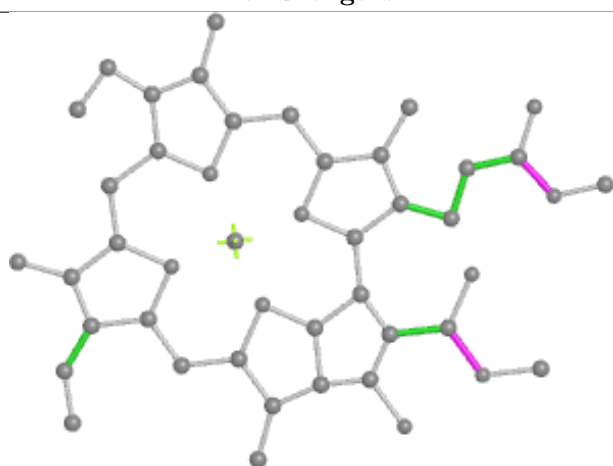
Ligand CLA 5 305



Bond lengths



Bond angles

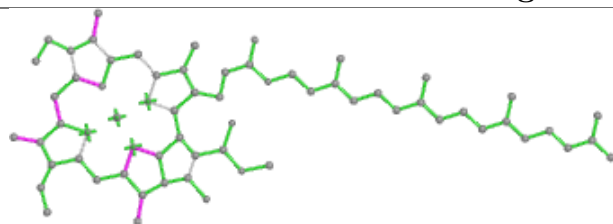


Torsions

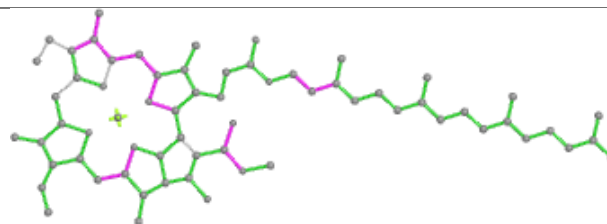


Rings

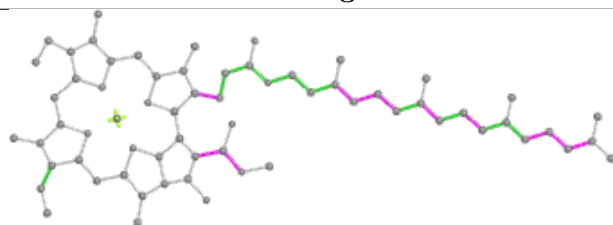
Ligand CLA b 814



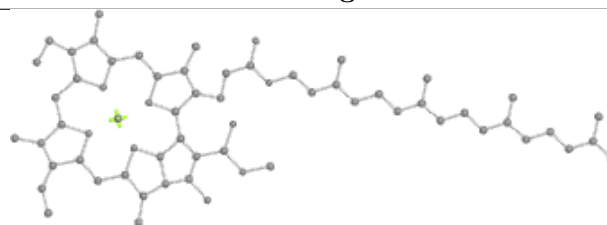
Bond lengths



Bond angles

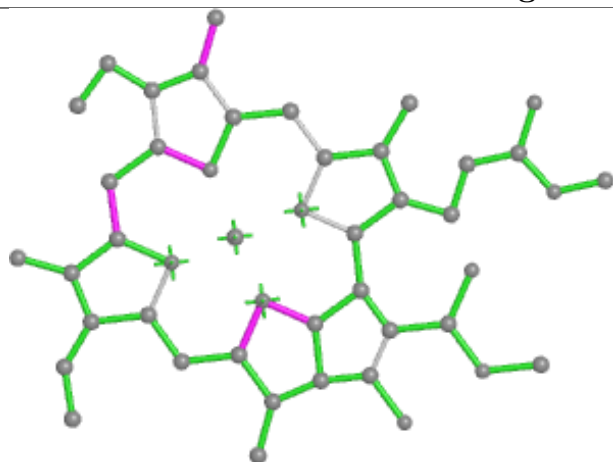


Torsions

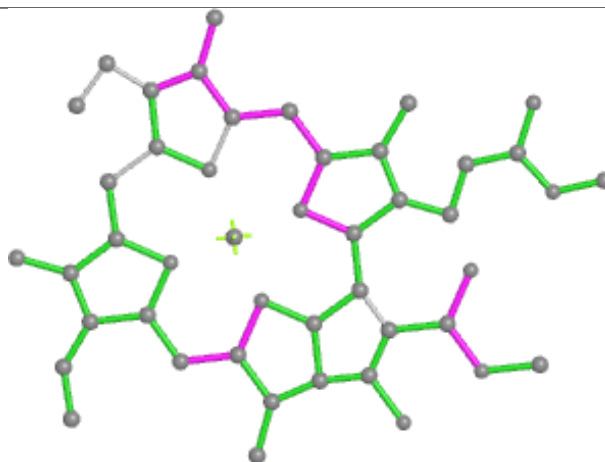


Rings

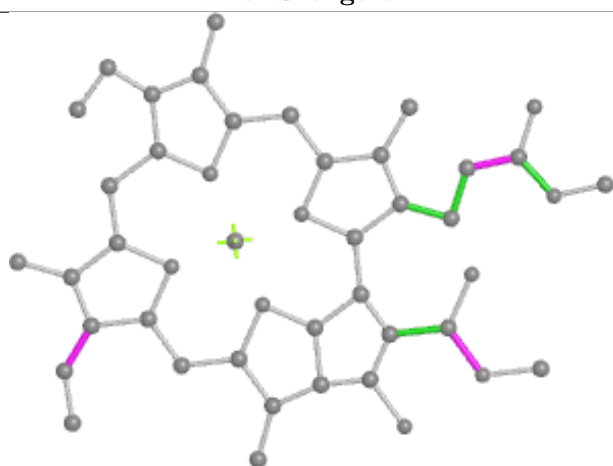
Ligand CLA 5 315



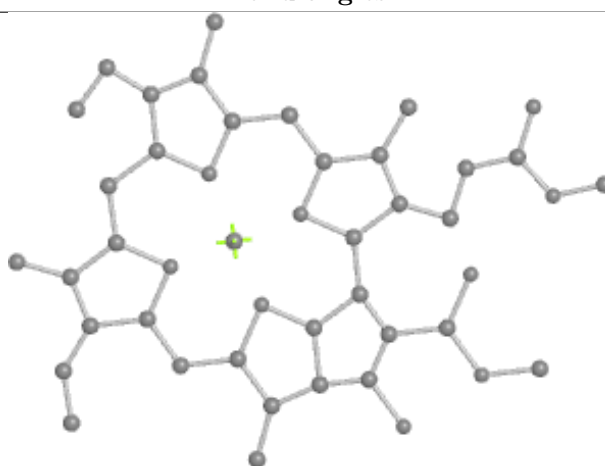
Bond lengths



Bond angles

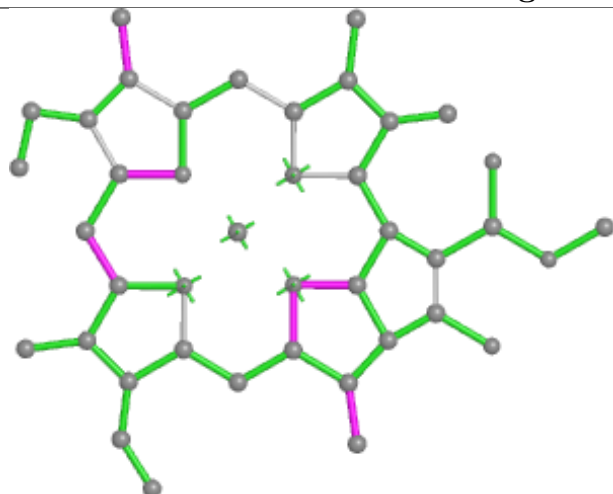


Torsions

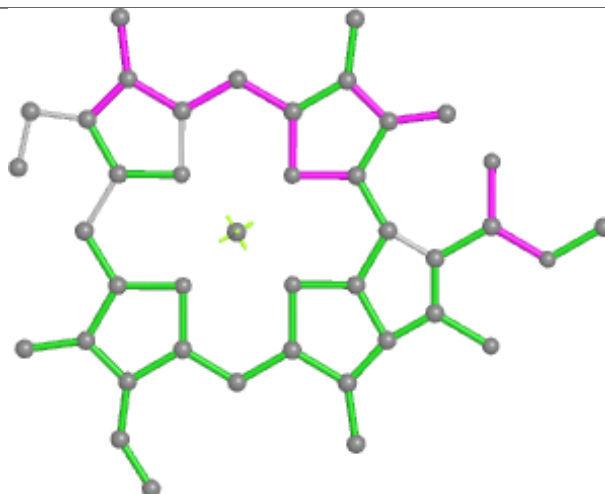


Rings

Ligand CLA 1 313



Bond lengths



Bond angles

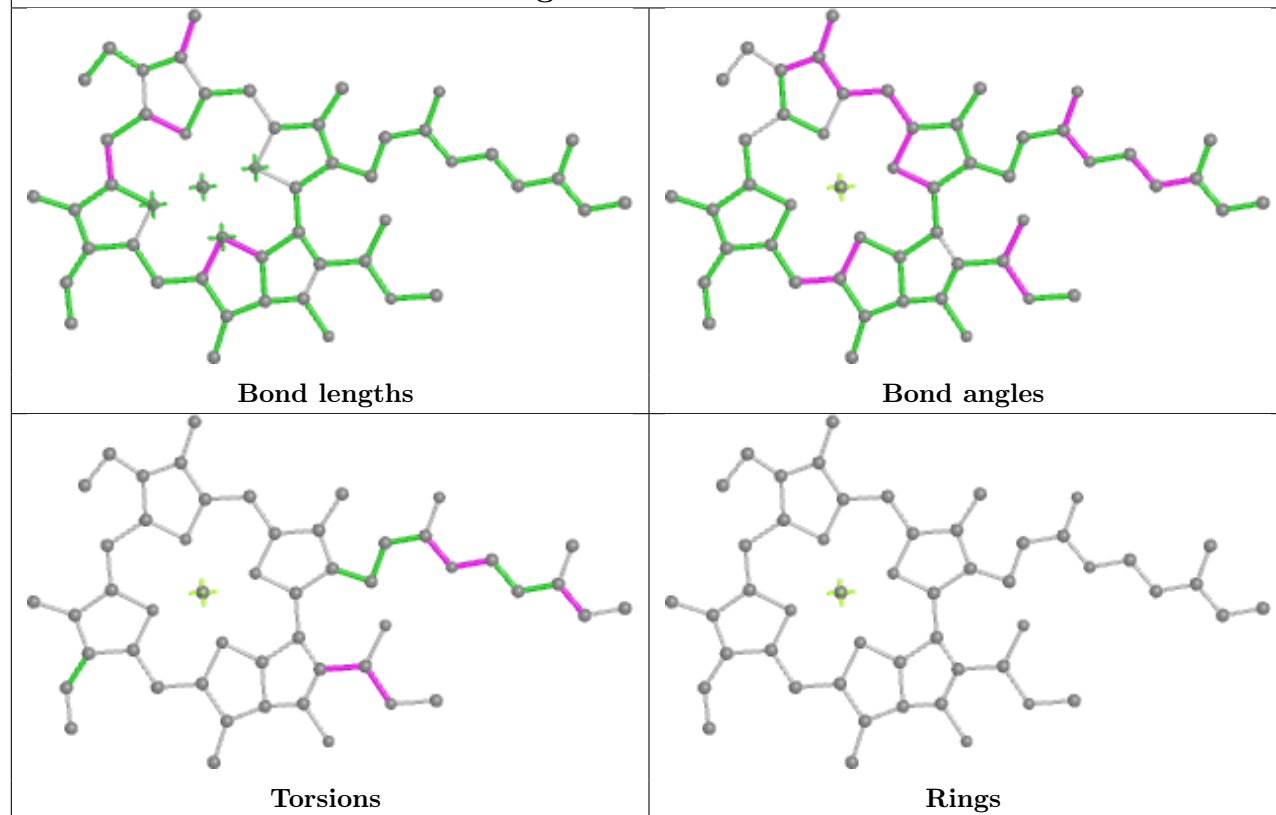


Torsions

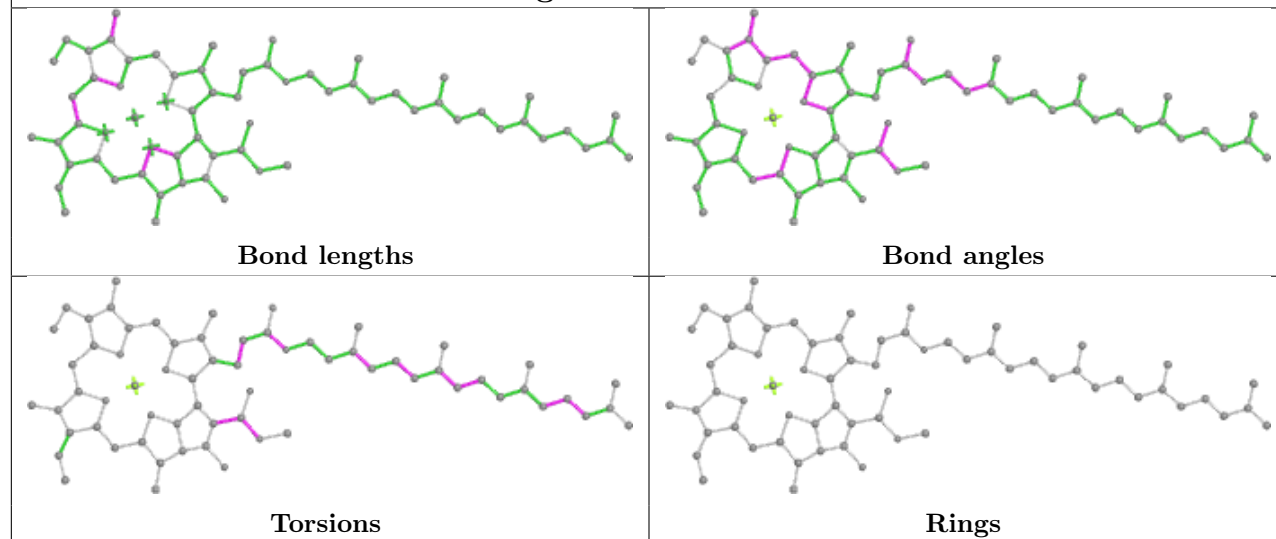


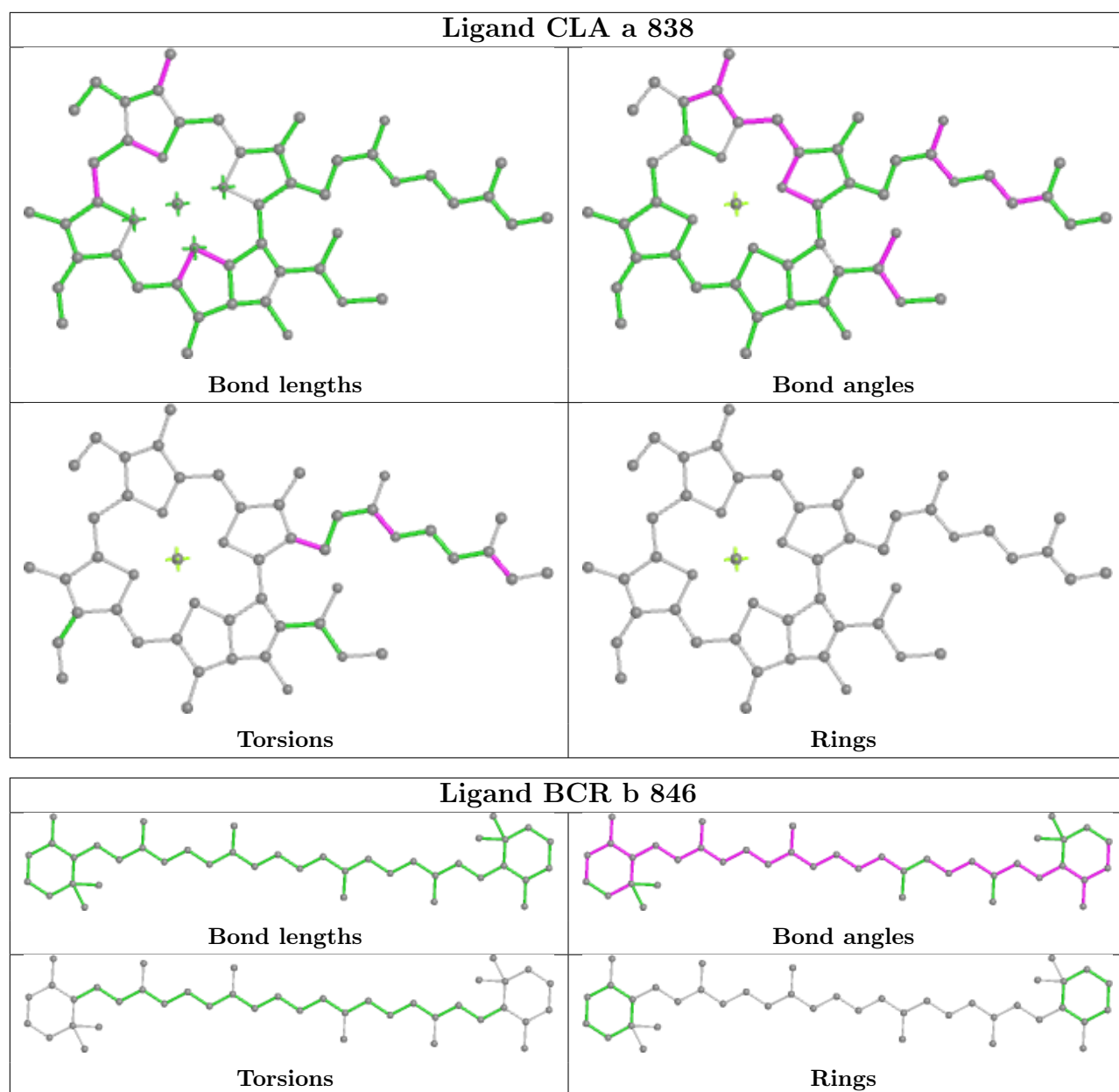
Rings

Ligand CLA 5 311

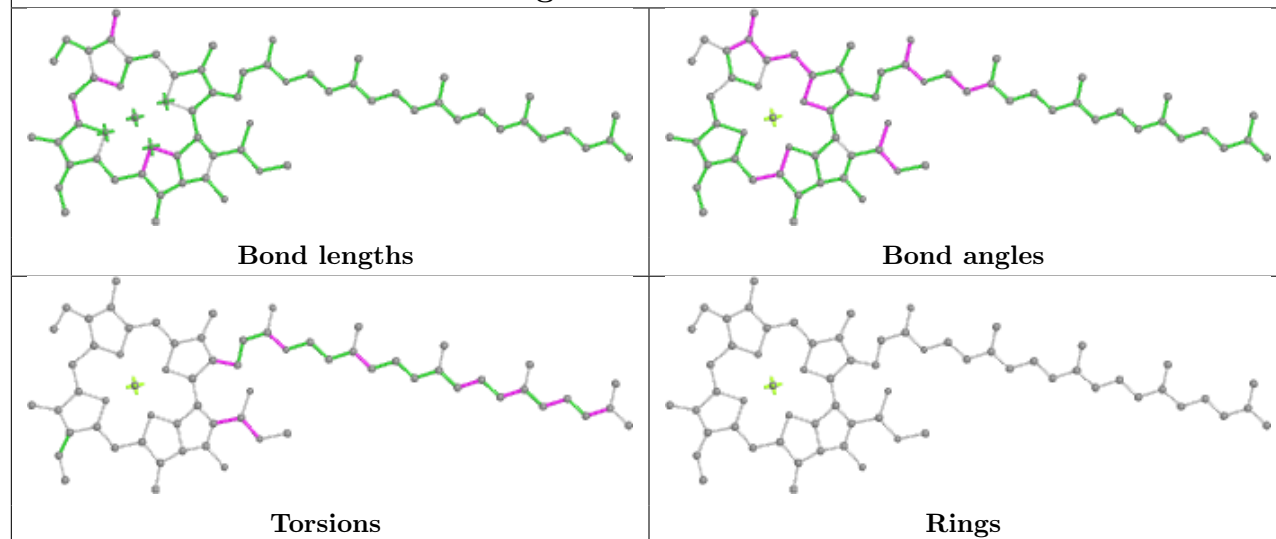


Ligand CLA a 841

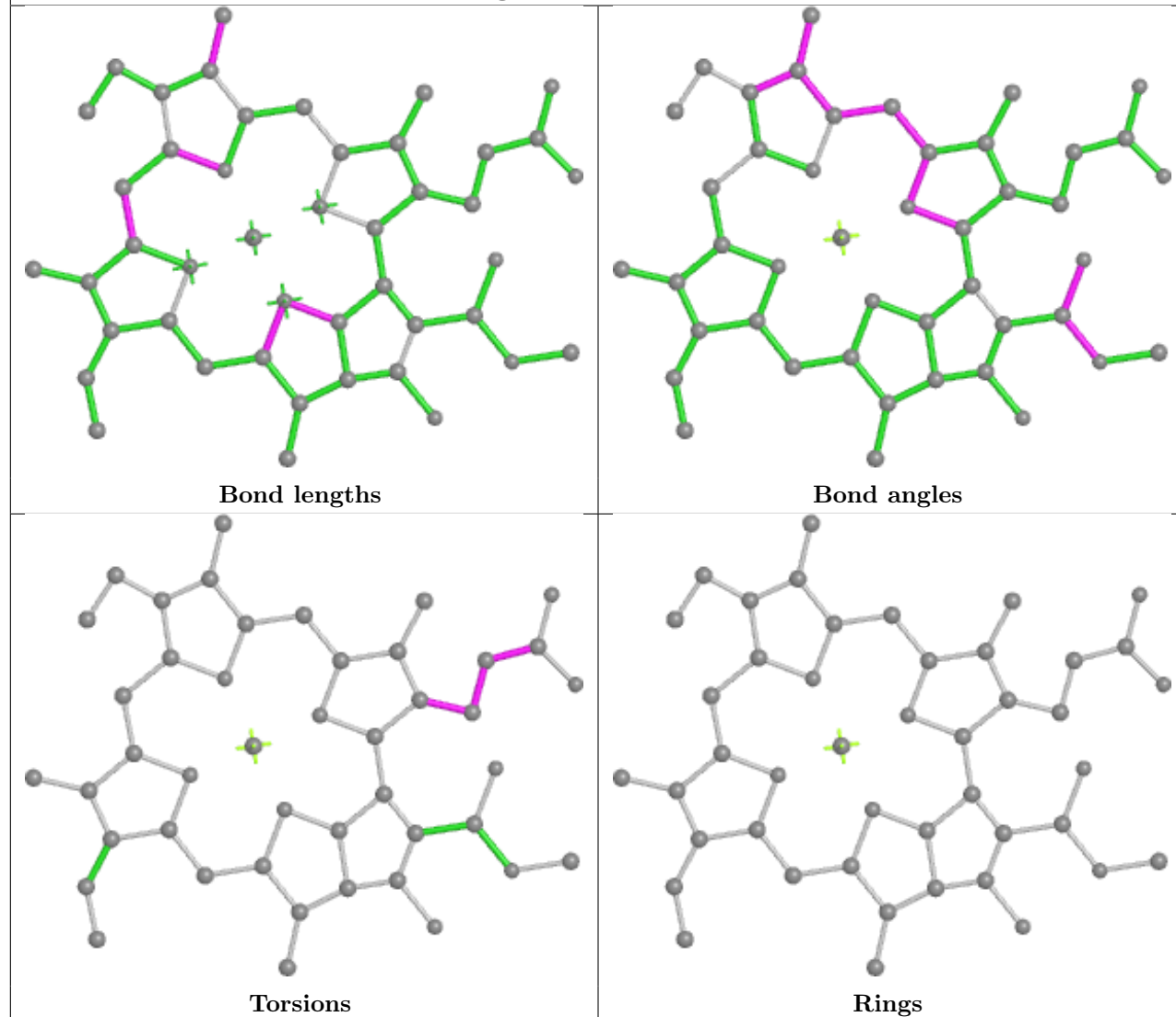




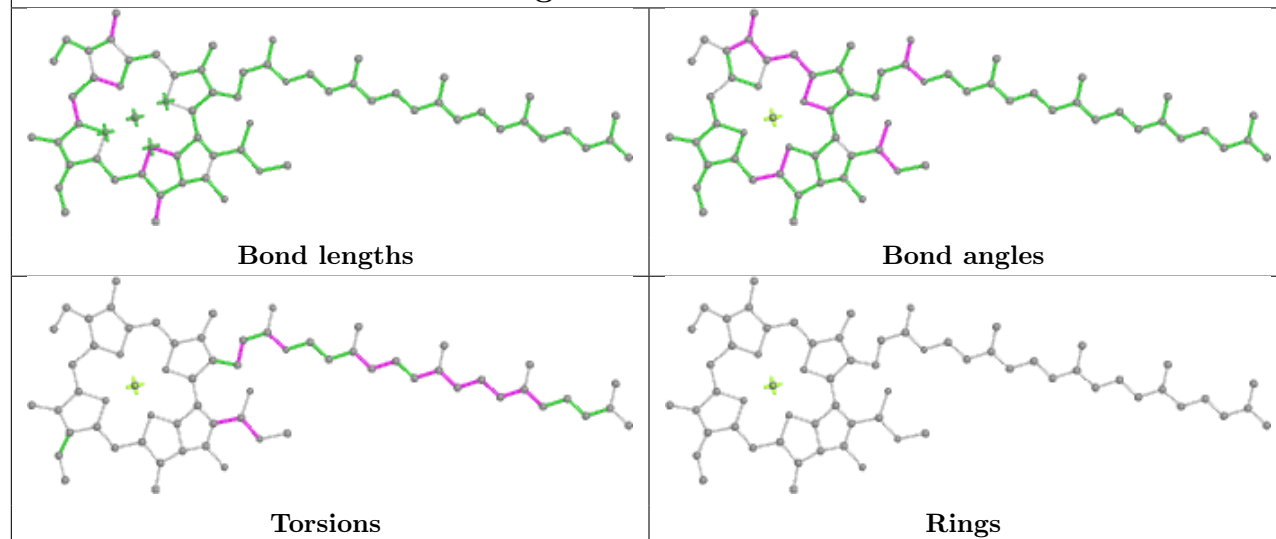
Ligand CLA a 820



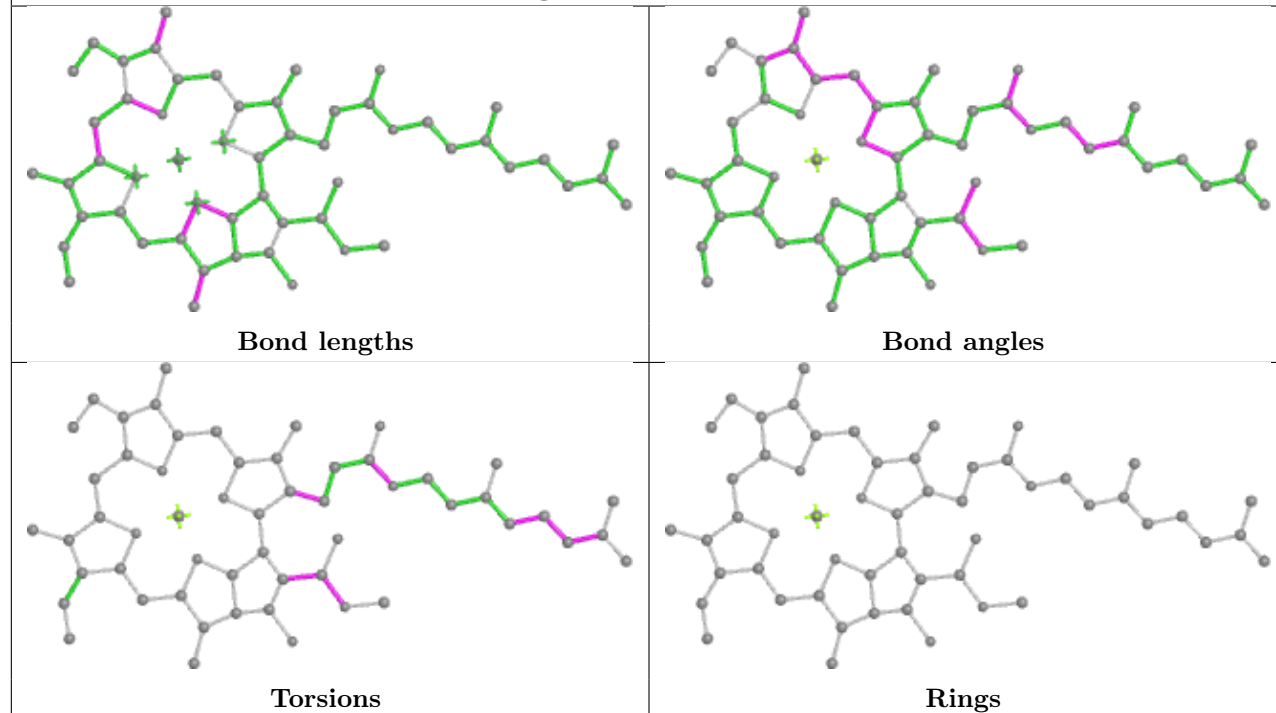
Ligand CLA 1 314



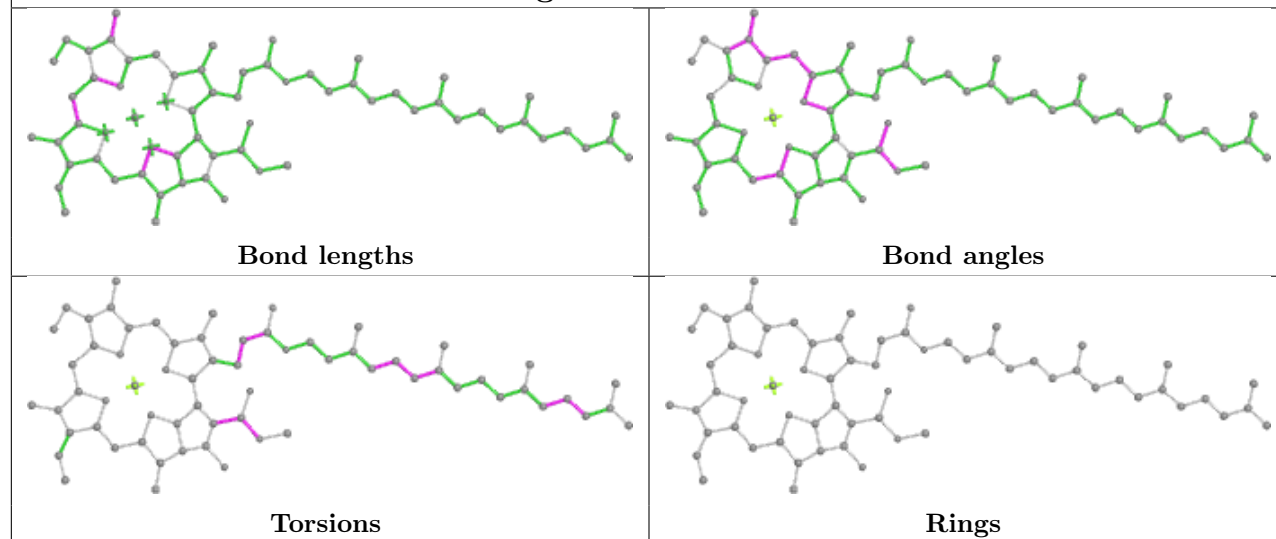
Ligand CLA b 802



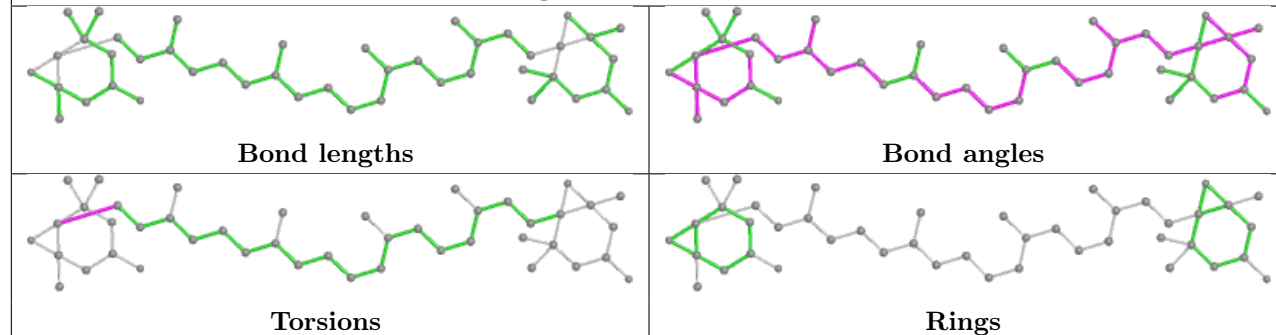
Ligand CLA b 815



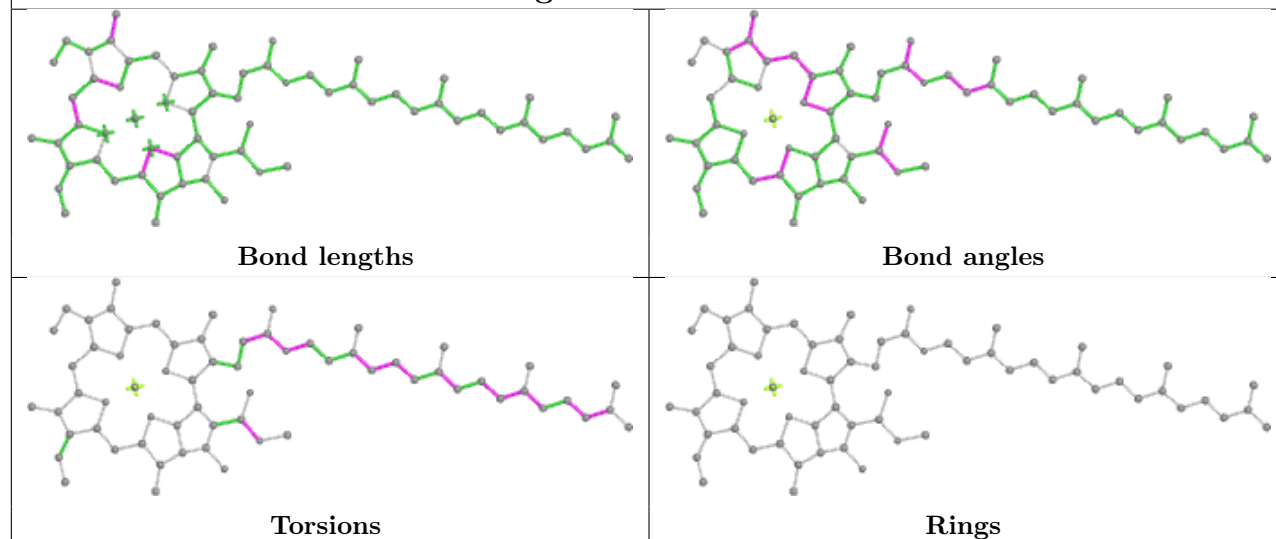
Ligand CLA 5 309

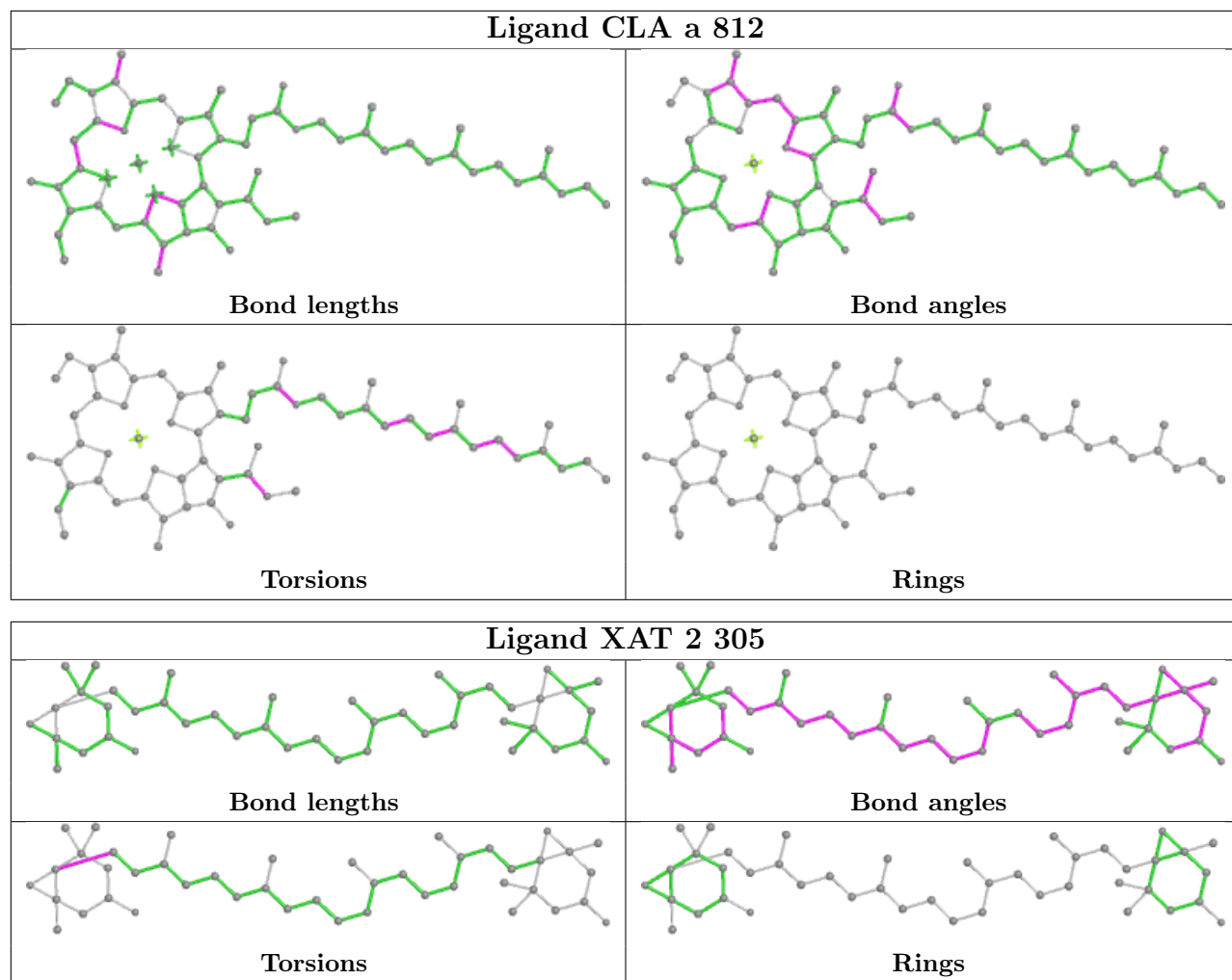


Ligand XAT 5 304

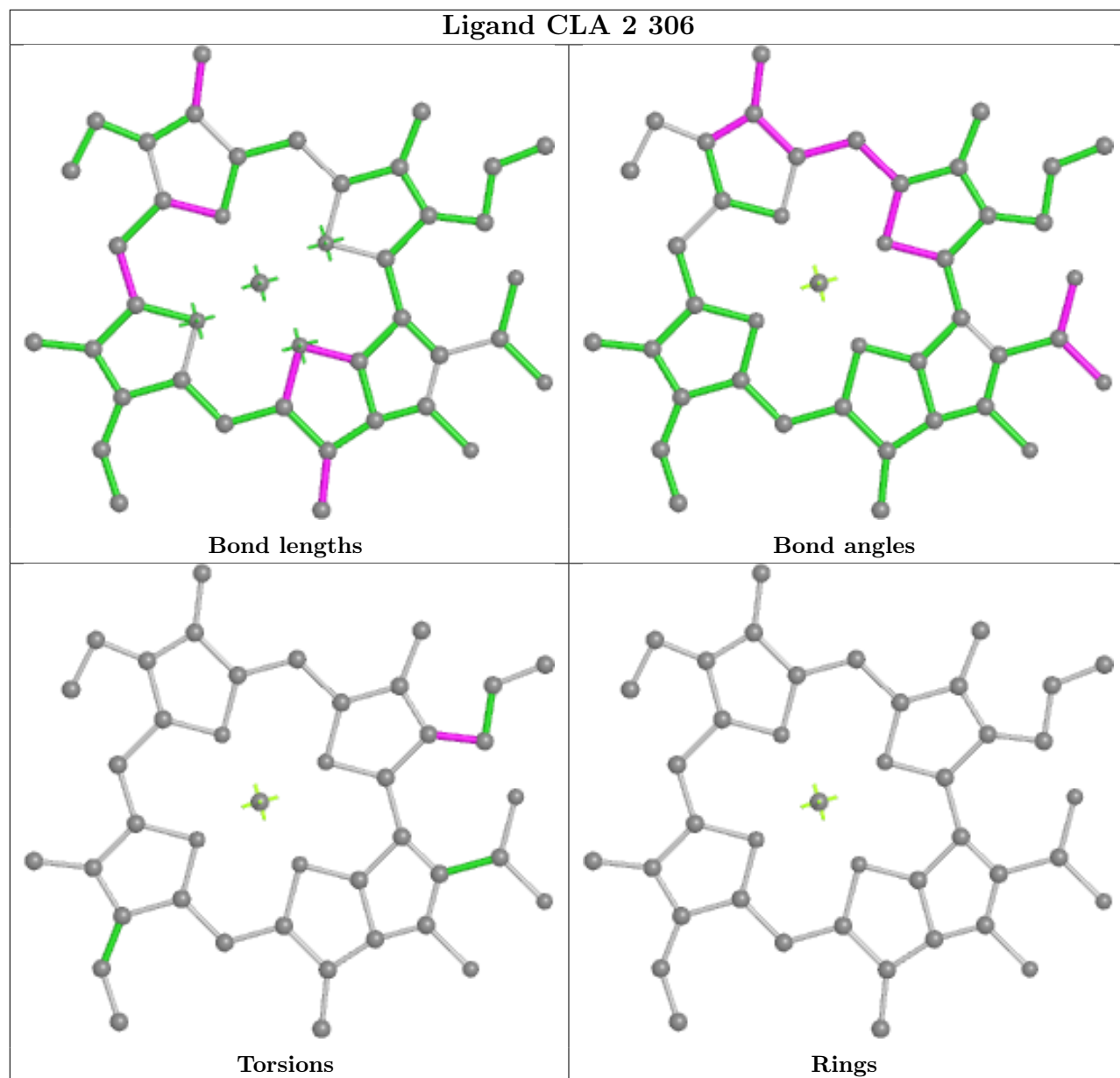


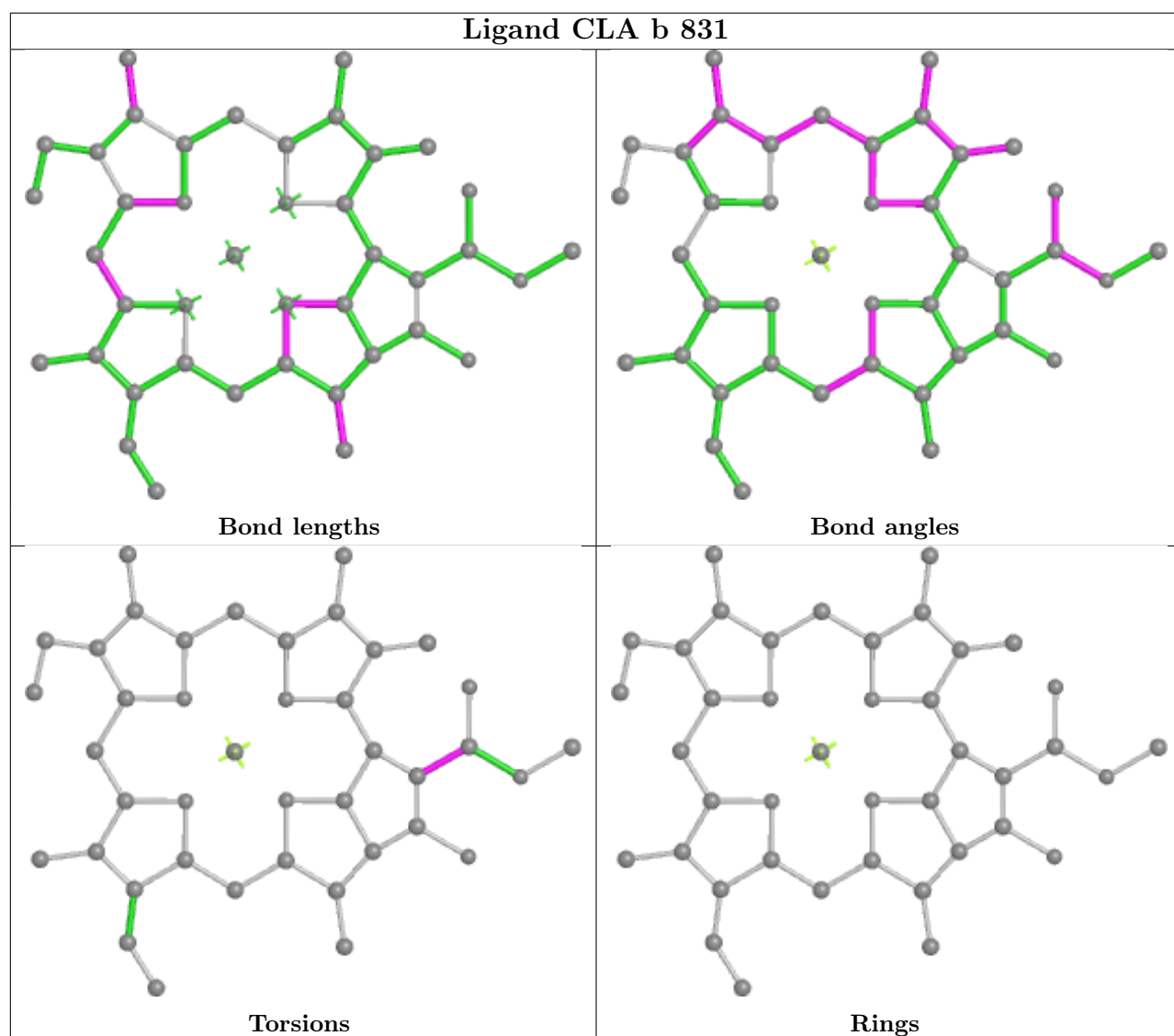
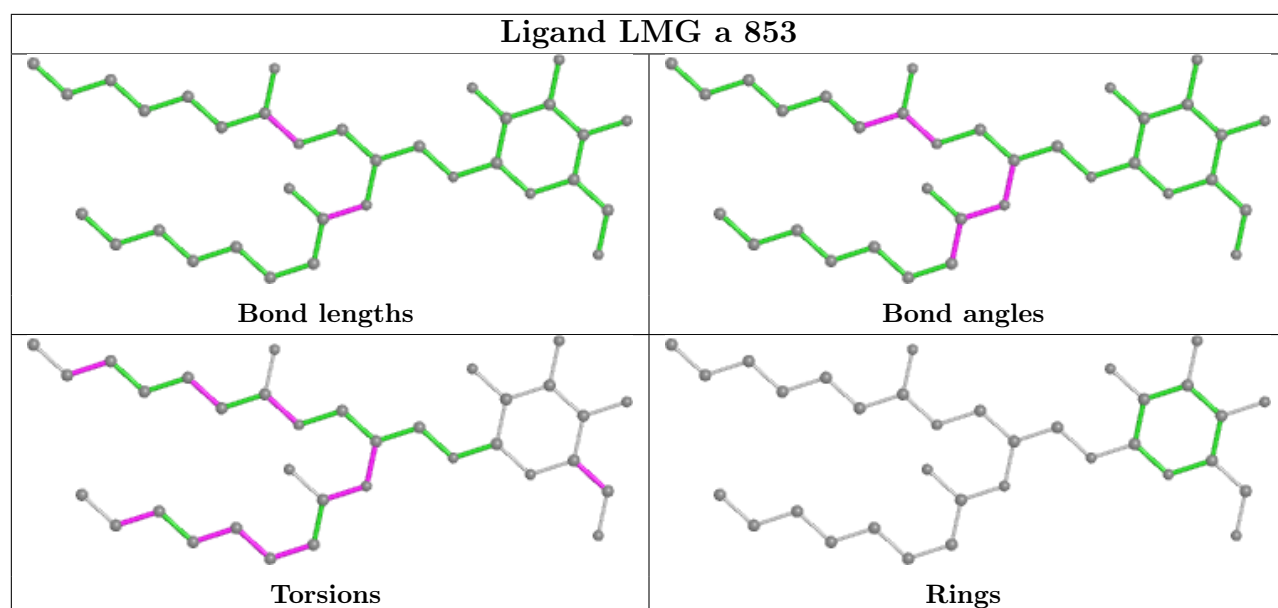
Ligand CLA b 807



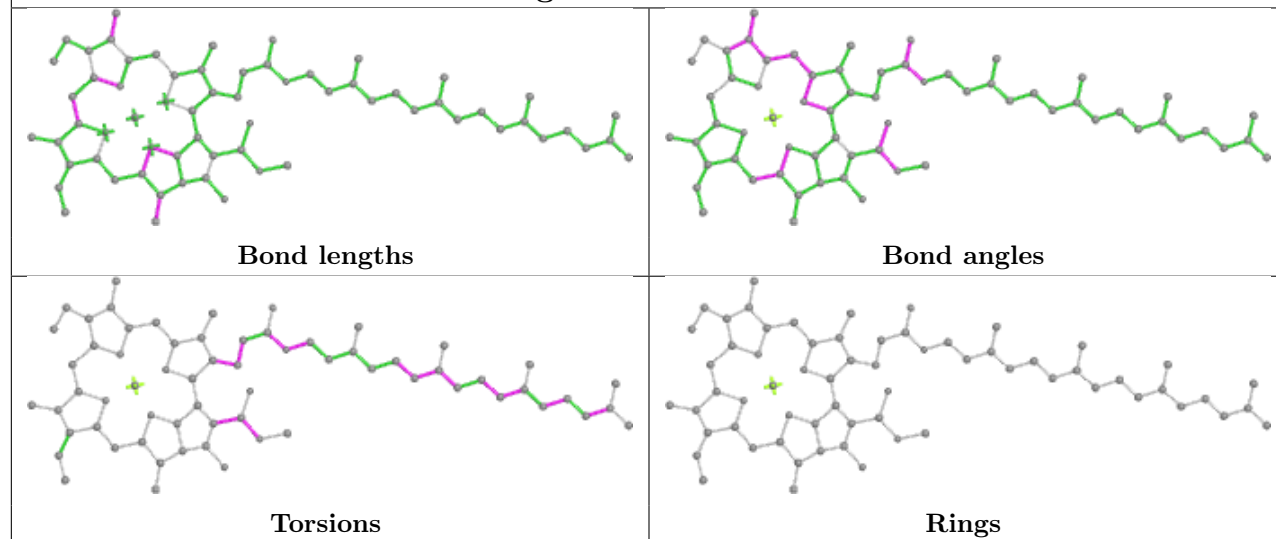


Ligand CLA 2 306

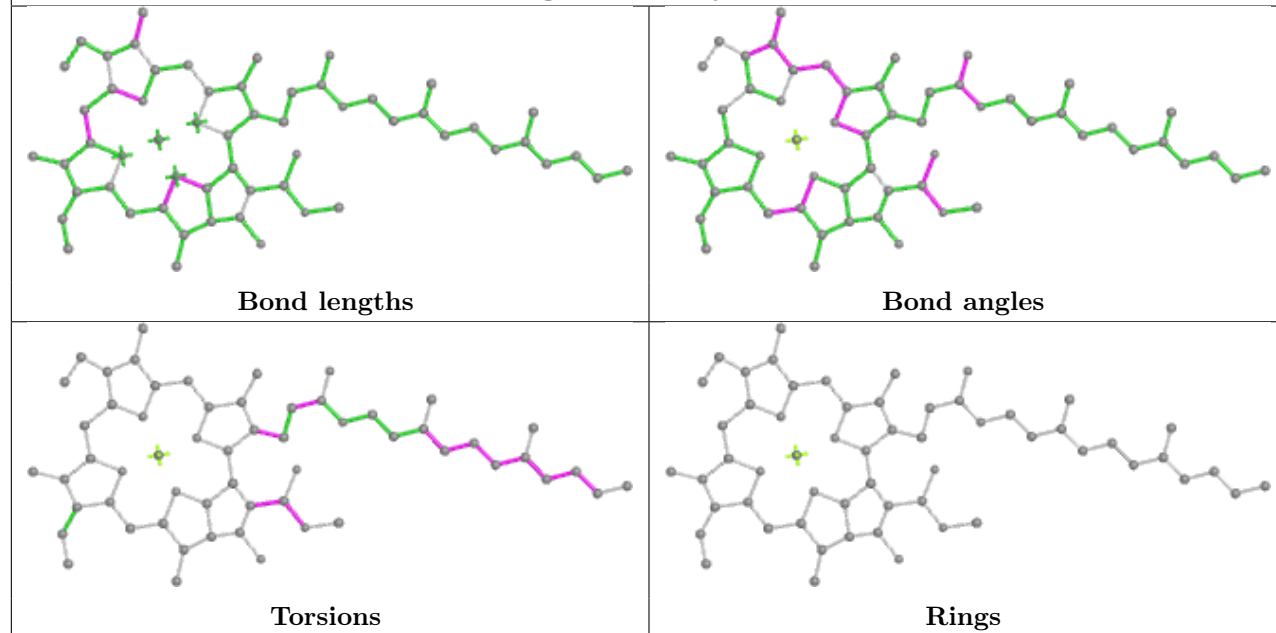




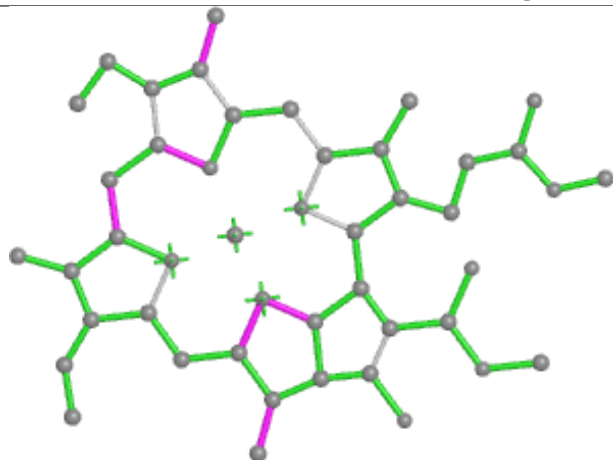
Ligand CLA a 814



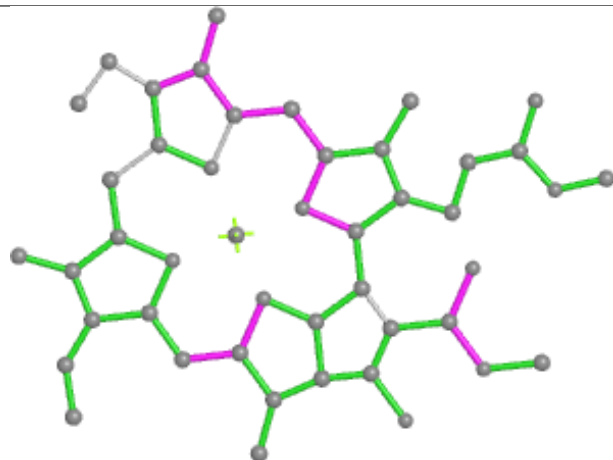
Ligand CLA j 102



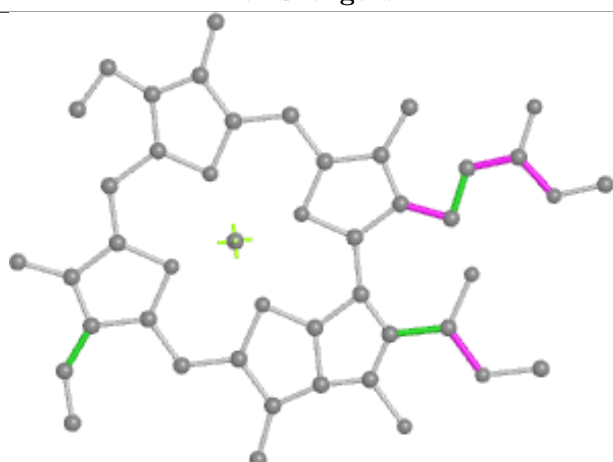
Ligand CLA 3 315



Bond lengths



Bond angles

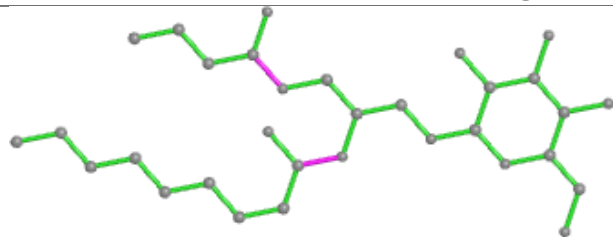


Torsions

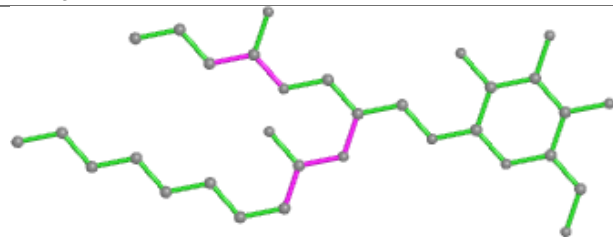


Rings

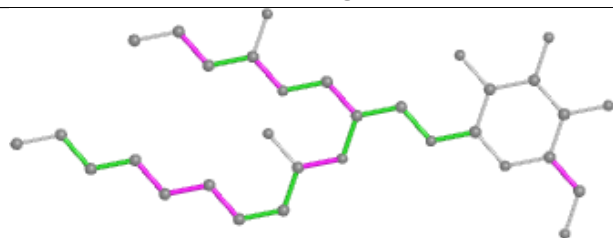
Ligand LMG j 105



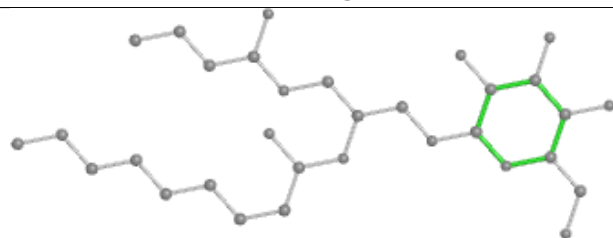
Bond lengths



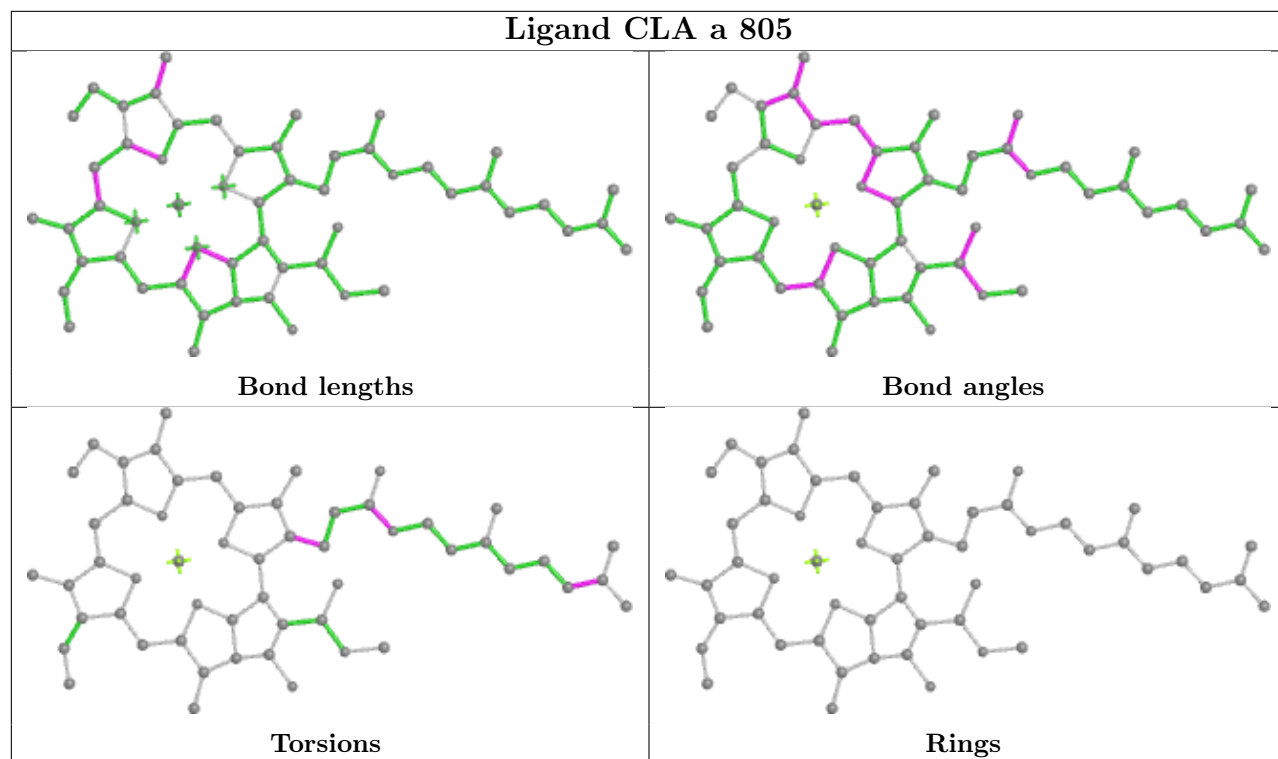
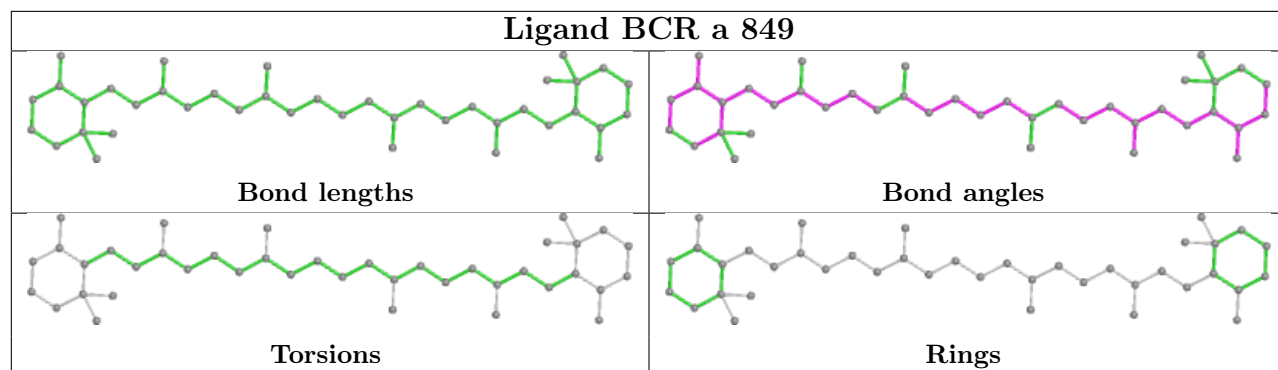
Bond angles



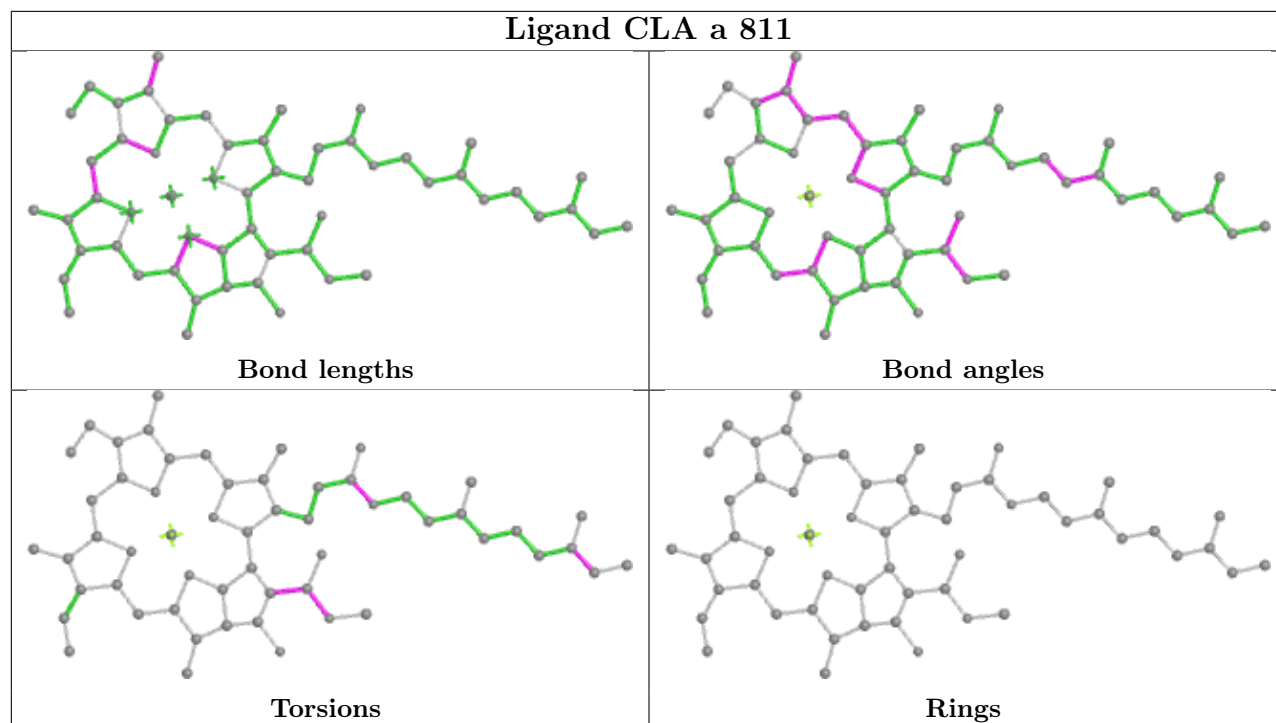
Torsions



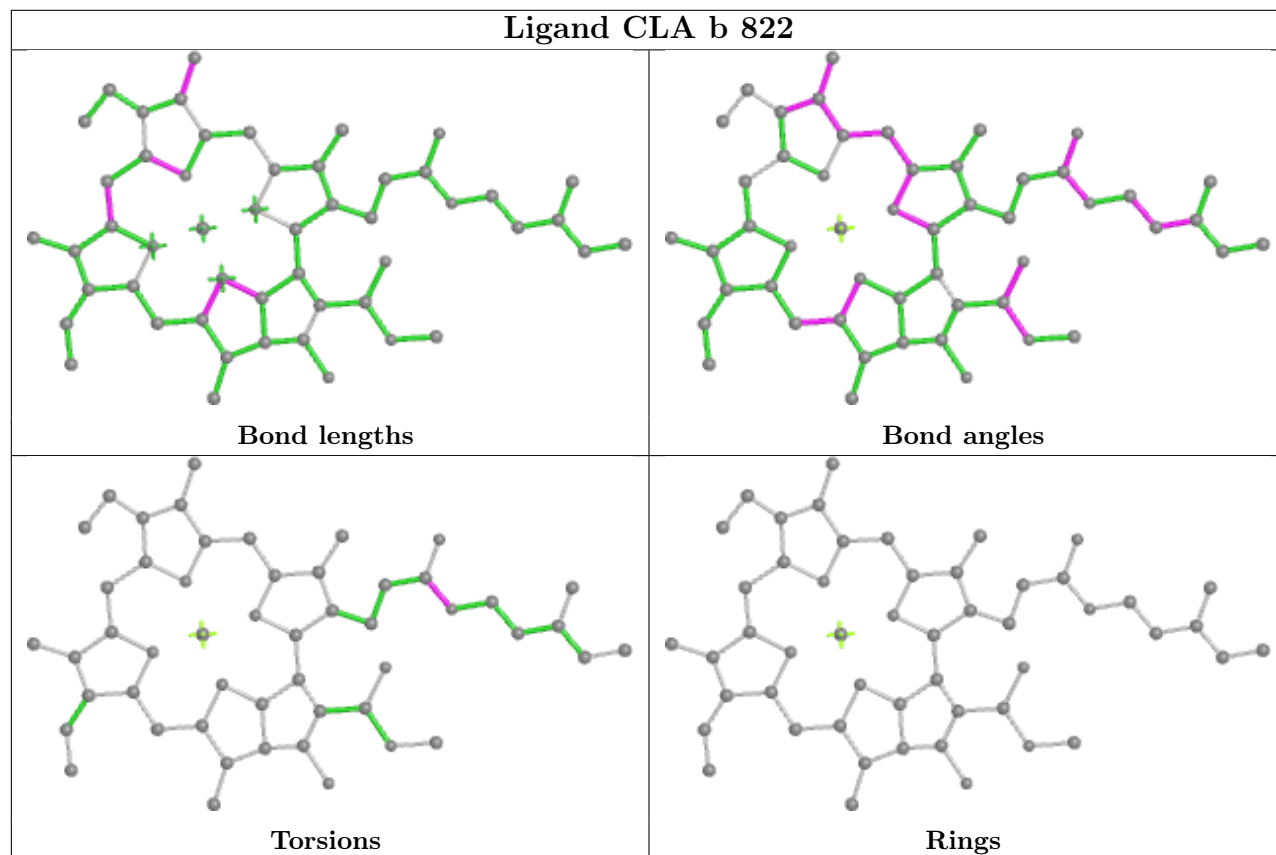
Rings

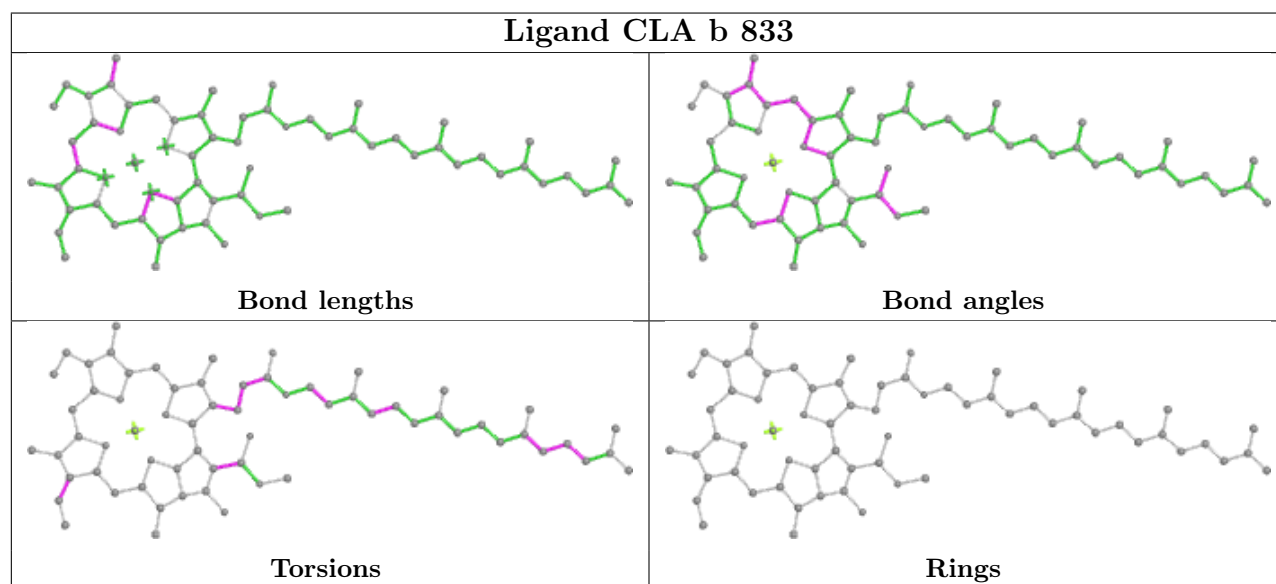
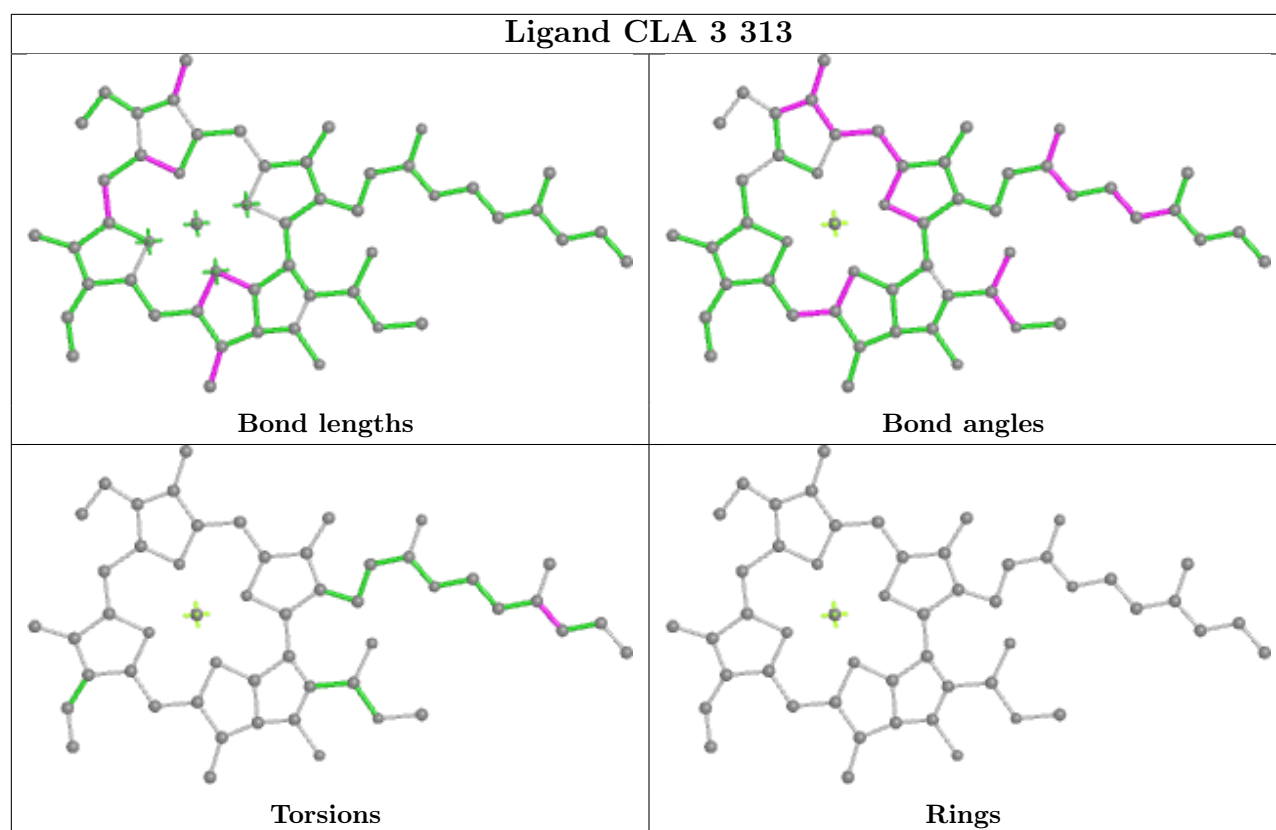


Ligand CLA a 811

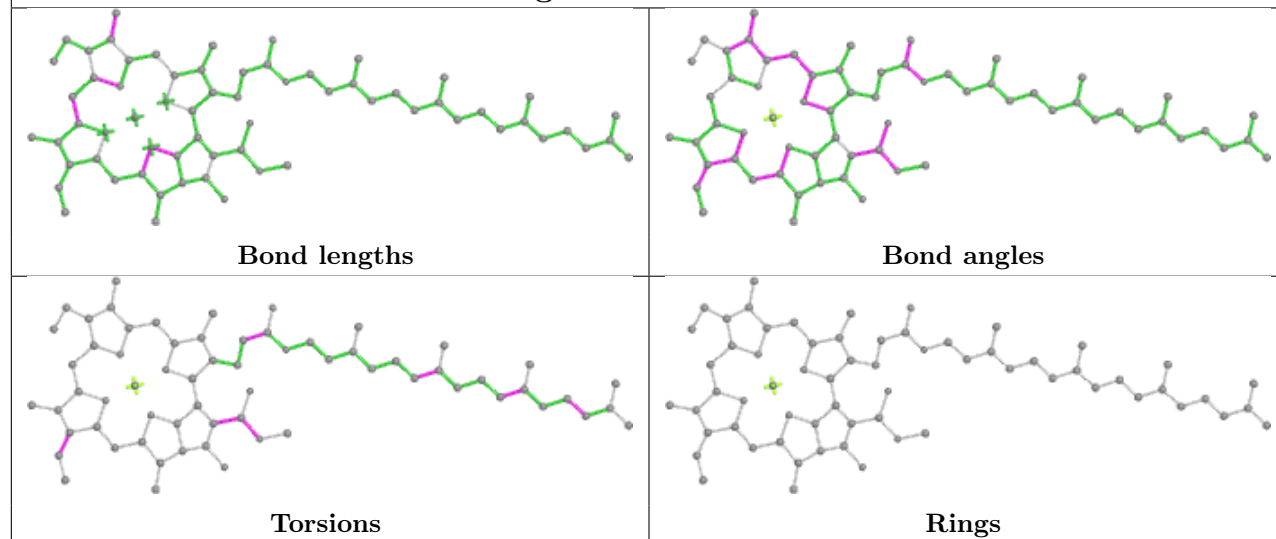


Ligand CLA b 822

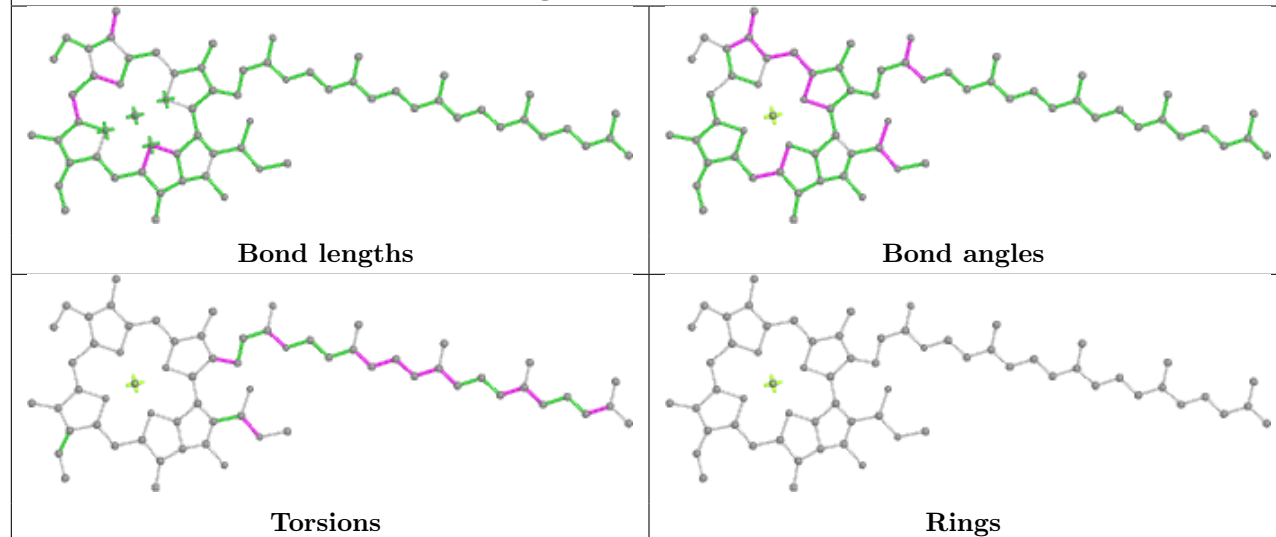




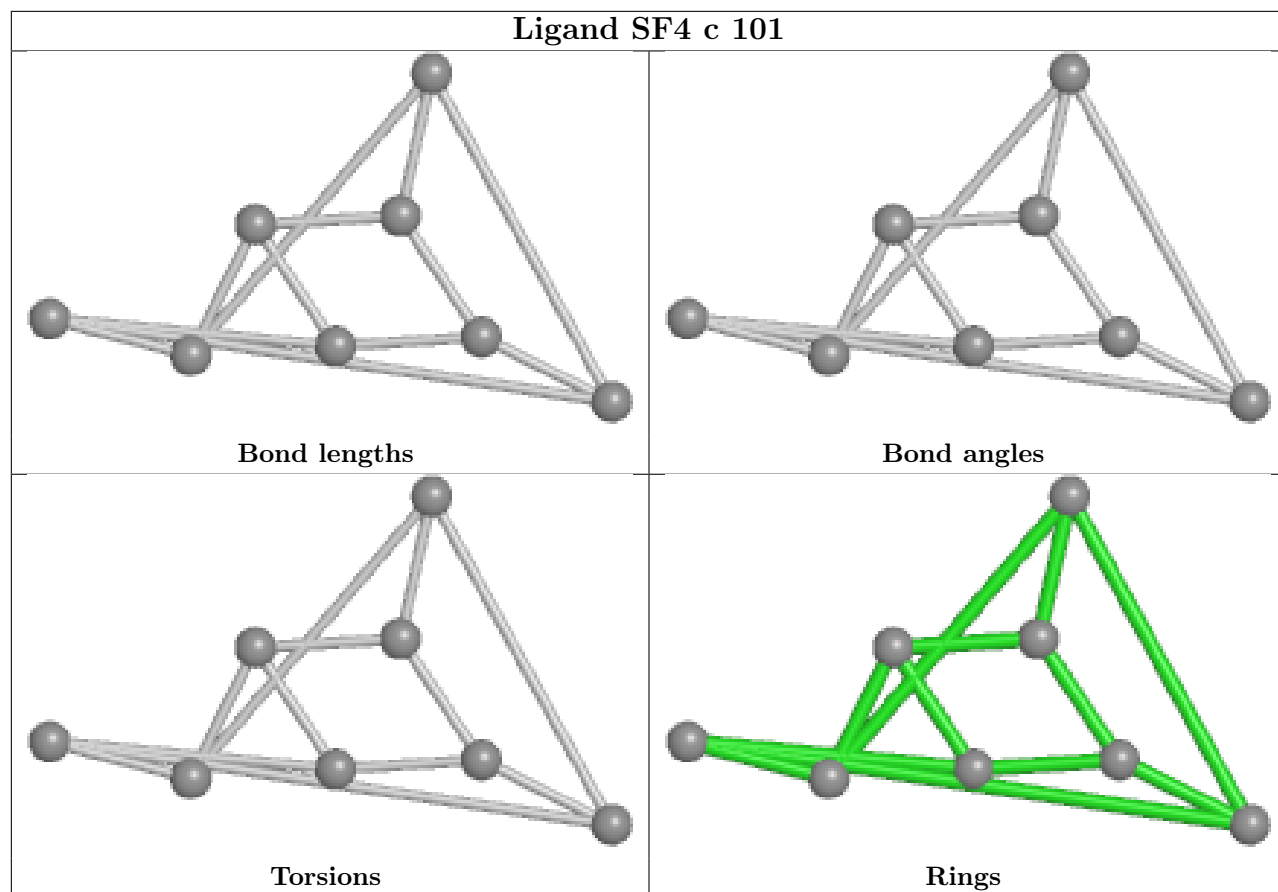
Ligand CLA b 804



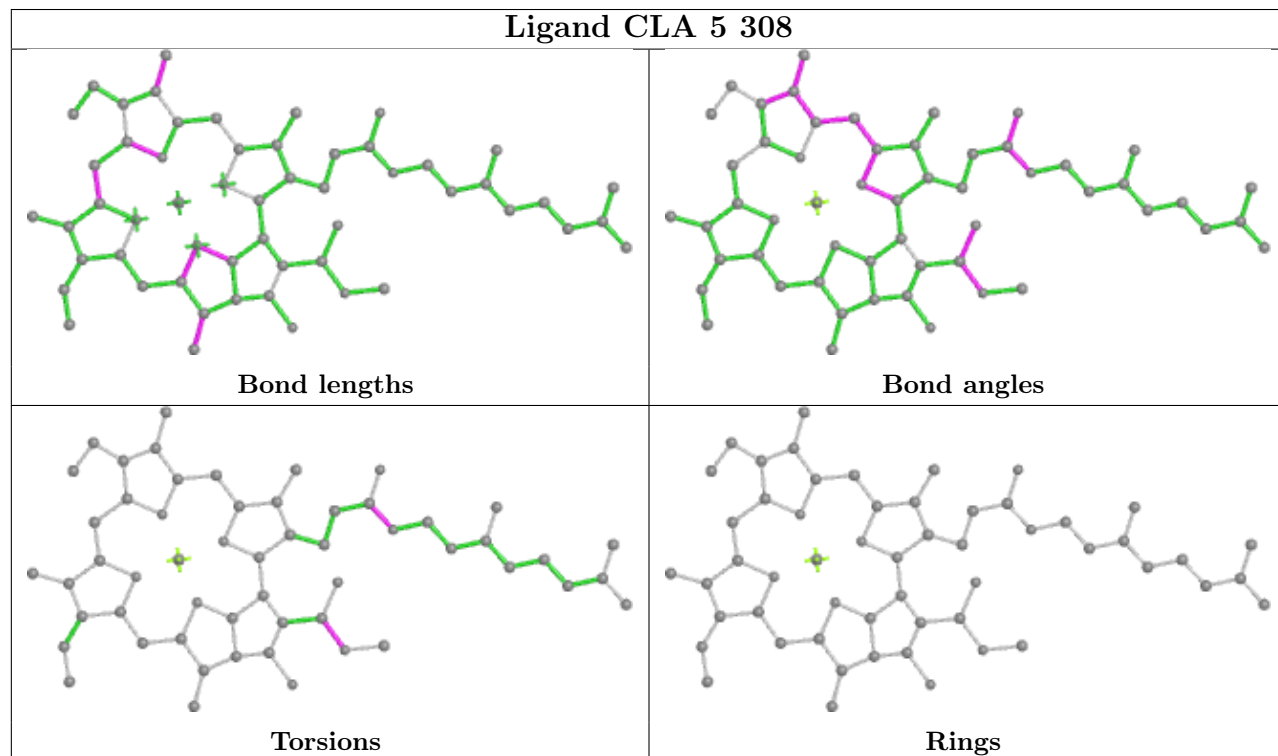
Ligand CLA 1 310



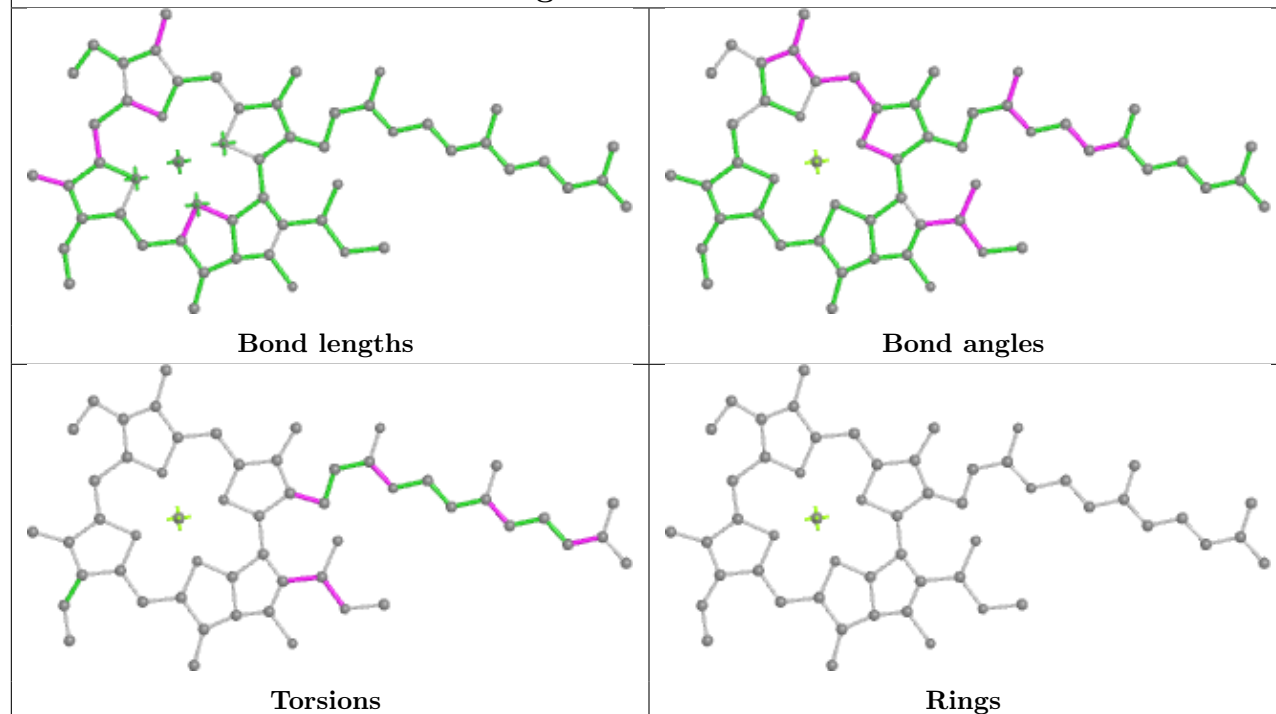
Ligand SF4 c 101



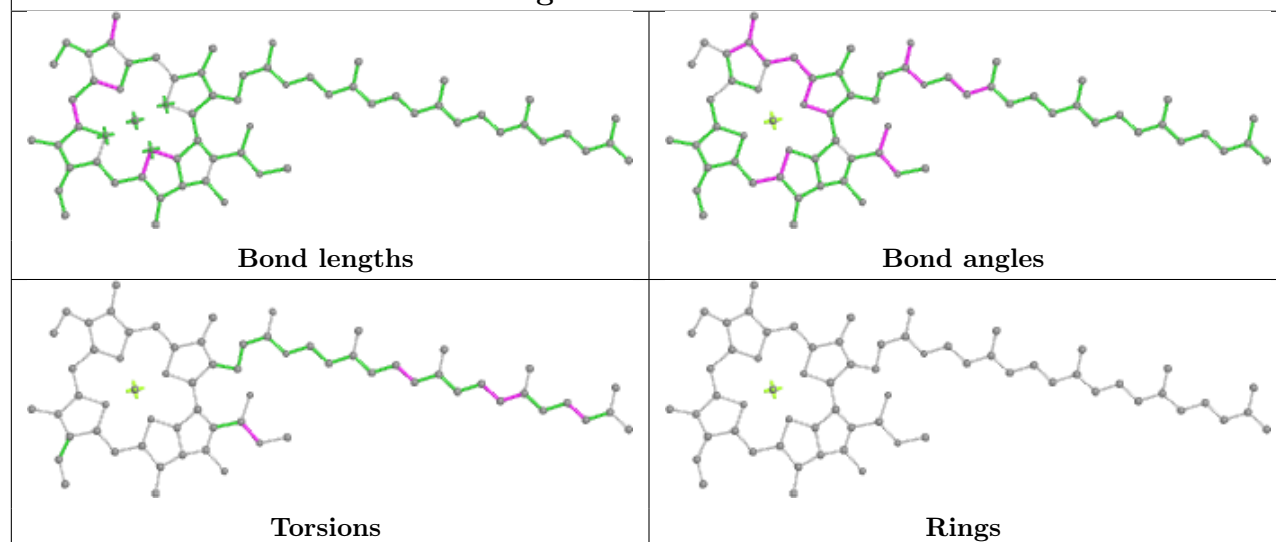
Ligand CLA 5 308



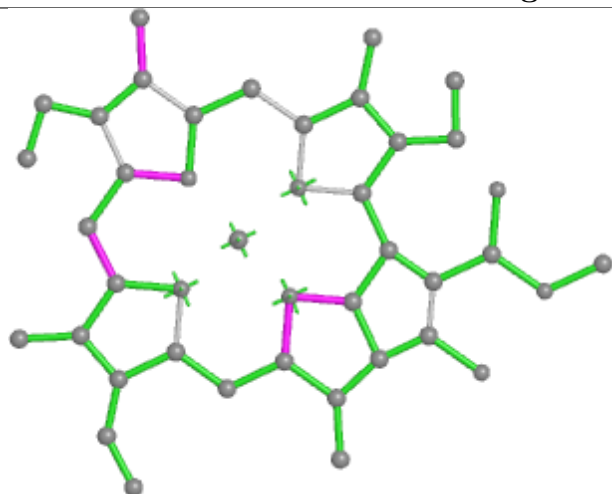
Ligand CLA a 804



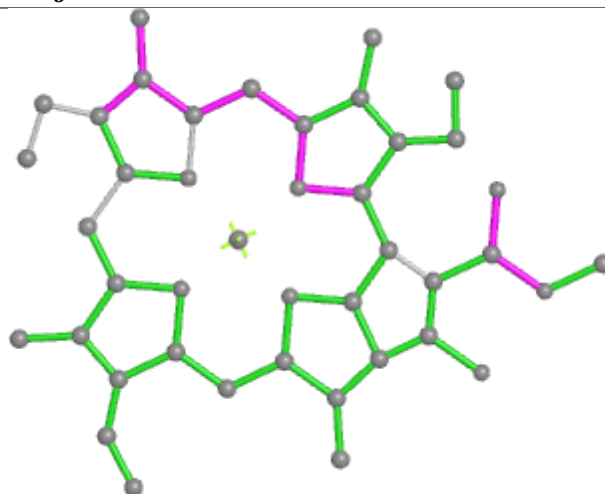
Ligand CLA a 834



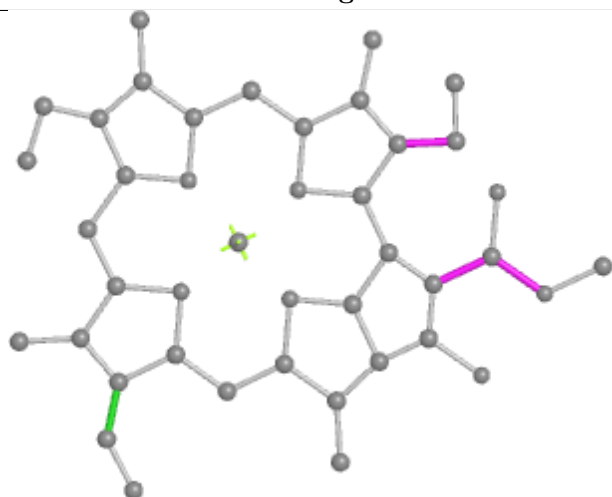
Ligand CLA j 103



Bond lengths



Bond angles

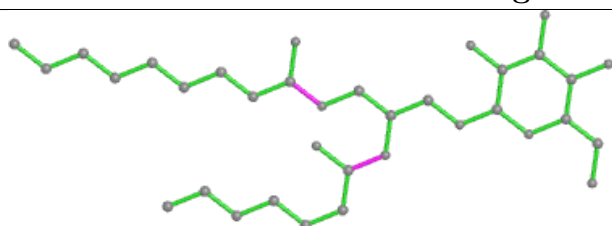


Torsions

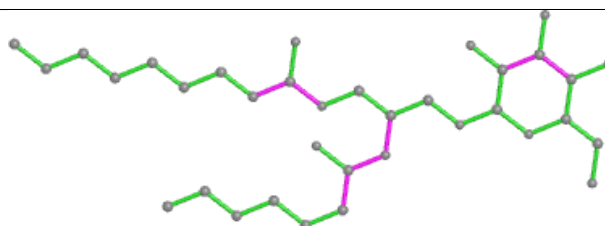


Rings

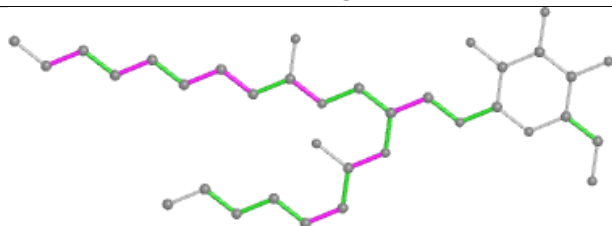
Ligand LMG 2 317



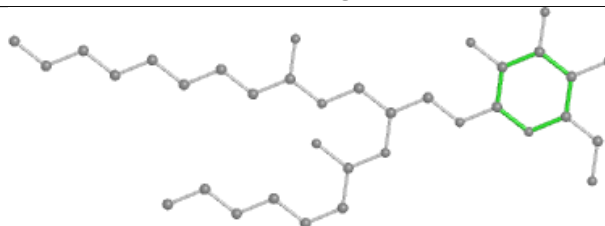
Bond lengths



Bond angles

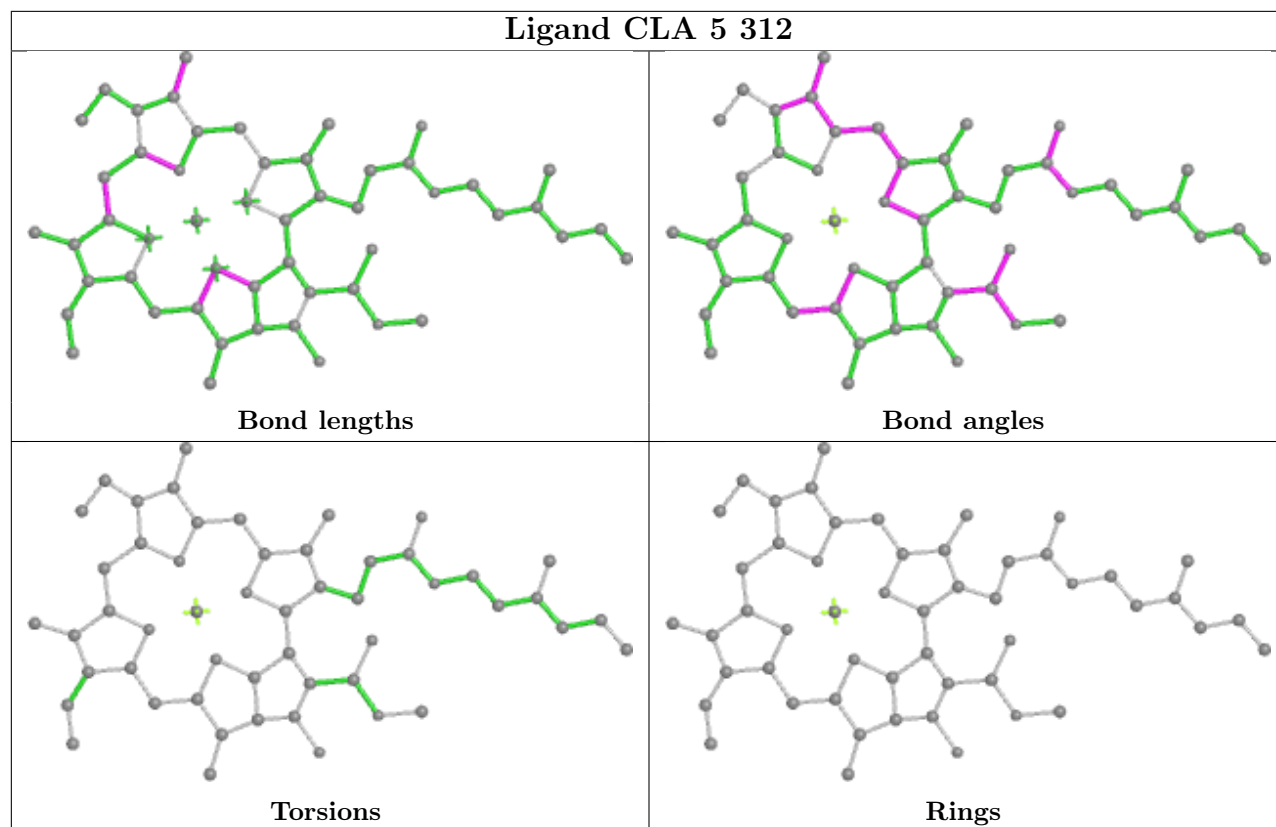


Torsions

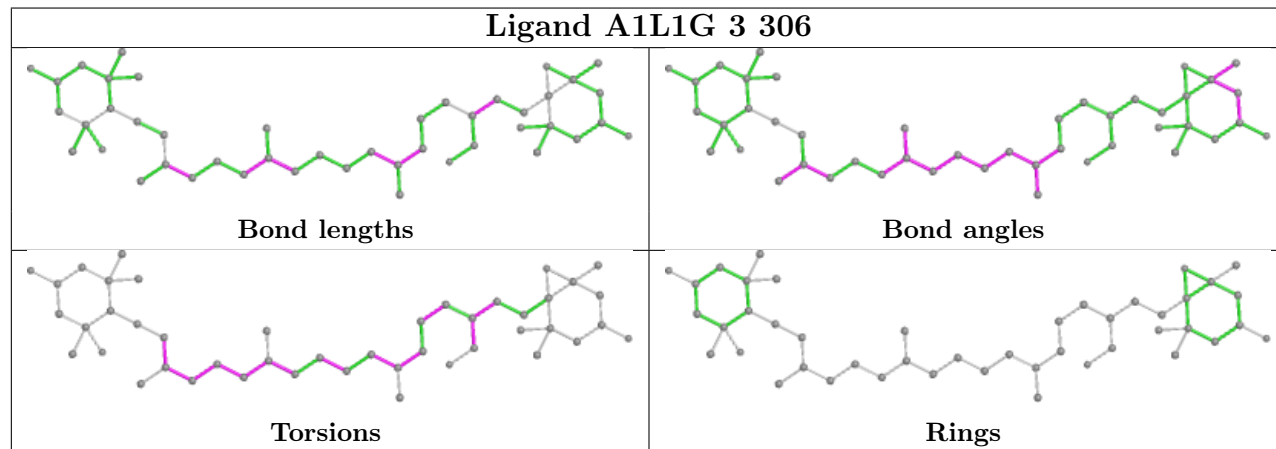


Rings

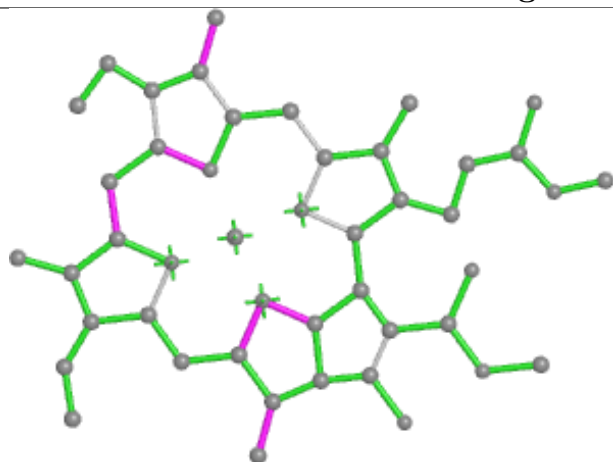
Ligand CLA 5 312



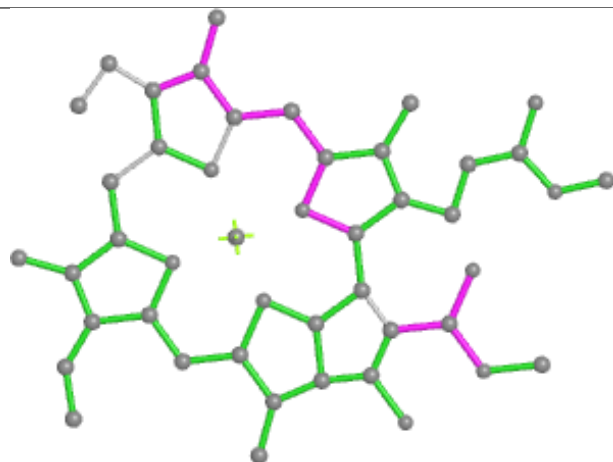
Ligand A1L1G 3 306



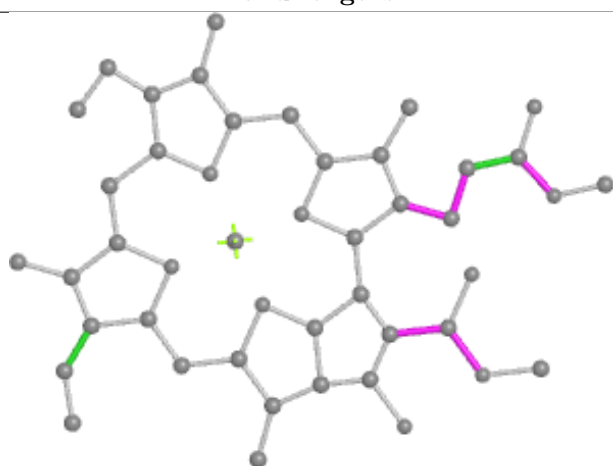
Ligand CLA 4 311



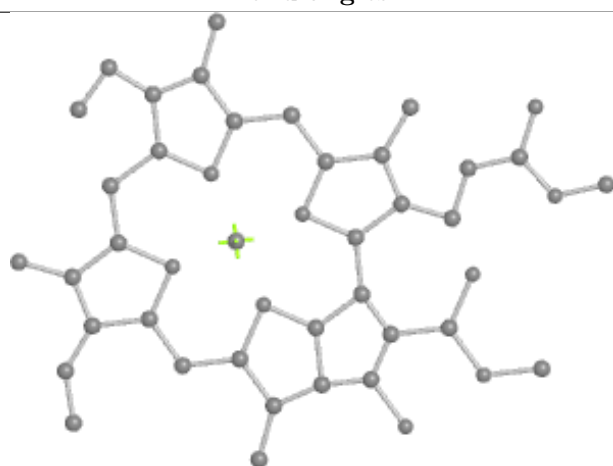
Bond lengths



Bond angles

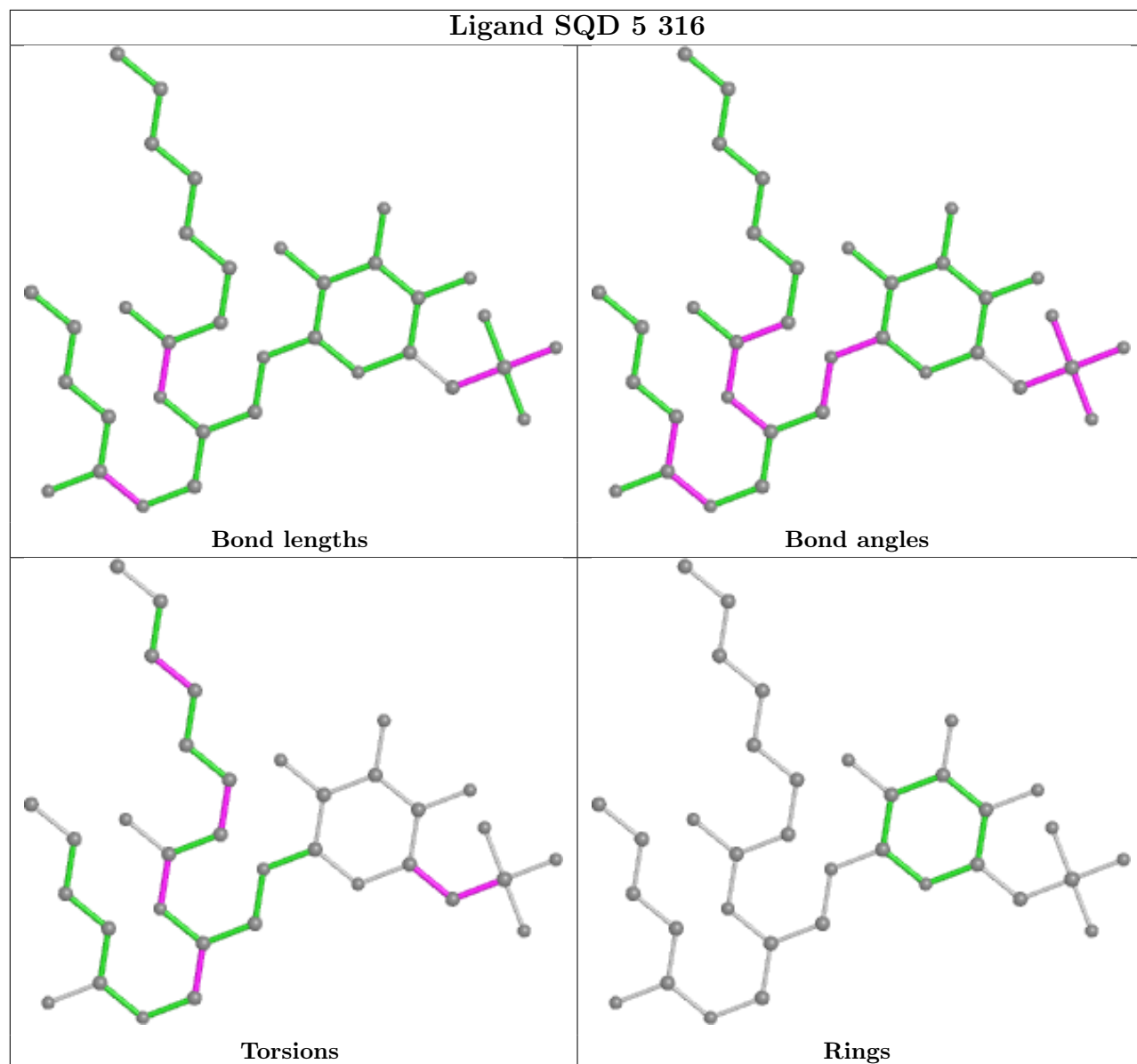


Torsions

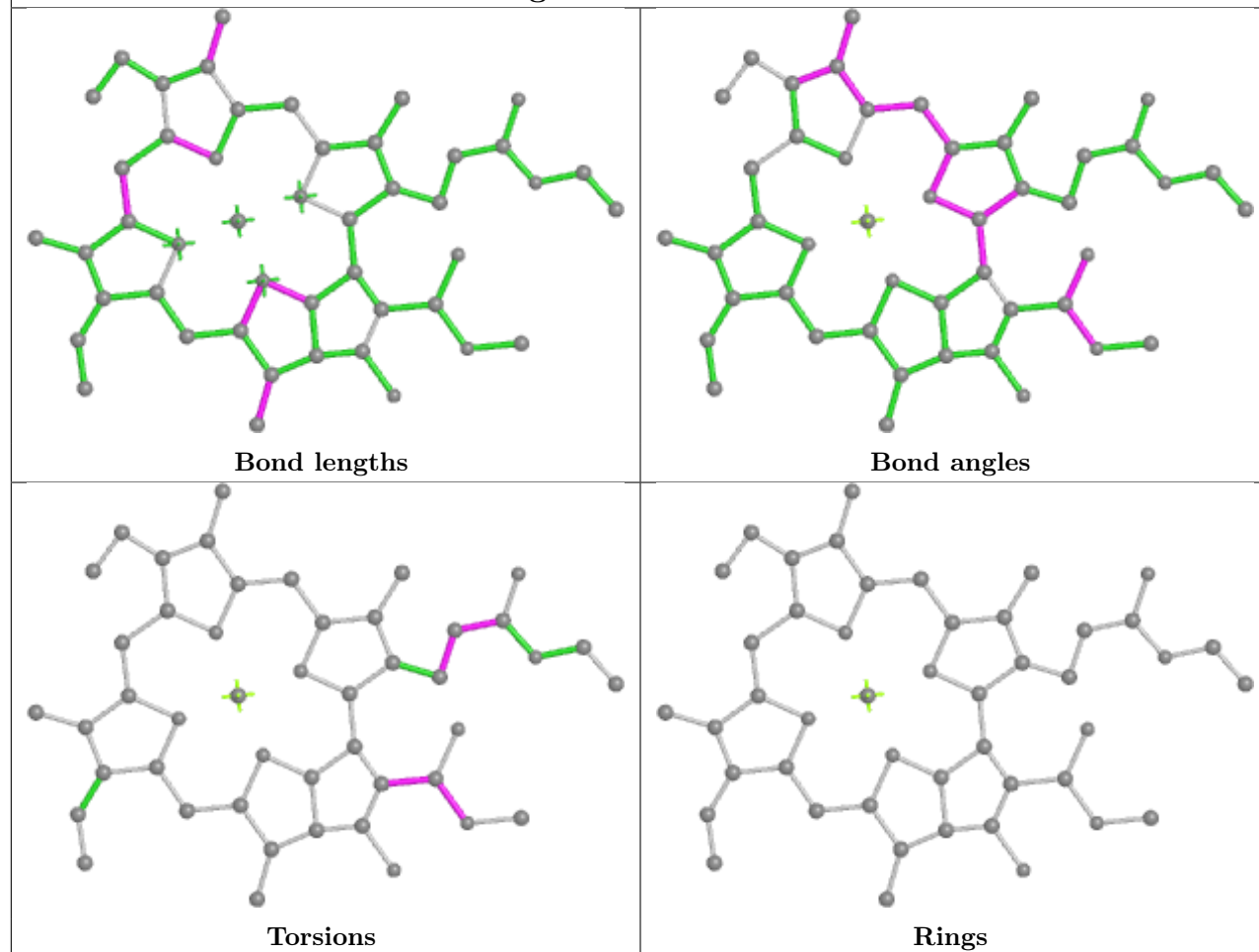


Rings

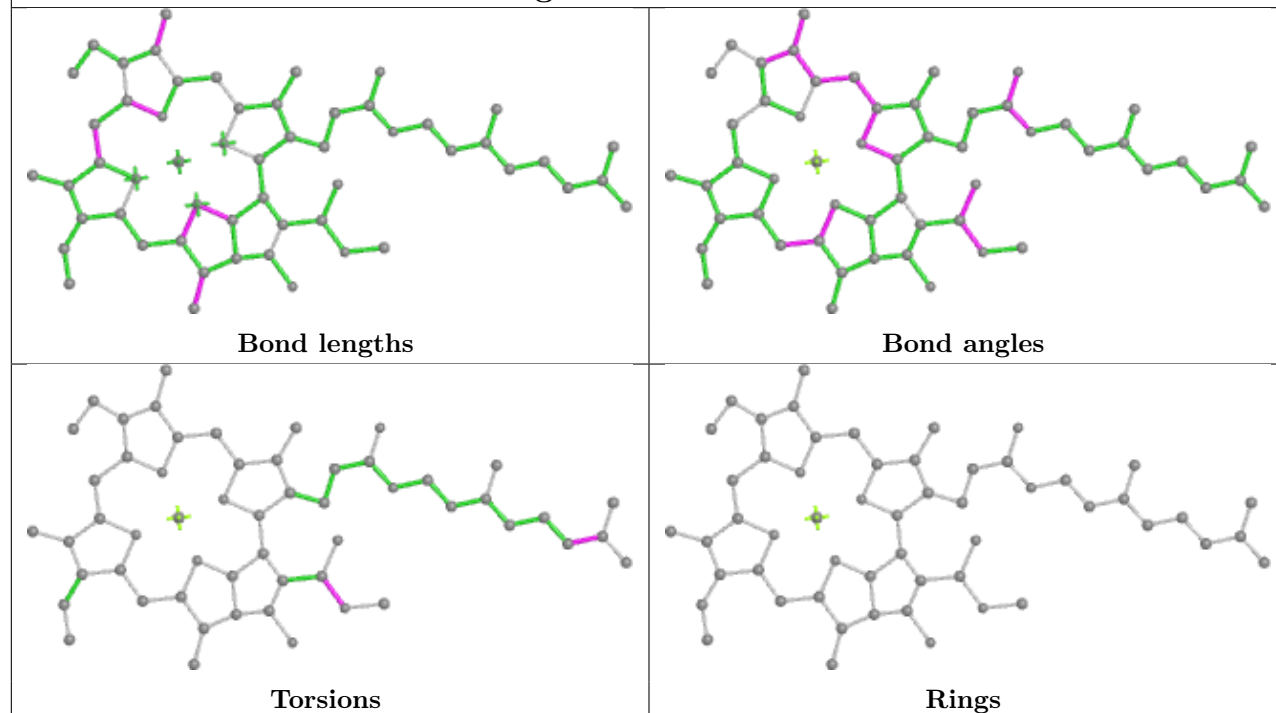
Ligand SQD 5 316



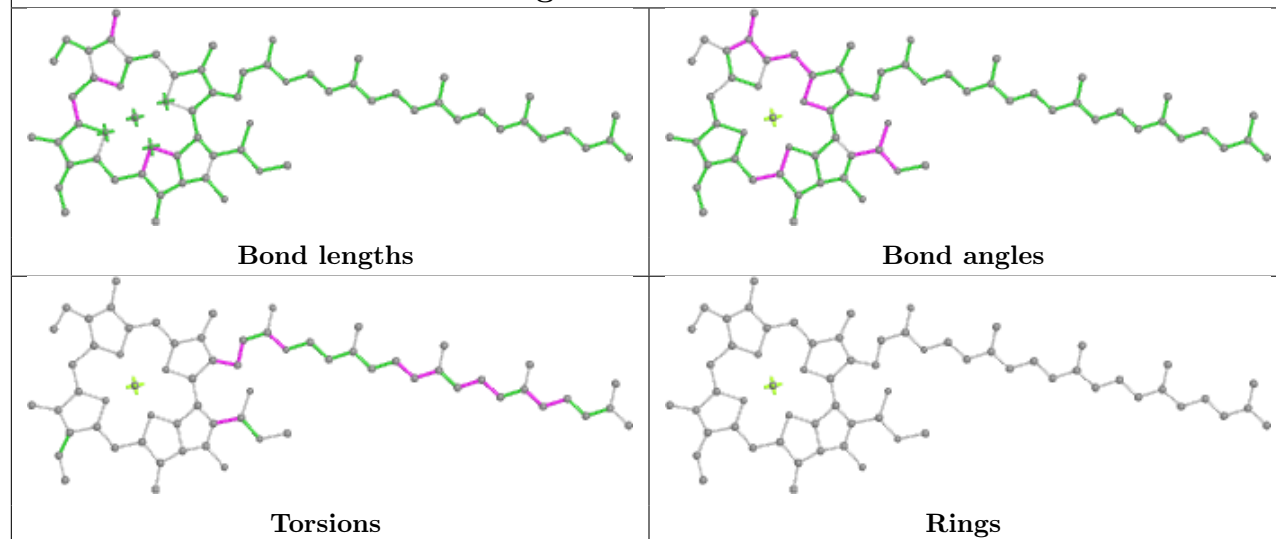
Ligand CLA 2 307



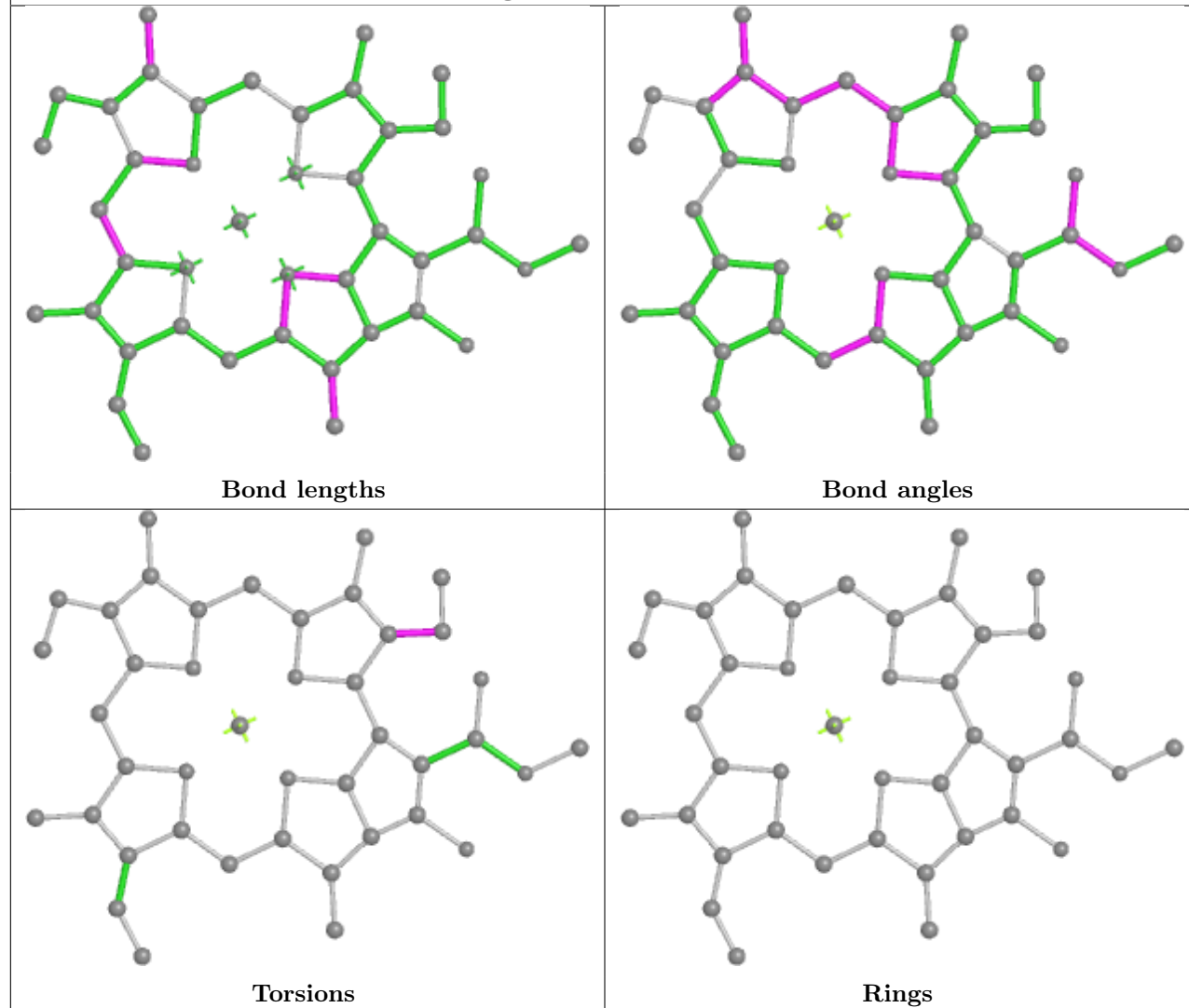
Ligand CLA b 820



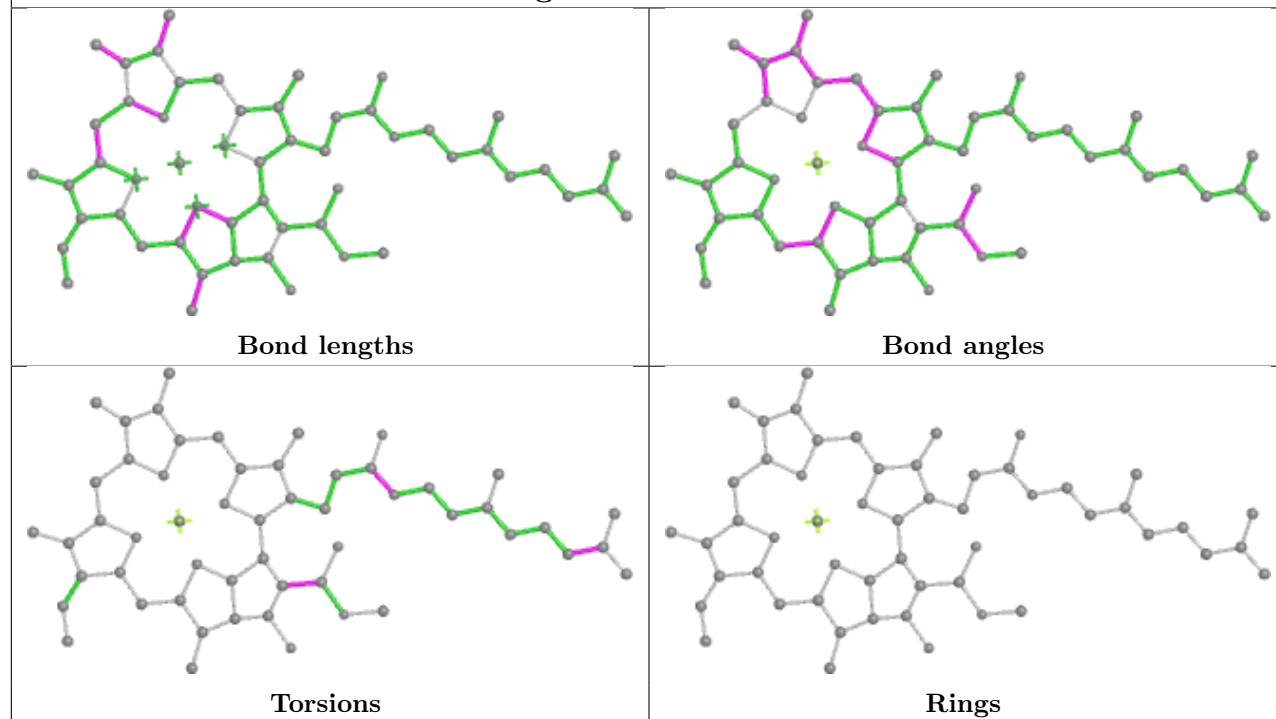
Ligand CLA a 809



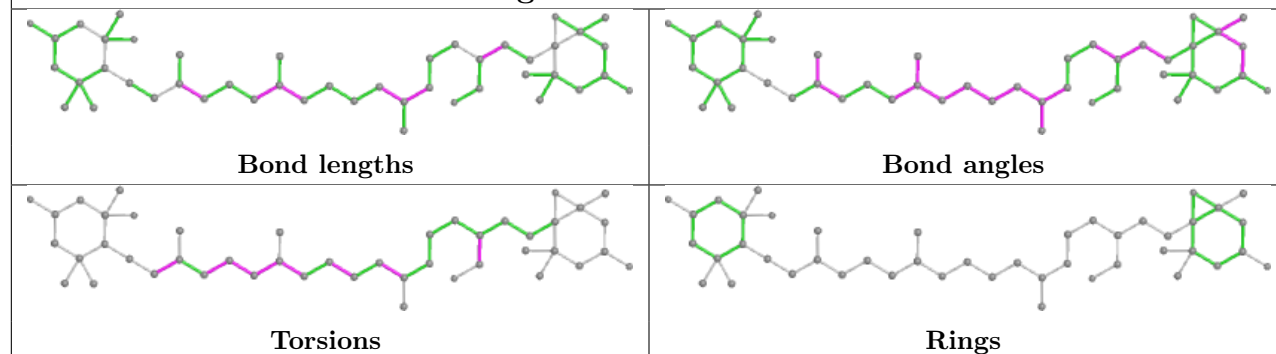
Ligand CLA 2 315



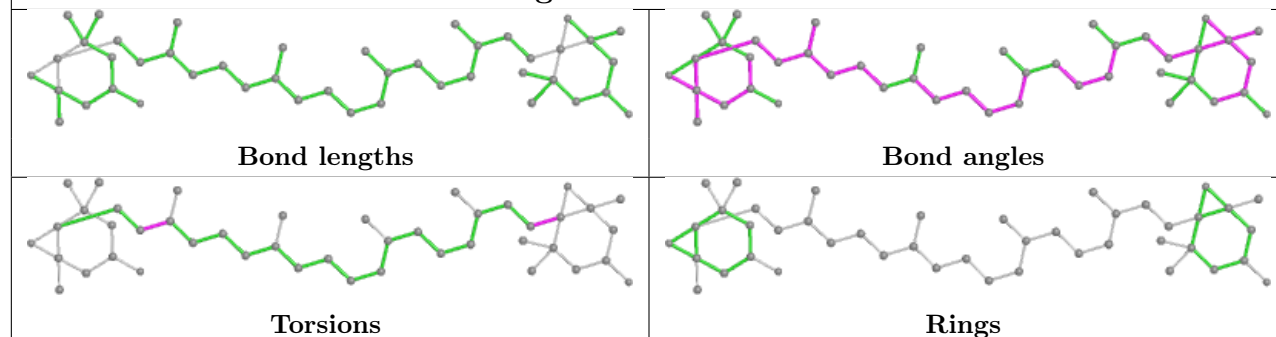
Ligand CLA b 812



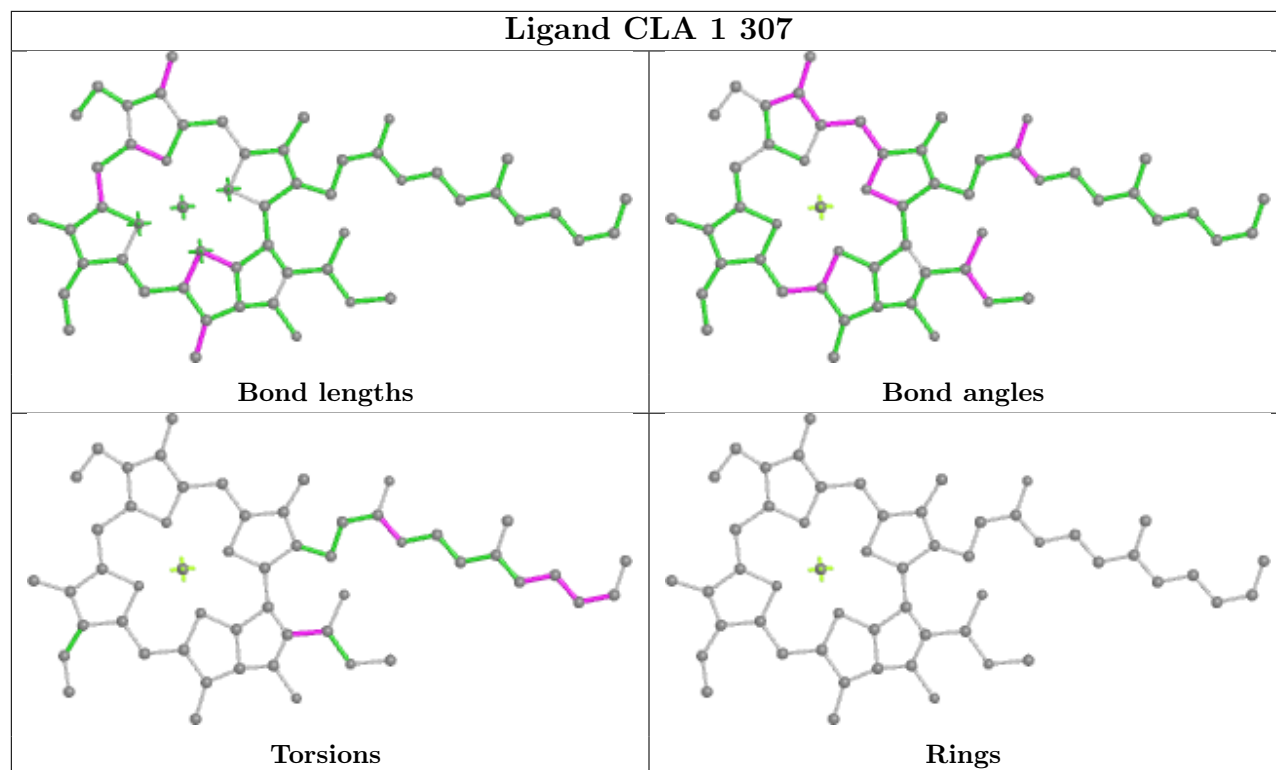
Ligand A1L1G 1 301



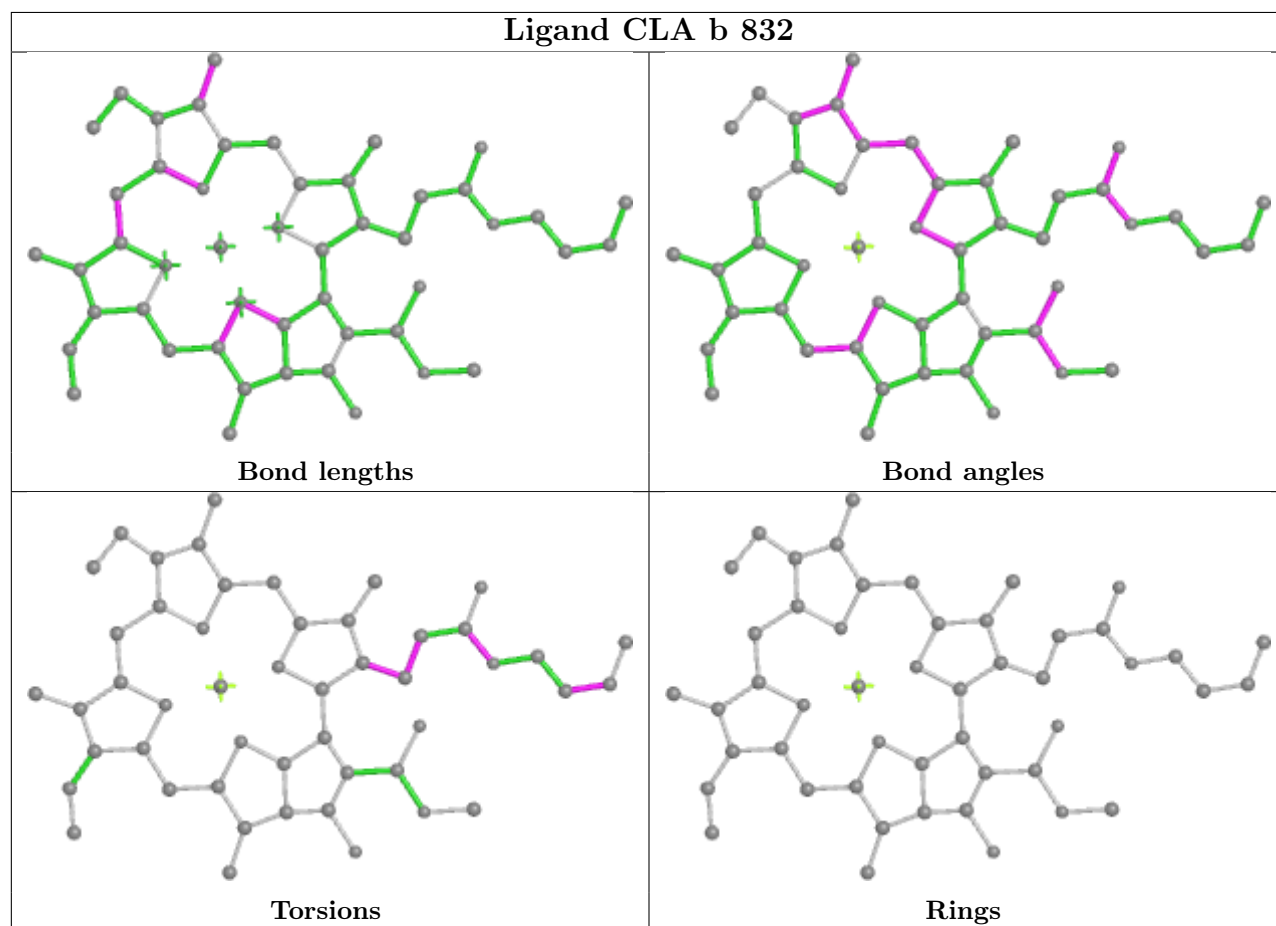
Ligand XAT 3 303

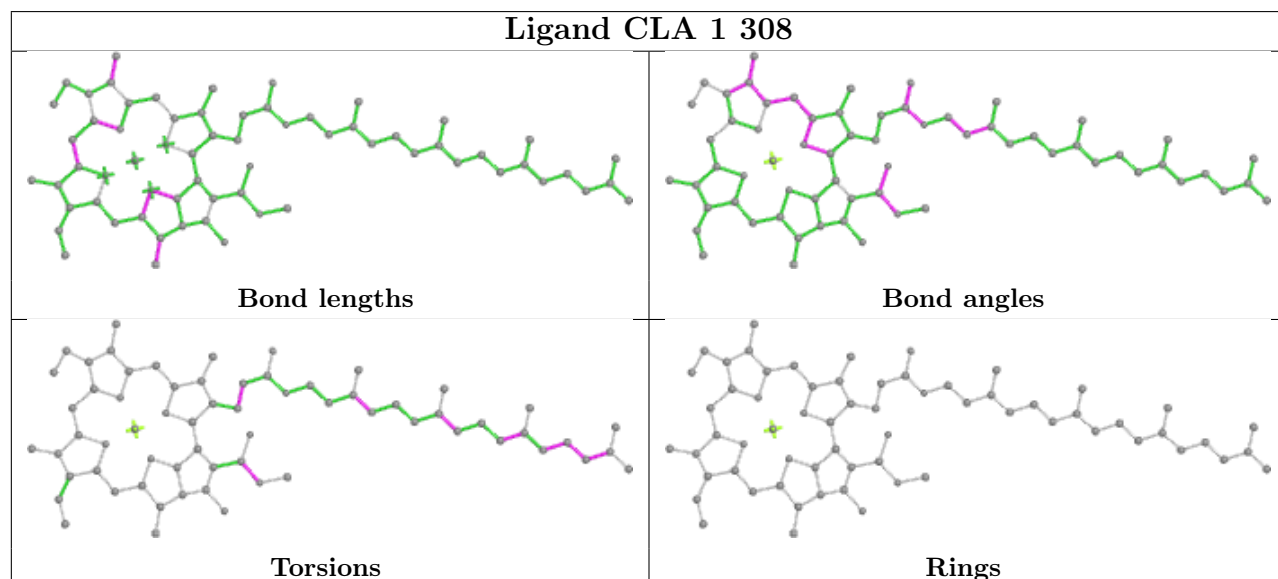
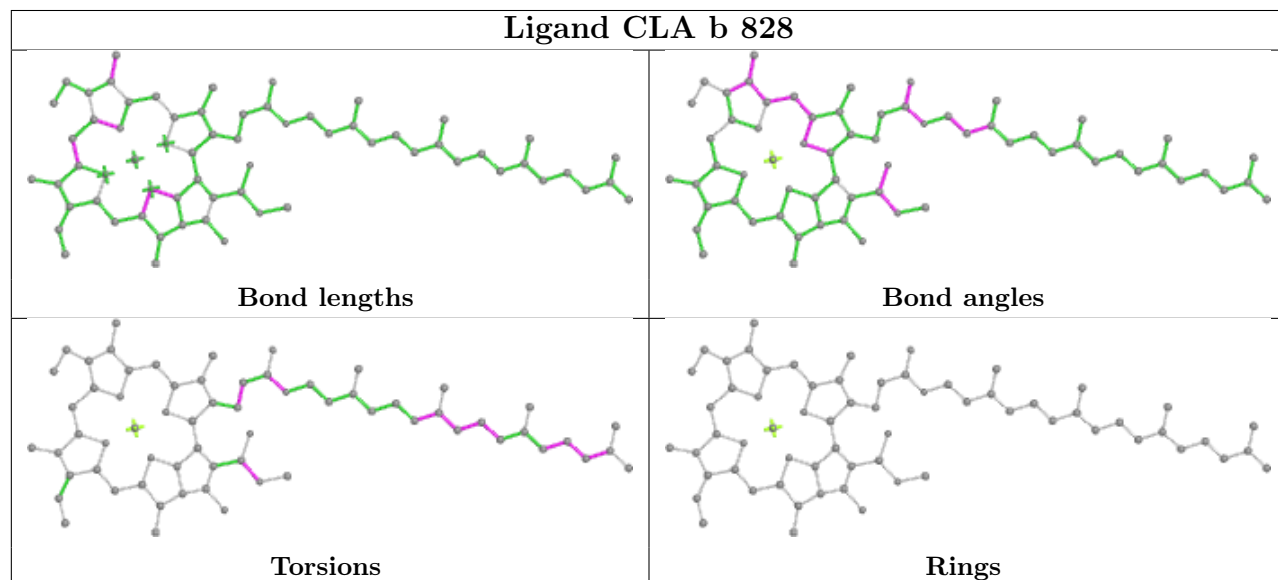
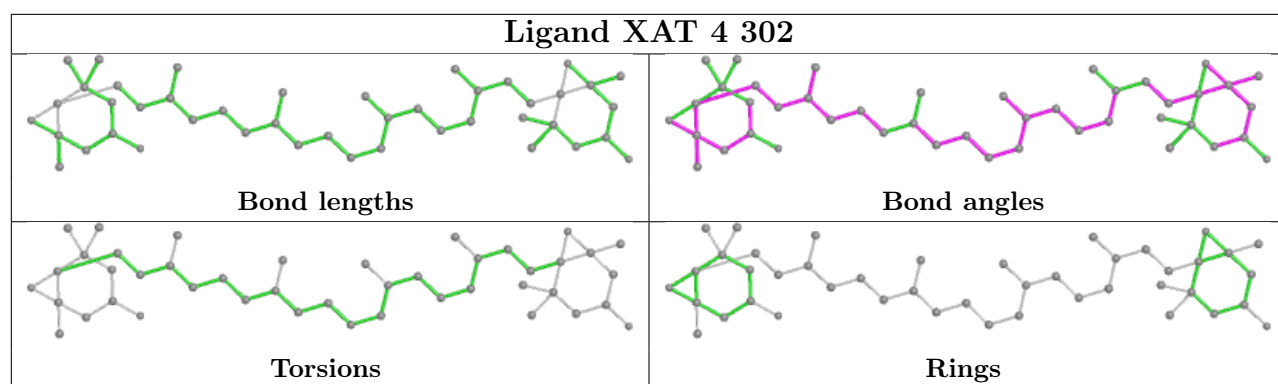


Ligand CLA 1 307

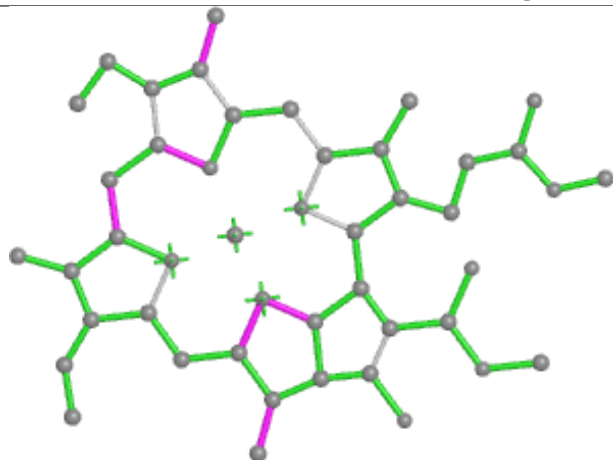


Ligand CLA b 832

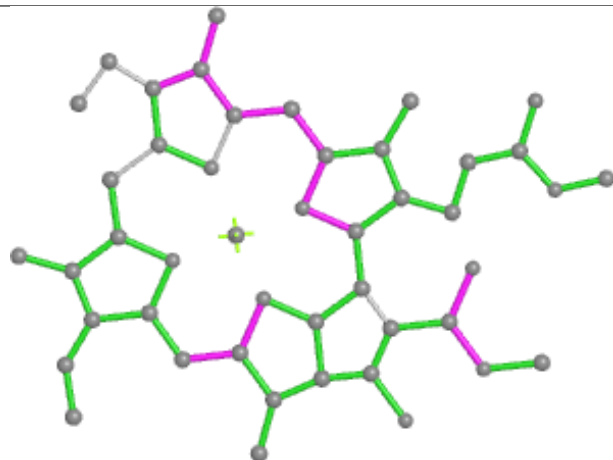




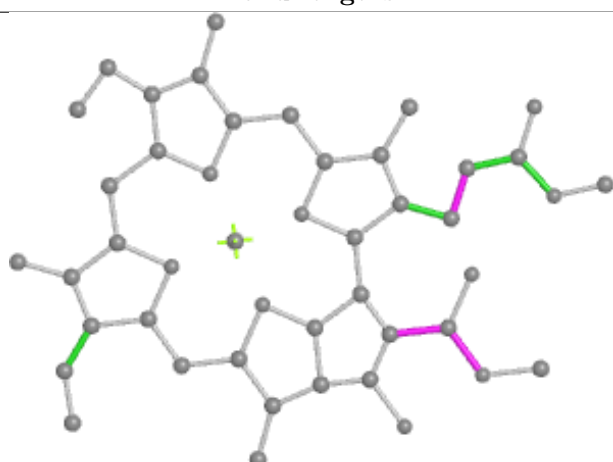
Ligand CLA 2 309



Bond lengths



Bond angles

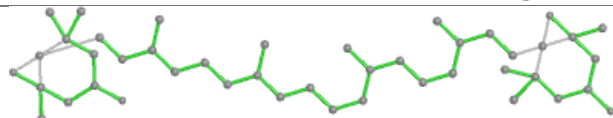


Torsions

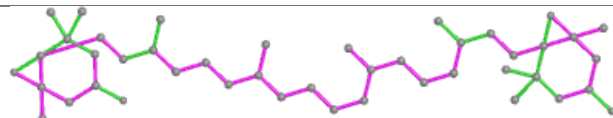


Rings

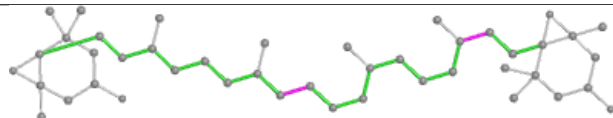
Ligand XAT 2 304



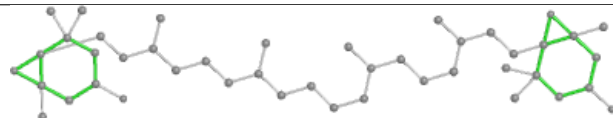
Bond lengths



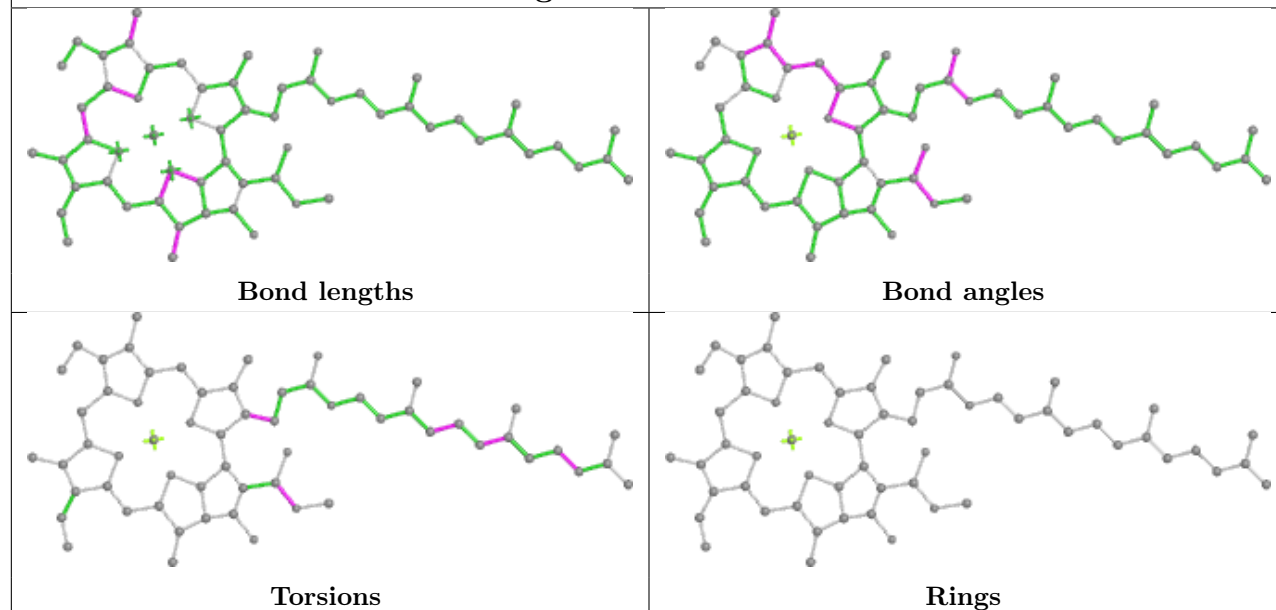
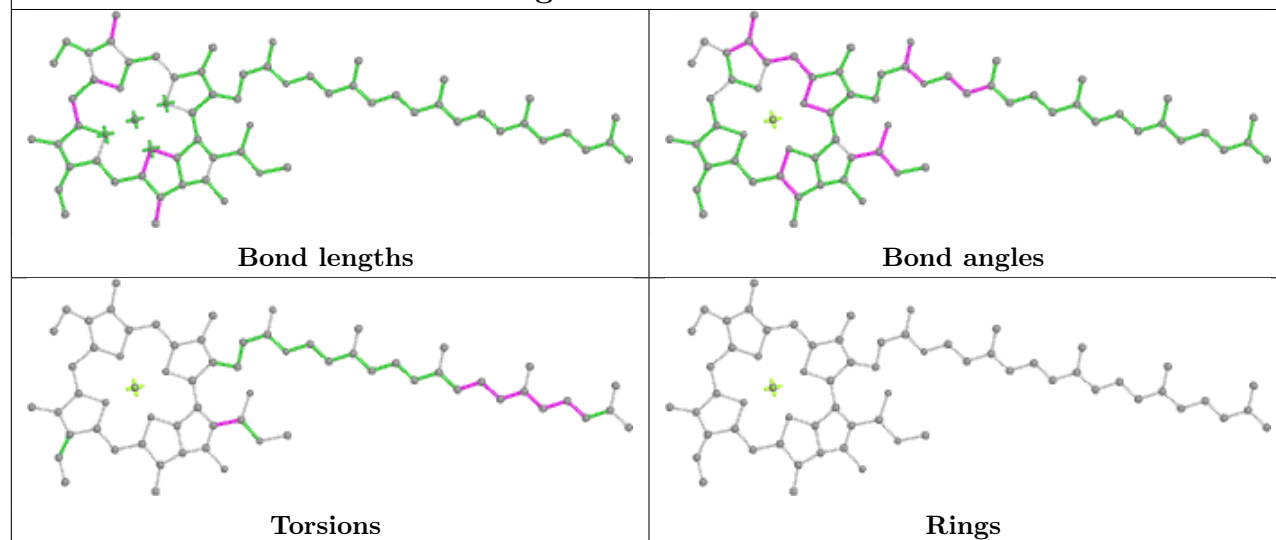
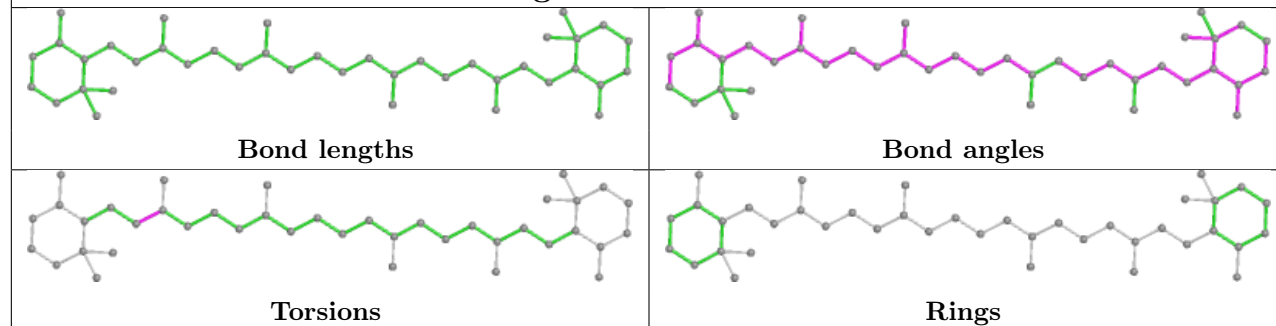
Bond angles

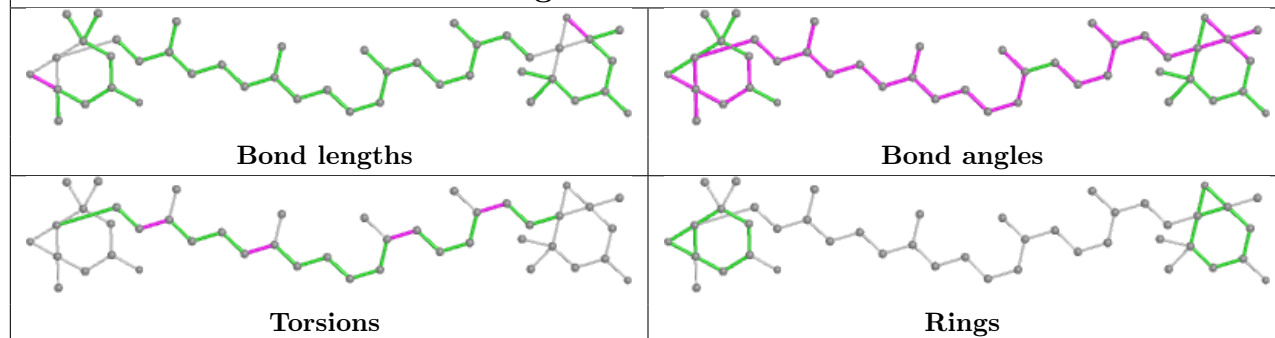
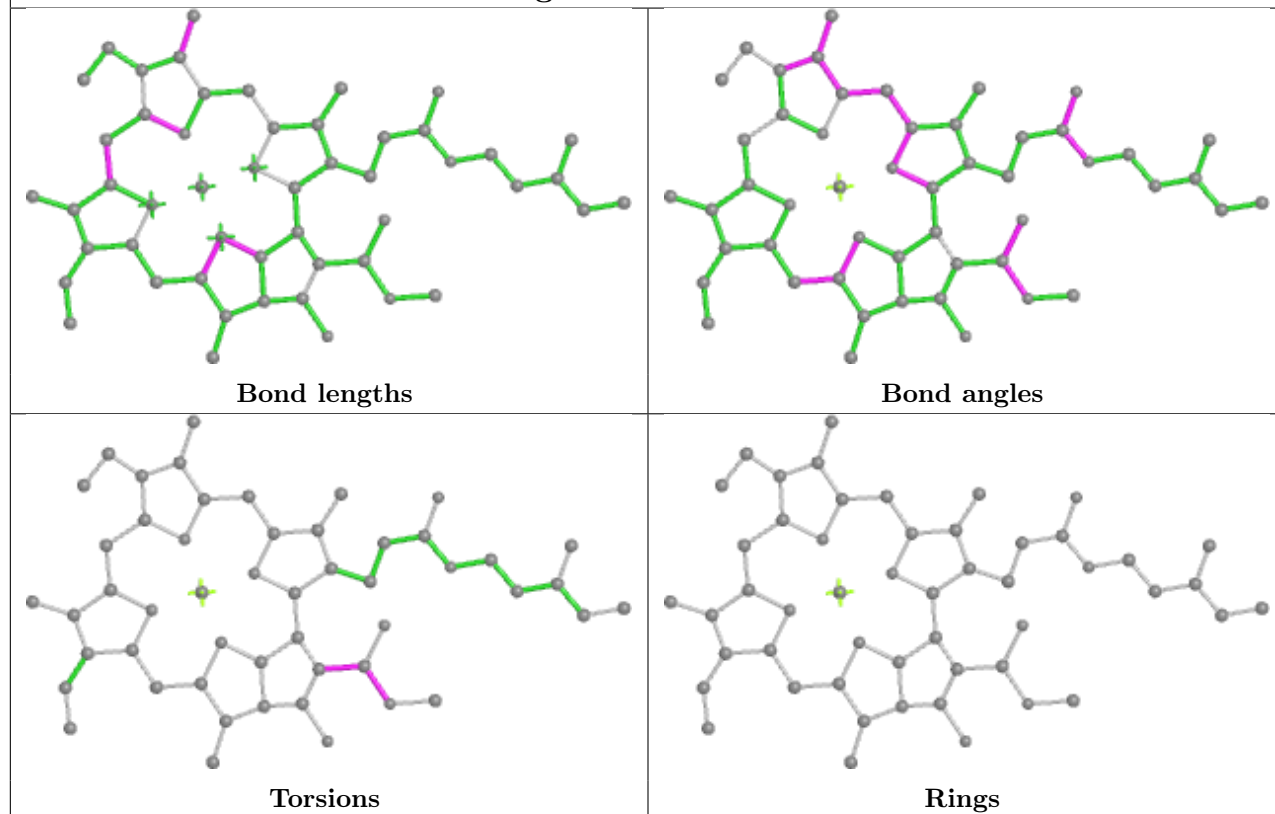
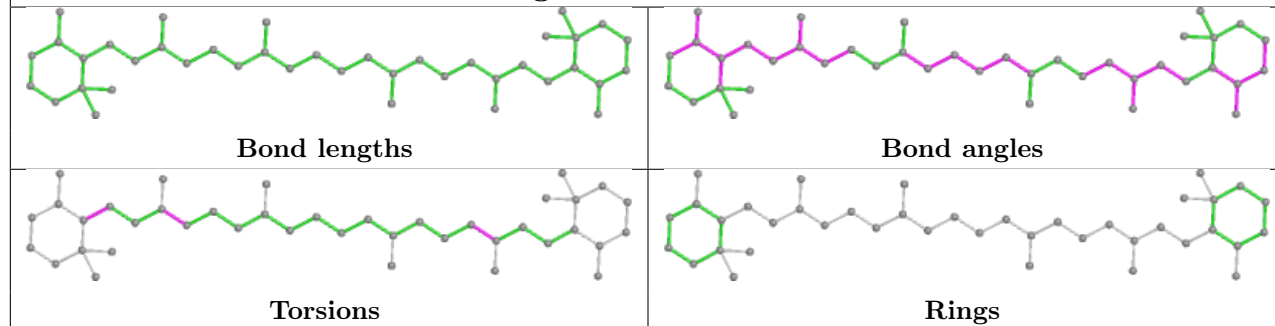


Torsions

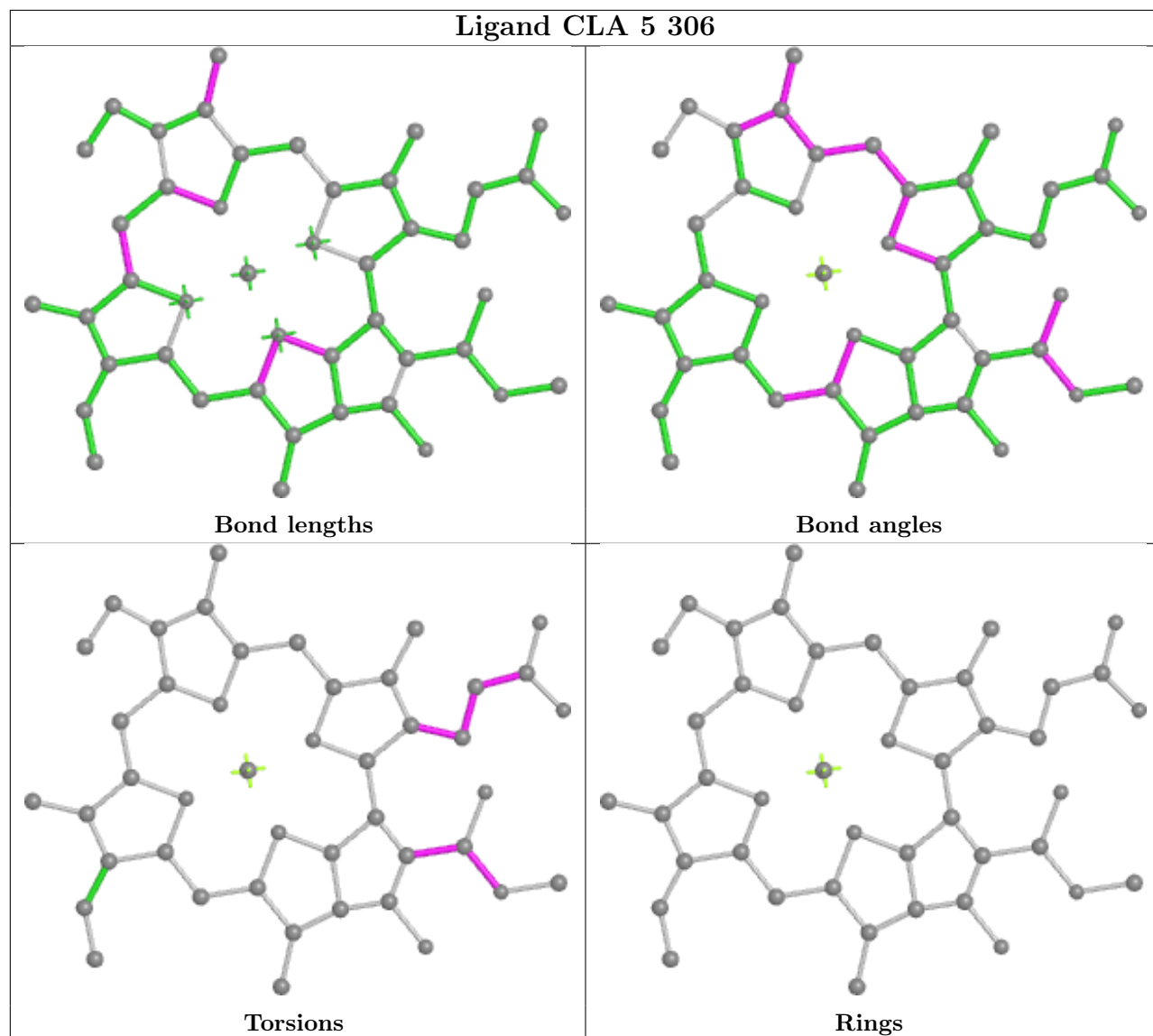


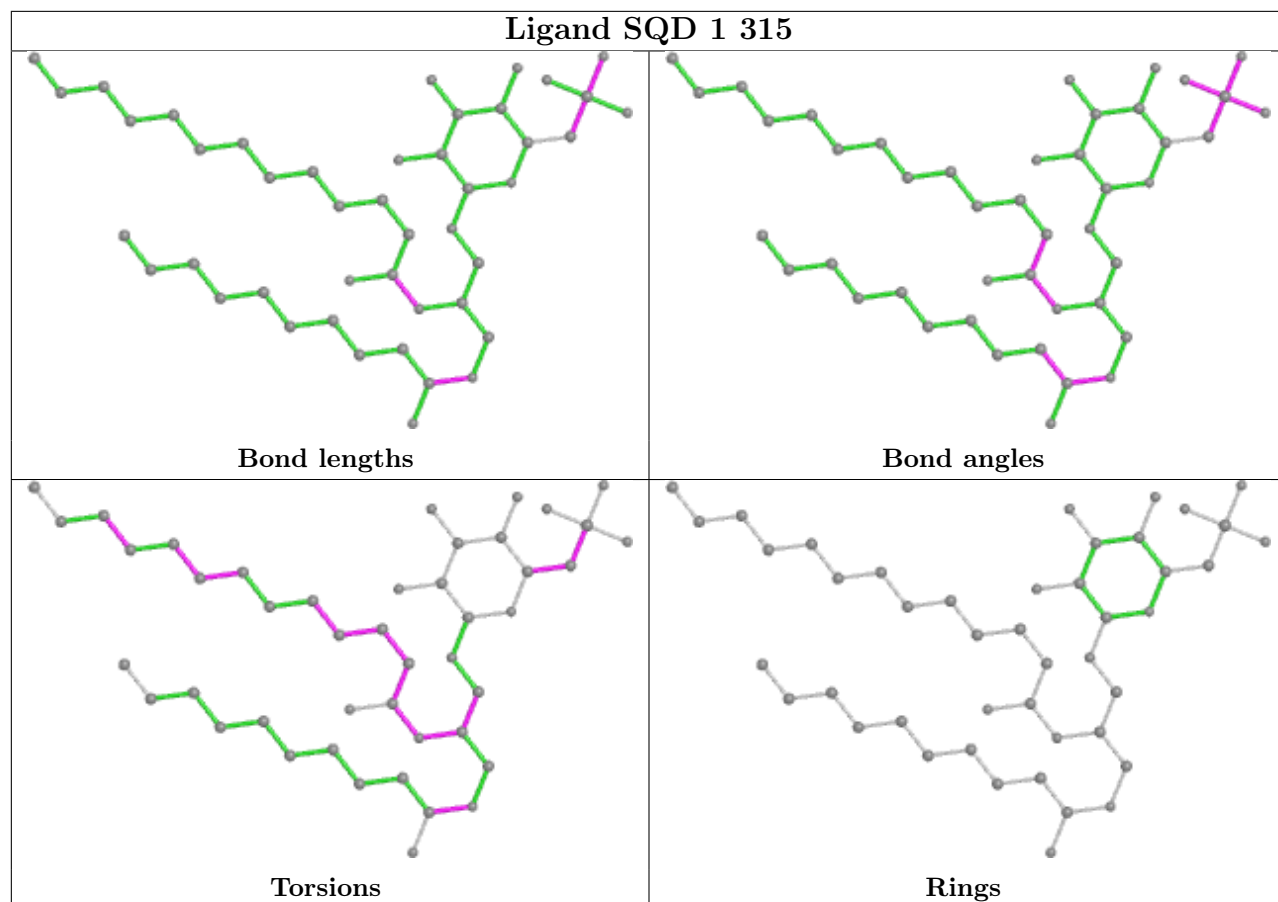
Rings

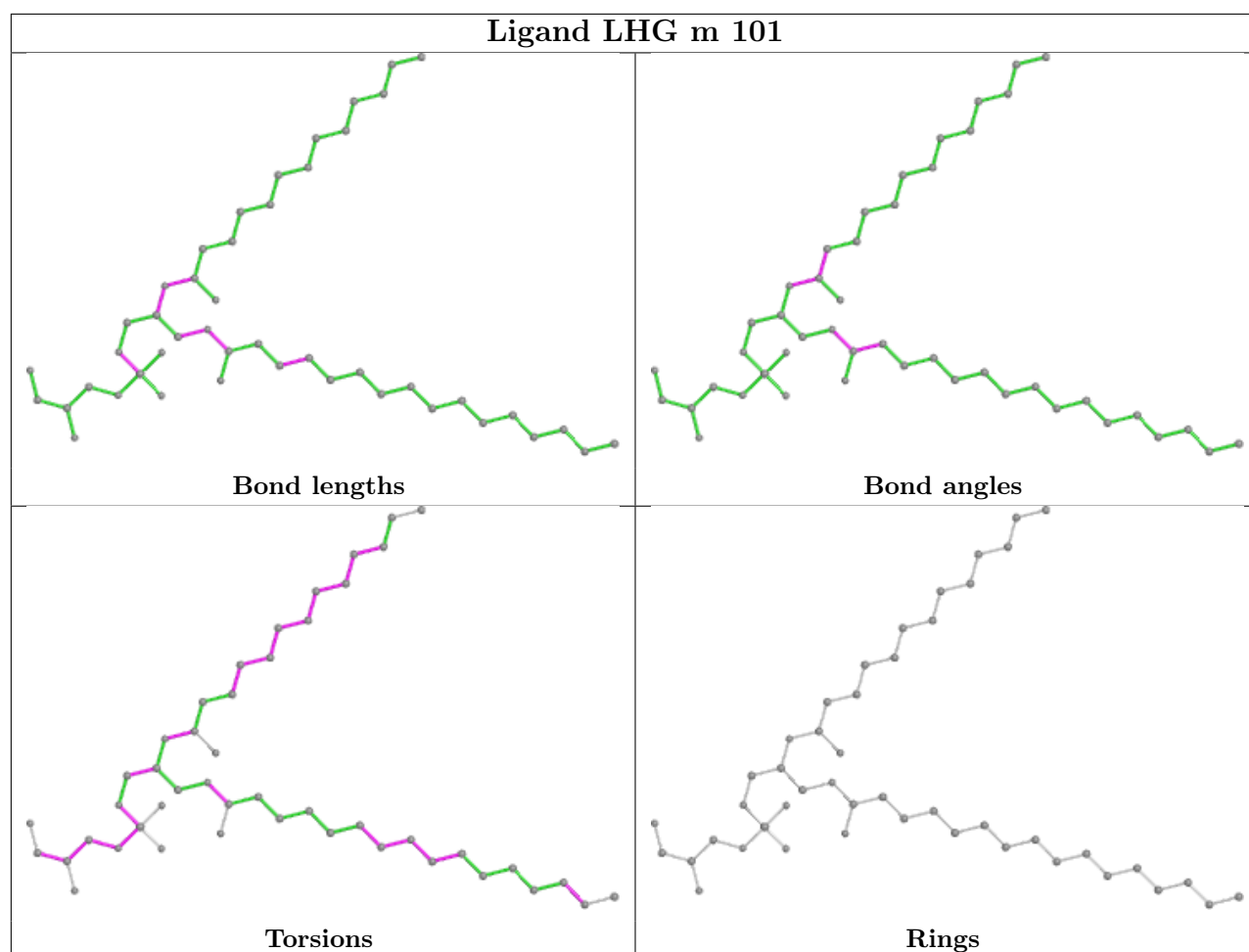
Ligand CLA b 823**Ligand CLA b 830****Ligand BCR b 847**

Ligand XAT a 852**Ligand CLA a 808****Ligand BCR b 845**

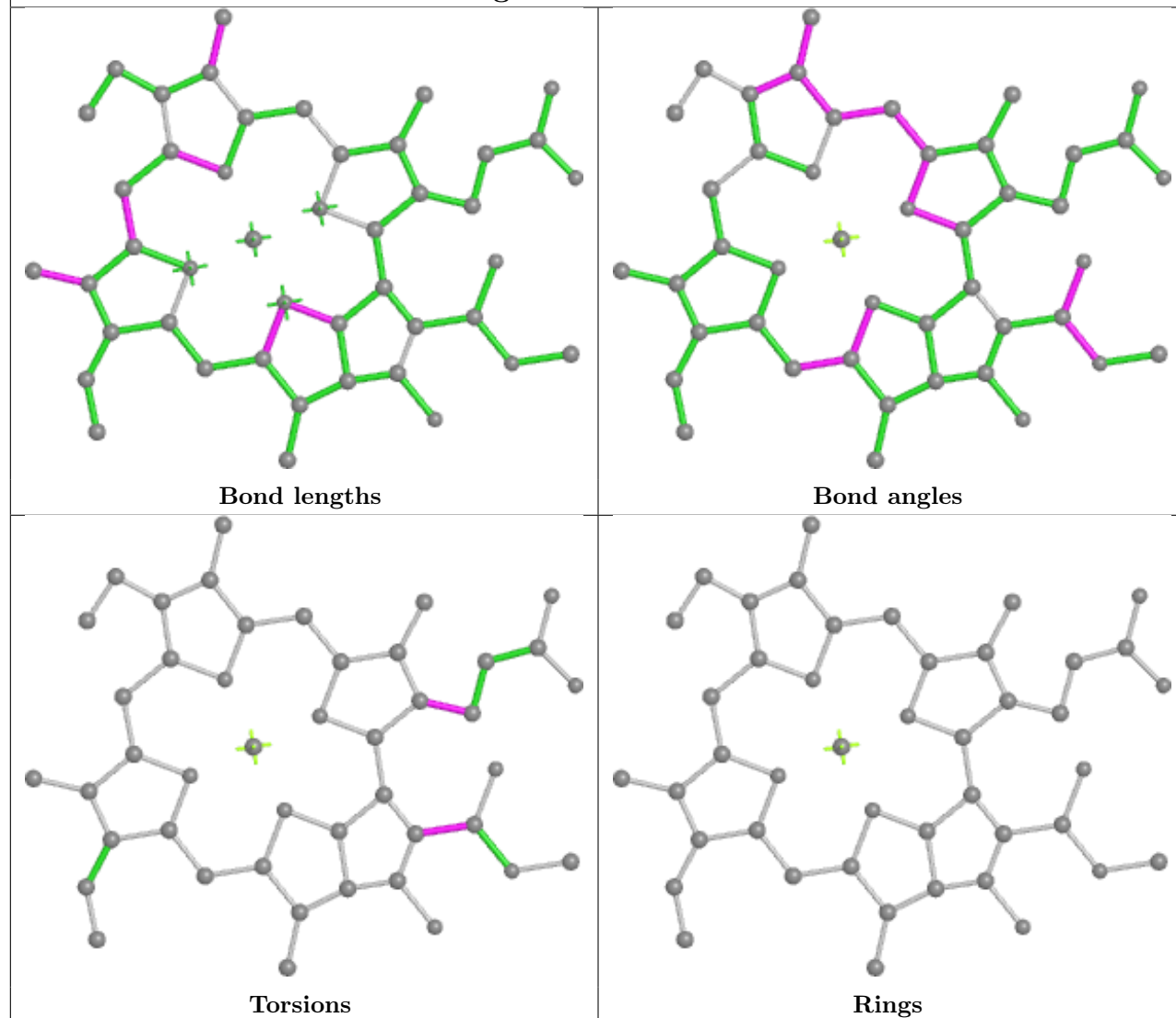
Ligand CLA 5 306



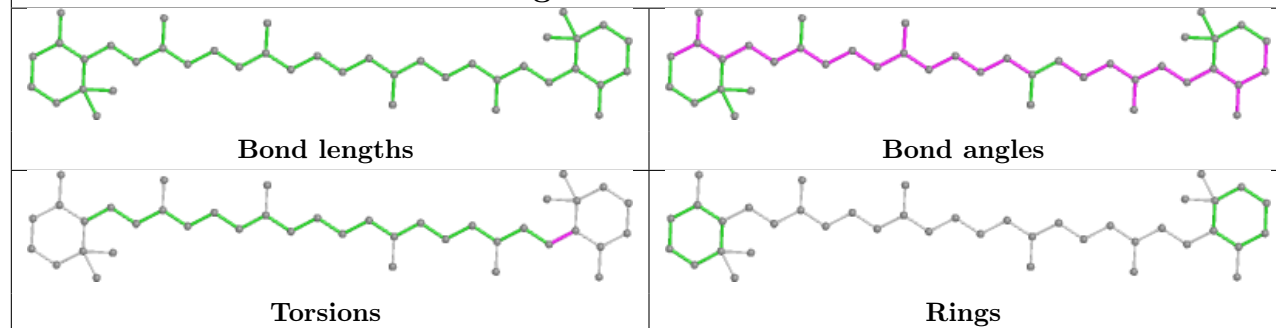


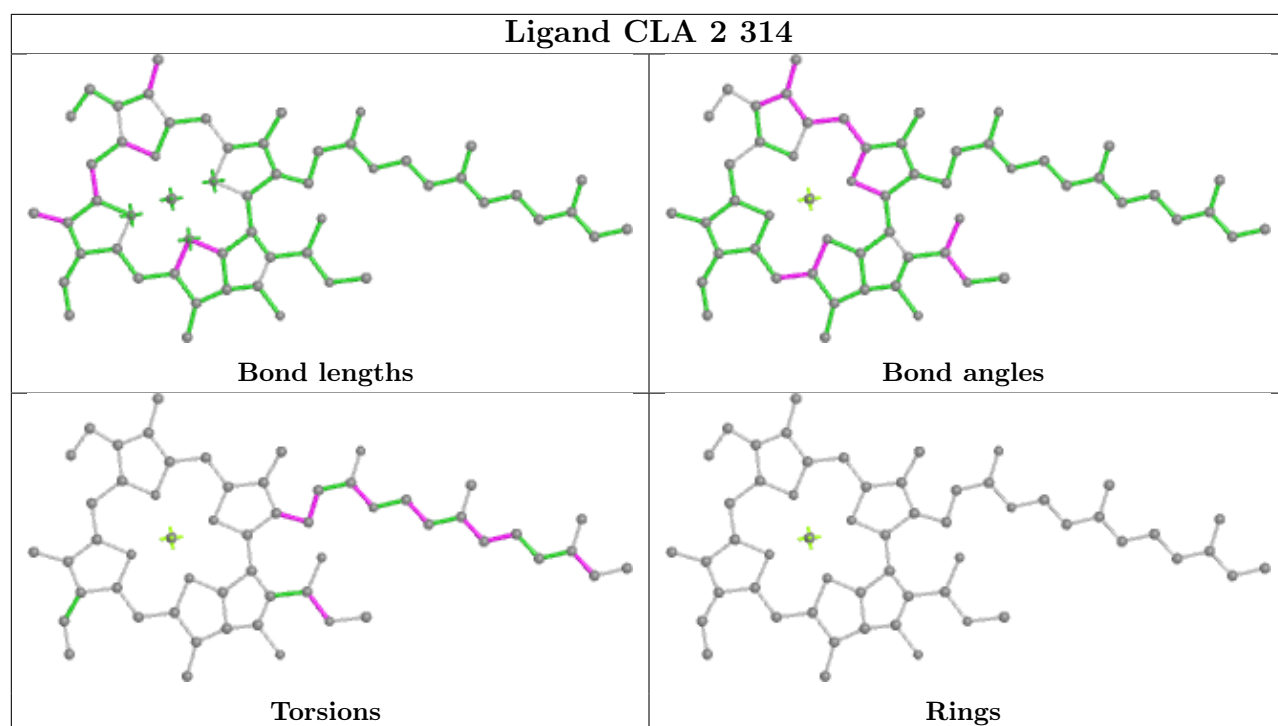


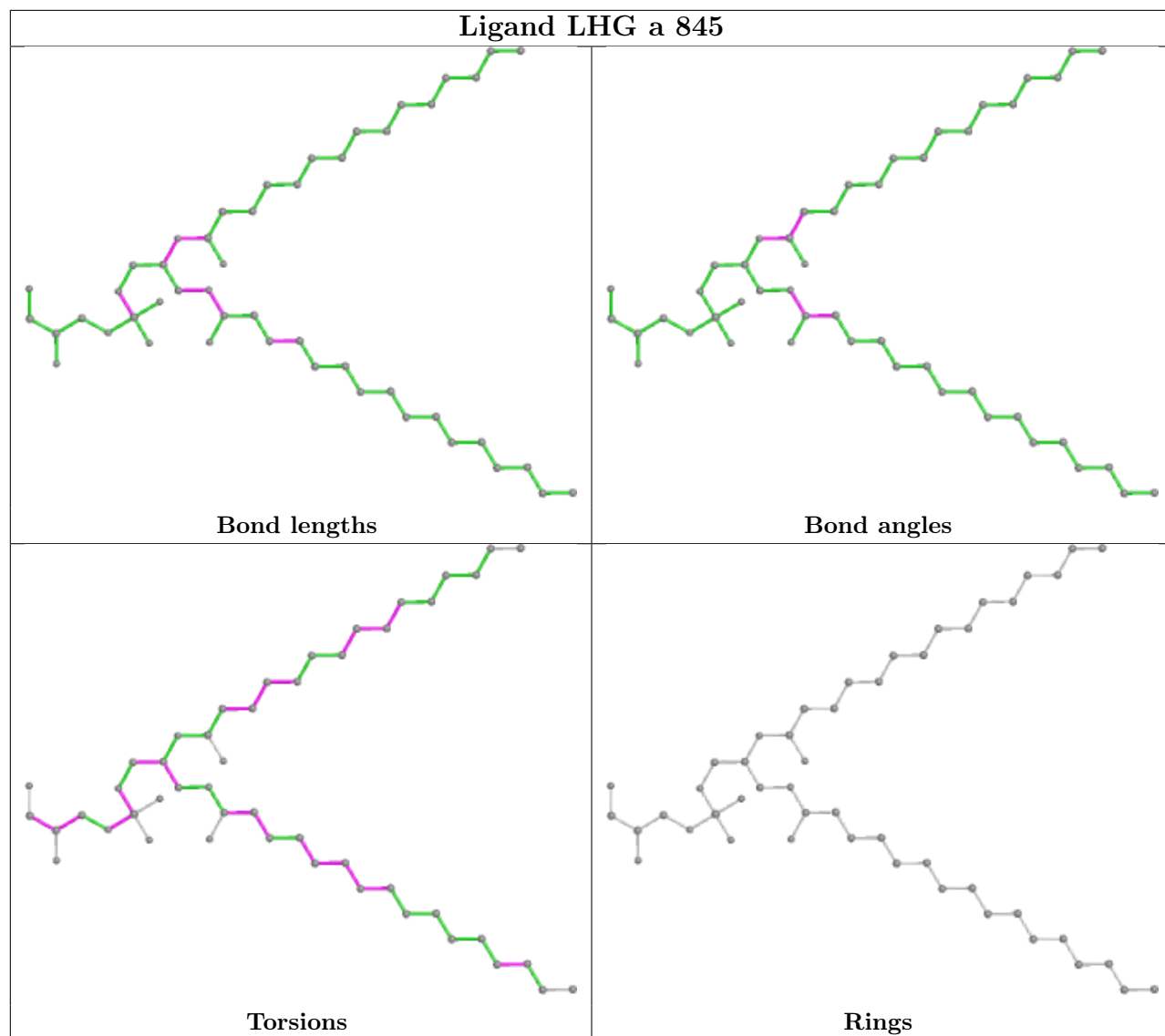
Ligand CLA b 816



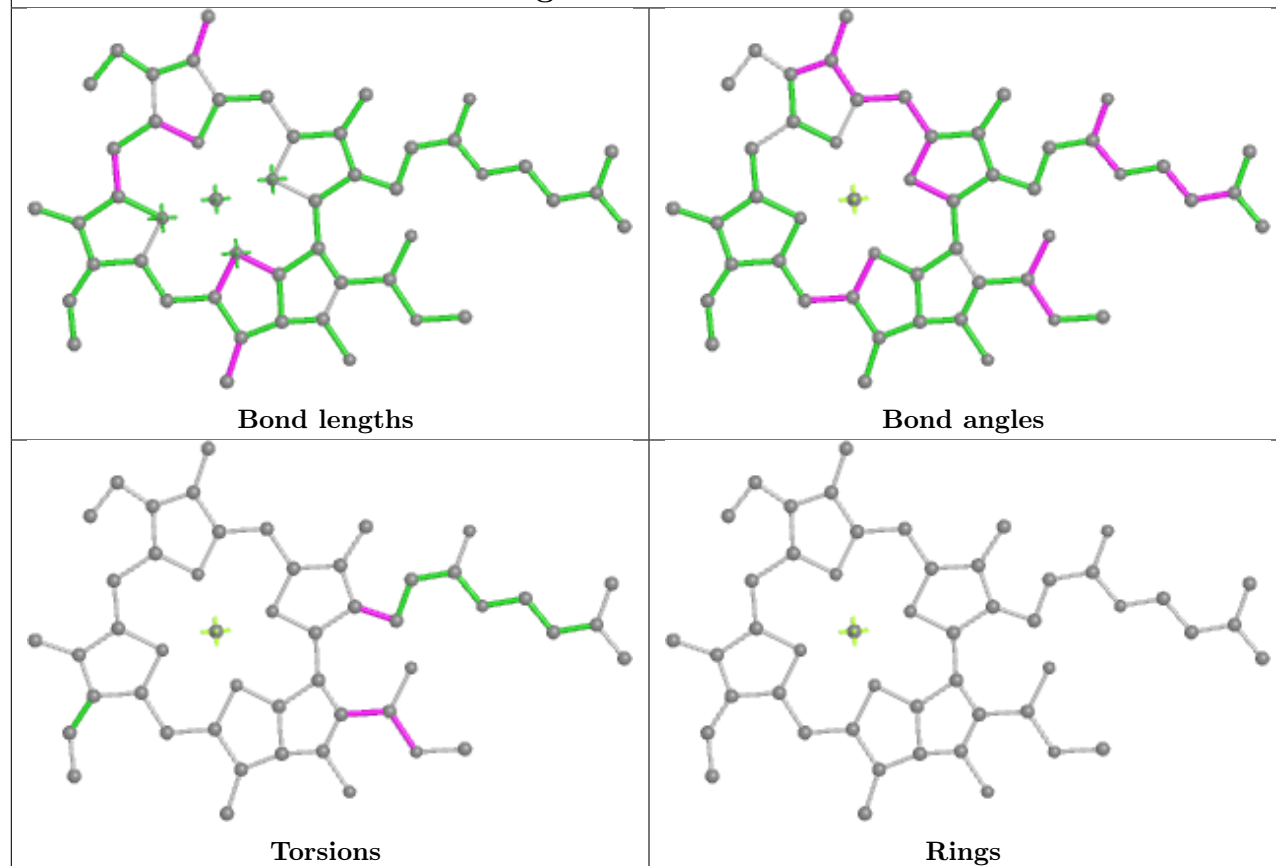
Ligand BCR b 850



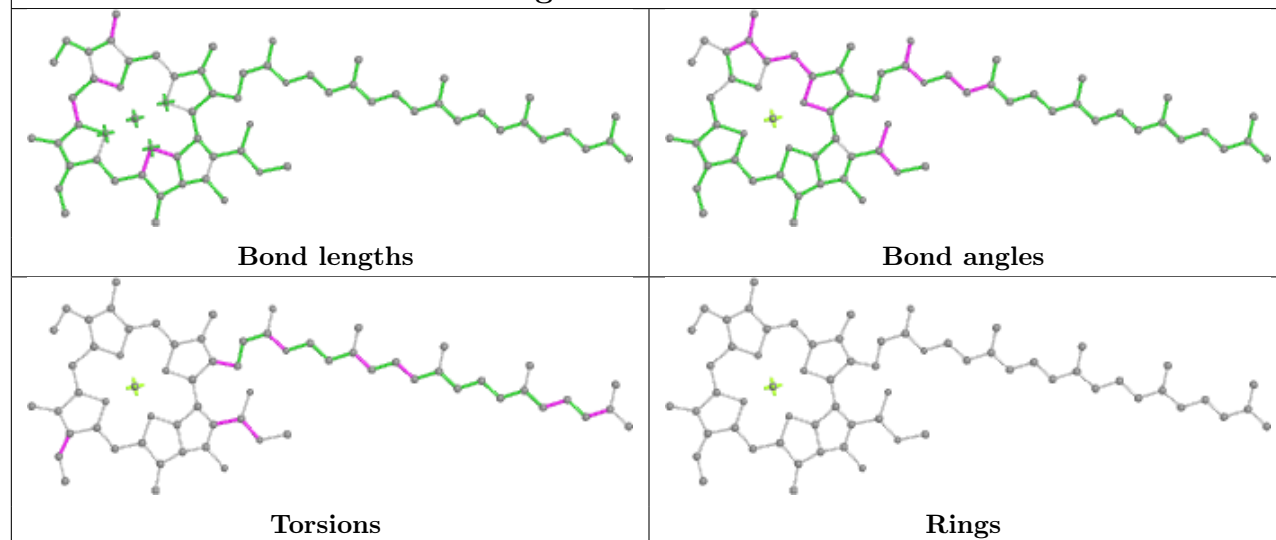


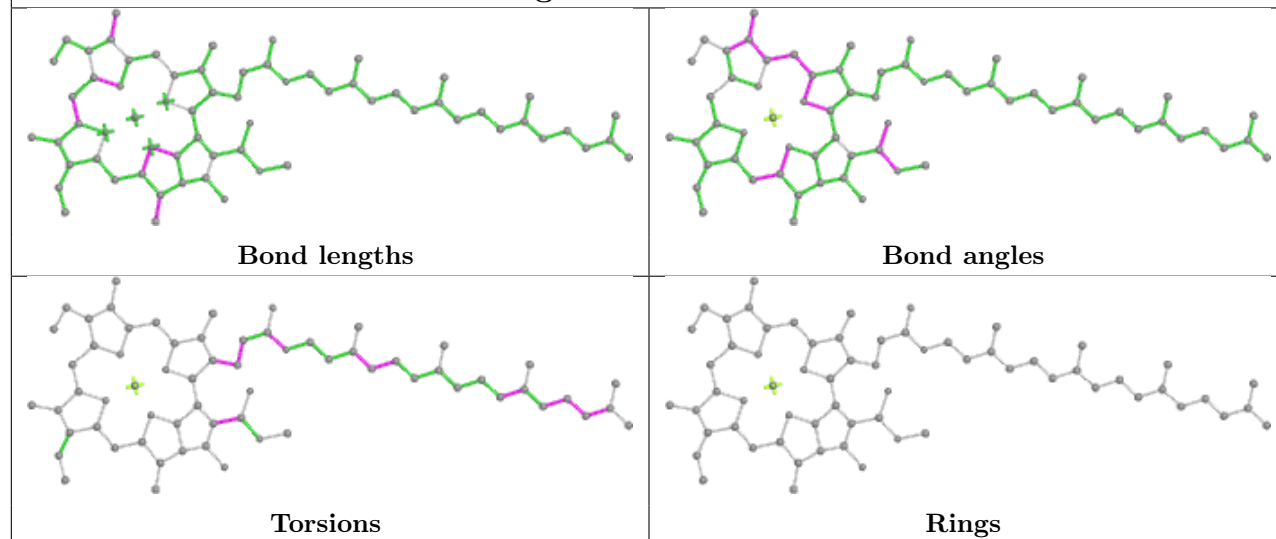
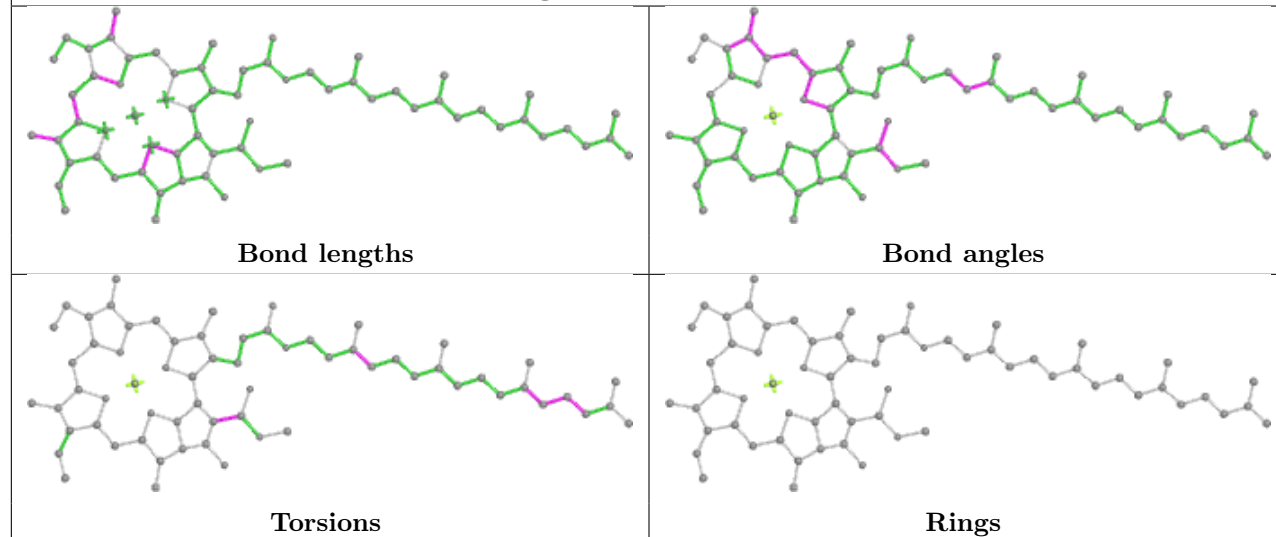


Ligand CLA a 832

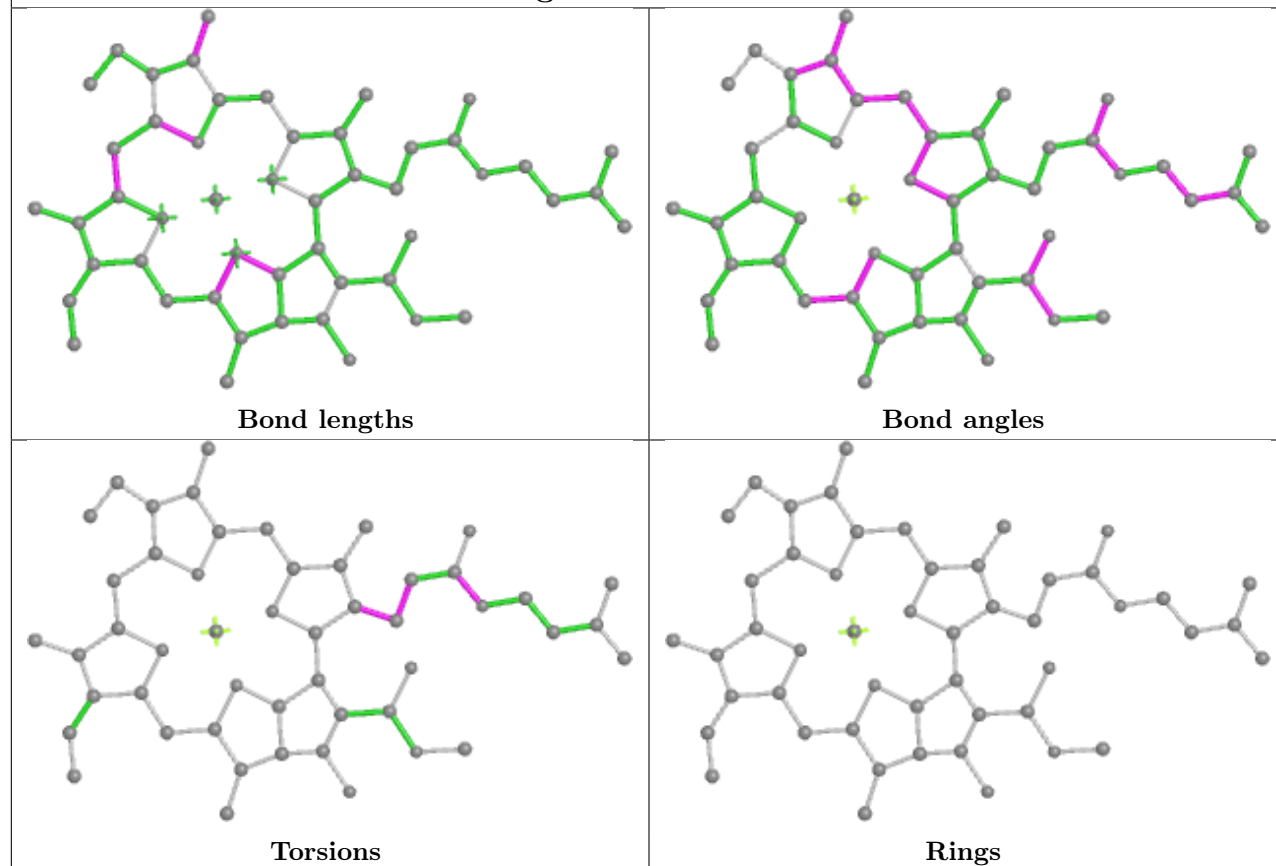


Ligand CLA b 840

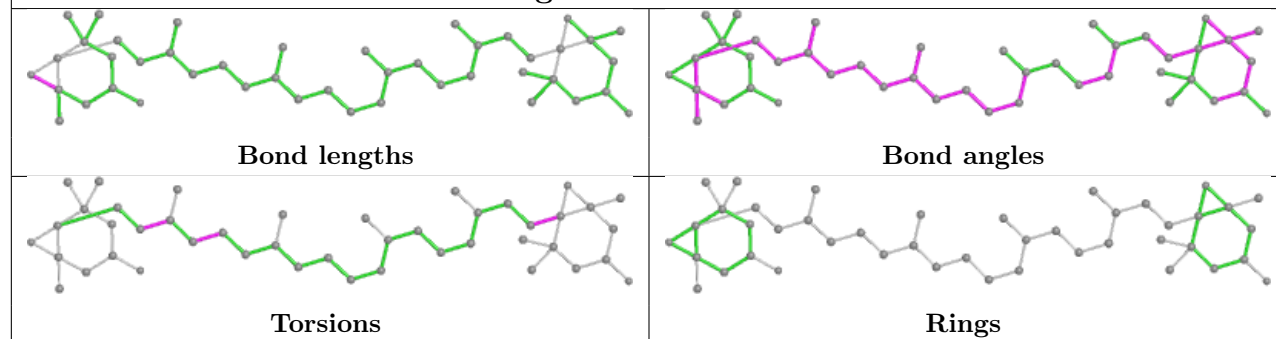


Ligand CLA b 834**Ligand CLA a 828**

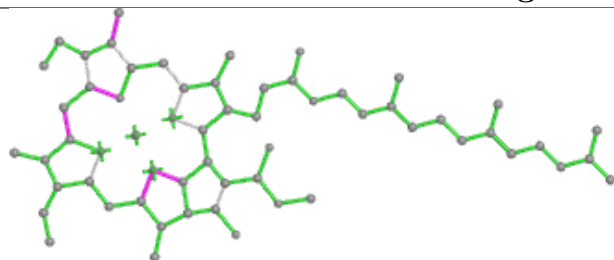
Ligand CLA 3 311



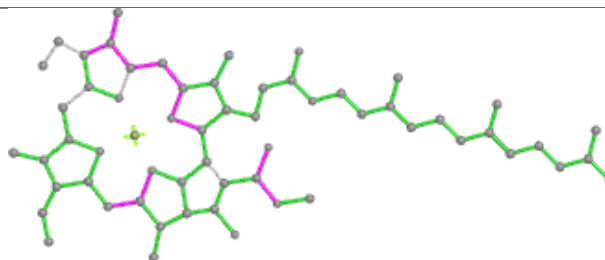
Ligand XAT 4 301



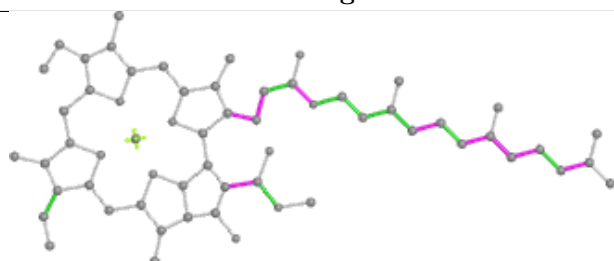
Ligand CLA b 819



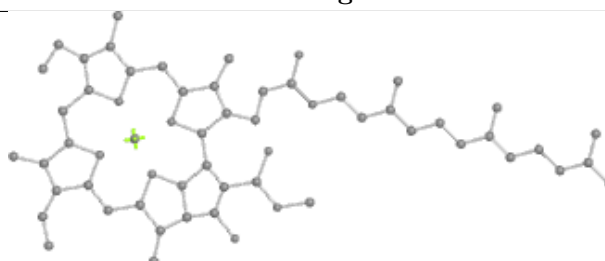
Bond lengths



Bond angles

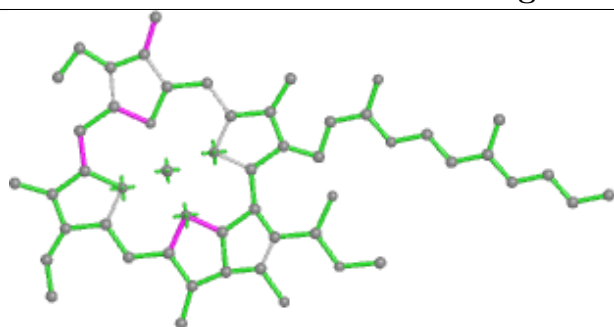


Torsions

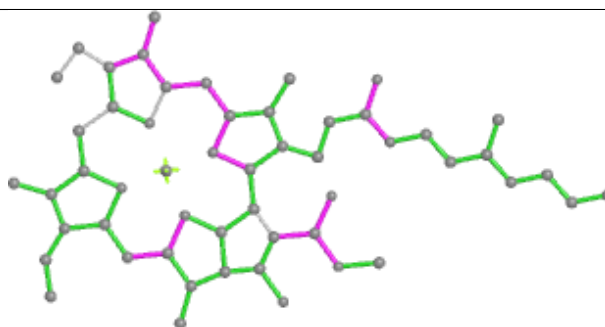


Rings

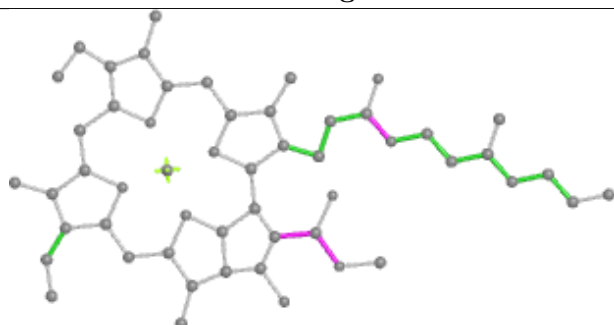
Ligand CLA 1 311



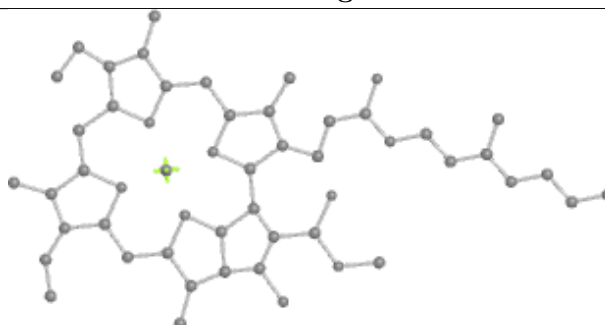
Bond lengths



Bond angles

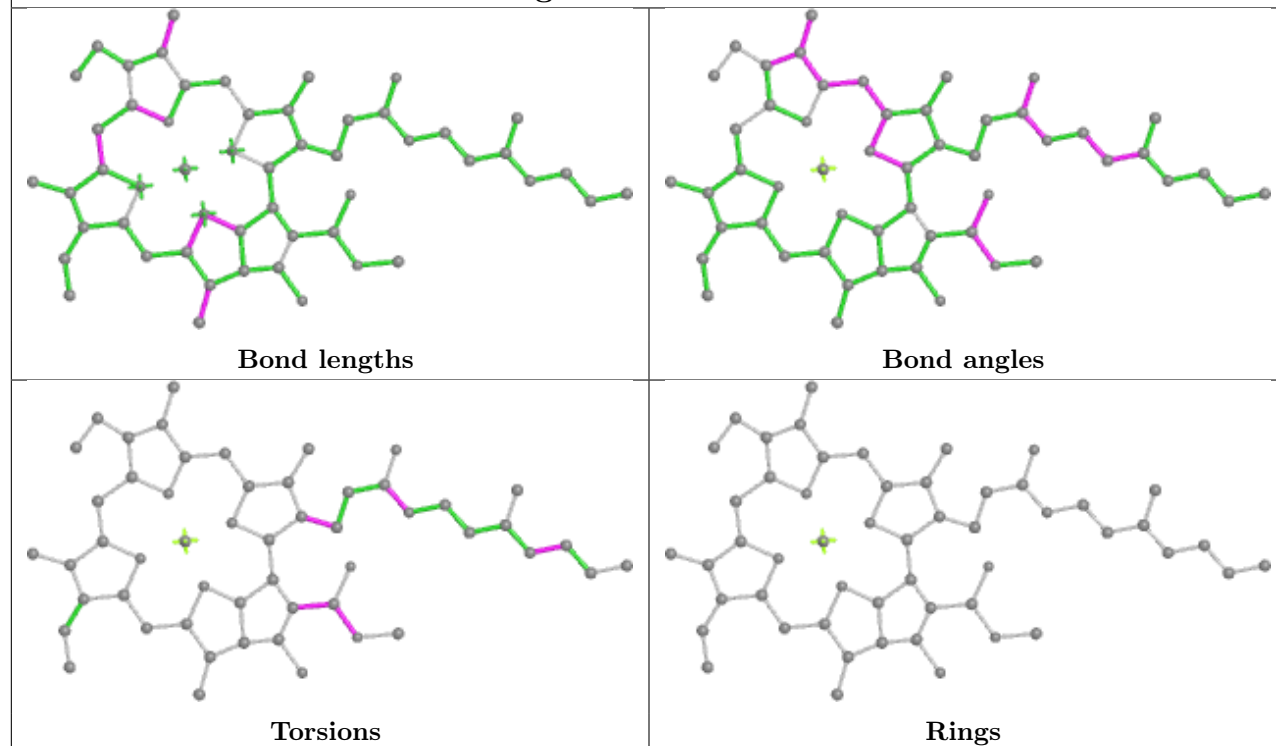


Torsions

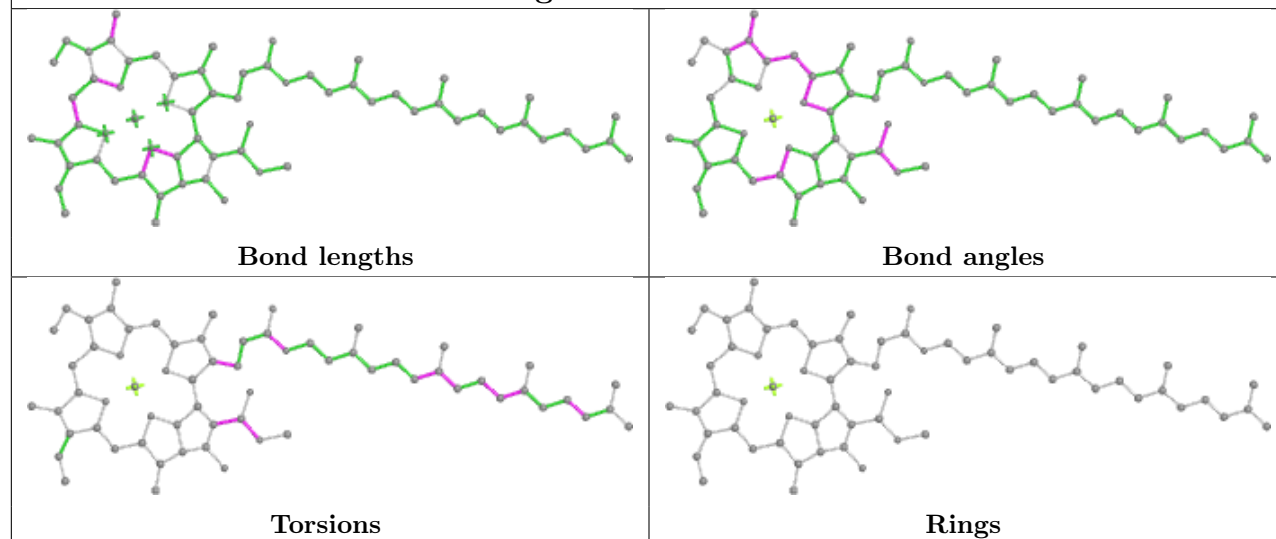


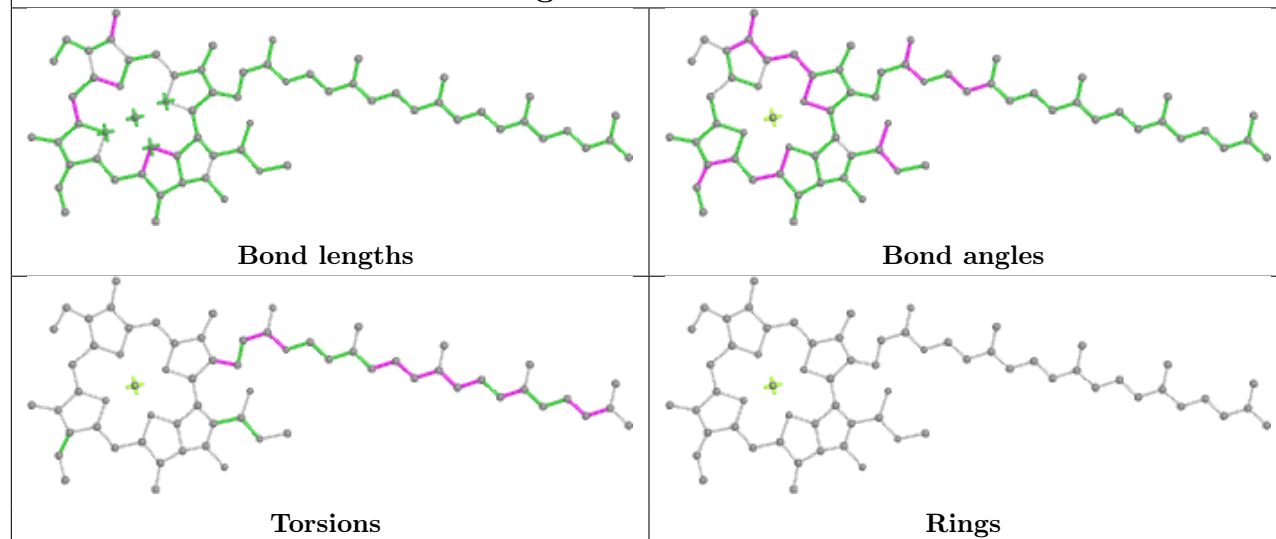
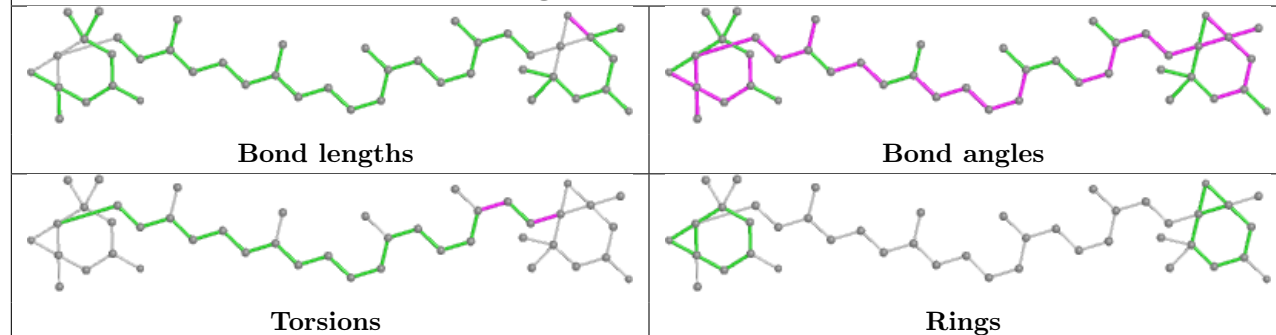
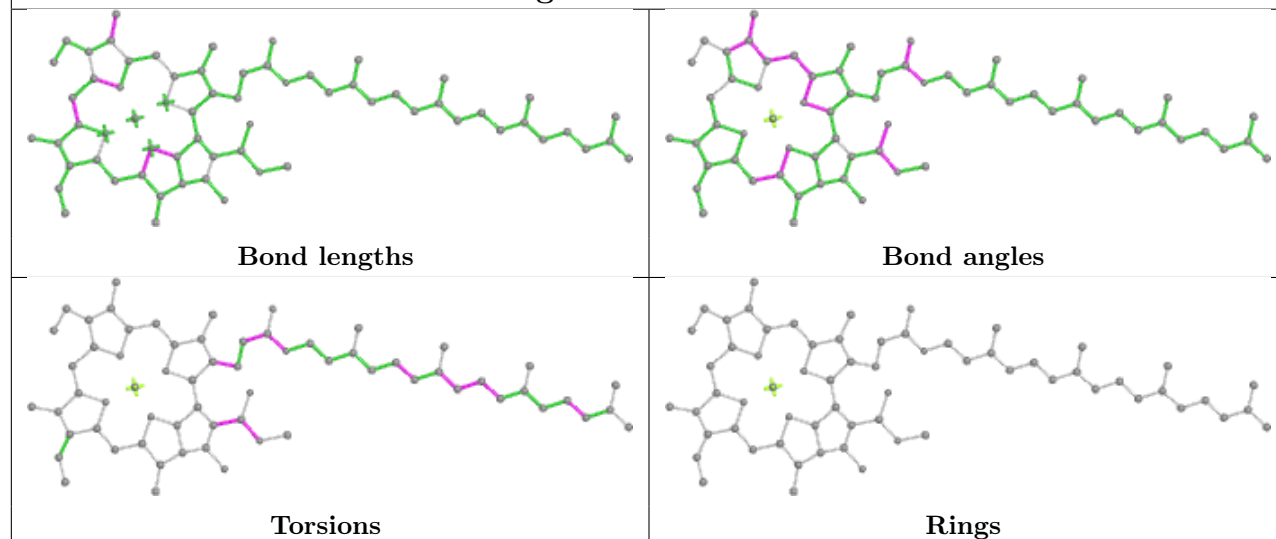
Rings

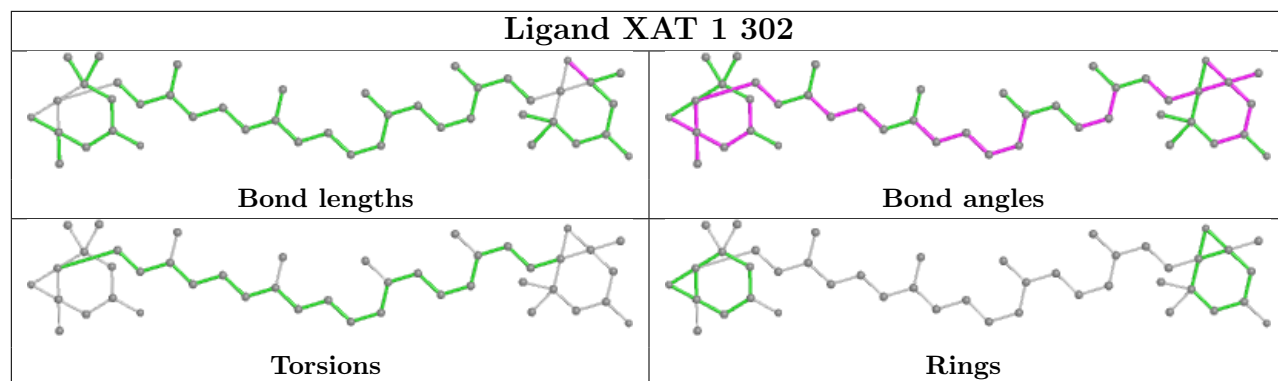
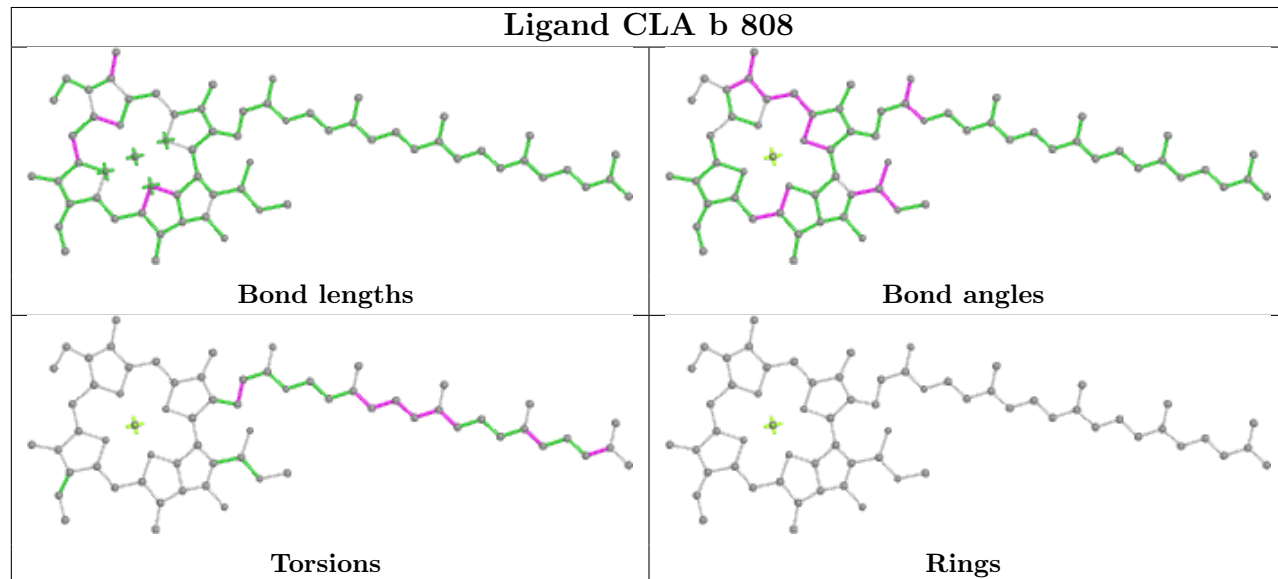
Ligand CLA b 824



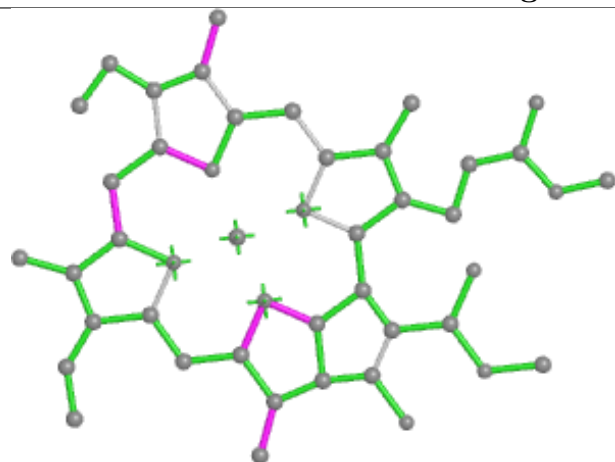
Ligand CLA b 806



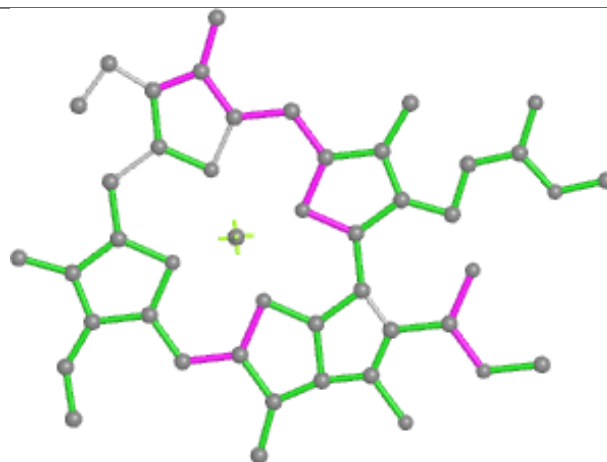
Ligand CLA 1 306**Ligand XAT 4 303****Ligand CLA a 854**

Ligand XAT 1 302**Ligand CLA b 808**

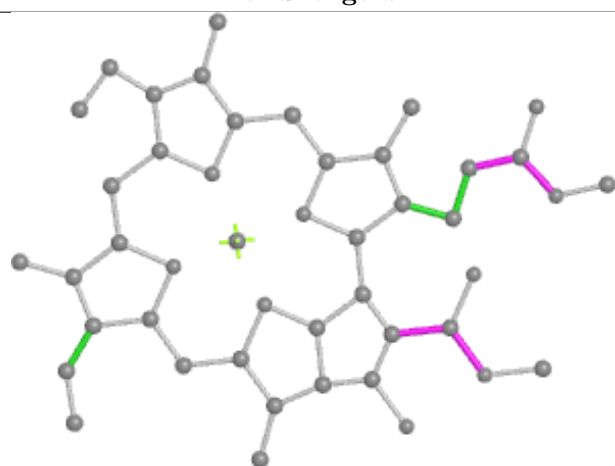
Ligand CLA 1 309



Bond lengths



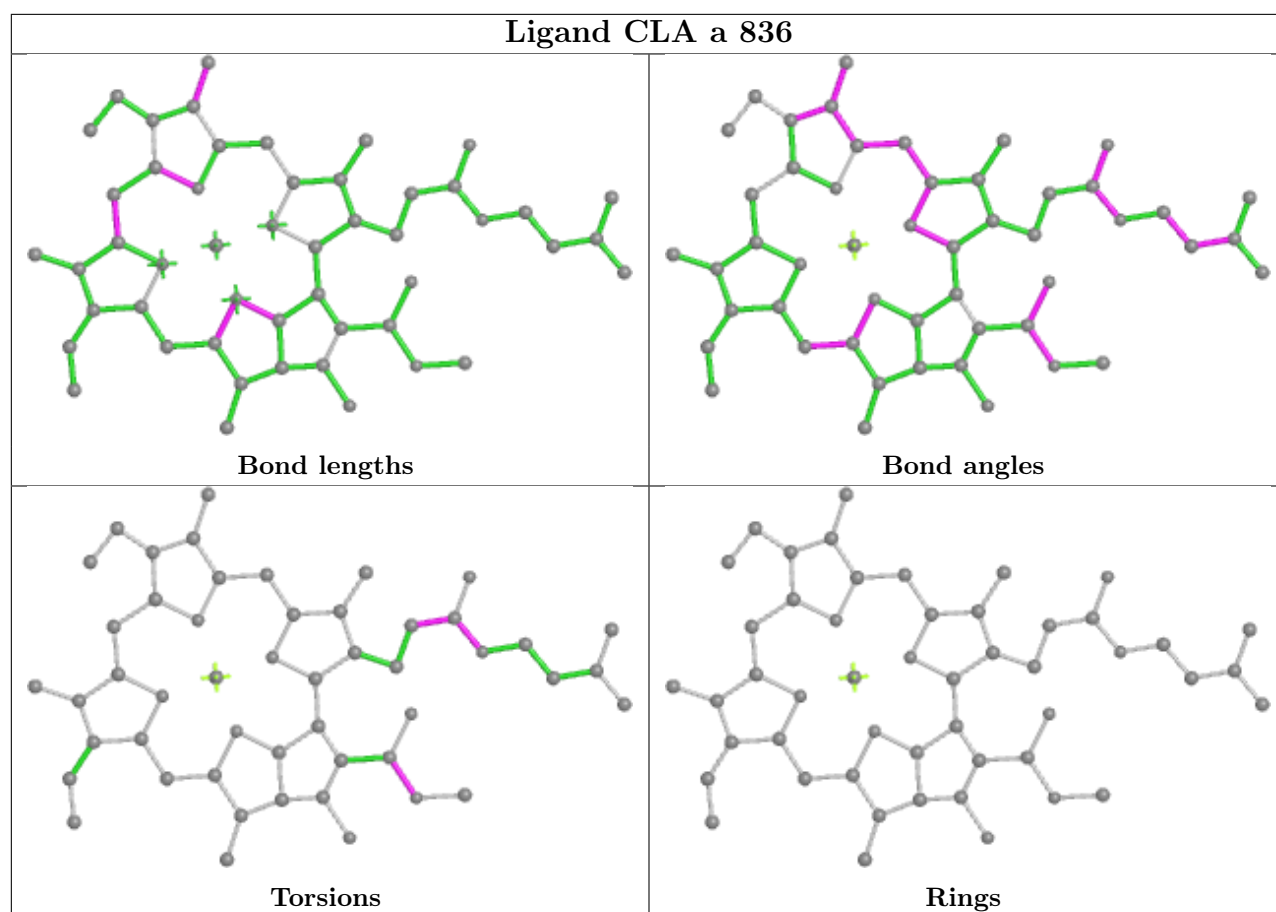
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

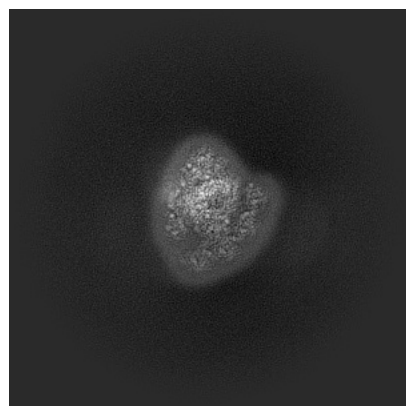
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60287. These allow visual inspection of the internal detail of the map and identification of artifacts.

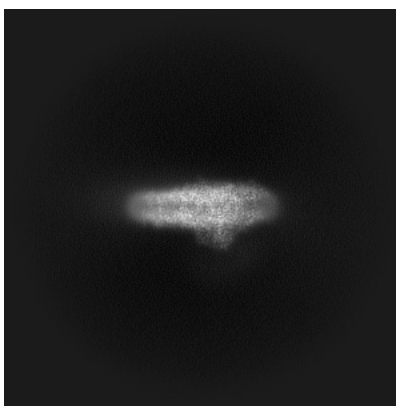
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

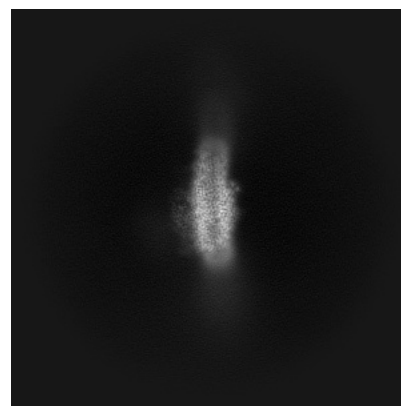
6.1.1 Primary map



X

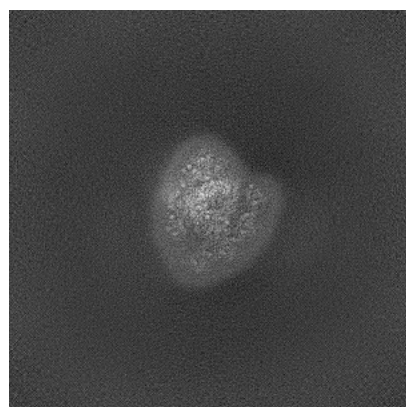


Y

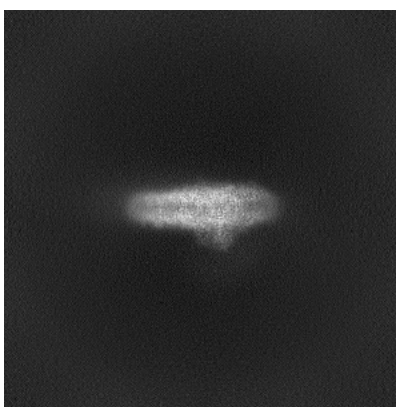


Z

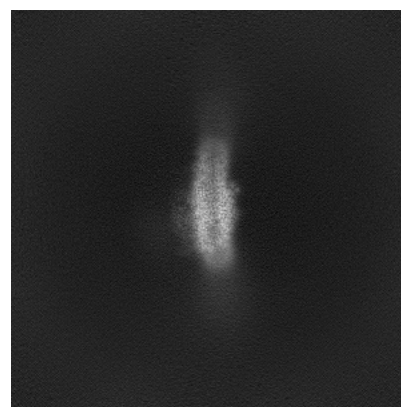
6.1.2 Raw map



X



Y

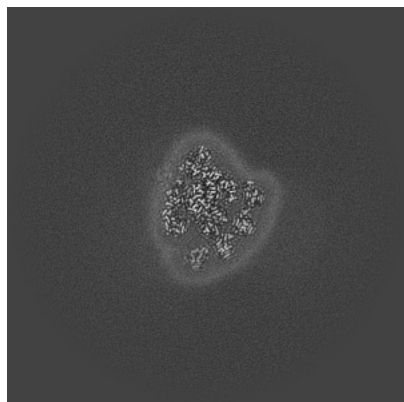


Z

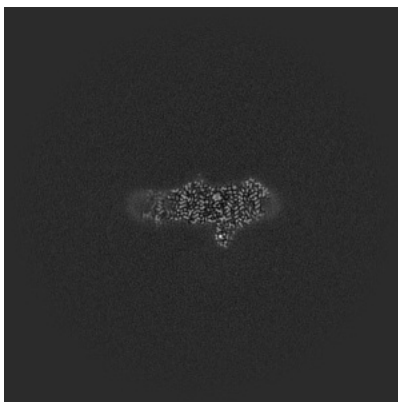
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

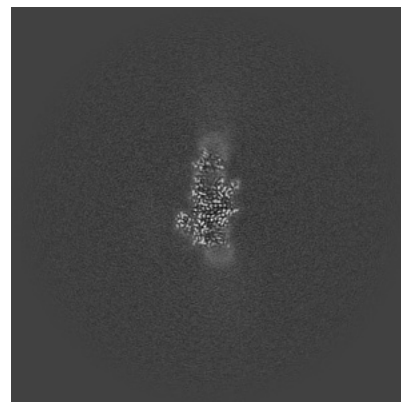
6.2.1 Primary map



X Index: 256

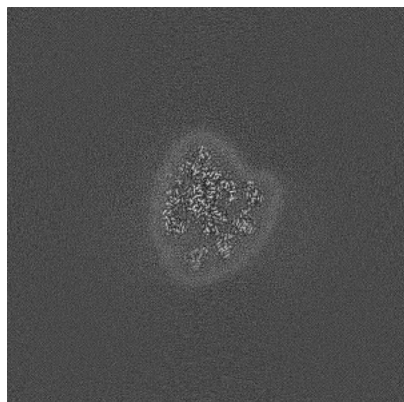


Y Index: 256

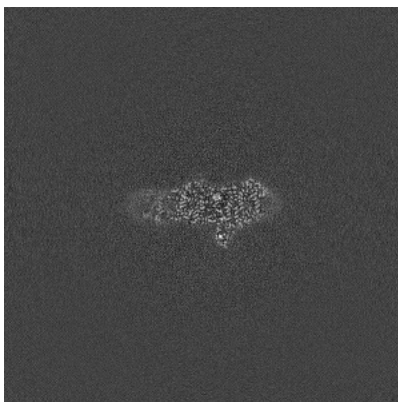


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

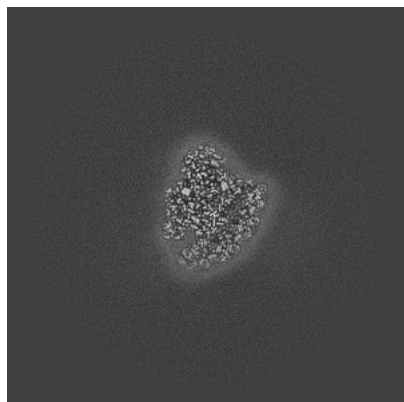


Z Index: 256

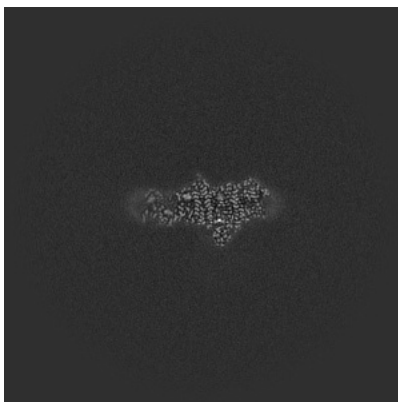
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

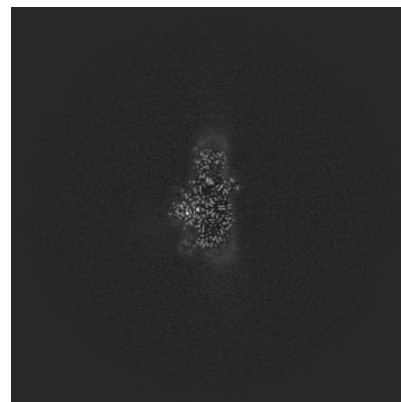
6.3.1 Primary map



X Index: 246

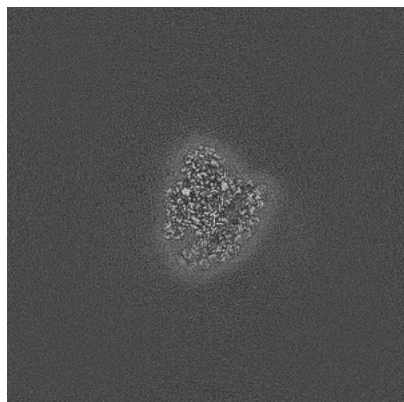


Y Index: 252

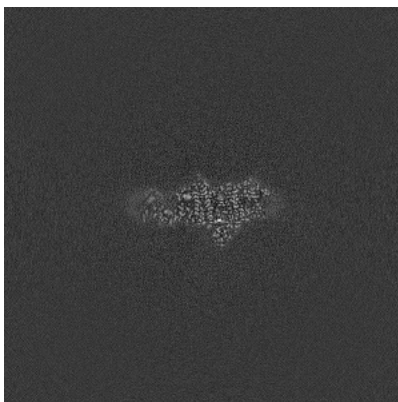


Z Index: 275

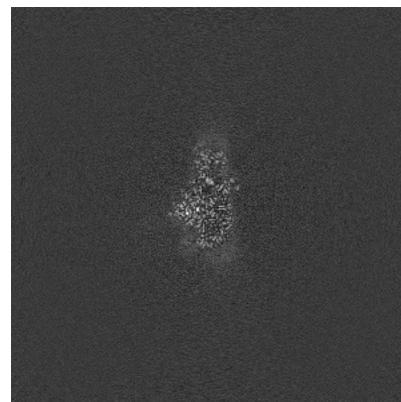
6.3.2 Raw map



X Index: 246



Y Index: 252

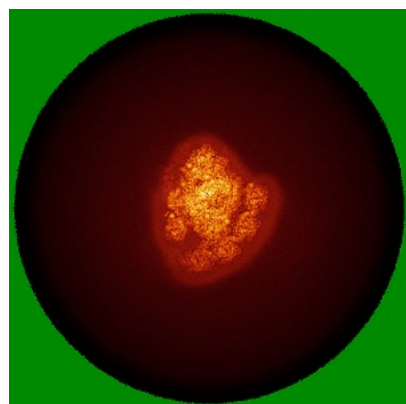


Z Index: 275

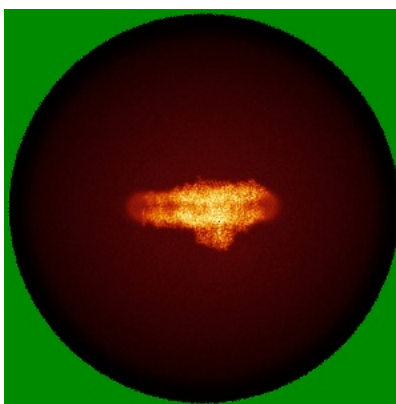
The images above show the largest variance slices of the map in three orthogonal directions.

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

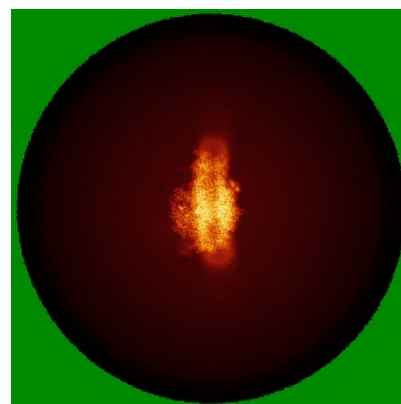
6.4.1 Primary map



X

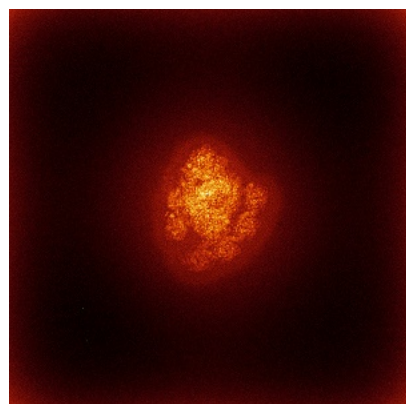


Y

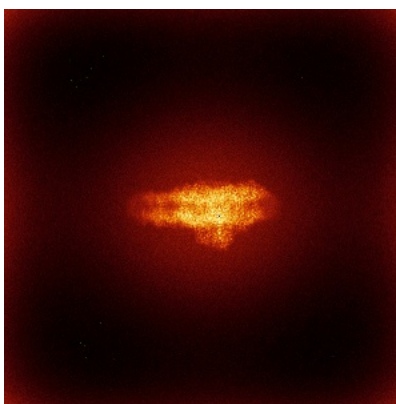


Z

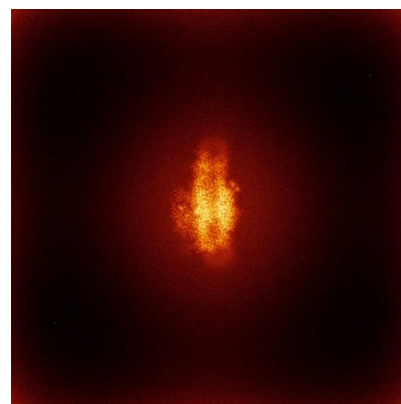
6.4.2 Raw map



X



Y

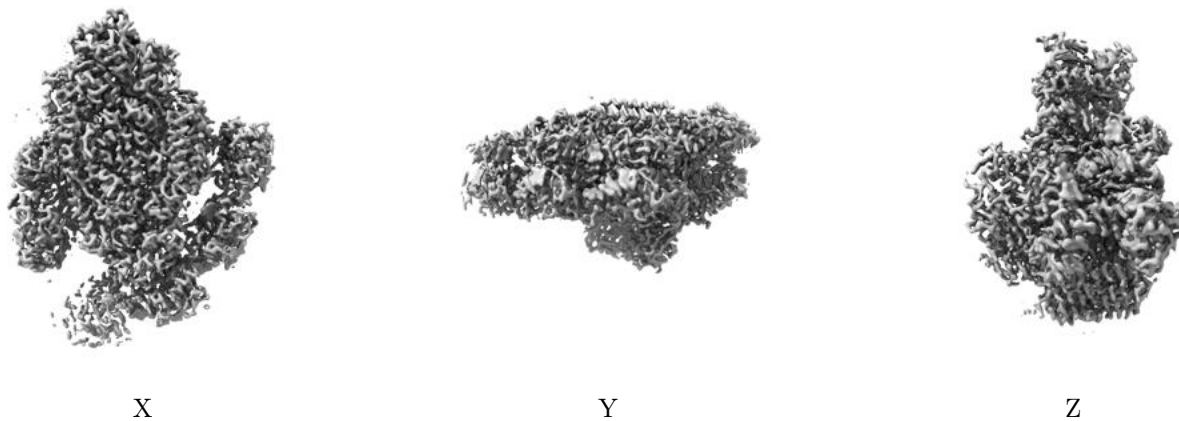


Z

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.

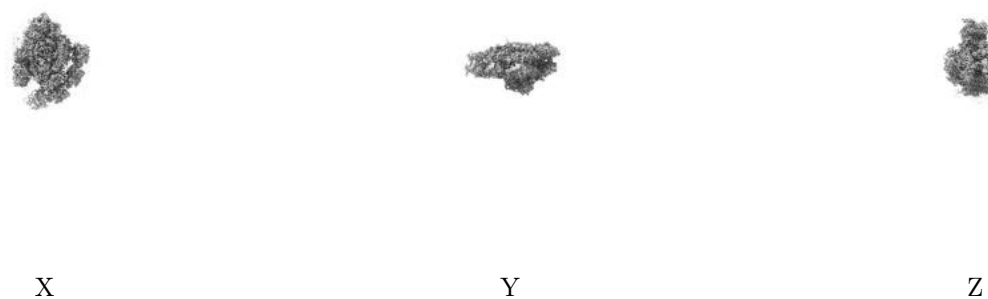
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.367. 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.

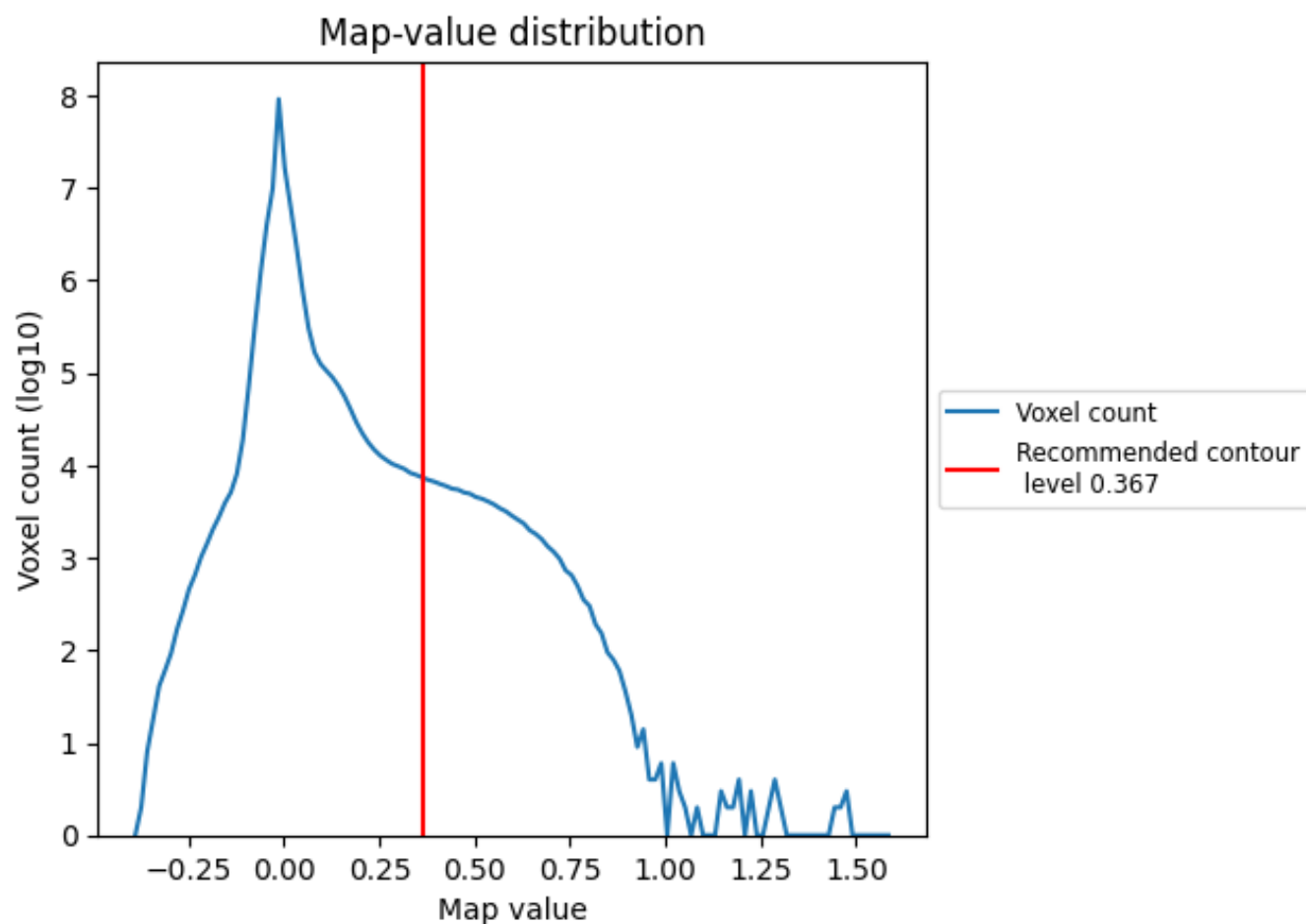
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

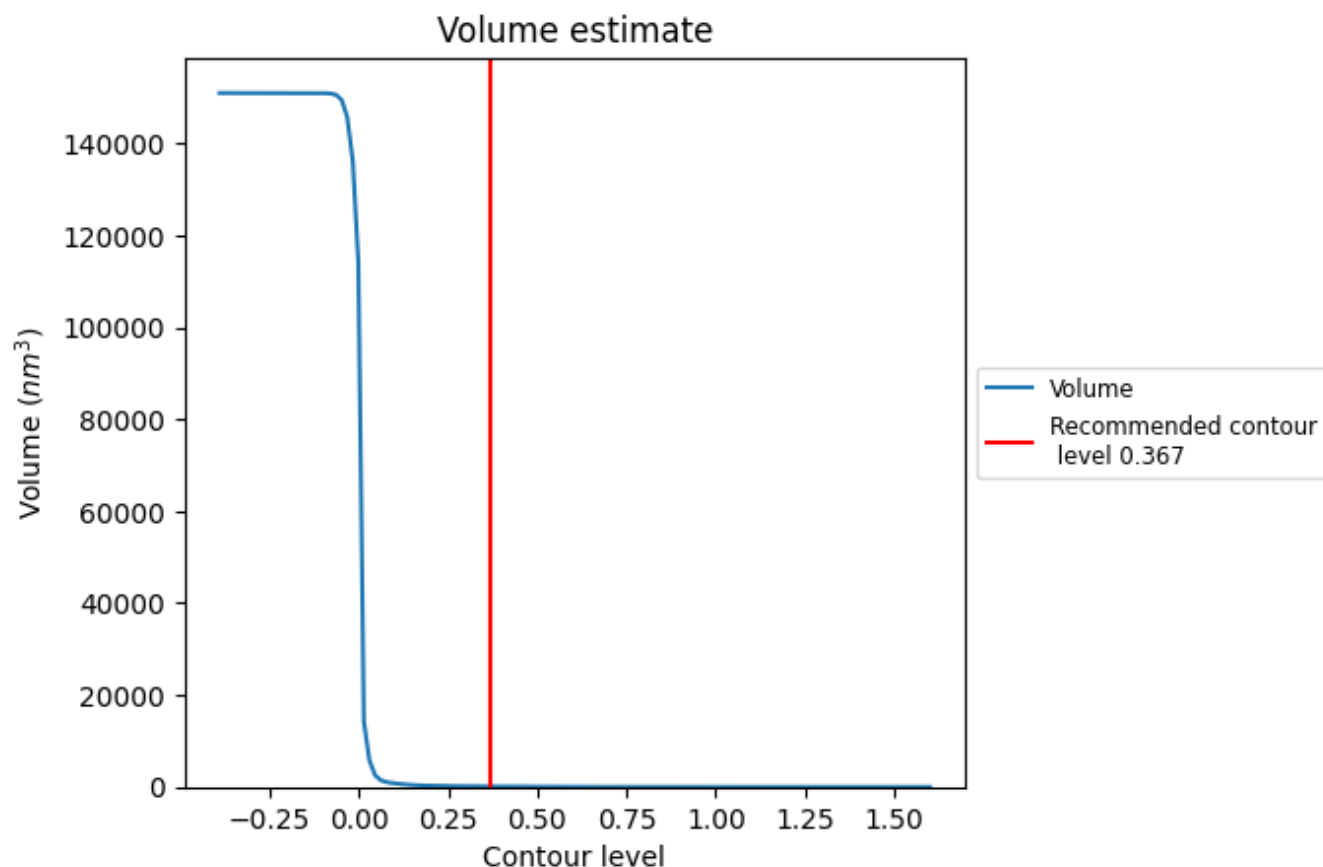
This section contains the results of statistical analysis of the map.

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.

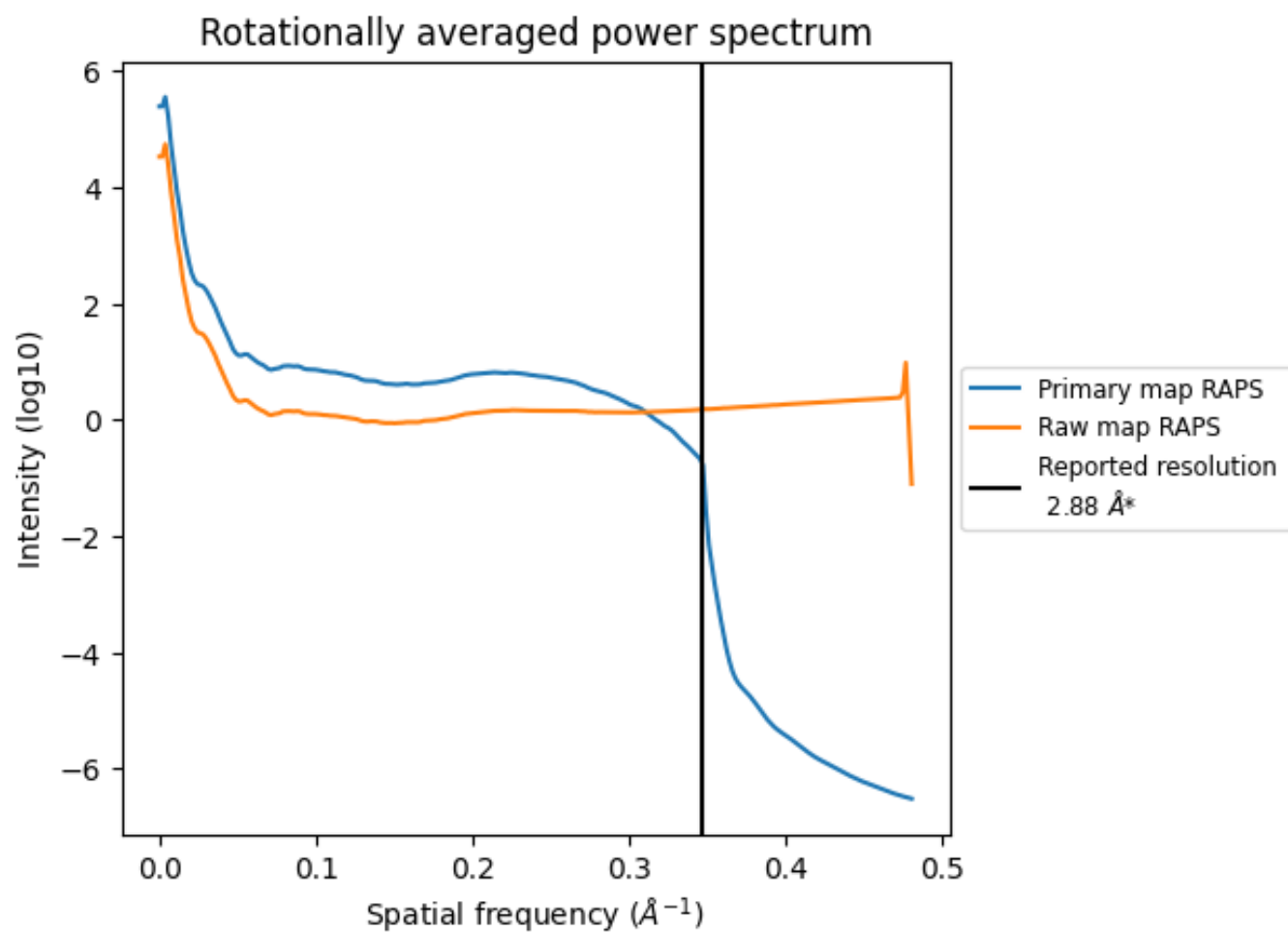
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm^3 ; this corresponds to an approximate mass of 97 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 ⓘ

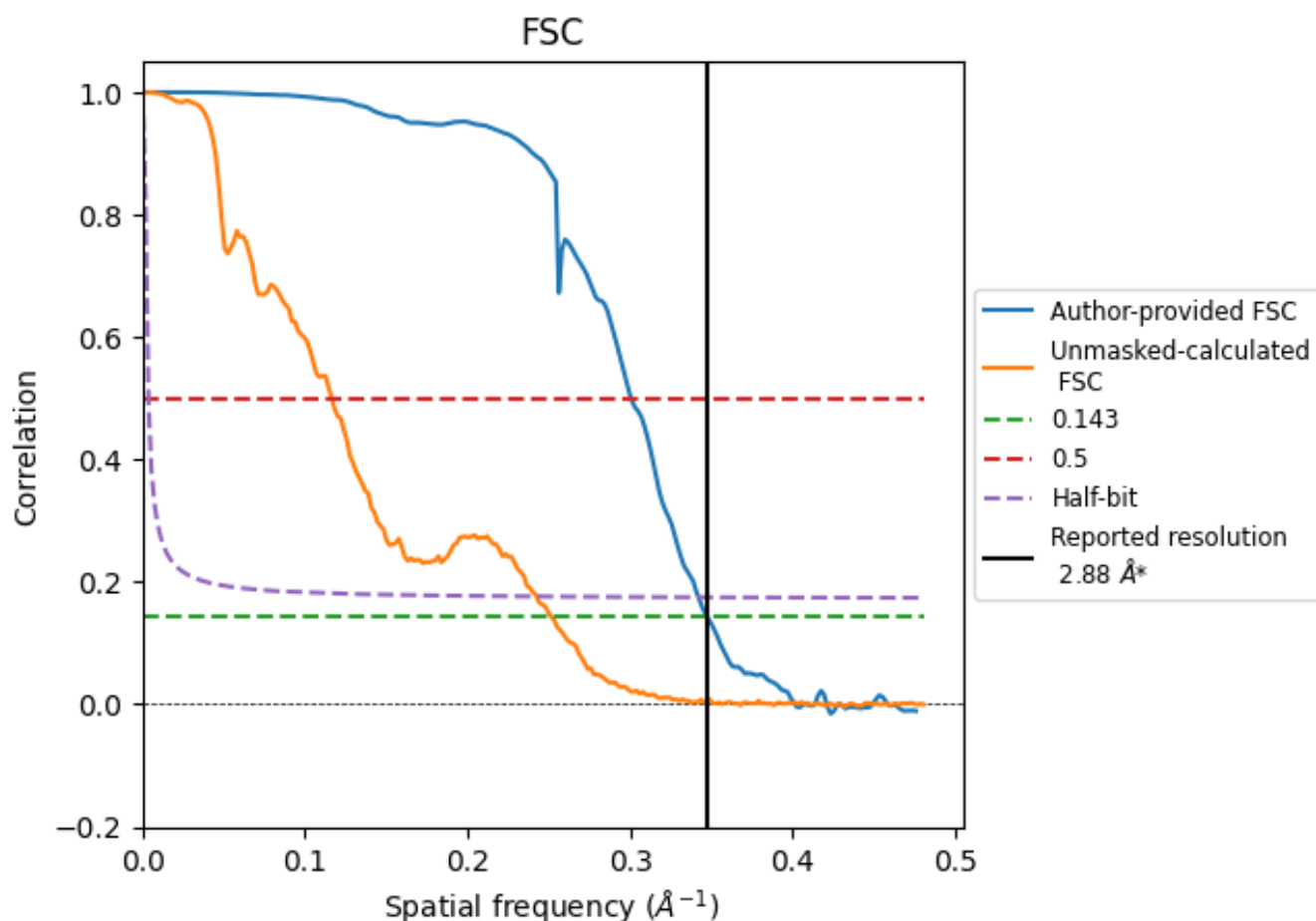


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.347 \AA^{-1}

8.2 Resolution estimates [i](#)

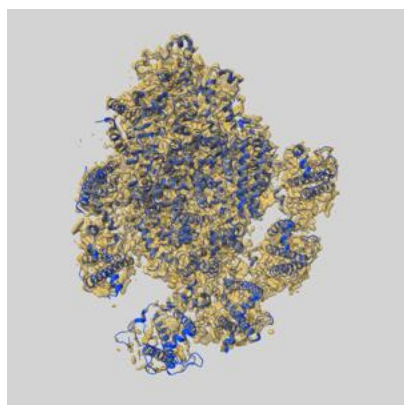
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.32	2.92
Unmasked-calculated*	3.98	8.57	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.88 by more than 10 %

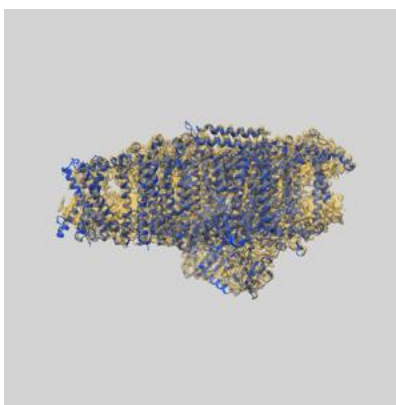
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60287 and PDB model 8ZOB. Per-residue inclusion information can be found in section 3 on page 26.

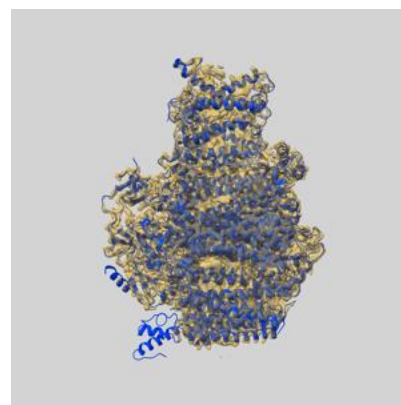
9.1 Map-model overlay [i](#)



X



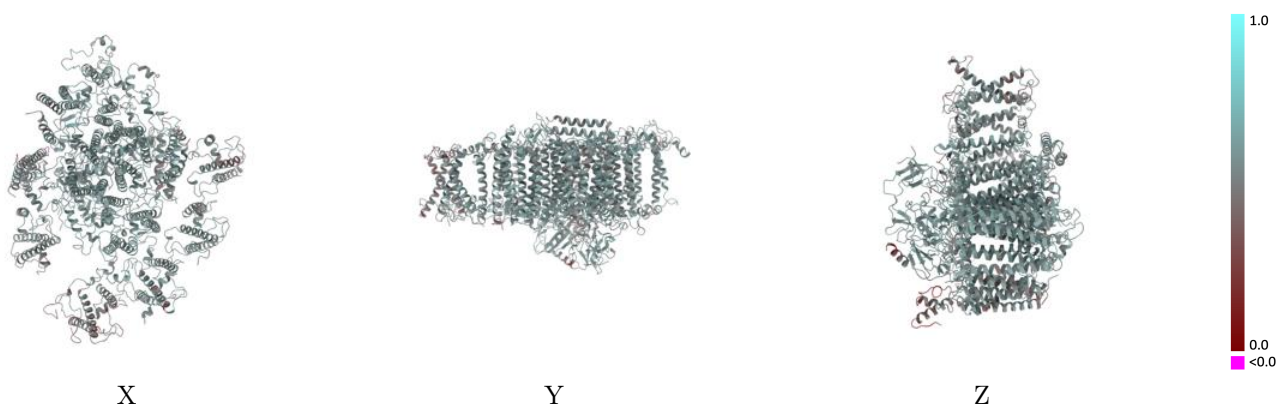
Y



Z

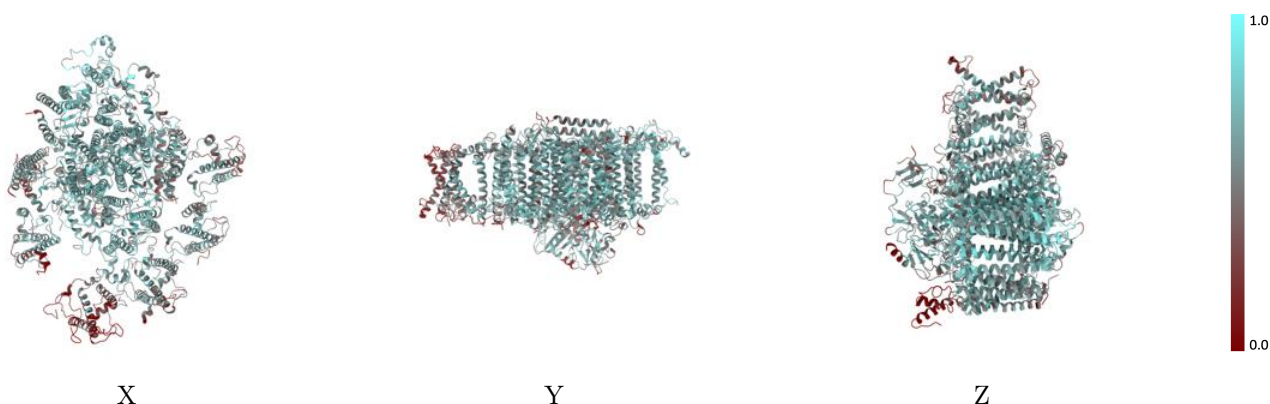
The images above show the 3D surface view of the map at the recommended contour level 0.367 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



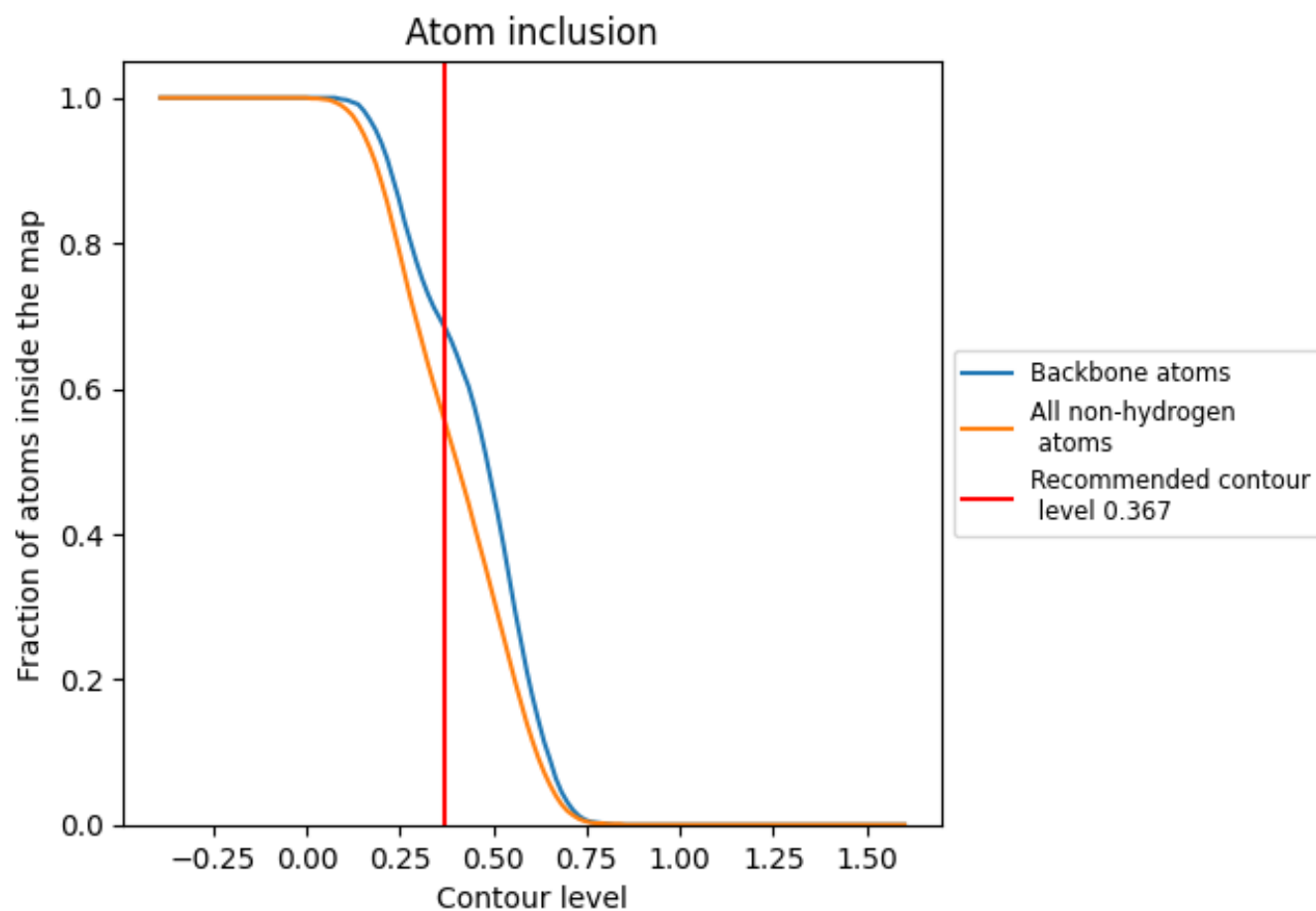
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.367).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 56% 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 (0.367) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5610	<div></div> 0.5480
1	<div></div> 0.5230	<div></div> 0.5330
2	<div></div> 0.2340	<div></div> 0.4590
3	<div></div> 0.5010	<div></div> 0.5440
4	<div></div> 0.5250	<div></div> 0.5390
5	<div></div> 0.4910	<div></div> 0.5200
a	<div></div> 0.6480	<div></div> 0.5800
b	<div></div> 0.6240	<div></div> 0.5620
c	<div></div> 0.6960	<div></div> 0.5620
d	<div></div> 0.5800	<div></div> 0.5580
e	<div></div> 0.5590	<div></div> 0.5580
f	<div></div> 0.5440	<div></div> 0.5390
g	<div></div> 0.2620	<div></div> 0.4280
i	<div></div> 0.4210	<div></div> 0.5210
j	<div></div> 0.5440	<div></div> 0.5650
l	<div></div> 0.5290	<div></div> 0.5250
m	<div></div> 0.4160	<div></div> 0.4900

