



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 8ZO9 / pdb_00008zo9
EMDB ID : EMD-60285
Title : Structure of the wild-type PSI-9VCPI supercomplex in *Nannochloropsis oceanica*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.75 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

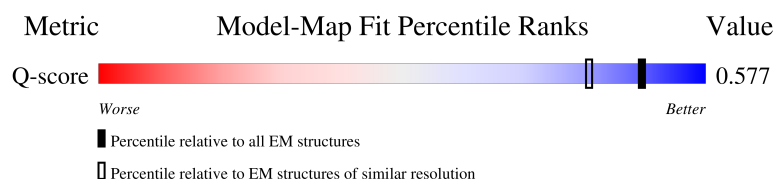
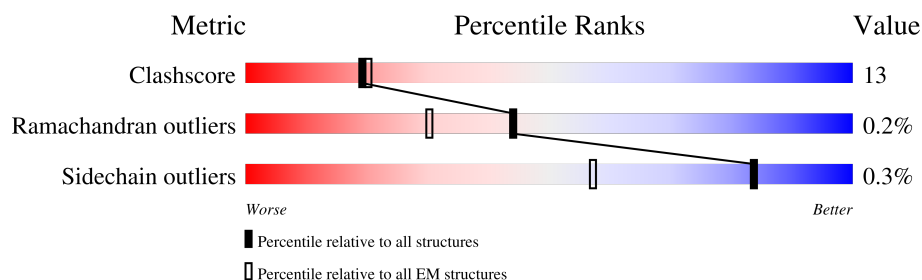
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	 52% 17% 31%
2	9	232	 65% 20% 13%
3	8	200	 62% 18% 18%
4	4	202	 72% 11% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	7	202	
5	3	220	
6	6	259	
7	2	223	
8	1	208	
9	a	745	
10	b	737	
11	d	136	
12	e	67	
13	f	185	
14	h	128	
15	i	45	
16	j	41	
17	l	172	
18	m	30	
19	g	55	
20	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
23	CLA	1	305	X	-	-	-
23	CLA	1	306	X	-	-	-
23	CLA	1	307	X	-	-	-
23	CLA	1	308	X	-	-	-
23	CLA	1	309	X	-	-	-
23	CLA	1	310	X	-	-	-
23	CLA	1	311	X	-	-	-
23	CLA	1	312	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	1	313	X	-	-	-
23	CLA	1	314	X	-	-	-
23	CLA	2	306	X	-	-	-
23	CLA	2	307	X	-	-	-
23	CLA	2	308	X	-	-	-
23	CLA	2	309	X	-	-	-
23	CLA	2	310	X	-	-	-
23	CLA	2	311	X	-	-	-
23	CLA	2	312	X	-	-	-
23	CLA	2	313	X	-	-	-
23	CLA	2	314	X	-	-	-
23	CLA	2	315	X	-	-	-
23	CLA	2	316	X	-	-	-
23	CLA	3	307	X	-	-	-
23	CLA	3	308	X	-	-	-
23	CLA	3	309	X	-	-	-
23	CLA	3	310	X	-	-	-
23	CLA	3	311	X	-	-	-
23	CLA	3	312	X	-	-	-
23	CLA	3	313	X	-	-	-
23	CLA	3	314	X	-	-	-
23	CLA	3	315	X	-	-	-
23	CLA	4	306	X	-	-	-
23	CLA	4	307	X	-	-	-
23	CLA	4	308	X	-	-	-
23	CLA	4	309	X	-	-	-
23	CLA	4	310	X	-	-	-
23	CLA	4	311	X	-	-	-
23	CLA	4	312	X	-	-	-
23	CLA	4	313	X	-	-	-
23	CLA	4	314	X	-	-	-
23	CLA	4	315	X	-	-	-
23	CLA	4	316	X	-	-	-
23	CLA	4	317	X	-	-	-
23	CLA	5	305	X	-	-	-
23	CLA	5	306	X	-	-	-
23	CLA	5	307	X	-	-	-
23	CLA	5	308	X	-	-	-
23	CLA	5	309	X	-	-	-
23	CLA	5	310	X	-	-	-
23	CLA	5	311	X	-	-	-
23	CLA	5	312	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	5	313	X	-	-	-
23	CLA	5	314	X	-	-	-
23	CLA	5	315	X	-	-	-
23	CLA	6	307	X	-	-	-
23	CLA	6	308	X	-	-	-
23	CLA	6	309	X	-	-	-
23	CLA	6	310	X	-	-	-
23	CLA	6	311	X	-	-	-
23	CLA	6	312	X	-	-	-
23	CLA	6	313	X	-	-	-
23	CLA	6	314	X	-	-	-
23	CLA	6	315	X	-	-	-
23	CLA	6	316	X	-	-	-
23	CLA	6	317	X	-	-	-
23	CLA	7	306	X	-	-	-
23	CLA	7	307	X	-	-	-
23	CLA	7	308	X	-	-	-
23	CLA	7	309	X	-	-	-
23	CLA	7	310	X	-	-	-
23	CLA	7	311	X	-	-	-
23	CLA	7	312	X	-	-	-
23	CLA	7	313	X	-	-	-
23	CLA	7	314	X	-	-	-
23	CLA	7	315	X	-	-	-
23	CLA	7	316	X	-	-	-
23	CLA	7	317	X	-	-	-
23	CLA	8	305	X	-	-	-
23	CLA	8	306	X	-	-	-
23	CLA	8	307	X	-	-	-
23	CLA	8	308	X	-	-	-
23	CLA	8	309	X	-	-	-
23	CLA	8	310	X	-	-	-
23	CLA	8	311	X	-	-	-
23	CLA	8	312	X	-	-	-
23	CLA	8	313	X	-	-	-
23	CLA	8	314	X	-	-	-
23	CLA	9	308	X	-	-	-
23	CLA	9	309	X	-	-	-
23	CLA	9	310	X	-	-	-
23	CLA	9	311	X	-	-	-
23	CLA	9	312	X	-	-	-
23	CLA	9	313	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	9	314	X	-	-	-
23	CLA	9	315	X	-	-	-
23	CLA	9	316	X	-	-	-
23	CLA	9	318	X	-	-	-
23	CLA	a	801	X	-	-	-
23	CLA	a	802	X	-	-	-
23	CLA	a	803	X	-	-	-
23	CLA	a	804	X	-	-	-
23	CLA	a	805	X	-	-	-
23	CLA	a	806	X	-	-	-
23	CLA	a	807	X	-	-	-
23	CLA	a	808	X	-	-	-
23	CLA	a	809	X	-	-	-
23	CLA	a	810	X	-	-	-
23	CLA	a	811	X	-	-	-
23	CLA	a	812	X	-	-	-
23	CLA	a	813	X	-	-	-
23	CLA	a	814	X	-	-	-
23	CLA	a	815	X	-	-	-
23	CLA	a	816	X	-	-	-
23	CLA	a	817	X	-	-	-
23	CLA	a	818	X	-	-	-
23	CLA	a	819	X	-	-	-
23	CLA	a	820	X	-	-	-
23	CLA	a	821	X	-	-	-
23	CLA	a	822	X	-	-	-
23	CLA	a	823	X	-	-	-
23	CLA	a	824	X	-	-	-
23	CLA	a	825	X	-	-	-
23	CLA	a	826	X	-	-	-
23	CLA	a	827	X	-	-	-
23	CLA	a	828	X	-	-	-
23	CLA	a	829	X	-	-	-
23	CLA	a	830	X	-	-	-
23	CLA	a	831	X	-	-	-
23	CLA	a	832	X	-	-	-
23	CLA	a	833	X	-	-	-
23	CLA	a	834	X	-	-	-
23	CLA	a	835	X	-	-	-
23	CLA	a	836	X	-	-	-
23	CLA	a	837	X	-	-	-
23	CLA	a	838	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	a	839	X	-	-	-
23	CLA	a	840	X	-	-	-
23	CLA	a	841	X	-	-	-
23	CLA	a	842	X	-	-	-
23	CLA	a	844	X	-	-	-
23	CLA	a	854	X	-	-	-
23	CLA	b	801	X	-	-	-
23	CLA	b	802	X	-	-	-
23	CLA	b	803	X	-	-	-
23	CLA	b	804	X	-	-	-
23	CLA	b	805	X	-	-	-
23	CLA	b	806	X	-	-	-
23	CLA	b	807	X	-	-	-
23	CLA	b	808	X	-	-	-
23	CLA	b	809	X	-	-	-
23	CLA	b	810	X	-	-	-
23	CLA	b	811	X	-	-	-
23	CLA	b	812	X	-	-	-
23	CLA	b	813	X	-	-	-
23	CLA	b	814	X	-	-	-
23	CLA	b	815	X	-	-	-
23	CLA	b	816	X	-	-	-
23	CLA	b	817	X	-	-	-
23	CLA	b	818	X	-	-	-
23	CLA	b	819	X	-	-	-
23	CLA	b	820	X	-	-	-
23	CLA	b	821	X	-	-	-
23	CLA	b	822	X	-	-	-
23	CLA	b	823	X	-	-	-
23	CLA	b	824	X	-	-	-
23	CLA	b	825	X	-	-	-
23	CLA	b	826	X	-	-	-
23	CLA	b	827	X	-	-	-
23	CLA	b	828	X	-	-	-
23	CLA	b	829	X	-	-	-
23	CLA	b	830	X	-	-	-
23	CLA	b	831	X	-	-	-
23	CLA	b	832	X	-	-	-
23	CLA	b	833	X	-	-	-
23	CLA	b	834	X	-	-	-
23	CLA	b	835	X	-	-	-
23	CLA	b	836	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	b	837	X	-	-	-
23	CLA	b	838	X	-	-	-
23	CLA	b	839	X	-	-	-
23	CLA	b	840	X	-	-	-
23	CLA	f	802	X	-	-	-
23	CLA	f	803	X	-	-	-
23	CLA	h	204	X	-	-	-
23	CLA	j	102	X	-	-	-
23	CLA	j	103	X	-	-	-
23	CLA	l	202	X	-	-	-
23	CLA	l	203	X	-	-	-
23	CLA	l	204	X	-	-	-
31	SF4	c	102	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 43774 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VCPI-5.

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

- Molecule 2 is a protein called VCPI-9.

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

- Molecule 3 is a protein called VCPI-8.

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

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

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

- Molecule 5 is a protein called VCPI-3.

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

- Molecule 6 is a protein called VCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	180	Total	C	N	O	S	0	0
			1352	880	223	244	5		

- Molecule 7 is a protein called VCPI-2.

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

- Molecule 8 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

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

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

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

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

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

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

- Molecule 14 is a protein called PsaR.

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

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

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

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 17 is a protein called PSI subunit V.

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

- Molecule 18 is a protein called PsaM.

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

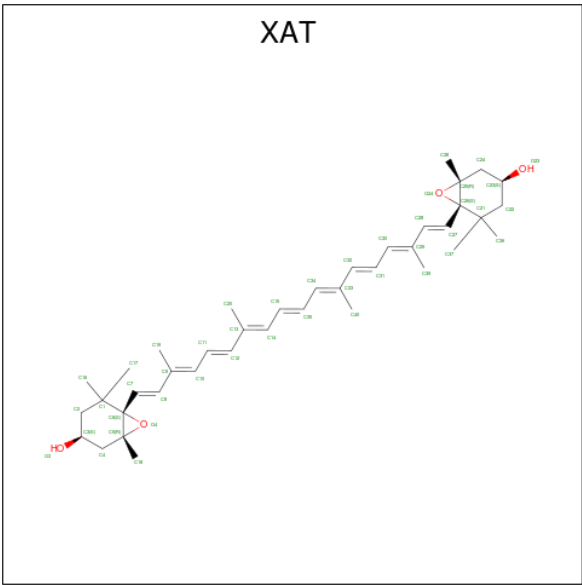
- Molecule 19 is a protein called PsaS.

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

- Molecule 20 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 21 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
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

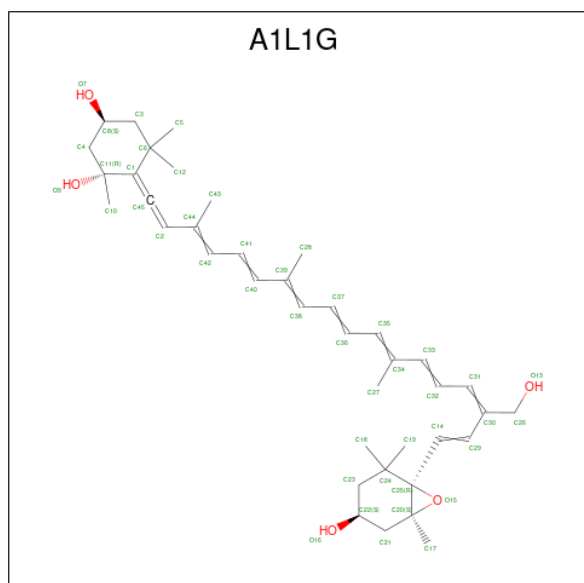
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			44	40	4	
21	a	1	Total	C	O	0
			44	40	4	
21	j	1	Total	C	O	0
			44	40	4	

- Molecule 22 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-cyclo hexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



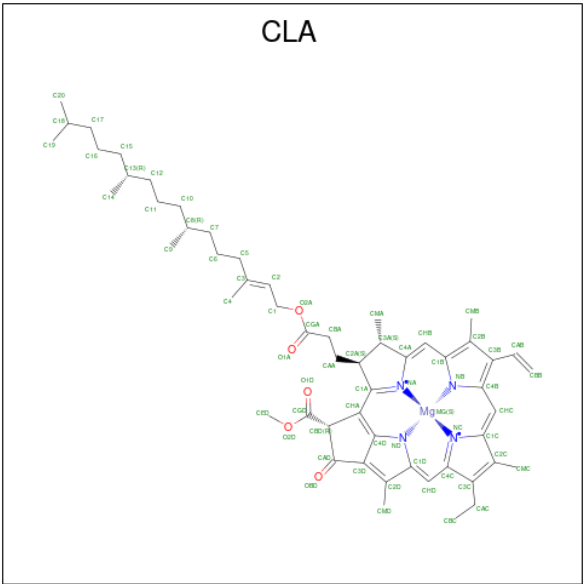
Mol	Chain	Residues	Atoms			AltConf
22	5	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
22	7	1	Total	C	O	0
			45	40	5	
22	1	1	Total	C	O	0
			45	40	5	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	8	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
23	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	2	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
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	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
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

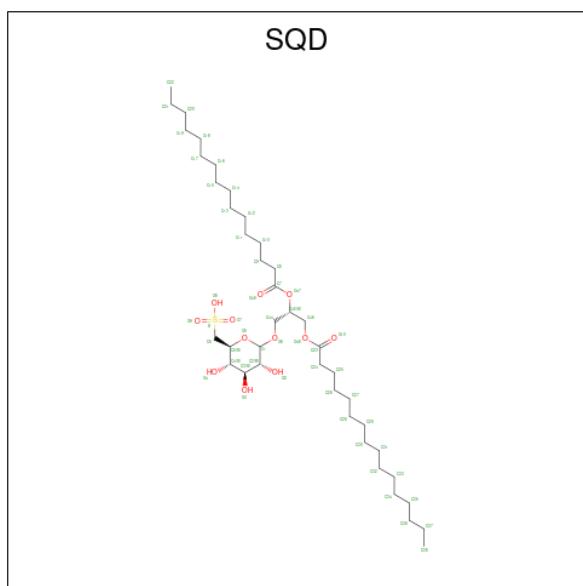
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

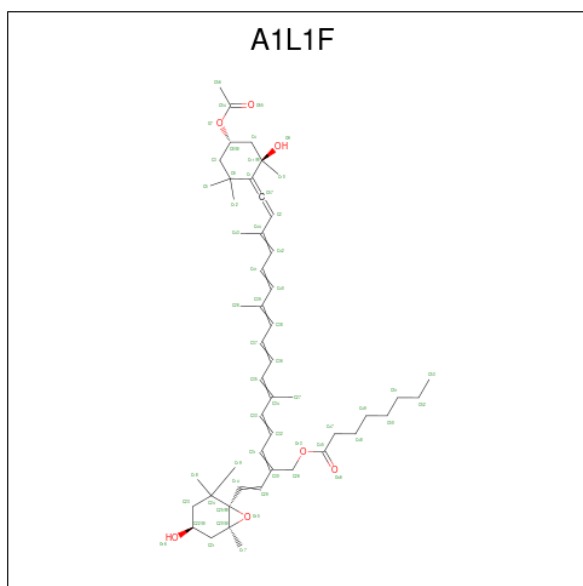
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	j	1	Total	C	Mg	N	O	0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

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



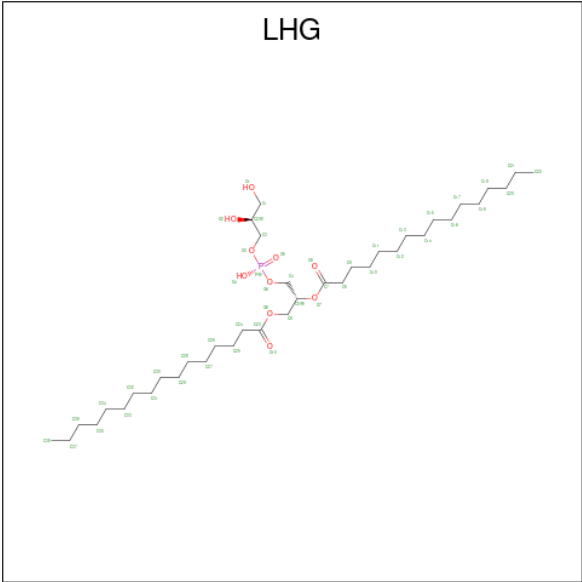
Mol	Chain	Residues	Atoms				AltConf
24	5	1	Total	C	O	S	0
			35	22	12	1	
24	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 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: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



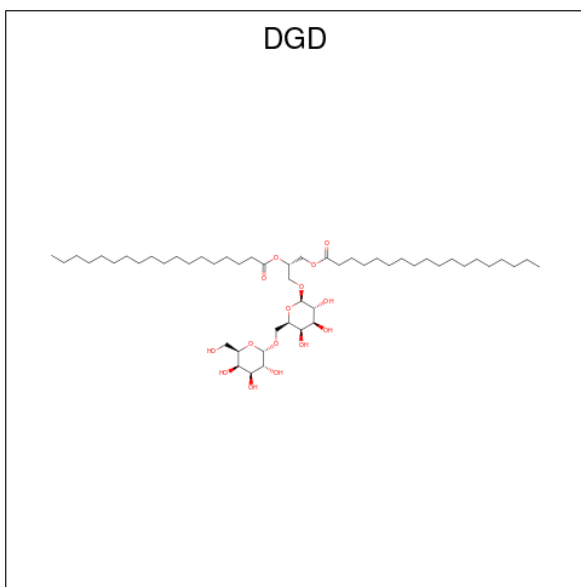
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O		0
			57	50	7		
25	8	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			53	46	7		
25	1	1	Total	C	O		0
			57	50	7		
25	h	1	Total	C	O		0
			57	50	7		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



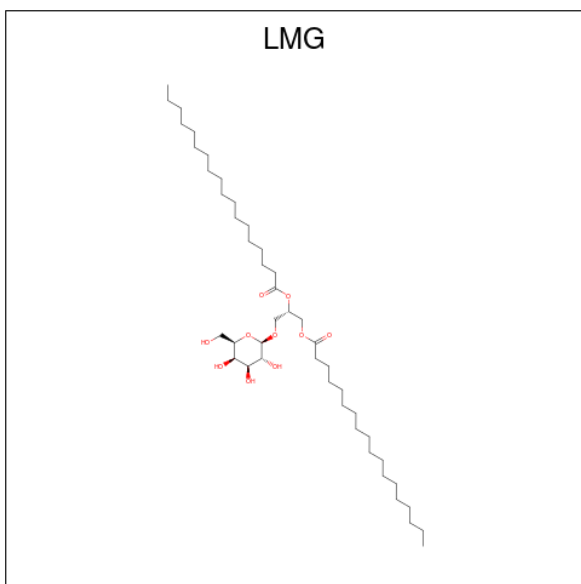
Mol	Chain	Residues	Atoms				AltConf
26	9	1	Total	C	O	P	0
			36	25	10	1	
26	9	1	Total	C	O	P	0
			46	35	10	1	
26	a	1	Total	C	O	P	0
			48	37	10	1	
26	a	1	Total	C	O	P	0
			27	16	10	1	
26	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



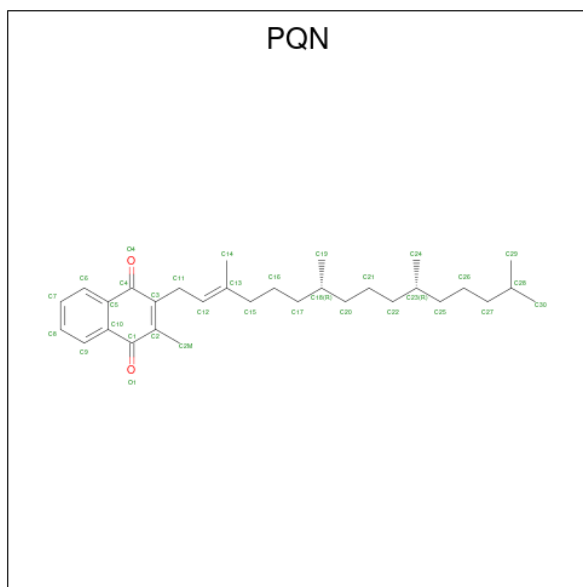
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	8	1	40	25	15	0
27	4	1	40	25	15	0
27	b	1	57	42	15	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



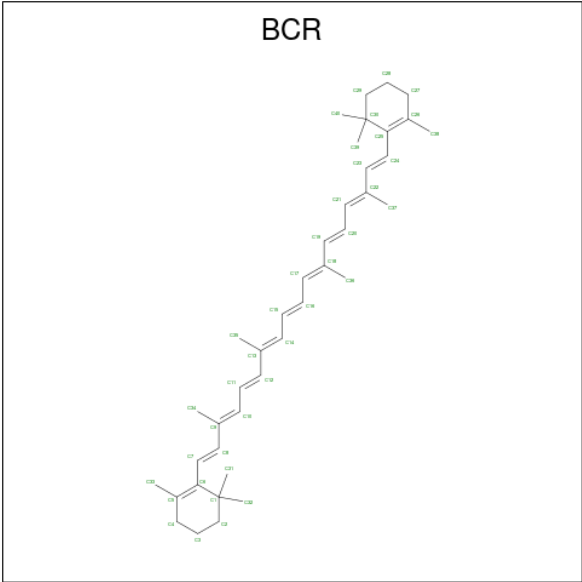
Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			35	25	10	
28	a	1	Total	C	O	0
			34	24	10	
28	j	1	Total	C	O	0
			32	22	10	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



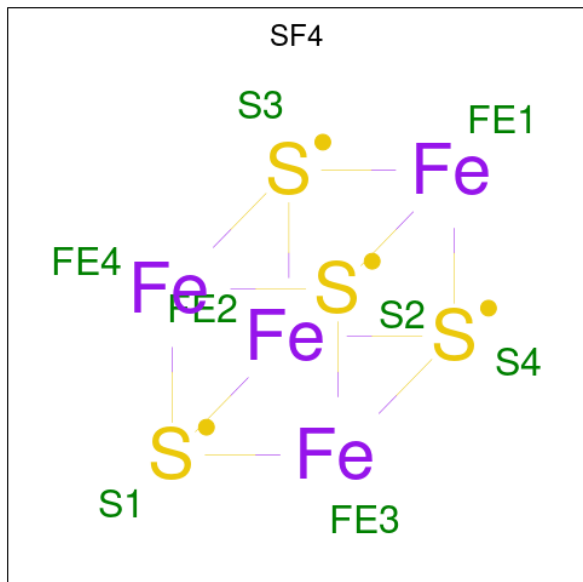
Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	f	1	Total C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

Continued on next page...

Continued from previous page...

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

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

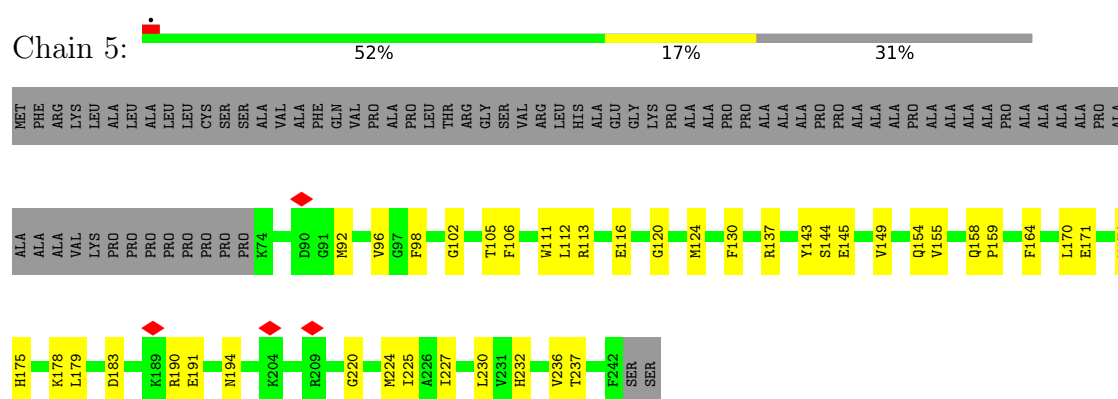


Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0

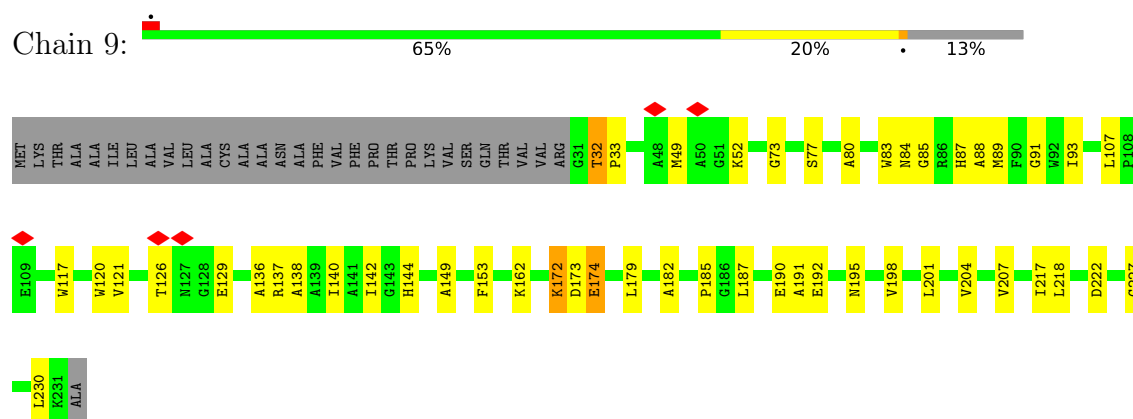
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

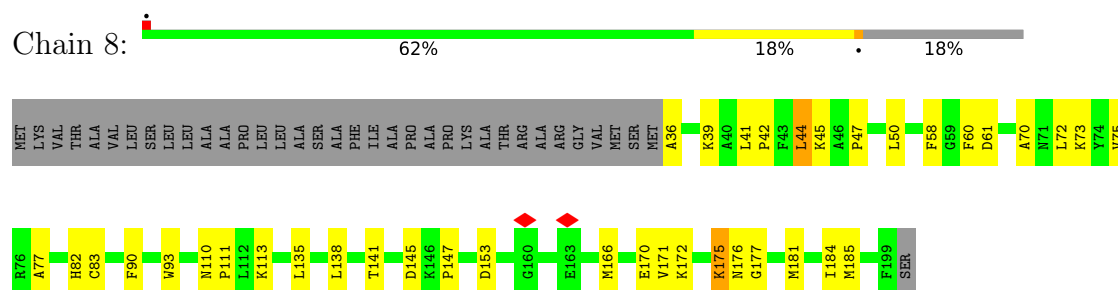
• Molecule 1: VCPI-5



• Molecule 2: VCPI-9

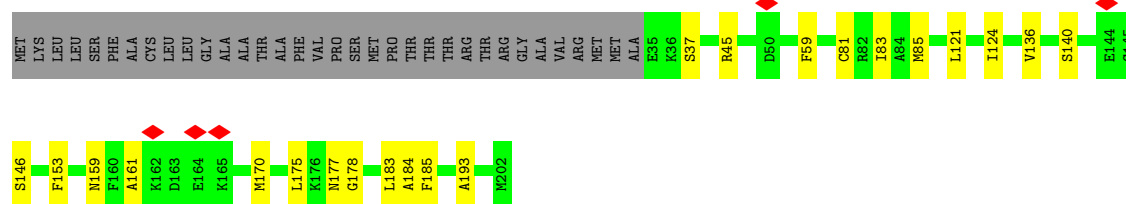


• Molecule 3: VCPI-8



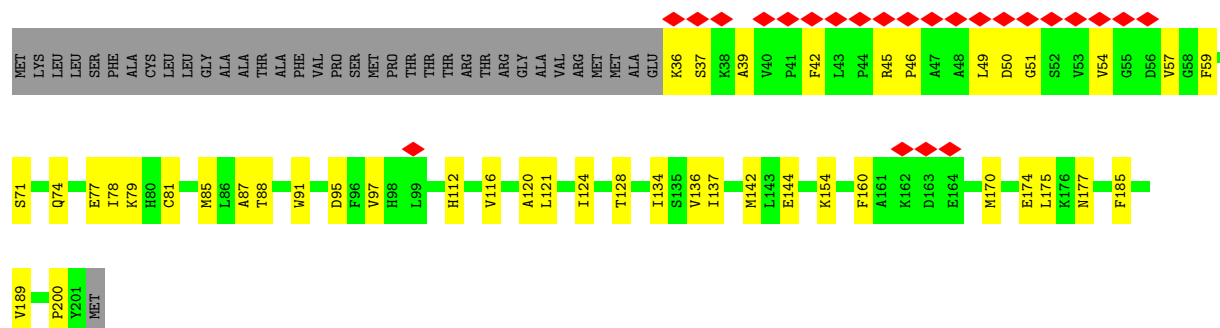
- Molecule 4: VCPI-4/7

Chain 4:  72% 11% 17%



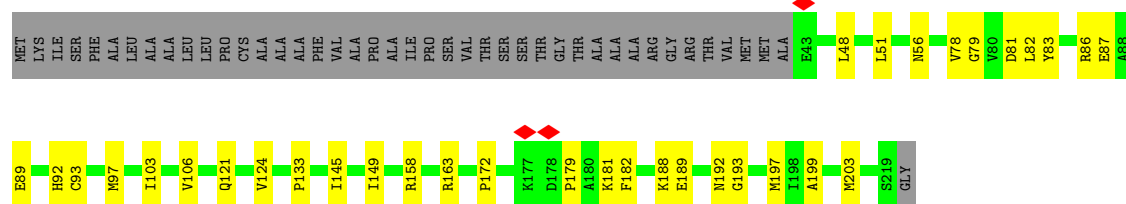
- Molecule 4: VCPI-4/7

Chain 7:  12% 60% 22% 18%



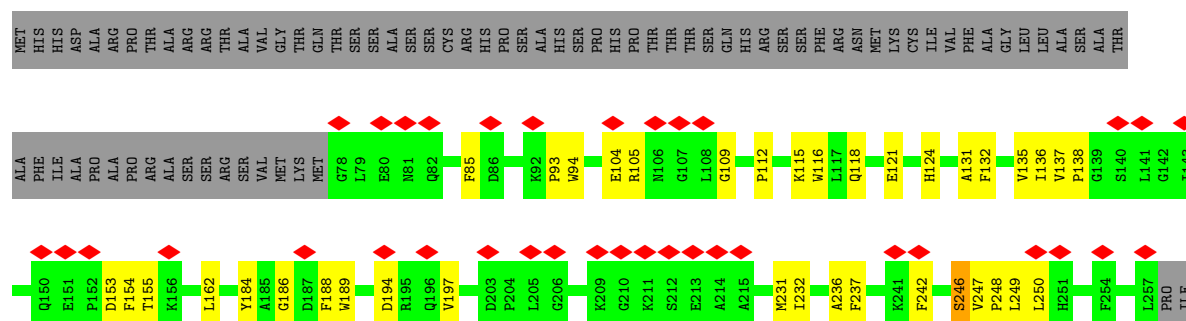
- Molecule 5: VCPI-3

Chain 3:  65% 15% 20%

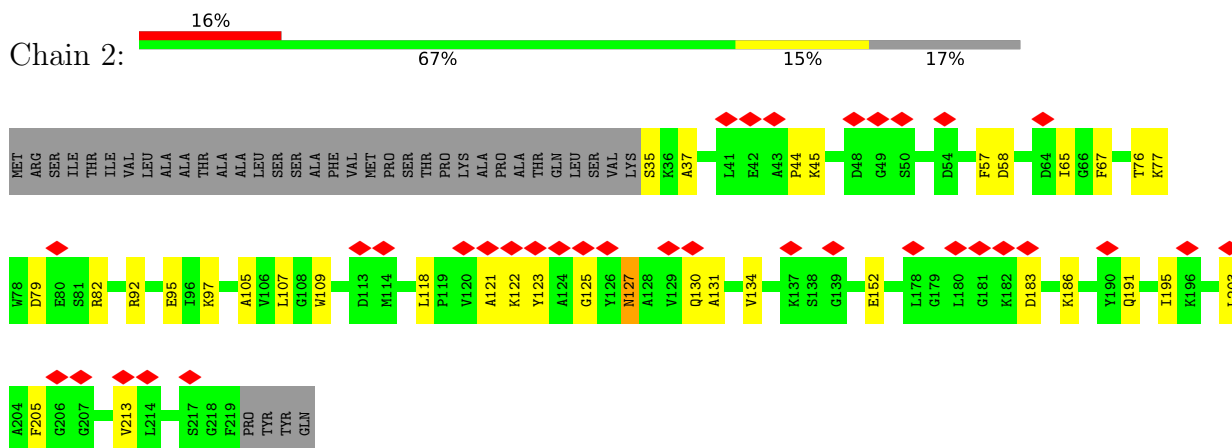


- Molecule 6: VCPI-6

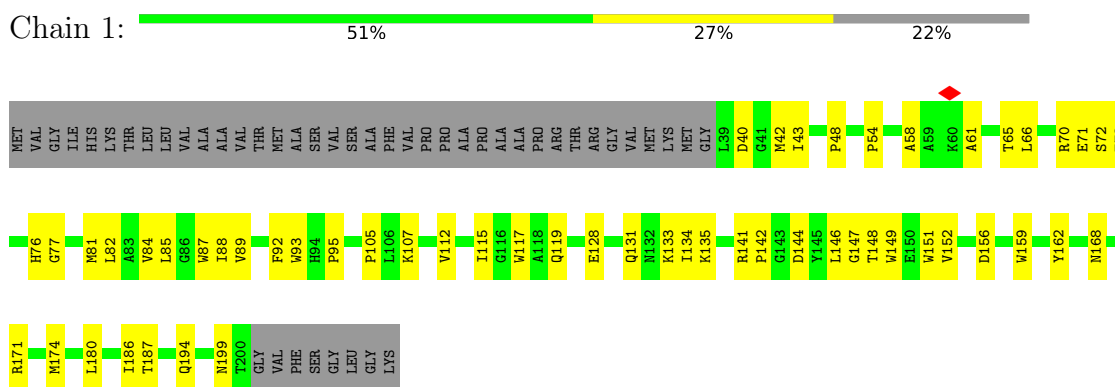
Chain 6:  14% 55% 14% 31%



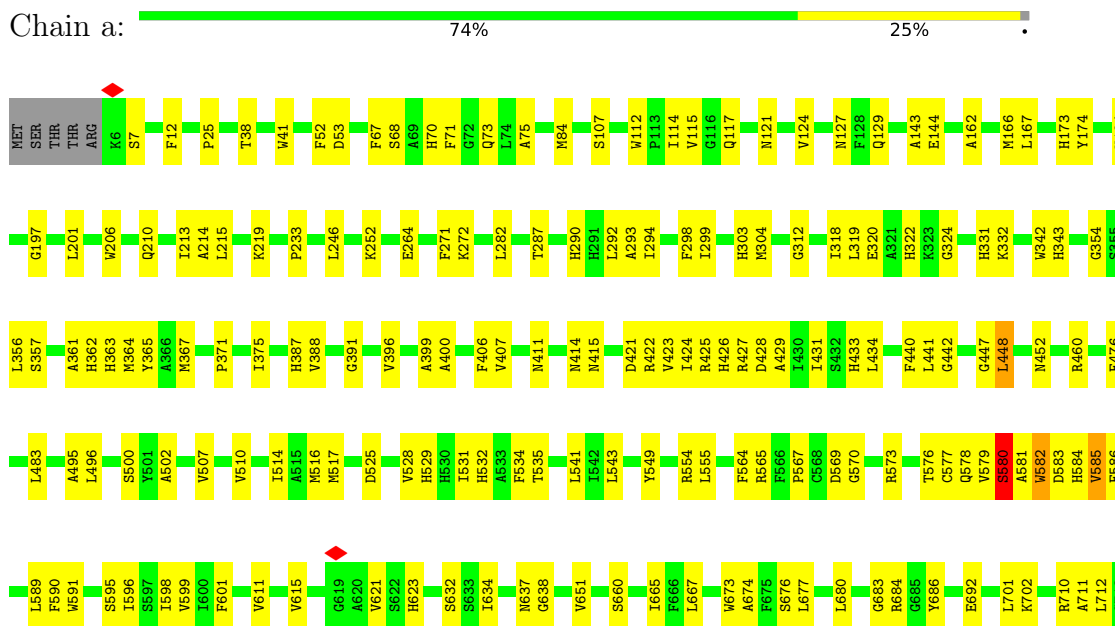
- Molecule 7: VCPI-2

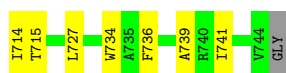


- Molecule 8: VCPI-1



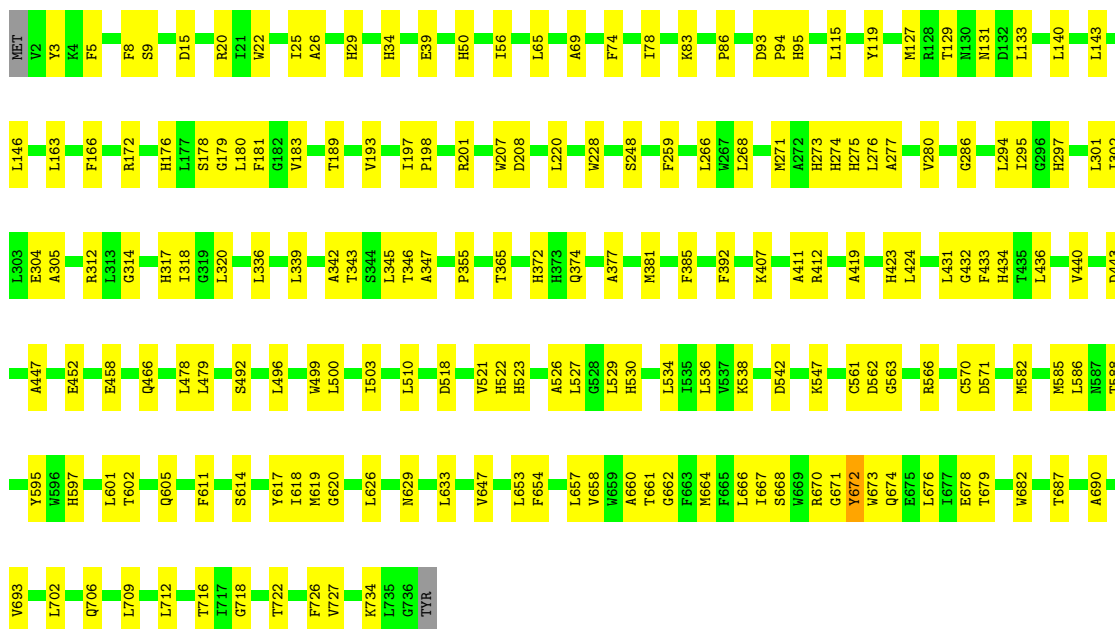
- Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1





• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 75% 25%



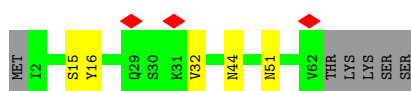
• Molecule 11: Photosystem I reaction center subunit II

Chain d: 76% 19%



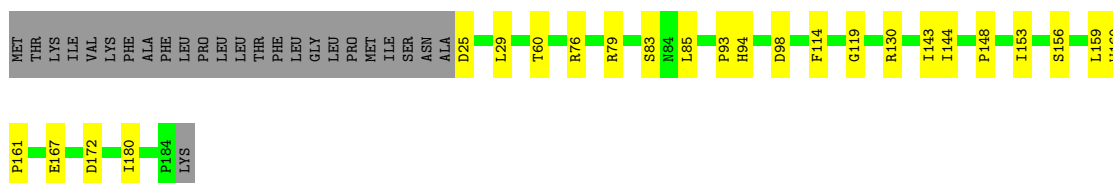
• Molecule 12: Photosystem I reaction center subunit IV

Chain e: 84% 7% 9%



• Molecule 13: Photosystem I reaction center subunit III

Chain f: 74% 13% 14%



● Molecule 20: Photosystem I iron-sulfur center

Chain c: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96367	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	1.565	Depositor
Minimum map value	-0.443	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.271	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	5	0.14	0/1353	0.29	0/1823
2	9	0.34	0/1496	0.33	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.16	0/1298	0.31	0/1761
4	7	0.18	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	6	0.17	0/1390	0.31	0/1883
7	2	0.14	0/1405	0.36	0/1904
8	1	0.13	0/1293	0.33	0/1759
9	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
10	b	0.20	0/6080	0.32	1/8302 (0.0%)
11	d	0.11	0/1040	0.32	0/1402
12	e	0.08	0/502	0.20	0/681
13	f	0.14	0/1297	0.31	0/1762
14	h	0.52	1/667 (0.1%)	0.52	0/915
15	i	0.14	0/278	0.33	0/378
16	j	0.15	0/351	0.36	0/478
17	l	0.14	0/1315	0.31	0/1796
18	m	0.08	0/210	0.28	0/288
20	c	0.12	0/606	0.34	0/822
All	All	0.23	5/30489 (0.0%)	0.33	8/41469 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	580	SER	CA-C	-7.03	1.43	1.52
3	8	44	LEU	C-O	-6.13	1.15	1.23
9	a	581	ALA	CA-C	-5.43	1.45	1.52
14	h	114	TRP	C-O	-5.33	1.18	1.24
9	a	582	TRP	CA-C	-5.02	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	581	ALA	N-CA-C	-8.62	102.51	113.72
3	8	39	LYS	N-CA-C	-6.09	105.67	113.23
9	a	448	LEU	N-CA-C	-6.09	104.20	111.69
9	a	584	HIS	N-CA-C	-5.83	106.51	113.97
10	b	672	TYR	N-CA-C	-5.59	106.30	113.23
3	8	41	LEU	CA-C-N	5.07	124.78	119.82
3	8	41	LEU	C-N-CA	5.07	124.78	119.82
9	a	585	VAL	N-CA-C	-5.06	105.47	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	36	0
2	9	1466	0	1470	49	0
3	8	1258	0	1280	32	0
4	4	1268	0	1288	23	0
4	7	1220	0	1209	42	0
5	3	1324	0	1340	23	0
6	6	1352	0	1334	31	0
7	2	1372	0	1347	23	0
8	1	1262	0	1237	41	0
9	a	5827	0	5697	140	0
10	b	5865	0	5710	151	0
11	d	1014	0	1015	20	0
12	e	494	0	495	5	0
13	f	1266	0	1262	21	0
14	h	646	0	649	18	0
15	i	271	0	292	12	0
16	j	339	0	342	21	0
17	l	1283	0	1278	27	0
18	m	210	0	226	3	0
19	g	275	0	62	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	c	596	0	583	19	0
21	1	88	0	112	5	0
21	2	220	0	280	19	0
21	3	176	0	224	18	0
21	4	220	0	280	27	0
21	5	132	0	168	16	0
21	6	176	0	224	20	0
21	7	176	0	224	29	0
21	8	132	0	168	17	0
21	9	132	0	168	17	0
21	a	44	0	56	4	0
21	j	44	0	56	5	0
22	1	45	0	0	1	0
22	3	90	0	0	0	0
22	5	45	0	0	1	0
22	7	45	0	0	2	0
22	9	90	0	0	3	0
23	1	547	0	508	15	0
23	2	544	0	452	10	0
23	3	458	0	378	10	0
23	4	613	0	522	30	0
23	5	563	0	472	23	0
23	6	564	0	485	14	0
23	7	576	0	444	24	0
23	8	507	0	429	24	0
23	9	519	0	452	39	0
23	a	2579	0	2562	137	0
23	b	2410	0	2464	122	0
23	f	117	0	115	2	0
23	h	55	0	49	3	0
23	j	100	0	86	9	0
23	l	148	0	123	3	0
24	1	45	0	54	3	0
24	5	35	0	34	1	0
25	1	57	0	0	2	0
25	6	110	0	0	6	0
25	8	57	0	0	2	0
25	9	57	0	0	2	0
25	h	57	0	0	4	0
26	9	82	0	110	6	0
26	a	75	0	93	6	0
26	b	31	0	32	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	40	0	38	11	0
27	8	40	0	38	2	0
27	b	57	0	72	6	0
28	2	35	0	40	3	0
28	a	34	0	38	11	0
28	j	32	0	34	7	0
29	a	33	0	46	3	0
29	b	33	0	46	2	0
30	a	160	0	224	13	0
30	b	240	0	336	28	0
30	f	80	0	112	13	0
30	h	80	0	112	6	0
30	i	40	0	56	3	0
30	j	40	0	56	10	0
30	l	80	0	112	12	0
30	m	40	0	56	1	0
31	a	8	0	0	0	0
31	c	16	0	0	3	0
All	All	43774	0	42674	1097	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 (1097) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:193:ALA:HB1	27:4:318:DGD:HE62	1.13	1.09
4:4:193:ALA:HB1	27:4:318:DGD:C6E	1.84	1.06
21:2:303:XAT:H32	23:2:308:CLA:HAB	1.52	0.90
21:5:302:XAT:H12	23:5:307:CLA:HAB	1.53	0.89
27:4:318:DGD:O4E	27:4:318:DGD:O5E	1.61	0.84
23:a:806:CLA:O1A	23:a:814:CLA:HBA1	1.81	0.80
9:a:531:ILE:HD12	23:a:801:CLA:H172	1.63	0.79
23:b:825:CLA:HMA1	30:b:845:BCR:H17C	1.66	0.77
21:8:303:XAT:H12	23:8:312:CLA:HAB	1.67	0.77
21:4:303:XAT:H12	23:4:308:CLA:HAB	1.67	0.76
23:1:312:CLA:HHC	23:1:312:CLA:HBB1	1.69	0.74
4:4:193:ALA:CB	27:4:318:DGD:HE62	2.07	0.74
21:2:303:XAT:H181	23:2:314:CLA:HBB1	1.70	0.72
23:b:833:CLA:H72	30:b:845:BCR:H391	1.72	0.70
13:f:167:GLU:HG3	13:f:172:ASP:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:43:ILE:O	8:1:70:ARG:NH2	2.25	0.69
16:j:22:THR:HA	16:j:25:PHE:CE1	2.28	0.69
10:b:273:HIS:HD1	23:b:817:CLA:HAB	1.58	0.69
1:5:179:LEU:HD12	13:f:159:LEU:HD11	1.75	0.69
23:4:317:CLA:H2A	27:4:318:DGD:HE62	1.73	0.69
30:a:847:BCR:H362	30:a:848:BCR:H21C	1.73	0.68
9:a:363:HIS:ND1	23:a:819:CLA:OBD	2.26	0.68
9:a:569:ASP:OD2	9:a:573:ARG:NH2	2.27	0.68
23:b:807:CLA:H151	23:b:828:CLA:HBB2	1.74	0.68
23:4:317:CLA:HAA2	27:4:318:DGD:HE5	1.77	0.67
23:a:804:CLA:HED1	16:j:15:LEU:HD22	1.76	0.66
10:b:336:LEU:HD21	23:b:829:CLA:HAB	1.78	0.66
21:4:302:XAT:H14	23:4:310:CLA:H12	1.76	0.66
21:6:303:XAT:H30	23:6:308:CLA:HAB	1.77	0.66
8:1:146:LEU:HD13	23:a:844:CLA:H91	1.77	0.66
8:1:70:ARG:NH1	8:1:73:GLU:OE1	2.28	0.66
10:b:295:ILE:HG13	23:b:820:CLA:HED1	1.77	0.66
10:b:304:GLU:HG2	10:b:318:ILE:HG13	1.78	0.66
9:a:112:TRP:HB3	21:j:101:XAT:H373	1.77	0.66
21:4:303:XAT:H193	23:4:308:CLA:H142	1.78	0.65
8:1:194:GLN:HG3	8:1:199:ASN:HB3	1.77	0.65
9:a:356:LEU:HD11	23:a:820:CLA:H71	1.79	0.65
10:b:9:SER:HB2	27:b:848:DGD:HE62	1.78	0.65
23:a:834:CLA:H142	30:b:846:BCR:H15C	1.79	0.65
23:b:823:CLA:HBB1	23:b:837:CLA:H151	1.79	0.65
9:a:197:GLY:O	9:a:201:LEU:HB2	1.97	0.65
14:h:114:TRP:HA	14:h:117:HIS:NE2	2.11	0.65
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.64
13:f:25:ASP:N	13:f:29:LEU:O	2.30	0.64
6:6:236:ALA:HB1	6:6:247:VAL:HG21	1.77	0.64
16:j:31:ARG:HD3	21:j:101:XAT:H222	1.78	0.64
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.64
23:a:808:CLA:HMB2	30:j:104:BCR:HC8	1.79	0.64
10:b:115:LEU:HA	10:b:365:THR:HG22	1.80	0.64
2:9:191:ALA:O	2:9:195:ASN:ND2	2.30	0.64
4:7:120:ALA:HB1	23:7:311:CLA:HMD1	1.79	0.64
23:b:813:CLA:H121	23:b:818:CLA:H72	1.79	0.64
21:4:305:XAT:H363	21:3:301:XAT:H10	1.80	0.64
21:3:305:XAT:H32	23:3:313:CLA:HAB	1.79	0.64
13:f:79:ARG:NH1	16:j:35:ASP:O	2.30	0.64
15:i:29:TYR:HA	15:i:32:LYS:HE2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:29:HIS:ND1	23:b:807:CLA:O1A	2.28	0.63
6:6:162:LEU:HG	23:h:204:CLA:HBC2	1.80	0.63
21:4:304:XAT:H32	23:4:313:CLA:HAB	1.80	0.63
16:j:26:VAL:HG11	30:j:104:BCR:H24C	1.81	0.63
16:j:21:PHE:HA	23:j:103:CLA:HBB2	1.80	0.63
9:a:362:HIS:HA	9:a:365:TYR:CE1	2.33	0.63
4:7:50:ASP:OD1	4:7:51:GLY:N	2.32	0.63
9:a:298:PHE:HE1	23:a:822:CLA:HAB	1.64	0.63
10:b:129:THR:HG22	10:b:131:ASN:H	1.63	0.63
4:7:136:VAL:HG22	23:7:312:CLA:HMA1	1.81	0.63
4:7:136:VAL:HG11	23:b:820:CLA:HBA1	1.81	0.63
10:b:561:CYS:SG	10:b:563:GLY:N	2.71	0.63
9:a:684:ARG:H	10:b:570:CYS:HB2	1.63	0.62
9:a:429:ALA:O	9:a:433:HIS:ND1	2.31	0.62
23:8:305:CLA:CGA	27:8:315:DGD:HE5	2.29	0.62
6:6:246:SER:HB2	23:6:315:CLA:CAA	2.28	0.62
11:d:86:ARG:HB2	11:d:96:LEU:HD11	1.82	0.62
9:a:298:PHE:CE1	23:a:822:CLA:HAB	2.35	0.62
21:5:302:XAT:H162	23:5:307:CLA:H2	1.82	0.62
24:5:316:SQD:H2	21:4:301:XAT:H373	1.82	0.62
21:7:303:XAT:H362	23:7:308:CLA:H51	1.81	0.62
23:a:818:CLA:C3D	28:a:853:LMG:HC91	2.30	0.62
9:a:114:ILE:HB	21:j:101:XAT:H372	1.81	0.62
1:5:130:PHE:CE1	21:5:302:XAT:O24	2.52	0.61
9:a:589:LEU:HD21	23:a:831:CLA:HBC1	1.81	0.61
4:7:144:GLU:HB2	10:b:294:LEU:HD11	1.82	0.61
8:1:186:ILE:HG13	8:1:187:THR:HG23	1.83	0.61
9:a:70:HIS:ND1	23:a:814:CLA:OBD	2.31	0.61
10:b:15:ASP:HB3	10:b:20:ARG:HB2	1.82	0.61
23:4:317:CLA:H2A	27:4:318:DGD:C6E	2.30	0.61
9:a:121:ASN:HB3	9:a:129:GLN:HB3	1.83	0.61
25:h:203:A1L1F:C12	25:h:203:A1L1F:C4	2.78	0.61
6:6:109:GLY:O	10:b:312:ARG:NH1	2.34	0.61
23:8:305:CLA:HAA2	27:8:315:DGD:HE5	1.82	0.61
10:b:424:LEU:HD13	10:b:534:LEU:HA	1.81	0.61
11:d:12:LYS:HB2	11:d:51:LYS:HB3	1.82	0.61
9:a:167:LEU:HD11	23:a:810:CLA:H193	1.83	0.61
10:b:660:ALA:HB3	23:b:804:CLA:HBB2	1.83	0.61
5:3:199:ALA:O	5:3:203:MET:HG3	2.01	0.60
11:d:88:TYR:HB2	11:d:92:ASP:HB2	1.81	0.60
23:a:833:CLA:HBC2	23:a:840:CLA:HMC2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.60
7:2:76:THR:O	7:2:82:ARG:NH1	2.33	0.60
25:1:304:A1L1F:C2	23:a:844:CLA:H11	2.31	0.60
3:8:185:MET:HE2	23:8:308:CLA:HBB2	1.83	0.60
1:5:225:ILE:HG22	23:5:314:CLA:HAB	1.82	0.60
5:3:92:HIS:HB3	5:3:197:MET:SD	2.42	0.60
23:b:830:CLA:HAB	23:b:837:CLA:HBB2	1.82	0.60
4:4:170:MET:HE1	23:4:313:CLA:H43	1.84	0.60
23:a:820:CLA:H92	23:a:830:CLA:H91	1.84	0.60
2:9:182:ALA:HB3	2:9:190:GLU:HG2	1.82	0.60
9:a:53:ASP:OD2	9:a:343:HIS:NE2	2.35	0.60
5:3:83:TYR:OH	5:3:163:ARG:NH1	2.35	0.59
8:1:72:SER:O	8:1:76:HIS:ND1	2.28	0.59
9:a:162:ALA:O	9:a:166:MET:HG2	2.00	0.59
23:a:804:CLA:ND	16:j:12:PRO:HG3	2.17	0.59
10:b:412:ARG:NH2	23:b:830:CLA:O1D	2.35	0.59
9:a:507:VAL:HG22	9:a:517:MET:HG3	1.85	0.59
23:b:831:CLA:HBC3	30:f:804:BCR:H362	1.83	0.59
17:l:38:ARG:O	17:l:46:ARG:NH2	2.35	0.59
21:8:302:XAT:H32	23:8:307:CLA:HAB	1.85	0.59
4:4:185:PHE:CZ	21:4:303:XAT:H30	2.37	0.59
2:9:185:PRO:HA	23:9:313:CLA:HBA2	1.85	0.58
22:1:301:A1L1G:C18	23:1:306:CLA:HAC2	2.32	0.58
23:a:818:CLA:C1D	28:a:853:LMG:H291	2.34	0.58
4:7:88:THR:HG21	21:7:304:XAT:H12	1.85	0.58
9:a:734:TRP:NE1	23:a:829:CLA:O1A	2.36	0.58
21:6:305:XAT:H373	26:b:847:LHG:HC61	1.86	0.58
7:2:44:PRO:HG3	7:2:58:ASP:HB3	1.83	0.58
23:6:317:CLA:C2	23:b:840:CLA:HBB2	2.34	0.58
30:b:842:BCR:H23C	30:h:202:BCR:H323	1.86	0.58
9:a:107:SER:HB2	9:a:124:VAL:HG11	1.85	0.58
1:5:111:TRP:NE1	23:5:308:CLA:O1A	2.33	0.58
21:2:303:XAT:H363	23:2:308:CLA:H2	1.84	0.58
9:a:292:LEU:HD21	23:a:818:CLA:CAB	2.34	0.58
10:b:74:PHE:O	10:b:78:ILE:HG12	2.04	0.58
1:5:112:LEU:HD22	23:5:307:CLA:H12	1.86	0.58
21:9:303:XAT:H363	3:8:135:LEU:HD12	1.86	0.57
23:6:317:CLA:HAA1	14:h:121:TRP:CD1	2.39	0.57
9:a:517:MET:HE1	9:a:623:HIS:NE2	2.19	0.57
23:b:804:CLA:CGA	23:b:804:CLA:H3A	2.34	0.57
5:3:87:GLU:OE2	5:3:163:ARG:NH2	2.31	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:185:PHE:CD2	21:7:303:XAT:H12	2.40	0.57
11:d:97:HIS:HB3	11:d:98:PRO:HD3	1.86	0.57
21:5:301:XAT:H14	23:5:309:CLA:H12	1.86	0.57
2:9:222:ASP:HB2	2:9:230:LEU:HD13	1.86	0.57
9:a:598:ILE:HG13	23:a:801:CLA:H192	1.86	0.57
10:b:69:ALA:HB2	10:b:133:LEU:HB2	1.86	0.57
9:a:324:GLY:HA3	26:a:846:LHG:HC32	1.87	0.57
23:a:826:CLA:HBA1	23:a:830:CLA:H193	1.86	0.57
10:b:178:SER:HB3	10:b:286:GLY:HA3	1.86	0.57
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
23:3:312:CLA:H42	30:a:848:BCR:H272	1.85	0.57
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.57
6:6:248:PRO:HG2	23:6:315:CLA:HBC2	1.87	0.57
9:a:7:SER:H	9:a:12:PHE:HE2	1.53	0.57
21:2:303:XAT:C36	23:2:308:CLA:H2	2.35	0.56
9:a:114:ILE:HG13	9:a:115:VAL:HG13	1.86	0.56
9:a:213:ILE:HG23	9:a:233:PRO:HB3	1.87	0.56
10:b:582:MET:HG3	10:b:712:LEU:HD21	1.87	0.56
15:i:26:LEU:HD13	30:l:205:BCR:HC8	1.86	0.56
1:5:155:VAL:HG21	23:5:309:CLA:HAA2	1.86	0.56
2:9:107:LEU:HD11	2:9:140:ILE:HD11	1.87	0.56
5:3:86:ARG:NH1	5:3:89:GLU:OE1	2.38	0.56
23:a:802:CLA:CGA	23:a:802:CLA:H3A	2.35	0.56
28:a:853:LMG:H112	28:a:853:LMG:C9	2.35	0.56
9:a:660:SER:HB2	10:b:447:ALA:HB1	1.88	0.56
23:a:822:CLA:HBC3	23:a:828:CLA:H172	1.87	0.56
23:b:805:CLA:H18	15:i:14:VAL:HG22	1.87	0.56
30:f:801:BCR:HC32	23:j:102:CLA:H43	1.86	0.56
17:l:54:HIS:HA	17:l:57:PHE:CE2	2.41	0.56
9:a:651:VAL:HG22	9:a:739:ALA:HB3	1.87	0.56
23:a:841:CLA:H72	30:f:801:BCR:H17C	1.88	0.56
10:b:39:GLU:HB3	10:b:163:LEU:HD11	1.87	0.56
23:b:821:CLA:HHB	23:b:822:CLA:H2	1.88	0.56
11:d:105:GLU:HG2	20:c:19:ARG:HB3	1.88	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
4:4:136:VAL:HG22	23:4:312:CLA:HMA1	1.87	0.56
5:3:182:PHE:HZ	23:3:313:CLA:HED3	1.70	0.56
23:a:854:CLA:H112	16:j:14:LEU:HD22	1.88	0.56
9:a:290:HIS:HB2	23:a:819:CLA:C1B	2.37	0.56
2:9:85:GLY:O	2:9:89:MET:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:88:ILE:HG22	8:1:92:PHE:HE1	1.71	0.55
5:3:48:LEU:HD13	5:3:51:LEU:HD12	1.87	0.55
23:a:818:CLA:CHD	28:a:853:LMG:H291	2.36	0.55
23:b:806:CLA:HBA1	23:b:813:CLA:HBA1	1.87	0.55
17:l:92:LEU:HB3	30:l:205:BCR:H401	1.88	0.55
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.55
10:b:693:VAL:HG11	23:b:801:CLA:HAB	1.87	0.55
6:6:248:PRO:HD2	25:6:304:A1L1F:C56	2.36	0.55
9:a:441:LEU:HB3	9:a:534:PHE:HB2	1.88	0.55
16:j:14:LEU:HD21	28:j:105:LMG:H141	1.89	0.55
7:2:35:SER:OG	7:2:37:ALA:O	2.22	0.55
2:9:153:PHE:HA	17:l:151:PHE:HE2	1.71	0.55
9:a:651:VAL:HG21	9:a:736:PHE:HA	1.87	0.55
10:b:5:PHE:HB2	15:i:30:ILE:HA	1.89	0.55
3:8:60:PHE:HE1	23:8:305:CLA:HBC3	1.70	0.55
28:a:853:LMG:H112	28:a:853:LMG:O8	2.05	0.55
20:c:15:THR:HG22	20:c:28:MET:HG3	1.89	0.55
23:a:825:CLA:H12	30:a:849:BCR:H14C	1.88	0.55
2:9:117:TRP:O	2:9:120:TRP:CD1	2.60	0.55
23:a:841:CLA:H92	30:f:801:BCR:H15C	1.88	0.55
2:9:149:ALA:O	2:9:153:PHE:HD1	1.90	0.54
3:8:75:VAL:HG23	23:8:307:CLA:HMA2	1.89	0.54
2:9:93:ILE:HG13	21:9:304:XAT:H8	1.89	0.54
8:1:115:ILE:O	8:1:119:GLN:NE2	2.40	0.54
12:e:32:VAL:HG11	20:c:35:LYS:HD3	1.89	0.54
9:a:197:GLY:HA3	23:a:814:CLA:HBB1	1.89	0.54
9:a:210:GLN:HA	9:a:214:ALA:HB3	1.89	0.54
6:6:153:ASP:OD1	6:6:155:THR:OG1	2.26	0.54
23:b:823:CLA:HBB2	23:b:840:CLA:H52	1.90	0.54
11:d:63:ARG:NH2	11:d:65:GLU:OE1	2.41	0.54
4:7:200:PRO:O	21:7:304:XAT:O3	2.26	0.54
8:1:61:ALA:HB1	8:1:65:THR:HB	1.90	0.54
9:a:591:TRP:HE1	23:b:804:CLA:C1D	2.21	0.54
25:8:304:A1L1F:C2	18:m:23:ARG:HD3	2.38	0.54
4:4:83:ILE:HD11	21:4:302:XAT:H362	1.90	0.54
9:a:702:LYS:HB3	13:f:130:ARG:HD3	1.89	0.54
10:b:355:PRO:HG3	23:b:818:CLA:HBA1	1.90	0.54
10:b:633:LEU:HD22	10:b:726:PHE:HA	1.89	0.54
22:5:303:A1L1G:C41	23:5:312:CLA:HMC1	2.37	0.54
4:4:185:PHE:CE2	21:4:303:XAT:H30	2.42	0.54
10:b:521:VAL:HG21	10:b:595:TYR:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:661:THR:O	10:b:664:MET:HB3	2.08	0.53
4:4:121:LEU:HD23	4:4:124:ILE:HD12	1.90	0.53
4:7:46:PRO:HG2	4:7:49:LEU:HD12	1.90	0.53
9:a:388:VAL:HG12	9:a:596:ILE:HG23	1.89	0.53
9:a:396:VAL:HG11	9:a:589:LEU:HG	1.91	0.53
9:a:667:LEU:HD11	10:b:619:MET:HB2	1.89	0.53
23:a:825:CLA:HMA3	23:a:844:CLA:HAB	1.91	0.53
10:b:317:HIS:HB3	10:b:320:LEU:HD12	1.89	0.53
3:8:36:ALA:N	3:8:44:LEU:O	2.42	0.53
6:6:154:PHE:HB2	21:6:303:XAT:H22	1.89	0.53
23:a:829:CLA:H101	30:j:104:BCR:H341	1.89	0.53
10:b:189:THR:HG21	10:b:276:LEU:HB2	1.91	0.53
9:a:686:TYR:OH	23:a:802:CLA:OBD	2.21	0.53
10:b:140:LEU:HG	30:b:844:BCR:H382	1.90	0.53
23:9:312:CLA:HBA1	23:9:312:CLA:HBD	1.89	0.53
4:7:128:THR:HG23	22:7:302:A1L1G:C17	2.39	0.53
4:4:140:SER:OG	16:j:1:MET:SD	2.57	0.53
23:b:829:CLA:H42	27:b:848:DGD:HB42	1.91	0.53
4:4:81:CYS:HB3	4:4:178:GLY:HA3	1.91	0.53
23:4:317:CLA:O2D	27:4:318:DGD:HE61	2.09	0.53
9:a:573:ARG:HG3	20:c:78:GLY:HA3	1.90	0.53
23:a:809:CLA:CHC	23:a:810:CLA:HMD2	2.39	0.53
23:a:820:CLA:HAB	23:a:820:CLA:H8	1.90	0.53
10:b:443:ASP:OD1	10:b:617:TYR:HB2	2.08	0.53
23:a:831:CLA:H42	26:a:845:LHG:H251	1.90	0.53
23:b:836:CLA:HBC3	30:f:804:BCR:H292	1.91	0.53
3:8:175:LYS:HB3	23:8:306:CLA:HMD2	1.90	0.53
10:b:718:GLY:O	10:b:722:THR:HG22	2.09	0.53
2:9:107:LEU:HG	2:9:136:ALA:HB1	1.91	0.52
3:8:70:ALA:H	23:b:811:CLA:HED1	1.75	0.52
6:6:232:ILE:HD13	25:6:301:A1L1F:C31	2.39	0.52
23:a:835:CLA:O2D	23:a:835:CLA:H2A	2.09	0.52
10:b:22:TRP:CG	10:b:706:GLN:HE22	2.26	0.52
10:b:709:LEU:HD11	27:b:848:DGD:HB41	1.90	0.52
21:5:302:XAT:C16	23:5:307:CLA:H2	2.39	0.52
5:3:79:GLY:O	5:3:158:ARG:NH1	2.43	0.52
2:9:179:LEU:HD23	23:9:308:CLA:HMD3	1.90	0.52
11:d:95:LEU:HD22	19:g:75:UNK:HA	1.91	0.52
3:8:177:GLY:O	3:8:181:MET:HG3	2.09	0.52
23:8:305:CLA:HBC2	4:7:134:ILE:HG13	1.91	0.52
9:a:219:LYS:HD3	9:a:246:LEU:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:411:ASN:ND2	9:a:414:ASN:OD1	2.37	0.52
23:a:810:CLA:HAB	23:j:102:CLA:HMD2	1.91	0.52
23:b:801:CLA:H101	23:b:801:CLA:HBB1	1.91	0.52
10:b:466:GLN:NE2	23:b:835:CLA:OBD	2.34	0.52
19:g:51:UNK:O	19:g:53:UNK:N	2.42	0.52
4:4:193:ALA:O	27:4:318:DGD:O6E	2.28	0.52
23:a:834:CLA:H151	29:b:841:PQN:H202	1.91	0.52
13:f:143:ILE:HG13	13:f:144:ILE:HG13	1.92	0.52
17:l:109:ASN:OD1	17:l:110:ALA:N	2.35	0.52
6:6:124:HIS:HB3	6:6:231:MET:HE2	1.92	0.52
6:6:184:TYR:CZ	6:6:186:GLY:HA3	2.44	0.52
6:6:249:LEU:HB2	25:6:304:A1L1F:O55	2.10	0.52
7:2:77:LYS:O	7:2:79:ASP:N	2.43	0.52
8:1:85:LEU:HB3	23:1:308:CLA:HMC2	1.92	0.52
20:c:11:CYS:SG	20:c:39:ILE:HG13	2.50	0.52
2:9:192:GLU:HB2	23:9:312:CLA:C1B	2.40	0.51
4:7:121:LEU:HD13	23:7:316:CLA:HBC3	1.92	0.51
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
6:6:131:ALA:HB2	21:6:303:XAT:H10	1.92	0.51
8:1:77:GLY:O	8:1:81:MET:HG3	2.09	0.51
23:b:807:CLA:H52	27:b:848:DGD:HB72	1.93	0.51
23:b:816:CLA:H91	14:h:105:LEU:HG	1.91	0.51
23:b:823:CLA:HAB	23:b:830:CLA:HMD1	1.93	0.51
23:b:836:CLA:HBC3	30:f:804:BCR:H401	1.91	0.51
25:h:203:A1L1F:O46	23:h:204:CLA:H52	2.11	0.51
3:8:172:LYS:O	3:8:176:ASN:ND2	2.39	0.51
9:a:431:ILE:HG13	9:a:549:TYR:HE1	1.74	0.51
10:b:26:ALA:HA	23:b:829:CLA:H43	1.93	0.51
10:b:342:ALA:O	10:b:346:THR:HG23	2.11	0.51
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.92	0.51
23:a:827:CLA:H93	23:a:840:CLA:H52	1.92	0.51
28:a:853:LMG:HC92	28:a:853:LMG:C11	2.41	0.51
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.51
25:1:304:A1L1F:C56	26:a:846:LHG:H241	2.41	0.51
9:a:460:ARG:NH2	23:a:835:CLA:O1D	2.44	0.51
10:b:722:THR:HG23	23:b:803:CLA:O1D	2.11	0.51
4:7:45:ARG:NH1	4:7:49:LEU:O	2.42	0.51
21:7:301:XAT:H10	23:7:315:CLA:HMD1	1.93	0.51
10:b:50:HIS:ND1	23:b:813:CLA:OBD	2.38	0.51
10:b:179:GLY:O	10:b:183:VAL:HB	2.10	0.51
10:b:208:ASP:OD1	10:b:208:ASP:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:434:HIS:CD2	30:b:849:BCR:H333	2.46	0.51
23:5:312:CLA:CGA	23:5:312:CLA:H3A	2.41	0.51
10:b:93:ASP:OD1	10:b:95:HIS:ND1	2.33	0.51
2:9:218:LEU:HG	23:9:314:CLA:HMA2	1.92	0.50
10:b:273:HIS:ND1	23:b:817:CLA:HAB	2.25	0.50
11:d:33:ILE:HG22	11:d:58:VAL:HG22	1.92	0.50
20:c:58:CYS:SG	20:c:63:LEU:HA	2.51	0.50
21:4:303:XAT:C16	23:4:308:CLA:H2	2.41	0.50
6:6:104:GLU:OE2	6:6:105:ARG:NH1	2.45	0.50
10:b:602:THR:HG21	10:b:611:PHE:HB2	1.92	0.50
13:f:85:LEU:HD13	13:f:93:PRO:HB3	1.92	0.50
17:l:38:ARG:NH1	17:l:49:GLU:OE1	2.40	0.50
9:a:577:CYS:O	10:b:671:GLY:HA3	2.11	0.50
20:c:13:GLY:O	20:c:38:GLN:NE2	2.44	0.50
3:8:50:LEU:HD11	3:8:61:ASP:HB2	1.93	0.50
5:3:93:CYS:HB3	5:3:193:GLY:HA3	1.93	0.50
23:a:818:CLA:O1A	28:a:853:LMG:O10	2.30	0.50
13:f:160:TRP:CD1	13:f:161:PRO:HD3	2.46	0.50
20:c:17:CYS:SG	20:c:18:VAL:N	2.85	0.50
9:a:440:PHE:HE2	23:a:839:CLA:HAB	1.76	0.50
10:b:274:HIS:HB2	23:b:817:CLA:C1B	2.41	0.50
10:b:662:GLY:O	10:b:666:LEU:HG	2.10	0.50
7:2:121:ALA:O	7:2:122:LYS:HG2	2.10	0.50
23:a:818:CLA:HHC	23:a:818:CLA:HBB1	1.93	0.50
1:5:130:PHE:HE1	21:5:302:XAT:O24	1.94	0.50
2:9:162:LYS:NZ	23:9:312:CLA:O1A	2.40	0.50
6:6:112:PRO:HB3	6:6:116:TRP:CD1	2.47	0.50
23:b:811:CLA:H72	23:b:812:CLA:HBC3	1.93	0.50
23:3:308:CLA:HED2	23:3:308:CLA:H2A	1.94	0.50
22:9:301:A1L1G:C44	23:9:315:CLA:HBC3	2.41	0.49
4:7:54:VAL:HG21	4:7:74:GLN:HE21	1.77	0.49
9:a:422:ARG:O	9:a:426:HIS:ND1	2.41	0.49
9:a:712:LEU:N	29:a:843:PQN:O4	2.45	0.49
10:b:478:LEU:HG	10:b:479:LEU:HG	1.93	0.49
17:l:106:VAL:H	17:l:140:VAL:HG23	1.77	0.49
21:5:301:XAT:H193	23:5:310:CLA:HBA2	1.94	0.49
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.49
2:9:117:TRP:O	2:9:120:TRP:NE1	2.45	0.49
7:2:107:LEU:HB3	23:2:310:CLA:HMC2	1.94	0.49
8:1:112:VAL:HB	8:1:117:TRP:NE1	2.27	0.49
30:b:849:BCR:H23C	16:j:33:TYR:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:191:ALA:HB1	23:9:313:CLA:HAA1	1.93	0.49
4:4:159:ASN:C	4:4:161:ALA:H	2.21	0.49
4:7:185:PHE:O	4:7:189:VAL:HG22	2.13	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
3:8:60:PHE:CE1	23:8:305:CLA:HBC3	2.47	0.49
23:6:317:CLA:HBA1	23:6:317:CLA:HBD	1.93	0.49
23:a:818:CLA:CHD	23:a:819:CLA:HBB2	2.43	0.49
10:b:25:ILE:HG12	30:l:205:BCR:H312	1.94	0.49
10:b:305:ALA:HB2	14:h:46:THR:HB	1.93	0.49
10:b:419:ALA:O	10:b:423:HIS:ND1	2.40	0.49
23:b:832:CLA:HBB2	30:f:801:BCR:HC41	1.94	0.49
20:c:17:CYS:HB3	31:c:102:SF4:S4	2.52	0.49
9:a:423:VAL:HA	9:a:426:HIS:CE1	2.47	0.49
9:a:425:ARG:NH2	11:d:15:GLY:O	2.44	0.49
10:b:492:SER:HA	10:b:496:LEU:HD12	1.94	0.49
17:l:43:PRO:HD3	17:l:136:GLU:CD	2.38	0.49
19:g:46:UNK:O	19:g:50:UNK:N	2.45	0.49
23:4:309:CLA:HAC1	23:4:316:CLA:HAB	1.95	0.49
7:2:183:ASP:O	7:2:186:LYS:N	2.44	0.49
4:7:42:PHE:HE2	23:7:306:CLA:HAB	1.77	0.49
9:a:554:ARG:HB2	10:b:678:GLU:OE1	2.13	0.49
23:a:803:CLA:H2	10:b:657:LEU:HD22	1.95	0.49
10:b:407:LYS:HB3	10:b:411:ALA:HB3	1.95	0.49
9:a:565:ARG:HG2	9:a:715:THR:HG21	1.93	0.49
9:a:674:ALA:HB3	23:a:802:CLA:HBB2	1.94	0.49
2:9:91:GLY:HA3	21:9:303:XAT:H173	1.94	0.49
23:a:802:CLA:H41	10:b:436:LEU:HD22	1.95	0.49
28:a:853:LMG:H131	28:a:853:LMG:H292	1.94	0.49
10:b:562:ASP:OD2	10:b:566:ARG:NH2	2.38	0.49
15:i:26:LEU:HD22	30:l:205:BCR:H323	1.94	0.49
25:6:304:A1L1F:C33	23:6:313:CLA:HAB	2.43	0.49
4:7:91:TRP:CE3	21:7:303:XAT:H22	2.48	0.49
10:b:181:PHE:HE2	23:b:819:CLA:HAB	1.78	0.49
23:a:839:CLA:H62	23:a:839:CLA:H41	1.54	0.48
10:b:166:PHE:O	10:b:172:ARG:NH2	2.46	0.48
11:d:95:LEU:HD11	11:d:98:PRO:HD2	1.95	0.48
2:9:137:ARG:NH1	23:9:318:CLA:OBD	2.41	0.48
28:a:853:LMG:C9	28:a:853:LMG:C11	2.91	0.48
10:b:277:ALA:HA	23:b:816:CLA:HMC2	1.95	0.48
10:b:597:HIS:CE1	10:b:601:LEU:HD11	2.48	0.48
23:b:839:CLA:H13	30:i:101:BCR:H19C	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:124:ILE:HA	23:7:311:CLA:HBC3	1.95	0.48
10:b:3:TYR:HB2	15:i:33:GLU:HA	1.95	0.48
16:j:2:LYS:O	28:j:105:LMG:HC61	2.13	0.48
4:7:97:VAL:O	4:7:97:VAL:HG13	2.13	0.48
23:b:812:CLA:H62	23:b:812:CLA:H41	1.62	0.48
2:9:32:THR:H	2:9:33:PRO:HD2	1.77	0.48
23:2:316:CLA:C2C	28:2:317:LMG:H111	2.44	0.48
23:a:841:CLA:H61	23:b:832:CLA:H42	1.95	0.48
10:b:266:LEU:HD22	23:b:817:CLA:HBA1	1.95	0.48
23:b:823:CLA:H2A	23:b:823:CLA:HED3	1.95	0.48
23:b:824:CLA:H141	23:b:824:CLA:H193	1.95	0.48
23:b:839:CLA:H92	23:b:839:CLA:H61	1.73	0.48
23:9:311:CLA:H2A	23:9:311:CLA:O2D	2.14	0.48
9:a:712:LEU:HD21	29:a:843:PQN:H151	1.96	0.48
10:b:412:ARG:HH21	23:b:830:CLA:CGD	2.27	0.48
14:h:72:PRO:HG3	25:h:203:A1L1F:C56	2.43	0.48
1:5:171:GLU:HG3	23:5:311:CLA:NB	2.28	0.48
21:5:304:XAT:C10	23:5:315:CLA:HBC3	2.44	0.48
2:9:172:LYS:HB3	2:9:172:LYS:HE2	1.45	0.48
21:6:302:XAT:H191	21:6:302:XAT:H11	1.65	0.48
23:a:825:CLA:H71	23:a:840:CLA:H62	1.96	0.48
10:b:8:PHE:HB2	10:b:34:HIS:CG	2.49	0.48
23:b:830:CLA:HAB	23:b:837:CLA:CBB	2.44	0.48
23:3:308:CLA:H2A	23:3:308:CLA:CED	2.44	0.48
21:2:305:XAT:H391	21:2:305:XAT:H31	1.71	0.48
9:a:290:HIS:HB2	23:a:819:CLA:CHB	2.44	0.48
23:b:818:CLA:H3A	23:b:818:CLA:HBA2	1.37	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.48
10:b:595:TYR:CZ	23:b:835:CLA:HBC3	2.49	0.48
21:8:303:XAT:H34	23:8:313:CLA:HBB1	1.96	0.48
5:3:145:ILE:O	5:3:149:ILE:HG12	2.13	0.48
5:3:203:MET:HE2	21:3:305:XAT:O4	2.13	0.48
23:7:316:CLA:HBA1	23:7:316:CLA:H3A	1.59	0.48
9:a:114:ILE:HG23	9:a:115:VAL:HG22	1.95	0.48
9:a:637:ASN:HB2	10:b:653:LEU:HD11	1.94	0.48
30:b:849:BCR:H23C	16:j:33:TYR:HD2	1.78	0.48
3:8:36:ALA:HB3	3:8:45:LYS:HZ2	1.79	0.47
25:8:304:A1L1F:C36	23:8:311:CLA:H51	2.43	0.47
21:7:301:XAT:H35	21:7:301:XAT:H401	1.71	0.47
9:a:287:THR:HG23	23:a:820:CLA:HMA3	1.96	0.47
9:a:292:LEU:HD12	23:a:816:CLA:HMC3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:476:PHE:HB3	23:a:838:CLA:H11	1.96	0.47
10:b:443:ASP:OD1	10:b:618:ILE:N	2.46	0.47
12:e:51:ASN:CG	20:c:61:ASP:HB2	2.39	0.47
14:h:89:ASN:O	14:h:91:PHE:N	2.46	0.47
16:j:5:LEU:HB3	28:j:105:LMG:HC72	1.96	0.47
6:6:118:GLN:O	6:6:121:GLU:HB2	2.14	0.47
7:2:92:ARG:NH1	7:2:95:GLU:OE1	2.47	0.47
8:1:88:ILE:HG22	8:1:92:PHE:CE1	2.49	0.47
21:1:302:XAT:H35	21:1:302:XAT:H401	1.72	0.47
9:a:68:SER:OG	9:a:174:TYR:HB2	2.14	0.47
9:a:570:GLY:O	9:a:576:THR:OG1	2.32	0.47
9:a:615:VAL:HG22	9:a:621:VAL:HG22	1.95	0.47
10:b:670:ARG:C	10:b:672:TYR:H	2.22	0.47
23:b:822:CLA:H43	14:h:115:GLY:C	2.40	0.47
23:b:838:CLA:HAB	29:b:841:PQN:H172	1.96	0.47
14:h:114:TRP:HA	14:h:117:HIS:CD2	2.49	0.47
4:7:81:CYS:O	4:7:85:MET:HG3	2.13	0.47
9:a:400:ALA:HB2	9:a:585:VAL:HG11	1.96	0.47
10:b:271:MET:O	10:b:275:HIS:ND1	2.47	0.47
23:b:821:CLA:CHB	23:b:822:CLA:H2	2.44	0.47
3:8:171:VAL:HG13	3:8:175:LYS:HE3	1.97	0.47
21:3:303:XAT:H401	21:3:303:XAT:H35	1.79	0.47
10:b:176:HIS:O	10:b:180:LEU:HB3	2.14	0.47
2:9:88:ALA:HA	21:9:303:XAT:H8	1.95	0.47
23:a:818:CLA:HBA2	23:a:818:CLA:H3A	1.57	0.47
10:b:538:LYS:O	10:b:542:ASP:HB2	2.15	0.47
10:b:586:LEU:HD21	10:b:716:THR:HG23	1.96	0.47
11:d:20:TRP:CZ2	17:l:14:VAL:HG12	2.50	0.47
23:j:102:CLA:NB	30:j:104:BCR:H281	2.30	0.47
5:3:78:VAL:HG12	5:3:78:VAL:O	2.13	0.47
6:6:118:GLN:HB3	6:6:197:VAL:HG11	1.96	0.47
6:6:194:ASP:OD1	6:6:194:ASP:N	2.48	0.47
8:1:84:VAL:O	8:1:88:ILE:HG12	2.14	0.47
9:a:354:GLY:HA2	9:a:391:GLY:HA2	1.97	0.47
9:a:375:ILE:HG21	9:a:510:VAL:HB	1.96	0.47
10:b:65:LEU:HD11	30:b:844:BCR:H281	1.95	0.47
30:b:844:BCR:H371	30:b:844:BCR:H24C	1.70	0.47
23:8:307:CLA:H203	23:8:307:CLA:H162	1.74	0.47
23:8:311:CLA:HBB1	23:8:311:CLA:HMB3	1.97	0.47
4:4:184:ALA:HA	23:4:315:CLA:HBB1	1.96	0.47
4:4:185:PHE:CZ	21:4:303:XAT:H28	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:185:PHE:HE1	21:7:303:XAT:H162	1.79	0.47
21:7:303:XAT:H191	21:7:303:XAT:H11	1.70	0.47
9:a:127:ASN:HD21	13:f:60:THR:HG21	1.79	0.47
9:a:144:GLU:HG2	9:a:206:TRP:HH2	1.80	0.47
9:a:673:TRP:O	9:a:676:SER:OG	2.32	0.47
10:b:297:HIS:HB3	10:b:302:ILE:HD11	1.97	0.47
23:b:825:CLA:HBA2	23:b:825:CLA:H3A	1.73	0.47
2:9:49:MET:HA	2:9:52:LYS:HD3	1.97	0.47
3:8:73:LYS:HD3	3:8:145:ASP:HA	1.95	0.47
6:6:131:ALA:CB	21:6:303:XAT:H10	2.44	0.47
8:1:73:GLU:HB2	23:1:306:CLA:C1B	2.45	0.47
30:b:844:BCR:HC8	30:b:844:BCR:H311	1.97	0.47
7:2:65:ILE:HG22	7:2:67:PHE:H	1.80	0.47
23:a:834:CLA:CAD	30:l:201:BCR:H10C	2.45	0.47
1:5:96:VAL:HG12	23:5:307:CLA:OBD	2.15	0.47
23:9:316:CLA:H202	17:l:90:LEU:HD22	1.96	0.47
23:a:832:CLA:HAB	23:a:840:CLA:HBB2	1.96	0.47
21:5:304:XAT:H35	21:5:304:XAT:H401	1.80	0.46
2:9:187:LEU:HA	23:9:312:CLA:HMB1	1.96	0.46
23:9:314:CLA:CED	23:9:314:CLA:H2A	2.45	0.46
23:9:316:CLA:HBC3	23:a:803:CLA:H151	1.97	0.46
3:8:110:ASN:HB3	3:8:113:LYS:HB2	1.96	0.46
5:3:81:ASP:N	5:3:81:ASP:OD1	2.46	0.46
21:6:305:XAT:H401	21:6:305:XAT:H35	1.64	0.46
7:2:191:GLN:O	7:2:195:ILE:HD12	2.15	0.46
8:1:40:ASP:HB2	8:1:42:MET:HG3	1.98	0.46
9:a:514:ILE:HD11	9:a:621:VAL:HG13	1.96	0.46
23:b:807:CLA:H161	23:b:807:CLA:H192	1.73	0.46
17:l:168:TYR:O	17:l:172:LEU:HB2	2.16	0.46
2:9:201:LEU:HD21	21:9:304:XAT:H371	1.96	0.46
5:3:179:PRO:C	5:3:181:LYS:H	2.24	0.46
6:6:94:TRP:CZ3	21:6:303:XAT:H383	2.50	0.46
23:6:314:CLA:O1A	23:6:314:CLA:H2A	2.15	0.46
7:2:118:LEU:N	23:2:310:CLA:OBD	2.47	0.46
8:1:42:MET:HE1	8:1:66:LEU:HD22	1.96	0.46
23:b:811:CLA:H51	23:b:812:CLA:H43	1.97	0.46
21:7:305:XAT:H15	21:7:305:XAT:H201	1.69	0.46
23:a:801:CLA:H61	23:a:803:CLA:O1D	2.15	0.46
10:b:432:GLY:HA2	10:b:527:LEU:HD22	1.96	0.46
10:b:687:THR:HG23	10:b:690:ALA:HB3	1.97	0.46
23:b:817:CLA:H41	23:b:833:CLA:HAA2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:232:HIS:HE1	21:5:304:XAT:H14	1.81	0.46
3:8:82:HIS:HB3	3:8:181:MET:SD	2.56	0.46
4:7:37:SER:HB2	4:7:45:ARG:HA	1.97	0.46
9:a:677:LEU:HB2	23:a:802:CLA:HMC2	1.97	0.46
10:b:127:MET:HE1	30:b:844:BCR:H282	1.97	0.46
15:i:26:LEU:HB3	30:l:205:BCR:H323	1.96	0.46
23:4:317:CLA:CGD	27:4:318:DGD:HE61	2.45	0.46
21:7:303:XAT:H32	23:7:308:CLA:HAB	1.97	0.46
21:7:304:XAT:H191	23:7:314:CLA:HAB	1.97	0.46
23:a:818:CLA:NC	28:a:853:LMG:H302	2.31	0.46
23:a:820:CLA:H203	23:a:828:CLA:H3A	1.96	0.46
23:a:834:CLA:H201	30:l:205:BCR:H343	1.98	0.46
22:9:301:A1L1G:O13	21:9:304:XAT:H28	2.16	0.46
23:9:316:CLA:HBA2	17:l:67:PRO:HG3	1.97	0.46
23:9:318:CLA:H91	23:9:318:CLA:H112	1.69	0.46
21:4:302:XAT:H30	23:4:310:CLA:H151	1.98	0.46
23:6:308:CLA:CGA	23:6:308:CLA:H3A	2.45	0.46
10:b:50:HIS:HE1	23:b:806:CLA:H171	1.81	0.46
23:b:817:CLA:H3A	23:b:817:CLA:HBA2	1.26	0.46
28:j:105:LMG:H292	28:j:105:LMG:H111	1.98	0.46
21:6:302:XAT:H15	21:6:302:XAT:H201	1.71	0.46
7:2:105:ALA:HB1	21:2:303:XAT:H161	1.97	0.46
23:2:316:CLA:C1C	28:2:317:LMG:H111	2.46	0.46
23:b:823:CLA:HBA1	30:h:201:BCR:H16C	1.98	0.46
3:8:141:THR:HA	3:8:147:PRO:HB3	1.97	0.46
23:4:310:CLA:H141	23:4:310:CLA:H162	1.69	0.46
4:7:120:ALA:O	4:7:124:ILE:HG13	2.16	0.46
23:1:306:CLA:H91	23:1:306:CLA:H112	1.69	0.46
23:a:801:CLA:CED	23:a:801:CLA:HAA2	2.46	0.46
28:a:853:LMG:H112	28:a:853:LMG:HC92	1.98	0.46
10:b:143:LEU:HD23	10:b:146:LEU:HD12	1.97	0.46
10:b:372:HIS:HB2	23:b:827:CLA:C1B	2.45	0.46
10:b:392:PHE:CE2	30:b:845:BCR:HC42	2.51	0.46
23:b:825:CLA:HAA2	23:b:826:CLA:OBD	2.16	0.46
23:b:827:CLA:H61	23:b:827:CLA:H102	1.85	0.46
30:b:843:BCR:H15C	30:b:843:BCR:H351	1.78	0.46
14:h:112:ILE:O	14:h:115:GLY:N	2.49	0.46
30:j:104:BCR:H341	30:j:104:BCR:H11C	1.72	0.46
23:9:316:CLA:H71	17:l:83:LEU:HG	1.97	0.46
3:8:83:CYS:HB3	3:8:177:GLY:HA3	1.97	0.46
21:6:302:XAT:H31	21:6:302:XAT:H391	1.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:105:PRO:C	8:1:107:LYS:H	2.24	0.46
23:1:306:CLA:H202	23:1:306:CLA:H162	1.69	0.46
10:b:339:LEU:O	10:b:343:THR:HG22	2.16	0.46
10:b:678:GLU:HG2	20:c:81:TYR:HE1	1.81	0.46
15:i:28:LEU:O	15:i:32:LYS:HG3	2.15	0.46
30:i:101:BCR:H351	30:i:101:BCR:H15C	1.85	0.46
1:5:143:TYR:OH	23:5:310:CLA:OBD	2.23	0.45
22:9:306:A1L1G:C31	23:9:310:CLA:HBD	2.46	0.45
9:a:282:LEU:HD21	9:a:367:MET:HB3	1.98	0.45
10:b:385:PHE:HB3	10:b:536:LEU:HB3	1.97	0.45
20:c:3:HIS:HB2	20:c:48:CYS:SG	2.56	0.45
26:9:307:LHG:H341	17:l:91:ILE:HD11	1.96	0.45
3:8:166:MET:O	3:8:170:GLU:HG3	2.16	0.45
23:b:832:CLA:H18	30:f:804:BCR:H17C	1.97	0.45
23:h:204:CLA:H2A	23:h:204:CLA:HED3	1.97	0.45
21:4:303:XAT:H11	21:4:303:XAT:H191	1.74	0.45
23:4:311:CLA:H2A	23:4:311:CLA:O2D	2.16	0.45
10:b:26:ALA:HB1	27:b:848:DGD:O1B	2.17	0.45
23:b:838:CLA:H12	30:l:205:BCR:H15C	1.98	0.45
14:h:65:ILE:O	14:h:123:GLN:NE2	2.49	0.45
9:a:38:THR:HB	9:a:710:ARG:HG3	1.97	0.45
9:a:114:ILE:O	9:a:117:GLN:HG2	2.16	0.45
23:b:822:CLA:HHC	23:b:840:CLA:HED1	1.98	0.45
13:f:119:GLY:HA3	13:f:160:TRP:CE2	2.51	0.45
21:5:301:XAT:H35	21:5:301:XAT:H401	1.77	0.45
3:8:58:PHE:HZ	3:8:175:LYS:HZ1	1.64	0.45
3:8:93:TRP:CE2	3:8:111:PRO:HG2	2.51	0.45
23:8:308:CLA:HBA1	23:8:308:CLA:H11	1.78	0.45
4:4:37:SER:HB3	4:4:45:ARG:HA	1.98	0.45
7:2:127:ASN:OD1	7:2:130:GLN:N	2.46	0.45
4:7:160:PHE:HE2	21:7:304:XAT:H373	1.81	0.45
23:a:827:CLA:H13	23:a:827:CLA:H172	1.77	0.45
23:b:813:CLA:H141	23:b:813:CLA:H161	1.77	0.45
2:9:80:ALA:O	2:9:84:ASN:ND2	2.49	0.45
21:4:303:XAT:H15	21:4:303:XAT:H201	1.82	0.45
6:6:132:PHE:O	6:6:136:ILE:HG12	2.17	0.45
21:6:305:XAT:H31	21:6:305:XAT:H391	1.69	0.45
21:7:304:XAT:H32	23:7:313:CLA:HAB	1.98	0.45
21:7:304:XAT:H171	23:7:315:CLA:HBB1	1.99	0.45
9:a:665:ILE:HG23	23:a:809:CLA:H171	1.99	0.45
10:b:433:PHE:HZ	30:f:801:BCR:H372	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:j:26:VAL:CG1	30:j:104:BCR:H403	2.47	0.45
3:8:138:LEU:HB2	23:8:311:CLA:HMA1	1.99	0.45
21:3:305:XAT:H35	21:3:305:XAT:H401	1.77	0.45
21:6:305:XAT:H15	21:6:305:XAT:H201	1.87	0.45
21:2:301:XAT:H15	21:2:301:XAT:H201	1.77	0.45
4:7:78:ILE:HG12	4:7:175:LEU:HD21	1.99	0.45
9:a:71:PHE:HD1	9:a:166:MET:HE3	1.82	0.45
9:a:342:TRP:CD1	23:a:826:CLA:H192	2.51	0.45
9:a:686:TYR:CE1	10:b:538:LYS:HD2	2.52	0.45
23:a:820:CLA:H3A	23:a:820:CLA:HBA2	1.48	0.45
23:a:829:CLA:HBB1	23:a:829:CLA:HMB1	1.97	0.45
10:b:585:MET:HE3	10:b:585:MET:HB3	1.83	0.45
13:f:153:ILE:O	13:f:156:SER:OG	2.31	0.45
21:5:304:XAT:H15	21:5:304:XAT:H201	1.76	0.45
23:9:308:CLA:H93	23:9:308:CLA:H111	1.70	0.45
4:4:193:ALA:HB1	27:4:318:DGD:O5E	2.16	0.45
23:4:308:CLA:H192	23:4:308:CLA:H161	1.77	0.45
23:4:310:CLA:H142	23:4:310:CLA:H112	1.79	0.45
23:a:806:CLA:H72	30:a:848:BCR:HC8	1.98	0.45
23:a:854:CLA:H143	28:j:105:LMG:H142	1.97	0.45
10:b:228:TRP:HZ3	30:h:202:BCR:H363	1.81	0.45
10:b:268:LEU:HD23	10:b:271:MET:HE3	1.98	0.45
15:i:14:VAL:O	15:i:19:PRO:HD2	2.17	0.45
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.45
1:5:116:GLU:HB2	23:5:307:CLA:C1B	2.46	0.45
21:8:302:XAT:H15	21:8:302:XAT:H201	1.73	0.45
21:4:301:XAT:H11	21:4:301:XAT:H191	1.86	0.45
7:2:131:ALA:HA	7:2:134:VAL:HG12	1.98	0.45
9:a:312:GLY:HA2	23:a:823:CLA:HMD2	1.99	0.45
9:a:502:ALA:HB2	9:a:516:MET:HE2	1.97	0.45
10:b:605:GLN:HE21	10:b:734:LYS:HB3	1.82	0.45
23:b:827:CLA:H143	23:b:827:CLA:H161	1.78	0.45
11:d:83:LYS:HG2	11:d:98:PRO:HG2	1.97	0.45
13:f:160:TRP:CG	13:f:161:PRO:HD3	2.52	0.45
16:j:30:ASN:ND2	23:j:102:CLA:O1A	2.47	0.45
21:4:301:XAT:H15	21:4:301:XAT:H201	1.80	0.45
7:2:125:GLY:O	7:2:127:ASN:N	2.44	0.45
9:a:580:SER:HB2	9:a:582:TRP:H	1.82	0.45
23:b:822:CLA:H42	14:h:62:LEU:HD11	1.97	0.45
23:b:823:CLA:HHB	23:b:840:CLA:O1D	2.16	0.45
2:9:93:ILE:CG1	21:9:304:XAT:H8	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:303:XAT:H15	21:6:303:XAT:H201	1.65	0.44
8:1:89:VAL:O	8:1:93:TRP:N	2.49	0.44
9:a:447:GLY:HA3	23:a:835:CLA:HAB	1.99	0.44
23:a:813:CLA:H62	23:a:813:CLA:H41	1.85	0.44
30:a:847:BCR:H11C	30:a:847:BCR:H341	1.84	0.44
14:h:72:PRO:CG	25:h:203:A1L1F:C56	2.96	0.44
21:8:301:XAT:H35	21:8:301:XAT:H401	1.78	0.44
4:7:170:MET:HE2	23:7:313:CLA:H12	1.99	0.44
21:7:301:XAT:H31	21:7:301:XAT:H391	1.79	0.44
21:7:303:XAT:H31	21:7:303:XAT:H391	1.73	0.44
21:1:303:XAT:H183	23:1:308:CLA:C2B	2.47	0.44
9:a:25:PRO:HB2	9:a:41:TRP:HH2	1.81	0.44
9:a:407:VAL:HG11	9:a:564:PHE:N	2.32	0.44
23:a:833:CLA:H72	23:l:203:CLA:H12	2.00	0.44
14:h:107:SER:O	14:h:110:THR:OG1	2.32	0.44
1:5:164:PHE:HE1	23:f:802:CLA:H121	1.81	0.44
26:9:317:LHG:H291	26:9:317:LHG:H321	1.65	0.44
4:7:112:HIS:O	4:7:116:VAL:HG13	2.18	0.44
9:a:532:HIS:CE1	9:a:599:VAL:HA	2.53	0.44
10:b:526:ALA:O	10:b:530:HIS:ND1	2.37	0.44
30:l:205:BCR:H15C	30:l:205:BCR:H351	1.74	0.44
2:9:73:GLY:O	2:9:77:SER:OG	2.23	0.44
21:9:305:XAT:H31	21:9:305:XAT:H391	1.83	0.44
4:4:170:MET:CE	23:4:313:CLA:H12	2.47	0.44
5:3:189:GLU:HB2	23:3:313:CLA:C1B	2.47	0.44
21:2:305:XAT:H35	21:2:305:XAT:H401	1.74	0.44
4:7:85:MET:HE3	4:7:177:ASN:HB3	1.98	0.44
23:a:826:CLA:HMB3	23:a:826:CLA:HBB1	1.99	0.44
10:b:201:ARG:HG2	10:b:248:SER:HB2	1.99	0.44
10:b:280:VAL:HG21	23:b:816:CLA:HAB	1.98	0.44
10:b:302:ILE:HD13	23:b:822:CLA:HMD2	1.99	0.44
1:5:106:PHE:HB2	13:f:148:PRO:HG3	1.99	0.44
2:9:126:THR:OG1	2:9:129:GLU:OE2	2.34	0.44
3:8:47:PRO:HG2	3:8:50:LEU:HG	2.00	0.44
7:2:118:LEU:HB2	7:2:123:TYR:HD2	1.83	0.44
9:a:304:MET:HG3	23:a:823:CLA:C3C	2.47	0.44
23:a:804:CLA:H41	23:a:841:CLA:HMC1	1.98	0.44
23:a:840:CLA:H152	23:a:840:CLA:H112	1.80	0.44
10:b:343:THR:HG23	10:b:377:ALA:HB2	2.00	0.44
30:b:842:BCR:H11C	30:b:842:BCR:H341	1.74	0.44
2:9:153:PHE:CG	17:l:151:PHE:HE2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:9:316:CLA:HBB1	23:9:316:CLA:HMB3	1.99	0.44
21:8:301:XAT:H382	23:8:312:CLA:HAC2	1.99	0.44
6:6:121:GLU:OE2	23:6:308:CLA:C1B	2.65	0.44
4:7:77:GLU:HB2	23:7:308:CLA:CHB	2.48	0.44
4:7:185:PHE:CE1	21:7:303:XAT:H162	2.53	0.44
23:a:835:CLA:H61	30:l:201:BCR:H363	1.99	0.44
10:b:172:ARG:HD2	23:b:824:CLA:OBD	2.18	0.44
10:b:259:PHE:CZ	10:b:510:LEU:HD12	2.52	0.44
10:b:654:PHE:O	10:b:658:VAL:HG23	2.17	0.44
13:f:79:ARG:O	13:f:83:SER:HB2	2.17	0.44
17:l:116:VAL:HG11	17:l:128:LEU:C	2.43	0.44
1:5:124:MET:HE3	23:5:312:CLA:HMC2	1.98	0.44
2:9:120:TRP:CD1	2:9:121:VAL:HG13	2.53	0.44
23:9:316:CLA:H112	23:9:318:CLA:HAB	1.99	0.44
3:8:72:LEU:HD13	23:8:307:CLA:HED1	1.99	0.44
21:8:303:XAT:H201	21:8:303:XAT:H15	1.72	0.44
21:4:302:XAT:H11	21:4:302:XAT:H191	1.89	0.44
21:4:302:XAT:H401	21:4:302:XAT:H35	1.76	0.44
21:3:301:XAT:H31	21:3:301:XAT:H391	1.83	0.44
6:6:85:PHE:HB3	6:6:93:PRO:HA	1.99	0.44
21:2:304:XAT:H31	21:2:304:XAT:H391	1.85	0.44
28:2:317:LMG:H321	28:2:317:LMG:H292	1.35	0.44
8:1:171:ARG:HA	8:1:174:MET:HE3	2.00	0.44
9:a:367:MET:HG2	9:a:500:SER:HB2	1.99	0.44
9:a:578:GLN:HA	9:a:583:ASP:OD2	2.18	0.44
9:a:683:GLY:HA3	10:b:571:ASP:HB2	1.99	0.44
23:a:822:CLA:H12	23:a:825:CLA:HBA2	1.99	0.44
10:b:518:ASP:O	10:b:522:HIS:ND1	2.38	0.44
14:h:112:ILE:O	14:h:113:SER:C	2.60	0.44
21:5:302:XAT:H383	23:5:309:CLA:C2B	2.48	0.44
2:9:207:VAL:HG21	23:9:308:CLA:H191	1.99	0.44
26:9:307:LHG:H352	15:i:16:LEU:HD22	1.99	0.44
4:4:59:PHE:HE1	23:4:306:CLA:HBC3	1.83	0.44
23:4:306:CLA:CHA	23:4:306:CLA:HBA1	2.48	0.44
8:1:152:VAL:HG11	8:1:159:TRP:CD1	2.53	0.44
9:a:52:PHE:CD2	23:a:806:CLA:HMC2	2.53	0.44
9:a:73:GLN:HG2	23:a:806:CLA:H3A	2.00	0.44
9:a:565:ARG:HD2	26:a:845:LHG:HC61	2.00	0.44
23:a:806:CLA:H141	23:a:806:CLA:H162	1.59	0.44
23:a:829:CLA:H91	23:a:831:CLA:H192	2.00	0.44
23:j:103:CLA:O1D	23:j:103:CLA:H2A	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:144:HIS:CD2	23:9:314:CLA:HBC3	2.53	0.44
9:a:84:MET:SD	23:a:829:CLA:HED1	2.58	0.44
9:a:701:LEU:HD12	23:a:841:CLA:HMA2	2.00	0.44
10:b:83:LYS:HE3	10:b:83:LYS:HB3	1.85	0.44
10:b:647:VAL:HG21	23:b:809:CLA:HAC1	2.00	0.44
23:b:835:CLA:H12	23:b:836:CLA:O1A	2.18	0.44
23:4:309:CLA:H3A	23:4:309:CLA:HBA1	1.77	0.43
5:3:172:PRO:HD2	21:3:305:XAT:H242	2.00	0.43
21:3:301:XAT:H15	21:3:301:XAT:H201	1.79	0.43
23:1:312:CLA:HMA2	24:1:315:SQD:H141	1.99	0.43
9:a:415:ASN:O	9:a:421:ASP:HB2	2.18	0.43
6:6:124:HIS:CB	6:6:231:MET:HE2	2.47	0.43
4:7:36:LYS:HB2	4:7:45:ARG:H	1.83	0.43
21:7:301:XAT:H201	21:7:301:XAT:H15	1.81	0.43
23:7:308:CLA:H142	23:7:308:CLA:H111	1.77	0.43
23:a:834:CLA:H202	23:a:834:CLA:H162	1.79	0.43
30:a:849:BCR:H15C	30:a:849:BCR:H351	1.79	0.43
30:a:849:BCR:H24C	30:a:849:BCR:H371	1.86	0.43
23:b:824:CLA:H62	23:b:824:CLA:H41	1.79	0.43
30:b:845:BCR:H15C	30:b:845:BCR:H351	1.85	0.43
25:9:302:A1L1F:C42	23:9:311:CLA:O1A	2.66	0.43
23:4:310:CLA:C1A	23:4:310:CLA:CGA	2.96	0.43
5:3:121:GLN:HA	5:3:124:VAL:HG12	1.99	0.43
21:2:303:XAT:H35	21:2:303:XAT:H401	1.71	0.43
21:7:304:XAT:H401	21:7:304:XAT:H35	1.74	0.43
9:a:442:GLY:HA3	23:b:804:CLA:O1A	2.18	0.43
20:c:59:PRO:HD2	31:c:102:SF4:S2	2.58	0.43
23:3:310:CLA:H61	23:3:310:CLA:H41	1.86	0.43
8:1:95:PRO:HD2	23:1:308:CLA:HMD3	1.99	0.43
8:1:151:TRP:CH2	17:l:20:PRO:HA	2.54	0.43
23:a:801:CLA:HED2	23:a:801:CLA:HBD	1.48	0.43
23:a:820:CLA:CAD	23:a:830:CLA:H41	2.48	0.43
23:a:822:CLA:OBD	23:a:824:CLA:HMD3	2.19	0.43
10:b:274:HIS:HB2	23:b:817:CLA:CHB	2.49	0.43
23:b:820:CLA:H3A	23:b:820:CLA:HBA2	1.33	0.43
11:d:81:ASN:H	11:d:81:ASN:ND2	2.16	0.43
20:c:25:VAL:HG21	20:c:48:CYS:HA	1.99	0.43
2:9:153:PHE:HA	17:l:151:PHE:CE2	2.51	0.43
2:9:153:PHE:CE2	17:l:155:LEU:HD22	2.53	0.43
26:9:317:LHG:H272	26:9:317:LHG:H302	1.86	0.43
21:8:302:XAT:H191	21:8:302:XAT:H11	1.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:309:CLA:HED2	23:4:309:CLA:HBD	1.83	0.43
6:6:242:PHE:HZ	21:6:305:XAT:H183	1.83	0.43
21:6:306:XAT:H11	21:6:306:XAT:H191	1.89	0.43
8:1:141:ARG:HD3	8:1:149:TRP:HB3	1.99	0.43
8:1:156:ASP:OD2	17:l:2:VAL:N	2.51	0.43
23:b:835:CLA:H51	23:b:835:CLA:H11	1.73	0.43
30:b:849:BCR:H15C	30:b:849:BCR:H351	1.91	0.43
30:j:104:BCR:H15C	30:j:104:BCR:H351	1.78	0.43
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.43
23:9:314:CLA:H2A	23:9:314:CLA:O2D	2.18	0.43
23:a:807:CLA:H43	26:a:845:LHG:H252	2.00	0.43
23:b:816:CLA:CHD	23:b:817:CLA:HBB2	2.49	0.43
23:b:838:CLA:H161	17:l:92:LEU:HD21	1.99	0.43
21:4:304:XAT:H11	21:4:304:XAT:H191	1.90	0.43
25:6:301:A1L1F:C42	23:6:315:CLA:O1D	2.67	0.43
21:7:305:XAT:H191	21:7:305:XAT:H11	1.84	0.43
9:a:75:ALA:HB2	9:a:166:MET:HB2	2.01	0.43
9:a:364:MET:HE1	23:a:830:CLA:CAD	2.49	0.43
23:a:831:CLA:H92	23:a:831:CLA:H61	1.70	0.43
30:a:850:BCR:H15C	30:a:850:BCR:H351	1.77	0.43
10:b:424:LEU:HG	23:b:837:CLA:CBB	2.49	0.43
23:b:813:CLA:H143	23:b:824:CLA:H51	1.99	0.43
14:h:82:SER:O	14:h:86:HIS:ND1	2.27	0.43
23:8:307:CLA:H122	23:8:307:CLA:H161	1.87	0.43
21:3:304:XAT:H12	23:3:309:CLA:HAB	2.01	0.43
8:1:133:LYS:HA	8:1:133:LYS:HD2	1.81	0.43
23:1:306:CLA:H93	23:1:306:CLA:H61	1.70	0.43
23:a:810:CLA:HBB1	30:j:104:BCR:H23C	2.00	0.43
23:a:819:CLA:HBA2	23:a:819:CLA:H3A	1.53	0.43
10:b:207:TRP:HE1	23:b:814:CLA:H11	1.84	0.43
10:b:452:GLU:OE2	13:f:76:ARG:NE	2.42	0.43
10:b:526:ALA:HB2	23:b:836:CLA:HMA1	2.00	0.43
23:b:809:CLA:H143	23:b:809:CLA:H161	1.83	0.43
23:b:812:CLA:H3A	23:b:812:CLA:HBA2	1.61	0.43
11:d:20:TRP:HB2	11:d:24:ALA:HB3	1.99	0.43
11:d:107:VAL:HG21	20:c:38:GLN:HB3	2.01	0.43
21:9:303:XAT:H7	23:9:309:CLA:HAB	2.01	0.43
21:4:304:XAT:H31	21:4:304:XAT:H391	1.92	0.43
21:4:305:XAT:H35	21:4:305:XAT:H401	1.78	0.43
9:a:483:LEU:HD23	9:a:483:LEU:HA	1.87	0.43
9:a:567:PRO:HB3	9:a:714:ILE:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:835:CLA:H141	23:a:835:CLA:H161	1.84	0.43
11:d:70:LEU:O	11:d:74:LEU:HG	2.19	0.43
21:9:303:XAT:H15	21:9:303:XAT:H201	1.71	0.43
21:8:303:XAT:C34	23:8:313:CLA:HBB1	2.49	0.43
6:6:189:TRP:CZ3	21:6:305:XAT:H363	2.53	0.43
21:7:303:XAT:H35	21:7:303:XAT:H401	1.76	0.43
24:1:315:SQD:H311	24:1:315:SQD:H282	1.84	0.43
9:a:361:ALA:HB2	9:a:387:HIS:HB2	2.01	0.43
9:a:517:MET:HE2	9:a:611:VAL:HA	2.00	0.43
10:b:220:LEU:HD21	30:b:842:BCR:H391	2.01	0.43
10:b:440:VAL:HG12	23:j:102:CLA:HAC1	2.01	0.43
23:b:816:CLA:C9	14:h:105:LEU:HG	2.49	0.43
11:d:32:ILE:HG21	11:d:70:LEU:HD23	2.00	0.43
12:e:16:TYR:CD2	12:e:44:ASN:HA	2.54	0.43
13:f:143:ILE:O	16:j:11:ALA:N	2.48	0.43
26:9:317:LHG:HC81	26:9:317:LHG:HC5	1.97	0.42
21:4:301:XAT:H35	21:4:301:XAT:H401	1.66	0.42
4:7:71:SER:HB3	4:7:142:MET:CE	2.49	0.42
21:7:304:XAT:H30	23:7:313:CLA:H71	2.01	0.42
8:1:128:GLU:HG3	21:1:302:XAT:H372	2.01	0.42
8:1:144:ASP:OD2	8:1:148:THR:OG1	2.23	0.42
8:1:171:ARG:HA	8:1:174:MET:CE	2.49	0.42
9:a:357:SER:HB2	23:a:830:CLA:HMC2	2.01	0.42
9:a:555:LEU:HD11	10:b:674:GLN:HB3	2.01	0.42
23:a:807:CLA:H161	23:a:807:CLA:H192	1.82	0.42
23:a:834:CLA:H142	30:b:846:BCR:H17C	2.01	0.42
23:a:844:CLA:C1C	26:a:846:LHG:HC31	2.48	0.42
30:a:850:BCR:H361	30:a:850:BCR:H20C	1.80	0.42
10:b:140:LEU:HD23	10:b:143:LEU:HD12	2.01	0.42
23:b:802:CLA:H122	23:b:802:CLA:H162	1.60	0.42
13:f:114:PHE:HB2	30:f:801:BCR:C32	2.49	0.42
16:j:14:LEU:CD2	28:j:105:LMG:H141	2.49	0.42
2:9:198:VAL:HG12	21:9:304:XAT:H34	2.01	0.42
23:9:318:CLA:HMC2	15:i:17:VAL:HG21	2.01	0.42
3:8:47:PRO:HG3	3:8:61:ASP:HB3	2.01	0.42
4:4:183:LEU:HD11	23:4:308:CLA:HAC1	2.00	0.42
5:3:133:PRO:HB2	21:3:301:XAT:H23	2.00	0.42
4:7:142:MET:C	4:7:144:GLU:H	2.26	0.42
9:a:684:ARG:NH1	9:a:711:ALA:O	2.52	0.42
23:a:823:CLA:CHD	21:a:852:XAT:H183	2.49	0.42
10:b:518:ASP:OD2	10:b:595:TYR:OH	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:682:TRP:NE1	17:l:15:GLY:O	2.43	0.42
23:b:805:CLA:H141	23:b:805:CLA:H162	1.67	0.42
30:h:201:BCR:H24C	30:h:201:BCR:H371	1.87	0.42
23:j:102:CLA:H61	23:j:102:CLA:H41	1.64	0.42
17:l:53:THR:HG22	23:l:202:CLA:C1B	2.49	0.42
23:5:307:CLA:HBC1	21:4:301:XAT:H383	2.01	0.42
2:9:222:ASP:OD1	2:9:227:GLY:HA2	2.19	0.42
5:3:56:ASN:HB3	5:3:82:LEU:HD22	2.01	0.42
7:2:205:PHE:HE1	21:2:303:XAT:H162	1.84	0.42
4:7:81:CYS:SG	4:7:175:LEU:HD23	2.59	0.42
23:a:807:CLA:H92	23:a:807:CLA:H61	1.69	0.42
10:b:529:LEU:HD23	10:b:588:THR:HG21	2.00	0.42
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.42
21:6:302:XAT:H35	21:6:302:XAT:H401	1.74	0.42
21:6:306:XAT:H31	21:6:306:XAT:H391	1.84	0.42
21:7:303:XAT:C36	23:7:308:CLA:H2	2.49	0.42
9:a:143:ALA:HB2	9:a:371:PRO:HD2	2.00	0.42
9:a:680:LEU:HB3	10:b:667:ILE:HG12	2.02	0.42
17:l:96:LEU:HG	30:l:205:BCR:H24C	2.01	0.42
1:5:98:PHE:HE1	23:5:305:CLA:HBC3	1.84	0.42
2:9:217:ILE:HG21	23:9:314:CLA:HHB	2.01	0.42
21:3:303:XAT:H15	21:3:303:XAT:H201	1.79	0.42
21:2:303:XAT:H191	21:2:303:XAT:H11	1.66	0.42
23:7:308:CLA:H91	23:7:308:CLA:H112	1.67	0.42
9:a:194:HIS:HE1	23:a:826:CLA:H72	1.83	0.42
9:a:727:LEU:HD22	23:a:842:CLA:HMA3	2.01	0.42
23:a:803:CLA:O1A	23:a:803:CLA:H3A	2.19	0.42
23:a:807:CLA:H161	23:a:807:CLA:H102	2.00	0.42
23:a:816:CLA:C4B	21:a:852:XAT:H242	2.50	0.42
23:a:840:CLA:H72	30:a:850:BCR:H373	2.00	0.42
20:c:54:CYS:SG	20:c:55:GLU:N	2.91	0.42
1:5:149:VAL:HG22	21:5:304:XAT:H182	2.02	0.42
2:9:120:TRP:HB3	10:b:94:PRO:HA	2.02	0.42
23:9:316:CLA:H2	23:9:316:CLA:H61	1.88	0.42
4:4:85:MET:HE3	4:4:177:ASN:HB3	2.00	0.42
23:2:307:CLA:H3A	23:2:307:CLA:HBA2	1.76	0.42
4:7:87:ALA:HB1	21:7:303:XAT:H161	2.01	0.42
21:7:303:XAT:H362	23:7:308:CLA:H2	2.01	0.42
9:a:342:TRP:HB3	23:a:806:CLA:HAC1	2.02	0.42
9:a:427:ARG:NH2	11:d:46:THR:O	2.53	0.42
9:a:692:GLU:CD	10:b:547:LYS:HB2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:172:ARG:HB2	23:b:813:CLA:HBC2	2.00	0.42
10:b:702:LEU:HD22	10:b:706:GLN:NE2	2.35	0.42
30:j:104:BCR:H24C	30:j:104:BCR:H371	1.85	0.42
30:l:201:BCR:H352	23:l:203:CLA:HAB	2.01	0.42
2:9:91:GLY:HA3	21:9:303:XAT:O4	2.19	0.42
3:8:184:ILE:HG21	21:8:302:XAT:H12	2.01	0.42
23:4:307:CLA:HBD	23:4:314:CLA:OBD	2.20	0.42
21:3:304:XAT:H15	21:3:304:XAT:H201	1.78	0.42
8:1:168:ASN:HA	8:1:171:ARG:HD2	2.01	0.42
9:a:252:LYS:NZ	9:a:264:GLU:OE1	2.41	0.42
9:a:399:ALA:HB1	9:a:543:LEU:HB3	2.02	0.42
10:b:56:ILE:HD11	30:m:101:BCR:HC7	2.02	0.42
10:b:458:GLU:OE1	13:f:94:HIS:ND1	2.46	0.42
10:b:597:HIS:CE1	10:b:727:VAL:HG23	2.54	0.42
30:b:843:BCR:H341	30:b:843:BCR:H11C	1.76	0.42
30:b:844:BCR:H351	30:b:844:BCR:H15C	1.78	0.42
15:i:29:TYR:HE1	18:m:30:ASN:HD21	1.67	0.42
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.42
2:9:217:ILE:HB	23:9:314:CLA:H3A	2.02	0.42
21:4:302:XAT:H31	21:4:302:XAT:H391	1.90	0.42
7:2:203:LEU:HD13	21:2:301:XAT:C10	2.50	0.42
9:a:525:ASP:HA	9:a:528:VAL:HG12	2.01	0.42
23:a:841:CLA:HED3	23:a:841:CLA:H2A	2.01	0.42
10:b:345:LEU:CD1	23:b:826:CLA:HAA1	2.49	0.42
23:b:816:CLA:CBB	30:h:202:BCR:H14C	2.50	0.42
28:j:105:LMG:H122	28:j:105:LMG:H151	1.56	0.42
2:9:173:ASP:O	2:9:174:GLU:C	2.63	0.42
21:9:303:XAT:H35	21:9:303:XAT:H401	1.85	0.42
3:8:172:LYS:HD3	23:8:313:CLA:HAA2	2.01	0.42
5:3:103:ILE:HD11	21:3:304:XAT:H363	2.01	0.42
5:3:188:LYS:O	5:3:192:ASN:ND2	2.45	0.42
21:3:304:XAT:H31	21:3:304:XAT:H391	1.78	0.42
6:6:135:VAL:HG13	21:6:303:XAT:H163	2.02	0.42
4:7:174:GLU:HB2	23:7:313:CLA:C1B	2.50	0.42
22:7:302:A1L1G:O9	23:7:311:CLA:O1A	2.37	0.42
8:1:71:GLU:HG2	8:1:142:PRO:O	2.20	0.42
9:a:67:PHE:HE2	9:a:173:HIS:CG	2.38	0.42
23:a:842:CLA:H12	29:a:843:PQN:H301	2.02	0.42
10:b:676:LEU:O	10:b:679:THR:OG1	2.33	0.42
11:d:88:TYR:HB3	11:d:89:PRO:HD2	2.01	0.42
23:5:314:CLA:H62	23:5:314:CLA:H41	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:138:ALA:O	2:9:142:ILE:HG12	2.20	0.42
23:9:314:CLA:H51	23:9:314:CLA:C1C	2.50	0.42
26:9:317:LHG:H312	18:m:22:ILE:HD12	2.02	0.42
21:6:306:XAT:H35	21:6:306:XAT:H401	1.71	0.42
4:7:79:LYS:HE3	4:7:79:LYS:HB2	1.79	0.42
8:1:82:LEU:HD11	23:1:311:CLA:HBC1	2.01	0.42
9:a:299:ILE:O	9:a:303:HIS:ND1	2.53	0.42
30:b:842:BCR:H20C	30:b:842:BCR:H361	1.92	0.42
14:h:104:VAL:HG22	30:h:202:BCR:H383	2.02	0.42
3:8:42:PRO:HB2	4:7:154:LYS:HB2	2.01	0.41
6:6:115:LYS:HE2	6:6:188:PHE:CE1	2.55	0.41
7:2:109:TRP:CE3	21:2:303:XAT:H22	2.54	0.41
7:2:205:PHE:CD2	21:2:303:XAT:H12	2.54	0.41
23:a:804:CLA:C4D	16:j:12:PRO:HG3	2.50	0.41
23:a:826:CLA:H202	23:a:826:CLA:H162	1.79	0.41
23:b:814:CLA:CHA	23:b:814:CLA:HBA1	2.49	0.41
30:f:804:BCR:H11C	30:f:804:BCR:H341	1.73	0.41
2:9:204:VAL:HG22	23:9:308:CLA:H203	2.01	0.41
21:4:303:XAT:H163	23:4:308:CLA:H2	2.02	0.41
7:2:57:PHE:CZ	21:2:305:XAT:H172	2.56	0.41
9:a:271:PHE:HE2	9:a:495:ALA:HB2	1.84	0.41
23:a:809:CLA:HBA2	23:a:809:CLA:H3A	1.67	0.41
23:a:827:CLA:HBA2	23:a:827:CLA:H3A	1.79	0.41
10:b:197:ILE:HB	10:b:198:PRO:HD3	2.02	0.41
21:5:302:XAT:H11	21:5:302:XAT:H191	1.65	0.41
21:4:305:XAT:H15	21:4:305:XAT:H201	1.71	0.41
21:2:303:XAT:H373	21:2:303:XAT:H23	1.87	0.41
8:1:162:TYR:CE2	23:a:844:CLA:HBD	2.56	0.41
23:1:306:CLA:H3A	23:1:306:CLA:O2A	2.20	0.41
24:1:315:SQD:H161	24:1:315:SQD:H132	1.72	0.41
9:a:293:ALA:HB1	23:a:818:CLA:HBC2	2.03	0.41
23:a:806:CLA:H161	23:a:806:CLA:H202	1.70	0.41
10:b:193:VAL:O	10:b:198:PRO:HD3	2.20	0.41
10:b:301:LEU:HB3	14:h:46:THR:HG21	2.02	0.41
23:b:814:CLA:H2	23:b:814:CLA:H61	1.77	0.41
16:j:12:PRO:HB2	21:j:101:XAT:H21	2.01	0.41
21:j:101:XAT:H31	21:j:101:XAT:H391	1.92	0.41
21:8:302:XAT:H31	21:8:302:XAT:H391	1.88	0.41
23:a:841:CLA:HAA2	23:b:831:CLA:HMB1	2.02	0.41
21:a:852:XAT:H11	21:a:852:XAT:H191	1.91	0.41
10:b:347:ALA:HB3	10:b:374:GLN:HE21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:836:CLA:H102	23:b:836:CLA:H62	1.77	0.41
21:5:302:XAT:H173	21:5:302:XAT:H3	1.86	0.41
21:9:305:XAT:H35	21:9:305:XAT:H401	1.74	0.41
23:9:314:CLA:H41	23:9:314:CLA:H61	1.84	0.41
23:9:318:CLA:H142	23:9:318:CLA:H111	1.61	0.41
23:7:307:CLA:C3D	23:7:314:CLA:HMA3	2.50	0.41
8:1:58:ALA:HB1	8:1:66:LEU:HD21	2.01	0.41
23:a:828:CLA:H122	23:a:828:CLA:H162	1.66	0.41
2:9:83:TRP:O	2:9:87:HIS:ND1	2.51	0.41
25:6:304:A1L1F:C33	23:6:313:CLA:HHC	2.51	0.41
8:1:54:PRO:HD2	21:1:303:XAT:H242	2.02	0.41
8:1:131:GLN:O	8:1:135:LYS:HG3	2.21	0.41
8:1:147:GLY:HA2	8:1:149:TRP:CZ3	2.55	0.41
9:a:601:PHE:CZ	23:a:801:CLA:HED3	2.55	0.41
23:a:805:CLA:HBA1	23:a:805:CLA:H3A	1.89	0.41
23:a:825:CLA:H62	23:a:825:CLA:H41	1.84	0.41
23:a:831:CLA:H93	23:a:842:CLA:HED3	2.01	0.41
30:a:847:BCR:H15C	30:a:847:BCR:H351	1.84	0.41
10:b:381:MET:HE1	30:b:845:BCR:H352	2.02	0.41
23:b:805:CLA:H2	23:b:805:CLA:H61	1.62	0.41
23:b:807:CLA:H161	23:b:807:CLA:H102	2.01	0.41
13:f:114:PHE:HB2	30:f:801:BCR:H321	2.02	0.41
23:5:305:CLA:HAB	4:4:153:PHE:O	2.21	0.41
21:9:305:XAT:H15	21:9:305:XAT:H201	1.81	0.41
21:8:302:XAT:H403	23:8:307:CLA:H202	2.02	0.41
4:4:175:LEU:HD23	4:4:175:LEU:HA	1.87	0.41
9:a:272:LYS:HG2	9:a:496:LEU:HD12	2.02	0.41
9:a:406:PHE:HE2	9:a:424:ILE:HD11	1.86	0.41
23:a:806:CLA:H72	30:a:848:BCR:C8	2.50	0.41
10:b:629:ASN:HA	10:b:734:LYS:HE2	2.02	0.41
10:b:709:LEU:CD1	27:b:848:DGD:HB41	2.51	0.41
23:b:802:CLA:HMA1	23:b:803:CLA:H161	2.02	0.41
23:b:808:CLA:H93	23:b:808:CLA:H61	1.71	0.41
23:b:828:CLA:H3A	23:b:828:CLA:HBA2	1.76	0.41
20:c:32:ASP:OD1	20:c:32:ASP:N	2.53	0.41
2:9:120:TRP:CH2	23:9:318:CLA:H43	2.56	0.41
23:6:317:CLA:H162	23:6:317:CLA:H141	1.77	0.41
21:2:304:XAT:H11	21:2:304:XAT:H191	1.89	0.41
4:7:39:ALA:HB2	4:7:57:VAL:HG23	2.03	0.41
23:7:307:CLA:CAD	23:7:314:CLA:HMA3	2.51	0.41
9:a:290:HIS:O	9:a:294:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:452:ASN:HD22	9:a:634:ILE:HB	1.85	0.41
21:a:852:XAT:H3	21:a:852:XAT:H173	1.83	0.41
10:b:523:HIS:CE1	30:b:849:BCR:H322	2.56	0.41
10:b:626:LEU:HD22	23:b:803:CLA:HMD3	2.01	0.41
30:b:845:BCR:H361	30:b:845:BCR:H20C	1.86	0.41
12:e:51:ASN:ND2	20:c:61:ASP:HB2	2.35	0.41
30:i:101:BCR:H20C	30:i:101:BCR:H361	1.87	0.41
3:8:44:LEU:HD22	4:7:137:ILE:HG22	2.03	0.41
3:8:77:ALA:HB2	3:8:147:PRO:HB2	2.02	0.41
21:8:301:XAT:H15	21:8:301:XAT:H201	1.84	0.41
23:4:317:CLA:HMB3	21:3:301:XAT:H392	2.03	0.41
5:3:106:VAL:HG11	23:3:311:CLA:HED1	2.03	0.41
6:6:237:PHE:CE1	6:6:250:LEU:HD11	2.55	0.41
7:2:97:LYS:NZ	7:2:152:GLU:OE1	2.38	0.41
23:1:311:CLA:H72	17:l:21:ILE:HG12	2.02	0.41
9:a:194:HIS:ND1	23:a:826:CLA:OBD	2.48	0.41
30:a:847:BCR:H361	30:a:847:BCR:H20C	1.80	0.41
10:b:181:PHE:CE2	23:b:819:CLA:HAB	2.56	0.41
10:b:431:LEU:HD11	23:b:836:CLA:HMB1	2.03	0.41
23:b:824:CLA:H92	23:b:824:CLA:H61	1.72	0.41
23:b:840:CLA:H161	23:b:840:CLA:H141	1.74	0.41
23:f:802:CLA:H11	23:j:102:CLA:H122	2.03	0.41
2:9:91:GLY:CA	21:9:303:XAT:H173	2.51	0.41
2:9:185:PRO:HA	23:9:313:CLA:CBA	2.51	0.41
2:9:201:LEU:HD13	23:9:308:CLA:HBC1	2.03	0.41
21:8:303:XAT:H383	23:8:314:CLA:C3B	2.51	0.41
21:4:305:XAT:H363	21:3:301:XAT:C10	2.49	0.41
5:3:97:MET:HG3	5:3:193:GLY:HA2	2.03	0.41
6:6:121:GLU:OE2	23:6:308:CLA:C2B	2.68	0.41
4:7:160:PHE:CE2	21:7:304:XAT:H373	2.56	0.41
8:1:87:TRP:CG	8:1:180:LEU:HD13	2.56	0.41
9:a:215:LEU:HD23	9:a:215:LEU:HA	1.88	0.41
9:a:440:PHE:CE2	23:a:839:CLA:HAB	2.55	0.41
9:a:632:SER:O	9:a:638:GLY:HA3	2.21	0.41
23:a:818:CLA:OBD	23:a:837:CLA:HED2	2.21	0.41
10:b:433:PHE:CZ	30:f:801:BCR:H372	2.56	0.41
23:b:801:CLA:H51	23:b:838:CLA:H102	2.01	0.41
23:b:827:CLA:H13	23:b:829:CLA:H141	2.02	0.41
30:b:842:BCR:H15C	30:b:842:BCR:H351	1.73	0.41
16:j:14:LEU:HD23	16:j:14:LEU:HA	1.83	0.41
23:9:308:CLA:H61	23:9:308:CLA:H92	1.76	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:302:XAT:H8	23:8:309:CLA:HBB1	2.04	0.40
21:3:301:XAT:H35	21:3:301:XAT:H401	1.81	0.40
4:7:59:PHE:HE1	23:7:306:CLA:HBC3	1.85	0.40
9:a:434:LEU:HG	9:a:541:LEU:HB2	2.03	0.40
9:a:586:PHE:CE1	9:a:590:PHE:HE2	2.39	0.40
9:a:741:ILE:HD12	9:a:741:ILE:HA	1.93	0.40
23:a:832:CLA:HBA1	23:a:832:CLA:H3A	1.80	0.40
10:b:86:PRO:HB3	10:b:119:TYR:CD2	2.56	0.40
10:b:314:GLY:HA3	10:b:412:ARG:HD2	2.02	0.40
10:b:342:ALA:HB2	23:b:824:CLA:H43	2.02	0.40
23:b:835:CLA:HBB1	23:b:835:CLA:HMB1	2.02	0.40
30:b:845:BCR:H24C	30:b:845:BCR:H371	1.83	0.40
11:d:27:GLU:O	11:d:89:PRO:HD3	2.21	0.40
30:j:104:BCR:H20C	30:j:104:BCR:H361	1.91	0.40
17:l:56:TYR:CD2	17:l:161:ALA:HB2	2.56	0.40
25:9:302:A1L1F:C28	23:9:310:CLA:HMC1	2.51	0.40
21:2:302:XAT:H11	21:2:302:XAT:H191	1.93	0.40
21:7:301:XAT:H11	21:7:301:XAT:H191	1.91	0.40
23:a:839:CLA:H143	23:a:839:CLA:H111	1.90	0.40
10:b:346:THR:HG21	23:b:828:CLA:HHD	2.03	0.40
10:b:499:TRP:CD1	23:b:833:CLA:HED2	2.57	0.40
10:b:668:SER:OG	10:b:673:TRP:NE1	2.52	0.40
23:b:826:CLA:HED1	30:b:845:BCR:H21C	2.02	0.40
13:f:98:ASP:OD1	13:f:98:ASP:N	2.54	0.40
20:c:64:SER:HB2	31:c:102:SF4:S3	2.62	0.40
1:5:98:PHE:CD2	23:5:305:CLA:HMD2	2.56	0.40
21:9:304:XAT:H35	21:9:304:XAT:H401	1.86	0.40
7:2:92:ARG:NH2	23:2:308:CLA:HED3	2.36	0.40
21:7:303:XAT:H15	21:7:303:XAT:H201	1.78	0.40
8:1:186:ILE:HG13	8:1:187:THR:N	2.36	0.40
9:a:529:HIS:CG	23:a:839:CLA:HED2	2.56	0.40
9:a:535:THR:HB	9:a:595:SER:HB2	2.04	0.40
23:a:826:CLA:HMD2	23:a:826:CLA:H143	2.03	0.40
10:b:500:LEU:HA	10:b:503:ILE:HG22	2.02	0.40
23:b:802:CLA:H93	23:b:802:CLA:H112	1.70	0.40
3:8:90:PHE:CE1	21:8:303:XAT:H30	2.57	0.40
21:3:304:XAT:H401	21:3:304:XAT:H35	1.68	0.40
6:6:137:VAL:HB	6:6:138:PRO:HD3	2.03	0.40
8:1:134:ILE:HD11	17:l:26:PHE:HA	2.03	0.40
23:1:308:CLA:H121	23:1:308:CLA:H8	1.96	0.40
9:a:356:LEU:HB2	23:a:828:CLA:H41	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:826:CLA:HMB2	23:b:833:CLA:HBA1	2.03	0.40
3:8:153:ASP:OD1	21:8:303:XAT:O3	2.28	0.40
23:4:308:CLA:H143	23:4:308:CLA:H112	1.66	0.40
23:3:312:CLA:HBA1	23:3:312:CLA:H3A	1.93	0.40
8:1:48:PRO:HG3	23:1:305:CLA:C4B	2.52	0.40
21:1:302:XAT:H31	21:1:302:XAT:H391	1.88	0.40
9:a:114:ILE:HD12	9:a:114:ILE:HA	1.93	0.40
9:a:318:ILE:O	9:a:322:HIS:ND1	2.54	0.40
9:a:319:LEU:O	9:a:331:HIS:HB2	2.21	0.40
9:a:320:GLU:HG2	9:a:332:LYS:HG3	2.04	0.40
10:b:547:LYS:HE2	13:f:180:ILE:HD11	2.03	0.40
10:b:547:LYS:NZ	12:e:15:SER:O	2.45	0.40
10:b:614:SER:O	10:b:620:GLY:HA3	2.21	0.40
23:b:805:CLA:HHC	23:b:807:CLA:OBD	2.22	0.40
23:b:809:CLA:C4A	23:b:809:CLA:HBA2	2.50	0.40
23:b:828:CLA:H61	23:b:828:CLA:H41	1.75	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	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	24	43
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	21	38
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
6	6	178/259 (69%)	158 (89%)	20 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	7	14
8	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
9	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	71
10	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
11	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
12	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
13	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
14	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	10	20
15	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
16	j	39/41 (95%)	39 (100%)	0	0	100	100
17	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	20
18	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3798/4357 (87%)	3551 (94%)	238 (6%)	9 (0%)	44	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
7	2	45	LYS
17	1	120	VAL
7	2	127	ASN
7	2	213	VAL
9	a	580	SER
17	l	131	ILE
4	4	146	SER
14	h	90	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	133/182 (73%)	133 (100%)	0	100	100
2	9	141/167 (84%)	139 (99%)	2 (1%)	59	75
3	8	132/160 (82%)	131 (99%)	1 (1%)	73	84
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	73	84
5	3	136/164 (83%)	136 (100%)	0	100	100
6	6	135/201 (67%)	134 (99%)	1 (1%)	76	86
7	2	134/172 (78%)	134 (100%)	0	100	100
8	1	128/165 (78%)	128 (100%)	0	100	100
9	a	607/613 (99%)	603 (99%)	4 (1%)	76	86
10	b	599/602 (100%)	599 (100%)	0	100	100
11	d	107/113 (95%)	107 (100%)	0	100	100
12	e	56/62 (90%)	56 (100%)	0	100	100
13	f	138/162 (85%)	138 (100%)	0	100	100
14	h	71/107 (66%)	70 (99%)	1 (1%)	59	75
15	i	32/43 (74%)	32 (100%)	0	100	100
16	j	36/36 (100%)	36 (100%)	0	100	100
17	l	130/141 (92%)	130 (100%)	0	100	100
18	m	21/24 (88%)	21 (100%)	0	100	100
20	c	67/68 (98%)	67 (100%)	0	100	100
All	All	3058/3500 (87%)	3048 (100%)	10 (0%)	84	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	9	172	LYS
2	9	174	GLU
3	8	175	LYS
6	6	246	SER
4	7	95	ASP
9	a	428	ASP
9	a	448	LEU
9	a	579	VAL
9	a	580	SER
14	h	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
3	8	156	ASN
5	3	156	GLN
5	3	169	ASN
6	6	226	ASN
8	1	63	GLN
8	1	119	GLN
8	1	132	ASN
8	1	194	GLN
9	a	127	ASN
9	a	186	ASN
9	a	435	ASN
10	b	80	ASN
10	b	112	ASN
10	b	169	ASN
10	b	326	ASN
10	b	605	GLN
10	b	629	ASN
10	b	706	GLN
11	d	7	GLN
13	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](#)

273 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
23	CLA	6	316	6	50,54,73	1.36	7 (14%)	59,90,113	1.43	4 (6%)
22	A1L1G	5	303	-	40,47,47	1.15	4 (10%)	49,71,71	1.37	7 (14%)
23	CLA	a	836	-	54,58,73	1.32	7 (12%)	64,95,113	1.38	6 (9%)
26	LHG	a	846	23	26,26,48	1.30	5 (19%)	29,32,54	1.18	2 (6%)
23	CLA	a	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.28	5 (6%)
23	CLA	8	313	-	50,54,73	1.38	9 (18%)	59,90,113	1.40	4 (6%)
23	CLA	a	805	23	59,63,73	1.26	6 (10%)	70,101,113	1.35	6 (8%)
23	CLA	5	310	-	50,54,73	1.37	8 (16%)	59,90,113	1.40	4 (6%)
25	A1L1F	9	302	-	52,59,59	1.48	6 (11%)	63,85,85	2.55	20 (31%)
26	LHG	b	847	23	30,30,48	1.38	6 (20%)	33,36,54	1.16	2 (6%)
24	SQD	1	315	-	43,45,54	1.22	3 (6%)	53,56,65	1.13	2 (3%)
30	BCR	1	201	-	41,41,41	0.67	0	56,56,56	1.98	17 (30%)
21	XAT	3	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.55	19 (35%)
23	CLA	a	833	-	59,63,73	1.25	6 (10%)	70,101,113	1.39	8 (11%)
25	A1L1F	6	301	-	52,59,59	1.42	6 (11%)	63,85,85	2.49	21 (33%)
23	CLA	b	829	-	69,73,73	1.20	8 (11%)	82,113,113	1.31	9 (10%)
21	XAT	5	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.60	19 (35%)
23	CLA	9	311	-	50,54,73	1.36	6 (12%)	59,90,113	1.45	5 (8%)
23	CLA	7	310	-	50,54,73	1.37	7 (14%)	59,90,113	1.40	4 (6%)
23	CLA	b	812	-	57,61,73	1.29	8 (14%)	67,98,113	1.35	5 (7%)
23	CLA	9	316	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	8 (9%)
30	BCR	b	846	-	41,41,41	0.69	0	56,56,56	1.80	14 (25%)
23	CLA	b	821	-	55,59,73	1.31	7 (12%)	64,96,113	1.42	7 (10%)
23	CLA	a	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
23	CLA	3	308	-	51,55,73	1.36	8 (15%)	60,91,113	1.42	6 (10%)
23	CLA	9	312	-	50,54,73	1.37	7 (14%)	59,90,113	1.49	5 (8%)
23	CLA	b	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	8 (9%)
23	CLA	5	314	-	56,60,73	1.30	7 (12%)	65,97,113	1.40	5 (7%)
23	CLA	b	817	-	63,67,73	1.23	8 (12%)	74,105,113	1.36	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	j	105	-	32,32,55	1.13	2 (6%)	40,40,63	1.15	4 (10%)
23	CLA	6	311	6	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
29	PQN	a	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.16	4 (9%)
23	CLA	a	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
23	CLA	4	306	4	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
23	CLA	5	309	1	69,73,73	1.17	6 (8%)	82,113,113	1.25	4 (4%)
23	CLA	a	804	-	59,63,73	1.27	8 (13%)	70,101,113	1.41	8 (11%)
23	CLA	a	806	-	69,73,73	1.21	11 (15%)	82,113,113	1.55	12 (14%)
23	CLA	b	818	-	64,68,73	1.22	8 (12%)	76,107,113	1.27	5 (6%)
24	SQD	5	316	23	33,35,54	1.39	3 (9%)	43,46,65	1.31	5 (11%)
23	CLA	6	312	6	55,59,73	1.32	8 (14%)	64,96,113	1.40	6 (9%)
23	CLA	b	830	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
23	CLA	a	814	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
21	XAT	7	304	-	41,47,47	0.94	2 (4%)	54,74,74	2.67	17 (31%)
23	CLA	2	306	-	45,50,73	1.42	8 (17%)	52,85,113	1.39	4 (7%)
23	CLA	a	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.41	7 (10%)
30	BCR	b	842	-	41,41,41	0.64	0	56,56,56	2.31	21 (37%)
23	CLA	7	307	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
27	DGD	b	848	-	58,58,67	1.13	5 (8%)	72,72,81	1.50	10 (13%)
30	BCR	f	804	-	41,41,41	0.69	0	56,56,56	2.05	14 (25%)
26	LHG	a	845	-	47,47,48	1.16	6 (12%)	50,53,54	0.98	2 (4%)
23	CLA	6	313	-	56,60,73	1.30	8 (14%)	65,97,113	1.35	6 (9%)
23	CLA	6	314	-	50,54,73	1.36	7 (14%)	59,90,113	1.43	6 (10%)
22	A1L1G	9	306	-	40,47,47	1.14	5 (12%)	49,71,71	1.44	7 (14%)
23	CLA	1	309	8	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
23	CLA	1	311	-	57,61,73	1.29	8 (14%)	67,98,113	1.36	7 (10%)
30	BCR	i	101	-	41,41,41	0.72	0	56,56,56	2.14	13 (23%)
23	CLA	f	802	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
23	CLA	a	838	-	55,59,73	1.31	8 (14%)	64,96,113	1.41	6 (9%)
23	CLA	6	310	-	56,60,73	1.30	6 (10%)	65,97,113	1.40	6 (9%)
23	CLA	a	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
31	SF4	c	102	-	0,12,12	-	-	-	-	-
23	CLA	3	312	5	63,67,73	1.23	8 (12%)	74,105,113	1.29	4 (5%)
30	BCR	h	202	-	41,41,41	0.67	0	56,56,56	1.90	17 (30%)
23	CLA	b	808	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	2	308	7	58,62,73	1.28	7 (12%)	68,99,113	1.28	6 (8%)
23	CLA	b	824	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
23	CLA	a	809	9	69,73,73	1.15	7 (10%)	82,113,113	1.29	8 (9%)
23	CLA	b	831	-	53,57,73	1.33	6 (11%)	61,93,113	1.39	5 (8%)
23	CLA	4	314	4	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
23	CLA	1	310	8	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
23	CLA	3	310	-	60,64,73	1.25	7 (11%)	71,102,113	1.29	5 (7%)
23	CLA	6	317	-	69,73,73	1.18	6 (8%)	82,113,113	1.33	6 (7%)
23	CLA	a	837	9	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
23	CLA	b	834	-	57,61,73	1.30	8 (14%)	67,98,113	1.36	6 (8%)
30	BCR	m	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.25	6 (10%)
23	CLA	6	307	-	50,54,73	1.37	6 (12%)	59,90,113	1.39	4 (6%)
23	CLA	2	315	-	46,50,73	1.42	8 (17%)	53,85,113	1.38	4 (7%)
23	CLA	4	309	-	54,58,73	1.31	7 (12%)	64,95,113	1.39	5 (7%)
23	CLA	4	315	4	45,49,73	1.43	7 (15%)	54,84,113	1.48	5 (9%)
21	XAT	3	303	-	41,47,47	0.89	2 (4%)	54,74,74	2.61	20 (37%)
30	BCR	a	848	-	41,41,41	0.67	0	56,56,56	1.95	18 (32%)
23	CLA	6	309	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
23	CLA	8	311	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	8 (11%)
21	XAT	2	305	-	41,47,47	0.95	2 (4%)	54,74,74	2.43	17 (31%)
21	XAT	9	303	-	41,47,47	0.95	2 (4%)	54,74,74	2.62	19 (35%)
21	XAT	a	852	-	41,47,47	0.92	2 (4%)	54,74,74	2.71	18 (33%)
23	CLA	a	830	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
23	CLA	a	812	23	66,70,73	1.19	7 (10%)	78,109,113	1.31	5 (6%)
21	XAT	6	302	-	41,47,47	0.92	2 (4%)	54,74,74	2.82	18 (33%)
23	CLA	b	801	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
26	LHG	9	317	-	45,45,48	1.19	6 (13%)	48,51,54	0.96	2 (4%)
21	XAT	9	305	-	41,47,47	1.03	3 (7%)	54,74,74	2.33	16 (29%)
21	XAT	3	304	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	17 (31%)
23	CLA	1	306	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
23	CLA	b	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.25	7 (8%)
23	CLA	b	823	-	57,61,73	1.29	8 (14%)	67,98,113	1.35	6 (8%)
23	CLA	3	314	5	51,55,73	1.36	8 (15%)	60,91,113	1.40	4 (6%)
23	CLA	j	103	16	46,50,73	1.40	7 (15%)	53,85,113	1.48	4 (7%)
23	CLA	b	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	b	844	-	41,41,41	0.66	0	56,56,56	2.10	16 (28%)
23	CLA	7	309	-	50,55,73	1.36	7 (14%)	58,91,113	1.36	5 (8%)
23	CLA	b	805	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
23	CLA	3	307	5	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
23	CLA	b	837	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	6 (7%)
23	CLA	a	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
30	BCR	f	801	-	41,41,41	0.66	0	56,56,56	2.16	15 (26%)
23	CLA	8	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.47	5 (9%)
23	CLA	1	307	-	58,62,73	1.28	8 (13%)	68,99,113	1.36	6 (8%)
30	BCR	b	843	-	41,41,41	0.68	0	56,56,56	1.93	16 (28%)
21	XAT	1	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.53	19 (35%)
23	CLA	7	314	-	49,53,73	1.40	8 (16%)	58,89,113	1.49	5 (8%)
23	CLA	2	307	-	51,55,73	1.36	8 (15%)	60,91,113	1.45	8 (13%)
23	CLA	a	840	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
30	BCR	b	849	-	41,41,41	0.71	0	56,56,56	2.06	13 (23%)
31	SF4	a	851	-	0,12,12	-	-	-	-	-
23	CLA	9	315	2	46,50,73	1.40	6 (13%)	53,85,113	1.42	4 (7%)
30	BCR	a	849	-	41,41,41	0.67	0	56,56,56	2.19	22 (39%)
21	XAT	8	303	-	41,47,47	0.88	2 (4%)	54,74,74	2.66	18 (33%)
23	CLA	a	819	-	58,62,73	1.28	9 (15%)	68,99,113	1.34	5 (7%)
23	CLA	4	307	-	60,64,73	1.27	6 (10%)	71,102,113	1.32	6 (8%)
27	DGD	8	315	23	41,41,67	1.06	2 (4%)	55,55,81	1.12	5 (9%)
21	XAT	2	304	-	41,47,47	0.88	2 (4%)	54,74,74	2.55	20 (37%)
23	CLA	a	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
23	CLA	5	307	1	64,68,73	1.21	7 (10%)	76,107,113	1.28	6 (7%)
21	XAT	6	306	-	41,47,47	0.94	2 (4%)	54,74,74	2.62	19 (35%)
23	CLA	5	306	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
23	CLA	9	310	-	50,54,73	1.36	7 (14%)	59,90,113	1.48	4 (6%)
23	CLA	8	305	3	47,51,73	1.39	7 (14%)	55,86,113	1.45	6 (10%)
23	CLA	b	825	-	68,72,73	1.18	8 (11%)	80,111,113	1.30	8 (10%)
23	CLA	1	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.47	5 (9%)
23	CLA	a	820	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
21	XAT	4	303	-	41,47,47	0.92	2 (4%)	54,74,74	2.58	17 (31%)
29	PQN	b	841	-	34,34,34	1.58	2 (5%)	43,45,45	1.24	5 (11%)
23	CLA	b	833	-	69,73,73	1.18	6 (8%)	82,113,113	1.24	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	A1L1G	3	306	-	40,47,47	1.17	4 (10%)	49,71,71	1.41	8 (16%)
23	CLA	7	306	4	52,56,73	1.36	7 (13%)	61,92,113	1.37	5 (8%)
25	A1L1F	h	203	-	52,59,59	1.47	6 (11%)	63,85,85	2.59	22 (34%)
23	CLA	a	802	-	62,66,73	1.22	9 (14%)	73,104,113	1.35	7 (9%)
23	CLA	9	309	2	50,54,73	1.36	8 (16%)	59,90,113	1.36	5 (8%)
21	XAT	4	305	-	41,47,47	0.92	2 (4%)	54,74,74	2.75	18 (33%)
23	CLA	a	839	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	h	204	-	59,63,73	1.27	7 (11%)	70,101,113	1.34	7 (10%)
23	CLA	8	312	3	56,60,73	1.29	7 (12%)	65,97,113	1.38	5 (7%)
21	XAT	3	305	-	41,47,47	0.89	2 (4%)	54,74,74	2.58	18 (33%)
23	CLA	2	311	-	62,66,73	1.24	7 (11%)	73,104,113	1.28	5 (6%)
23	CLA	4	310	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	5 (6%)
23	CLA	3	309	5	60,64,73	1.25	7 (11%)	71,102,113	1.30	5 (7%)
23	CLA	3	315	5	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
21	XAT	5	304	-	41,47,47	0.86	2 (4%)	54,74,74	2.85	20 (37%)
23	CLA	a	841	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
23	CLA	4	308	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	7 (8%)
23	CLA	b	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.23	5 (6%)
30	BCR	l	205	-	41,41,41	0.65	0	56,56,56	2.04	15 (26%)
23	CLA	b	806	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
23	CLA	5	313	1	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
23	CLA	a	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
23	CLA	6	315	6	45,49,73	1.44	8 (17%)	54,84,113	1.48	5 (9%)
23	CLA	b	802	-	69,73,73	1.16	6 (8%)	82,113,113	1.18	5 (6%)
23	CLA	9	308	2	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
22	A1L1G	7	302	-	40,47,47	1.14	3 (7%)	49,71,71	1.41	8 (16%)
23	CLA	l	204	-	50,54,73	1.36	9 (18%)	59,90,113	1.40	4 (6%)
21	XAT	7	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	19 (35%)
23	CLA	b	822	-	64,68,73	1.21	7 (10%)	76,107,113	1.26	5 (6%)
23	CLA	5	311	-	55,59,73	1.30	7 (12%)	64,96,113	1.37	7 (10%)
23	CLA	5	315	-	50,54,73	1.36	7 (14%)	59,90,113	1.41	4 (6%)
23	CLA	b	813	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
23	CLA	2	313	7	45,49,73	1.43	7 (15%)	54,84,113	1.50	5 (9%)
25	A1L1F	1	304	-	52,59,59	1.40	6 (11%)	63,85,85	2.26	18 (28%)
23	CLA	7	312	-	52,56,73	1.34	7 (13%)	61,92,113	1.38	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	XAT	1	302	-	41,47,47	0.91	2 (4%)	54,74,74	2.61	18 (33%)
31	SF4	c	101	-	0,12,12	-	-	-		
23	CLA	b	820	-	54,58,73	1.31	7 (12%)	64,95,113	1.44	7 (10%)
23	CLA	9	318	-	66,70,73	1.21	8 (12%)	78,109,113	1.27	6 (7%)
21	XAT	4	301	-	41,47,47	0.95	2 (4%)	54,74,74	2.63	19 (35%)
23	CLA	a	810	9	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
23	CLA	2	316	7	50,54,73	1.37	8 (16%)	59,90,113	1.40	4 (6%)
23	CLA	2	310	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
23	CLA	b	815	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
23	CLA	a	829	-	66,70,73	1.19	6 (9%)	78,109,113	1.24	7 (8%)
25	A1L1F	8	304	-	52,59,59	1.40	5 (9%)	63,85,85	2.75	23 (36%)
23	CLA	4	317	-	59,63,73	1.28	8 (13%)	70,101,113	1.34	5 (7%)
22	A1L1G	1	301	-	40,47,47	1.14	5 (12%)	49,71,71	1.46	10 (20%)
23	CLA	b	836	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	b	839	-	69,73,73	1.18	7 (10%)	82,113,113	1.32	6 (7%)
30	BCR	a	847	-	41,41,41	0.67	0	56,56,56	1.95	16 (28%)
21	XAT	2	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.72	18 (33%)
23	CLA	1	305	-	65,69,73	1.21	8 (12%)	77,108,113	1.28	4 (5%)
21	XAT	4	304	-	41,47,47	0.90	2 (4%)	54,74,74	2.57	19 (35%)
21	XAT	7	303	-	41,47,47	0.99	2 (4%)	54,74,74	2.60	18 (33%)
23	CLA	8	310	-	50,54,73	1.37	8 (16%)	59,90,113	1.39	5 (8%)
23	CLA	7	315	4	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
22	A1L1G	9	301	-	40,47,47	1.16	5 (12%)	49,71,71	1.48	9 (18%)
23	CLA	5	308	-	59,63,73	1.27	7 (11%)	70,101,113	1.35	6 (8%)
28	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.17	3 (7%)
23	CLA	7	316	-	55,59,73	1.31	7 (12%)	64,96,113	1.44	7 (10%)
23	CLA	9	314	-	59,63,73	1.26	7 (11%)	70,101,113	1.34	6 (8%)
21	XAT	j	101	-	41,47,47	0.86	2 (4%)	54,74,74	2.74	18 (33%)
21	XAT	8	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.55	18 (33%)
23	CLA	a	811	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	6 (8%)
21	XAT	7	305	-	41,47,47	0.86	2 (4%)	54,74,74	2.65	19 (35%)
23	CLA	5	312	-	56,60,73	1.30	8 (14%)	65,97,113	1.39	6 (9%)
23	CLA	a	823	-	53,57,73	1.32	7 (13%)	61,93,113	1.42	6 (9%)
23	CLA	a	813	-	58,62,73	1.28	6 (10%)	68,99,113	1.31	5 (7%)
30	BCR	h	201	-	41,41,41	0.66	0	56,56,56	1.99	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	9	313	2	50,54,73	1.37	6 (12%)	59,90,113	1.47	4 (6%)
21	XAT	4	302	-	41,47,47	0.90	2 (4%)	54,74,74	2.59	19 (35%)
23	CLA	a	808	-	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
23	CLA	a	824	-	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
23	CLA	a	825	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	5 (7%)
23	CLA	b	811	-	58,62,73	1.35	9 (15%)	71,100,113	1.34	7 (9%)
23	CLA	4	316	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	4 (6%)
23	CLA	b	832	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
23	CLA	2	309	-	50,54,73	1.36	7 (14%)	59,90,113	1.40	4 (6%)
23	CLA	b	840	26	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
23	CLA	7	313	-	58,62,73	1.29	7 (12%)	68,99,113	1.35	6 (8%)
23	CLA	6	308	-	62,66,73	1.26	7 (11%)	73,104,113	1.30	4 (5%)
23	CLA	7	317	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
23	CLA	a	831	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
23	CLA	a	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
23	CLA	8	308	-	59,63,73	1.28	8 (13%)	70,101,113	1.35	8 (11%)
23	CLA	4	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	5 (8%)
26	LHG	9	307	-	35,35,48	1.27	6 (17%)	38,41,54	0.91	2 (5%)
23	CLA	8	309	-	61,65,73	1.25	7 (11%)	72,103,113	1.33	6 (8%)
23	CLA	a	815	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
22	A1L1G	3	302	-	40,47,47	1.16	5 (12%)	49,71,71	1.32	7 (14%)
23	CLA	b	827	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
21	XAT	6	303	-	41,47,47	0.91	2 (4%)	54,74,74	2.67	18 (33%)
30	BCR	b	845	-	41,41,41	0.65	0	56,56,56	2.22	22 (39%)
23	CLA	a	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
23	CLA	b	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	5 (6%)
25	A1L1F	6	304	-	48,55,59	1.43	5 (10%)	59,81,85	2.48	21 (35%)
28	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
23	CLA	1	312	8	56,60,73	1.32	7 (12%)	65,97,113	1.36	5 (7%)
23	CLA	a	818	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	7 (9%)
23	CLA	b	816	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	6 (8%)
23	CLA	b	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
21	XAT	5	302	-	41,47,47	0.95	2 (4%)	54,74,74	2.59	19 (35%)
21	XAT	6	305	-	41,47,47	0.89	2 (4%)	54,74,74	2.74	18 (33%)
23	CLA	1	203	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	2	312	-	51,55,73	1.36	8 (15%)	60,91,113	1.40	5 (8%)
23	CLA	4	313	-	57,61,73	1.29	7 (12%)	67,98,113	1.32	7 (10%)
21	XAT	9	304	-	41,47,47	0.96	2 (4%)	54,74,74	2.43	18 (33%)
23	CLA	7	308	-	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)
23	CLA	b	809	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
23	CLA	b	838	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
30	BCR	j	104	-	41,41,41	0.68	0	56,56,56	2.09	17 (30%)
23	CLA	3	311	-	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
23	CLA	1	314	-	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
21	XAT	8	302	-	41,47,47	0.94	2 (4%)	54,74,74	2.67	18 (33%)
23	CLA	1	308	8	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	f	803	13	56,60,73	1.30	8 (14%)	65,97,113	1.37	5 (7%)
23	CLA	8	307	3	69,73,73	1.17	6 (8%)	82,113,113	1.25	5 (6%)
23	CLA	2	314	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	4 (5%)
23	CLA	a	832	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
23	CLA	b	835	-	62,66,73	1.24	7 (11%)	73,104,113	1.37	8 (10%)
23	CLA	a	821	-	49,53,73	1.38	7 (14%)	58,89,113	1.46	4 (6%)
23	CLA	j	102	-	62,66,73	1.24	7 (11%)	73,104,113	1.30	5 (6%)
23	CLA	l	202	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
23	CLA	8	306	27	50,54,73	1.36	7 (14%)	59,90,113	1.39	4 (6%)
23	CLA	b	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
23	CLA	a	817	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
23	CLA	a	844	26	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
23	CLA	4	312	-	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
30	BCR	a	850	-	41,41,41	0.69	0	56,56,56	2.17	14 (25%)
23	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
21	XAT	2	303	-	41,47,47	1.01	2 (4%)	54,74,74	2.63	17 (31%)
23	CLA	b	814	-	59,63,73	1.27	6 (10%)	70,101,113	1.40	8 (11%)
27	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.79	6 (10%)
23	CLA	3	313	-	56,60,73	1.30	8 (14%)	65,97,113	1.38	6 (9%)
23	CLA	5	305	1	50,54,73	1.37	7 (14%)	59,90,113	1.39	4 (6%)
23	CLA	a	834	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
21	XAT	2	302	-	41,47,47	0.93	2 (4%)	54,74,74	2.52	18 (33%)
23	CLA	7	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	5 (8%)

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
23	CLA	6	316	6	1/1/11/20	9/17/93/115	-
23	CLA	a	836	-	1/1/12/20	8/21/97/115	-
22	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
21	XAT	2	302	-	-	0/31/93/93	0/4/4/4
23	CLA	a	801	-	1/1/15/20	22/39/115/115	-
26	LHG	a	846	23	-	15/31/31/53	-
23	CLA	8	313	-	1/1/11/20	5/17/93/115	-
23	CLA	a	805	23	1/1/13/20	6/27/103/115	-
23	CLA	5	310	-	1/1/11/20	8/17/93/115	-
25	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
26	LHG	b	847	23	-	20/35/35/53	-
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
30	BCR	1	201	-	-	4/29/63/63	0/2/2/2
21	XAT	3	301	-	-	3/31/93/93	0/4/4/4
23	CLA	a	833	-	1/1/13/20	2/27/103/115	-
25	A1L1F	6	301	-	-	10/43/99/99	0/3/3/3
23	CLA	b	829	-	1/1/15/20	11/39/115/115	-
21	XAT	5	301	-	-	3/31/93/93	0/4/4/4
23	CLA	9	311	-	1/1/11/20	6/17/93/115	-
23	CLA	7	310	-	1/1/11/20	6/17/93/115	-
23	CLA	b	812	-	1/1/12/20	5/25/101/115	-
23	CLA	9	316	-	1/1/15/20	16/39/115/115	-
30	BCR	b	846	-	-	2/29/63/63	0/2/2/2
23	CLA	b	821	-	1/1/12/20	4/23/99/115	-
23	CLA	a	807	-	1/1/15/20	18/39/115/115	-
23	CLA	3	308	-	1/1/11/20	7/18/94/115	-
23	CLA	9	312	-	1/1/11/20	7/17/93/115	-
23	CLA	b	804	-	1/1/15/20	7/39/115/115	-
23	CLA	5	314	-	1/1/12/20	4/24/100/115	-
23	CLA	b	817	-	1/1/13/20	11/32/108/115	-
28	LMG	j	105	-	-	11/27/47/70	0/1/1/1
23	CLA	6	311	6	1/1/10/20	5/12/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	CLA	a	803	-	1/1/15/20	3/39/115/115	-
23	CLA	4	306	4	1/1/11/20	9/15/91/115	-
23	CLA	5	309	1	1/1/15/20	10/39/115/115	-
23	CLA	a	804	-	1/1/13/20	9/27/103/115	-
23	CLA	a	806	-	1/1/15/20	11/39/115/115	-
23	CLA	b	818	-	1/1/14/20	15/33/109/115	-
24	SQD	5	316	23	-	11/30/50/69	0/1/1/1
23	CLA	6	312	6	1/1/12/20	4/23/99/115	-
23	CLA	b	830	-	1/1/10/20	2/10/86/115	-
23	CLA	a	814	-	1/1/15/20	19/39/115/115	-
23	CLA	2	306	-	1/1/10/20	4/11/87/115	-
21	XAT	7	304	-	-	6/31/93/93	0/4/4/4
23	CLA	a	816	-	1/1/12/20	4/21/97/115	-
30	BCR	b	842	-	-	2/29/63/63	0/2/2/2
23	CLA	7	307	-	1/1/11/20	6/15/91/115	-
27	DGD	b	848	-	-	20/46/86/95	0/2/2/2
30	BCR	f	804	-	-	4/29/63/63	0/2/2/2
26	LHG	a	845	-	-	26/52/52/53	-
23	CLA	6	313	-	1/1/12/20	2/24/100/115	-
23	CLA	6	314	-	1/1/11/20	4/17/93/115	-
23	CLA	1	309	8	1/1/11/20	7/17/93/115	-
22	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
23	CLA	1	311	-	1/1/12/20	4/25/101/115	-
30	BCR	i	101	-	-	3/29/63/63	0/2/2/2
23	CLA	f	802	-	1/1/15/20	13/39/115/115	-
23	CLA	a	838	-	1/1/12/20	6/23/99/115	-
23	CLA	6	310	-	1/1/12/20	6/24/100/115	-
23	CLA	a	828	-	1/1/15/20	8/39/115/115	-
31	SF4	c	102	-	-	-	0/6/5/5
23	CLA	3	312	5	1/1/13/20	10/32/108/115	-
30	BCR	h	202	-	-	0/29/63/63	0/2/2/2
23	CLA	b	808	-	1/1/15/20	11/39/115/115	-
23	CLA	2	308	7	1/1/12/20	3/26/102/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	824	-	1/1/15/20	15/39/115/115	-
23	CLA	a	809	9	1/1/15/20	15/39/115/115	-
23	CLA	b	831	-	1/1/11/20	5/20/96/115	-
23	CLA	4	314	4	1/1/11/20	6/15/91/115	-
23	CLA	1	310	8	1/1/15/20	17/39/115/115	-
23	CLA	3	310	-	1/1/13/20	3/29/105/115	-
23	CLA	6	317	-	1/1/15/20	9/39/115/115	-
23	CLA	a	837	9	1/1/11/20	4/15/91/115	-
23	CLA	b	834	-	1/1/12/20	9/25/101/115	-
30	BCR	m	101	-	-	8/29/63/63	0/2/2/2
23	CLA	6	307	-	1/1/11/20	3/17/93/115	-
23	CLA	2	315	-	1/1/10/20	3/12/88/115	-
23	CLA	4	309	-	1/1/12/20	4/21/97/115	-
23	CLA	4	315	4	1/1/10/20	6/10/86/115	-
21	XAT	3	303	-	-	3/31/93/93	0/4/4/4
30	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	CLA	6	309	-	1/1/15/20	10/39/115/115	-
23	CLA	8	311	-	1/1/13/20	7/29/105/115	-
21	XAT	2	305	-	-	2/31/93/93	0/4/4/4
21	XAT	9	303	-	-	4/31/93/93	0/4/4/4
21	XAT	a	852	-	-	7/31/93/93	0/4/4/4
23	CLA	a	830	-	1/1/15/20	13/39/115/115	-
23	CLA	a	812	23	1/1/14/20	9/36/112/115	-
23	CLA	b	801	-	1/1/15/20	20/39/115/115	-
21	XAT	6	302	-	-	7/31/93/93	0/4/4/4
26	LHG	9	317	-	-	28/50/50/53	-
23	CLA	1	306	-	1/1/15/20	15/39/115/115	-
21	XAT	9	305	-	-	3/31/93/93	0/4/4/4
23	CLA	j	103	16	1/1/10/20	7/12/88/115	-
23	CLA	b	803	-	1/1/15/20	17/39/115/115	-
23	CLA	b	823	-	1/1/12/20	6/25/101/115	-
23	CLA	3	314	5	1/1/11/20	8/18/94/115	-
21	XAT	3	304	-	-	3/31/93/93	0/4/4/4
23	CLA	b	810	-	1/1/15/20	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	b	844	-	-	6/29/63/63	0/2/2/2
23	CLA	7	309	-	1/1/11/20	5/17/93/115	-
23	CLA	b	805	-	1/1/15/20	11/39/115/115	-
23	CLA	3	307	5	1/1/11/20	2/15/91/115	-
23	CLA	b	837	-	1/1/15/20	9/39/115/115	-
23	CLA	a	822	-	1/1/15/20	5/39/115/115	-
30	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	CLA	8	314	-	1/1/10/20	6/10/86/115	-
23	CLA	1	307	-	1/1/12/20	5/26/102/115	-
30	BCR	b	843	-	-	2/29/63/63	0/2/2/2
21	XAT	1	303	-	-	0/31/93/93	0/4/4/4
23	CLA	7	314	-	1/1/11/20	5/15/91/115	-
23	CLA	2	307	-	1/1/11/20	7/18/94/115	-
23	CLA	a	840	-	1/1/15/20	7/39/115/115	-
30	BCR	b	849	-	-	4/29/63/63	0/2/2/2
31	SF4	a	851	-	-	-	0/6/5/5
23	CLA	9	315	2	1/1/10/20	5/12/88/115	-
30	BCR	a	849	-	-	0/29/63/63	0/2/2/2
21	XAT	8	303	-	-	0/31/93/93	0/4/4/4
23	CLA	a	819	-	1/1/12/20	6/26/102/115	-
23	CLA	4	307	-	1/1/13/20	9/29/105/115	-
27	DGD	8	315	23	-	10/29/69/95	0/2/2/2
23	CLA	a	826	-	1/1/15/20	8/39/115/115	-
21	XAT	2	304	-	-	3/31/93/93	0/4/4/4
23	CLA	5	307	1	1/1/14/20	5/33/109/115	-
23	CLA	8	305	3	1/1/10/20	2/13/89/115	-
23	CLA	5	306	24	1/1/11/20	8/15/91/115	-
23	CLA	9	310	-	1/1/11/20	6/17/93/115	-
23	CLA	b	825	-	1/1/14/20	4/38/114/115	-
21	XAT	6	306	-	-	4/31/93/93	0/4/4/4
23	CLA	1	313	-	1/1/10/20	6/10/86/115	-
23	CLA	a	820	-	1/1/15/20	12/39/115/115	-
21	XAT	4	303	-	-	3/31/93/93	0/4/4/4
29	PQN	b	841	-	-	1/23/43/43	0/2/2/2
23	CLA	b	833	-	1/1/15/20	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	A1L1G	3	306	-	-	19/29/85/85	0/3/3/3
23	CLA	7	306	4	1/1/11/20	10/19/95/115	-
25	A1L1F	h	203	-	-	11/43/99/99	1/3/3/3
23	CLA	a	802	-	1/1/13/20	5/31/107/115	-
23	CLA	9	309	2	1/1/11/20	5/17/93/115	-
23	CLA	a	839	-	1/1/15/20	14/39/115/115	-
21	XAT	4	305	-	-	4/31/93/93	0/4/4/4
23	CLA	h	204	-	1/1/13/20	9/27/103/115	-
23	CLA	8	312	3	1/1/12/20	2/24/100/115	-
23	CLA	2	311	-	1/1/13/20	5/31/107/115	-
21	XAT	3	305	-	-	0/31/93/93	0/4/4/4
23	CLA	4	310	-	1/1/15/20	15/39/115/115	-
23	CLA	3	309	5	1/1/13/20	3/29/105/115	-
23	CLA	3	315	5	1/1/11/20	9/17/93/115	-
21	XAT	5	304	-	-	1/31/93/93	0/4/4/4
23	CLA	a	841	-	1/1/15/20	15/39/115/115	-
23	CLA	4	308	-	1/1/15/20	13/39/115/115	-
23	CLA	b	826	-	1/1/15/20	3/39/115/115	-
30	BCR	l	205	-	-	8/29/63/63	0/2/2/2
23	CLA	b	806	-	1/1/15/20	13/39/115/115	-
23	CLA	a	842	-	1/1/15/20	8/39/115/115	-
23	CLA	6	315	6	1/1/10/20	5/10/86/115	-
23	CLA	b	802	-	1/1/15/20	15/39/115/115	-
23	CLA	9	308	2	1/1/15/20	14/39/115/115	-
23	CLA	l	204	-	1/1/11/20	3/17/93/115	-
22	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
21	XAT	7	301	-	-	6/31/93/93	0/4/4/4
23	CLA	b	822	-	1/1/14/20	7/33/109/115	-
23	CLA	5	311	-	1/1/12/20	7/23/99/115	-
23	CLA	5	315	-	1/1/11/20	5/17/93/115	-
23	CLA	b	813	-	1/1/15/20	13/39/115/115	-
23	CLA	2	313	7	1/1/10/20	2/10/86/115	-
25	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
23	CLA	7	312	-	1/1/11/20	3/19/95/115	-
21	XAT	1	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
31	SF4	c	101	-	-	-	0/6/5/5
23	CLA	b	820	-	1/1/12/20	5/21/97/115	-
23	CLA	9	318	-	1/1/14/20	11/36/112/115	-
23	CLA	a	810	9	1/1/15/20	14/39/115/115	-
23	CLA	b	815	-	1/1/11/20	3/15/91/115	-
23	CLA	2	316	7	1/1/11/20	6/17/93/115	-
23	CLA	2	310	-	1/1/15/20	14/39/115/115	-
21	XAT	4	301	-	-	4/31/93/93	0/4/4/4
23	CLA	a	829	-	1/1/14/20	13/36/112/115	-
25	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
23	CLA	4	317	-	1/1/13/20	9/27/103/115	-
23	CLA	b	836	-	1/1/15/20	7/39/115/115	-
23	CLA	b	839	-	1/1/15/20	15/39/115/115	-
22	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
30	BCR	a	847	-	-	0/29/63/63	0/2/2/2
21	XAT	2	301	-	-	3/31/93/93	0/4/4/4
23	CLA	1	305	-	1/1/14/20	9/35/111/115	-
21	XAT	4	304	-	-	0/31/93/93	0/4/4/4
23	CLA	7	315	4	1/1/10/20	4/10/86/115	-
23	CLA	8	310	-	1/1/11/20	6/17/93/115	-
21	XAT	7	303	-	-	7/31/93/93	0/4/4/4
23	CLA	5	308	-	1/1/13/20	6/27/103/115	-
22	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
28	LMG	a	853	-	-	13/29/49/70	0/1/1/1
23	CLA	7	316	-	1/1/12/20	10/23/99/115	-
23	CLA	9	314	-	1/1/13/20	10/27/103/115	-
23	CLA	a	811	-	1/1/13/20	6/29/105/115	-
21	XAT	8	301	-	-	3/31/93/93	0/4/4/4
23	CLA	a	823	-	1/1/11/20	7/20/96/115	-
21	XAT	7	305	-	-	2/31/93/93	0/4/4/4
23	CLA	5	312	-	1/1/12/20	0/24/100/115	-
21	XAT	j	101	-	-	5/31/93/93	0/4/4/4
23	CLA	a	813	-	1/1/12/20	10/26/102/115	-
30	BCR	h	201	-	-	0/29/63/63	0/2/2/2
23	CLA	9	313	2	1/1/11/20	12/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	808	-	1/1/12/20	4/23/99/115	-
21	XAT	4	302	-	-	0/31/93/93	0/4/4/4
23	CLA	a	824	-	1/1/11/20	5/17/93/115	-
23	CLA	a	825	-	1/1/13/20	8/27/103/115	-
23	CLA	b	811	-	1/1/13/20	4/25/101/115	-
23	CLA	4	316	-	1/1/11/20	7/17/93/115	-
23	CLA	b	832	-	1/1/15/20	13/39/115/115	-
23	CLA	2	309	-	1/1/11/20	3/17/93/115	-
23	CLA	b	840	26	1/1/15/20	11/39/115/115	-
23	CLA	7	313	-	1/1/12/20	5/26/102/115	-
23	CLA	6	308	-	1/1/13/20	6/31/107/115	-
23	CLA	7	317	-	1/1/11/20	7/15/91/115	-
23	CLA	a	831	-	1/1/15/20	11/39/115/115	-
23	CLA	a	827	-	1/1/15/20	6/39/115/115	-
23	CLA	8	308	-	1/1/13/20	7/27/103/115	-
23	CLA	4	311	-	1/1/11/20	9/17/93/115	-
26	LHG	9	307	-	-	20/40/40/53	-
23	CLA	8	309	-	1/1/13/20	7/30/106/115	-
23	CLA	a	815	-	1/1/11/20	0/15/91/115	-
23	CLA	b	827	-	1/1/15/20	14/39/115/115	-
22	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
21	XAT	6	303	-	-	5/31/93/93	0/4/4/4
30	BCR	b	845	-	-	0/29/63/63	0/2/2/2
23	CLA	a	854	-	1/1/15/20	14/39/115/115	-
23	CLA	b	828	-	1/1/15/20	13/39/115/115	-
25	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
28	LMG	2	317	-	-	11/30/50/70	0/1/1/1
23	CLA	1	312	8	1/1/12/20	3/24/100/115	-
23	CLA	a	818	-	1/1/13/20	11/29/105/115	-
23	CLA	b	816	-	1/1/13/20	3/27/103/115	-
23	CLA	b	819	-	1/1/13/20	5/27/103/115	-
23	CLA	1	203	-	1/1/14/20	4/33/109/115	-
21	XAT	5	302	-	-	3/31/93/93	0/4/4/4
21	XAT	6	305	-	-	4/31/93/93	0/4/4/4
23	CLA	2	312	-	1/1/11/20	4/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	4	313	-	1/1/12/20	4/25/101/115	-
21	XAT	9	304	-	-	1/31/93/93	0/4/4/4
23	CLA	7	308	-	1/1/14/20	12/33/109/115	-
23	CLA	b	809	-	1/1/15/20	13/39/115/115	-
23	CLA	b	838	-	1/1/15/20	15/39/115/115	-
30	BCR	j	104	-	-	2/29/63/63	0/2/2/2
23	CLA	3	311	-	1/1/12/20	4/21/97/115	-
23	CLA	1	314	-	1/1/11/20	7/15/91/115	-
23	CLA	1	308	8	1/1/15/20	13/39/115/115	-
23	CLA	l	202	-	1/1/10/20	0/12/88/115	-
23	CLA	f	803	13	1/1/12/20	5/24/100/115	-
23	CLA	8	307	3	1/1/15/20	11/39/115/115	-
23	CLA	2	314	-	1/1/13/20	14/29/105/115	-
23	CLA	a	832	-	1/1/12/20	7/21/97/115	-
23	CLA	b	835	-	1/1/13/20	10/31/107/115	-
23	CLA	a	821	-	1/1/11/20	1/15/91/115	-
23	CLA	j	102	-	1/1/13/20	18/31/107/115	-
21	XAT	8	302	-	-	4/31/93/93	0/4/4/4
23	CLA	8	306	27	1/1/11/20	4/17/93/115	-
23	CLA	b	807	-	1/1/15/20	18/39/115/115	-
23	CLA	a	817	-	1/1/11/20	8/15/91/115	-
23	CLA	a	844	26	1/1/15/20	15/39/115/115	-
23	CLA	4	312	-	1/1/11/20	6/17/93/115	-
30	BCR	a	850	-	-	4/29/63/63	0/2/2/2
23	CLA	a	835	-	1/1/15/20	11/39/115/115	-
23	CLA	b	814	-	1/1/13/20	10/27/103/115	-
21	XAT	2	303	-	-	6/31/93/93	0/4/4/4
27	DGD	4	318	-	-	10/29/69/95	0/2/2/2
23	CLA	3	313	-	1/1/12/20	1/24/100/115	-
23	CLA	5	305	1	1/1/11/20	6/17/93/115	-
23	CLA	a	834	-	1/1/15/20	9/39/115/115	-
23	CLA	5	313	1	1/1/11/20	6/15/91/115	-
23	CLA	7	311	-	1/1/11/20	4/17/93/115	-

All (1591) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	843	PQN	C3-C2	7.75	1.49	1.35
29	b	841	PQN	C3-C2	7.50	1.48	1.35
29	b	841	PQN	C10-C5	4.93	1.48	1.40
29	a	843	PQN	C10-C5	4.88	1.48	1.40
25	h	203	A1L1F	O7-C54	4.68	1.45	1.35
25	9	302	A1L1F	O7-C54	4.68	1.45	1.35
25	8	304	A1L1F	O7-C54	4.65	1.45	1.35
25	6	304	A1L1F	O7-C54	4.59	1.45	1.35
25	1	304	A1L1F	O7-C54	4.58	1.45	1.35
25	6	301	A1L1F	O7-C54	4.51	1.45	1.35
24	5	316	SQD	O8-S	4.46	1.64	1.47
25	9	302	A1L1F	C57-C1	-4.45	1.25	1.30
24	1	315	SQD	O8-S	4.42	1.63	1.47
25	h	203	A1L1F	C57-C1	-4.39	1.25	1.30
27	8	315	DGD	O1G-C1A	4.30	1.45	1.33
24	1	315	SQD	O48-C23	4.30	1.45	1.33
25	8	304	A1L1F	C57-C1	-4.26	1.25	1.30
28	a	853	LMG	O8-C28	4.24	1.45	1.33
24	5	316	SQD	O48-C23	4.23	1.45	1.33
25	1	304	A1L1F	O13-C45	4.22	1.45	1.33
25	1	304	A1L1F	C57-C1	-4.19	1.25	1.30
24	1	315	SQD	O47-C7	4.19	1.46	1.34
25	6	301	A1L1F	C57-C1	-4.18	1.25	1.30
28	a	853	LMG	O7-C10	4.15	1.46	1.34
25	h	203	A1L1F	O13-C45	4.15	1.45	1.33
25	6	304	A1L1F	O13-C45	4.12	1.45	1.33
25	6	301	A1L1F	O13-C45	4.12	1.45	1.33
28	j	105	LMG	O8-C28	4.10	1.45	1.33
25	6	304	A1L1F	C57-C1	-4.10	1.25	1.30
25	8	304	A1L1F	O13-C45	4.09	1.45	1.33
24	5	316	SQD	O47-C7	4.08	1.45	1.34
28	2	317	LMG	O8-C28	4.05	1.45	1.33
27	4	318	DGD	O1G-C1A	4.04	1.45	1.33
27	b	848	DGD	O2G-C1B	3.99	1.45	1.34
27	b	848	DGD	O1G-C1A	3.97	1.44	1.33
28	2	317	LMG	O7-C10	3.97	1.45	1.34
30	m	101	BCR	C1-C6	-3.94	1.48	1.53
25	9	302	A1L1F	O13-C45	3.93	1.44	1.33
25	8	304	A1L1F	C57-C2	-3.92	1.25	1.31
25	h	203	A1L1F	C57-C2	-3.91	1.25	1.31
28	j	105	LMG	O7-C10	3.87	1.45	1.34
25	9	302	A1L1F	C57-C2	-3.87	1.25	1.31
27	4	318	DGD	O2G-C1B	3.85	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	304	A1L1F	C57-C2	-3.77	1.25	1.31
25	6	301	A1L1F	C57-C2	-3.76	1.25	1.31
27	8	315	DGD	O2G-C1B	3.74	1.44	1.34
23	6	315	CLA	C1D-ND	3.71	1.42	1.37
23	6	317	CLA	C1D-ND	3.68	1.42	1.37
23	a	804	CLA	C1D-ND	3.67	1.42	1.37
23	6	308	CLA	C1D-ND	3.66	1.42	1.37
23	2	313	CLA	C1D-ND	3.65	1.42	1.37
25	1	304	A1L1F	C57-C2	-3.65	1.26	1.31
23	3	308	CLA	C1D-ND	3.65	1.42	1.37
23	9	312	CLA	C1D-ND	3.62	1.42	1.37
23	7	306	CLA	C1D-ND	3.62	1.42	1.37
23	1	312	CLA	C1D-ND	3.62	1.42	1.37
23	9	313	CLA	C1D-ND	3.61	1.42	1.37
23	8	314	CLA	C1D-ND	3.61	1.42	1.37
23	8	313	CLA	C1D-ND	3.61	1.42	1.37
23	3	314	CLA	C1D-ND	3.60	1.42	1.37
23	8	308	CLA	C1D-ND	3.60	1.42	1.37
23	a	828	CLA	C1D-ND	3.59	1.42	1.37
23	7	315	CLA	C1D-ND	3.59	1.42	1.37
23	4	314	CLA	C1D-ND	3.59	1.42	1.37
23	a	837	CLA	C1D-ND	3.59	1.42	1.37
23	a	840	CLA	C1D-ND	3.58	1.42	1.37
23	2	307	CLA	C1D-ND	3.58	1.42	1.37
23	8	305	CLA	C1D-ND	3.58	1.42	1.37
23	3	315	CLA	C1D-ND	3.58	1.42	1.37
23	8	310	CLA	C1D-ND	3.58	1.42	1.37
23	b	826	CLA	C1D-ND	3.58	1.42	1.37
23	4	316	CLA	C1D-ND	3.57	1.42	1.37
23	2	306	CLA	C1D-ND	3.57	1.42	1.37
23	2	315	CLA	C1D-ND	3.56	1.42	1.37
23	4	307	CLA	C1D-ND	3.56	1.42	1.37
23	b	818	CLA	C1D-ND	3.56	1.42	1.37
23	b	840	CLA	C1D-ND	3.56	1.42	1.37
23	b	824	CLA	C1D-ND	3.56	1.42	1.37
23	7	307	CLA	C1D-ND	3.56	1.42	1.37
23	7	311	CLA	C1D-ND	3.56	1.42	1.37
23	j	103	CLA	C1D-ND	3.56	1.42	1.37
23	5	314	CLA	C1D-ND	3.56	1.42	1.37
23	9	310	CLA	C1D-ND	3.56	1.42	1.37
23	7	310	CLA	C1D-ND	3.56	1.42	1.37
23	2	314	CLA	C1D-ND	3.56	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	814	CLA	C1D-ND	3.56	1.42	1.37
23	5	310	CLA	C1D-ND	3.55	1.42	1.37
23	6	316	CLA	C1D-ND	3.55	1.42	1.37
23	5	305	CLA	C1D-ND	3.55	1.42	1.37
23	1	204	CLA	C1D-ND	3.55	1.42	1.37
23	b	833	CLA	C1D-ND	3.55	1.42	1.37
23	2	311	CLA	C1D-ND	3.55	1.42	1.37
23	5	308	CLA	C1D-ND	3.55	1.42	1.37
23	1	310	CLA	C1D-ND	3.55	1.42	1.37
23	9	314	CLA	C1D-ND	3.54	1.42	1.37
23	7	317	CLA	C1D-ND	3.54	1.42	1.37
23	a	839	CLA	C1D-ND	3.54	1.42	1.37
23	b	820	CLA	C1D-ND	3.54	1.42	1.37
23	6	307	CLA	C1D-ND	3.54	1.42	1.37
23	5	311	CLA	C1D-ND	3.54	1.42	1.37
23	6	313	CLA	C1D-ND	3.54	1.42	1.37
23	b	839	CLA	C1D-ND	3.54	1.42	1.37
23	3	311	CLA	C1D-ND	3.53	1.42	1.37
23	a	811	CLA	C1D-ND	3.53	1.42	1.37
23	f	802	CLA	C1D-ND	3.53	1.42	1.37
23	8	309	CLA	C1D-ND	3.53	1.42	1.37
23	6	309	CLA	C1D-ND	3.53	1.42	1.37
23	3	313	CLA	C1D-ND	3.53	1.42	1.37
23	b	805	CLA	C1D-ND	3.53	1.42	1.37
23	2	312	CLA	C1D-ND	3.53	1.42	1.37
23	4	315	CLA	C1D-ND	3.53	1.42	1.37
23	a	835	CLA	C1D-ND	3.53	1.42	1.37
23	b	834	CLA	C1D-ND	3.53	1.42	1.37
23	5	309	CLA	C1D-ND	3.52	1.42	1.37
23	9	315	CLA	C1D-ND	3.52	1.42	1.37
23	4	306	CLA	C1D-ND	3.52	1.42	1.37
23	a	838	CLA	C1D-ND	3.52	1.42	1.37
23	5	313	CLA	C1D-ND	3.52	1.42	1.37
23	6	310	CLA	C1D-ND	3.52	1.42	1.37
23	3	312	CLA	C1D-ND	3.52	1.42	1.37
23	5	306	CLA	C1D-ND	3.51	1.42	1.37
23	7	313	CLA	C1D-ND	3.51	1.42	1.37
23	b	807	CLA	C1D-ND	3.51	1.42	1.37
23	8	307	CLA	C1D-ND	3.51	1.42	1.37
23	a	819	CLA	C1D-ND	3.51	1.42	1.37
23	1	314	CLA	C1D-ND	3.51	1.42	1.37
23	b	831	CLA	C1D-ND	3.51	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	825	CLA	C1D-ND	3.51	1.42	1.37
23	7	308	CLA	C1D-ND	3.50	1.42	1.37
23	6	312	CLA	C1D-ND	3.50	1.42	1.37
23	6	314	CLA	C1D-ND	3.50	1.42	1.37
23	1	309	CLA	C1D-ND	3.50	1.42	1.37
23	a	829	CLA	C1D-ND	3.50	1.42	1.37
23	b	812	CLA	C1D-ND	3.50	1.42	1.37
23	a	813	CLA	C1D-ND	3.50	1.42	1.37
23	b	835	CLA	C1D-ND	3.50	1.42	1.37
23	b	817	CLA	C1D-ND	3.50	1.42	1.37
23	4	317	CLA	C1D-ND	3.50	1.42	1.37
23	a	817	CLA	C1D-ND	3.50	1.42	1.37
23	8	306	CLA	C1D-ND	3.49	1.42	1.37
23	7	316	CLA	C1D-ND	3.49	1.42	1.37
23	1	307	CLA	C1D-ND	3.49	1.42	1.37
23	a	815	CLA	C1D-ND	3.49	1.42	1.37
23	a	809	CLA	C1D-ND	3.49	1.42	1.37
23	b	813	CLA	C1D-ND	3.49	1.42	1.37
23	4	312	CLA	C1D-ND	3.49	1.42	1.37
23	2	309	CLA	C1D-ND	3.49	1.42	1.37
23	7	314	CLA	C1D-ND	3.49	1.42	1.37
23	l	202	CLA	C1D-ND	3.48	1.42	1.37
23	b	814	CLA	C1D-ND	3.48	1.42	1.37
23	a	826	CLA	C1D-ND	3.48	1.42	1.37
23	b	816	CLA	C1D-ND	3.48	1.42	1.37
23	1	311	CLA	C1D-ND	3.48	1.42	1.37
23	a	844	CLA	C1D-ND	3.48	1.42	1.37
23	4	310	CLA	C1D-ND	3.48	1.42	1.37
23	6	311	CLA	C1D-ND	3.48	1.42	1.37
23	1	306	CLA	C1D-ND	3.48	1.42	1.37
23	b	837	CLA	C1D-ND	3.48	1.42	1.37
23	a	816	CLA	C1D-ND	3.48	1.42	1.37
23	9	318	CLA	C1D-ND	3.47	1.42	1.37
23	b	821	CLA	C1D-ND	3.47	1.42	1.37
23	3	310	CLA	C1D-ND	3.47	1.42	1.37
23	a	821	CLA	C1D-ND	3.47	1.42	1.37
23	a	854	CLA	C1D-ND	3.47	1.42	1.37
23	j	102	CLA	C1D-ND	3.47	1.42	1.37
23	a	820	CLA	C1D-ND	3.47	1.42	1.37
23	a	834	CLA	C1D-ND	3.47	1.42	1.37
23	b	828	CLA	C1D-ND	3.47	1.42	1.37
23	a	842	CLA	C1D-ND	3.47	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	815	CLA	C1D-ND	3.47	1.42	1.37
23	a	807	CLA	C1D-ND	3.46	1.42	1.37
23	h	204	CLA	C1D-ND	3.46	1.42	1.37
23	a	822	CLA	C1D-ND	3.46	1.42	1.37
23	b	838	CLA	C1D-ND	3.46	1.42	1.37
23	a	832	CLA	C1D-ND	3.46	1.42	1.37
23	7	312	CLA	C1D-ND	3.46	1.42	1.37
23	a	836	CLA	C1D-ND	3.46	1.42	1.37
23	b	808	CLA	C1D-ND	3.46	1.42	1.37
23	3	309	CLA	C1D-ND	3.45	1.42	1.37
23	2	308	CLA	C1D-ND	3.45	1.42	1.37
23	a	818	CLA	C1D-ND	3.45	1.42	1.37
23	a	841	CLA	C1D-ND	3.45	1.42	1.37
23	5	315	CLA	C1D-ND	3.45	1.42	1.37
23	4	308	CLA	C1D-ND	3.45	1.42	1.37
23	4	313	CLA	C1D-ND	3.45	1.42	1.37
23	b	819	CLA	C1D-ND	3.45	1.42	1.37
23	9	316	CLA	C1D-ND	3.44	1.42	1.37
23	1	305	CLA	C1D-ND	3.44	1.42	1.37
23	a	823	CLA	C1D-ND	3.44	1.42	1.37
23	a	808	CLA	C1D-ND	3.44	1.42	1.37
23	b	801	CLA	C1D-ND	3.43	1.42	1.37
23	f	803	CLA	C1D-ND	3.43	1.42	1.37
23	b	829	CLA	C1D-ND	3.43	1.42	1.37
23	1	313	CLA	C1D-ND	3.43	1.42	1.37
23	8	311	CLA	C1D-ND	3.43	1.42	1.37
23	5	312	CLA	C1D-ND	3.42	1.42	1.37
23	4	309	CLA	C1D-ND	3.42	1.42	1.37
23	1	308	CLA	C1D-ND	3.42	1.42	1.37
23	a	805	CLA	C1D-ND	3.42	1.42	1.37
23	a	824	CLA	C1D-ND	3.42	1.42	1.37
23	a	810	CLA	C1D-ND	3.42	1.42	1.37
23	b	822	CLA	C1D-ND	3.42	1.42	1.37
23	b	827	CLA	C1D-ND	3.42	1.42	1.37
23	9	311	CLA	C1D-ND	3.41	1.42	1.37
23	b	825	CLA	C1D-ND	3.41	1.42	1.37
23	a	831	CLA	C1D-ND	3.41	1.42	1.37
23	b	810	CLA	C1D-ND	3.40	1.42	1.37
23	9	308	CLA	C1D-ND	3.40	1.42	1.37
23	7	309	CLA	C1D-ND	3.40	1.42	1.37
23	a	803	CLA	C1D-ND	3.40	1.42	1.37
23	2	316	CLA	C1D-ND	3.40	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	307	CLA	C1D-ND	3.39	1.42	1.37
23	a	812	CLA	C1D-ND	3.39	1.42	1.37
23	a	827	CLA	C1D-ND	3.39	1.42	1.37
23	b	836	CLA	C1D-ND	3.38	1.42	1.37
23	b	806	CLA	C1D-ND	3.38	1.42	1.37
23	2	310	CLA	C1D-ND	3.38	1.42	1.37
23	a	830	CLA	C1D-ND	3.38	1.42	1.37
23	1	203	CLA	C1D-ND	3.37	1.42	1.37
23	5	307	CLA	C1D-ND	3.37	1.42	1.37
23	4	311	CLA	C1D-ND	3.37	1.42	1.37
23	1	312	CLA	C4B-NB	3.37	1.42	1.37
23	b	809	CLA	C1D-ND	3.36	1.42	1.37
30	m	101	BCR	C30-C25	-3.36	1.49	1.53
23	8	312	CLA	C1D-ND	3.35	1.42	1.37
23	b	823	CLA	C1D-ND	3.35	1.42	1.37
23	9	309	CLA	C1D-ND	3.35	1.42	1.37
23	b	802	CLA	C1D-ND	3.33	1.42	1.37
23	b	811	CLA	C1D-ND	3.32	1.42	1.37
23	b	832	CLA	C1D-ND	3.32	1.42	1.37
23	a	802	CLA	C1D-ND	3.32	1.42	1.37
23	b	803	CLA	C1D-ND	3.31	1.42	1.37
23	b	830	CLA	C1D-ND	3.29	1.42	1.37
26	a	845	LHG	C26-C25	-3.27	1.35	1.51
23	a	801	CLA	C1D-ND	3.26	1.42	1.37
23	a	818	CLA	C4B-NB	3.25	1.42	1.37
26	9	317	LHG	C26-C25	-3.24	1.35	1.51
23	a	842	CLA	C4B-NB	3.23	1.42	1.37
23	a	840	CLA	C4B-NB	3.23	1.42	1.37
23	2	315	CLA	C4B-NB	3.23	1.42	1.37
26	b	847	LHG	C26-C25	-3.21	1.35	1.51
23	3	315	CLA	C4B-NB	3.21	1.42	1.37
26	9	307	LHG	C26-C25	-3.20	1.35	1.51
23	b	837	CLA	C4B-NB	3.19	1.42	1.37
23	6	317	CLA	C4B-NB	3.19	1.42	1.37
23	a	833	CLA	C1D-ND	3.19	1.42	1.37
23	4	315	CLA	C4B-NB	3.18	1.42	1.37
23	1	309	CLA	C4B-NB	3.17	1.42	1.37
23	b	829	CLA	C4B-NB	3.16	1.42	1.37
23	4	306	CLA	C4B-NB	3.15	1.42	1.37
23	5	313	CLA	C4B-NB	3.15	1.42	1.37
23	4	314	CLA	C4B-NB	3.15	1.42	1.37
23	4	307	CLA	C4B-NB	3.15	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	313	CLA	C4B-NB	3.14	1.42	1.37
23	6	311	CLA	C4B-NB	3.14	1.42	1.37
23	6	307	CLA	C4B-NB	3.14	1.42	1.37
23	b	820	CLA	C4B-NB	3.14	1.42	1.37
23	6	308	CLA	C4B-NB	3.14	1.42	1.37
23	4	311	CLA	C4B-NB	3.14	1.42	1.37
23	b	834	CLA	C4B-NB	3.14	1.42	1.37
23	4	312	CLA	C4B-NB	3.14	1.42	1.37
23	a	813	CLA	C4B-NB	3.13	1.42	1.37
23	2	311	CLA	C4B-NB	3.13	1.42	1.37
23	j	102	CLA	C4B-NB	3.13	1.42	1.37
23	8	313	CLA	C4B-NB	3.13	1.42	1.37
23	a	808	CLA	C4B-NB	3.13	1.42	1.37
23	1	314	CLA	C4B-NB	3.13	1.42	1.37
23	7	311	CLA	C4B-NB	3.12	1.42	1.37
23	5	310	CLA	C4B-NB	3.12	1.42	1.37
23	2	308	CLA	C4B-NB	3.12	1.42	1.37
23	2	312	CLA	C4B-NB	3.12	1.42	1.37
23	a	817	CLA	C4B-NB	3.11	1.42	1.37
23	7	315	CLA	C4B-NB	3.11	1.42	1.37
23	a	825	CLA	C4B-NB	3.11	1.42	1.37
23	b	839	CLA	C4B-NB	3.11	1.42	1.37
23	9	318	CLA	C4B-NB	3.11	1.41	1.37
23	2	314	CLA	C4B-NB	3.11	1.41	1.37
23	5	305	CLA	C4B-NB	3.11	1.41	1.37
23	b	811	CLA	CAB-C3B	-3.10	1.44	1.50
23	b	802	CLA	C4B-NB	3.10	1.41	1.37
23	6	312	CLA	C4B-NB	3.10	1.41	1.37
23	a	831	CLA	C4B-NB	3.10	1.41	1.37
23	1	313	CLA	C4B-NB	3.10	1.41	1.37
23	3	311	CLA	C4B-NB	3.10	1.41	1.37
23	4	317	CLA	C4B-NB	3.10	1.41	1.37
23	a	824	CLA	C4B-NB	3.10	1.41	1.37
23	7	307	CLA	C4B-NB	3.09	1.41	1.37
23	b	818	CLA	C4B-NB	3.09	1.41	1.37
23	1	305	CLA	C4B-NB	3.09	1.41	1.37
23	b	801	CLA	C4B-NB	3.09	1.41	1.37
23	5	306	CLA	C4B-NB	3.09	1.41	1.37
23	9	314	CLA	C4B-NB	3.09	1.41	1.37
23	4	316	CLA	C4B-NB	3.09	1.41	1.37
23	b	828	CLA	C4B-NB	3.09	1.41	1.37
23	f	803	CLA	C4B-NB	3.08	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	316	CLA	C4B-NB	3.08	1.41	1.37
23	7	317	CLA	C4B-NB	3.08	1.41	1.37
23	2	310	CLA	C4B-NB	3.08	1.41	1.37
23	a	804	CLA	C4B-NB	3.07	1.41	1.37
23	b	826	CLA	C4B-NB	3.07	1.41	1.37
23	b	840	CLA	C4B-NB	3.07	1.41	1.37
23	8	314	CLA	C4B-NB	3.07	1.41	1.37
23	1	202	CLA	C4B-NB	3.07	1.41	1.37
23	6	310	CLA	C4B-NB	3.06	1.41	1.37
23	2	309	CLA	C4B-NB	3.06	1.41	1.37
23	8	308	CLA	C4B-NB	3.06	1.41	1.37
23	a	820	CLA	C4B-NB	3.06	1.41	1.37
23	a	841	CLA	C4B-NB	3.06	1.41	1.37
23	4	313	CLA	C4B-NB	3.06	1.41	1.37
23	b	805	CLA	C4B-NB	3.06	1.41	1.37
23	3	307	CLA	C4B-NB	3.06	1.41	1.37
23	b	816	CLA	C4B-NB	3.06	1.41	1.37
23	2	306	CLA	C4B-NB	3.05	1.41	1.37
23	4	309	CLA	C4B-NB	3.05	1.41	1.37
23	3	308	CLA	C4B-NB	3.05	1.41	1.37
23	1	310	CLA	C4B-NB	3.05	1.41	1.37
23	2	313	CLA	C4B-NB	3.05	1.41	1.37
23	3	312	CLA	C4B-NB	3.05	1.41	1.37
23	b	827	CLA	C4B-NB	3.05	1.41	1.37
23	9	309	CLA	C4B-NB	3.05	1.41	1.37
23	a	805	CLA	C4B-NB	3.05	1.41	1.37
23	3	310	CLA	C4B-NB	3.04	1.41	1.37
23	4	310	CLA	C4B-NB	3.04	1.41	1.37
23	a	810	CLA	C4B-NB	3.04	1.41	1.37
23	5	315	CLA	C4B-NB	3.04	1.41	1.37
23	6	309	CLA	C4B-NB	3.04	1.41	1.37
23	1	307	CLA	C4B-NB	3.04	1.41	1.37
23	a	837	CLA	C4B-NB	3.04	1.41	1.37
23	b	831	CLA	C4B-NB	3.04	1.41	1.37
23	a	822	CLA	C4B-NB	3.03	1.41	1.37
23	a	834	CLA	C4B-NB	3.03	1.41	1.37
23	b	822	CLA	C4B-NB	3.03	1.41	1.37
23	7	310	CLA	C4B-NB	3.03	1.41	1.37
23	7	306	CLA	C4B-NB	3.03	1.41	1.37
23	b	836	CLA	C4B-NB	3.03	1.41	1.37
23	8	309	CLA	C4B-NB	3.02	1.41	1.37
23	b	804	CLA	C1D-ND	3.02	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	312	CLA	C4B-NB	3.02	1.41	1.37
23	a	829	CLA	C4B-NB	3.02	1.41	1.37
23	a	854	CLA	C4B-NB	3.02	1.41	1.37
23	b	824	CLA	C4B-NB	3.02	1.41	1.37
23	j	103	CLA	C4B-NB	3.02	1.41	1.37
23	7	308	CLA	C4B-NB	3.02	1.41	1.37
23	b	814	CLA	C4B-NB	3.02	1.41	1.37
23	5	309	CLA	C4B-NB	3.02	1.41	1.37
23	9	308	CLA	C4B-NB	3.01	1.41	1.37
23	8	306	CLA	C4B-NB	3.01	1.41	1.37
23	b	804	CLA	C4B-NB	3.01	1.41	1.37
23	6	316	CLA	C4B-NB	3.01	1.41	1.37
23	b	809	CLA	C4B-NB	3.01	1.41	1.37
23	3	313	CLA	C4B-NB	3.01	1.41	1.37
23	9	310	CLA	C4B-NB	3.01	1.41	1.37
23	a	836	CLA	C4B-NB	3.00	1.41	1.37
23	6	314	CLA	C4B-NB	3.00	1.41	1.37
23	7	314	CLA	C4B-NB	3.00	1.41	1.37
23	1	308	CLA	C4B-NB	3.00	1.41	1.37
23	8	310	CLA	C4B-NB	3.00	1.41	1.37
23	b	838	CLA	C4B-NB	3.00	1.41	1.37
23	7	309	CLA	C4B-NB	3.00	1.41	1.37
23	b	811	CLA	C4B-NB	2.99	1.41	1.37
23	a	812	CLA	C4B-NB	2.99	1.41	1.37
23	6	315	CLA	C4B-NB	2.99	1.41	1.37
23	a	816	CLA	C4B-NB	2.99	1.41	1.37
23	b	833	CLA	C4B-NB	2.99	1.41	1.37
23	l	203	CLA	C4B-NB	2.99	1.41	1.37
23	5	308	CLA	C4B-NB	2.99	1.41	1.37
23	8	305	CLA	C4B-NB	2.99	1.41	1.37
23	b	819	CLA	C4B-NB	2.98	1.41	1.37
23	b	803	CLA	C4B-NB	2.98	1.41	1.37
23	9	313	CLA	C4B-NB	2.98	1.41	1.37
23	f	802	CLA	C4B-NB	2.98	1.41	1.37
23	9	311	CLA	C4B-NB	2.98	1.41	1.37
23	1	306	CLA	C4B-NB	2.98	1.41	1.37
23	a	819	CLA	C4B-NB	2.98	1.41	1.37
23	b	832	CLA	C4B-NB	2.98	1.41	1.37
23	7	312	CLA	C4B-NB	2.97	1.41	1.37
23	3	314	CLA	C4B-NB	2.97	1.41	1.37
23	a	815	CLA	C4B-NB	2.97	1.41	1.37
23	5	307	CLA	C4B-NB	2.97	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	312	CLA	C4B-NB	2.97	1.41	1.37
23	9	315	CLA	C4B-NB	2.97	1.41	1.37
23	a	826	CLA	C4B-NB	2.97	1.41	1.37
23	b	808	CLA	C4B-NB	2.97	1.41	1.37
25	h	203	A1L1F	O15-C20	-2.97	1.42	1.46
23	5	314	CLA	C4B-NB	2.96	1.41	1.37
23	a	823	CLA	C4B-NB	2.96	1.41	1.37
23	a	811	CLA	C4B-NB	2.96	1.41	1.37
23	h	204	CLA	C4B-NB	2.96	1.41	1.37
23	a	827	CLA	C4B-NB	2.96	1.41	1.37
23	a	821	CLA	C4B-NB	2.96	1.41	1.37
23	a	839	CLA	C4B-NB	2.96	1.41	1.37
23	b	812	CLA	C4B-NB	2.96	1.41	1.37
23	a	830	CLA	C4B-NB	2.95	1.41	1.37
23	8	311	CLA	C4B-NB	2.95	1.41	1.37
23	b	810	CLA	C4B-NB	2.95	1.41	1.37
23	6	313	CLA	C4B-NB	2.95	1.41	1.37
23	l	204	CLA	C4B-NB	2.95	1.41	1.37
23	3	309	CLA	C4B-NB	2.94	1.41	1.37
23	a	802	CLA	C4B-NB	2.94	1.41	1.37
23	a	832	CLA	C4B-NB	2.94	1.41	1.37
23	a	833	CLA	C4B-NB	2.94	1.41	1.37
23	b	803	CLA	C1B-C2B	2.93	1.50	1.43
25	9	302	A1L1F	C6-C1	-2.93	1.49	1.54
23	a	803	CLA	C4B-NB	2.93	1.41	1.37
23	a	835	CLA	C4B-NB	2.93	1.41	1.37
23	5	311	CLA	C4B-NB	2.93	1.41	1.37
23	9	312	CLA	C4B-NB	2.93	1.41	1.37
23	b	806	CLA	C4B-NB	2.93	1.41	1.37
23	b	825	CLA	C4B-NB	2.92	1.41	1.37
23	b	813	CLA	C4B-NB	2.92	1.41	1.37
23	a	814	CLA	C4B-NB	2.92	1.41	1.37
23	b	835	CLA	C4B-NB	2.91	1.41	1.37
23	b	815	CLA	C4B-NB	2.91	1.41	1.37
23	a	844	CLA	C4B-NB	2.91	1.41	1.37
23	1	311	CLA	C4B-NB	2.91	1.41	1.37
23	2	307	CLA	C4B-NB	2.90	1.41	1.37
23	b	823	CLA	C4B-NB	2.90	1.41	1.37
23	8	307	CLA	C4B-NB	2.90	1.41	1.37
23	b	817	CLA	C4B-NB	2.90	1.41	1.37
23	9	316	CLA	C4B-NB	2.89	1.41	1.37
23	a	807	CLA	C4B-NB	2.89	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	807	CLA	C4B-NB	2.88	1.41	1.37
23	b	821	CLA	C4B-NB	2.87	1.41	1.37
23	6	308	CLA	C1B-C2B	2.86	1.49	1.43
23	a	801	CLA	C4B-NB	2.86	1.41	1.37
23	4	308	CLA	C4B-NB	2.86	1.41	1.37
25	6	301	A1L1F	O15-C20	-2.86	1.42	1.46
23	a	838	CLA	C4B-NB	2.85	1.41	1.37
23	7	316	CLA	C4B-NB	2.85	1.41	1.37
23	b	830	CLA	C4B-NB	2.85	1.41	1.37
23	b	839	CLA	C1B-C2B	2.84	1.49	1.43
23	a	823	CLA	C1B-C2B	2.84	1.49	1.43
23	6	312	CLA	C1B-C2B	2.83	1.49	1.43
23	3	308	CLA	C1B-C2B	2.81	1.49	1.43
23	1	305	CLA	C1B-C2B	2.81	1.49	1.43
23	6	310	CLA	C1B-C2B	2.81	1.49	1.43
23	a	828	CLA	C4B-NB	2.81	1.41	1.37
23	3	311	CLA	C1B-C2B	2.81	1.49	1.43
23	9	316	CLA	C1B-C2B	2.80	1.49	1.43
23	1	306	CLA	C1B-C2B	2.80	1.49	1.43
23	7	315	CLA	C1B-C2B	2.80	1.49	1.43
23	b	823	CLA	C1B-C2B	2.80	1.49	1.43
23	7	308	CLA	C1B-C2B	2.79	1.49	1.43
23	b	827	CLA	C1B-C2B	2.78	1.49	1.43
23	a	809	CLA	C4B-NB	2.78	1.41	1.37
23	6	309	CLA	C1B-C2B	2.78	1.49	1.43
22	9	301	A1L1G	C33-C34	-2.78	1.40	1.46
23	b	808	CLA	C1B-C2B	2.78	1.49	1.43
23	7	309	CLA	C1B-C2B	2.78	1.49	1.43
23	b	807	CLA	C1B-C2B	2.78	1.49	1.43
23	a	830	CLA	C1B-C2B	2.78	1.49	1.43
23	2	316	CLA	C1B-C2B	2.78	1.49	1.43
23	3	314	CLA	C1B-C2B	2.78	1.49	1.43
23	b	821	CLA	C1B-C2B	2.78	1.49	1.43
23	6	316	CLA	C1B-C2B	2.77	1.49	1.43
23	a	844	CLA	C1B-C2B	2.77	1.49	1.43
23	b	820	CLA	C1B-C2B	2.77	1.49	1.43
23	2	313	CLA	C1B-C2B	2.77	1.49	1.43
23	1	311	CLA	C1B-C2B	2.77	1.49	1.43
23	6	314	CLA	C1B-C2B	2.77	1.49	1.43
23	7	316	CLA	C1B-C2B	2.77	1.49	1.43
23	a	821	CLA	C1B-C2B	2.77	1.49	1.43
23	1	308	CLA	C1B-C2B	2.77	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	832	CLA	C1B-C2B	2.77	1.49	1.43
23	8	307	CLA	C1B-C2B	2.76	1.49	1.43
23	7	306	CLA	C1B-C2B	2.76	1.49	1.43
23	8	305	CLA	C1B-C2B	2.76	1.49	1.43
23	j	103	CLA	C1B-C2B	2.76	1.49	1.43
23	a	810	CLA	C1B-C2B	2.76	1.49	1.43
23	2	315	CLA	C1B-C2B	2.76	1.49	1.43
23	b	812	CLA	C1B-C2B	2.76	1.49	1.43
23	3	310	CLA	C1B-C2B	2.75	1.49	1.43
23	4	310	CLA	C1B-C2B	2.75	1.49	1.43
23	j	102	CLA	C1B-C2B	2.75	1.49	1.43
23	l	204	CLA	C1B-C2B	2.75	1.49	1.43
23	4	316	CLA	C1B-C2B	2.75	1.49	1.43
23	3	309	CLA	C1B-C2B	2.75	1.49	1.43
23	a	834	CLA	C1B-C2B	2.75	1.49	1.43
23	7	310	CLA	C1B-C2B	2.75	1.49	1.43
23	a	817	CLA	C1B-C2B	2.74	1.49	1.43
23	a	812	CLA	C1B-C2B	2.74	1.49	1.43
21	9	303	XAT	O4-C5	-2.74	1.42	1.46
23	7	312	CLA	C1B-C2B	2.74	1.49	1.43
23	a	838	CLA	C1B-C2B	2.74	1.49	1.43
23	f	802	CLA	C1B-C2B	2.74	1.49	1.43
23	b	836	CLA	C1B-C2B	2.74	1.49	1.43
23	5	315	CLA	C1B-C2B	2.74	1.49	1.43
23	b	833	CLA	C1B-C2B	2.74	1.49	1.43
23	8	309	CLA	C1B-C2B	2.74	1.49	1.43
23	a	842	CLA	C1B-C2B	2.74	1.49	1.43
23	7	317	CLA	C1B-C2B	2.74	1.49	1.43
23	9	313	CLA	C1B-C2B	2.74	1.49	1.43
23	a	828	CLA	C1B-C2B	2.74	1.49	1.43
23	4	312	CLA	C1B-C2B	2.74	1.49	1.43
23	8	314	CLA	C1B-C2B	2.73	1.49	1.43
23	a	835	CLA	C1B-C2B	2.73	1.49	1.43
23	b	811	CLA	C4B-C3B	2.73	1.49	1.43
23	5	310	CLA	C1B-C2B	2.73	1.49	1.43
23	4	314	CLA	C1B-C2B	2.73	1.49	1.43
23	4	317	CLA	C1B-C2B	2.73	1.49	1.43
23	a	806	CLA	MG-NB	-2.73	2.00	2.05
23	9	311	CLA	C1B-C2B	2.73	1.49	1.43
23	a	809	CLA	C1B-C2B	2.73	1.49	1.43
23	7	307	CLA	C1B-C2B	2.73	1.49	1.43
23	3	313	CLA	C1B-C2B	2.73	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	h	204	CLA	C1B-C2B	2.73	1.49	1.43
23	8	306	CLA	C1B-C2B	2.73	1.49	1.43
23	1	313	CLA	C1B-C2B	2.73	1.49	1.43
23	5	309	CLA	C1B-C2B	2.73	1.49	1.43
23	9	315	CLA	C1B-C2B	2.73	1.49	1.43
23	4	307	CLA	C1B-C2B	2.72	1.49	1.43
23	2	309	CLA	C1B-C2B	2.72	1.49	1.43
23	8	311	CLA	C1B-C2B	2.72	1.49	1.43
23	9	310	CLA	C1B-C2B	2.72	1.49	1.43
23	2	306	CLA	C1B-C2B	2.72	1.49	1.43
23	b	805	CLA	C1B-C2B	2.72	1.49	1.43
23	2	311	CLA	C1B-C2B	2.72	1.49	1.43
23	a	824	CLA	C1B-C2B	2.72	1.49	1.43
23	4	308	CLA	C1B-C2B	2.72	1.49	1.43
23	5	311	CLA	C1B-C2B	2.72	1.49	1.43
23	4	306	CLA	C1B-C2B	2.72	1.49	1.43
23	a	818	CLA	C3B-C4B	2.72	1.50	1.42
23	a	811	CLA	C1B-C2B	2.71	1.49	1.43
23	2	308	CLA	C1B-C2B	2.71	1.49	1.43
23	9	312	CLA	C1B-C2B	2.71	1.49	1.43
23	6	311	CLA	C1B-C2B	2.71	1.49	1.43
23	1	314	CLA	C1B-C2B	2.71	1.49	1.43
23	2	312	CLA	C1B-C2B	2.71	1.49	1.43
23	1	309	CLA	C1B-C2B	2.71	1.49	1.43
23	a	829	CLA	C1B-C2B	2.71	1.49	1.43
23	9	318	CLA	C1B-C2B	2.71	1.49	1.43
23	3	312	CLA	C1B-C2B	2.71	1.49	1.43
23	b	822	CLA	C1B-C2B	2.71	1.49	1.43
23	a	805	CLA	C1B-C2B	2.71	1.49	1.43
23	9	308	CLA	C1B-C2B	2.71	1.49	1.43
23	a	825	CLA	C1B-C2B	2.71	1.49	1.43
23	a	807	CLA	C1B-C2B	2.70	1.49	1.43
23	l	202	CLA	C1B-C2B	2.70	1.49	1.43
23	6	315	CLA	C1B-C2B	2.70	1.49	1.43
23	7	314	CLA	C1B-C2B	2.70	1.49	1.43
23	5	313	CLA	C1B-C2B	2.70	1.49	1.43
23	a	826	CLA	C1B-C2B	2.70	1.49	1.43
23	f	803	CLA	C1B-C2B	2.70	1.49	1.43
23	6	307	CLA	C1B-C2B	2.70	1.49	1.43
23	a	854	CLA	C1B-C2B	2.70	1.49	1.43
23	a	839	CLA	C1B-C2B	2.70	1.49	1.43
23	5	306	CLA	C1B-C2B	2.69	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	801	CLA	C1B-C2B	2.69	1.49	1.43
23	a	814	CLA	C1B-C2B	2.69	1.49	1.43
23	a	840	CLA	C1B-C2B	2.69	1.49	1.43
23	4	309	CLA	C1B-C2B	2.69	1.49	1.43
23	a	804	CLA	C1B-C2B	2.69	1.49	1.43
23	2	310	CLA	C1B-C2B	2.69	1.49	1.43
23	b	831	CLA	C1B-C2B	2.69	1.49	1.43
23	b	837	CLA	C1B-C2B	2.69	1.49	1.43
23	b	811	CLA	C1B-C2B	2.69	1.49	1.43
23	b	815	CLA	C1B-C2B	2.69	1.49	1.43
23	5	305	CLA	C1B-C2B	2.69	1.49	1.43
23	1	307	CLA	C1B-C2B	2.69	1.49	1.43
23	a	816	CLA	C1B-C2B	2.68	1.49	1.43
23	b	806	CLA	C1B-C2B	2.68	1.49	1.43
23	4	311	CLA	C1B-C2B	2.68	1.49	1.43
23	b	813	CLA	C1B-C2B	2.68	1.49	1.43
23	5	312	CLA	C1B-C2B	2.68	1.49	1.43
23	8	308	CLA	C1B-C2B	2.68	1.49	1.43
23	b	826	CLA	C1B-C2B	2.68	1.49	1.43
23	8	313	CLA	C1B-C2B	2.68	1.49	1.43
23	a	813	CLA	C1B-C2B	2.68	1.49	1.43
23	1	312	CLA	C3B-C4B	2.68	1.50	1.42
23	6	317	CLA	C1B-C2B	2.68	1.49	1.43
23	b	809	CLA	C1B-C2B	2.68	1.49	1.43
23	5	314	CLA	C1B-C2B	2.67	1.49	1.43
23	b	840	CLA	C1B-C2B	2.67	1.49	1.43
23	5	307	CLA	C1B-C2B	2.67	1.49	1.43
23	b	802	CLA	C1B-C2B	2.67	1.49	1.43
25	h	203	A1L1F	C6-C1	-2.67	1.50	1.54
23	4	315	CLA	C1B-C2B	2.66	1.49	1.43
23	a	815	CLA	C1B-C2B	2.66	1.49	1.43
23	b	835	CLA	C1B-C2B	2.66	1.49	1.43
23	3	307	CLA	C1B-C2B	2.66	1.49	1.43
23	b	810	CLA	C1B-C2B	2.66	1.49	1.43
23	a	827	CLA	C1B-C2B	2.66	1.49	1.43
23	8	312	CLA	C1B-C2B	2.66	1.49	1.43
23	a	819	CLA	C1B-C2B	2.66	1.49	1.43
23	a	836	CLA	C1B-C2B	2.65	1.49	1.43
23	2	314	CLA	C1B-C2B	2.65	1.49	1.43
22	5	303	A1L1G	C33-C34	-2.65	1.40	1.46
23	a	837	CLA	C1B-C2B	2.65	1.49	1.43
23	5	308	CLA	C1B-C2B	2.65	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	808	CLA	C1B-C2B	2.65	1.49	1.43
23	b	829	CLA	CMB-C2B	-2.65	1.45	1.50
23	a	801	CLA	C1B-C2B	2.64	1.49	1.43
23	3	315	CLA	C1B-C2B	2.64	1.49	1.43
22	3	306	A1L1G	C40-C39	-2.64	1.40	1.46
23	b	814	CLA	C1B-C2B	2.64	1.49	1.43
23	b	816	CLA	C1B-C2B	2.64	1.49	1.43
23	a	832	CLA	C1B-C2B	2.63	1.49	1.43
23	l	203	CLA	C1B-C2B	2.63	1.49	1.43
23	a	831	CLA	CMB-C2B	-2.63	1.45	1.50
23	1	310	CLA	C1B-C2B	2.63	1.49	1.43
23	b	838	CLA	C1B-C2B	2.63	1.49	1.43
23	6	313	CLA	C1B-C2B	2.63	1.49	1.43
23	b	825	CLA	C1B-C2B	2.62	1.49	1.43
23	9	314	CLA	C1B-C2B	2.62	1.49	1.43
23	7	311	CLA	C1B-C2B	2.62	1.49	1.43
23	b	824	CLA	C1B-C2B	2.62	1.49	1.43
23	1	312	CLA	C1B-C2B	2.62	1.49	1.43
23	a	833	CLA	C1B-C2B	2.61	1.49	1.43
22	3	306	A1L1G	C33-C34	-2.61	1.40	1.46
23	b	818	CLA	C1B-C2B	2.61	1.49	1.43
23	8	310	CLA	C1B-C2B	2.60	1.49	1.43
23	a	841	CLA	C1B-C2B	2.60	1.49	1.43
23	b	828	CLA	C1B-C2B	2.60	1.49	1.43
23	a	822	CLA	C1B-C2B	2.60	1.49	1.43
25	9	302	A1L1F	O15-C20	-2.60	1.42	1.46
23	7	313	CLA	C1B-C2B	2.58	1.49	1.43
23	b	834	CLA	C1B-C2B	2.58	1.49	1.43
22	9	306	A1L1G	C33-C34	-2.57	1.40	1.46
23	9	309	CLA	C1B-C2B	2.57	1.49	1.43
23	b	819	CLA	C1B-C2B	2.56	1.49	1.43
22	7	302	A1L1G	C33-C34	-2.55	1.40	1.46
23	9	314	CLA	C3B-C4B	2.54	1.50	1.42
23	b	830	CLA	C1B-C2B	2.54	1.49	1.43
22	3	302	A1L1G	C33-C34	-2.53	1.40	1.46
23	a	818	CLA	C1B-C2B	2.53	1.49	1.43
23	a	806	CLA	CMD-C2D	-2.53	1.45	1.50
23	b	829	CLA	CMD-C2D	-2.52	1.45	1.50
23	4	313	CLA	C3B-C4B	2.52	1.50	1.42
22	5	303	A1L1G	C40-C39	-2.51	1.40	1.46
23	3	315	CLA	C3B-C4B	2.51	1.50	1.42
25	1	304	A1L1F	O15-C20	-2.50	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	313	CLA	CHC-C1C	2.49	1.43	1.38
23	4	315	CLA	C3B-C4B	2.48	1.50	1.42
23	a	831	CLA	C1B-C2B	2.48	1.49	1.43
23	7	313	CLA	C3B-C4B	2.48	1.49	1.42
23	5	313	CLA	C3B-C4B	2.48	1.49	1.42
23	a	820	CLA	C1B-C2B	2.48	1.48	1.43
23	a	803	CLA	C1B-C2B	2.47	1.48	1.43
23	a	842	CLA	C3B-C4B	2.47	1.49	1.42
23	4	313	CLA	C1B-C2B	2.47	1.48	1.43
23	b	814	CLA	C3B-C4B	2.46	1.49	1.42
22	3	302	A1L1G	C40-C39	-2.46	1.40	1.46
22	1	301	A1L1G	C33-C34	-2.46	1.40	1.46
23	b	804	CLA	C3B-C4B	2.46	1.49	1.42
23	a	830	CLA	CMC-C2C	-2.45	1.45	1.50
23	a	802	CLA	C1B-C2B	2.45	1.48	1.43
23	a	801	CLA	CMD-C2D	-2.45	1.45	1.50
23	2	314	CLA	C3B-C4B	2.45	1.49	1.42
23	7	313	CLA	CHC-C1C	2.44	1.43	1.38
23	a	827	CLA	C3B-C4B	2.44	1.49	1.42
22	9	306	A1L1G	C40-C39	-2.44	1.40	1.46
23	6	308	CLA	C3B-C4B	2.44	1.49	1.42
23	a	841	CLA	C3B-C4B	2.44	1.49	1.42
23	a	840	CLA	C3B-C4B	2.44	1.49	1.42
23	a	813	CLA	C3B-C4B	2.44	1.49	1.42
23	4	307	CLA	C3B-C4B	2.43	1.49	1.42
23	a	806	CLA	CMC-C2C	-2.43	1.45	1.50
23	6	307	CLA	C3B-C4B	2.43	1.49	1.42
23	b	816	CLA	C3B-C4B	2.43	1.49	1.42
23	2	307	CLA	C1B-C2B	2.43	1.48	1.43
23	a	822	CLA	C3B-C4B	2.43	1.49	1.42
23	a	802	CLA	C3B-C4B	2.43	1.49	1.42
23	9	311	CLA	C3B-C4B	2.43	1.49	1.42
23	a	814	CLA	C3B-C4B	2.43	1.49	1.42
26	a	846	LHG	O8-C6	-2.43	1.39	1.45
23	b	829	CLA	C1B-C2B	2.43	1.48	1.43
23	b	806	CLA	C3B-C4B	2.43	1.49	1.42
22	7	302	A1L1G	C40-C39	-2.43	1.40	1.46
23	b	834	CLA	C3B-C4B	2.42	1.49	1.42
23	b	809	CLA	C3B-C4B	2.42	1.49	1.42
23	9	318	CLA	C3B-C4B	2.42	1.49	1.42
23	2	311	CLA	C3B-C4B	2.42	1.49	1.42
23	b	813	CLA	C3B-C4B	2.41	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	822	CLA	CHC-C1C	2.41	1.43	1.38
23	5	306	CLA	C3B-C4B	2.41	1.49	1.42
23	a	802	CLA	CHC-C1C	2.41	1.43	1.38
23	b	816	CLA	CHC-C1C	2.41	1.43	1.38
23	a	819	CLA	C3B-C4B	2.41	1.49	1.42
23	a	817	CLA	C3B-C4B	2.41	1.49	1.42
23	a	829	CLA	C3B-C4B	2.41	1.49	1.42
26	b	847	LHG	O8-C6	-2.41	1.39	1.45
23	a	806	CLA	CMB-C2B	-2.41	1.45	1.50
23	5	305	CLA	C3B-C4B	2.40	1.49	1.42
23	b	817	CLA	C1B-C2B	2.40	1.48	1.43
26	a	846	LHG	O7-C5	-2.40	1.41	1.46
23	6	311	CLA	C3B-C4B	2.40	1.49	1.42
23	a	804	CLA	C3B-C4B	2.40	1.49	1.42
23	a	816	CLA	C3B-C4B	2.40	1.49	1.42
23	2	315	CLA	C3B-C4B	2.40	1.49	1.42
23	4	308	CLA	C3B-C4B	2.40	1.49	1.42
23	f	803	CLA	C3B-C4B	2.40	1.49	1.42
26	a	845	LHG	O8-C6	-2.40	1.39	1.45
23	b	828	CLA	C3B-C4B	2.40	1.49	1.42
23	8	313	CLA	C3B-C4B	2.39	1.49	1.42
23	b	835	CLA	C3B-C4B	2.39	1.49	1.42
23	4	316	CLA	C3B-C4B	2.39	1.49	1.42
23	6	314	CLA	C3B-C4B	2.39	1.49	1.42
21	3	305	XAT	O4-C5	-2.39	1.43	1.46
23	b	838	CLA	CHC-C1C	2.39	1.43	1.38
23	a	828	CLA	C3B-C4B	2.39	1.49	1.42
23	4	312	CLA	C3B-C4B	2.39	1.49	1.42
23	b	802	CLA	C3B-C4B	2.39	1.49	1.42
23	a	837	CLA	C3B-C4B	2.39	1.49	1.42
23	b	831	CLA	C3B-C4B	2.39	1.49	1.42
23	2	306	CLA	C3B-C4B	2.39	1.49	1.42
23	1	309	CLA	C3B-C4B	2.39	1.49	1.42
23	2	308	CLA	C3B-C4B	2.39	1.49	1.42
23	7	307	CLA	C3B-C4B	2.39	1.49	1.42
23	h	204	CLA	C3B-C4B	2.39	1.49	1.42
23	4	312	CLA	CHC-C1C	2.39	1.43	1.38
23	5	312	CLA	C3B-C4B	2.38	1.49	1.42
23	6	308	CLA	CHC-C1C	2.38	1.43	1.38
26	9	317	LHG	O8-C6	-2.38	1.39	1.45
23	5	315	CLA	C3B-C4B	2.38	1.49	1.42
23	9	308	CLA	C3B-C4B	2.38	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	805	CLA	C3B-C4B	2.38	1.49	1.42
23	a	818	CLA	CHC-C1C	2.38	1.43	1.38
23	b	804	CLA	C1B-C2B	2.38	1.48	1.43
23	j	103	CLA	C3B-C4B	2.38	1.49	1.42
23	a	808	CLA	C3B-C4B	2.38	1.49	1.42
23	a	826	CLA	C3B-C4B	2.38	1.49	1.42
23	b	837	CLA	C3B-C4B	2.38	1.49	1.42
23	8	312	CLA	C3B-C4B	2.38	1.49	1.42
23	2	308	CLA	CHC-C1C	2.38	1.43	1.38
23	2	316	CLA	C3B-C4B	2.38	1.49	1.42
23	8	311	CLA	C3B-C4B	2.38	1.49	1.42
26	9	307	LHG	O8-C6	-2.38	1.39	1.45
23	7	317	CLA	C3B-C4B	2.38	1.49	1.42
23	9	309	CLA	C3B-C4B	2.38	1.49	1.42
23	9	318	CLA	CHC-C1C	2.38	1.43	1.38
23	2	313	CLA	C3B-C4B	2.37	1.49	1.42
23	5	307	CLA	C3B-C4B	2.37	1.49	1.42
23	5	314	CLA	C3B-C4B	2.37	1.49	1.42
23	b	815	CLA	C3B-C4B	2.37	1.49	1.42
23	4	311	CLA	CMD-C2D	-2.37	1.45	1.50
23	1	314	CLA	C3B-C4B	2.37	1.49	1.42
23	5	310	CLA	C3B-C4B	2.37	1.49	1.42
23	a	833	CLA	C3B-C4B	2.37	1.49	1.42
23	4	306	CLA	C3B-C4B	2.37	1.49	1.42
23	a	844	CLA	C3B-C4B	2.37	1.49	1.42
23	3	307	CLA	C3B-C4B	2.37	1.49	1.42
23	7	311	CLA	C3B-C4B	2.37	1.49	1.42
21	4	301	XAT	O24-C25	-2.37	1.43	1.46
23	9	308	CLA	CHC-C1C	2.37	1.43	1.38
23	5	309	CLA	C3B-C4B	2.37	1.49	1.42
23	b	811	CLA	CHC-C1C	2.37	1.43	1.38
23	a	809	CLA	C3B-C4B	2.37	1.49	1.42
23	l	203	CLA	C3B-C4B	2.37	1.49	1.42
21	1	302	XAT	O4-C5	-2.36	1.43	1.46
26	b	847	LHG	O7-C5	-2.36	1.41	1.46
23	9	311	CLA	CHC-C1C	2.36	1.43	1.38
23	a	819	CLA	CHC-C1C	2.36	1.43	1.38
23	b	814	CLA	CHC-C1C	2.36	1.43	1.38
23	6	313	CLA	C3B-C4B	2.36	1.49	1.42
23	8	307	CLA	C3B-C4B	2.36	1.49	1.42
23	4	314	CLA	C3B-C4B	2.36	1.49	1.42
23	7	306	CLA	C3B-C4B	2.36	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	805	CLA	C3B-C4B	2.36	1.49	1.42
23	b	825	CLA	C3B-C4B	2.36	1.49	1.42
23	j	102	CLA	C3B-C4B	2.36	1.49	1.42
23	3	313	CLA	C3B-C4B	2.36	1.49	1.42
23	7	312	CLA	C3B-C4B	2.36	1.49	1.42
23	a	820	CLA	C3B-C4B	2.36	1.49	1.42
23	b	836	CLA	C3B-C4B	2.36	1.49	1.42
23	3	312	CLA	C3B-C4B	2.36	1.49	1.42
23	a	839	CLA	C3B-C4B	2.36	1.49	1.42
23	b	821	CLA	C3B-C4B	2.36	1.49	1.42
23	b	833	CLA	C3B-C4B	2.36	1.49	1.42
23	8	314	CLA	C3B-C4B	2.36	1.49	1.42
23	8	305	CLA	C3B-C4B	2.36	1.49	1.42
23	b	838	CLA	C3B-C4B	2.35	1.49	1.42
23	8	311	CLA	CHC-C1C	2.35	1.43	1.38
23	4	317	CLA	C3B-C4B	2.35	1.49	1.42
23	a	811	CLA	C3B-C4B	2.35	1.49	1.42
23	8	309	CLA	C3B-C4B	2.35	1.49	1.42
23	4	310	CLA	C3B-C4B	2.35	1.49	1.42
23	6	317	CLA	C3B-C4B	2.35	1.49	1.42
23	8	312	CLA	CHC-C1C	2.35	1.43	1.38
23	a	841	CLA	CHC-C1C	2.35	1.43	1.38
23	7	311	CLA	CHC-C1C	2.35	1.43	1.38
23	2	309	CLA	CHC-C1C	2.35	1.43	1.38
21	4	304	XAT	O24-C25	-2.35	1.43	1.46
23	2	309	CLA	C3B-C4B	2.35	1.49	1.42
23	a	835	CLA	C3B-C4B	2.35	1.49	1.42
23	3	315	CLA	CHC-C1C	2.35	1.43	1.38
23	1	313	CLA	C3B-C4B	2.35	1.49	1.42
23	l	204	CLA	C3B-C4B	2.35	1.49	1.42
23	a	829	CLA	CHC-C1C	2.35	1.43	1.38
26	a	845	LHG	O7-C5	-2.35	1.41	1.46
23	a	825	CLA	C3B-C4B	2.35	1.49	1.42
23	1	308	CLA	CHC-C1C	2.35	1.43	1.38
23	b	824	CLA	C3B-C4B	2.35	1.49	1.42
23	b	822	CLA	C3B-C4B	2.34	1.49	1.42
23	b	836	CLA	CHC-C1C	2.34	1.43	1.38
26	9	317	LHG	O8-C23	2.34	1.40	1.33
25	8	304	A1L1F	O15-C20	-2.34	1.43	1.46
23	9	312	CLA	C3B-C4B	2.34	1.49	1.42
23	a	815	CLA	C3B-C4B	2.34	1.49	1.42
23	5	311	CLA	C3B-C4B	2.34	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	832	CLA	C3B-C4B	2.34	1.49	1.42
23	a	854	CLA	C3B-C4B	2.34	1.49	1.42
23	b	805	CLA	CHC-C1C	2.34	1.43	1.38
23	9	310	CLA	C3B-C4B	2.34	1.49	1.42
23	b	807	CLA	C3B-C4B	2.34	1.49	1.42
23	a	804	CLA	CHC-C1C	2.34	1.43	1.38
23	1	308	CLA	C3B-C4B	2.34	1.49	1.42
23	b	835	CLA	CHC-C1C	2.34	1.43	1.38
23	f	802	CLA	C3B-C4B	2.34	1.49	1.42
23	b	802	CLA	CHC-C1C	2.34	1.43	1.38
23	a	801	CLA	CMB-C2B	-2.34	1.46	1.50
23	8	313	CLA	CHC-C1C	2.34	1.43	1.38
23	a	834	CLA	C3B-C4B	2.34	1.49	1.42
23	b	801	CLA	C3B-C4B	2.34	1.49	1.42
23	3	309	CLA	C3B-C4B	2.34	1.49	1.42
23	1	310	CLA	C3B-C4B	2.34	1.49	1.42
23	a	837	CLA	CHC-C1C	2.34	1.43	1.38
23	b	817	CLA	C3B-C4B	2.33	1.49	1.42
23	a	823	CLA	C3B-C4B	2.33	1.49	1.42
26	9	307	LHG	O7-C7	2.33	1.40	1.34
23	a	836	CLA	C3B-C4B	2.33	1.49	1.42
21	5	302	XAT	O4-C5	-2.33	1.43	1.46
23	a	812	CLA	C3B-C4B	2.33	1.49	1.42
23	b	806	CLA	CHC-C1C	2.33	1.43	1.38
23	8	308	CLA	C3B-C4B	2.33	1.49	1.42
23	a	824	CLA	C3B-C4B	2.33	1.49	1.42
22	3	302	A1L1G	C29-C30	-2.33	1.40	1.45
21	9	305	XAT	O4-C5	-2.33	1.43	1.46
23	5	311	CLA	CHC-C1C	2.33	1.43	1.38
23	a	820	CLA	CHC-C1C	2.33	1.43	1.38
23	b	828	CLA	CHC-C1C	2.33	1.43	1.38
23	9	308	CLA	CMC-C2C	-2.33	1.46	1.50
26	9	317	LHG	O7-C5	-2.33	1.41	1.46
23	9	315	CLA	C3B-C4B	2.33	1.49	1.42
23	a	813	CLA	CHC-C1C	2.33	1.43	1.38
23	b	815	CLA	CHC-C1C	2.33	1.43	1.38
26	b	847	LHG	O8-C23	2.33	1.40	1.33
23	8	314	CLA	CHC-C1C	2.33	1.43	1.38
23	a	827	CLA	CHC-C1C	2.33	1.43	1.38
23	a	833	CLA	CHC-C1C	2.33	1.43	1.38
23	b	813	CLA	CHC-C1C	2.33	1.43	1.38
23	5	308	CLA	C3B-C4B	2.33	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	310	CLA	C3B-C4B	2.33	1.49	1.42
23	7	314	CLA	C3B-C4B	2.33	1.49	1.42
21	a	852	XAT	O4-C5	-2.33	1.43	1.46
23	6	313	CLA	CHC-C1C	2.32	1.43	1.38
23	4	311	CLA	C3B-C4B	2.32	1.49	1.42
23	3	311	CLA	C3B-C4B	2.32	1.49	1.42
23	1	202	CLA	C3B-C4B	2.32	1.49	1.42
23	7	312	CLA	CHC-C1C	2.32	1.43	1.38
23	a	826	CLA	CHC-C1C	2.32	1.43	1.38
23	1	311	CLA	C3B-C4B	2.32	1.49	1.42
23	2	312	CLA	C3B-C4B	2.32	1.49	1.42
23	9	313	CLA	C3B-C4B	2.32	1.49	1.42
23	a	830	CLA	C3B-C4B	2.32	1.49	1.42
23	6	311	CLA	CHC-C1C	2.32	1.43	1.38
23	f	803	CLA	CHC-C1C	2.32	1.43	1.38
23	4	309	CLA	C3B-C4B	2.32	1.49	1.42
21	7	301	XAT	O24-C25	-2.32	1.43	1.46
23	7	306	CLA	CHC-C1C	2.32	1.43	1.38
23	a	854	CLA	CHC-C1C	2.32	1.43	1.38
23	5	312	CLA	CHC-C1C	2.32	1.43	1.38
23	2	315	CLA	CHC-C1C	2.32	1.43	1.38
23	7	308	CLA	CHC-C1C	2.32	1.43	1.38
23	7	308	CLA	C3B-C4B	2.32	1.49	1.42
23	2	307	CLA	C3B-C4B	2.32	1.49	1.42
22	1	301	A1L1G	C40-C39	-2.32	1.41	1.46
23	8	310	CLA	C3B-C4B	2.32	1.49	1.42
23	a	844	CLA	CHC-C1C	2.32	1.43	1.38
23	b	825	CLA	CHC-C1C	2.32	1.43	1.38
23	b	839	CLA	C3B-C4B	2.32	1.49	1.42
23	5	314	CLA	CHC-C1C	2.32	1.43	1.38
23	1	310	CLA	CHC-C1C	2.31	1.43	1.38
23	a	832	CLA	CHC-C1C	2.31	1.43	1.38
23	6	310	CLA	C3B-C4B	2.31	1.49	1.42
23	1	307	CLA	C3B-C4B	2.31	1.49	1.42
23	5	306	CLA	CHC-C1C	2.31	1.43	1.38
23	2	313	CLA	CHC-C1C	2.31	1.43	1.38
23	a	809	CLA	CHC-C1C	2.31	1.43	1.38
23	7	315	CLA	C3B-C4B	2.31	1.49	1.42
23	a	821	CLA	C3B-C4B	2.31	1.49	1.42
23	8	309	CLA	CHC-C1C	2.31	1.43	1.38
23	4	314	CLA	CHC-C1C	2.31	1.43	1.38
23	b	812	CLA	C3B-C4B	2.31	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	819	CLA	CMB-C2B	-2.31	1.46	1.50
23	b	832	CLA	CHC-C1C	2.31	1.43	1.38
26	9	307	LHG	O8-C23	2.31	1.40	1.33
23	3	311	CLA	CHC-C1C	2.31	1.43	1.38
23	b	834	CLA	CHC-C1C	2.31	1.43	1.38
23	b	831	CLA	CHC-C1C	2.31	1.43	1.38
23	b	833	CLA	CHC-C1C	2.31	1.43	1.38
23	a	832	CLA	C3B-C4B	2.31	1.49	1.42
21	9	304	XAT	O4-C5	-2.31	1.43	1.46
23	8	305	CLA	CHC-C1C	2.31	1.43	1.38
23	8	306	CLA	CHC-C1C	2.31	1.43	1.38
23	4	315	CLA	CHC-C1C	2.30	1.43	1.38
23	h	204	CLA	CHC-C1C	2.30	1.43	1.38
26	a	845	LHG	O7-C7	2.30	1.40	1.34
23	b	817	CLA	CHC-C1C	2.30	1.43	1.38
26	9	317	LHG	O7-C7	2.30	1.40	1.34
23	1	314	CLA	CHC-C1C	2.30	1.43	1.38
23	a	816	CLA	CHC-C1C	2.30	1.43	1.38
23	3	308	CLA	C3B-C4B	2.30	1.49	1.42
23	6	309	CLA	C3B-C4B	2.30	1.49	1.42
23	7	314	CLA	CHC-C1C	2.30	1.43	1.38
23	b	820	CLA	C3B-C4B	2.30	1.49	1.42
23	b	809	CLA	CMD-C2D	-2.30	1.46	1.50
23	5	309	CLA	CHC-C1C	2.30	1.43	1.38
23	b	812	CLA	CHC-C1C	2.30	1.43	1.38
23	2	310	CLA	C3B-C4B	2.30	1.49	1.42
23	5	313	CLA	CHC-C1C	2.30	1.43	1.38
21	2	303	XAT	O4-C5	-2.30	1.43	1.46
23	5	315	CLA	CHC-C1C	2.30	1.43	1.38
21	2	302	XAT	O4-C5	-2.30	1.43	1.46
23	8	306	CLA	C3B-C4B	2.30	1.49	1.42
23	a	828	CLA	CHC-C1C	2.30	1.43	1.38
23	1	312	CLA	CHC-C1C	2.30	1.43	1.38
23	1	306	CLA	C3B-C4B	2.30	1.49	1.42
23	3	310	CLA	C3B-C4B	2.29	1.49	1.42
23	3	313	CLA	CHC-C1C	2.29	1.43	1.38
23	b	823	CLA	CHC-C1C	2.29	1.43	1.38
23	a	808	CLA	CHC-C1C	2.29	1.43	1.38
23	2	310	CLA	CHC-C1C	2.29	1.43	1.38
23	b	809	CLA	CHC-C1C	2.29	1.43	1.38
23	a	806	CLA	C1D-ND	2.29	1.40	1.37
23	b	827	CLA	C3B-C4B	2.29	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	309	CLA	CHC-C1C	2.29	1.43	1.38
26	9	307	LHG	O7-C5	-2.29	1.41	1.46
23	6	316	CLA	C3B-C4B	2.29	1.49	1.42
23	b	826	CLA	C3B-C4B	2.29	1.49	1.42
23	a	805	CLA	CHC-C1C	2.29	1.43	1.38
23	2	316	CLA	CHC-C1C	2.29	1.43	1.38
23	a	842	CLA	CHC-C1C	2.29	1.43	1.38
23	b	822	CLA	CMD-C2D	-2.29	1.46	1.50
23	1	311	CLA	CHC-C1C	2.29	1.43	1.38
23	7	309	CLA	C3B-C4B	2.29	1.49	1.42
23	b	817	CLA	MG-NB	-2.28	2.01	2.05
23	a	814	CLA	CHC-C1C	2.28	1.43	1.38
26	a	845	LHG	O8-C23	2.28	1.40	1.33
23	4	317	CLA	CHC-C1C	2.28	1.43	1.38
21	3	301	XAT	O24-C25	-2.28	1.43	1.46
23	2	311	CLA	CHC-C1C	2.28	1.43	1.38
23	7	310	CLA	CHC-C1C	2.28	1.43	1.38
23	3	314	CLA	C3B-C4B	2.28	1.49	1.42
23	a	823	CLA	CHC-C1C	2.28	1.43	1.38
21	6	305	XAT	O4-C5	-2.28	1.43	1.46
23	b	822	CLA	CHC-C1C	2.28	1.43	1.38
23	1	305	CLA	C3B-C4B	2.28	1.49	1.42
25	1	304	AIL1F	C6-C1	-2.28	1.50	1.54
21	8	303	XAT	O4-C5	-2.28	1.43	1.46
23	9	314	CLA	CHC-C1C	2.28	1.43	1.38
23	a	824	CLA	CHC-C1C	2.28	1.43	1.38
23	a	810	CLA	C3B-C4B	2.28	1.49	1.42
23	1	309	CLA	CHC-C1C	2.28	1.43	1.38
23	1	202	CLA	CHC-C1C	2.28	1.43	1.38
23	1	203	CLA	CHC-C1C	2.28	1.43	1.38
23	9	316	CLA	C3B-C4B	2.28	1.49	1.42
23	b	827	CLA	CHC-C1C	2.28	1.43	1.38
23	1	204	CLA	CHC-C1C	2.28	1.43	1.38
23	b	808	CLA	C3B-C4B	2.27	1.49	1.42
23	2	312	CLA	CHC-C1C	2.27	1.43	1.38
21	5	301	XAT	O4-C5	-2.27	1.43	1.46
23	9	313	CLA	CHC-C1C	2.27	1.43	1.38
23	1	307	CLA	CHC-C1C	2.27	1.43	1.38
26	a	846	LHG	O8-C23	2.27	1.40	1.33
23	a	838	CLA	C3B-C4B	2.27	1.49	1.42
23	b	819	CLA	C3B-C4B	2.27	1.49	1.42
23	4	308	CLA	CHC-C1C	2.27	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	815	CLA	CHC-C1C	2.27	1.43	1.38
23	a	834	CLA	CHC-C1C	2.27	1.43	1.38
23	j	102	CLA	CHC-C1C	2.27	1.43	1.38
23	6	315	CLA	C3B-C4B	2.27	1.49	1.42
23	f	802	CLA	CHC-C1C	2.27	1.43	1.38
23	6	312	CLA	C3B-C4B	2.27	1.49	1.42
23	b	837	CLA	CHC-C1C	2.27	1.43	1.38
23	9	312	CLA	CHC-C1C	2.27	1.43	1.38
23	3	312	CLA	CHC-C1C	2.27	1.43	1.38
23	b	830	CLA	C3B-C4B	2.27	1.49	1.42
23	8	310	CLA	CHC-C1C	2.27	1.43	1.38
23	3	309	CLA	CHC-C1C	2.27	1.43	1.38
23	b	807	CLA	CHC-C1C	2.27	1.43	1.38
26	a	846	LHG	O7-C7	2.27	1.40	1.34
23	6	307	CLA	CHC-C1C	2.27	1.43	1.38
23	b	818	CLA	C3B-C4B	2.27	1.49	1.42
21	4	305	XAT	O4-C5	-2.27	1.43	1.46
23	b	830	CLA	CMD-C2D	-2.27	1.46	1.50
22	9	301	A1L1G	C40-C39	-2.27	1.41	1.46
23	9	309	CLA	CHC-C1C	2.27	1.43	1.38
23	6	314	CLA	CHC-C1C	2.27	1.43	1.38
23	3	307	CLA	CHC-C1C	2.27	1.43	1.38
23	4	310	CLA	CHC-C1C	2.26	1.43	1.38
23	2	314	CLA	CHC-C1C	2.26	1.43	1.38
23	b	830	CLA	CHC-C1C	2.26	1.43	1.38
23	b	830	CLA	MG-NB	-2.26	2.01	2.05
23	5	310	CLA	CHC-C1C	2.26	1.43	1.38
23	9	310	CLA	CHC-C1C	2.26	1.43	1.38
23	b	823	CLA	C3B-C4B	2.26	1.49	1.42
21	8	302	XAT	O4-C5	-2.26	1.43	1.46
21	a	852	XAT	O24-C25	-2.26	1.43	1.46
23	3	310	CLA	CHC-C1C	2.26	1.43	1.38
23	a	830	CLA	CHC-C1C	2.26	1.43	1.38
23	a	839	CLA	CHC-C1C	2.26	1.43	1.38
21	1	303	XAT	O4-C5	-2.26	1.43	1.46
23	a	803	CLA	CHC-C1C	2.26	1.43	1.38
21	5	302	XAT	O24-C25	-2.25	1.43	1.46
21	7	305	XAT	O4-C5	-2.25	1.43	1.46
23	4	307	CLA	CHC-C1C	2.25	1.43	1.38
23	a	836	CLA	CHC-C1C	2.25	1.43	1.38
21	7	303	XAT	O4-C5	-2.25	1.43	1.46
23	b	803	CLA	C3B-C4B	2.25	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	305	XAT	O4-C5	-2.25	1.43	1.46
23	a	812	CLA	CHC-C1C	2.25	1.43	1.38
21	3	304	XAT	O4-C5	-2.25	1.43	1.46
23	a	817	CLA	CHC-C1C	2.25	1.43	1.38
23	b	823	CLA	CMD-C2D	-2.25	1.46	1.50
23	b	840	CLA	CHC-C1C	2.25	1.43	1.38
26	b	847	LHG	O7-C7	2.25	1.40	1.34
23	6	309	CLA	CHC-C1C	2.25	1.43	1.38
23	a	824	CLA	CMD-C2D	-2.25	1.46	1.50
21	2	301	XAT	O4-C5	-2.24	1.43	1.46
23	7	315	CLA	CHC-C1C	2.24	1.43	1.38
22	9	301	A1L1G	C29-C30	-2.24	1.40	1.45
23	1	305	CLA	CHC-C1C	2.24	1.43	1.38
23	b	810	CLA	CMB-C2B	-2.24	1.46	1.50
23	5	307	CLA	CHC-C1C	2.24	1.43	1.38
23	6	316	CLA	CHC-C1C	2.24	1.43	1.38
23	a	811	CLA	CHC-C1C	2.24	1.43	1.38
23	b	821	CLA	CHC-C1C	2.24	1.43	1.38
23	3	314	CLA	CHC-C1C	2.24	1.43	1.38
23	b	801	CLA	CMB-C2B	-2.24	1.46	1.50
23	7	316	CLA	C3B-C4B	2.24	1.49	1.42
23	a	803	CLA	C3B-C4B	2.24	1.49	1.42
23	1	313	CLA	CHC-C1C	2.24	1.43	1.38
21	3	301	XAT	O4-C5	-2.24	1.43	1.46
23	6	317	CLA	CHC-C1C	2.24	1.43	1.38
23	b	824	CLA	CHC-C1C	2.24	1.43	1.38
23	9	315	CLA	CHC-C1C	2.24	1.43	1.38
23	2	307	CLA	CMB-C2B	-2.24	1.46	1.50
23	7	307	CLA	CHC-C1C	2.23	1.43	1.38
21	4	303	XAT	O4-C5	-2.23	1.43	1.46
23	7	317	CLA	CHC-C1C	2.23	1.43	1.38
23	5	305	CLA	CHC-C1C	2.23	1.43	1.38
23	a	835	CLA	CHC-C1C	2.23	1.43	1.38
23	a	810	CLA	CMD-C2D	-2.23	1.46	1.50
23	b	840	CLA	C3B-C4B	2.23	1.49	1.42
23	a	807	CLA	C3B-C4B	2.23	1.49	1.42
21	7	304	XAT	O4-C5	-2.23	1.43	1.46
23	5	308	CLA	CHC-C1C	2.23	1.43	1.38
23	b	839	CLA	CMB-C2B	-2.23	1.46	1.50
23	b	804	CLA	CHC-C1C	2.23	1.43	1.38
21	8	301	XAT	O4-C5	-2.23	1.43	1.46
21	6	306	XAT	O4-C5	-2.23	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	304	XAT	O24-C25	-2.23	1.43	1.46
25	6	304	A1L1F	O15-C20	-2.23	1.43	1.46
23	4	311	CLA	CMB-C2B	-2.23	1.46	1.50
21	4	304	XAT	O4-C5	-2.23	1.43	1.46
21	4	301	XAT	O4-C5	-2.23	1.43	1.46
23	3	307	CLA	CMD-C2D	-2.23	1.46	1.50
23	7	309	CLA	CHC-C1C	2.22	1.42	1.38
23	a	801	CLA	CMC-C2C	-2.22	1.46	1.50
21	3	303	XAT	O4-C5	-2.22	1.43	1.46
23	a	828	CLA	CMC-C2C	-2.22	1.46	1.50
21	6	306	XAT	O24-C25	-2.22	1.43	1.46
23	7	314	CLA	CMD-C2D	-2.22	1.46	1.50
21	3	304	XAT	O24-C25	-2.22	1.43	1.46
23	8	307	CLA	CHC-C1C	2.22	1.42	1.38
23	3	308	CLA	CHC-C1C	2.22	1.42	1.38
23	a	810	CLA	CHC-C1C	2.22	1.42	1.38
23	b	810	CLA	C3B-C4B	2.22	1.49	1.42
23	a	831	CLA	C3B-C4B	2.22	1.49	1.42
23	a	830	CLA	CMD-C2D	-2.22	1.46	1.50
23	a	821	CLA	CHC-C1C	2.22	1.42	1.38
23	7	316	CLA	CMD-C2D	-2.22	1.46	1.50
23	a	840	CLA	CHC-C1C	2.22	1.42	1.38
22	1	301	A1L1G	C38-C39	2.21	1.40	1.35
21	3	303	XAT	O24-C25	-2.21	1.43	1.46
23	6	315	CLA	CHC-C1C	2.21	1.42	1.38
23	b	820	CLA	CHC-C1C	2.21	1.42	1.38
23	4	306	CLA	CHC-C1C	2.21	1.42	1.38
23	6	310	CLA	CHC-C1C	2.21	1.42	1.38
23	a	825	CLA	CHC-C1C	2.21	1.42	1.38
23	a	833	CLA	MG-NB	-2.21	2.01	2.05
23	b	803	CLA	CMD-C2D	-2.21	1.46	1.50
21	6	303	XAT	O24-C25	-2.21	1.43	1.46
23	b	803	CLA	CHC-C1C	2.21	1.42	1.38
21	6	303	XAT	O4-C5	-2.21	1.43	1.46
23	4	311	CLA	CHC-C1C	2.21	1.42	1.38
23	4	316	CLA	CHC-C1C	2.21	1.42	1.38
23	a	838	CLA	CHC-C1C	2.20	1.42	1.38
23	a	832	CLA	MG-NB	-2.20	2.01	2.05
23	b	819	CLA	CHC-C1C	2.20	1.42	1.38
23	8	308	CLA	CHC-C1C	2.20	1.42	1.38
23	5	305	CLA	CMD-C2D	-2.20	1.46	1.50
23	b	829	CLA	C3B-C4B	2.20	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	310	CLA	MG-NB	-2.20	2.01	2.05
23	a	806	CLA	CAA-C2A	-2.20	1.50	1.54
23	1	306	CLA	CHC-C1C	2.20	1.42	1.38
23	a	804	CLA	CMC-C2C	-2.19	1.46	1.50
21	6	302	XAT	O4-C5	-2.19	1.43	1.46
21	9	305	XAT	O24-C25	-2.19	1.43	1.46
23	2	306	CLA	CHC-C1C	2.19	1.42	1.38
23	b	801	CLA	CHC-C1C	2.19	1.42	1.38
23	a	832	CLA	CMB-C2B	-2.19	1.46	1.50
23	b	808	CLA	CHC-C1C	2.19	1.42	1.38
23	6	313	CLA	MG-NB	-2.19	2.01	2.05
21	j	101	XAT	O4-C5	-2.19	1.43	1.46
22	3	306	A1L1G	C29-C30	-2.19	1.40	1.45
23	8	310	CLA	CMB-C2B	-2.19	1.46	1.50
23	b	830	CLA	CMB-C2B	-2.19	1.46	1.50
23	a	801	CLA	C3B-C4B	2.19	1.49	1.42
23	9	309	CLA	MG-NB	-2.19	2.01	2.05
21	4	303	XAT	O24-C25	-2.19	1.43	1.46
22	1	301	A1L1G	C29-C30	-2.19	1.40	1.45
23	a	803	CLA	MG-NB	-2.19	2.01	2.05
23	9	309	CLA	CMD-C2D	-2.19	1.46	1.50
23	2	310	CLA	CMB-C2B	-2.18	1.46	1.50
21	1	302	XAT	O24-C25	-2.18	1.43	1.46
23	a	807	CLA	CHC-C1C	2.18	1.42	1.38
23	b	829	CLA	MG-NB	-2.18	2.01	2.05
21	6	305	XAT	O24-C25	-2.18	1.43	1.46
21	8	303	XAT	O24-C25	-2.18	1.43	1.46
25	6	301	A1L1F	C6-C1	-2.18	1.50	1.54
23	a	806	CLA	C1B-NB	-2.18	1.35	1.37
23	9	316	CLA	CHC-C1C	2.18	1.42	1.38
23	a	836	CLA	CMB-C2B	-2.17	1.46	1.50
23	2	307	CLA	CHC-C1C	2.17	1.42	1.38
21	4	302	XAT	O24-C25	-2.17	1.43	1.46
23	a	831	CLA	MG-NB	-2.17	2.01	2.05
23	b	814	CLA	CMD-C2D	-2.17	1.46	1.50
23	b	826	CLA	CHC-C1C	2.17	1.42	1.38
23	a	807	CLA	MG-NB	-2.17	2.01	2.05
21	8	302	XAT	O24-C25	-2.17	1.43	1.46
23	2	310	CLA	CMD-C2D	-2.17	1.46	1.50
23	a	801	CLA	CHC-C1C	2.16	1.42	1.38
23	b	817	CLA	CMB-C2B	-2.16	1.46	1.50
23	b	804	CLA	MG-NB	-2.16	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	305	XAT	O24-C25	-2.16	1.43	1.46
23	a	820	CLA	CMB-C2B	-2.16	1.46	1.50
21	2	304	XAT	O4-C5	-2.16	1.43	1.46
23	b	838	CLA	CMD-C2D	-2.16	1.46	1.50
23	b	834	CLA	CMB-C2B	-2.16	1.46	1.50
23	b	819	CLA	MG-NB	-2.16	2.01	2.05
23	b	801	CLA	CMD-C2D	-2.16	1.46	1.50
23	j	103	CLA	CHC-C1C	2.16	1.42	1.38
23	b	837	CLA	CMD-C2D	-2.15	1.46	1.50
21	2	304	XAT	O24-C25	-2.15	1.43	1.46
23	b	828	CLA	CMD-C2D	-2.15	1.46	1.50
23	7	316	CLA	CHC-C1C	2.15	1.42	1.38
23	a	820	CLA	MG-NB	-2.15	2.01	2.05
21	2	302	XAT	O24-C25	-2.15	1.43	1.46
22	5	303	A1L1G	C29-C30	-2.15	1.40	1.45
21	4	302	XAT	O4-C5	-2.15	1.43	1.46
23	8	310	CLA	MG-NB	-2.15	2.01	2.05
21	j	101	XAT	O24-C25	-2.15	1.43	1.46
21	5	301	XAT	O24-C25	-2.15	1.43	1.46
21	2	301	XAT	O24-C25	-2.15	1.43	1.46
23	b	811	CLA	CMD-C2D	-2.15	1.46	1.50
23	5	312	CLA	MG-NB	-2.15	2.01	2.05
21	5	304	XAT	O24-C25	-2.15	1.43	1.46
23	2	316	CLA	CMD-C2D	-2.15	1.46	1.50
23	b	823	CLA	MG-NB	-2.14	2.01	2.05
21	5	304	XAT	O4-C5	-2.14	1.43	1.46
22	1	301	A1L1G	C35-C34	2.14	1.40	1.35
23	a	828	CLA	MG-NB	-2.14	2.01	2.05
23	b	818	CLA	CMB-C2B	-2.14	1.46	1.50
23	b	832	CLA	MG-NB	-2.14	2.01	2.05
23	a	802	CLA	MG-NB	-2.13	2.01	2.05
23	a	821	CLA	CMD-C2D	-2.13	1.46	1.50
23	2	307	CLA	MG-NB	-2.13	2.01	2.05
23	9	312	CLA	CMD-C2D	-2.13	1.46	1.50
23	a	812	CLA	CMD-C2D	-2.13	1.46	1.50
23	1	307	CLA	MG-NB	-2.13	2.01	2.05
23	b	835	CLA	MG-NB	-2.13	2.01	2.05
21	2	303	XAT	O24-C25	-2.13	1.43	1.46
23	a	803	CLA	CMB-C2B	-2.13	1.46	1.50
23	9	309	CLA	CMB-C2B	-2.13	1.46	1.50
23	9	318	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	816	CLA	MG-NB	-2.13	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	828	CLA	CMB-C2B	-2.13	1.46	1.50
22	9	301	A1L1G	C38-C39	2.13	1.40	1.35
23	6	312	CLA	CMD-C2D	-2.13	1.46	1.50
23	a	801	CLA	MG-NB	-2.13	2.01	2.05
23	6	312	CLA	CHC-C1C	2.12	1.42	1.38
23	b	818	CLA	CHC-C1C	2.12	1.42	1.38
23	a	802	CLA	CMB-C2B	-2.12	1.46	1.50
23	8	312	CLA	MG-NB	-2.12	2.01	2.05
23	a	824	CLA	CMB-C2B	-2.12	1.46	1.50
23	7	311	CLA	CMB-C2B	-2.12	1.46	1.50
26	9	317	LHG	P-O6	2.12	1.67	1.59
23	a	832	CLA	CMD-C2D	-2.12	1.46	1.50
21	8	301	XAT	O24-C25	-2.12	1.43	1.46
23	b	824	CLA	MG-NB	-2.12	2.01	2.05
23	b	809	CLA	CMC-C2C	-2.12	1.46	1.50
26	9	307	LHG	P-O6	2.12	1.67	1.59
23	3	307	CLA	MG-NB	-2.12	2.01	2.05
23	a	842	CLA	CMD-C2D	-2.12	1.46	1.50
23	7	310	CLA	MG-NB	-2.11	2.01	2.05
23	a	838	CLA	MG-NB	-2.11	2.01	2.05
23	b	825	CLA	MG-NB	-2.11	2.01	2.05
23	a	810	CLA	MG-NB	-2.11	2.01	2.05
22	7	302	A1L1G	C38-C39	2.11	1.40	1.35
23	2	309	CLA	MG-NB	-2.11	2.01	2.05
23	a	822	CLA	CMB-C2B	-2.11	1.46	1.50
23	5	308	CLA	MG-NB	-2.11	2.01	2.05
23	6	315	CLA	MG-NB	-2.11	2.01	2.05
23	b	822	CLA	MG-NB	-2.11	2.01	2.05
26	b	847	LHG	P-O6	2.11	1.67	1.59
23	4	317	CLA	CMB-C2B	-2.11	1.46	1.50
23	7	309	CLA	MG-NB	-2.11	2.01	2.05
23	a	806	CLA	C4B-NB	2.11	1.40	1.37
23	b	810	CLA	CHC-C1C	2.11	1.42	1.38
23	3	310	CLA	MG-NB	-2.11	2.01	2.05
23	3	309	CLA	CMD-C2D	-2.10	1.46	1.50
21	3	305	XAT	O24-C25	-2.10	1.43	1.46
26	a	845	LHG	P-O6	2.10	1.67	1.59
21	7	301	XAT	O4-C5	-2.10	1.43	1.46
21	7	303	XAT	O24-C25	-2.10	1.43	1.46
23	5	307	CLA	MG-NB	-2.10	2.01	2.05
23	3	307	CLA	CMB-C2B	-2.10	1.46	1.50
23	a	816	CLA	CMD-C2D	-2.10	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	312	CLA	CMB-C2B	-2.10	1.46	1.50
21	9	303	XAT	O24-C25	-2.10	1.43	1.46
22	9	306	A1L1G	C29-C30	-2.10	1.40	1.45
23	b	808	CLA	MG-NB	-2.10	2.01	2.05
23	b	840	CLA	MG-NB	-2.10	2.01	2.05
23	1	313	CLA	CMD-C2D	-2.10	1.46	1.50
23	a	816	CLA	MG-NB	-2.10	2.01	2.05
23	1	313	CLA	MG-NB	-2.10	2.01	2.05
23	b	825	CLA	CMD-C2D	-2.10	1.46	1.50
23	l	203	CLA	CMB-C2B	-2.10	1.46	1.50
23	7	316	CLA	MG-NB	-2.10	2.01	2.05
23	b	810	CLA	MG-NB	-2.10	2.01	2.05
23	4	308	CLA	MG-NB	-2.10	2.01	2.05
23	7	312	CLA	CMD-C2D	-2.10	1.46	1.50
23	a	826	CLA	CMD-C2D	-2.10	1.46	1.50
23	1	310	CLA	MG-NB	-2.10	2.01	2.05
23	4	309	CLA	MG-NB	-2.10	2.01	2.05
23	b	813	CLA	MG-NB	-2.10	2.01	2.05
23	8	305	CLA	MG-NB	-2.09	2.01	2.05
22	9	301	A1L1G	C35-C34	2.09	1.40	1.35
23	a	807	CLA	CMD-C2D	-2.09	1.46	1.50
23	9	315	CLA	MG-NB	-2.09	2.01	2.05
22	9	306	A1L1G	C35-C34	2.09	1.40	1.35
22	3	302	A1L1G	C35-C34	2.09	1.40	1.35
23	4	308	CLA	CMD-C2D	-2.09	1.46	1.50
23	a	837	CLA	CMB-C2B	-2.09	1.46	1.50
23	8	306	CLA	MG-NB	-2.09	2.01	2.05
23	3	309	CLA	MG-NB	-2.09	2.01	2.05
23	b	809	CLA	CMB-C2B	-2.09	1.46	1.50
23	4	311	CLA	MG-NB	-2.09	2.01	2.05
23	8	308	CLA	MG-NB	-2.09	2.01	2.05
23	4	314	CLA	MG-NB	-2.09	2.01	2.05
23	a	808	CLA	CMB-C2B	-2.09	1.46	1.50
23	a	834	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	834	CLA	MG-NB	-2.09	2.01	2.05
23	7	311	CLA	CMD-C2D	-2.09	1.46	1.50
23	5	308	CLA	CMD-C2D	-2.09	1.46	1.50
23	3	315	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	826	CLA	MG-NB	-2.09	2.01	2.05
21	1	303	XAT	O24-C25	-2.09	1.43	1.46
23	8	313	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	831	CLA	MG-NB	-2.08	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	822	CLA	MG-NB	-2.08	2.01	2.05
23	b	838	CLA	MG-NB	-2.08	2.01	2.05
23	1	309	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	815	CLA	CMC-C2C	-2.08	1.46	1.50
23	2	306	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	803	CLA	CMC-C2C	-2.08	1.46	1.50
23	a	826	CLA	MG-NB	-2.08	2.01	2.05
23	1	204	CLA	CMC-C2C	-2.08	1.46	1.50
23	b	812	CLA	MG-NB	-2.08	2.01	2.05
23	b	807	CLA	MG-NB	-2.08	2.01	2.05
21	9	305	XAT	C26-C27	2.08	1.54	1.50
23	b	834	CLA	CMD-C2D	-2.08	1.46	1.50
23	6	309	CLA	MG-NB	-2.08	2.01	2.05
23	j	102	CLA	CMD-C2D	-2.08	1.46	1.50
23	8	310	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	819	CLA	CMD-C2D	-2.08	1.46	1.50
23	8	307	CLA	MG-NB	-2.08	2.01	2.05
23	1	202	CLA	MG-NB	-2.08	2.01	2.05
23	1	307	CLA	CMB-C2B	-2.08	1.46	1.50
23	a	806	CLA	MG-ND	-2.08	2.01	2.05
23	6	313	CLA	CMB-C2B	-2.07	1.46	1.50
23	b	802	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	833	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	818	CLA	CMB-C2B	-2.07	1.46	1.50
23	1	306	CLA	MG-NB	-2.07	2.01	2.05
23	a	827	CLA	MG-NB	-2.07	2.01	2.05
23	a	827	CLA	CMD-C2D	-2.07	1.46	1.50
23	4	313	CLA	CMB-C2B	-2.07	1.46	1.50
23	6	317	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	839	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	815	CLA	MG-NB	-2.07	2.01	2.05
23	b	827	CLA	CMD-C2D	-2.07	1.46	1.50
23	7	312	CLA	MG-NB	-2.07	2.01	2.05
23	6	308	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	808	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	828	CLA	MG-NB	-2.07	2.01	2.05
23	7	314	CLA	MG-NB	-2.07	2.01	2.05
23	5	310	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	807	CLA	CMD-C2D	-2.07	1.46	1.50
23	1	203	CLA	CMC-C2C	-2.07	1.46	1.50
23	a	808	CLA	MG-NB	-2.07	2.01	2.05
23	a	814	CLA	MG-NB	-2.07	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	854	CLA	MG-NB	-2.07	2.01	2.05
23	7	306	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	820	CLA	CMD-C2D	-2.07	1.46	1.50
23	5	312	CLA	CMB-C2B	-2.06	1.46	1.50
23	7	313	CLA	MG-NB	-2.06	2.01	2.05
23	a	825	CLA	MG-NB	-2.06	2.01	2.05
27	b	848	DGD	C1E-C2E	2.06	1.58	1.52
23	7	308	CLA	MG-NB	-2.06	2.01	2.05
23	b	811	CLA	MG-NB	-2.06	2.01	2.05
21	9	304	XAT	O24-C25	-2.06	1.43	1.46
23	2	314	CLA	CMC-C2C	-2.06	1.46	1.50
23	b	811	CLA	CMB-C2B	-2.06	1.46	1.50
21	6	302	XAT	O24-C25	-2.06	1.43	1.46
22	3	302	A1L1G	C38-C39	2.06	1.40	1.35
23	a	819	CLA	CMD-C2D	-2.06	1.46	1.50
23	7	311	CLA	MG-NB	-2.06	2.01	2.05
22	3	306	A1L1G	C38-C39	2.06	1.40	1.35
23	2	314	CLA	CMD-C2D	-2.06	1.46	1.50
23	4	312	CLA	CMD-C2D	-2.06	1.46	1.50
23	2	312	CLA	MG-NB	-2.06	2.01	2.05
23	1	202	CLA	CMB-C2B	-2.06	1.46	1.50
21	4	305	XAT	O24-C25	-2.06	1.43	1.46
23	8	311	CLA	MG-NB	-2.06	2.01	2.05
23	2	308	CLA	MG-NB	-2.06	2.01	2.05
23	a	824	CLA	MG-NB	-2.06	2.01	2.05
23	6	315	CLA	CMD-C2D	-2.06	1.46	1.50
23	a	854	CLA	CMB-C2B	-2.06	1.46	1.50
23	a	811	CLA	MG-NB	-2.06	2.01	2.05
23	a	817	CLA	CMB-C2B	-2.06	1.46	1.50
23	4	312	CLA	MG-NB	-2.06	2.01	2.05
23	3	314	CLA	MG-NB	-2.06	2.01	2.05
23	b	801	CLA	MG-NB	-2.06	2.01	2.05
23	9	316	CLA	MG-NB	-2.05	2.01	2.05
21	7	305	XAT	O24-C25	-2.05	1.43	1.46
23	9	316	CLA	CMD-C2D	-2.05	1.46	1.50
23	3	314	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	804	CLA	CMD-C2D	-2.05	1.46	1.50
23	h	204	CLA	MG-NB	-2.05	2.01	2.05
23	9	314	CLA	CMD-C2D	-2.05	1.46	1.50
23	7	315	CLA	CMD-C2D	-2.05	1.46	1.50
23	9	310	CLA	MG-NB	-2.05	2.01	2.05
23	a	830	CLA	MG-NB	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	l	203	CLA	MG-NB	-2.05	2.01	2.05
23	b	832	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	817	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	823	CLA	MG-NB	-2.05	2.01	2.05
23	a	810	CLA	CMB-C2B	-2.05	1.46	1.50
23	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	825	CLA	CMB-C2B	-2.05	1.46	1.50
23	9	308	CLA	MG-NB	-2.05	2.01	2.05
23	b	837	CLA	MG-NB	-2.05	2.01	2.05
23	b	835	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	818	CLA	MG-NB	-2.05	2.01	2.05
23	8	308	CLA	CMD-C2D	-2.05	1.46	1.50
23	2	312	CLA	CMD-C2D	-2.05	1.46	1.50
23	2	316	CLA	MG-NB	-2.05	2.01	2.05
23	5	311	CLA	MG-NB	-2.05	2.01	2.05
23	a	802	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	813	CLA	CMD-C2D	-2.05	1.46	1.50
23	6	312	CLA	MG-NB	-2.05	2.01	2.05
23	1	305	CLA	MG-NB	-2.05	2.01	2.05
23	a	829	CLA	CMD-C2D	-2.05	1.46	1.50
26	a	846	LHG	P-O6	2.05	1.67	1.59
23	a	805	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	817	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	820	CLA	MG-NB	-2.05	2.01	2.05
23	b	827	CLA	MG-NB	-2.05	2.01	2.05
23	f	802	CLA	MG-NB	-2.05	2.01	2.05
23	4	317	CLA	CMD-C2D	-2.05	1.46	1.50
23	3	308	CLA	CMD-C2D	-2.05	1.46	1.50
23	7	313	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	810	CLA	CMD-C2D	-2.05	1.46	1.50
23	2	309	CLA	CMD-C2D	-2.05	1.46	1.50
23	1	309	CLA	CMB-C2B	-2.05	1.46	1.50
23	7	315	CLA	CMB-C2B	-2.04	1.46	1.50
23	a	831	CLA	CMD-C2D	-2.04	1.46	1.50
23	l	202	CLA	CMD-C2D	-2.04	1.46	1.50
23	6	311	CLA	CMD-C2D	-2.04	1.46	1.50
23	b	839	CLA	CMD-C2D	-2.04	1.46	1.50
23	8	309	CLA	MG-NB	-2.04	2.01	2.05
23	a	823	CLA	CMD-C2D	-2.04	1.46	1.50
23	a	837	CLA	CMD-C2D	-2.04	1.46	1.50
23	l	204	CLA	CMB-C2B	-2.04	1.46	1.50
23	7	306	CLA	MG-NB	-2.04	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	815	CLA	MG-NB	-2.04	2.01	2.05
23	1	307	CLA	CMD-C2D	-2.04	1.46	1.50
23	6	311	CLA	MG-NB	-2.04	2.01	2.05
23	8	308	CLA	CMB-C2B	-2.04	1.46	1.50
23	a	811	CLA	CMD-C2D	-2.04	1.46	1.50
23	5	309	CLA	MG-NB	-2.04	2.01	2.05
23	a	839	CLA	MG-NB	-2.04	2.01	2.05
23	3	313	CLA	MG-NB	-2.04	2.01	2.05
23	a	844	CLA	MG-NB	-2.04	2.01	2.05
23	4	307	CLA	CMD-C2D	-2.04	1.46	1.50
23	5	305	CLA	MG-NB	-2.04	2.01	2.05
23	9	312	CLA	MG-NB	-2.04	2.01	2.05
23	9	313	CLA	MG-NB	-2.04	2.01	2.05
23	b	821	CLA	MG-NB	-2.04	2.01	2.05
23	a	813	CLA	CMD-C2D	-2.04	1.46	1.50
23	a	819	CLA	CMC-C2C	-2.04	1.46	1.50
23	b	824	CLA	CMB-C2B	-2.04	1.46	1.50
23	1	309	CLA	MG-NB	-2.04	2.01	2.05
23	a	819	CLA	MG-NB	-2.04	2.01	2.05
23	a	831	CLA	CHC-C1C	2.04	1.42	1.38
23	3	312	CLA	CMD-C2D	-2.04	1.46	1.50
23	7	310	CLA	CMD-C2D	-2.04	1.46	1.50
23	a	844	CLA	CMD-C2D	-2.04	1.46	1.50
23	3	311	CLA	MG-NB	-2.04	2.01	2.05
23	7	315	CLA	MG-NB	-2.04	2.01	2.05
23	a	812	CLA	MG-NB	-2.04	2.01	2.05
23	4	315	CLA	CMD-C2D	-2.04	1.46	1.50
23	8	311	CLA	CMD-C2D	-2.04	1.46	1.50
23	a	803	CLA	CMD-C2D	-2.04	1.46	1.50
23	4	317	CLA	MG-NB	-2.04	2.01	2.05
23	2	311	CLA	CMC-C2C	-2.04	1.46	1.50
23	b	809	CLA	MG-NB	-2.04	2.01	2.05
23	9	310	CLA	CMD-C2D	-2.04	1.46	1.50
23	4	306	CLA	CMD-C2D	-2.04	1.46	1.50
23	6	307	CLA	CMD-C2D	-2.04	1.46	1.50
23	2	315	CLA	CMD-C2D	-2.04	1.46	1.50
23	2	313	CLA	MG-NB	-2.04	2.01	2.05
23	4	314	CLA	CMD-C2D	-2.04	1.46	1.50
23	2	311	CLA	CMD-C2D	-2.04	1.46	1.50
23	7	317	CLA	CMD-C2D	-2.04	1.46	1.50
23	h	204	CLA	CMC-C2C	-2.04	1.46	1.50
23	j	103	CLA	CMB-C2B	-2.04	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	808	CLA	CMD-C2D	-2.03	1.46	1.50
23	1	311	CLA	MG-NB	-2.03	2.01	2.05
23	a	814	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	842	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	809	CLA	MG-NB	-2.03	2.01	2.05
23	9	308	CLA	CMD-C2D	-2.03	1.46	1.50
23	7	314	CLA	CMB-C2B	-2.03	1.46	1.50
23	2	308	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	809	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	836	CLA	MG-NB	-2.03	2.01	2.05
23	b	813	CLA	CMC-C2C	-2.03	1.46	1.50
23	a	838	CLA	CMD-C2D	-2.03	1.46	1.50
23	5	311	CLA	CMD-C2D	-2.03	1.46	1.50
23	2	307	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	816	CLA	CMC-C2C	-2.03	1.46	1.50
23	5	315	CLA	MG-NB	-2.03	2.01	2.05
23	3	311	CLA	CMB-C2B	-2.03	1.46	1.50
23	3	313	CLA	CMD-C2D	-2.03	1.46	1.50
23	7	308	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	804	CLA	MG-NB	-2.03	2.01	2.05
23	8	313	CLA	CMC-C2C	-2.03	1.46	1.50
23	7	307	CLA	CMD-C2D	-2.03	1.46	1.50
23	1	204	CLA	CMD-C2D	-2.03	1.46	1.50
23	2	312	CLA	CMC-C2C	-2.03	1.46	1.50
23	a	841	CLA	CMC-C2C	-2.03	1.46	1.50
23	b	805	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	812	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	840	CLA	CMD-C2D	-2.03	1.46	1.50
23	4	312	CLA	CMB-C2B	-2.03	1.46	1.50
23	6	309	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	835	CLA	CMD-C2D	-2.03	1.46	1.50
23	6	310	CLA	CMD-C2D	-2.03	1.46	1.50
23	5	314	CLA	CMD-C2D	-2.03	1.46	1.50
23	8	313	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	822	CLA	CMD-C2D	-2.03	1.46	1.50
23	1	204	CLA	MG-NB	-2.03	2.01	2.05
23	4	306	CLA	MG-NB	-2.03	2.01	2.05
23	a	828	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	826	CLA	CMD-C2D	-2.03	1.46	1.50
23	8	309	CLA	CMD-C2D	-2.03	1.46	1.50
23	1	305	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	840	CLA	CMB-C2B	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	842	CLA	MG-NB	-2.03	2.01	2.05
23	b	812	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	815	CLA	CMD-C2D	-2.03	1.46	1.50
23	l	203	CLA	CMD-C2D	-2.03	1.46	1.50
23	5	314	CLA	MG-NB	-2.03	2.01	2.05
23	7	307	CLA	CMB-C2B	-2.03	1.46	1.50
23	1	314	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	815	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	838	CLA	CMB-C2B	-2.03	1.46	1.50
23	4	315	CLA	CMB-C2B	-2.02	1.46	1.50
23	a	814	CLA	CMC-C2C	-2.02	1.46	1.50
23	a	815	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	821	CLA	MG-NB	-2.02	2.01	2.05
23	8	305	CLA	CMD-C2D	-2.02	1.46	1.50
23	6	308	CLA	MG-NB	-2.02	2.01	2.05
23	1	310	CLA	CMB-C2B	-2.02	1.46	1.50
23	f	803	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	829	CLA	CHC-C1C	2.02	1.42	1.38
23	1	314	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	835	CLA	CMB-C2B	-2.02	1.46	1.50
23	7	307	CLA	MG-NB	-2.02	2.01	2.05
23	2	313	CLA	CMD-C2D	-2.02	1.46	1.50
23	7	309	CLA	CMD-C2D	-2.02	1.46	1.50
23	1	305	CLA	CMB-C2B	-2.02	1.46	1.50
23	1	308	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	824	CLA	CMD-C2D	-2.02	1.46	1.50
23	4	313	CLA	CMD-C2D	-2.02	1.46	1.50
23	3	308	CLA	MG-NB	-2.02	2.01	2.05
23	9	311	CLA	CMB-C2B	-2.02	1.46	1.50
23	6	316	CLA	CMD-C2D	-2.02	1.46	1.50
23	f	802	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	805	CLA	MG-NB	-2.02	2.01	2.05
23	a	818	CLA	CMD-C2D	-2.02	1.46	1.50
23	9	318	CLA	MG-NB	-2.02	2.01	2.05
23	4	314	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	816	CLA	CMD-C2D	-2.02	1.46	1.50
23	2	315	CLA	MG-NB	-2.02	2.01	2.05
23	b	839	CLA	MG-NB	-2.02	2.01	2.05
23	a	818	CLA	CMC-C2C	-2.02	1.46	1.50
23	a	819	CLA	CMB-C2B	-2.02	1.46	1.50
23	a	838	CLA	CMB-C2B	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	854	CLA	CMD-C2D	-2.02	1.46	1.50
23	1	308	CLA	MG-NB	-2.02	2.01	2.05
23	a	837	CLA	MG-NB	-2.02	2.01	2.05
23	a	835	CLA	MG-NB	-2.02	2.01	2.05
23	3	308	CLA	CMB-C2B	-2.02	1.46	1.50
23	1	312	CLA	CMD-C2D	-2.02	1.46	1.50
23	5	307	CLA	CMD-C2D	-2.02	1.46	1.50
23	1	306	CLA	CMC-C2C	-2.02	1.46	1.50
23	1	313	CLA	CMB-C2B	-2.02	1.46	1.50
23	b	804	CLA	CMC-C2C	-2.02	1.46	1.50
23	2	315	CLA	CMB-C2B	-2.02	1.46	1.50
23	1	311	CLA	CMD-C2D	-2.02	1.46	1.50
23	5	312	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	804	CLA	CMD-C2D	-2.01	1.46	1.50
23	5	313	CLA	CMD-C2D	-2.01	1.46	1.50
23	5	306	CLA	CMB-C2B	-2.01	1.46	1.50
23	6	315	CLA	CMB-C2B	-2.01	1.46	1.50
23	6	316	CLA	CMB-C2B	-2.01	1.46	1.50
23	2	314	CLA	CMB-C2B	-2.01	1.46	1.50
30	m	101	BCR	C33-C5	-2.01	1.47	1.50
23	5	310	CLA	CMB-C2B	-2.01	1.46	1.50
23	3	312	CLA	CMB-C2B	-2.01	1.46	1.50
23	2	316	CLA	CMC-C2C	-2.01	1.46	1.50
23	b	821	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	310	CLA	MG-NB	-2.01	2.01	2.05
23	2	306	CLA	MG-NB	-2.01	2.01	2.05
23	6	311	CLA	CMB-C2B	-2.01	1.46	1.50
23	3	312	CLA	MG-NB	-2.01	2.01	2.05
23	b	823	CLA	CMC-C2C	-2.01	1.46	1.50
23	3	314	CLA	CMC-C2C	-2.01	1.46	1.50
23	a	834	CLA	CMB-C2B	-2.01	1.46	1.50
23	b	818	CLA	CMD-C2D	-2.01	1.46	1.50
23	8	313	CLA	MG-NB	-2.01	2.01	2.05
23	8	314	CLA	CMD-C2D	-2.01	1.46	1.50
23	7	317	CLA	CMB-C2B	-2.01	1.46	1.50
23	5	306	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	314	CLA	CMB-C2B	-2.01	1.46	1.50
23	a	831	CLA	CMC-C2C	-2.01	1.46	1.50
23	b	836	CLA	CMD-C2D	-2.01	1.46	1.50
23	5	310	CLA	MG-NB	-2.01	2.01	2.05
23	3	315	CLA	CMB-C2B	-2.01	1.46	1.50
23	6	313	CLA	CMD-C2D	-2.01	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	827	CLA	CMB-C2B	-2.01	1.46	1.50
27	b	848	DGD	O3D-C3D	-2.01	1.38	1.43
23	a	806	CLA	C1B-C2B	2.01	1.47	1.43
23	b	806	CLA	MG-NB	-2.01	2.01	2.05
23	a	841	CLA	CMB-C2B	-2.01	1.46	1.50
23	a	836	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	841	CLA	MG-NB	-2.01	2.01	2.05
23	3	310	CLA	CMD-C2D	-2.01	1.46	1.50
23	9	308	CLA	CMB-C2B	-2.01	1.46	1.50
23	2	306	CLA	CMB-C2B	-2.01	1.46	1.50
23	5	313	CLA	CMC-C2C	-2.01	1.46	1.50
23	8	306	CLA	CMD-C2D	-2.01	1.46	1.50
23	j	103	CLA	CMD-C2D	-2.01	1.46	1.50
23	f	803	CLA	MG-NB	-2.01	2.01	2.05
22	9	306	A1L1G	C38-C39	2.01	1.40	1.35
23	b	837	CLA	CMB-C2B	-2.00	1.46	1.50
23	5	306	CLA	MG-NB	-2.00	2.01	2.05
23	a	806	CLA	CHC-C1C	2.00	1.42	1.38
22	5	303	A1L1G	C38-C39	2.00	1.40	1.35
23	j	102	CLA	CMB-C2B	-2.00	1.46	1.50
23	6	314	CLA	MG-NB	-2.00	2.01	2.05
23	a	802	CLA	CMC-C2C	-2.00	1.46	1.50
23	9	318	CLA	CMB-C2B	-2.00	1.46	1.50
27	b	848	DGD	O4D-C4D	-2.00	1.38	1.43
23	4	316	CLA	CMB-C2B	-2.00	1.46	1.50
23	9	314	CLA	CMB-C2B	-2.00	1.46	1.50
23	1	310	CLA	CMD-C2D	-2.00	1.46	1.50
23	8	312	CLA	CMB-C2B	-2.00	1.46	1.50
23	6	314	CLA	CMD-C2D	-2.00	1.46	1.50
23	1	311	CLA	CMB-C2B	-2.00	1.46	1.50
23	a	840	CLA	CMB-C2B	-2.00	1.46	1.50
23	f	803	CLA	CMB-C2B	-2.00	1.46	1.50
23	5	315	CLA	CMD-C2D	-2.00	1.46	1.50
23	4	309	CLA	CMD-C2D	-2.00	1.46	1.50
23	3	313	CLA	CMB-C2B	-2.00	1.46	1.50
23	b	806	CLA	CMD-C2D	-2.00	1.46	1.50

All (2232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	302	A1L1F	O15-C20-C21	10.43	123.27	113.49
27	4	318	DGD	C6E-C5E-C4E	-8.97	90.99	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	301	A1L1F	C17-C20-C25	-8.66	108.06	122.30
25	9	302	A1L1F	C17-C20-C25	-8.65	108.07	122.30
25	h	203	A1L1F	C17-C20-C25	-8.53	108.27	122.30
25	6	304	A1L1F	C17-C20-C25	-8.43	108.42	122.30
25	8	304	A1L1F	C17-C20-C25	-8.40	108.47	122.30
25	1	304	A1L1F	C17-C20-C25	-8.27	108.69	122.30
25	8	304	A1L1F	C37-C38-C39	-7.98	116.08	127.28
21	6	305	XAT	C18-C5-C4	7.69	122.88	114.24
21	6	303	XAT	C38-C25-C26	-7.57	109.84	122.30
21	9	303	XAT	C38-C25-C24	7.34	122.49	114.24
23	7	314	CLA	C4A-NA-C1A	7.29	110.00	106.68
23	b	839	CLA	C4A-NA-C1A	7.27	109.99	106.68
23	9	310	CLA	C4A-NA-C1A	7.26	109.99	106.68
21	4	305	XAT	C38-C25-C24	7.24	122.38	114.24
21	3	305	XAT	C38-C25-C24	7.24	122.38	114.24
23	9	313	CLA	C4A-NA-C1A	7.24	109.98	106.68
21	5	304	XAT	C38-C25-C24	7.23	122.36	114.24
21	1	303	XAT	C38-C25-C24	7.23	122.36	114.24
21	a	852	XAT	C15-C14-C13	-7.20	117.19	127.28
21	7	304	XAT	C38-C25-C24	7.19	122.32	114.24
23	b	803	CLA	C4A-NA-C1A	7.18	109.95	106.68
23	a	806	CLA	C4A-NA-C1A	7.15	109.94	106.68
30	f	801	BCR	C24-C23-C22	-7.15	115.66	126.23
21	j	101	XAT	C38-C25-C24	7.14	122.26	114.24
21	7	305	XAT	C38-C25-C24	7.14	122.26	114.24
21	9	304	XAT	C38-C25-C24	7.13	122.25	114.24
23	l	203	CLA	C4A-NA-C1A	7.13	109.93	106.68
21	4	304	XAT	C38-C25-C24	7.05	122.16	114.24
23	b	809	CLA	C4A-NA-C1A	7.05	109.89	106.68
21	5	304	XAT	C18-C5-C4	7.05	122.16	114.24
23	a	835	CLA	C4A-NA-C1A	7.04	109.89	106.68
23	4	310	CLA	C4A-NA-C1A	7.03	109.89	106.68
21	3	304	XAT	C38-C25-C24	7.01	122.12	114.24
21	5	301	XAT	C38-C25-C26	-7.01	110.76	122.30
23	6	312	CLA	C4A-NA-C1A	7.01	109.88	106.68
23	a	833	CLA	C4A-NA-C1A	7.00	109.87	106.68
21	2	301	XAT	C18-C5-C6	-7.00	110.78	122.30
21	6	305	XAT	C38-C25-C24	7.00	122.10	114.24
23	a	821	CLA	C4A-NA-C1A	6.99	109.87	106.68
21	4	305	XAT	C38-C25-C26	-6.97	110.82	122.30
23	9	308	CLA	C4A-NA-C1A	6.97	109.86	106.68
21	9	303	XAT	C38-C25-C26	-6.96	110.85	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	820	CLA	C4A-NA-C1A	6.95	109.85	106.68
23	a	823	CLA	C4A-NA-C1A	6.95	109.85	106.68
23	j	103	CLA	C4A-NA-C1A	6.95	109.85	106.68
23	a	810	CLA	C4A-NA-C1A	6.94	109.85	106.68
21	8	301	XAT	C38-C25-C24	6.94	122.03	114.24
21	8	301	XAT	C38-C25-C26	-6.93	110.89	122.30
21	3	304	XAT	C38-C25-C26	-6.93	110.90	122.30
21	6	302	XAT	C38-C25-C24	6.91	122.00	114.24
21	1	302	XAT	C38-C25-C24	6.91	122.00	114.24
23	7	317	CLA	C4A-NA-C1A	6.89	109.82	106.68
23	a	826	CLA	C4A-NA-C1A	6.88	109.82	106.68
21	8	303	XAT	C18-C5-C6	-6.88	110.97	122.30
25	6	301	A1L1F	O15-C20-C21	6.88	119.94	113.49
21	4	303	XAT	C38-C25-C24	6.85	121.94	114.24
21	5	304	XAT	C6-C7-C8	-6.84	111.53	125.99
21	9	304	XAT	C38-C25-C26	-6.83	111.05	122.30
21	8	303	XAT	C38-C25-C24	6.83	121.91	114.24
23	4	316	CLA	C4A-NA-C1A	6.83	109.80	106.68
25	6	304	A1L1F	O15-C20-C21	6.83	119.89	113.49
21	2	304	XAT	C38-C25-C24	6.83	121.91	114.24
23	6	310	CLA	C4A-NA-C1A	6.83	109.79	106.68
23	b	821	CLA	C4A-NA-C1A	6.83	109.79	106.68
23	a	828	CLA	C4A-NA-C1A	6.82	109.79	106.68
21	5	304	XAT	C18-C5-C6	-6.82	111.08	122.30
23	b	801	CLA	C4A-NA-C1A	6.82	109.79	106.68
21	a	852	XAT	C38-C25-C24	6.81	121.89	114.24
21	7	304	XAT	C18-C5-C6	-6.80	111.10	122.30
23	b	805	CLA	C4A-NA-C1A	6.80	109.78	106.68
23	b	814	CLA	C4A-NA-C1A	6.80	109.78	106.68
23	4	317	CLA	C4A-NA-C1A	6.79	109.78	106.68
21	3	304	XAT	C18-C5-C6	-6.79	111.12	122.30
23	6	316	CLA	C4A-NA-C1A	6.79	109.78	106.68
23	b	827	CLA	C4A-NA-C1A	6.78	109.77	106.68
21	7	301	XAT	C18-C5-C6	-6.78	111.14	122.30
21	6	302	XAT	C38-C25-C26	-6.78	111.15	122.30
21	6	302	XAT	C11-C10-C9	-6.78	117.78	127.28
21	j	101	XAT	C38-C25-C26	-6.77	111.15	122.30
23	f	802	CLA	C4A-NA-C1A	6.77	109.77	106.68
21	6	303	XAT	C38-C25-C24	6.77	121.85	114.24
23	a	801	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	3	308	CLA	C4A-NA-C1A	6.76	109.76	106.68
21	8	302	XAT	C38-C25-C24	6.76	121.83	114.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	101	BCR	C24-C23-C22	-6.76	116.24	126.23
21	7	303	XAT	C38-C25-C26	-6.76	111.18	122.30
23	a	807	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	6	314	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	b	810	CLA	C4A-NA-C1A	6.74	109.76	106.68
21	4	302	XAT	C38-C25-C24	6.74	121.81	114.24
23	b	806	CLA	C4A-NA-C1A	6.73	109.75	106.68
23	1	306	CLA	C4A-NA-C1A	6.73	109.75	106.68
21	2	304	XAT	C18-C5-C4	6.73	121.80	114.24
21	5	302	XAT	C18-C5-C6	-6.73	111.23	122.30
21	8	302	XAT	C38-C25-C26	-6.72	111.24	122.30
21	7	304	XAT	C38-C25-C26	-6.72	111.25	122.30
21	8	302	XAT	C18-C5-C6	-6.71	111.25	122.30
25	8	304	A1L1F	O15-C20-C21	6.71	119.78	113.49
23	9	316	CLA	C4A-NA-C1A	6.71	109.74	106.68
23	7	316	CLA	C4A-NA-C1A	6.71	109.74	106.68
21	2	301	XAT	C18-C5-C4	6.71	121.78	114.24
23	5	306	CLA	C4A-NA-C1A	6.71	109.74	106.68
23	5	310	CLA	C4A-NA-C1A	6.71	109.74	106.68
23	1	308	CLA	C4A-NA-C1A	6.71	109.74	106.68
23	6	317	CLA	C4A-NA-C1A	6.71	109.74	106.68
21	2	303	XAT	C18-C5-C6	-6.70	111.27	122.30
21	3	303	XAT	C38-C25-C24	6.70	121.77	114.24
23	4	311	CLA	C4A-NA-C1A	6.70	109.73	106.68
21	6	305	XAT	C38-C25-C26	-6.69	111.29	122.30
23	a	817	CLA	C4A-NA-C1A	6.69	109.73	106.68
23	a	805	CLA	C4A-NA-C1A	6.68	109.73	106.68
23	a	825	CLA	C4A-NA-C1A	6.68	109.73	106.68
23	2	316	CLA	C4A-NA-C1A	6.68	109.72	106.68
21	3	301	XAT	C18-C5-C4	6.68	121.74	114.24
21	7	301	XAT	C18-C5-C4	6.68	121.74	114.24
23	b	812	CLA	C4A-NA-C1A	6.67	109.72	106.68
23	b	836	CLA	C4A-NA-C1A	6.67	109.72	106.68
21	4	303	XAT	C18-C5-C6	-6.67	111.32	122.30
21	4	301	XAT	C18-C5-C6	-6.67	111.33	122.30
23	b	824	CLA	C4A-NA-C1A	6.67	109.72	106.68
21	5	304	XAT	C38-C25-C26	-6.66	111.33	122.30
21	7	305	XAT	C38-C25-C26	-6.66	111.33	122.30
23	a	809	CLA	C4A-NA-C1A	6.66	109.72	106.68
21	3	305	XAT	C38-C25-C26	-6.66	111.34	122.30
23	3	313	CLA	C4A-NA-C1A	6.66	109.72	106.68
23	8	312	CLA	C4A-NA-C1A	6.66	109.72	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	309	CLA	C4A-NA-C1A	6.66	109.72	106.68
23	a	834	CLA	C4A-NA-C1A	6.65	109.71	106.68
21	4	301	XAT	C31-C30-C29	-6.65	117.96	127.28
23	5	311	CLA	C4A-NA-C1A	6.65	109.71	106.68
23	1	305	CLA	C4A-NA-C1A	6.65	109.71	106.68
23	a	812	CLA	C4A-NA-C1A	6.65	109.71	106.68
23	b	832	CLA	C4A-NA-C1A	6.64	109.71	106.68
23	a	831	CLA	C4A-NA-C1A	6.64	109.71	106.68
21	6	303	XAT	C18-C5-C6	-6.64	111.38	122.30
23	2	312	CLA	C4A-NA-C1A	6.64	109.71	106.68
23	9	314	CLA	C4A-NA-C1A	6.63	109.71	106.68
30	a	850	BCR	C24-C23-C22	-6.63	116.42	126.23
21	7	303	XAT	C18-C5-C6	-6.63	111.39	122.30
25	h	203	A1L1F	O15-C20-C21	6.63	119.71	113.49
21	4	303	XAT	C38-C25-C26	-6.63	111.39	122.30
23	3	314	CLA	C4A-NA-C1A	6.63	109.70	106.68
23	a	838	CLA	C4A-NA-C1A	6.63	109.70	106.68
21	2	305	XAT	C18-C5-C6	-6.63	111.39	122.30
21	5	301	XAT	C38-C25-C24	6.62	121.68	114.24
21	2	303	XAT	C38-C25-C26	-6.62	111.40	122.30
23	2	311	CLA	C4A-NA-C1A	6.62	109.70	106.68
23	a	840	CLA	C4A-NA-C1A	6.62	109.70	106.68
23	a	841	CLA	C4A-NA-C1A	6.61	109.70	106.68
23	1	202	CLA	C4A-NA-C1A	6.61	109.70	106.68
23	1	204	CLA	C4A-NA-C1A	6.61	109.69	106.68
23	3	312	CLA	C4A-NA-C1A	6.61	109.69	106.68
23	5	314	CLA	C4A-NA-C1A	6.60	109.69	106.68
23	4	315	CLA	C4A-NA-C1A	6.60	109.69	106.68
21	6	306	XAT	C18-C5-C6	-6.59	111.45	122.30
21	4	301	XAT	C18-C5-C4	6.59	121.65	114.24
23	8	313	CLA	C4A-NA-C1A	6.59	109.69	106.68
23	a	842	CLA	C4A-NA-C1A	6.59	109.69	106.68
23	7	315	CLA	C4A-NA-C1A	6.59	109.69	106.68
21	2	304	XAT	C38-C25-C26	-6.59	111.46	122.30
23	a	837	CLA	C4A-NA-C1A	6.59	109.68	106.68
21	2	304	XAT	C18-C5-C6	-6.59	111.46	122.30
21	7	303	XAT	C38-C25-C24	6.58	121.64	114.24
23	b	808	CLA	C4A-NA-C1A	6.58	109.68	106.68
23	4	307	CLA	C4A-NA-C1A	6.58	109.68	106.68
23	a	804	CLA	C4A-NA-C1A	6.58	109.68	106.68
21	3	303	XAT	C18-C5-C6	-6.57	111.48	122.30
23	a	830	CLA	C4A-NA-C1A	6.57	109.68	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	307	CLA	C4A-NA-C1A	6.57	109.68	106.68
23	a	811	CLA	C4A-NA-C1A	6.56	109.67	106.68
23	f	803	CLA	C4A-NA-C1A	6.56	109.67	106.68
23	a	839	CLA	C4A-NA-C1A	6.56	109.67	106.68
23	6	315	CLA	C4A-NA-C1A	6.55	109.67	106.68
21	8	303	XAT	C18-C5-C4	6.55	121.60	114.24
23	5	313	CLA	C4A-NA-C1A	6.55	109.67	106.68
23	4	306	CLA	C4A-NA-C1A	6.55	109.67	106.68
21	6	302	XAT	C18-C5-C6	-6.55	111.53	122.30
23	8	305	CLA	C4A-NA-C1A	6.54	109.66	106.68
23	b	807	CLA	C4A-NA-C1A	6.54	109.66	106.68
23	a	854	CLA	C4A-NA-C1A	6.54	109.66	106.68
21	4	302	XAT	C18-C5-C4	6.54	121.58	114.24
23	j	102	CLA	C4A-NA-C1A	6.54	109.66	106.68
23	7	310	CLA	C4A-NA-C1A	6.53	109.66	106.68
23	b	822	CLA	C4A-NA-C1A	6.53	109.66	106.68
21	j	101	XAT	C18-C5-C6	-6.53	111.55	122.30
21	6	303	XAT	C18-C5-C4	6.53	121.57	114.24
23	5	312	CLA	C4A-NA-C1A	6.53	109.66	106.68
23	1	307	CLA	C4A-NA-C1A	6.53	109.66	106.68
21	3	301	XAT	C18-C5-C6	-6.53	111.56	122.30
23	8	311	CLA	C4A-NA-C1A	6.53	109.66	106.68
23	4	314	CLA	C4A-NA-C1A	6.53	109.66	106.68
21	1	302	XAT	C38-C25-C26	-6.52	111.57	122.30
23	b	815	CLA	C4A-NA-C1A	6.52	109.65	106.68
21	3	303	XAT	C38-C25-C26	-6.52	111.57	122.30
23	2	313	CLA	C4A-NA-C1A	6.52	109.65	106.68
21	7	305	XAT	C18-C5-C6	-6.52	111.58	122.30
23	3	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
23	a	829	CLA	C4A-NA-C1A	6.51	109.65	106.68
23	3	315	CLA	C4A-NA-C1A	6.51	109.65	106.68
23	a	844	CLA	C4A-NA-C1A	6.50	109.64	106.68
23	8	307	CLA	C4A-NA-C1A	6.50	109.64	106.68
21	4	302	XAT	C18-C5-C6	-6.50	111.61	122.30
23	5	308	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	6	308	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	b	835	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	8	309	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	b	818	CLA	C4A-NA-C1A	6.48	109.64	106.68
21	9	303	XAT	C18-C5-C6	-6.48	111.64	122.30
23	6	311	CLA	C4A-NA-C1A	6.48	109.63	106.68
23	a	832	CLA	C4A-NA-C1A	6.48	109.63	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	838	CLA	C4A-NA-C1A	6.47	109.63	106.68
21	4	304	XAT	C18-C5-C6	-6.47	111.65	122.30
23	b	833	CLA	C4A-NA-C1A	6.47	109.63	106.68
23	8	314	CLA	C4A-NA-C1A	6.46	109.63	106.68
23	b	826	CLA	C4A-NA-C1A	6.46	109.62	106.68
23	a	836	CLA	C4A-NA-C1A	6.45	109.62	106.68
23	3	309	CLA	C4A-NA-C1A	6.45	109.62	106.68
23	2	307	CLA	C4A-NA-C1A	6.45	109.62	106.68
23	b	823	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	b	831	CLA	C4A-NA-C1A	6.44	109.62	106.68
21	1	302	XAT	C18-C5-C6	-6.44	111.70	122.30
23	1	312	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	7	312	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	a	818	CLA	C4A-NA-C1A	6.44	109.61	106.68
23	a	827	CLA	C4A-NA-C1A	6.44	109.61	106.68
23	b	813	CLA	C4A-NA-C1A	6.43	109.61	106.68
21	4	305	XAT	C18-C5-C6	-6.43	111.72	122.30
23	9	318	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	a	816	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	2	309	CLA	C4A-NA-C1A	6.42	109.61	106.68
21	2	302	XAT	C18-C5-C6	-6.42	111.74	122.30
23	6	307	CLA	C4A-NA-C1A	6.42	109.61	106.68
23	2	314	CLA	C4A-NA-C1A	6.42	109.61	106.68
23	a	808	CLA	C4A-NA-C1A	6.42	109.61	106.68
23	1	313	CLA	C4A-NA-C1A	6.41	109.60	106.68
21	4	302	XAT	C38-C25-C26	-6.41	111.75	122.30
21	4	305	XAT	C31-C30-C29	-6.41	118.29	127.28
21	5	302	XAT	C26-C27-C28	-6.41	112.44	125.99
21	3	305	XAT	C18-C5-C6	-6.41	111.75	122.30
23	9	312	CLA	C4A-NA-C1A	6.41	109.60	106.68
21	6	306	XAT	C38-C25-C26	-6.41	111.76	122.30
21	8	301	XAT	C18-C5-C6	-6.40	111.76	122.30
21	2	303	XAT	C38-C25-C24	6.40	121.43	114.24
21	4	304	XAT	C38-C25-C26	-6.40	111.77	122.30
23	5	315	CLA	C4A-NA-C1A	6.40	109.60	106.68
21	3	301	XAT	C38-C25-C26	-6.40	111.77	122.30
21	2	302	XAT	C38-C25-C24	6.40	121.43	114.24
23	4	308	CLA	C4A-NA-C1A	6.39	109.60	106.68
23	a	815	CLA	C4A-NA-C1A	6.39	109.60	106.68
23	2	315	CLA	C4A-NA-C1A	6.39	109.59	106.68
23	a	822	CLA	C4A-NA-C1A	6.39	109.59	106.68
21	8	303	XAT	C38-C25-C26	-6.39	111.79	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	j	101	XAT	C18-C5-C4	6.39	121.42	114.24
23	7	306	CLA	C4A-NA-C1A	6.39	109.59	106.68
21	1	303	XAT	C18-C5-C6	-6.38	111.79	122.30
23	7	311	CLA	C4A-NA-C1A	6.38	109.59	106.68
21	7	305	XAT	C18-C5-C4	6.38	121.41	114.24
21	a	852	XAT	C38-C25-C26	-6.38	111.80	122.30
23	4	309	CLA	C4A-NA-C1A	6.38	109.59	106.68
23	2	306	CLA	C4A-NA-C1A	6.37	109.59	106.68
23	h	204	CLA	C4A-NA-C1A	6.37	109.59	106.68
21	3	305	XAT	C18-C5-C4	6.37	121.40	114.24
21	8	302	XAT	C11-C10-C9	-6.37	118.35	127.28
23	3	307	CLA	C4A-NA-C1A	6.37	109.58	106.68
23	7	308	CLA	C4A-NA-C1A	6.37	109.58	106.68
23	1	311	CLA	C4A-NA-C1A	6.37	109.58	106.68
23	5	309	CLA	C4A-NA-C1A	6.36	109.58	106.68
23	a	819	CLA	C4A-NA-C1A	6.36	109.58	106.68
21	1	302	XAT	C18-C5-C4	6.36	121.39	114.24
23	3	310	CLA	C4A-NA-C1A	6.36	109.58	106.68
23	8	306	CLA	C4A-NA-C1A	6.36	109.58	106.68
23	a	814	CLA	C4A-NA-C1A	6.35	109.58	106.68
21	1	303	XAT	C38-C25-C26	-6.35	111.84	122.30
21	5	301	XAT	C18-C5-C6	-6.35	111.85	122.30
21	3	303	XAT	C18-C5-C4	6.35	121.38	114.24
21	9	305	XAT	C18-C5-C6	-6.34	111.86	122.30
23	9	311	CLA	C4A-NA-C1A	6.34	109.57	106.68
30	i	101	BCR	C20-C21-C22	-6.34	118.39	127.28
23	8	308	CLA	C4A-NA-C1A	6.34	109.57	106.68
21	2	302	XAT	C38-C25-C26	-6.33	111.88	122.30
21	3	304	XAT	C18-C5-C4	6.32	121.34	114.24
23	a	824	CLA	C4A-NA-C1A	6.32	109.56	106.68
21	4	303	XAT	C18-C5-C4	6.32	121.33	114.24
23	2	310	CLA	C4A-NA-C1A	6.31	109.56	106.68
23	b	819	CLA	C4A-NA-C1A	6.31	109.56	106.68
23	5	305	CLA	C4A-NA-C1A	6.31	109.56	106.68
23	1	314	CLA	C4A-NA-C1A	6.31	109.56	106.68
23	5	307	CLA	C4A-NA-C1A	6.30	109.55	106.68
23	4	312	CLA	C4A-NA-C1A	6.30	109.55	106.68
21	2	301	XAT	C38-C25-C24	6.29	121.31	114.24
21	9	305	XAT	C11-C10-C9	-6.29	118.46	127.28
23	7	309	CLA	C4A-NA-C1A	6.29	109.55	106.68
23	b	825	CLA	C4A-NA-C1A	6.29	109.55	106.68
25	8	304	AI1L1F	O15-C20-C17	6.29	122.07	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	813	CLA	C4A-NA-C1A	6.28	109.55	106.68
23	b	834	CLA	C4A-NA-C1A	6.28	109.55	106.68
23	7	313	CLA	C4A-NA-C1A	6.28	109.54	106.68
23	a	802	CLA	C4A-NA-C1A	6.28	109.54	106.68
21	6	306	XAT	C18-C5-C4	6.26	121.27	114.24
23	1	309	CLA	C4A-NA-C1A	6.25	109.53	106.68
21	4	304	XAT	C18-C5-C4	6.24	121.25	114.24
21	6	306	XAT	C38-C25-C24	6.23	121.24	114.24
23	b	829	CLA	C4A-NA-C1A	6.23	109.52	106.68
21	3	301	XAT	C38-C25-C24	6.23	121.23	114.24
23	b	840	CLA	C4A-NA-C1A	6.22	109.52	106.68
21	6	305	XAT	C35-C34-C33	-6.22	118.56	127.28
23	1	310	CLA	C4A-NA-C1A	6.21	109.51	106.68
21	6	302	XAT	C18-C5-C4	6.21	121.21	114.24
21	2	301	XAT	C38-C25-C26	-6.20	112.09	122.30
21	5	302	XAT	C38-C25-C24	6.20	121.21	114.24
23	9	315	CLA	C4A-NA-C1A	6.19	109.50	106.68
21	1	303	XAT	C18-C5-C4	6.17	121.17	114.24
23	6	313	CLA	C4A-NA-C1A	6.16	109.49	106.68
23	b	811	CLA	C4A-NA-C1A	6.16	109.49	106.68
23	a	820	CLA	C4A-NA-C1A	6.15	109.48	106.68
23	b	837	CLA	C4A-NA-C1A	6.13	109.47	106.68
21	2	301	XAT	C31-C30-C29	-6.12	118.69	127.28
21	6	303	XAT	C15-C14-C13	-6.10	118.73	127.28
21	a	852	XAT	C26-C27-C28	-6.10	113.10	125.99
21	7	304	XAT	C18-C5-C4	6.09	121.08	114.24
21	2	305	XAT	C18-C5-C4	6.08	121.08	114.24
30	b	842	BCR	C7-C8-C9	-6.08	117.24	126.23
21	4	305	XAT	C18-C5-C4	6.08	121.07	114.24
23	b	804	CLA	C4A-NA-C1A	6.07	109.45	106.68
23	b	828	CLA	C4A-NA-C1A	6.07	109.45	106.68
25	1	304	A1L1F	O15-C20-C17	6.06	121.82	115.05
23	2	308	CLA	C4A-NA-C1A	6.05	109.44	106.68
23	9	309	CLA	C4A-NA-C1A	6.04	109.44	106.68
21	2	302	XAT	C18-C5-C4	6.02	121.00	114.24
23	b	816	CLA	C4A-NA-C1A	6.01	109.42	106.68
23	8	310	CLA	C4A-NA-C1A	6.00	109.42	106.68
23	b	817	CLA	C4A-NA-C1A	6.00	109.42	106.68
21	5	302	XAT	C18-C5-C4	5.98	120.96	114.24
23	4	313	CLA	C4A-NA-C1A	5.96	109.40	106.68
21	8	301	XAT	C18-C5-C4	5.96	120.94	114.24
21	7	301	XAT	C38-C25-C24	5.95	120.93	114.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	303	XAT	C18-C5-C4	5.95	120.93	114.24
25	h	203	A1L1F	C37-C38-C39	-5.95	118.94	127.28
21	5	304	XAT	C26-C27-C28	-5.94	113.43	125.99
30	b	849	BCR	C16-C17-C18	-5.94	118.95	127.28
21	8	302	XAT	C18-C5-C4	5.93	120.91	114.24
21	5	302	XAT	C38-C25-C26	-5.92	112.56	122.30
23	b	802	CLA	C4A-NA-C1A	5.92	109.38	106.68
21	7	301	XAT	C38-C25-C26	-5.92	112.56	122.30
23	b	830	CLA	C4A-NA-C1A	5.90	109.37	106.68
21	5	301	XAT	C18-C5-C4	5.89	120.86	114.24
21	7	301	XAT	C31-C30-C29	-5.89	119.02	127.28
25	h	203	A1L1F	O15-C20-C17	5.87	121.61	115.05
25	6	301	A1L1F	O15-C20-C17	5.86	121.60	115.05
21	j	101	XAT	C6-C7-C8	-5.86	113.61	125.99
21	2	303	XAT	C18-C5-C4	5.85	120.81	114.24
21	9	303	XAT	C18-C5-C4	5.82	120.78	114.24
30	a	850	BCR	C20-C21-C22	-5.79	119.16	127.28
21	4	301	XAT	C35-C34-C33	-5.76	119.20	127.28
30	b	844	BCR	C24-C23-C22	-5.76	117.72	126.23
21	5	302	XAT	C11-C10-C9	-5.75	119.21	127.28
30	b	842	BCR	C11-C10-C9	-5.71	119.27	127.28
25	1	304	A1L1F	O15-C20-C21	5.71	118.84	113.49
30	f	801	BCR	C16-C17-C18	-5.71	119.27	127.28
21	4	301	XAT	C38-C25-C24	5.70	120.64	114.24
21	6	305	XAT	C18-C5-C6	-5.67	112.96	122.30
21	9	304	XAT	C26-C27-C28	-5.66	114.03	125.99
30	b	844	BCR	C7-C8-C9	-5.63	117.91	126.23
21	6	305	XAT	C31-C30-C29	-5.61	119.41	127.28
21	7	305	XAT	C15-C14-C13	-5.59	119.44	127.28
30	b	845	BCR	C16-C17-C18	-5.54	119.50	127.28
21	9	303	XAT	C15-C14-C13	-5.51	119.56	127.28
30	f	801	BCR	C20-C21-C22	-5.49	119.58	127.28
21	8	303	XAT	C26-C27-C28	-5.49	114.39	125.99
30	f	804	BCR	C15-C14-C13	-5.47	119.61	127.28
21	6	306	XAT	C31-C30-C29	-5.47	119.61	127.28
21	3	304	XAT	C35-C34-C33	-5.46	119.61	127.28
21	4	301	XAT	C38-C25-C26	-5.45	113.33	122.30
30	j	104	BCR	C28-C27-C26	-5.45	104.33	114.06
21	a	852	XAT	C18-C5-C6	-5.45	113.33	122.30
30	b	844	BCR	C33-C5-C6	-5.44	118.54	124.48
21	2	303	XAT	C35-C34-C33	-5.44	119.65	127.28
23	a	803	CLA	C4A-NA-C1A	5.43	109.16	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	302	XAT	C15-C14-C13	-5.43	119.67	127.28
21	3	301	XAT	C6-C7-C8	-5.42	114.52	125.99
25	6	304	A1L1F	O15-C20-C17	5.42	121.11	115.05
21	2	303	XAT	C31-C30-C29	-5.41	119.69	127.28
21	4	305	XAT	C15-C14-C13	-5.35	119.78	127.28
30	b	842	BCR	C15-C14-C13	-5.35	119.78	127.28
30	l	201	BCR	C7-C8-C9	-5.34	118.33	126.23
21	2	305	XAT	C31-C30-C29	-5.33	119.81	127.28
25	8	304	A1L1F	O7-C54-C56	5.32	120.58	111.09
21	7	301	XAT	C35-C34-C33	-5.31	119.83	127.28
21	2	302	XAT	C35-C34-C33	-5.31	119.83	127.28
30	b	842	BCR	C3-C4-C5	-5.31	104.59	114.06
25	6	301	A1L1F	C36-C37-C38	-5.30	112.67	123.52
21	7	304	XAT	C11-C10-C9	-5.30	119.84	127.28
25	8	304	A1L1F	C41-C42-C44	-5.30	119.85	127.28
21	2	303	XAT	C11-C10-C9	-5.29	119.85	127.28
21	6	302	XAT	C31-C30-C29	-5.29	119.86	127.28
21	6	306	XAT	C35-C34-C33	-5.29	119.86	127.28
21	4	303	XAT	C26-C27-C28	-5.28	114.82	125.99
27	b	848	DGD	O2G-C1B-C2B	5.28	122.91	111.48
21	a	852	XAT	C18-C5-C4	5.28	120.17	114.24
30	a	849	BCR	C3-C4-C5	-5.27	104.66	114.06
21	2	301	XAT	C35-C34-C33	-5.27	119.89	127.28
21	4	304	XAT	C26-C27-C28	-5.25	114.90	125.99
21	9	305	XAT	C18-C5-C4	5.24	120.13	114.24
21	a	852	XAT	C6-C7-C8	-5.24	114.92	125.99
30	l	205	BCR	C24-C23-C22	-5.23	118.50	126.23
21	8	303	XAT	C15-C14-C13	-5.21	119.97	127.28
21	9	303	XAT	C26-C27-C28	-5.20	115.00	125.99
21	2	304	XAT	C6-C7-C8	-5.19	115.02	125.99
21	j	101	XAT	C26-C27-C28	-5.18	115.05	125.99
21	2	305	XAT	C35-C34-C33	-5.12	120.09	127.28
21	1	302	XAT	C35-C34-C33	-5.12	120.10	127.28
30	h	201	BCR	C3-C4-C5	-5.11	104.95	114.06
30	a	847	BCR	C16-C17-C18	-5.08	120.16	127.28
21	6	302	XAT	C35-C34-C33	-5.05	120.19	127.28
21	3	305	XAT	C26-C27-C28	-5.04	115.33	125.99
21	8	303	XAT	C6-C7-C8	-5.04	115.34	125.99
30	b	849	BCR	C11-C10-C9	-5.04	120.21	127.28
21	7	305	XAT	C26-C27-C28	-5.04	115.34	125.99
30	b	849	BCR	C20-C21-C22	-5.01	120.25	127.28
30	f	804	BCR	C11-C10-C9	-5.01	120.25	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	850	BCR	C16-C17-C18	-5.01	120.25	127.28
21	5	301	XAT	C26-C27-C28	-5.00	115.42	125.99
21	4	304	XAT	C6-C7-C8	-4.98	115.46	125.99
21	1	302	XAT	C26-C27-C28	-4.98	115.47	125.99
21	2	301	XAT	C15-C14-C13	-4.96	120.32	127.28
30	a	849	BCR	C16-C17-C18	-4.96	120.33	127.28
21	3	305	XAT	C6-C7-C8	-4.95	115.52	125.99
21	7	303	XAT	C31-C30-C29	-4.94	120.35	127.28
30	j	104	BCR	C11-C10-C9	-4.91	120.39	127.28
30	b	849	BCR	C38-C26-C25	-4.90	119.13	124.48
21	4	303	XAT	C11-C10-C9	-4.90	120.41	127.28
21	1	303	XAT	C6-C7-C8	-4.90	115.64	125.99
21	j	101	XAT	C11-C10-C9	-4.89	120.42	127.28
21	7	304	XAT	C26-C27-C28	-4.88	115.67	125.99
21	2	305	XAT	C6-C7-C8	-4.87	115.69	125.99
21	5	302	XAT	C15-C14-C13	-4.86	120.46	127.28
21	2	301	XAT	C6-C7-C8	-4.85	115.74	125.99
21	5	304	XAT	C15-C14-C13	-4.85	120.48	127.28
30	l	205	BCR	C15-C14-C13	-4.85	120.48	127.28
21	9	305	XAT	C35-C34-C33	-4.84	120.49	127.28
30	i	101	BCR	C16-C17-C18	-4.84	120.50	127.28
30	h	202	BCR	C16-C17-C18	-4.83	120.51	127.28
21	1	302	XAT	C6-C7-C8	-4.80	115.84	125.99
30	b	849	BCR	C7-C8-C9	-4.79	119.14	126.23
21	7	304	XAT	C35-C34-C33	-4.78	120.57	127.28
21	7	301	XAT	C6-C7-C8	-4.77	115.91	125.99
21	7	304	XAT	C15-C14-C13	-4.75	120.62	127.28
21	4	302	XAT	C26-C27-C28	-4.74	115.97	125.99
21	9	304	XAT	C15-C14-C13	-4.74	120.63	127.28
25	9	302	A1L1F	O7-C54-C56	4.71	119.49	111.09
21	8	301	XAT	C26-C27-C28	-4.71	116.03	125.99
21	7	305	XAT	C6-C7-C8	-4.70	116.06	125.99
21	4	302	XAT	C6-C7-C8	-4.67	116.11	125.99
25	6	304	A1L1F	O7-C54-C56	4.67	119.42	111.09
21	3	303	XAT	C26-C27-C28	-4.67	116.12	125.99
21	4	302	XAT	C35-C34-C33	-4.66	120.75	127.28
21	7	303	XAT	C11-C10-C9	-4.66	120.75	127.28
21	8	302	XAT	C15-C14-C13	-4.65	120.75	127.28
30	b	846	BCR	C16-C17-C18	-4.65	120.76	127.28
21	9	305	XAT	C38-C25-C24	4.64	119.46	114.24
25	h	203	A1L1F	O7-C54-C56	4.64	119.37	111.09
30	b	843	BCR	C7-C8-C9	-4.64	119.38	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	301	XAT	C35-C34-C33	-4.63	120.78	127.28
30	b	843	BCR	C11-C10-C9	-4.63	120.78	127.28
21	3	304	XAT	C6-C7-C8	-4.60	116.26	125.99
21	2	305	XAT	C15-C14-C13	-4.60	120.83	127.28
25	6	301	A1L1F	O7-C54-C56	4.58	119.26	111.09
21	7	301	XAT	C27-C28-C29	-4.56	118.45	125.53
21	7	303	XAT	C35-C34-C33	-4.55	120.90	127.28
21	8	302	XAT	C26-C27-C28	-4.54	116.38	125.99
21	4	305	XAT	C26-C27-C28	-4.54	116.39	125.99
21	8	302	XAT	C35-C34-C33	-4.54	120.91	127.28
21	3	303	XAT	C6-C7-C8	-4.50	116.47	125.99
21	6	306	XAT	C6-C7-C8	-4.50	116.48	125.99
21	3	305	XAT	C35-C34-C33	-4.50	120.97	127.28
21	2	302	XAT	C6-C7-C8	-4.50	116.48	125.99
30	a	848	BCR	C16-C17-C18	-4.50	120.97	127.28
21	2	304	XAT	C26-C27-C28	-4.49	116.50	125.99
25	9	302	A1L1F	C36-C35-C34	-4.49	120.99	127.28
21	7	303	XAT	C26-C27-C28	-4.47	116.54	125.99
25	h	203	A1L1F	O15-C25-C14	-4.46	104.09	116.88
30	a	848	BCR	C15-C14-C13	-4.46	121.02	127.28
25	6	304	A1L1F	C26-C30-C31	-4.46	119.31	124.97
30	a	850	BCR	C15-C14-C13	-4.45	121.04	127.28
30	j	104	BCR	C15-C14-C13	-4.44	121.05	127.28
30	a	849	BCR	C15-C14-C13	-4.44	121.06	127.28
30	b	844	BCR	C16-C17-C18	-4.41	121.09	127.28
30	b	846	BCR	C33-C5-C6	-4.41	119.67	124.48
21	3	303	XAT	C35-C34-C33	-4.40	121.11	127.28
30	b	842	BCR	C16-C17-C18	-4.40	121.11	127.28
21	3	303	XAT	C15-C14-C13	-4.39	121.12	127.28
21	8	301	XAT	C35-C34-C33	-4.38	121.13	127.28
25	9	302	A1L1F	C14-C29-C30	-4.38	118.02	125.47
21	j	101	XAT	C35-C34-C33	-4.36	121.16	127.28
30	j	104	BCR	C16-C17-C18	-4.36	121.16	127.28
27	4	318	DGD	O6E-C5E-C6E	4.36	117.25	106.44
25	h	203	A1L1F	C25-C14-C29	-4.36	116.78	125.99
21	6	306	XAT	C15-C14-C13	-4.35	121.17	127.28
28	2	317	LMG	O7-C10-C11	4.35	120.90	111.48
21	5	304	XAT	C35-C34-C33	-4.35	121.18	127.28
21	3	304	XAT	C31-C30-C29	-4.33	121.21	127.28
25	1	304	A1L1F	O7-C54-C56	4.31	118.78	111.09
21	6	302	XAT	C6-C7-C8	-4.29	116.92	125.99
30	f	804	BCR	C24-C23-C22	-4.29	119.89	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	301	XAT	C6-C7-C8	-4.29	116.92	125.99
30	b	843	BCR	C15-C14-C13	-4.29	121.27	127.28
30	h	202	BCR	C33-C5-C6	-4.28	119.81	124.48
21	9	304	XAT	C18-C5-C4	4.28	119.04	114.24
25	6	301	A1L1F	O15-C25-C14	-4.28	104.63	116.88
21	3	301	XAT	C15-C14-C13	-4.27	121.28	127.28
21	7	303	XAT	C15-C14-C13	-4.27	121.29	127.28
30	b	845	BCR	C24-C23-C22	-4.27	119.92	126.23
21	4	304	XAT	C35-C34-C33	-4.27	121.29	127.28
21	2	305	XAT	C38-C25-C24	4.27	119.03	114.24
30	j	104	BCR	C7-C8-C9	-4.26	119.93	126.23
30	b	844	BCR	C15-C14-C13	-4.26	121.31	127.28
25	1	304	A1L1F	C37-C38-C39	-4.24	121.33	127.28
25	h	203	A1L1F	C41-C42-C44	-4.24	121.33	127.28
30	l	201	BCR	C33-C5-C6	-4.23	119.87	124.48
30	l	201	BCR	C15-C14-C13	-4.23	121.35	127.28
27	4	318	DGD	O2G-C1B-C2B	4.23	120.62	111.48
21	4	305	XAT	C35-C34-C33	-4.22	121.35	127.28
25	8	304	A1L1F	C41-C40-C39	-4.22	114.78	126.36
30	l	205	BCR	C20-C21-C22	-4.22	121.36	127.28
30	h	201	BCR	C16-C17-C18	-4.20	121.38	127.28
30	a	850	BCR	C38-C26-C25	-4.20	119.90	124.48
25	8	304	A1L1F	C32-C31-C30	-4.20	121.38	127.23
22	9	301	A1L1G	C37-C36-C35	4.20	132.11	123.52
26	a	845	LHG	O7-C7-C8	4.19	120.55	111.48
21	7	305	XAT	C11-C10-C9	-4.18	121.41	127.28
21	3	304	XAT	C15-C14-C13	-4.18	121.41	127.28
30	f	804	BCR	C7-C8-C9	-4.18	120.05	126.23
30	b	845	BCR	C20-C21-C22	-4.18	121.42	127.28
21	6	305	XAT	C27-C28-C29	-4.17	119.05	125.53
25	1	304	A1L1F	C17-C20-C21	4.17	118.92	114.24
25	6	301	A1L1F	C8-O7-C54	-4.16	110.50	117.85
30	b	845	BCR	C7-C8-C9	-4.16	120.08	126.23
21	5	301	XAT	C11-C10-C9	-4.14	121.47	127.28
30	l	205	BCR	C38-C26-C25	-4.13	119.97	124.48
30	a	847	BCR	C38-C26-C25	-4.13	119.98	124.48
30	a	848	BCR	C11-C10-C9	-4.11	121.51	127.28
29	b	841	PQN	C11-C12-C13	-4.11	119.75	126.83
28	a	853	LMG	O7-C10-C11	4.10	120.34	111.48
21	4	301	XAT	C15-C14-C13	-4.09	121.54	127.28
26	b	847	LHG	O7-C7-C8	4.09	120.32	111.48
30	f	801	BCR	C3-C4-C5	-4.08	106.78	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	845	BCR	C16-C15-C14	-4.07	115.20	123.52
30	f	804	BCR	C33-C5-C6	-4.05	120.06	124.48
21	9	304	XAT	C18-C5-C6	-4.04	115.65	122.30
30	b	842	BCR	C28-C27-C26	-4.04	106.85	114.06
25	9	302	A1L1F	O15-C20-C17	4.04	119.56	115.05
30	i	101	BCR	C7-C8-C9	-4.02	120.28	126.23
21	3	301	XAT	C35-C34-C33	-4.02	121.64	127.28
21	7	303	XAT	C6-C7-C8	-4.02	117.50	125.99
25	6	301	A1L1F	C37-C38-C39	-4.01	121.66	127.28
25	6	304	A1L1F	C36-C35-C34	-4.01	121.66	127.28
21	4	305	XAT	C6-C7-C8	-4.00	117.54	125.99
30	b	845	BCR	C15-C14-C13	-4.00	121.67	127.28
21	4	305	XAT	C11-C10-C9	-4.00	121.67	127.28
21	a	852	XAT	C31-C30-C29	-3.99	121.68	127.28
25	8	304	A1L1F	C37-C36-C35	-3.99	115.35	123.52
30	l	201	BCR	C11-C10-C9	-3.98	121.70	127.28
30	b	845	BCR	C28-C27-C26	-3.98	106.97	114.06
21	4	303	XAT	C15-C14-C13	-3.97	121.71	127.28
21	2	302	XAT	C31-C30-C29	-3.97	121.71	127.28
26	9	317	LHG	O7-C7-C8	3.97	120.06	111.48
26	a	846	LHG	O7-C7-C8	3.97	120.06	111.48
25	6	304	A1L1F	C37-C38-C39	-3.96	121.72	127.28
30	f	804	BCR	C38-C26-C25	-3.95	120.17	124.48
28	j	105	LMG	O7-C10-C11	3.95	120.03	111.48
25	6	301	A1L1F	C42-C41-C40	-3.94	111.77	123.20
21	1	303	XAT	C26-C27-C28	-3.94	117.67	125.99
21	j	101	XAT	C15-C14-C13	-3.94	121.76	127.28
21	6	303	XAT	C26-C27-C28	-3.93	117.68	125.99
21	2	303	XAT	C15-C14-C13	-3.93	121.76	127.28
30	a	847	BCR	C20-C21-C22	-3.93	121.77	127.28
30	l	205	BCR	C33-C5-C6	-3.92	120.20	124.48
23	b	804	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
21	2	302	XAT	C15-C14-C13	-3.91	121.79	127.28
25	6	304	A1L1F	C17-C20-C21	3.91	118.64	114.24
30	f	804	BCR	C20-C21-C22	-3.90	121.81	127.28
21	7	301	XAT	C15-C14-C13	-3.88	121.83	127.28
21	2	305	XAT	C27-C28-C29	-3.88	119.51	125.53
30	l	201	BCR	C16-C17-C18	-3.88	121.84	127.28
30	l	205	BCR	C16-C17-C18	-3.87	121.85	127.28
21	2	302	XAT	C26-C27-C28	-3.85	117.86	125.99
27	8	315	DGD	O2G-C1B-C2B	3.84	119.80	111.48
30	f	804	BCR	C16-C17-C18	-3.84	121.89	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	306	A1L1G	C36-C37-C38	3.84	131.38	123.52
30	b	846	BCR	C15-C14-C13	-3.84	121.90	127.28
21	5	301	XAT	C15-C14-C13	-3.82	121.92	127.28
22	1	301	A1L1G	C37-C36-C35	3.82	131.34	123.52
21	6	306	XAT	C27-C28-C29	-3.81	119.62	125.53
25	h	203	A1L1F	C36-C35-C34	-3.80	121.95	127.28
21	8	301	XAT	C15-C14-C13	-3.80	121.95	127.28
27	b	848	DGD	O5D-C6D-C5D	-3.80	100.86	109.42
21	1	303	XAT	C35-C34-C33	-3.80	121.95	127.28
23	a	806	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
30	f	801	BCR	C16-C15-C14	-3.78	115.78	123.52
30	h	201	BCR	C15-C14-C13	-3.78	121.98	127.28
30	j	104	BCR	C20-C21-C22	-3.78	121.98	127.28
30	a	850	BCR	C33-C5-C6	-3.78	120.36	124.48
30	a	849	BCR	C28-C27-C26	-3.77	107.33	114.06
21	9	305	XAT	C15-C14-C13	-3.77	121.99	127.28
24	1	315	SQD	O47-C7-C8	3.75	119.60	111.48
21	a	852	XAT	C35-C34-C33	-3.75	122.02	127.28
21	3	301	XAT	C31-C30-C29	-3.73	122.05	127.28
22	5	303	A1L1G	C36-C37-C38	3.73	131.15	123.52
21	2	303	XAT	C26-C27-C28	-3.72	118.12	125.99
30	a	849	BCR	C4-C5-C6	-3.72	117.68	122.70
30	h	202	BCR	C7-C8-C9	-3.70	120.76	126.23
30	a	849	BCR	C20-C21-C22	-3.70	122.09	127.28
30	b	843	BCR	C3-C4-C5	-3.69	107.47	114.06
25	9	302	A1L1F	C32-C31-C30	-3.69	122.09	127.23
21	3	301	XAT	C26-C27-C28	-3.69	118.19	125.99
21	8	301	XAT	C11-C10-C9	-3.68	122.11	127.28
22	9	306	A1L1G	C37-C36-C35	3.67	131.03	123.52
21	9	305	XAT	C31-C30-C29	-3.67	122.13	127.28
21	2	303	XAT	C6-C7-C8	-3.66	118.25	125.99
21	2	301	XAT	C27-C28-C29	-3.66	119.85	125.53
21	7	304	XAT	C6-C7-C8	-3.66	118.25	125.99
21	6	302	XAT	C26-C27-C28	-3.65	118.28	125.99
30	a	847	BCR	C33-C5-C6	-3.65	120.51	124.48
21	1	302	XAT	C11-C10-C9	-3.64	122.17	127.28
22	7	302	A1L1G	C37-C36-C35	3.64	130.96	123.52
21	4	302	XAT	C35-C15-C14	-3.63	116.09	123.52
30	a	849	BCR	C11-C10-C9	-3.63	122.19	127.28
21	8	303	XAT	C30-C31-C32	-3.62	112.71	123.20
21	8	301	XAT	C6-C7-C8	-3.62	118.34	125.99
30	b	845	BCR	C3-C4-C5	-3.62	107.61	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	304	A1L1F	C32-C31-C30	-3.61	122.20	127.23
30	b	845	BCR	C10-C11-C12	-3.61	112.73	123.20
30	b	843	BCR	C33-C5-C6	-3.61	120.54	124.48
30	i	101	BCR	C33-C5-C6	-3.61	120.55	124.48
30	a	847	BCR	C7-C8-C9	-3.60	120.91	126.23
23	a	806	CLA	CAA-CBA-CGA	-3.60	103.00	113.21
21	j	101	XAT	C10-C11-C12	-3.59	112.79	123.20
30	l	205	BCR	C11-C10-C9	-3.58	122.25	127.28
21	9	303	XAT	C11-C10-C9	-3.58	122.26	127.28
25	8	304	A1L1F	C31-C32-C33	-3.58	112.83	123.20
21	6	305	XAT	C15-C14-C13	-3.58	122.26	127.28
30	h	201	BCR	C24-C23-C22	-3.57	120.96	126.23
21	6	305	XAT	C11-C10-C9	-3.57	122.28	127.28
30	a	847	BCR	C15-C14-C13	-3.56	122.28	127.28
21	8	303	XAT	C15-C35-C34	-3.56	116.24	123.52
21	2	305	XAT	C24-C23-C22	-3.55	104.14	110.79
30	a	848	BCR	C24-C23-C22	-3.55	120.99	126.23
21	4	303	XAT	C35-C34-C33	-3.55	122.30	127.28
23	9	312	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
30	h	202	BCR	C38-C26-C25	-3.55	120.61	124.48
21	1	303	XAT	C15-C14-C13	-3.54	122.31	127.28
30	l	205	BCR	C3-C4-C5	-3.53	107.76	114.06
25	1	304	A1L1F	C8-O7-C54	-3.53	111.61	117.85
21	9	303	XAT	C35-C34-C33	-3.53	122.33	127.28
21	6	303	XAT	C35-C34-C33	-3.53	122.33	127.28
21	6	303	XAT	C7-C8-C9	-3.53	120.06	125.53
21	4	302	XAT	C11-C10-C9	-3.52	122.34	127.28
30	a	849	BCR	C7-C8-C9	-3.52	121.02	126.23
21	8	302	XAT	C31-C30-C29	-3.51	122.35	127.28
22	9	301	A1L1G	C36-C37-C38	3.51	130.70	123.52
23	a	806	CLA	C3B-C4B-NB	-3.50	107.40	110.53
30	a	847	BCR	C24-C23-C22	-3.50	121.06	126.23
21	6	303	XAT	C31-C30-C29	-3.50	122.37	127.28
22	9	306	A1L1G	C36-C37-C38	3.49	130.66	123.52
24	5	316	SQD	O47-C7-C8	3.49	119.03	111.48
22	7	302	A1L1G	C36-C37-C38	3.48	130.65	123.52
21	2	304	XAT	C11-C10-C9	-3.48	122.39	127.28
21	3	303	XAT	C11-C10-C9	-3.48	122.40	127.28
30	i	101	BCR	C28-C27-C26	-3.48	107.86	114.06
25	h	203	A1L1F	C31-C32-C33	-3.47	113.13	123.20
21	3	305	XAT	C15-C14-C13	-3.47	122.41	127.28
21	7	304	XAT	C31-C30-C29	-3.47	122.42	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	304	XAT	C31-C30-C29	-3.46	122.42	127.28
30	a	848	BCR	C20-C21-C22	-3.46	122.42	127.28
30	a	847	BCR	C11-C10-C9	-3.46	122.42	127.28
23	9	314	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
21	a	852	XAT	C10-C11-C12	-3.45	113.20	123.20
23	b	804	CLA	CHB-C4A-NA	3.45	129.38	124.40
30	a	849	BCR	C24-C23-C22	-3.44	121.14	126.23
22	3	302	A1L1G	C36-C37-C38	3.44	130.56	123.52
21	1	303	XAT	C24-C23-C22	-3.44	104.36	110.79
25	9	302	A1L1F	C37-C38-C39	-3.43	122.47	127.28
21	9	304	XAT	C35-C34-C33	-3.42	122.48	127.28
25	8	304	A1L1F	C14-C29-C30	-3.42	119.65	125.47
22	3	302	A1L1G	C37-C36-C35	3.42	130.51	123.52
25	6	304	A1L1F	C14-C29-C30	-3.41	119.68	125.47
21	5	302	XAT	C6-C7-C8	-3.40	118.80	125.99
27	b	848	DGD	C2G-O2G-C1B	-3.39	109.67	117.80
21	5	304	XAT	C24-C23-C22	-3.38	104.47	110.79
21	5	301	XAT	C7-C8-C9	-3.38	120.29	125.53
21	5	301	XAT	C24-C23-C22	-3.37	104.48	110.79
30	b	846	BCR	C10-C11-C12	-3.37	113.44	123.20
30	h	202	BCR	C11-C10-C9	-3.36	122.56	127.28
21	1	303	XAT	C31-C30-C29	-3.36	122.57	127.28
21	5	304	XAT	C4-C3-C2	-3.35	104.52	110.79
30	j	104	BCR	C24-C23-C22	-3.35	121.28	126.23
21	5	301	XAT	C6-C7-C8	-3.35	118.91	125.99
21	6	303	XAT	C11-C10-C9	-3.35	122.58	127.28
30	i	101	BCR	C15-C14-C13	-3.35	122.58	127.28
21	9	305	XAT	C38-C25-C26	-3.34	116.80	122.30
22	5	303	A1L1G	C37-C36-C35	3.34	130.36	123.52
25	1	304	A1L1F	C14-C29-C30	-3.33	119.80	125.47
30	a	847	BCR	C3-C4-C5	-3.33	108.11	114.06
23	5	312	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
21	4	301	XAT	C11-C10-C9	-3.33	122.61	127.28
23	b	804	CLA	C3B-C4B-NB	-3.31	107.58	110.53
25	9	302	A1L1F	C25-C14-C29	-3.31	119.00	125.99
25	8	304	A1L1F	C26-C30-C31	-3.30	120.78	124.97
30	a	850	BCR	C7-C8-C9	-3.30	121.35	126.23
23	9	311	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
25	6	301	A1L1F	C26-C30-C31	-3.30	120.78	124.97
21	4	303	XAT	C6-C7-C8	-3.29	119.03	125.99
22	1	301	A1L1G	C36-C37-C38	3.29	130.26	123.52
21	6	303	XAT	C24-C23-C22	-3.29	104.64	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	203	A1L1F	C17-C20-C21	3.28	117.92	114.24
30	i	101	BCR	C11-C10-C9	-3.27	122.69	127.28
25	9	302	A1L1F	C42-C41-C40	-3.27	113.72	123.20
30	l	201	BCR	C38-C26-C25	-3.27	120.91	124.48
21	9	304	XAT	C11-C10-C9	-3.27	122.69	127.28
30	a	848	BCR	C33-C5-C6	-3.27	120.92	124.48
22	9	301	A1L1G	C33-C34-C35	3.27	124.15	119.01
23	j	103	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
21	6	305	XAT	C7-C8-C9	-3.26	120.47	125.53
30	b	849	BCR	C24-C23-C22	-3.26	121.41	126.23
21	4	303	XAT	C24-C23-C22	-3.26	104.70	110.79
21	9	304	XAT	C24-C23-C22	-3.26	104.70	110.79
21	9	305	XAT	C24-C23-C22	-3.26	104.70	110.79
21	9	303	XAT	C24-C23-C22	-3.25	104.71	110.79
21	4	304	XAT	C24-C23-C22	-3.25	104.71	110.79
21	3	303	XAT	C24-C23-C22	-3.25	104.71	110.79
23	b	809	CLA	O2A-CGA-O1A	-3.25	115.50	123.63
29	a	843	PQN	C14-C13-C15	3.24	120.86	115.23
21	4	304	XAT	C15-C14-C13	-3.24	122.73	127.28
21	a	852	XAT	C11-C10-C9	-3.23	122.75	127.28
25	9	302	A1L1F	O15-C25-C14	-3.23	107.62	116.88
25	6	301	A1L1F	C25-C14-C29	-3.23	119.16	125.99
30	h	201	BCR	C20-C21-C22	-3.23	122.75	127.28
21	3	304	XAT	C26-C27-C28	-3.23	119.17	125.99
23	b	820	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
21	l	302	XAT	C15-C14-C13	-3.22	122.76	127.28
30	a	848	BCR	C38-C26-C25	-3.22	120.97	124.48
27	4	318	DGD	O1G-C1A-C2A	3.22	121.65	111.83
21	8	301	XAT	C24-C23-C22	-3.22	104.77	110.79
25	h	203	A1L1F	C37-C36-C35	-3.22	116.94	123.52
30	l	201	BCR	C24-C23-C22	-3.21	121.48	126.23
23	b	830	CLA	C3B-C4B-NB	-3.20	107.67	110.53
30	a	850	BCR	C11-C10-C9	-3.20	122.79	127.28
21	7	304	XAT	C24-C23-C22	-3.20	104.81	110.79
30	b	843	BCR	C16-C17-C18	-3.19	122.80	127.28
23	a	835	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
21	3	304	XAT	C11-C10-C9	-3.19	122.81	127.28
23	a	804	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
30	b	849	BCR	C33-C5-C6	-3.18	121.02	124.48
21	2	301	XAT	C11-C10-C9	-3.18	122.82	127.28
21	7	305	XAT	C35-C34-C33	-3.17	122.83	127.28
23	b	817	CLA	C3B-C4B-NB	-3.17	107.70	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	316	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
27	8	315	DGD	O1G-C1A-C2A	3.16	121.48	111.83
30	a	849	BCR	C38-C26-C25	-3.16	121.03	124.48
23	1	313	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
23	a	818	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
21	6	303	XAT	C6-C7-C8	-3.16	119.32	125.99
22	3	306	A1L1G	C37-C36-C35	3.15	129.97	123.52
21	3	304	XAT	C4-C3-C2	-3.15	104.90	110.79
30	a	848	BCR	C3-C4-C5	-3.15	108.44	114.06
21	9	303	XAT	C6-C7-C8	-3.14	119.35	125.99
23	b	832	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
30	h	201	BCR	C38-C26-C25	-3.13	121.06	124.48
21	4	303	XAT	C30-C31-C32	-3.13	114.14	123.20
30	l	205	BCR	C8-C7-C6	-3.13	118.65	127.00
23	a	819	CLA	C3B-C4B-NB	-3.13	107.74	110.53
22	9	306	A1L1G	C33-C34-C35	3.12	123.92	119.01
25	8	304	A1L1F	C36-C35-C34	-3.12	122.90	127.28
21	4	305	XAT	C24-C23-C22	-3.12	104.95	110.79
21	2	301	XAT	C26-C27-C28	-3.12	119.39	125.99
25	9	302	A1L1F	C26-C30-C31	-3.12	121.01	124.97
21	8	302	XAT	C24-C23-C22	-3.12	104.96	110.79
30	a	848	BCR	C8-C7-C6	-3.12	118.68	127.00
30	b	845	BCR	C11-C10-C9	-3.11	122.91	127.28
30	b	842	BCR	C20-C21-C22	-3.11	122.92	127.28
21	6	305	XAT	C24-C23-C22	-3.10	104.98	110.79
21	a	852	XAT	C35-C15-C14	-3.10	117.17	123.52
21	3	305	XAT	C4-C3-C2	-3.10	104.99	110.79
30	f	801	BCR	C8-C7-C6	-3.10	118.72	127.00
21	5	301	XAT	C31-C30-C29	-3.10	122.93	127.28
21	1	302	XAT	C31-C30-C29	-3.10	122.94	127.28
23	4	311	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
23	4	316	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
21	8	303	XAT	C24-C23-C22	-3.09	105.02	110.79
21	4	304	XAT	C35-C15-C14	-3.09	117.20	123.52
21	7	305	XAT	C4-C3-C2	-3.09	105.02	110.79
25	8	304	A1L1F	O15-C25-C14	-3.08	108.04	116.88
23	a	809	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
21	a	852	XAT	C31-C32-C33	-3.08	117.92	126.36
23	3	308	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
22	1	301	A1L1G	C33-C34-C35	3.08	123.85	119.01
23	b	809	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
23	a	802	CLA	C3B-C4B-NB	-3.07	107.79	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	807	CLA	C3B-C4B-NB	-3.07	107.79	110.53
21	6	306	XAT	C11-C10-C9	-3.07	122.98	127.28
22	5	303	A1L1G	C40-C39-C38	3.06	123.83	119.01
25	8	304	A1L1F	C25-C14-C29	-3.06	119.52	125.99
23	6	308	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	8	308	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
30	h	202	BCR	C15-C14-C13	-3.06	122.99	127.28
23	4	307	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
21	9	305	XAT	C8-C9-C10	3.06	123.82	119.01
23	9	311	CLA	C3B-C4B-NB	-3.05	107.80	110.53
23	9	318	CLA	C3B-C4B-NB	-3.05	107.81	110.53
21	6	306	XAT	C26-C27-C28	-3.05	119.55	125.99
26	a	846	LHG	O8-C23-C24	3.05	120.40	111.15
21	6	302	XAT	C24-C23-C22	-3.05	105.09	110.79
30	h	201	BCR	C4-C5-C6	-3.05	118.59	122.70
23	a	832	CLA	C3B-C4B-NB	-3.05	107.81	110.53
30	b	846	BCR	C8-C7-C6	-3.04	118.87	127.00
23	3	307	CLA	C3B-C4B-NB	-3.04	107.81	110.53
21	4	304	XAT	C4-C3-C2	-3.04	105.11	110.79
23	3	315	CLA	C3B-C4B-NB	-3.04	107.82	110.53
21	7	305	XAT	C24-C23-C22	-3.04	105.11	110.79
30	h	202	BCR	C16-C15-C14	-3.03	117.31	123.52
21	3	305	XAT	C24-C23-C22	-3.03	105.12	110.79
23	b	816	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
23	a	831	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
21	8	303	XAT	C4-C3-C2	-3.03	105.13	110.79
21	3	301	XAT	C4-C3-C2	-3.02	105.13	110.79
23	7	314	CLA	C3B-C4B-NB	-3.02	107.83	110.53
21	6	305	XAT	C35-C15-C14	-3.02	117.33	123.52
22	9	301	A1L1G	C27-C34-C35	-3.02	117.92	122.82
23	4	312	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	a	854	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	9	313	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
23	9	310	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
30	b	846	BCR	C21-C20-C19	-3.02	114.46	123.20
30	h	201	BCR	C8-C7-C6	-3.01	118.95	127.00
23	9	314	CLA	O2D-CGD-CBD	3.01	116.50	111.23
21	2	303	XAT	C4-C3-C2	-3.01	105.16	110.79
25	6	301	A1L1F	C17-C20-C21	3.01	117.62	114.24
21	3	305	XAT	C31-C30-C29	-3.01	123.06	127.28
21	1	302	XAT	C4-C3-C2	-3.01	105.16	110.79
23	6	311	CLA	C3B-C4B-NB	-3.01	107.85	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	302	XAT	C11-C12-C13	-3.01	118.12	126.36
21	4	301	XAT	C31-C32-C33	-3.00	118.12	126.36
23	a	822	CLA	C3B-C4B-NB	-3.00	107.85	110.53
21	2	304	XAT	C24-C23-C22	-3.00	105.18	110.79
25	h	203	A1L1F	C12-C6-C1	-3.00	107.79	110.47
23	a	813	CLA	C3B-C4B-NB	-3.00	107.85	110.53
21	5	302	XAT	C24-C23-C22	-3.00	105.18	110.79
21	7	301	XAT	C4-C3-C2	-3.00	105.19	110.79
23	b	808	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
21	4	302	XAT	C24-C23-C22	-3.00	105.19	110.79
29	b	841	PQN	C16-C15-C13	-3.00	106.17	113.47
23	a	830	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
22	1	301	A1L1G	C40-C39-C38	3.00	123.72	119.01
23	1	314	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
23	b	811	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
23	6	315	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	a	818	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	b	836	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	4	315	CLA	C3B-C4B-NB	-2.99	107.86	110.53
30	b	843	BCR	C38-C26-C25	-2.99	121.22	124.48
21	9	304	XAT	C30-C31-C32	-2.99	114.55	123.20
22	3	302	A1L1G	C33-C34-C35	2.99	123.71	119.01
23	a	841	CLA	C3B-C4B-NB	-2.99	107.86	110.53
21	9	305	XAT	C27-C28-C29	-2.98	120.90	125.53
21	8	302	XAT	C6-C7-C8	-2.98	119.69	125.99
22	7	302	A1L1G	C33-C34-C35	2.98	123.70	119.01
23	a	820	CLA	C1-C2-C3	-2.98	121.31	126.20
23	4	309	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
23	2	309	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
23	b	814	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	7	302	A1L1G	C40-C39-C38	2.98	123.69	119.01
23	b	834	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
30	b	849	BCR	C16-C15-C14	-2.97	117.43	123.52
22	9	306	A1L1G	C40-C39-C38	2.97	123.68	119.01
23	6	309	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
23	a	839	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
23	1	311	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	2	313	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
30	b	843	BCR	C21-C20-C19	-2.97	114.60	123.20
21	1	302	XAT	C35-C15-C14	-2.96	117.45	123.52
21	1	302	XAT	C24-C23-C22	-2.96	105.25	110.79
22	3	306	A1L1G	C40-C39-C38	2.96	123.67	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	809	CLA	C3B-C4B-NB	-2.96	107.89	110.53
23	6	307	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
23	7	308	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	7	313	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	b	839	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	a	812	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	3	309	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
23	4	308	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	3	301	XAT	C10-C11-C12	-2.95	114.64	123.20
23	b	829	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
23	7	314	CLA	CHB-C4A-NA	2.95	128.66	124.40
30	b	844	BCR	C38-C26-C25	-2.95	121.27	124.48
21	4	302	XAT	C4-C3-C2	-2.95	105.27	110.79
21	a	852	XAT	C24-C23-C22	-2.95	105.27	110.79
30	a	850	BCR	C28-C27-C26	-2.95	108.80	114.06
23	6	317	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
21	6	305	XAT	C31-C32-C33	-2.95	118.28	126.36
23	b	824	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	8	313	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	9	301	A1L1G	C40-C39-C38	2.95	123.64	119.01
30	h	202	BCR	C23-C24-C25	-2.95	119.13	127.00
23	8	314	CLA	C3B-C4B-NB	-2.94	107.90	110.53
21	3	303	XAT	C4-C3-C2	-2.94	105.28	110.79
23	b	818	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
23	f	803	CLA	C3B-C4B-NB	-2.94	107.91	110.53
23	2	309	CLA	C3B-C4B-NB	-2.94	107.91	110.53
23	3	307	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
30	a	849	BCR	C2-C1-C6	2.94	114.71	110.44
23	b	819	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	1	304	A1L1F	C26-O13-C45	2.93	121.79	115.64
27	b	848	DGD	O3E-C3E-C2E	-2.93	103.46	110.38
30	f	801	BCR	C20-C19-C18	-2.93	118.32	126.36
22	7	302	A1L1G	C27-C34-C35	-2.93	118.06	122.82
23	b	814	CLA	CHB-C4A-NA	2.93	128.63	124.40
21	2	304	XAT	C4-C3-C2	-2.93	105.31	110.79
23	a	817	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	j	102	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
21	4	301	XAT	C4-C3-C2	-2.93	105.32	110.79
23	6	316	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
30	b	842	BCR	C4-C5-C6	-2.92	118.75	122.70
30	a	848	BCR	C7-C8-C9	-2.92	121.91	126.23
23	6	317	CLA	C1-C2-C3	-2.92	121.41	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	314	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	a	808	CLA	C3B-C4B-NB	-2.92	107.92	110.53
21	1	303	XAT	C4-C3-C2	-2.92	105.32	110.79
22	5	303	A1L1G	C28-C39-C38	-2.92	118.08	122.82
23	7	315	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	a	842	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	b	805	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
21	5	304	XAT	C19-C9-C8	2.92	122.55	118.09
23	b	817	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
23	b	838	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	9	306	A1L1G	C27-C34-C35	-2.92	118.09	122.82
23	5	312	CLA	O2D-CGD-CBD	2.92	116.33	111.23
22	9	306	A1L1G	C28-C39-C38	-2.92	118.09	122.82
21	j	101	XAT	C4-C3-C2	-2.92	105.34	110.79
23	a	828	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	4	312	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
30	b	845	BCR	C33-C5-C6	-2.91	121.30	124.48
23	7	317	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	6	313	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	a	840	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	9	309	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	5	315	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	2	316	CLA	C3B-C4B-NB	-2.91	107.94	110.53
23	a	813	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	4	317	CLA	C3B-C4B-NB	-2.91	107.94	110.53
23	2	316	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
23	b	826	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	1	202	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	1	312	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	1	303	XAT	C10-C11-C12	-2.90	114.79	123.20
23	1	310	CLA	C3B-C4B-NB	-2.90	107.94	110.53
23	2	310	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	5	307	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	7	312	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	2	301	XAT	C4-C3-C2	-2.90	105.37	110.79
22	9	301	A1L1G	C28-C39-C38	-2.90	118.12	122.82
21	3	304	XAT	C24-C23-C22	-2.90	105.37	110.79
23	a	820	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
30	f	801	BCR	C33-C5-C6	-2.90	121.32	124.48
23	a	804	CLA	C1-C2-C3	-2.90	121.45	126.20
23	a	836	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	1	301	A1L1G	C27-C34-C35	-2.89	118.13	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	304	A1L1F	C11-C1-C6	2.89	122.57	119.70
23	4	314	CLA	C3B-C4B-NB	-2.89	107.95	110.53
23	8	310	CLA	C3B-C4B-NB	-2.89	107.95	110.53
23	b	816	CLA	C3B-C4B-NB	-2.89	107.95	110.53
21	2	305	XAT	C11-C10-C9	-2.89	123.23	127.28
21	9	304	XAT	C4-C3-C2	-2.89	105.39	110.79
23	6	308	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
22	3	302	A1L1G	C28-C39-C38	-2.89	118.14	122.82
22	3	306	A1L1G	C27-C34-C35	-2.89	118.14	122.82
22	1	301	A1L1G	C28-C39-C38	-2.89	118.14	122.82
22	3	302	A1L1G	C40-C39-C38	2.89	123.55	119.01
21	9	304	XAT	C15-C35-C34	-2.88	117.62	123.52
25	8	304	A1L1F	C17-C20-C21	2.88	117.48	114.24
23	a	837	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
23	8	306	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	7	315	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	a	825	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	b	834	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	a	833	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	2	314	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	7	307	CLA	C3B-C4B-NB	-2.88	107.96	110.53
27	b	848	DGD	O1G-C1A-C2A	2.88	120.61	111.83
23	8	311	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
23	6	307	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	2	317	LMG	O8-C28-C29	2.88	120.61	111.83
30	b	846	BCR	C15-C16-C17	-2.87	117.64	123.52
22	7	302	A1L1G	C28-C39-C38	-2.87	118.16	122.82
25	h	203	A1L1F	C26-C30-C31	-2.87	121.32	124.97
21	4	305	XAT	C4-C3-C2	-2.87	105.42	110.79
21	5	302	XAT	C35-C34-C33	-2.87	123.25	127.28
23	1	312	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	b	806	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	h	201	BCR	C10-C11-C12	-2.87	114.88	123.20
23	5	306	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	2	307	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	a	823	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
21	8	303	XAT	C11-C10-C9	-2.87	123.25	127.28
23	b	823	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	a	816	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
22	3	306	A1L1G	C33-C34-C35	2.87	123.52	119.01
23	b	837	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	6	311	CLA	O2D-CGD-O1D	-2.86	118.27	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	303	A1L1G	C33-C34-C35	2.86	123.51	119.01
23	5	305	CLA	C3B-C4B-NB	-2.86	107.97	110.53
23	6	314	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	8	310	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	5	309	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	3	311	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
23	7	311	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	1	307	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	4	318	DGD	O5E-C6E-C5E	-2.86	101.61	111.33
21	5	304	XAT	C10-C11-C12	-2.86	114.92	123.20
23	a	811	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
23	a	825	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
23	4	316	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	4	307	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	6	313	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	i	101	BCR	C29-C30-C25	2.85	114.58	110.44
23	9	315	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	a	817	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	5	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	9	313	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	8	309	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	a	826	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	8	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	8	307	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	8	312	CLA	C3B-C4B-NB	-2.85	107.99	110.53
23	j	102	CLA	C3B-C4B-NB	-2.85	107.99	110.53
23	5	315	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	7	315	CLA	CAA-C2A-C3A	-2.84	109.71	116.23
23	b	838	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
23	3	313	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
22	3	306	A1L1G	C28-C39-C38	-2.84	118.21	122.82
21	2	301	XAT	C24-C23-C22	-2.84	105.47	110.79
23	2	314	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	7	312	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	8	312	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	2	310	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	9	312	CLA	CHB-C4A-NA	2.84	128.50	124.40
23	9	308	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	3	302	A1L1G	C27-C34-C35	-2.84	118.22	122.82
23	a	833	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
23	1	305	CLA	C3B-C4B-NB	-2.84	108.00	110.53
23	8	313	CLA	O2D-CGD-O1D	-2.83	118.33	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	306	CLA	C3B-C4B-NB	-2.83	108.00	110.53
23	b	827	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
21	2	305	XAT	C38-C25-C26	-2.83	117.64	122.30
25	8	304	A1L1F	O13-C45-C47	2.83	120.47	111.83
28	a	853	LMG	O8-C28-C29	2.83	120.47	111.83
23	a	802	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	a	827	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	8	304	A1L1F	O7-C54-O55	-2.83	117.53	122.99
23	7	307	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	6	310	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
30	f	801	BCR	C10-C11-C12	-2.83	115.01	123.20
23	4	311	CLA	C3B-C4B-NB	-2.83	108.01	110.53
23	5	309	CLA	C3B-C4B-NB	-2.83	108.01	110.53
23	a	834	CLA	C3B-C4B-NB	-2.83	108.01	110.53
23	a	805	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
23	2	307	CLA	C3B-C4B-NB	-2.83	108.01	110.53
23	7	310	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	l	203	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
29	a	843	PQN	C11-C3-C2	-2.82	120.05	124.89
23	2	307	CLA	CHB-C4A-NA	2.82	128.47	124.40
21	4	304	XAT	C11-C10-C9	-2.82	123.32	127.28
23	b	828	CLA	C3B-C4B-NB	-2.82	108.01	110.53
30	b	842	BCR	C2-C1-C6	2.82	114.53	110.44
23	a	815	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
21	2	305	XAT	C4-C3-C2	-2.82	105.52	110.79
23	a	832	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	5	303	A1L1G	C27-C34-C35	-2.82	118.25	122.82
23	4	313	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	b	821	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
30	b	844	BCR	C20-C21-C22	-2.82	123.33	127.28
21	9	303	XAT	C15-C35-C34	-2.81	117.76	123.52
23	b	812	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	a	821	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
21	8	303	XAT	C39-C29-C28	2.81	122.38	118.09
30	h	202	BCR	C21-C20-C19	-2.81	115.06	123.20
23	7	306	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	h	203	A1L1F	O13-C45-C47	2.81	120.39	111.83
23	b	831	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	1	315	SQD	O48-C23-C24	2.81	120.39	111.83
25	h	203	A1L1F	C8-O7-C54	-2.81	112.89	117.85
25	9	302	A1L1F	O13-C45-C47	2.81	120.39	111.83
30	h	201	BCR	C33-C5-C4	2.81	119.58	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	j	101	XAT	C24-C23-C22	-2.81	105.54	110.79
23	1	310	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
23	a	836	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	4	306	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	b	813	CLA	C3B-C4B-NB	-2.80	108.03	110.53
21	7	305	XAT	C15-C35-C34	-2.80	117.78	123.52
23	1	305	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	8	309	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	3	314	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
25	1	304	A1L1F	C36-C35-C34	-2.80	123.35	127.28
23	a	831	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
23	h	204	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	1	308	CLA	C1-C2-C3	-2.80	121.61	126.20
30	m	101	BCR	C27-C26-C25	2.80	126.49	122.70
30	b	842	BCR	C38-C26-C25	-2.80	121.43	124.48
21	4	302	XAT	C31-C30-C29	-2.80	123.35	127.28
21	9	303	XAT	C30-C31-C32	-2.80	115.09	123.20
23	5	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	1	306	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	a	849	BCR	C33-C5-C4	2.80	119.56	113.60
23	6	316	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	7	317	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	j	103	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	l	203	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	b	840	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	b	828	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	a	837	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	a	844	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
21	6	305	XAT	C26-C27-C28	-2.79	120.09	125.99
23	2	308	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	6	312	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	a	803	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	3	312	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	3	313	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	b	801	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	2	306	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	3	315	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	5	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	1	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	7	306	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	a	824	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	b	801	CLA	O2D-CGD-O1D	-2.79	118.43	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	j	104	BCR	C23-C24-C25	-2.78	119.56	127.00
23	2	315	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	b	815	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
21	2	302	XAT	C24-C23-C22	-2.78	105.58	110.79
23	5	310	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	6	306	XAT	C4-C3-C2	-2.78	105.59	110.79
23	9	308	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	b	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	b	815	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	4	310	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	9	311	CLA	CHB-C4A-NA	2.78	128.41	124.40
23	9	312	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	9	316	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	a	839	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	a	828	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
26	9	317	LHG	O8-C23-C24	2.77	120.30	111.83
23	h	204	CLA	C3B-C4B-NB	-2.77	108.05	110.53
23	a	841	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
23	5	313	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	a	811	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	b	842	BCR	C24-C23-C22	-2.77	122.14	126.23
23	b	832	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	h	201	BCR	C2-C1-C6	2.77	114.46	110.44
23	8	314	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	a	819	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	b	830	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	5	316	SQD	O48-C23-C24	2.77	120.27	111.83
23	1	313	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	4	306	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	5	314	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
21	7	301	XAT	C11-C10-C9	-2.77	123.40	127.28
21	3	301	XAT	C19-C9-C8	2.77	122.31	118.09
21	5	302	XAT	C4-C3-C2	-2.77	105.62	110.79
23	b	825	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	i	101	BCR	C20-C19-C18	-2.76	118.78	126.36
23	a	841	CLA	CHB-C4A-NA	2.76	128.39	124.40
23	2	313	CLA	CAA-C2A-C3A	-2.76	109.89	116.23
23	b	836	CLA	C3B-C4B-NB	-2.76	108.06	110.53
23	b	819	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
21	6	303	XAT	C15-C35-C34	-2.76	117.87	123.52
23	5	314	CLA	C3B-C4B-NB	-2.76	108.07	110.53
23	a	816	CLA	C3B-C4B-NB	-2.76	108.07	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	805	CLA	C3B-C4B-NB	-2.76	108.07	110.53
21	2	301	XAT	C31-C32-C33	-2.76	118.80	126.36
23	b	829	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
21	4	301	XAT	C26-C27-C28	-2.76	120.16	125.99
23	b	806	CLA	C3B-C4B-NB	-2.76	108.07	110.53
23	a	838	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	b	849	BCR	C20-C19-C18	-2.75	118.81	126.36
23	a	820	CLA	C3B-C4B-NB	-2.75	108.07	110.53
30	b	842	BCR	C23-C24-C25	-2.75	119.65	127.00
23	f	802	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
30	h	202	BCR	C24-C23-C22	-2.75	122.17	126.23
23	b	822	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	3	314	CLA	C3B-C4B-NB	-2.75	108.08	110.53
23	9	310	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	6	301	A1L1F	O13-C45-C47	2.75	120.21	111.83
23	a	824	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	b	812	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	f	803	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	a	807	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	b	840	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	3	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	7	309	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	3	312	CLA	CHB-C4A-NA	2.74	128.36	124.40
21	6	302	XAT	C4-C3-C2	-2.74	105.66	110.79
21	3	305	XAT	C35-C15-C14	-2.74	117.91	123.52
23	a	815	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	1	301	A1L1G	C43-C44-C42	-2.74	118.38	122.82
23	l	204	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	a	827	CLA	C3B-C4B-NB	-2.74	108.08	110.53
30	b	845	BCR	C35-C13-C12	2.74	122.27	118.09
21	6	303	XAT	C4-C3-C2	-2.74	105.67	110.79
23	b	817	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
23	5	305	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	1	309	CLA	C3B-C4B-NB	-2.74	108.09	110.53
21	3	303	XAT	C31-C30-C29	-2.74	123.44	127.28
21	4	303	XAT	C4-C3-C2	-2.73	105.67	110.79
23	a	814	CLA	C3B-C4B-NB	-2.73	108.09	110.53
21	2	302	XAT	C35-C15-C14	-2.73	117.93	123.52
30	h	201	BCR	C7-C8-C9	-2.73	122.19	126.23
23	4	313	CLA	C3B-C4B-NB	-2.73	108.09	110.53
21	8	302	XAT	C4-C3-C2	-2.73	105.68	110.79
23	b	835	CLA	O2D-CGD-O1D	-2.73	118.53	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	304	XAT	C7-C8-C9	-2.73	121.29	125.53
23	7	311	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	2	313	CLA	C3B-C4B-NB	-2.73	108.09	110.53
23	4	314	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	5	308	CLA	C3B-C4B-NB	-2.73	108.09	110.53
23	b	810	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	2	312	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
21	7	303	XAT	C24-C23-C22	-2.72	105.70	110.79
23	a	841	CLA	C1-C2-C3	-2.72	121.73	126.20
21	j	101	XAT	C31-C30-C29	-2.72	123.46	127.28
23	b	830	CLA	CAA-C2A-C3A	-2.72	109.99	116.23
23	5	307	CLA	C3B-C4B-NB	-2.72	108.10	110.53
21	j	101	XAT	C15-C35-C34	-2.72	117.95	123.52
21	3	301	XAT	C24-C23-C22	-2.72	105.71	110.79
23	9	310	CLA	CHB-C4A-NA	2.72	128.32	124.40
21	7	304	XAT	C4-C3-C2	-2.71	105.72	110.79
21	j	101	XAT	C31-C32-C33	-2.71	118.93	126.36
23	9	315	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	a	808	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	1	304	A1L1F	C26-C30-C31	-2.71	121.53	124.97
23	a	802	CLA	C1-C2-C3	-2.71	121.76	126.20
21	4	305	XAT	C31-C32-C33	-2.71	118.94	126.36
30	h	202	BCR	C20-C21-C22	-2.70	123.49	127.28
30	b	844	BCR	C11-C10-C9	-2.70	123.49	127.28
23	3	312	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
23	9	309	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
21	4	303	XAT	C39-C29-C28	2.70	122.22	118.09
26	b	847	LHG	O8-C23-C24	2.70	120.06	111.83
23	a	812	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	b	831	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	5	312	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	7	313	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	4	315	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
23	a	814	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
23	a	810	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	b	824	CLA	C3B-C4B-NB	-2.69	108.13	110.53
21	8	301	XAT	C7-C8-C9	-2.69	121.36	125.53
21	7	303	XAT	C4-C3-C2	-2.69	105.76	110.79
28	j	105	LMG	O8-C28-C29	2.69	120.04	111.83
23	2	311	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	l	202	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	9	307	LHG	O8-C23-C24	2.69	120.03	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	315	CLA	CAA-C2A-C3A	-2.68	110.08	116.23
21	4	302	XAT	C15-C14-C13	-2.68	123.52	127.28
23	a	801	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	b	814	CLA	C3B-C4B-NB	-2.68	108.14	110.53
21	8	301	XAT	C4-C3-C2	-2.68	105.77	110.79
23	7	317	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	6	301	A1L1F	C31-C32-C33	-2.68	115.43	123.20
23	a	822	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
23	a	805	CLA	CHB-C4A-NA	2.68	128.27	124.40
23	4	310	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
23	b	807	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
25	1	304	A1L1F	O15-C25-C14	-2.67	109.22	116.88
21	5	304	XAT	C31-C30-C29	-2.67	123.53	127.28
21	8	303	XAT	C35-C34-C33	-2.67	123.53	127.28
21	9	303	XAT	C4-C3-C2	-2.67	105.79	110.79
29	b	841	PQN	C2M-C2-C3	-2.67	120.06	124.45
25	1	304	A1L1F	O13-C45-C47	2.67	119.98	111.83
23	8	307	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	a	845	LHG	O8-C23-C24	2.67	119.97	111.83
30	m	101	BCR	C33-C5-C6	-2.67	121.58	124.48
23	2	315	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	f	801	BCR	C2-C1-C6	2.66	114.31	110.44
23	b	833	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	a	847	BCR	C16-C15-C14	-2.66	118.07	123.52
23	4	309	CLA	C3B-C4B-NB	-2.66	108.15	110.53
23	b	837	CLA	C3B-C4B-NB	-2.66	108.15	110.53
21	2	304	XAT	C15-C14-C13	-2.66	123.55	127.28
21	5	304	XAT	C30-C31-C32	-2.66	115.49	123.20
23	4	315	CLA	CHB-C4A-NA	2.66	128.24	124.40
23	a	835	CLA	CHB-C4A-NA	2.66	128.24	124.40
21	2	305	XAT	C31-C32-C33	-2.66	119.07	126.36
21	6	306	XAT	C24-C23-C22	-2.66	105.82	110.79
23	b	825	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	a	840	CLA	C3B-C4B-NB	-2.66	108.16	110.53
21	5	301	XAT	C35-C15-C14	-2.66	118.09	123.52
23	a	829	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	5	316	SQD	C44-O6-C1	-2.65	108.11	113.80
23	a	834	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
21	3	301	XAT	C27-C28-C29	-2.65	121.42	125.53
30	j	104	BCR	C27-C26-C25	-2.65	119.12	122.70
23	5	306	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	5	311	CLA	C3B-C4B-NB	-2.65	108.17	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	826	CLA	CHB-C4A-NA	2.64	128.22	124.40
21	6	305	XAT	C6-C7-C8	-2.64	120.40	125.99
23	l	203	CLA	CHB-C4A-NA	2.64	128.21	124.40
21	2	302	XAT	C4-C3-C2	-2.64	105.85	110.79
23	7	310	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	b	803	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	a	810	CLA	C1-C2-C3	-2.64	121.87	126.20
23	a	810	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	1	308	CLA	C3B-C4B-NB	-2.64	108.18	110.53
21	4	304	XAT	C31-C30-C29	-2.64	123.58	127.28
23	6	315	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
23	8	311	CLA	C3B-C4B-NB	-2.63	108.18	110.53
23	5	314	CLA	CHB-C4A-NA	2.63	128.20	124.40
23	a	842	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
23	a	821	CLA	CHB-C4A-NA	2.63	128.20	124.40
21	4	305	XAT	C7-C8-C9	-2.63	121.45	125.53
30	h	201	BCR	C21-C20-C19	-2.63	115.58	123.20
23	6	310	CLA	C3B-C4B-NB	-2.63	108.18	110.53
21	4	301	XAT	C27-C28-C29	-2.63	121.45	125.53
23	4	317	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	b	846	BCR	C24-C23-C22	-2.63	122.35	126.23
27	b	848	DGD	C1E-O6E-C5E	2.62	118.84	113.72
30	a	849	BCR	C16-C15-C14	-2.62	118.15	123.52
23	1	307	CLA	C3B-C4B-NB	-2.62	108.19	110.53
23	b	802	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
23	8	314	CLA	CAA-C2A-C3A	-2.62	110.22	116.23
23	a	838	CLA	C3B-C4B-NB	-2.62	108.19	110.53
23	b	801	CLA	CHB-C4A-NA	2.62	128.18	124.40
30	l	201	BCR	C21-C20-C19	-2.62	115.62	123.20
23	a	821	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	b	845	BCR	C8-C7-C6	-2.62	120.01	127.00
21	2	304	XAT	C35-C15-C14	-2.62	118.17	123.52
30	a	849	BCR	C23-C24-C25	-2.61	120.01	127.00
25	6	304	A1L1F	C42-C41-C40	-2.61	115.62	123.20
23	6	317	CLA	CHB-C4A-NA	2.61	128.17	124.40
23	b	824	CLA	CHB-C4A-NA	2.61	128.17	124.40
30	m	101	BCR	C15-C16-C17	-2.61	118.18	123.52
23	9	318	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
23	b	822	CLA	C3B-C4B-NB	-2.61	108.20	110.53
30	b	846	BCR	C34-C9-C8	2.61	122.07	118.09
23	1	309	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
23	a	835	CLA	C3B-C4B-NB	-2.60	108.21	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	202	BCR	C28-C27-C26	-2.60	109.42	114.06
30	l	201	BCR	C20-C21-C22	-2.60	123.63	127.28
23	a	807	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	6	304	A1L1F	O13-C45-C47	2.60	119.76	111.83
23	b	833	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
23	b	806	CLA	CHB-C4A-NA	2.60	128.15	124.40
23	5	311	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
28	a	853	LMG	C8-O7-C10	-2.60	111.58	117.80
23	3	310	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
30	j	104	BCR	C33-C5-C6	-2.59	121.65	124.48
23	a	804	CLA	C3B-C4B-NB	-2.59	108.21	110.53
23	b	813	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
23	4	317	CLA	CHB-C4A-NA	2.59	128.14	124.40
23	2	311	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
30	b	845	BCR	C38-C26-C25	-2.59	121.66	124.48
23	7	309	CLA	O2D-CGD-O1D	-2.59	118.20	124.08
22	9	306	A1L1G	C43-C44-C42	-2.59	118.62	122.82
23	a	814	CLA	CHB-C4A-NA	2.59	128.14	124.40
23	b	809	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	8	302	XAT	C11-C12-C13	-2.59	119.26	126.36
23	b	820	CLA	C1-C2-C3	-2.59	122.57	126.76
23	a	819	CLA	CHB-C4A-NA	2.59	128.13	124.40
23	9	316	CLA	CHB-C4A-NA	2.59	128.13	124.40
30	l	205	BCR	C28-C27-C26	-2.59	109.44	114.06
23	l	204	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	a	833	CLA	CHB-C4A-NA	2.58	128.13	124.40
23	a	854	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
23	1	311	CLA	C3B-C4B-NB	-2.58	108.22	110.53
21	2	303	XAT	C19-C9-C10	-2.58	118.63	122.82
23	j	103	CLA	CHB-C4A-NA	2.58	128.12	124.40
21	4	302	XAT	C10-C11-C12	-2.58	115.73	123.20
30	b	842	BCR	C21-C20-C19	-2.58	115.73	123.20
30	b	843	BCR	C24-C23-C22	-2.58	122.42	126.23
21	5	304	XAT	C8-C9-C10	-2.58	114.96	119.01
23	3	308	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	a	832	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	a	844	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	a	801	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
23	a	809	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	2	312	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	3	305	XAT	C10-C11-C12	-2.57	115.75	123.20
23	4	310	CLA	CHB-C4A-NA	2.57	128.10	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	309	CLA	C3B-C4B-NB	-2.57	108.24	110.53
23	a	805	CLA	C3B-C4B-NB	-2.57	108.24	110.53
23	3	315	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	1	314	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	4	311	CLA	CHB-C4A-NA	2.56	128.10	124.40
23	6	316	CLA	CHB-C4A-NA	2.56	128.10	124.40
23	6	314	CLA	C3B-C4B-NB	-2.56	108.24	110.53
30	a	850	BCR	C10-C11-C12	-2.56	115.78	123.20
21	6	302	XAT	C27-C28-C29	-2.56	121.56	125.53
30	b	842	BCR	C29-C30-C25	2.56	114.16	110.44
23	b	808	CLA	C3B-C4B-NB	-2.56	108.24	110.53
25	h	203	A1L1F	C27-C34-C33	2.56	122.00	118.09
21	8	301	XAT	C31-C30-C29	-2.56	123.69	127.28
25	h	203	A1L1F	C29-C30-C31	-2.56	115.02	119.00
23	7	316	CLA	CHB-C4A-NA	2.56	128.09	124.40
21	1	303	XAT	C35-C15-C14	-2.56	118.29	123.52
23	1	306	CLA	CHB-C4A-NA	2.55	128.09	124.40
23	a	828	CLA	C1-C2-C3	-2.55	122.01	126.20
23	b	821	CLA	C3B-C4B-NB	-2.55	108.25	110.53
23	2	306	CLA	O2D-CGD-O1D	-2.55	118.29	124.08
23	9	313	CLA	CHB-C4A-NA	2.55	128.09	124.40
30	b	849	BCR	C15-C14-C13	-2.55	123.70	127.28
23	b	807	CLA	C1-C2-C3	-2.55	122.02	126.20
21	2	302	XAT	C11-C10-C9	-2.55	123.70	127.28
21	5	301	XAT	C4-C3-C2	-2.55	106.03	110.79
27	b	848	DGD	O2G-C1B-O1B	-2.55	117.75	123.70
23	8	311	CLA	CHB-C4A-NA	2.55	128.08	124.40
25	6	304	A1L1F	C31-C32-C33	-2.55	115.82	123.20
23	b	813	CLA	CHB-C4A-NA	2.55	128.07	124.40
23	b	820	CLA	O2D-CGD-CBD	2.54	115.68	111.23
23	a	804	CLA	CHB-C4A-NA	2.54	128.07	124.40
21	5	304	XAT	C39-C29-C28	2.54	121.97	118.09
21	5	304	XAT	C15-C35-C34	-2.54	118.32	123.52
23	a	832	CLA	C1-C2-C3	-2.54	122.65	126.76
22	7	302	A1L1G	C43-C44-C42	-2.54	118.70	122.82
22	3	306	A1L1G	C43-C44-C42	-2.54	118.70	122.82
23	b	803	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
23	5	306	CLA	CHB-C4A-NA	2.54	128.06	124.40
23	a	830	CLA	C1-C2-C3	-2.54	122.04	126.20
23	b	835	CLA	CHB-C4A-NA	2.54	128.06	124.40
23	b	807	CLA	C3B-C4B-NB	-2.53	108.27	110.53
21	4	302	XAT	C30-C31-C32	-2.53	115.86	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	302	XAT	C31-C32-C33	-2.53	119.42	126.36
30	l	205	BCR	C15-C16-C17	-2.53	118.34	123.52
23	b	817	CLA	CHB-C4A-NA	2.53	128.05	124.40
30	f	804	BCR	C15-C16-C17	-2.53	118.34	123.52
23	5	313	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	4	306	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	b	820	CLA	C3B-C4B-NB	-2.53	108.27	110.53
26	9	307	LHG	O7-C7-C8	2.53	120.22	110.93
23	3	308	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	6	314	CLA	CHB-C4A-NA	2.53	128.05	124.40
30	h	202	BCR	C10-C11-C12	-2.53	115.87	123.20
30	b	846	BCR	C20-C21-C22	-2.53	123.73	127.28
21	3	303	XAT	C30-C31-C32	-2.53	115.87	123.20
21	8	301	XAT	C35-C15-C14	-2.53	118.35	123.52
30	j	104	BCR	C38-C26-C27	2.53	118.98	113.60
23	a	806	CLA	O1D-CGD-CBD	2.52	129.50	124.52
23	1	306	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	1	312	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	5	312	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	f	802	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	5	308	CLA	CHB-C4A-NA	2.52	128.03	124.40
30	b	842	BCR	C33-C5-C4	2.52	118.96	113.60
23	3	314	CLA	CHB-C4A-NA	2.51	128.03	124.40
23	2	313	CLA	CHB-C4A-NA	2.51	128.03	124.40
23	a	838	CLA	CHB-C4A-NA	2.51	128.03	124.40
21	9	303	XAT	C7-C8-C9	-2.51	121.63	125.53
23	b	812	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	a	806	CLA	C6-C5-C3	-2.51	107.35	113.47
23	f	803	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	a	836	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	b	835	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	a	825	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	9	312	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	l	204	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	6	312	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	8	313	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	4	314	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	b	831	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	9	305	XAT	C19-C9-C10	-2.50	118.76	122.82
23	a	802	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
25	1	304	A1L1F	C31-C32-C33	-2.50	115.95	123.20
23	a	802	CLA	CHB-C4A-NA	2.50	128.01	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	822	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	b	833	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	8	308	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	a	806	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	4	307	CLA	CHB-C4A-NA	2.50	128.00	124.40
23	a	840	CLA	CHB-C4A-NA	2.50	128.00	124.40
21	9	304	XAT	C39-C29-C28	2.50	121.90	118.09
25	1	304	A1L1F	C27-C34-C33	2.50	121.90	118.09
23	a	816	CLA	CHB-C4A-NA	2.50	128.00	124.40
27	b	848	DGD	C6D-O5D-C1E	2.50	119.15	113.80
25	h	203	A1L1F	C23-C22-C21	-2.49	106.12	110.79
30	l	201	BCR	C28-C27-C26	-2.49	109.61	114.06
23	8	312	CLA	CHB-C4A-NA	2.49	128.00	124.40
21	6	303	XAT	O24-C25-C38	2.49	117.83	115.05
30	a	848	BCR	C10-C11-C12	-2.49	115.98	123.20
23	a	827	CLA	CHB-C4A-NA	2.49	128.00	124.40
23	b	836	CLA	CHB-C4A-NA	2.49	128.00	124.40
23	b	820	CLA	CHB-C4A-NA	2.49	128.00	124.40
30	b	843	BCR	C15-C16-C17	-2.49	118.42	123.52
23	5	310	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	7	307	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	a	817	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	b	805	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	5	305	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	8	305	CLA	C3B-C4B-NB	-2.49	108.31	110.53
23	6	312	CLA	C3B-C4B-NB	-2.49	108.31	110.53
22	3	306	A1L1G	C17-C20-C21	2.49	117.03	114.24
21	4	301	XAT	C35-C15-C14	-2.49	118.43	123.52
23	2	312	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	6	311	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	1	308	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	8	307	CLA	CHB-C4A-NA	2.49	127.99	124.40
21	2	301	XAT	C10-C11-C12	-2.49	116.00	123.20
23	1	307	CLA	CHB-C4A-NA	2.48	127.99	124.40
25	9	302	A1L1F	C36-C37-C38	-2.48	118.44	123.52
30	j	104	BCR	C15-C16-C17	-2.48	118.44	123.52
23	a	810	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	b	845	BCR	C39-C30-C25	-2.48	106.35	110.24
23	3	313	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	7	301	XAT	C35-C15-C14	-2.48	118.44	123.52
23	a	804	CLA	O2D-CGD-CBD	2.48	115.57	111.23
21	7	304	XAT	C11-C12-C13	-2.48	119.56	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	826	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	8	304	A1L1F	C12-C6-C1	-2.48	108.25	110.47
23	a	815	CLA	CHB-C4A-NA	2.48	127.98	124.40
23	8	309	CLA	C1-C2-C3	-2.48	122.14	126.20
25	h	203	A1L1F	C41-C40-C39	-2.48	119.57	126.36
23	6	310	CLA	CHB-C4A-NA	2.48	127.97	124.40
23	3	307	CLA	CHB-C4A-NA	2.48	127.97	124.40
23	1	313	CLA	CAA-C2A-C3A	-2.47	110.56	116.23
23	8	305	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	7	313	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	a	837	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	5	315	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	l	202	CLA	CHB-C4A-NA	2.47	127.97	124.40
30	a	850	BCR	C38-C26-C27	2.47	118.86	113.60
23	7	315	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	b	839	CLA	CHB-C4A-NA	2.47	127.97	124.40
21	2	303	XAT	C24-C23-C22	-2.47	106.17	110.79
23	a	812	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	5	303	A1L1G	C43-C44-C42	-2.47	118.82	122.82
21	7	303	XAT	C19-C9-C10	-2.47	118.82	122.82
23	b	819	CLA	CHB-C4A-NA	2.47	127.96	124.40
23	b	827	CLA	C3B-C4B-NB	-2.47	108.33	110.53
30	b	842	BCR	C15-C16-C17	-2.46	118.48	123.52
23	a	811	CLA	CHB-C4A-NA	2.46	127.96	124.40
23	b	811	CLA	CMB-C2B-C3B	2.46	130.08	123.53
23	b	807	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	7	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
30	b	846	BCR	C38-C26-C25	-2.46	121.80	124.48
23	a	808	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	a	830	CLA	C3B-C4B-NB	-2.46	108.33	110.53
23	8	308	CLA	C1-C2-C3	-2.46	122.17	126.20
23	9	314	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	5	302	XAT	C31-C30-C29	-2.46	123.83	127.28
23	4	316	CLA	CHB-C4A-NA	2.46	127.95	124.40
21	2	302	XAT	C10-C11-C12	-2.46	116.08	123.20
25	8	304	A1L1F	C23-C22-C21	-2.46	106.19	110.79
23	2	308	CLA	C3B-C4B-NB	-2.46	108.34	110.53
23	6	315	CLA	CHB-C4A-NA	2.46	127.94	124.40
23	9	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	a	850	BCR	C8-C7-C6	-2.45	120.44	127.00
23	f	802	CLA	C3B-C4B-NB	-2.45	108.34	110.53
23	4	308	CLA	C3B-C4B-NB	-2.45	108.34	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	309	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	2	314	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	2	316	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	7	306	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	1	310	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	b	821	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	a	835	CLA	O2D-CGD-CBD	2.45	115.51	111.23
23	b	838	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	b	821	CLA	C1-C2-C3	-2.45	122.19	126.20
28	j	105	LMG	C8-O7-C10	-2.45	111.94	117.80
23	2	306	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	h	204	CLA	CHB-C4A-NA	2.45	127.93	124.40
21	9	305	XAT	C35-C15-C14	-2.45	118.51	123.52
25	h	203	A1L1F	O7-C54-O55	-2.45	118.27	122.99
23	b	810	CLA	C1-C2-C3	-2.45	122.19	126.20
23	9	311	CLA	O2D-CGD-CBD	2.44	115.50	111.23
23	8	314	CLA	CHB-C4A-NA	2.44	127.93	124.40
23	a	809	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	a	828	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	b	839	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	h	201	BCR	C33-C5-C6	-2.44	121.82	124.48
25	6	304	A1L1F	C25-C14-C29	-2.44	120.84	125.99
21	3	304	XAT	C31-C32-C33	-2.44	119.68	126.36
30	b	845	BCR	C21-C20-C19	-2.44	116.14	123.20
23	a	823	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	a	820	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	6	309	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	a	818	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	b	815	CLA	CHB-C4A-NA	2.43	127.91	124.40
29	b	841	PQN	C11-C3-C2	-2.43	120.72	124.89
23	7	308	CLA	C3B-C4B-NB	-2.43	108.36	110.53
21	7	305	XAT	C31-C30-C29	-2.43	123.87	127.28
21	8	303	XAT	C28-C29-C30	-2.43	115.19	119.01
23	2	309	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	h	202	BCR	C8-C7-C6	-2.43	120.52	127.00
25	9	302	A1L1F	O7-C54-O55	-2.42	118.31	122.99
23	b	808	CLA	CHB-C4A-NA	2.42	127.90	124.40
23	6	307	CLA	CHB-C4A-NA	2.42	127.90	124.40
27	8	315	DGD	C2G-O2G-C1B	-2.42	112.00	117.80
25	6	304	A1L1F	O7-C54-O55	-2.42	118.31	122.99
21	6	303	XAT	C11-C12-C13	-2.42	119.73	126.36
23	b	834	CLA	CHB-C4A-NA	2.42	127.89	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	839	CLA	CHB-C4A-NA	2.42	127.89	124.40
30	j	104	BCR	C38-C26-C25	-2.42	121.85	124.48
23	7	314	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
23	a	829	CLA	C3B-C4B-NB	-2.42	108.37	110.53
29	b	841	PQN	C14-C13-C15	2.41	119.42	115.23
23	b	811	CLA	CAB-C3B-C2B	2.41	129.94	123.53
23	a	833	CLA	C1-C2-C3	-2.41	122.25	126.20
22	9	301	A1L1G	C43-C44-C42	-2.41	118.91	122.82
23	3	311	CLA	C1-C2-C3	-2.41	122.86	126.76
23	7	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	a	803	CLA	C3B-C4B-NB	-2.41	108.38	110.53
23	9	314	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	5	311	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	2	311	CLA	CHB-C4A-NA	2.41	127.87	124.40
30	a	848	BCR	C21-C20-C19	-2.40	116.23	123.20
30	a	850	BCR	C16-C15-C14	-2.40	118.60	123.52
30	a	847	BCR	C23-C24-C25	-2.40	120.58	127.00
21	8	301	XAT	C30-C31-C32	-2.40	116.24	123.20
23	7	308	CLA	CHB-C4A-NA	2.40	127.87	124.40
23	7	316	CLA	C3B-C4B-NB	-2.40	108.39	110.53
30	f	804	BCR	C28-C27-C26	-2.40	109.77	114.06
23	b	813	CLA	C1-C2-C3	-2.40	122.26	126.20
23	3	311	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	8	303	XAT	C40-C33-C32	2.40	121.75	118.09
23	4	309	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	8	310	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	4	312	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	b	827	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	9	302	A1L1F	C26-O13-C45	2.40	120.67	115.64
23	b	810	CLA	C3B-C4B-NB	-2.39	108.39	110.53
21	5	301	XAT	O24-C25-C38	2.39	117.72	115.05
23	5	309	CLA	CHB-C4A-NA	2.39	127.86	124.40
23	4	313	CLA	CHB-C4A-NA	2.39	127.86	124.40
23	9	309	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	h	201	BCR	C16-C15-C14	-2.39	118.62	123.52
23	9	315	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	7	302	A1L1G	C17-C20-C21	2.39	116.92	114.24
21	8	302	XAT	C7-C8-C9	-2.39	121.83	125.53
23	1	311	CLA	CHB-C4A-NA	2.39	127.84	124.40
30	b	843	BCR	C23-C24-C25	-2.38	120.63	127.00
23	7	312	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	6	301	A1L1F	O7-C54-O55	-2.38	118.39	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	844	BCR	C28-C27-C26	-2.38	109.81	114.06
23	4	308	CLA	CHB-C4A-NA	2.38	127.84	124.40
23	1	313	CLA	CHB-C4A-NA	2.38	127.84	124.40
30	a	848	BCR	C15-C16-C17	-2.38	118.65	123.52
23	b	825	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	6	301	A1L1F	C14-C29-C30	-2.38	121.42	125.47
23	6	313	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	3	302	A1L1G	C43-C44-C42	-2.38	118.96	122.82
23	a	834	CLA	CHB-C4A-NA	2.38	127.83	124.40
23	b	822	CLA	CHB-C4A-NA	2.38	127.83	124.40
23	b	835	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
30	b	844	BCR	C34-C9-C10	-2.38	118.97	122.82
30	f	801	BCR	C33-C5-C4	2.38	118.66	113.60
23	3	309	CLA	CHB-C4A-NA	2.37	127.83	124.40
23	a	854	CLA	CHB-C4A-NA	2.37	127.83	124.40
23	b	811	CLA	CHB-C4A-NA	2.37	127.83	124.40
25	6	304	A1L1F	C11-C1-C6	2.37	122.05	119.70
21	j	101	XAT	C39-C29-C28	2.37	121.71	118.09
23	9	318	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	7	314	CLA	C2A-C1A-CHA	2.37	127.98	123.87
30	a	849	BCR	C21-C20-C19	-2.37	116.33	123.20
23	b	832	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	a	842	CLA	CHB-C4A-NA	2.37	127.82	124.40
21	9	303	XAT	C39-C29-C28	2.37	121.70	118.09
23	a	813	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	a	834	CLA	C1-C2-C3	-2.37	122.32	126.20
21	6	306	XAT	C31-C32-C33	-2.37	119.87	126.36
23	b	810	CLA	CHB-C4A-NA	2.37	127.81	124.40
23	b	818	CLA	CHB-C4A-NA	2.37	127.81	124.40
21	7	301	XAT	C31-C32-C33	-2.37	119.88	126.36
23	j	102	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	8	306	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	6	317	CLA	C3B-C4B-NB	-2.36	108.42	110.53
23	b	816	CLA	CHB-C4A-NA	2.36	127.81	124.40
21	5	301	XAT	C30-C31-C32	-2.36	116.36	123.20
21	3	303	XAT	O24-C25-C38	2.36	117.69	115.05
21	7	304	XAT	O24-C25-C38	2.36	117.68	115.05
23	b	811	CLA	C3B-C4B-NB	-2.36	107.88	110.33
23	a	823	CLA	C3B-C4B-NB	-2.36	108.43	110.53
30	m	101	BCR	C8-C7-C6	-2.36	120.71	127.00
25	9	302	A1L1F	C31-C32-C33	-2.35	116.38	123.20
23	a	841	CLA	O2A-CGA-O1A	-2.35	117.74	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	804	BCR	C11-C12-C13	-2.35	119.91	126.36
23	7	316	CLA	O2D-CGD-CBD	2.35	115.34	111.23
30	b	843	BCR	C28-C27-C26	-2.35	109.86	114.06
21	9	303	XAT	O24-C25-C38	2.35	117.68	115.05
23	6	308	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	l	201	BCR	C29-C30-C25	2.35	113.85	110.44
23	1	305	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	l	201	BCR	C15-C16-C17	-2.35	118.71	123.52
23	b	835	CLA	C1-C2-C3	-2.35	122.35	126.20
30	b	842	BCR	C11-C12-C13	-2.35	119.92	126.36
21	7	305	XAT	C30-C31-C32	-2.35	116.40	123.20
25	6	304	A1L1F	C5-C6-C1	-2.35	108.37	110.47
21	a	852	XAT	C19-C9-C8	2.34	121.67	118.09
23	3	310	CLA	CHB-C4A-NA	2.34	127.78	124.40
30	b	844	BCR	C7-C6-C5	-2.34	116.17	121.56
23	a	831	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	1	304	A1L1F	O7-C54-O55	-2.34	118.48	122.99
21	4	303	XAT	O24-C25-C38	2.34	117.66	115.05
23	2	307	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
25	6	301	A1L1F	C23-C22-C21	-2.33	106.42	110.79
30	b	849	BCR	C23-C24-C25	-2.33	120.77	127.00
23	7	309	CLA	CHB-C4A-NA	2.33	127.77	124.40
23	b	823	CLA	CHB-C4A-NA	2.33	127.77	124.40
23	b	837	CLA	C1-C2-C3	-2.33	122.38	126.20
23	b	839	CLA	C1-C2-C3	-2.33	122.38	126.20
23	2	315	CLA	CHB-C4A-NA	2.33	127.76	124.40
30	b	844	BCR	C37-C22-C21	-2.33	119.04	122.82
23	5	307	CLA	CHB-C4A-NA	2.33	127.76	124.40
30	i	101	BCR	C16-C15-C14	-2.33	118.76	123.52
23	a	824	CLA	CHB-C4A-NA	2.33	127.76	124.40
21	8	301	XAT	O24-C25-C38	2.33	117.65	115.05
21	8	302	XAT	O24-C25-C38	2.33	117.65	115.05
23	a	844	CLA	C1-C2-C3	-2.32	122.39	126.20
21	4	305	XAT	O24-C25-C38	2.32	117.64	115.05
21	8	303	XAT	O4-C5-C18	2.32	117.64	115.05
21	2	303	XAT	C8-C9-C10	2.32	122.66	119.01
23	a	810	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
21	2	304	XAT	C35-C34-C33	-2.32	124.03	127.28
23	6	314	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
23	b	840	CLA	CHB-C4A-NA	2.32	127.74	124.40
21	6	305	XAT	C10-C11-C12	-2.32	116.49	123.20
25	6	301	A1L1F	C36-C35-C34	-2.32	124.03	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	302	XAT	O24-C25-C38	2.32	117.64	115.05
23	9	316	CLA	C3B-C4B-NB	-2.32	108.46	110.53
23	5	314	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
23	b	823	CLA	C1-C2-C3	-2.31	122.41	126.20
23	8	308	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
23	7	313	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
23	6	309	CLA	C3B-C4B-NB	-2.31	108.47	110.53
22	1	301	A1L1G	C17-C20-C21	2.31	116.84	114.24
23	1	306	CLA	C1-C2-C3	-2.31	122.41	126.20
22	1	301	A1L1G	C14-C29-C30	-2.31	121.54	125.47
25	1	304	A1L1F	C37-C36-C35	-2.31	118.79	123.52
23	1	309	CLA	CHB-C4A-NA	2.31	127.73	124.40
23	b	829	CLA	C1-C2-C3	-2.31	122.41	126.20
30	m	101	BCR	C24-C23-C22	-2.31	122.82	126.23
23	b	830	CLA	CHB-C4A-NA	2.31	127.73	124.40
21	5	302	XAT	C15-C35-C34	-2.31	118.80	123.52
30	b	845	BCR	C34-C9-C8	2.31	121.61	118.09
23	a	805	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
30	l	201	BCR	C23-C24-C25	-2.31	120.84	127.00
21	7	303	XAT	C8-C9-C10	2.30	122.63	119.01
23	a	816	CLA	C1-C2-C3	-2.30	123.03	126.76
21	2	304	XAT	O24-C25-C38	2.30	117.62	115.05
23	a	836	CLA	C1-C2-C3	-2.30	123.04	126.76
30	b	845	BCR	C29-C30-C25	2.30	113.78	110.44
21	5	304	XAT	O24-C25-C38	2.30	117.62	115.05
21	3	304	XAT	O4-C5-C18	2.30	117.62	115.05
21	7	301	XAT	C24-C23-C22	-2.30	106.49	110.79
30	f	804	BCR	C3-C4-C5	-2.30	109.95	114.06
30	a	849	BCR	C10-C11-C12	-2.30	116.54	123.20
23	a	833	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
23	a	844	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
23	b	816	CLA	C1-C2-C3	-2.30	122.43	126.20
21	3	301	XAT	C15-C35-C34	-2.30	118.82	123.52
22	9	301	A1L1G	C14-C29-C30	-2.30	121.56	125.47
21	1	303	XAT	C27-C28-C29	-2.30	121.97	125.53
21	2	304	XAT	C20-C13-C12	2.29	121.59	118.09
30	a	848	BCR	C16-C15-C14	-2.29	118.83	123.52
21	7	305	XAT	O24-C25-C38	2.29	117.61	115.05
23	b	809	CLA	O2D-CGD-CBD	2.29	115.23	111.23
23	4	313	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
30	b	845	BCR	C33-C5-C4	2.29	118.48	113.60
21	9	304	XAT	C10-C11-C12	-2.29	116.57	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	308	CLA	C3B-C4B-NB	-2.29	108.49	110.53
23	a	844	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	5	316	SQD	C45-O47-C7	-2.29	112.33	117.80
23	4	310	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
21	9	304	XAT	O24-C25-C38	2.28	117.60	115.05
21	j	101	XAT	O24-C25-C38	2.28	117.60	115.05
21	2	303	XAT	O4-C5-C18	2.28	117.60	115.05
30	i	101	BCR	C10-C11-C12	-2.28	116.59	123.20
30	f	801	BCR	C34-C9-C8	2.28	121.57	118.09
23	b	804	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	b	821	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
21	2	305	XAT	O4-C5-C18	2.28	117.59	115.05
30	h	202	BCR	C37-C22-C23	2.28	121.57	118.09
23	b	818	CLA	C3B-C4B-NB	-2.28	108.50	110.53
21	7	305	XAT	O4-C5-C18	2.28	117.59	115.05
23	7	313	CLA	C1-C2-C3	-2.28	122.47	126.20
23	b	834	CLA	C1-C2-C3	-2.28	122.47	126.20
23	b	817	CLA	CMB-C2B-C3B	2.28	131.91	126.55
23	a	826	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
23	b	825	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
23	a	818	CLA	O2D-CGD-CBD	2.27	115.21	111.23
21	2	304	XAT	C10-C11-C12	-2.27	116.61	123.20
30	b	846	BCR	C35-C13-C12	2.27	121.56	118.09
30	f	801	BCR	C35-C13-C12	2.27	121.56	118.09
23	3	310	CLA	C3B-C4B-NB	-2.27	108.50	110.53
30	l	205	BCR	C38-C26-C27	2.27	118.43	113.60
23	2	310	CLA	CHB-C4A-NA	2.27	127.67	124.40
21	5	302	XAT	C11-C12-C13	-2.27	120.14	126.36
21	2	305	XAT	C19-C9-C8	2.27	121.55	118.09
21	3	304	XAT	C27-C28-C29	-2.27	122.02	125.53
21	5	302	XAT	O4-C5-C18	2.26	117.58	115.05
21	a	852	XAT	O24-C25-C38	2.26	117.58	115.05
21	4	301	XAT	C39-C29-C30	-2.26	119.15	122.82
21	7	301	XAT	C10-C11-C12	-2.26	116.64	123.20
21	3	303	XAT	C10-C11-C12	-2.26	116.65	123.20
25	6	301	A1L1F	C32-C31-C30	-2.26	124.08	127.23
21	5	304	XAT	O4-C5-C18	2.26	117.58	115.05
21	2	301	XAT	O24-C25-C38	2.26	117.58	115.05
23	b	837	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	b	803	CLA	CHB-C4A-NA	2.26	127.66	124.40
21	7	301	XAT	C26-C27-C28	-2.26	121.22	125.99
29	a	843	PQN	C11-C12-C13	-2.26	122.94	126.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	305	XAT	O24-C25-C38	2.25	117.57	115.05
23	9	308	CLA	C1-C2-C3	-2.25	122.50	126.20
30	l	205	BCR	C33-C5-C4	2.25	118.40	113.60
21	4	304	XAT	O4-C5-C18	2.25	117.56	115.05
23	a	827	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
21	1	303	XAT	C19-C9-C8	2.25	121.53	118.09
23	8	305	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
30	a	850	BCR	C20-C19-C18	-2.25	120.19	126.36
25	h	203	A1L1F	C26-O13-C45	2.25	120.36	115.64
21	4	305	XAT	C15-C35-C34	-2.25	118.92	123.52
23	3	313	CLA	C1-C2-C3	-2.25	122.51	126.20
23	a	840	CLA	C1-C2-C3	-2.25	122.51	126.20
25	9	302	A1L1F	C23-C22-C21	-2.25	106.59	110.79
21	7	303	XAT	O24-C25-C38	2.25	117.56	115.05
21	7	305	XAT	C39-C29-C28	2.24	121.52	118.09
21	1	302	XAT	O24-C25-C38	2.24	117.56	115.05
23	2	311	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
23	f	803	CLA	C1-C2-C3	-2.24	122.52	126.20
30	f	801	BCR	C28-C27-C26	-2.24	110.06	114.06
30	b	845	BCR	C23-C24-C25	-2.24	121.01	127.00
21	6	306	XAT	O24-C25-C38	2.24	117.55	115.05
23	f	802	CLA	C1-C2-C3	-2.24	122.52	126.20
23	a	820	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
21	3	301	XAT	O24-C25-C38	2.24	117.55	115.05
23	5	307	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
23	b	836	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
21	3	303	XAT	O4-C5-C18	2.24	117.55	115.05
23	a	806	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
23	a	838	CLA	C1-C2-C3	-2.24	122.53	126.20
23	7	308	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
21	6	306	XAT	C35-C15-C14	-2.24	118.94	123.52
21	3	305	XAT	C19-C9-C8	2.24	121.50	118.09
23	b	829	CLA	CHB-C4A-NA	2.24	127.63	124.40
23	b	814	CLA	C1-C2-C3	-2.23	122.54	126.20
23	a	811	CLA	C1-C2-C3	-2.23	122.54	126.20
23	a	819	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
23	8	311	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
23	b	804	CLA	O1D-CGD-CBD	2.23	128.92	124.52
30	h	201	BCR	C11-C10-C9	-2.23	124.15	127.28
21	5	302	XAT	C30-C31-C32	-2.23	116.74	123.20
21	3	301	XAT	O4-C5-C18	2.23	117.54	115.05
23	b	826	CLA	CHB-C4A-NA	2.23	127.61	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	801	BCR	C15-C14-C13	-2.23	124.16	127.28
21	3	303	XAT	C15-C35-C34	-2.23	118.97	123.52
23	a	820	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
21	8	303	XAT	O24-C25-C38	2.22	117.53	115.05
30	b	843	BCR	C36-C18-C19	2.22	121.49	118.09
30	b	843	BCR	C37-C22-C23	2.22	121.49	118.09
23	a	829	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
21	3	304	XAT	O24-C25-C38	2.22	117.53	115.05
23	5	311	CLA	C1-C2-C3	-2.22	122.56	126.20
21	3	305	XAT	O24-C25-C38	2.22	117.53	115.05
21	1	303	XAT	O24-C25-C38	2.22	117.53	115.05
23	a	809	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
23	b	835	CLA	CAC-C3C-C4C	2.22	127.67	124.79
21	2	302	XAT	O24-C25-C38	2.22	117.52	115.05
23	3	310	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
21	4	305	XAT	O4-C5-C18	2.21	117.52	115.05
23	1	312	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
30	h	201	BCR	C34-C9-C8	2.21	121.47	118.09
30	h	202	BCR	C35-C13-C12	2.21	121.47	118.09
21	a	852	XAT	C40-C33-C32	2.21	121.47	118.09
21	2	305	XAT	C15-C35-C34	-2.21	119.00	123.52
23	a	823	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
21	2	303	XAT	O24-C25-C38	2.21	117.52	115.05
25	6	304	A1L1F	C36-C37-C38	-2.21	119.00	123.52
23	a	829	CLA	CHB-C4A-NA	2.21	127.59	124.40
21	8	302	XAT	O4-C5-C18	2.21	117.52	115.05
23	b	817	CLA	C1-C2-C3	-2.21	122.58	126.20
23	a	831	CLA	O2D-CGD-CBD	2.21	115.09	111.23
21	4	302	XAT	C39-C29-C28	2.21	121.46	118.09
21	2	303	XAT	C31-C32-C33	-2.21	120.31	126.36
23	6	313	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
30	j	104	BCR	C29-C30-C25	2.21	113.64	110.44
30	l	201	BCR	C39-C30-C25	-2.21	106.78	110.24
23	9	316	CLA	C1-C2-C3	-2.21	122.58	126.20
21	4	302	XAT	O4-C5-C18	2.20	117.51	115.05
21	6	303	XAT	O4-C5-C18	2.20	117.51	115.05
21	4	305	XAT	C39-C29-C30	-2.20	119.25	122.82
30	a	848	BCR	C23-C24-C25	-2.20	121.11	127.00
21	8	301	XAT	O4-C5-C18	2.20	117.51	115.05
30	h	202	BCR	C33-C5-C4	2.20	118.29	113.60
23	6	309	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
21	5	301	XAT	O4-C5-C18	2.20	117.51	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	310	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
23	8	308	CLA	O2D-CGD-CBD	2.20	115.08	111.23
23	b	805	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
21	4	302	XAT	O24-C25-C38	2.20	117.50	115.05
23	h	204	CLA	C1-C2-C3	-2.20	122.59	126.20
28	2	317	LMG	C8-O7-C10	-2.20	112.54	117.80
30	a	849	BCR	C8-C7-C6	-2.20	121.13	127.00
23	8	312	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
23	a	804	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
21	7	301	XAT	O4-C5-C18	2.19	117.50	115.05
30	a	848	BCR	C33-C5-C4	2.19	118.27	113.60
21	3	305	XAT	O4-C5-C18	2.19	117.50	115.05
23	b	827	CLA	C1-C2-C3	-2.19	122.61	126.20
23	2	308	CLA	CHB-C4A-NA	2.19	127.56	124.40
21	1	302	XAT	O4-C5-C18	2.19	117.50	115.05
21	6	306	XAT	O4-C5-C18	2.19	117.50	115.05
21	3	303	XAT	C39-C29-C28	2.19	121.43	118.09
23	b	814	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
23	5	311	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
23	3	311	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
21	4	302	XAT	C20-C13-C12	2.19	121.43	118.09
21	3	303	XAT	C35-C15-C14	-2.19	119.05	123.52
23	a	806	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
21	4	303	XAT	O4-C5-C18	2.18	117.49	115.05
21	2	305	XAT	C10-C11-C12	-2.18	116.88	123.20
21	3	301	XAT	C8-C9-C10	-2.18	115.58	119.01
21	2	304	XAT	O4-C5-C18	2.18	117.49	115.05
30	f	804	BCR	C21-C20-C19	-2.18	116.88	123.20
23	b	828	CLA	CHB-C4A-NA	2.18	127.55	124.40
30	b	846	BCR	C37-C22-C23	2.18	121.42	118.09
30	b	843	BCR	C11-C12-C13	-2.18	120.39	126.36
23	a	831	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
29	a	843	PQN	C2M-C2-C3	-2.18	120.88	124.45
21	4	301	XAT	O4-C5-C18	2.18	117.48	115.05
23	a	834	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
23	1	308	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
21	6	306	XAT	C10-C11-C12	-2.17	116.90	123.20
23	a	830	CLA	CHB-C4A-NA	2.17	127.53	124.40
21	6	305	XAT	O4-C5-C4	2.17	115.53	113.49
23	5	308	CLA	C1-C2-C3	-2.17	122.64	126.20
30	h	201	BCR	C23-C24-C25	-2.17	121.20	127.00
30	a	847	BCR	C8-C7-C6	-2.17	121.21	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	304	XAT	O24-C25-C38	2.17	117.47	115.05
23	4	307	CLA	O2D-CGD-CBD	2.17	115.02	111.23
21	2	304	XAT	C30-C31-C32	-2.17	116.92	123.20
23	9	318	CLA	C1-C2-C3	-2.16	122.65	126.20
23	7	312	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	b	818	CLA	C1-C2-C3	-2.16	122.65	126.20
23	a	801	CLA	CHB-C4A-NA	2.16	127.52	124.40
23	b	830	CLA	CMA-C3A-C2A	-2.16	111.27	116.23
23	5	312	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	a	806	CLA	C5-C3-C2	-2.16	116.32	121.17
21	7	303	XAT	O4-C5-C18	2.16	117.46	115.05
23	b	840	CLA	C1-C2-C3	-2.16	122.66	126.20
30	m	101	BCR	C15-C14-C13	-2.16	124.25	127.28
23	f	802	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
27	8	315	DGD	O2G-C1B-O1B	-2.16	118.66	123.70
23	4	311	CLA	O2D-CGD-CBD	2.16	115.00	111.23
23	a	839	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
23	7	316	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
23	3	313	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
23	8	308	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
23	b	823	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
30	b	844	BCR	C1-C6-C7	2.15	121.49	115.65
21	5	302	XAT	O24-C25-C26	-2.15	57.22	58.93
23	a	812	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
23	4	308	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
21	7	304	XAT	O4-C5-C18	2.15	117.45	115.05
23	a	838	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	b	822	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	a	803	CLA	CMB-C2B-C3B	2.15	131.60	126.55
30	a	848	BCR	C34-C9-C8	2.15	121.37	118.09
23	4	308	CLA	O2D-CGD-CBD	2.15	114.98	111.23
30	l	201	BCR	C37-C22-C23	2.15	121.37	118.09
23	9	318	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
21	9	304	XAT	C40-C33-C32	2.15	121.36	118.09
30	j	104	BCR	C16-C15-C14	-2.15	119.13	123.52
21	9	305	XAT	C31-C32-C33	-2.14	120.48	126.36
23	8	309	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
30	h	201	BCR	C15-C16-C17	-2.14	119.14	123.52
21	1	302	XAT	C30-C31-C32	-2.14	117.00	123.20
23	b	820	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
30	l	201	BCR	C3-C4-C5	-2.14	110.24	114.06
21	1	303	XAT	O4-C5-C18	2.14	117.44	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	826	CLA	C1-C2-C3	-2.14	122.69	126.20
22	9	301	A1L1G	C29-C30-C31	2.14	122.32	119.00
23	b	807	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	j	101	XAT	O4-C5-C18	2.14	117.44	115.05
30	j	104	BCR	C21-C20-C19	-2.14	117.00	123.20
23	9	314	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	4	303	XAT	C7-C8-C9	-2.14	122.21	125.53
23	a	816	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
23	b	832	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
21	2	302	XAT	O4-C5-C18	2.14	117.44	115.05
23	a	842	CLA	C1-C2-C3	-2.14	122.70	126.20
30	b	842	BCR	C37-C22-C23	2.13	121.35	118.09
30	b	845	BCR	C2-C1-C6	2.13	113.54	110.44
21	1	302	XAT	C10-C11-C12	-2.13	117.02	123.20
23	6	309	CLA	C1-C2-C3	-2.13	122.70	126.20
24	5	316	SQD	O7-S-C6	2.13	109.94	106.76
23	b	825	CLA	C1-C2-C3	-2.13	122.71	126.20
30	a	849	BCR	C15-C16-C17	-2.13	119.16	123.52
23	b	838	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
21	8	302	XAT	C19-C9-C10	-2.13	119.37	122.82
23	b	801	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
21	5	302	XAT	O24-C25-C38	2.13	117.42	115.05
23	b	802	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	4	313	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	b	829	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	7	316	CLA	CMB-C2B-C1B	-2.12	122.18	125.42
30	b	849	BCR	C32-C1-C6	-2.12	106.91	110.24
23	1	307	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
21	7	301	XAT	O24-C25-C38	2.12	117.42	115.05
30	b	846	BCR	C23-C24-C25	-2.12	121.33	127.00
21	8	302	XAT	C8-C9-C10	2.12	122.35	119.01
21	7	301	XAT	C19-C9-C8	2.12	121.33	118.09
23	a	807	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	2	308	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	8	311	CLA	C1-C2-C3	-2.12	122.73	126.20
23	9	308	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	a	829	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
21	6	302	XAT	O4-C5-C18	2.12	117.41	115.05
27	b	848	DGD	O3D-C3D-C4D	-2.12	105.39	110.38
23	a	836	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	a	826	CLA	CMB-C2B-C3B	2.12	131.53	126.55
21	9	303	XAT	C11-C12-C13	-2.12	120.56	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	835	CLA	CMB-C2B-C3B	2.12	131.53	126.55
30	b	842	BCR	C38-C26-C27	2.11	118.10	113.60
30	b	843	BCR	C33-C5-C4	2.11	118.10	113.60
21	5	304	XAT	C35-C15-C14	-2.11	119.19	123.52
23	3	309	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
21	4	303	XAT	C35-C15-C14	-2.11	119.20	123.52
23	b	819	CLA	C1-C2-C3	-2.11	122.74	126.20
25	6	301	A1L1F	C5-C6-C1	-2.11	108.58	110.47
21	5	301	XAT	C39-C29-C28	2.11	121.31	118.09
23	b	812	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
23	6	310	CLA	C1-C2-C3	-2.11	122.74	126.20
23	h	204	CLA	O2D-CGD-CBD	2.11	114.91	111.23
21	a	852	XAT	C39-C29-C28	2.11	121.31	118.09
23	b	808	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
21	7	303	XAT	C15-C35-C34	-2.11	119.21	123.52
23	a	803	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
23	a	818	CLA	C1-C2-C3	-2.11	122.75	126.20
23	a	827	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
30	a	847	BCR	C33-C5-C4	2.10	118.08	113.60
30	j	104	BCR	C3-C4-C5	-2.10	110.30	114.06
23	a	809	CLA	O2D-CGD-CBD	2.10	114.91	111.23
23	b	819	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
23	a	802	CLA	CMB-C2B-C3B	2.10	131.50	126.55
23	a	825	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
21	3	304	XAT	C35-C15-C14	-2.10	119.22	123.52
23	1	310	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	9	302	A1L1F	C17-C20-C21	2.10	116.60	114.24
30	l	201	BCR	C34-C9-C10	-2.10	119.41	122.82
21	6	302	XAT	C19-C9-C10	-2.10	119.41	122.82
23	9	316	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
23	a	826	CLA	C1-C2-C3	-2.10	122.76	126.20
25	8	304	A1L1F	C27-C34-C33	2.10	121.29	118.09
23	4	309	CLA	C1-C2-C3	-2.10	123.37	126.76
23	a	804	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
21	2	304	XAT	C40-C33-C32	2.10	121.29	118.09
30	a	849	BCR	C37-C22-C23	2.10	121.29	118.09
23	b	829	CLA	CHB-C1B-NB	2.10	127.19	124.05
23	b	831	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
23	b	829	CLA	O2D-CGD-CBD	2.09	114.89	111.23
23	8	311	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	b	803	CLA	O2D-CGD-CBD	2.09	114.89	111.23
21	9	305	XAT	O4-C5-C18	2.09	117.39	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	837	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	b	840	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
23	9	316	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
21	2	302	XAT	C19-C9-C8	2.09	121.28	118.09
21	1	303	XAT	C20-C13-C12	2.09	121.28	118.09
21	9	303	XAT	O4-C5-C18	2.09	117.38	115.05
23	b	805	CLA	C1-C2-C3	-2.09	122.77	126.20
23	a	844	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
21	5	302	XAT	C19-C9-C10	-2.09	119.43	122.82
23	2	308	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
23	a	801	CLA	O1D-CGD-CBD	2.09	128.64	124.52
28	2	317	LMG	C4-C3-C2	-2.09	107.16	110.83
23	a	827	CLA	C1-C2-C3	-2.09	122.78	126.20
23	a	854	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
21	9	305	XAT	C11-C12-C13	-2.09	120.64	126.36
23	9	309	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
23	a	818	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
21	4	304	XAT	C30-C31-C32	-2.08	117.16	123.20
21	4	304	XAT	C19-C9-C8	2.08	121.27	118.09
23	1	311	CLA	O2D-CGD-CBD	2.08	114.87	111.23
23	b	827	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	b	829	CLA	C3B-C4B-NB	-2.08	108.67	110.53
23	5	308	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
30	b	844	BCR	C16-C15-C14	-2.08	119.27	123.52
23	2	312	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
23	a	822	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
30	a	847	BCR	C28-C27-C26	-2.08	110.35	114.06
30	i	101	BCR	C23-C22-C21	2.08	122.28	119.01
23	a	808	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
23	j	102	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
23	5	307	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
21	7	305	XAT	C7-C8-C9	-2.08	122.31	125.53
23	b	838	CLA	C1-C2-C3	-2.08	122.80	126.20
23	a	806	CLA	C6-C7-C8	-2.08	109.07	115.97
23	4	317	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
21	2	301	XAT	C19-C9-C8	2.07	121.26	118.09
23	a	805	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
23	b	804	CLA	O2D-CGD-CBD	2.07	114.85	111.23
21	7	304	XAT	C19-C9-C10	-2.07	119.46	122.82
21	9	304	XAT	C31-C30-C29	-2.07	124.37	127.28
23	a	832	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	b	816	CLA	O2D-CGD-CBD	2.07	114.85	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	303	XAT	C11-C10-C9	-2.07	124.38	127.28
23	1	311	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	b	839	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	6	301	A1L1F	C12-C6-C1	-2.07	108.62	110.47
23	3	308	CLA	O2D-CGD-CBD	2.07	114.85	111.23
23	a	806	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
30	h	201	BCR	C35-C13-C12	2.07	121.25	118.09
23	b	808	CLA	O2D-CGD-CBD	2.07	114.84	111.23
21	4	301	XAT	C10-C11-C12	-2.07	117.22	123.20
27	b	848	DGD	O5E-C6E-C5E	-2.07	104.30	111.33
21	8	301	XAT	C39-C29-C28	2.06	121.24	118.09
23	6	317	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
21	2	302	XAT	C27-C28-C29	-2.06	122.33	125.53
23	1	306	CLA	CAC-C3C-C4C	2.06	127.47	124.79
21	6	303	XAT	C27-C28-C29	-2.06	122.33	125.53
21	9	303	XAT	C19-C9-C8	2.06	121.24	118.09
21	2	304	XAT	C15-C35-C34	-2.06	119.30	123.52
23	a	814	CLA	C1-C2-C3	-2.06	122.82	126.20
30	a	847	BCR	C20-C19-C18	-2.06	120.71	126.36
23	1	307	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	a	814	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
21	2	301	XAT	O4-C5-C18	2.06	117.35	115.05
23	2	310	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	1	306	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	b	821	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
23	a	829	CLA	CMB-C2B-C3B	2.06	131.39	126.55
21	7	304	XAT	C31-C32-C33	-2.06	120.72	126.36
23	b	817	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	h	204	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	6	314	CLA	CMB-C2B-C3B	2.06	131.39	126.55
25	6	304	A1L1F	O15-C25-C14	-2.06	110.99	116.88
25	6	304	A1L1F	C12-C6-C1	-2.05	108.63	110.47
21	3	303	XAT	C19-C9-C8	2.05	121.23	118.09
21	4	301	XAT	C24-C23-C22	-2.05	106.95	110.79
23	b	802	CLA	C3B-C4B-NB	-2.05	108.70	110.53
21	7	305	XAT	C11-C12-C13	-2.05	120.73	126.36
23	7	311	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
21	1	302	XAT	C39-C29-C28	2.05	121.22	118.09
23	b	836	CLA	O2D-CGD-CBD	2.05	114.82	111.23
23	b	810	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
30	f	804	BCR	C8-C7-C6	-2.05	121.52	127.00
22	1	301	A1L1G	C29-C30-C31	2.05	122.18	119.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	307	CLA	CMB-C2B-C3B	2.05	131.37	126.55
23	2	307	CLA	C2A-C1A-CHA	2.05	127.42	123.87
23	b	806	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
23	a	831	CLA	C3B-C4B-NB	-2.05	108.70	110.53
23	a	823	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	4	307	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
21	4	304	XAT	C39-C29-C28	2.05	121.22	118.09
23	6	313	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	a	849	BCR	C38-C26-C27	2.05	117.96	113.60
30	b	844	BCR	C21-C20-C19	-2.05	117.27	123.20
23	a	839	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
23	5	311	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
23	a	830	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	6	315	CLA	CAA-C2A-C3A	-2.04	111.55	116.23
23	3	308	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	b	810	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	8	307	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
21	3	305	XAT	C20-C13-C12	2.04	121.20	118.09
23	a	854	CLA	C1-C2-C3	-2.04	122.86	126.20
23	a	844	CLA	CMB-C2B-C3B	2.04	131.34	126.55
23	1	311	CLA	C1-C2-C3	-2.04	122.86	126.20
30	a	849	BCR	C29-C30-C25	2.04	113.40	110.44
21	4	301	XAT	C28-C29-C30	2.04	122.21	119.01
23	l	203	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	b	849	BCR	C38-C26-C27	2.04	117.94	113.60
23	7	308	CLA	CMB-C2B-C3B	2.04	131.34	126.55
30	l	205	BCR	C10-C11-C12	-2.03	117.31	123.20
23	2	307	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
23	b	803	CLA	C1-C2-C3	-2.03	122.87	126.20
30	b	842	BCR	C33-C5-C6	-2.03	122.27	124.48
21	6	306	XAT	C19-C9-C8	2.03	121.19	118.09
23	b	824	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	a	809	CLA	CMB-C2B-C3B	2.03	131.33	126.55
23	a	833	CLA	CMB-C2B-C3B	2.03	131.33	126.55
23	b	814	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	a	809	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	b	825	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	b	809	CLA	C1-C2-C3	-2.03	122.87	126.20
23	b	826	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
21	5	301	XAT	C10-C11-C12	-2.03	117.32	123.20
23	b	817	CLA	CHB-C1B-NB	2.03	127.09	124.05
23	a	816	CLA	O2A-CGA-O1A	-2.03	118.56	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	201	BCR	C28-C27-C26	-2.03	110.44	114.06
28	j	105	LMG	O7-C10-O9	-2.03	118.97	123.70
23	b	804	CLA	CAC-C3C-C4C	2.02	127.42	124.79
23	8	305	CLA	CMB-C2B-C3B	2.02	131.31	126.55
30	a	849	BCR	C35-C13-C12	2.02	121.18	118.09
23	a	833	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
30	a	848	BCR	C28-C27-C26	-2.02	110.45	114.06
23	a	811	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
23	a	835	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	6	304	A1L1F	C8-O7-C54	-2.02	114.27	117.85
23	a	842	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
30	b	845	BCR	C38-C26-C27	2.02	117.91	113.60
30	a	847	BCR	C10-C11-C12	-2.02	117.34	123.20
25	8	304	A1L1F	C28-C39-C38	-2.02	119.54	122.82
23	6	312	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
30	b	842	BCR	C16-C15-C14	-2.02	119.39	123.52
23	7	306	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
21	7	303	XAT	C31-C32-C33	-2.02	120.83	126.36
30	b	844	BCR	C10-C11-C12	-2.02	117.35	123.20
23	4	313	CLA	CMB-C2B-C3B	2.02	131.30	126.55
23	8	311	CLA	CMB-C2B-C3B	2.02	131.29	126.55
21	4	304	XAT	C20-C13-C12	2.02	121.17	118.09
23	8	310	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
23	b	834	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
23	6	312	CLA	C1-C2-C3	-2.01	122.90	126.20
23	b	811	CLA	C1-C2-C3	-2.01	122.90	126.20
23	b	828	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
23	b	807	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
23	a	813	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
23	7	309	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
21	3	305	XAT	C39-C29-C28	2.01	121.16	118.09
23	b	806	CLA	C1-C2-C3	-2.01	122.91	126.20
23	b	814	CLA	CMB-C2B-C3B	2.01	131.28	126.55
23	b	825	CLA	CMB-C2B-C3B	2.01	131.27	126.55
25	1	304	A1L1F	C25-C14-C29	-2.01	121.75	125.99
23	b	803	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
27	8	315	DGD	C4D-C3D-C2D	-2.01	107.31	110.83
21	3	301	XAT	C30-C31-C32	-2.01	117.38	123.20
27	4	318	DGD	C4D-C3D-C2D	-2.01	107.31	110.83
23	b	802	CLA	C1-C2-C3	-2.00	122.91	126.20
23	a	803	CLA	CHB-C4A-NA	2.00	127.29	124.40
23	9	316	CLA	CMB-C2B-C3B	2.00	131.26	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	308	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
25	9	302	A1L1F	O13-C45-O46	-2.00	118.62	123.63
30	1	205	BCR	C7-C8-C9	-2.00	123.28	126.23
23	2	310	CLA	C1-C2-C3	-2.00	122.92	126.20

All (188) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	5	305	CLA	ND
23	5	306	CLA	ND
23	5	307	CLA	ND
23	5	308	CLA	ND
23	5	309	CLA	ND
23	5	310	CLA	ND
23	5	311	CLA	ND
23	5	312	CLA	ND
23	5	313	CLA	ND
23	5	314	CLA	ND
23	5	315	CLA	ND
23	9	308	CLA	ND
23	9	309	CLA	ND
23	9	310	CLA	ND
23	9	311	CLA	ND
23	9	312	CLA	ND
23	9	313	CLA	ND
23	9	314	CLA	ND
23	9	315	CLA	ND
23	9	316	CLA	ND
23	9	318	CLA	ND
23	8	305	CLA	ND
23	8	306	CLA	ND
23	8	307	CLA	ND
23	8	308	CLA	ND
23	8	309	CLA	ND
23	8	310	CLA	ND
23	8	311	CLA	ND
23	8	312	CLA	ND
23	8	313	CLA	ND
23	8	314	CLA	ND
23	4	306	CLA	ND
23	4	307	CLA	ND
23	4	308	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	4	309	CLA	ND
23	4	310	CLA	ND
23	4	311	CLA	ND
23	4	312	CLA	ND
23	4	313	CLA	ND
23	4	314	CLA	ND
23	4	315	CLA	ND
23	4	316	CLA	ND
23	4	317	CLA	ND
23	3	307	CLA	ND
23	3	308	CLA	ND
23	3	309	CLA	ND
23	3	310	CLA	ND
23	3	311	CLA	ND
23	3	312	CLA	ND
23	3	313	CLA	ND
23	3	314	CLA	ND
23	3	315	CLA	ND
23	6	307	CLA	ND
23	6	308	CLA	ND
23	6	309	CLA	ND
23	6	310	CLA	ND
23	6	311	CLA	ND
23	6	312	CLA	ND
23	6	313	CLA	ND
23	6	314	CLA	ND
23	6	315	CLA	ND
23	6	316	CLA	ND
23	6	317	CLA	ND
23	2	306	CLA	ND
23	2	307	CLA	ND
23	2	308	CLA	ND
23	2	309	CLA	ND
23	2	310	CLA	ND
23	2	311	CLA	ND
23	2	312	CLA	ND
23	2	313	CLA	ND
23	2	314	CLA	ND
23	2	315	CLA	ND
23	2	316	CLA	ND
23	7	306	CLA	ND
23	7	307	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	7	308	CLA	ND
23	7	309	CLA	ND
23	7	310	CLA	ND
23	7	311	CLA	ND
23	7	312	CLA	ND
23	7	313	CLA	ND
23	7	314	CLA	ND
23	7	315	CLA	ND
23	7	316	CLA	ND
23	7	317	CLA	ND
23	1	305	CLA	ND
23	1	306	CLA	ND
23	1	307	CLA	ND
23	1	308	CLA	ND
23	1	309	CLA	ND
23	1	310	CLA	ND
23	1	311	CLA	ND
23	1	312	CLA	ND
23	1	313	CLA	ND
23	1	314	CLA	ND
23	a	801	CLA	ND
23	a	802	CLA	ND
23	a	803	CLA	ND
23	a	804	CLA	ND
23	a	805	CLA	ND
23	a	806	CLA	ND
23	a	807	CLA	ND
23	a	808	CLA	ND
23	a	809	CLA	ND
23	a	810	CLA	ND
23	a	811	CLA	ND
23	a	812	CLA	ND
23	a	813	CLA	ND
23	a	814	CLA	ND
23	a	815	CLA	ND
23	a	816	CLA	ND
23	a	817	CLA	ND
23	a	818	CLA	ND
23	a	819	CLA	ND
23	a	820	CLA	ND
23	a	821	CLA	ND
23	a	822	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	a	823	CLA	ND
23	a	824	CLA	ND
23	a	825	CLA	ND
23	a	826	CLA	ND
23	a	827	CLA	ND
23	a	828	CLA	ND
23	a	829	CLA	ND
23	a	830	CLA	ND
23	a	831	CLA	ND
23	a	832	CLA	ND
23	a	833	CLA	ND
23	a	834	CLA	ND
23	a	835	CLA	ND
23	a	836	CLA	ND
23	a	837	CLA	ND
23	a	838	CLA	ND
23	a	839	CLA	ND
23	a	840	CLA	ND
23	a	841	CLA	ND
23	a	842	CLA	ND
23	a	844	CLA	ND
23	a	854	CLA	ND
23	b	801	CLA	ND
23	b	802	CLA	ND
23	b	803	CLA	ND
23	b	804	CLA	ND
23	b	805	CLA	ND
23	b	806	CLA	ND
23	b	807	CLA	ND
23	b	808	CLA	ND
23	b	809	CLA	ND
23	b	810	CLA	ND
23	b	811	CLA	ND
23	b	812	CLA	ND
23	b	813	CLA	ND
23	b	814	CLA	ND
23	b	815	CLA	ND
23	b	816	CLA	ND
23	b	817	CLA	ND
23	b	818	CLA	ND
23	b	819	CLA	ND
23	b	820	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	b	821	CLA	ND
23	b	822	CLA	ND
23	b	823	CLA	ND
23	b	824	CLA	ND
23	b	825	CLA	ND
23	b	826	CLA	ND
23	b	827	CLA	ND
23	b	828	CLA	ND
23	b	829	CLA	ND
23	b	830	CLA	ND
23	b	831	CLA	ND
23	b	832	CLA	ND
23	b	833	CLA	ND
23	b	834	CLA	ND
23	b	835	CLA	ND
23	b	836	CLA	ND
23	b	837	CLA	ND
23	b	838	CLA	ND
23	b	839	CLA	ND
23	b	840	CLA	ND
23	f	802	CLA	ND
23	f	803	CLA	ND
23	h	204	CLA	ND
23	j	102	CLA	ND
23	j	103	CLA	ND
23	l	202	CLA	ND
23	l	203	CLA	ND
23	l	204	CLA	ND

All (2060) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	5	302	XAT	O4-C6-C7-C8
21	5	302	XAT	C7-C8-C9-C10
21	5	302	XAT	C7-C8-C9-C19
21	9	303	XAT	O4-C6-C7-C8
21	9	304	XAT	O24-C26-C27-C28
21	9	305	XAT	O4-C6-C7-C8
21	9	305	XAT	C7-C8-C9-C10
21	9	305	XAT	C7-C8-C9-C19
21	8	302	XAT	O4-C6-C7-C8
21	8	302	XAT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	8	302	XAT	C7-C8-C9-C19
21	4	301	XAT	C27-C28-C29-C30
21	4	301	XAT	C27-C28-C29-C39
21	4	303	XAT	O4-C6-C7-C8
21	4	303	XAT	C7-C8-C9-C10
21	4	303	XAT	C7-C8-C9-C19
21	4	305	XAT	O24-C26-C27-C28
21	3	301	XAT	O4-C6-C7-C8
21	3	301	XAT	C27-C28-C29-C30
21	3	301	XAT	C27-C28-C29-C39
21	3	303	XAT	C27-C28-C29-C30
21	3	304	XAT	O24-C26-C27-C28
21	3	304	XAT	C27-C28-C29-C30
21	3	304	XAT	C27-C28-C29-C39
21	6	302	XAT	O24-C26-C27-C28
21	6	302	XAT	C27-C28-C29-C30
21	6	302	XAT	C27-C28-C29-C39
21	6	303	XAT	O4-C6-C7-C8
21	6	305	XAT	O24-C26-C27-C28
21	6	305	XAT	C27-C28-C29-C30
21	6	305	XAT	C27-C28-C29-C39
21	6	306	XAT	C27-C28-C29-C30
21	6	306	XAT	C27-C28-C29-C39
21	2	303	XAT	O4-C6-C7-C8
21	2	303	XAT	O24-C26-C27-C28
21	2	303	XAT	C27-C28-C29-C30
21	2	303	XAT	C27-C28-C29-C39
21	2	305	XAT	C25-C26-C27-C28
21	7	301	XAT	O4-C6-C7-C8
21	7	301	XAT	C27-C28-C29-C30
21	7	301	XAT	C27-C28-C29-C39
21	7	303	XAT	O4-C6-C7-C8
21	7	303	XAT	O24-C26-C27-C28
21	7	303	XAT	C27-C28-C29-C30
21	7	303	XAT	C27-C28-C29-C39
21	7	304	XAT	O4-C6-C7-C8
21	7	304	XAT	C11-C12-C13-C14
21	7	304	XAT	C11-C12-C13-C20
21	a	852	XAT	C7-C8-C9-C10
21	a	852	XAT	C7-C8-C9-C19
21	a	852	XAT	C11-C12-C13-C14
21	a	852	XAT	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	j	101	XAT	O4-C6-C7-C8
21	j	101	XAT	C7-C8-C9-C10
21	j	101	XAT	O24-C26-C27-C28
22	5	303	A1L1G	C26-C30-C31-C32
22	5	303	A1L1G	C31-C32-C33-C34
22	5	303	A1L1G	C32-C33-C34-C27
22	5	303	A1L1G	C32-C33-C34-C35
22	5	303	A1L1G	C41-C42-C44-C2
22	5	303	A1L1G	C41-C42-C44-C43
22	9	301	A1L1G	O13-C26-C30-C29
22	9	301	A1L1G	C26-C30-C31-C32
22	9	301	A1L1G	C31-C32-C33-C34
22	9	301	A1L1G	C38-C39-C40-C41
22	9	301	A1L1G	C39-C40-C41-C42
22	9	306	A1L1G	C45-C2-C44-C42
22	9	306	A1L1G	C45-C2-C44-C43
22	9	306	A1L1G	C29-C14-C25-C24
22	9	306	A1L1G	C25-C14-C29-C30
22	9	306	A1L1G	C35-C36-C37-C38
22	9	306	A1L1G	C37-C38-C39-C28
22	9	306	A1L1G	C37-C38-C39-C40
22	3	302	A1L1G	C25-C14-C29-C30
22	3	302	A1L1G	C14-C29-C30-C26
22	3	302	A1L1G	C26-C30-C31-C32
22	3	302	A1L1G	C29-C30-C31-C32
22	3	302	A1L1G	C41-C42-C44-C2
22	3	302	A1L1G	C41-C42-C44-C43
22	3	306	A1L1G	C45-C2-C44-C42
22	3	306	A1L1G	C45-C2-C44-C43
22	3	306	A1L1G	O13-C26-C30-C29
22	3	306	A1L1G	C37-C38-C39-C28
22	3	306	A1L1G	C37-C38-C39-C40
22	3	306	A1L1G	C39-C40-C41-C42
22	3	306	A1L1G	C41-C42-C44-C2
22	3	306	A1L1G	C41-C42-C44-C43
22	7	302	A1L1G	C45-C2-C44-C42
22	7	302	A1L1G	C29-C14-C25-C24
22	7	302	A1L1G	C35-C36-C37-C38
22	7	302	A1L1G	C37-C38-C39-C28
22	7	302	A1L1G	C37-C38-C39-C40
22	7	302	A1L1G	C39-C40-C41-C42
22	7	302	A1L1G	C41-C42-C44-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	7	302	A1L1G	C41-C42-C44-C43
22	1	301	A1L1G	C45-C2-C44-C42
22	1	301	A1L1G	C45-C2-C44-C43
22	1	301	A1L1G	O13-C26-C30-C29
22	1	301	A1L1G	C27-C34-C35-C36
22	1	301	A1L1G	C33-C34-C35-C36
22	1	301	A1L1G	C35-C36-C37-C38
22	1	301	A1L1G	C38-C39-C40-C41
22	1	301	A1L1G	C39-C40-C41-C42
23	5	308	CLA	CBD-CGD-O2D-CED
23	5	309	CLA	CAD-CBD-CGD-O1D
23	5	309	CLA	CAD-CBD-CGD-O2D
23	5	310	CLA	CBD-CGD-O2D-CED
23	5	314	CLA	C1A-C2A-CAA-CBA
23	5	314	CLA	C3A-C2A-CAA-CBA
23	5	315	CLA	CBD-CGD-O2D-CED
23	5	315	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	CBD-CGD-O2D-CED
23	9	310	CLA	CHA-CBD-CGD-O1D
23	9	310	CLA	CHA-CBD-CGD-O2D
23	9	311	CLA	CBD-CGD-O2D-CED
23	9	311	CLA	O1D-CGD-O2D-CED
23	9	314	CLA	CHA-CBD-CGD-O1D
23	9	314	CLA	CHA-CBD-CGD-O2D
23	9	315	CLA	CAD-CBD-CGD-O2D
23	9	315	CLA	CBD-CGD-O2D-CED
23	9	316	CLA	C1A-C2A-CAA-CBA
23	9	316	CLA	CAD-CBD-CGD-O1D
23	9	316	CLA	CAD-CBD-CGD-O2D
23	8	308	CLA	CHA-CBD-CGD-O1D
23	8	308	CLA	CHA-CBD-CGD-O2D
23	4	306	CLA	C1A-C2A-CAA-CBA
23	4	307	CLA	CHA-CBD-CGD-O1D
23	4	307	CLA	CHA-CBD-CGD-O2D
23	4	309	CLA	CBD-CGD-O2D-CED
23	4	310	CLA	C1A-C2A-CAA-CBA
23	4	311	CLA	CBA-CGA-O2A-C1
23	4	311	CLA	CBD-CGD-O2D-CED
23	4	312	CLA	C1A-C2A-CAA-CBA
23	4	312	CLA	C3A-C2A-CAA-CBA
23	4	315	CLA	CAD-CBD-CGD-O2D
23	4	316	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	317	CLA	CBD-CGD-O2D-CED
23	3	308	CLA	CHA-CBD-CGD-O1D
23	3	308	CLA	CHA-CBD-CGD-O2D
23	3	312	CLA	C1A-C2A-CAA-CBA
23	3	315	CLA	C1A-C2A-CAA-CBA
23	6	309	CLA	CHA-CBD-CGD-O1D
23	6	309	CLA	CHA-CBD-CGD-O2D
23	6	309	CLA	C6-C7-C8-C9
23	6	310	CLA	CAD-CBD-CGD-O2D
23	6	311	CLA	C1A-C2A-CAA-CBA
23	6	311	CLA	C3A-C2A-CAA-CBA
23	6	314	CLA	CBD-CGD-O2D-CED
23	6	315	CLA	CBD-CGD-O2D-CED
23	6	316	CLA	C1A-C2A-CAA-CBA
23	6	317	CLA	C1A-C2A-CAA-CBA
23	2	307	CLA	CHA-CBD-CGD-O2D
23	2	307	CLA	CBD-CGD-O2D-CED
23	2	309	CLA	CBD-CGD-O2D-CED
23	2	310	CLA	CHA-CBD-CGD-O1D
23	2	310	CLA	CHA-CBD-CGD-O2D
23	2	312	CLA	CBD-CGD-O2D-CED
23	2	313	CLA	CBD-CGD-O2D-CED
23	7	306	CLA	C3A-C2A-CAA-CBA
23	7	306	CLA	CBD-CGD-O2D-CED
23	7	307	CLA	CBD-CGD-O2D-CED
23	7	310	CLA	CBA-CGA-O2A-C1
23	7	311	CLA	CBA-CGA-O2A-C1
23	7	314	CLA	CBD-CGD-O2D-CED
23	7	315	CLA	C4B-C3B-CAB-CBB
23	7	315	CLA	CBD-CGD-O2D-CED
23	7	316	CLA	C1A-C2A-CAA-CBA
23	7	316	CLA	C3A-C2A-CAA-CBA
23	7	316	CLA	CHA-CBD-CGD-O1D
23	7	316	CLA	CHA-CBD-CGD-O2D
23	1	305	CLA	C11-C10-C8-C9
23	1	310	CLA	CBD-CGD-O2D-CED
23	1	313	CLA	CBD-CGD-O2D-CED
23	1	314	CLA	C1A-C2A-CAA-CBA
23	1	314	CLA	C3A-C2A-CAA-CBA
23	a	801	CLA	CBD-CGD-O2D-CED
23	a	804	CLA	CHA-CBD-CGD-O1D
23	a	804	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	805	CLA	C1A-C2A-CAA-CBA
23	a	805	CLA	C3A-C2A-CAA-CBA
23	a	806	CLA	CAD-CBD-CGD-O2D
23	a	809	CLA	C1A-C2A-CAA-CBA
23	a	809	CLA	C3A-C2A-CAA-CBA
23	a	809	CLA	CHA-CBD-CGD-O1D
23	a	809	CLA	CHA-CBD-CGD-O2D
23	a	811	CLA	CBD-CGD-O2D-CED
23	a	817	CLA	CHA-CBD-CGD-O1D
23	a	817	CLA	CHA-CBD-CGD-O2D
23	a	818	CLA	C1A-C2A-CAA-CBA
23	a	818	CLA	C3A-C2A-CAA-CBA
23	a	818	CLA	CHA-CBD-CGD-O1D
23	a	818	CLA	CHA-CBD-CGD-O2D
23	a	819	CLA	C3A-C2A-CAA-CBA
23	a	820	CLA	C1A-C2A-CAA-CBA
23	a	820	CLA	C3A-C2A-CAA-CBA
23	a	823	CLA	C1A-C2A-CAA-CBA
23	a	823	CLA	C3A-C2A-CAA-CBA
23	a	823	CLA	CHA-CBD-CGD-O1D
23	a	823	CLA	CHA-CBD-CGD-O2D
23	a	829	CLA	C1A-C2A-CAA-CBA
23	a	829	CLA	CBD-CGD-O2D-CED
23	a	831	CLA	CHA-CBD-CGD-O1D
23	a	831	CLA	CHA-CBD-CGD-O2D
23	a	832	CLA	C1A-C2A-CAA-CBA
23	a	832	CLA	C3A-C2A-CAA-CBA
23	a	834	CLA	C2B-C3B-CAB-CBB
23	a	834	CLA	C4B-C3B-CAB-CBB
23	a	838	CLA	C1A-C2A-CAA-CBA
23	a	838	CLA	C2-C3-C5-C6
23	a	838	CLA	C4-C3-C5-C6
23	a	854	CLA	C1A-C2A-CAA-CBA
23	a	854	CLA	C2B-C3B-CAB-CBB
23	a	854	CLA	C4B-C3B-CAB-CBB
23	b	803	CLA	CBD-CGD-O2D-CED
23	b	804	CLA	CBD-CGD-O2D-CED
23	b	805	CLA	CHA-CBD-CGD-O1D
23	b	805	CLA	CHA-CBD-CGD-O2D
23	b	806	CLA	C1A-C2A-CAA-CBA
23	b	806	CLA	C3A-C2A-CAA-CBA
23	b	806	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	806	CLA	CAD-CBD-CGD-O2D
23	b	809	CLA	CHA-CBD-CGD-O1D
23	b	809	CLA	CHA-CBD-CGD-O2D
23	b	810	CLA	C1A-C2A-CAA-CBA
23	b	812	CLA	C1A-C2A-CAA-CBA
23	b	812	CLA	C2-C3-C5-C6
23	b	812	CLA	C4-C3-C5-C6
23	b	814	CLA	C1A-C2A-CAA-CBA
23	b	814	CLA	CBD-CGD-O2D-CED
23	b	815	CLA	CHA-CBD-CGD-O1D
23	b	815	CLA	CHA-CBD-CGD-O2D
23	b	817	CLA	C3A-C2A-CAA-CBA
23	b	818	CLA	C1A-C2A-CAA-CBA
23	b	818	CLA	C3A-C2A-CAA-CBA
23	b	819	CLA	C4B-C3B-CAB-CBB
23	b	820	CLA	C1A-C2A-CAA-CBA
23	b	820	CLA	C3A-C2A-CAA-CBA
23	b	821	CLA	CHA-CBD-CGD-O2D
23	b	824	CLA	CHA-CBD-CGD-O1D
23	b	824	CLA	CHA-CBD-CGD-O2D
23	b	828	CLA	C1A-C2A-CAA-CBA
23	b	828	CLA	C3A-C2A-CAA-CBA
23	b	829	CLA	CHA-CBD-CGD-O1D
23	b	829	CLA	CHA-CBD-CGD-O2D
23	b	832	CLA	C1A-C2A-CAA-CBA
23	b	832	CLA	C3A-C2A-CAA-CBA
23	b	833	CLA	C1A-C2A-CAA-CBA
23	b	833	CLA	C3A-C2A-CAA-CBA
23	b	833	CLA	C11-C12-C13-C14
23	b	834	CLA	CHA-CBD-CGD-O1D
23	b	834	CLA	CHA-CBD-CGD-O2D
23	b	834	CLA	CBD-CGD-O2D-CED
23	b	838	CLA	C4B-C3B-CAB-CBB
23	b	839	CLA	C1A-C2A-CAA-CBA
23	b	839	CLA	C3A-C2A-CAA-CBA
23	b	839	CLA	CAD-CBD-CGD-O1D
23	b	839	CLA	CAD-CBD-CGD-O2D
23	b	839	CLA	CBD-CGD-O2D-CED
23	j	102	CLA	C1A-C2A-CAA-CBA
23	j	103	CLA	CAD-CBD-CGD-O1D
23	j	103	CLA	CAD-CBD-CGD-O2D
23	j	103	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	203	CLA	C6-C7-C8-C9
24	5	316	SQD	O49-C7-O47-C45
24	5	316	SQD	C8-C7-O47-C45
24	5	316	SQD	C5-C6-S-O7
24	5	316	SQD	C5-C6-S-O8
24	5	316	SQD	C5-C6-S-O9
24	1	315	SQD	O5-C5-C6-S
24	1	315	SQD	C5-C6-S-O7
24	1	315	SQD	C5-C6-S-O8
24	1	315	SQD	C5-C6-S-O9
25	9	302	A1L1F	O13-C26-C30-C31
25	9	302	A1L1F	C56-C54-O7-C8
25	8	304	A1L1F	C32-C33-C34-C35
25	8	304	A1L1F	C56-C54-O7-C8
25	8	304	A1L1F	O55-C54-O7-C8
25	6	304	A1L1F	C14-C29-C30-C31
25	6	304	A1L1F	C56-C54-O7-C8
25	1	304	A1L1F	C29-C14-C25-C24
25	1	304	A1L1F	C32-C33-C34-C35
25	1	304	A1L1F	C38-C39-C40-C41
25	h	203	A1L1F	C56-C54-O7-C8
25	h	203	A1L1F	O55-C54-O7-C8
26	9	307	LHG	C3-O3-P-O4
26	9	307	LHG	C3-O3-P-O5
26	9	307	LHG	C3-O3-P-O6
26	9	307	LHG	O9-C7-O7-C5
26	9	307	LHG	C8-C7-O7-C5
26	9	317	LHG	C1-C2-C3-O3
26	9	317	LHG	C3-O3-P-O4
26	9	317	LHG	O9-C7-O7-C5
26	9	317	LHG	C8-C7-O7-C5
26	a	845	LHG	O1-C1-C2-C3
26	a	845	LHG	C3-O3-P-O4
26	a	845	LHG	C3-O3-P-O6
26	a	845	LHG	C4-O6-P-O3
26	a	845	LHG	C4-O6-P-O5
26	a	845	LHG	O6-C4-C5-O7
26	a	845	LHG	O7-C5-C6-O8
26	a	846	LHG	O1-C1-C2-C3
26	a	846	LHG	O6-C4-C5-O7
26	b	847	LHG	O1-C1-C2-C3
26	b	847	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	b	847	LHG	O2-C2-C3-O3
26	b	847	LHG	C3-O3-P-O5
26	b	847	LHG	C3-O3-P-O6
26	b	847	LHG	C4-O6-P-O3
26	b	847	LHG	C4-O6-P-O4
26	b	847	LHG	C4-O6-P-O5
27	8	315	DGD	C2B-C1B-O2G-C2G
27	4	318	DGD	C2B-C1B-O2G-C2G
27	4	318	DGD	O1B-C1B-O2G-C2G
28	2	317	LMG	O1-C7-C8-O7
28	a	853	LMG	C11-C10-O7-C8
28	j	105	LMG	O9-C10-O7-C8
28	j	105	LMG	C11-C10-O7-C8
30	a	850	BCR	C23-C24-C25-C26
30	b	842	BCR	C7-C8-C9-C10
30	b	842	BCR	C7-C8-C9-C34
30	b	844	BCR	C1-C6-C7-C8
30	b	844	BCR	C5-C6-C7-C8
30	i	101	BCR	C21-C22-C23-C24
30	i	101	BCR	C37-C22-C23-C24
30	j	104	BCR	C7-C8-C9-C10
30	j	104	BCR	C7-C8-C9-C34
30	m	101	BCR	C21-C22-C23-C24
30	m	101	BCR	C37-C22-C23-C24
23	5	310	CLA	O1D-CGD-O2D-CED
23	9	315	CLA	O1D-CGD-O2D-CED
23	4	309	CLA	O1D-CGD-O2D-CED
23	2	314	CLA	O1D-CGD-O2D-CED
23	7	314	CLA	O1D-CGD-O2D-CED
25	9	302	A1L1F	O55-C54-O7-C8
23	9	308	CLA	O1D-CGD-O2D-CED
23	6	315	CLA	O1D-CGD-O2D-CED
23	2	307	CLA	O1D-CGD-O2D-CED
23	2	309	CLA	O1D-CGD-O2D-CED
23	2	313	CLA	O1D-CGD-O2D-CED
23	7	307	CLA	O1D-CGD-O2D-CED
23	1	313	CLA	O1D-CGD-O2D-CED
23	a	812	CLA	O1D-CGD-O2D-CED
23	b	803	CLA	O1D-CGD-O2D-CED
23	b	834	CLA	O1D-CGD-O2D-CED
25	6	304	A1L1F	O55-C54-O7-C8
23	5	313	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	9	318	CLA	CBD-CGD-O2D-CED
23	8	306	CLA	CBD-CGD-O2D-CED
23	4	306	CLA	CBD-CGD-O2D-CED
23	6	313	CLA	CBD-CGD-O2D-CED
23	2	314	CLA	CBD-CGD-O2D-CED
23	1	309	CLA	CBD-CGD-O2D-CED
23	a	812	CLA	CBD-CGD-O2D-CED
23	8	308	CLA	O1A-CGA-O2A-C1
23	4	310	CLA	O1A-CGA-O2A-C1
23	1	307	CLA	O1A-CGA-O2A-C1
23	a	806	CLA	O1A-CGA-O2A-C1
23	b	814	CLA	O1A-CGA-O2A-C1
25	6	304	A1L1F	O46-C45-O13-C26
26	9	317	LHG	O10-C23-O8-C6
28	2	317	LMG	O10-C28-O8-C9
23	7	310	CLA	O1A-CGA-O2A-C1
23	4	316	CLA	O1D-CGD-O2D-CED
23	7	315	CLA	O1D-CGD-O2D-CED
23	b	804	CLA	O1D-CGD-O2D-CED
25	9	302	A1L1F	C4-C8-O7-C54
23	a	801	CLA	O1D-CGD-O2D-CED
23	8	308	CLA	CBA-CGA-O2A-C1
23	1	307	CLA	CBA-CGA-O2A-C1
23	a	806	CLA	CBA-CGA-O2A-C1
23	b	814	CLA	CBA-CGA-O2A-C1
25	6	304	A1L1F	C47-C45-O13-C26
26	9	317	LHG	C24-C23-O8-C6
23	2	310	CLA	O1A-CGA-O2A-C1
23	2	311	CLA	O1A-CGA-O2A-C1
23	7	312	CLA	O1A-CGA-O2A-C1
23	a	805	CLA	O1A-CGA-O2A-C1
23	a	818	CLA	O1A-CGA-O2A-C1
23	b	821	CLA	O1A-CGA-O2A-C1
23	f	802	CLA	O1A-CGA-O2A-C1
25	6	301	A1L1F	O46-C45-O13-C26
26	b	847	LHG	O10-C23-O8-C6
27	8	315	DGD	O1A-C1A-O1G-C1G
28	a	853	LMG	O10-C28-O8-C9
23	4	311	CLA	O1A-CGA-O2A-C1
23	7	311	CLA	O1A-CGA-O2A-C1
23	2	312	CLA	O1D-CGD-O2D-CED
23	b	814	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	5	308	CLA	O1D-CGD-O2D-CED
23	4	317	CLA	O1D-CGD-O2D-CED
23	7	306	CLA	O1D-CGD-O2D-CED
23	1	310	CLA	O1D-CGD-O2D-CED
23	a	811	CLA	O1D-CGD-O2D-CED
23	a	829	CLA	O1D-CGD-O2D-CED
23	b	839	CLA	O1D-CGD-O2D-CED
23	j	103	CLA	O1D-CGD-O2D-CED
25	6	301	A1L1F	C56-C54-O7-C8
27	8	315	DGD	O1B-C1B-O2G-C2G
28	a	853	LMG	O9-C10-O7-C8
23	6	316	CLA	CBA-CGA-O2A-C1
23	1	309	CLA	CBA-CGA-O2A-C1
23	1	309	CLA	O1A-CGA-O2A-C1
23	1	204	CLA	O1A-CGA-O2A-C1
23	3	312	CLA	C3-C5-C6-C7
23	2	310	CLA	C3-C5-C6-C7
23	2	311	CLA	C3-C5-C6-C7
23	2	314	CLA	C3-C5-C6-C7
23	7	308	CLA	C3-C5-C6-C7
23	a	810	CLA	C3-C5-C6-C7
23	b	802	CLA	C3-C5-C6-C7
23	b	805	CLA	C3-C5-C6-C7
23	b	807	CLA	C3-C5-C6-C7
23	b	809	CLA	C3-C5-C6-C7
23	6	314	CLA	O1D-CGD-O2D-CED
23	2	310	CLA	CBA-CGA-O2A-C1
23	2	311	CLA	CBA-CGA-O2A-C1
23	7	312	CLA	CBA-CGA-O2A-C1
23	a	805	CLA	CBA-CGA-O2A-C1
23	a	818	CLA	CBA-CGA-O2A-C1
23	a	836	CLA	CBA-CGA-O2A-C1
23	b	821	CLA	CBA-CGA-O2A-C1
23	b	823	CLA	CBA-CGA-O2A-C1
23	f	802	CLA	CBA-CGA-O2A-C1
25	6	301	A1L1F	C47-C45-O13-C26
28	2	317	LMG	C29-C28-O8-C9
28	a	853	LMG	C29-C28-O8-C9
25	1	304	A1L1F	C56-C54-O7-C8
25	1	304	A1L1F	O55-C54-O7-C8
23	5	305	CLA	CBD-CGD-O2D-CED
23	5	309	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	9	312	CLA	CBD-CGD-O2D-CED
23	9	314	CLA	CBD-CGD-O2D-CED
23	8	309	CLA	CBD-CGD-O2D-CED
23	3	308	CLA	CBD-CGD-O2D-CED
23	6	310	CLA	CBD-CGD-O2D-CED
23	2	316	CLA	CBD-CGD-O2D-CED
23	7	310	CLA	CBD-CGD-O2D-CED
23	a	804	CLA	CBD-CGD-O2D-CED
23	a	814	CLA	CBD-CGD-O2D-CED
23	b	806	CLA	CBD-CGD-O2D-CED
23	b	819	CLA	CBD-CGD-O2D-CED
23	b	835	CLA	CBD-CGD-O2D-CED
23	h	204	CLA	CBD-CGD-O2D-CED
23	4	311	CLA	O1D-CGD-O2D-CED
23	7	306	CLA	O1A-CGA-O2A-C1
23	6	316	CLA	O1A-CGA-O2A-C1
23	8	311	CLA	C4-C3-C5-C6
23	3	310	CLA	C4-C3-C5-C6
23	a	825	CLA	C4-C3-C5-C6
23	a	831	CLA	C4-C3-C5-C6
23	a	839	CLA	C4-C3-C5-C6
23	j	102	CLA	C4-C3-C5-C6
23	8	311	CLA	C2-C3-C5-C6
23	3	310	CLA	C2-C3-C5-C6
23	a	831	CLA	C2-C3-C5-C6
23	a	839	CLA	C2-C3-C5-C6
23	j	102	CLA	C2-C3-C5-C6
23	9	309	CLA	CBA-CGA-O2A-C1
23	l	204	CLA	CBA-CGA-O2A-C1
23	5	306	CLA	CBD-CGD-O2D-CED
23	1	309	CLA	O1D-CGD-O2D-CED
23	a	817	CLA	C2A-CAA-CBA-CGA
23	b	810	CLA	C2A-CAA-CBA-CGA
23	9	308	CLA	C3-C5-C6-C7
23	8	308	CLA	C3-C5-C6-C7
23	1	307	CLA	C3-C5-C6-C7
23	1	310	CLA	C3-C5-C6-C7
23	b	818	CLA	C3-C5-C6-C7
23	9	316	CLA	CBA-CGA-O2A-C1
23	4	310	CLA	CBA-CGA-O2A-C1
23	1	305	CLA	CBA-CGA-O2A-C1
23	a	807	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	811	CLA	CBA-CGA-O2A-C1
23	b	806	CLA	CBA-CGA-O2A-C1
23	b	818	CLA	CBA-CGA-O2A-C1
26	9	307	LHG	C24-C23-O8-C6
26	b	847	LHG	C24-C23-O8-C6
27	8	315	DGD	C2A-C1A-O1G-C1G
28	j	105	LMG	C29-C28-O8-C9
28	j	105	LMG	C4-C5-C6-O5
22	9	301	A1L1G	C30-C31-C32-C33
22	9	301	A1L1G	C40-C41-C42-C44
22	3	302	A1L1G	C30-C31-C32-C33
22	7	302	A1L1G	C30-C31-C32-C33
25	8	304	A1L1F	C30-C31-C32-C33
25	6	301	A1L1F	C36-C37-C38-C39
23	5	311	CLA	O1A-CGA-O2A-C1
23	1	305	CLA	O1A-CGA-O2A-C1
23	a	811	CLA	O1A-CGA-O2A-C1
23	a	812	CLA	O1A-CGA-O2A-C1
23	a	820	CLA	O1A-CGA-O2A-C1
23	b	806	CLA	O1A-CGA-O2A-C1
23	b	818	CLA	O1A-CGA-O2A-C1
28	j	105	LMG	O10-C28-O8-C9
23	6	313	CLA	O1D-CGD-O2D-CED
23	4	307	CLA	CBD-CGD-O2D-CED
23	6	312	CLA	CBD-CGD-O2D-CED
23	7	308	CLA	CBD-CGD-O2D-CED
23	a	818	CLA	CBD-CGD-O2D-CED
23	a	837	CLA	CBD-CGD-O2D-CED
28	j	105	LMG	C12-C13-C14-C15
26	9	307	LHG	O2-C2-C3-O3
26	9	317	LHG	O2-C2-C3-O3
26	a	845	LHG	O2-C2-C3-O3
23	7	306	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	CBA-CGA-O2A-C1
23	b	839	CLA	CBA-CGA-O2A-C1
23	a	836	CLA	O1A-CGA-O2A-C1
23	b	823	CLA	O1A-CGA-O2A-C1
26	9	307	LHG	O10-C23-O8-C6
23	9	316	CLA	CBD-CGD-O2D-CED
23	3	309	CLA	CBD-CGD-O2D-CED
23	3	315	CLA	CBD-CGD-O2D-CED
23	9	312	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	6	314	CLA	CBA-CGA-O2A-C1
23	b	839	CLA	O1A-CGA-O2A-C1
23	9	318	CLA	O1D-CGD-O2D-CED
23	8	306	CLA	O1D-CGD-O2D-CED
23	5	309	CLA	C3-C5-C6-C7
23	a	807	CLA	C3-C5-C6-C7
23	a	835	CLA	C3-C5-C6-C7
23	a	841	CLA	CBD-CGD-O2D-CED
23	b	823	CLA	CBD-CGD-O2D-CED
23	b	827	CLA	CBD-CGD-O2D-CED
27	b	848	DGD	O6E-C5E-C6E-O5E
23	4	306	CLA	O1D-CGD-O2D-CED
23	5	311	CLA	CBA-CGA-O2A-C1
23	6	309	CLA	CBA-CGA-O2A-C1
23	a	820	CLA	CBA-CGA-O2A-C1
23	a	813	CLA	C4-C3-C5-C6
23	b	828	CLA	C4-C3-C5-C6
23	a	825	CLA	C2-C3-C5-C6
23	9	316	CLA	O1A-CGA-O2A-C1
23	a	807	CLA	O1A-CGA-O2A-C1
23	8	313	CLA	CBA-CGA-O2A-C1
23	7	317	CLA	CBD-CGD-O2D-CED
23	1	312	CLA	C3-C5-C6-C7
23	6	309	CLA	O1A-CGA-O2A-C1
27	8	315	DGD	O6E-C1E-O5D-C6D
27	4	318	DGD	O6E-C1E-O5D-C6D
23	7	316	CLA	CBA-CGA-O2A-C1
23	4	308	CLA	CBD-CGD-O2D-CED
23	a	807	CLA	CBD-CGD-O2D-CED
23	a	810	CLA	CBD-CGD-O2D-CED
23	a	834	CLA	CBD-CGD-O2D-CED
23	a	835	CLA	CBD-CGD-O2D-CED
23	b	840	CLA	CBD-CGD-O2D-CED
26	a	845	LHG	C23-C24-C25-C26
23	9	312	CLA	O1A-CGA-O2A-C1
28	a	853	LMG	O6-C5-C6-O5
28	j	105	LMG	O6-C5-C6-O5
23	5	313	CLA	O1D-CGD-O2D-CED
26	a	845	LHG	C12-C13-C14-C15
23	9	309	CLA	O1A-CGA-O2A-C1
22	5	303	A1L1G	C40-C41-C42-C44
25	8	304	A1L1F	C40-C41-C42-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	9	307	LHG	C1-C2-C3-O3
26	a	845	LHG	C1-C2-C3-O3
23	5	308	CLA	CBA-CGA-O2A-C1
23	8	311	CLA	CBA-CGA-O2A-C1
23	3	311	CLA	CBA-CGA-O2A-C1
23	6	317	CLA	CBA-CGA-O2A-C1
23	a	809	CLA	CBA-CGA-O2A-C1
23	a	839	CLA	CBA-CGA-O2A-C1
23	a	854	CLA	CBA-CGA-O2A-C1
23	b	820	CLA	CBA-CGA-O2A-C1
23	b	826	CLA	CBA-CGA-O2A-C1
23	b	833	CLA	CBA-CGA-O2A-C1
23	5	311	CLA	CBD-CGD-O2D-CED
23	b	822	CLA	CBD-CGD-O2D-CED
28	a	853	LMG	C4-C5-C6-O5
25	9	302	A1L1F	C47-C48-C49-C50
23	a	804	CLA	O1D-CGD-O2D-CED
26	a	845	LHG	C28-C29-C30-C31
23	a	813	CLA	C2-C3-C5-C6
23	9	318	CLA	C11-C10-C8-C9
23	9	318	CLA	C11-C12-C13-C14
23	8	307	CLA	C11-C10-C8-C9
23	8	311	CLA	C6-C7-C8-C9
23	2	310	CLA	C11-C12-C13-C14
23	1	306	CLA	C6-C7-C8-C9
23	1	306	CLA	C11-C12-C13-C14
23	1	310	CLA	C14-C13-C15-C16
23	a	829	CLA	C11-C10-C8-C9
23	b	801	CLA	C11-C10-C8-C9
23	b	801	CLA	C14-C13-C15-C16
23	b	805	CLA	C11-C10-C8-C9
23	b	818	CLA	C11-C10-C8-C9
23	b	824	CLA	C6-C7-C8-C9
23	b	829	CLA	C14-C13-C15-C16
23	b	838	CLA	C6-C7-C8-C9
23	f	802	CLA	C11-C12-C13-C14
28	2	317	LMG	C29-C30-C31-C32
23	9	312	CLA	O1D-CGD-O2D-CED
23	9	314	CLA	O1D-CGD-O2D-CED
23	7	310	CLA	O1D-CGD-O2D-CED
23	b	806	CLA	O1D-CGD-O2D-CED
27	8	315	DGD	C2E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	4	318	DGD	C2E-C1E-O5D-C6D
26	a	846	LHG	O2-C2-C3-O3
23	8	309	CLA	O1D-CGD-O2D-CED
23	b	835	CLA	O1D-CGD-O2D-CED
23	8	311	CLA	O1A-CGA-O2A-C1
23	a	809	CLA	O1A-CGA-O2A-C1
23	a	854	CLA	O1A-CGA-O2A-C1
23	h	204	CLA	O1D-CGD-O2D-CED
21	8	301	XAT	C7-C8-C9-C19
21	3	303	XAT	C27-C28-C29-C39
21	6	303	XAT	C7-C8-C9-C19
21	2	301	XAT	C27-C28-C29-C39
21	a	852	XAT	C11-C12-C13-C20
21	a	852	XAT	C27-C28-C29-C39
21	j	101	XAT	C7-C8-C9-C19
22	9	301	A1L1G	C28-C39-C40-C41
22	3	306	A1L1G	C28-C39-C40-C41
22	1	301	A1L1G	C28-C39-C40-C41
25	8	304	A1L1F	C32-C33-C34-C27
25	8	304	A1L1F	C28-C39-C40-C41
25	1	304	A1L1F	C32-C33-C34-C27
25	1	304	A1L1F	C28-C39-C40-C41
30	b	849	BCR	C7-C8-C9-C34
30	l	205	BCR	C7-C8-C9-C34
30	l	205	BCR	C37-C22-C23-C24
30	m	101	BCR	C7-C8-C9-C34
21	6	303	XAT	C7-C8-C9-C10
21	2	301	XAT	C27-C28-C29-C30
22	3	306	A1L1G	C38-C39-C40-C41
30	b	849	BCR	C7-C8-C9-C10
30	l	205	BCR	C7-C8-C9-C10
30	l	205	BCR	C21-C22-C23-C24
23	5	310	CLA	C2A-CAA-CBA-CGA
23	9	313	CLA	C2A-CAA-CBA-CGA
23	4	311	CLA	C2A-CAA-CBA-CGA
23	4	316	CLA	C2A-CAA-CBA-CGA
23	b	805	CLA	C2A-CAA-CBA-CGA
23	b	826	CLA	C2A-CAA-CBA-CGA
28	a	853	LMG	C28-C29-C30-C31
23	5	305	CLA	O1D-CGD-O2D-CED
23	3	311	CLA	O1A-CGA-O2A-C1
23	6	317	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	820	CLA	O1A-CGA-O2A-C1
23	9	313	CLA	CBA-CGA-O2A-C1
23	4	316	CLA	CBA-CGA-O2A-C1
23	2	312	CLA	CBA-CGA-O2A-C1
23	b	838	CLA	CBA-CGA-O2A-C1
23	a	810	CLA	C13-C15-C16-C17
23	5	308	CLA	O1A-CGA-O2A-C1
23	b	826	CLA	O1A-CGA-O2A-C1
23	2	316	CLA	O1D-CGD-O2D-CED
23	a	814	CLA	O1D-CGD-O2D-CED
23	6	308	CLA	CBD-CGD-O2D-CED
22	3	302	A1L1G	C35-C36-C37-C38
23	9	318	CLA	C8-C10-C11-C12
23	8	307	CLA	C5-C6-C7-C8
23	a	807	CLA	C5-C6-C7-C8
23	b	809	CLA	C5-C6-C7-C8
23	b	823	CLA	C3-C5-C6-C7
23	4	315	CLA	CBD-CGD-O2D-CED
23	6	317	CLA	CBD-CGD-O2D-CED
23	b	807	CLA	CBD-CGD-O2D-CED
23	1	310	CLA	C11-C10-C8-C7
23	a	801	CLA	C12-C13-C15-C16
23	a	809	CLA	C12-C13-C15-C16
23	a	828	CLA	C12-C13-C15-C16
23	a	844	CLA	C12-C13-C15-C16
23	b	808	CLA	C12-C13-C15-C16
23	b	833	CLA	C13-C15-C16-C17
27	b	848	DGD	C1A-C2A-C3A-C4A
25	6	301	A1L1F	C34-C35-C36-C37
25	6	301	A1L1F	O55-C54-O7-C8
23	5	309	CLA	O1D-CGD-O2D-CED
23	b	807	CLA	C15-C16-C17-C18
26	b	847	LHG	C7-C8-C9-C10
23	a	839	CLA	O1A-CGA-O2A-C1
23	b	833	CLA	O1A-CGA-O2A-C1
23	b	827	CLA	CBA-CGA-O2A-C1
23	2	310	CLA	C15-C16-C17-C18
23	a	809	CLA	C5-C6-C7-C8
23	b	801	CLA	C15-C16-C17-C18
23	9	311	CLA	C2A-CAA-CBA-CGA
23	9	312	CLA	C2A-CAA-CBA-CGA
23	7	317	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	825	CLA	C2A-CAA-CBA-CGA
23	a	830	CLA	C2A-CAA-CBA-CGA
23	a	842	CLA	C2A-CAA-CBA-CGA
23	b	820	CLA	C2A-CAA-CBA-CGA
23	b	833	CLA	C2A-CAA-CBA-CGA
23	b	838	CLA	C2A-CAA-CBA-CGA
22	9	306	A1L1G	C39-C40-C41-C42
22	3	302	A1L1G	C39-C40-C41-C42
23	9	308	CLA	C5-C6-C7-C8
23	9	318	CLA	C10-C11-C12-C13
23	4	308	CLA	C10-C11-C12-C13
23	a	802	CLA	C5-C6-C7-C8
23	a	814	CLA	C13-C15-C16-C17
23	a	834	CLA	C15-C16-C17-C18
23	b	832	CLA	C13-C15-C16-C17
23	b	840	CLA	C13-C15-C16-C17
25	1	304	A1L1F	C45-C47-C48-C49
26	a	846	LHG	C7-C8-C9-C10
28	a	853	LMG	C10-C11-C12-C13
23	a	801	CLA	C3-C5-C6-C7
25	1	304	A1L1F	C49-C50-C51-C52
23	3	308	CLA	O1D-CGD-O2D-CED
23	6	310	CLA	O1D-CGD-O2D-CED
23	b	819	CLA	O1D-CGD-O2D-CED
23	5	309	CLA	C13-C15-C16-C17
23	1	306	CLA	C5-C6-C7-C8
23	1	306	CLA	C8-C10-C11-C12
23	a	809	CLA	C8-C10-C11-C12
23	a	830	CLA	C13-C15-C16-C17
23	a	831	CLA	C5-C6-C7-C8
23	b	809	CLA	C8-C10-C11-C12
23	b	813	CLA	C15-C16-C17-C18
23	b	829	CLA	C8-C10-C11-C12
23	1	203	CLA	C10-C11-C12-C13
23	8	310	CLA	CBD-CGD-O2D-CED
23	7	316	CLA	O1A-CGA-O2A-C1
23	a	807	CLA	C15-C16-C17-C18
23	a	841	CLA	C5-C6-C7-C8
23	b	814	CLA	C5-C6-C7-C8
23	b	836	CLA	C5-C6-C7-C8
23	6	312	CLA	O1D-CGD-O2D-CED
23	5	305	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	5	306	CLA	O1D-CGD-O2D-CED
23	7	308	CLA	O1D-CGD-O2D-CED
23	a	837	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	C8-C10-C11-C12
23	f	802	CLA	CBD-CGD-O2D-CED
23	2	312	CLA	O1A-CGA-O2A-C1
23	1	306	CLA	C15-C16-C17-C18
23	a	841	CLA	C15-C16-C17-C18
23	b	840	CLA	C10-C11-C12-C13
23	4	317	CLA	CBA-CGA-O2A-C1
23	a	816	CLA	CBA-CGA-O2A-C1
23	b	802	CLA	CBA-CGA-O2A-C1
23	b	831	CLA	CBA-CGA-O2A-C1
27	b	848	DGD	C4E-C5E-C6E-O5E
23	b	802	CLA	CBD-CGD-O2D-CED
23	a	818	CLA	O1D-CGD-O2D-CED
23	4	313	CLA	C3-C5-C6-C7
23	7	313	CLA	C3-C5-C6-C7
22	9	306	A1L1G	C40-C41-C42-C44
23	b	801	CLA	C2A-CAA-CBA-CGA
23	4	307	CLA	O1D-CGD-O2D-CED
23	a	814	CLA	CBA-CGA-O2A-C1
23	a	838	CLA	CBA-CGA-O2A-C1
23	6	309	CLA	C10-C11-C12-C13
23	a	801	CLA	C8-C10-C11-C12
23	a	828	CLA	C13-C15-C16-C17
23	a	828	CLA	C15-C16-C17-C18
23	f	802	CLA	C13-C15-C16-C17
23	h	204	CLA	C5-C6-C7-C8
29	b	841	PQN	C23-C25-C26-C27
23	a	826	CLA	CBD-CGD-O2D-CED
23	7	316	CLA	C2C-C3C-CAC-CBC
23	3	315	CLA	O1D-CGD-O2D-CED
23	7	308	CLA	C10-C11-C12-C13
23	b	836	CLA	C8-C10-C11-C12
23	f	802	CLA	C5-C6-C7-C8
23	8	313	CLA	O1A-CGA-O2A-C1
23	6	314	CLA	O1A-CGA-O2A-C1
27	4	318	DGD	C3B-C4B-C5B-C6B
23	a	831	CLA	C15-C16-C17-C18
23	a	839	CLA	C13-C15-C16-C17
23	b	801	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	802	CLA	C8-C10-C11-C12
23	b	827	CLA	C13-C15-C16-C17
23	a	833	CLA	CBA-CGA-O2A-C1
23	a	844	CLA	CBA-CGA-O2A-C1
23	7	308	CLA	C4-C3-C5-C6
23	b	828	CLA	C2-C3-C5-C6
23	b	801	CLA	C8-C10-C11-C12
23	1	203	CLA	C8-C10-C11-C12
24	1	315	SQD	C8-C7-O47-C45
23	9	316	CLA	O1D-CGD-O2D-CED
24	1	315	SQD	O49-C7-O47-C45
23	7	306	CLA	O2A-C1-C2-C3
23	7	309	CLA	O2A-C1-C2-C3
23	9	310	CLA	CBA-CGA-O2A-C1
23	a	824	CLA	CBA-CGA-O2A-C1
24	1	315	SQD	C24-C23-O48-C46
23	9	316	CLA	C16-C17-C18-C20
23	a	801	CLA	C16-C17-C18-C20
23	b	838	CLA	O1A-CGA-O2A-C1
22	9	306	A1L1G	C14-C29-C30-C31
22	3	302	A1L1G	C14-C29-C30-C31
22	9	301	A1L1G	C41-C42-C44-C43
22	9	306	A1L1G	C41-C42-C44-C43
22	3	302	A1L1G	C37-C38-C39-C28
22	3	306	A1L1G	C27-C34-C35-C36
21	9	303	XAT	C7-C8-C9-C19
21	2	303	XAT	C7-C8-C9-C19
21	2	304	XAT	C7-C8-C9-C19
22	9	301	A1L1G	C32-C33-C34-C27
22	3	302	A1L1G	C32-C33-C34-C27
22	7	302	A1L1G	C32-C33-C34-C27
30	a	850	BCR	C37-C22-C23-C24
30	f	801	BCR	C37-C22-C23-C24
21	9	303	XAT	C7-C8-C9-C10
21	8	301	XAT	C7-C8-C9-C10
21	2	303	XAT	C7-C8-C9-C10
21	7	304	XAT	C7-C8-C9-C10
22	9	301	A1L1G	C32-C33-C34-C35
22	3	302	A1L1G	C32-C33-C34-C35
25	8	304	A1L1F	C38-C39-C40-C41
30	a	850	BCR	C21-C22-C23-C24
30	f	801	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	317	CLA	O1A-CGA-O2A-C1
23	a	816	CLA	O1A-CGA-O2A-C1
23	b	802	CLA	O1A-CGA-O2A-C1
23	2	310	CLA	C2A-CAA-CBA-CGA
23	7	310	CLA	C2A-CAA-CBA-CGA
23	b	831	CLA	C2A-CAA-CBA-CGA
23	h	204	CLA	C2A-CAA-CBA-CGA
23	b	829	CLA	C10-C11-C12-C13
23	b	839	CLA	C5-C6-C7-C8
23	3	309	CLA	O1D-CGD-O2D-CED
23	a	841	CLA	O1D-CGD-O2D-CED
23	a	806	CLA	O2A-C1-C2-C3
23	5	315	CLA	C2C-C3C-CAC-CBC
22	5	303	A1L1G	C29-C30-C31-C32
22	9	301	A1L1G	C29-C30-C31-C32
22	9	306	A1L1G	C29-C30-C31-C32
23	b	833	CLA	C16-C17-C18-C19
23	b	840	CLA	C16-C17-C18-C20
23	b	823	CLA	O1D-CGD-O2D-CED
23	a	814	CLA	O1A-CGA-O2A-C1
23	b	827	CLA	O1A-CGA-O2A-C1
22	9	301	A1L1G	C41-C42-C44-C2
22	9	306	A1L1G	C41-C42-C44-C2
22	3	302	A1L1G	C37-C38-C39-C40
22	3	306	A1L1G	C33-C34-C35-C36
23	b	824	CLA	C5-C6-C7-C8
23	a	835	CLA	O1D-CGD-O2D-CED
23	a	836	CLA	CBD-CGD-O2D-CED
23	7	317	CLA	O1D-CGD-O2D-CED
23	b	827	CLA	O1D-CGD-O2D-CED
23	a	818	CLA	C2-C1-O2A-CGA
23	9	316	CLA	C16-C17-C18-C19
23	4	308	CLA	C16-C17-C18-C20
23	a	854	CLA	C5-C6-C7-C8
27	b	848	DGD	C9B-CAB-CBB-CCB
22	9	301	A1L1G	C35-C36-C37-C38
22	3	306	A1L1G	C35-C36-C37-C38
30	m	101	BCR	C14-C15-C16-C17
26	a	845	LHG	C11-C10-C9-C8
23	a	834	CLA	O1D-CGD-O2D-CED
23	b	827	CLA	C8-C10-C11-C12
29	a	843	PQN	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	831	CLA	O1A-CGA-O2A-C1
23	b	816	CLA	CBA-CGA-O2A-C1
26	9	307	LHG	C28-C29-C30-C31
26	9	307	LHG	C31-C32-C33-C34
26	a	845	LHG	O1-C1-C2-O2
26	a	846	LHG	O1-C1-C2-O2
26	b	847	LHG	O1-C1-C2-O2
26	9	307	LHG	C34-C35-C36-C37
23	8	310	CLA	C4B-C3B-CAB-CBB
23	8	314	CLA	C4B-C3B-CAB-CBB
23	4	312	CLA	C4B-C3B-CAB-CBB
23	6	311	CLA	C4B-C3B-CAB-CBB
23	6	315	CLA	C4B-C3B-CAB-CBB
23	2	307	CLA	C4B-C3B-CAB-CBB
23	7	307	CLA	C4B-C3B-CAB-CBB
23	a	841	CLA	C4B-C3B-CAB-CBB
23	b	840	CLA	C4B-C3B-CAB-CBB
25	9	302	A1L1F	C45-C47-C48-C49
26	9	317	LHG	C9-C10-C11-C12
26	a	845	LHG	C27-C28-C29-C30
23	b	811	CLA	C6-C7-C8-C9
23	f	802	CLA	C16-C17-C18-C19
23	f	802	CLA	C16-C17-C18-C20
23	1	314	CLA	C2A-CAA-CBA-CGA
23	b	828	CLA	C2A-CAA-CBA-CGA
23	a	814	CLA	C10-C11-C12-C13
23	a	827	CLA	C8-C10-C11-C12
23	a	841	CLA	C8-C10-C11-C12
23	b	806	CLA	C15-C16-C17-C18
23	b	835	CLA	C5-C6-C7-C8
23	1	308	CLA	C11-C10-C8-C7
26	a	845	LHG	C13-C14-C15-C16
23	b	840	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	CBA-CGA-O2A-C1
23	b	809	CLA	C10-C11-C12-C13
26	9	307	LHG	C27-C28-C29-C30
23	9	310	CLA	C3A-C2A-CAA-CBA
23	9	313	CLA	C3A-C2A-CAA-CBA
23	4	310	CLA	C3A-C2A-CAA-CBA
23	3	312	CLA	C3A-C2A-CAA-CBA
23	3	314	CLA	C3A-C2A-CAA-CBA
23	6	317	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	306	CLA	C3A-C2A-CAA-CBA
23	7	311	CLA	C3A-C2A-CAA-CBA
23	a	807	CLA	C3A-C2A-CAA-CBA
23	a	838	CLA	C3A-C2A-CAA-CBA
23	a	854	CLA	C3A-C2A-CAA-CBA
23	b	810	CLA	C3A-C2A-CAA-CBA
23	b	812	CLA	C3A-C2A-CAA-CBA
23	b	814	CLA	C3A-C2A-CAA-CBA
23	f	803	CLA	C3A-C2A-CAA-CBA
23	6	317	CLA	C10-C11-C12-C13
28	2	317	LMG	C28-C29-C30-C31
23	b	811	CLA	C6-C7-C8-C10
23	b	833	CLA	C16-C17-C18-C20
23	a	833	CLA	O1A-CGA-O2A-C1
23	a	838	CLA	O1A-CGA-O2A-C1
23	a	844	CLA	O1A-CGA-O2A-C1
24	1	315	SQD	O10-C23-O48-C46
26	9	317	LHG	C28-C29-C30-C31
23	a	814	CLA	C5-C6-C7-C8
23	6	316	CLA	CBD-CGD-O2D-CED
23	a	823	CLA	CBA-CGA-O2A-C1
23	b	807	CLA	CBA-CGA-O2A-C1
23	b	835	CLA	CBA-CGA-O2A-C1
25	8	304	A1L1F	C45-C47-C48-C49
24	1	315	SQD	C11-C10-C9-C8
26	9	317	LHG	C14-C15-C16-C17
27	4	318	DGD	C2B-C3B-C4B-C5B
23	a	807	CLA	O1D-CGD-O2D-CED
27	b	848	DGD	C4A-C5A-C6A-C7A
23	b	801	CLA	C16-C17-C18-C20
23	8	314	CLA	C2B-C3B-CAB-CBB
23	4	311	CLA	C2B-C3B-CAB-CBB
23	4	312	CLA	C2B-C3B-CAB-CBB
23	4	314	CLA	C2B-C3B-CAB-CBB
23	6	311	CLA	C2B-C3B-CAB-CBB
23	2	307	CLA	C2B-C3B-CAB-CBB
23	7	307	CLA	C2B-C3B-CAB-CBB
23	7	315	CLA	C2B-C3B-CAB-CBB
23	a	808	CLA	C2B-C3B-CAB-CBB
23	a	836	CLA	C2B-C3B-CAB-CBB
23	b	819	CLA	C2B-C3B-CAB-CBB
23	b	838	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	850	BCR	C23-C24-C25-C30
30	l	205	BCR	C23-C24-C25-C26
30	l	205	BCR	C23-C24-C25-C30
23	3	314	CLA	CBD-CGD-O2D-CED
23	4	308	CLA	O1D-CGD-O2D-CED
23	a	810	CLA	O1D-CGD-O2D-CED
23	b	824	CLA	CBA-CGA-O2A-C1
23	b	808	CLA	C5-C6-C7-C8
23	b	808	CLA	C3-C5-C6-C7
23	5	306	CLA	C2A-CAA-CBA-CGA
23	a	814	CLA	C2A-CAA-CBA-CGA
26	9	317	LHG	C11-C12-C13-C14
27	b	848	DGD	C4B-C5B-C6B-C7B
23	9	308	CLA	O1A-CGA-O2A-C1
23	j	102	CLA	CBD-CGD-O2D-CED
23	a	811	CLA	C11-C10-C8-C7
23	1	308	CLA	C4-C3-C5-C6
23	1	310	CLA	C4-C3-C5-C6
27	b	848	DGD	C2B-C3B-C4B-C5B
22	5	303	A1L1G	C39-C40-C41-C42
22	7	302	A1L1G	C31-C32-C33-C34
23	7	308	CLA	C2-C3-C5-C6
27	b	848	DGD	C3B-C4B-C5B-C6B
23	a	825	CLA	CBA-CGA-O2A-C1
23	b	825	CLA	C11-C10-C8-C9
23	9	313	CLA	O1A-CGA-O2A-C1
27	4	318	DGD	O6D-C1D-O3G-C3G
23	b	816	CLA	O1A-CGA-O2A-C1
23	4	316	CLA	O1A-CGA-O2A-C1
23	a	840	CLA	C13-C15-C16-C17
25	h	203	A1L1F	C40-C41-C42-C44
26	a	846	LHG	C8-C7-O7-C5
27	b	848	DGD	C2B-C1B-O2G-C2G
23	b	838	CLA	C15-C16-C17-C18
25	6	304	A1L1F	C4-C8-O7-C54
23	a	809	CLA	C13-C15-C16-C17
21	6	303	XAT	C11-C12-C13-C20
21	7	304	XAT	C7-C8-C9-C19
26	9	307	LHG	C30-C31-C32-C33
23	b	804	CLA	C2C-C3C-CAC-CBC
25	9	302	A1L1F	C48-C49-C50-C51
23	a	810	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	832	CLA	C2A-CAA-CBA-CGA
23	2	314	CLA	C11-C10-C8-C9
23	b	801	CLA	C16-C17-C18-C19
23	4	310	CLA	C4-C3-C5-C6
23	b	834	CLA	C4-C3-C5-C6
23	b	839	CLA	C4-C3-C5-C6
25	1	304	A1L1F	C47-C48-C49-C50
23	8	307	CLA	C15-C16-C17-C18
23	b	829	CLA	C15-C16-C17-C18
26	a	845	LHG	C26-C27-C28-C29
25	h	203	A1L1F	C47-C48-C49-C50
23	a	823	CLA	O1A-CGA-O2A-C1
23	b	807	CLA	O1A-CGA-O2A-C1
23	4	307	CLA	C3-C5-C6-C7
23	b	805	CLA	C13-C15-C16-C17
23	b	810	CLA	C5-C6-C7-C8
23	j	102	CLA	C8-C10-C11-C12
28	2	317	LMG	C10-C11-C12-C13
26	b	847	LHG	O6-C4-C5-O7
23	b	832	CLA	C15-C16-C17-C18
23	a	806	CLA	C16-C17-C18-C19
23	b	840	CLA	C16-C17-C18-C19
24	1	315	SQD	C7-C8-C9-C10
23	4	308	CLA	C13-C15-C16-C17
23	4	308	CLA	C15-C16-C17-C18
23	2	308	CLA	C3-C5-C6-C7
27	4	318	DGD	O1G-C1G-C2G-O2G
23	b	835	CLA	O1A-CGA-O2A-C1
23	a	806	CLA	C13-C15-C16-C17
23	8	310	CLA	CBA-CGA-O2A-C1
23	3	315	CLA	CBA-CGA-O2A-C1
23	a	801	CLA	C16-C17-C18-C19
23	a	820	CLA	C16-C17-C18-C20
23	b	810	CLA	C10-C11-C12-C13
23	4	310	CLA	C2-C3-C5-C6
23	1	308	CLA	C2-C3-C5-C6
23	b	839	CLA	C2-C3-C5-C6
26	a	846	LHG	O9-C7-O7-C5
23	a	822	CLA	C2A-CAA-CBA-CGA
23	9	313	CLA	CBD-CGD-O2D-CED
23	a	808	CLA	CBD-CGD-O2D-CED
23	5	305	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	305	CLA	C8-C10-C11-C12
23	a	844	CLA	C10-C11-C12-C13
23	5	311	CLA	O1D-CGD-O2D-CED
23	b	824	CLA	O1A-CGA-O2A-C1
23	5	306	CLA	C1A-C2A-CAA-CBA
23	9	310	CLA	C1A-C2A-CAA-CBA
23	9	313	CLA	C1A-C2A-CAA-CBA
23	4	313	CLA	C1A-C2A-CAA-CBA
23	3	314	CLA	C1A-C2A-CAA-CBA
23	2	306	CLA	C1A-C2A-CAA-CBA
23	7	306	CLA	C1A-C2A-CAA-CBA
23	7	311	CLA	C1A-C2A-CAA-CBA
23	7	313	CLA	C1A-C2A-CAA-CBA
23	1	306	CLA	C1A-C2A-CAA-CBA
23	a	807	CLA	C1A-C2A-CAA-CBA
23	a	817	CLA	C1A-C2A-CAA-CBA
23	a	819	CLA	C1A-C2A-CAA-CBA
23	a	825	CLA	C1A-C2A-CAA-CBA
23	b	816	CLA	C1A-C2A-CAA-CBA
23	b	817	CLA	C1A-C2A-CAA-CBA
23	b	837	CLA	C1A-C2A-CAA-CBA
23	f	803	CLA	C1A-C2A-CAA-CBA
23	b	809	CLA	C15-C16-C17-C18
26	a	845	LHG	O6-C4-C5-C6
23	a	839	CLA	C3-C5-C6-C7
23	b	801	CLA	C3-C5-C6-C7
23	b	813	CLA	C3-C5-C6-C7
23	9	316	CLA	C11-C12-C13-C15
23	6	309	CLA	C11-C10-C8-C7
23	a	807	CLA	C12-C13-C15-C16
23	a	810	CLA	C12-C13-C15-C16
23	a	822	CLA	C6-C7-C8-C10
23	a	830	CLA	C12-C13-C15-C16
23	a	841	CLA	C11-C10-C8-C7
23	a	844	CLA	C11-C12-C13-C15
23	b	807	CLA	C11-C10-C8-C7
23	b	807	CLA	C12-C13-C15-C16
23	b	818	CLA	C6-C7-C8-C10
23	b	822	CLA	C6-C7-C8-C10
23	b	824	CLA	C11-C10-C8-C7
23	b	825	CLA	C6-C7-C8-C10
23	b	827	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	833	CLA	C11-C12-C13-C15
23	b	838	CLA	C6-C7-C8-C10
23	f	802	CLA	C11-C12-C13-C15
23	b	814	CLA	C6-C7-C8-C10
23	9	316	CLA	C2-C3-C5-C6
27	b	848	DGD	CAB-CBB-CCB-CDB
23	7	316	CLA	C4C-C3C-CAC-CBC
23	b	829	CLA	C13-C15-C16-C17
23	b	835	CLA	C2C-C3C-CAC-CBC
25	6	304	A1L1F	C45-C47-C48-C49
26	b	847	LHG	C8-C7-O7-C5
23	8	308	CLA	C2A-CAA-CBA-CGA
23	a	806	CLA	C2A-CAA-CBA-CGA
23	4	308	CLA	C11-C12-C13-C14
23	2	310	CLA	C14-C13-C15-C16
23	1	308	CLA	C11-C10-C8-C9
23	a	807	CLA	C11-C12-C13-C14
23	a	809	CLA	C14-C13-C15-C16
23	a	814	CLA	C11-C10-C8-C9
23	a	822	CLA	C6-C7-C8-C9
23	a	827	CLA	C11-C10-C8-C9
23	a	842	CLA	C11-C12-C13-C14
23	a	844	CLA	C11-C10-C8-C9
23	a	844	CLA	C14-C13-C15-C16
23	b	801	CLA	C11-C12-C13-C14
23	b	803	CLA	C11-C10-C8-C9
23	b	807	CLA	C14-C13-C15-C16
23	b	808	CLA	C11-C10-C8-C9
23	b	822	CLA	C6-C7-C8-C9
23	b	824	CLA	C11-C10-C8-C9
23	b	825	CLA	C6-C7-C8-C9
23	b	836	CLA	C14-C13-C15-C16
27	b	848	DGD	CBB-CCB-CDB-CEB
25	h	203	A1L1F	C4-C8-O7-C54
23	8	307	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	C10-C11-C12-C13
26	a	845	LHG	C4-C5-C6-O8
26	b	847	LHG	C4-C5-C6-O8
27	4	318	DGD	O1G-C1G-C2G-C3G
23	5	315	CLA	C4C-C3C-CAC-CBC
27	8	315	DGD	C2B-C3B-C4B-C5B
27	b	848	DGD	C6A-C7A-C8A-C9A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	807	CLA	O1D-CGD-O2D-CED
23	b	822	CLA	O1D-CGD-O2D-CED
23	a	835	CLA	CBA-CGA-O2A-C1
23	a	844	CLA	C16-C17-C18-C19
26	9	317	LHG	C29-C30-C31-C32
23	a	825	CLA	O1A-CGA-O2A-C1
23	4	315	CLA	O1D-CGD-O2D-CED
23	a	829	CLA	C10-C11-C12-C13
23	b	838	CLA	C4-C3-C5-C6
23	a	820	CLA	C8-C10-C11-C12
29	a	843	PQN	C23-C25-C26-C27
21	7	303	XAT	C7-C8-C9-C19
23	b	814	CLA	C6-C7-C8-C9
23	b	818	CLA	C11-C12-C13-C14
23	6	317	CLA	O1D-CGD-O2D-CED
26	9	317	LHG	C11-C10-C9-C8
21	4	305	XAT	C27-C28-C29-C30
23	1	308	CLA	C13-C15-C16-C17
23	a	854	CLA	C10-C11-C12-C13
23	b	839	CLA	C13-C15-C16-C17
23	4	307	CLA	CBA-CGA-O2A-C1
23	a	841	CLA	CBA-CGA-O2A-C1
23	1	310	CLA	C5-C6-C7-C8
25	9	302	A1L1F	C49-C50-C51-C52
23	a	844	CLA	C16-C17-C18-C20
23	7	313	CLA	C5-C6-C7-C8
23	9	314	CLA	C3-C5-C6-C7
23	6	308	CLA	O1D-CGD-O2D-CED
23	b	836	CLA	C2C-C3C-CAC-CBC
23	b	804	CLA	C15-C16-C17-C18
23	8	310	CLA	O1D-CGD-O2D-CED
27	b	848	DGD	C2A-C1A-O1G-C1G
23	8	307	CLA	O1A-CGA-O2A-C1
25	h	203	A1L1F	C48-C49-C50-C51
23	9	316	CLA	C4-C3-C5-C6
23	b	802	CLA	C4-C3-C5-C6
26	9	317	LHG	C12-C13-C14-C15
23	b	805	CLA	C16-C17-C18-C20
25	1	304	A1L1F	C50-C51-C52-C53
25	6	301	A1L1F	C50-C51-C52-C53
28	a	853	LMG	C14-C15-C16-C17
23	5	310	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	848	DGD	C3A-C4A-C5A-C6A
28	j	105	LMG	C13-C14-C15-C16
23	b	827	CLA	C15-C16-C17-C18
25	h	203	A1L1F	C3-C8-O7-C54
23	3	314	CLA	CBA-CGA-O2A-C1
23	1	306	CLA	CBA-CGA-O2A-C1
23	1	310	CLA	CBA-CGA-O2A-C1
23	b	828	CLA	CBA-CGA-O2A-C1
23	1	311	CLA	CBD-CGD-O2D-CED
23	4	317	CLA	C3-C5-C6-C7
23	f	802	CLA	O1D-CGD-O2D-CED
23	a	829	CLA	C8-C10-C11-C12
23	b	802	CLA	O1D-CGD-O2D-CED
23	a	811	CLA	C11-C10-C8-C9
23	a	805	CLA	C6-C7-C8-C9
23	9	310	CLA	O1A-CGA-O2A-C1
23	a	824	CLA	O1A-CGA-O2A-C1
23	a	801	CLA	C4-C3-C5-C6
23	a	804	CLA	C2-C3-C5-C6
23	b	803	CLA	C2-C3-C5-C6
23	a	831	CLA	CBA-CGA-O2A-C1
23	b	811	CLA	CBA-CGA-O2A-C1
23	9	316	CLA	C11-C12-C13-C14
23	4	310	CLA	C11-C10-C8-C9
23	7	308	CLA	C11-C10-C8-C9
23	a	810	CLA	C14-C13-C15-C16
23	a	814	CLA	C11-C12-C13-C14
23	a	830	CLA	C14-C13-C15-C16
23	a	835	CLA	C6-C7-C8-C9
23	a	841	CLA	C11-C10-C8-C9
23	a	844	CLA	C11-C12-C13-C14
23	b	803	CLA	C6-C7-C8-C9
23	b	810	CLA	C6-C7-C8-C9
23	b	818	CLA	C6-C7-C8-C9
23	b	828	CLA	C11-C12-C13-C14
23	b	837	CLA	C14-C13-C15-C16
23	j	102	CLA	C6-C7-C8-C9
23	a	810	CLA	C5-C6-C7-C8
23	a	826	CLA	C15-C16-C17-C18
26	9	317	LHG	C2-C3-O3-P
23	5	308	CLA	C4B-C3B-CAB-CBB
23	4	311	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	314	CLA	C4B-C3B-CAB-CBB
23	3	307	CLA	C4B-C3B-CAB-CBB
23	3	308	CLA	C4B-C3B-CAB-CBB
23	6	308	CLA	C4B-C3B-CAB-CBB
23	6	316	CLA	C4B-C3B-CAB-CBB
23	7	314	CLA	C4B-C3B-CAB-CBB
23	7	317	CLA	C4B-C3B-CAB-CBB
23	1	305	CLA	C4B-C3B-CAB-CBB
23	1	309	CLA	C4B-C3B-CAB-CBB
23	1	313	CLA	C4B-C3B-CAB-CBB
23	1	314	CLA	C4B-C3B-CAB-CBB
23	a	801	CLA	C4B-C3B-CAB-CBB
23	a	808	CLA	C4B-C3B-CAB-CBB
23	a	825	CLA	C4B-C3B-CAB-CBB
23	a	836	CLA	C4B-C3B-CAB-CBB
23	a	837	CLA	C4B-C3B-CAB-CBB
23	b	817	CLA	C4B-C3B-CAB-CBB
23	b	818	CLA	C4B-C3B-CAB-CBB
23	j	102	CLA	C4B-C3B-CAB-CBB
27	b	848	DGD	CCB-CDB-CEB-CFB
23	3	315	CLA	CAA-CBA-CGA-O2A
23	1	308	CLA	C15-C16-C17-C18
23	a	844	CLA	C15-C16-C17-C18
23	b	807	CLA	C10-C11-C12-C13
23	8	314	CLA	CBD-CGD-O2D-CED
23	a	819	CLA	C2A-CAA-CBA-CGA
27	4	318	DGD	C2D-C1D-O3G-C3G
25	6	301	A1L1F	C47-C48-C49-C50
23	b	832	CLA	C3-C5-C6-C7
23	b	833	CLA	C3-C5-C6-C7
23	h	204	CLA	C3-C5-C6-C7
26	b	847	LHG	C9-C10-C11-C12
26	b	847	LHG	O6-C4-C5-C6
22	9	306	A1L1G	C26-C30-C31-C32
23	8	307	CLA	C11-C10-C8-C7
23	4	308	CLA	C12-C13-C15-C16
23	4	310	CLA	C11-C10-C8-C7
23	6	309	CLA	C6-C7-C8-C10
23	1	308	CLA	C11-C12-C13-C15
23	a	807	CLA	C11-C12-C13-C15
23	a	809	CLA	C6-C7-C8-C10
23	a	812	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	814	CLA	C11-C12-C13-C15
23	a	827	CLA	C11-C10-C8-C7
23	a	829	CLA	C6-C7-C8-C10
23	a	835	CLA	C6-C7-C8-C10
23	a	842	CLA	C11-C12-C13-C15
23	a	844	CLA	C11-C10-C8-C7
23	b	801	CLA	C11-C12-C13-C15
23	b	803	CLA	C6-C7-C8-C10
23	b	803	CLA	C11-C10-C8-C7
23	b	803	CLA	C12-C13-C15-C16
23	b	808	CLA	C11-C10-C8-C7
23	b	810	CLA	C6-C7-C8-C10
23	b	828	CLA	C12-C13-C15-C16
23	b	829	CLA	C12-C13-C15-C16
23	b	836	CLA	C12-C13-C15-C16
23	b	837	CLA	C12-C13-C15-C16
23	b	838	CLA	C12-C13-C15-C16
23	j	102	CLA	C6-C7-C8-C10
23	a	812	CLA	C8-C10-C11-C12
26	a	845	LHG	C7-C8-C9-C10
23	4	311	CLA	C3A-C2A-CAA-CBA
23	3	315	CLA	C3A-C2A-CAA-CBA
23	2	314	CLA	C3A-C2A-CAA-CBA
23	a	804	CLA	C4-C3-C5-C6
23	a	820	CLA	C4-C3-C5-C6
23	a	829	CLA	C3A-C2A-CAA-CBA
23	a	840	CLA	C4-C3-C5-C6
23	b	803	CLA	C4-C3-C5-C6
23	j	102	CLA	C3A-C2A-CAA-CBA
23	a	828	CLA	C2-C3-C5-C6
23	a	835	CLA	O1A-CGA-O2A-C1
28	j	105	LMG	C28-C29-C30-C31
23	9	314	CLA	CBA-CGA-O2A-C1
26	9	307	LHG	C25-C26-C27-C28
22	9	306	A1L1G	C30-C31-C32-C33
22	3	306	A1L1G	C40-C41-C42-C44
22	7	302	A1L1G	C34-C35-C36-C37
23	b	801	CLA	C5-C6-C7-C8
21	5	301	XAT	C7-C8-C9-C19
21	4	305	XAT	C27-C28-C29-C39
22	9	306	A1L1G	C32-C33-C34-C27
23	4	307	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	826	CLA	O1D-CGD-O2D-CED
21	7	303	XAT	C7-C8-C9-C10
23	7	314	CLA	C2A-CAA-CBA-CGA
23	a	809	CLA	C2A-CAA-CBA-CGA
23	a	836	CLA	O1D-CGD-O2D-CED
24	1	315	SQD	O6-C44-C45-C46
26	a	846	LHG	C4-C5-C6-O8
28	2	317	LMG	O1-C7-C8-C9
23	b	812	CLA	C5-C6-C7-C8
23	b	835	CLA	C3-C5-C6-C7
23	a	805	CLA	C6-C7-C8-C10
23	b	818	CLA	C11-C12-C13-C15
23	j	102	CLA	C5-C6-C7-C8
23	a	828	CLA	C4-C3-C5-C6
23	b	813	CLA	C4-C3-C5-C6
23	a	801	CLA	C2-C3-C5-C6
23	b	807	CLA	C2-C3-C5-C6
23	a	827	CLA	C3-C5-C6-C7
23	4	308	CLA	C16-C17-C18-C19
23	1	310	CLA	C16-C17-C18-C20
27	b	848	DGD	O1B-C1B-O2G-C2G
23	3	307	CLA	C2B-C3B-CAB-CBB
23	6	315	CLA	C2B-C3B-CAB-CBB
23	7	317	CLA	C2B-C3B-CAB-CBB
23	1	309	CLA	C2B-C3B-CAB-CBB
23	a	825	CLA	C2B-C3B-CAB-CBB
23	a	837	CLA	C2B-C3B-CAB-CBB
23	a	841	CLA	C2B-C3B-CAB-CBB
23	b	817	CLA	C2B-C3B-CAB-CBB
23	j	102	CLA	C2B-C3B-CAB-CBB
30	b	843	BCR	C1-C6-C7-C8
30	m	101	BCR	C1-C6-C7-C8
23	a	830	CLA	C5-C6-C7-C8
26	9	307	LHG	C33-C34-C35-C36
23	a	806	CLA	C16-C17-C18-C20
23	b	822	CLA	C10-C11-C12-C13
26	a	845	LHG	C34-C35-C36-C37
23	b	807	CLA	C4-C3-C5-C6
22	9	306	A1L1G	C31-C32-C33-C34
23	5	309	CLA	C5-C6-C7-C8
23	a	820	CLA	C2-C3-C5-C6
23	b	813	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	6	301	A1L1F	C48-C49-C50-C51
23	a	820	CLA	C16-C17-C18-C19
23	4	317	CLA	C5-C6-C7-C8
23	a	803	CLA	C15-C16-C17-C18
23	6	316	CLA	O1D-CGD-O2D-CED
27	b	848	DGD	C7A-C8A-C9A-CAA
23	1	308	CLA	C11-C12-C13-C14
23	1	310	CLA	C6-C7-C8-C9
23	1	310	CLA	C11-C10-C8-C9
23	a	807	CLA	C14-C13-C15-C16
23	a	829	CLA	C6-C7-C8-C9
23	b	802	CLA	C11-C10-C8-C9
23	b	824	CLA	C11-C12-C13-C14
23	b	832	CLA	C14-C13-C15-C16
23	3	314	CLA	O1D-CGD-O2D-CED
23	a	841	CLA	O1A-CGA-O2A-C1
23	9	308	CLA	C16-C17-C18-C19
23	2	315	CLA	C1A-C2A-CAA-CBA
23	j	103	CLA	C1A-C2A-CAA-CBA
23	b	803	CLA	C13-C15-C16-C17
23	b	806	CLA	C10-C11-C12-C13
21	2	304	XAT	C33-C34-C35-C15
23	a	806	CLA	CBD-CGD-O2D-CED
25	1	304	A1L1F	C14-C29-C30-C31
23	b	811	CLA	O1A-CGA-O2A-C1
23	4	313	CLA	CBA-CGA-O2A-C1
26	9	317	LHG	O6-C4-C5-C6
26	a	846	LHG	O6-C4-C5-C6
23	a	854	CLA	C8-C10-C11-C12
21	6	302	XAT	C7-C8-C9-C19
22	3	306	A1L1G	C32-C33-C34-C27
25	h	203	A1L1F	C28-C39-C40-C41
23	9	308	CLA	C11-C12-C13-C15
23	9	318	CLA	C11-C10-C8-C7
23	8	309	CLA	C11-C10-C8-C7
23	1	306	CLA	C6-C7-C8-C10
23	a	801	CLA	C6-C7-C8-C10
23	a	802	CLA	C6-C7-C8-C10
23	a	814	CLA	C6-C7-C8-C10
23	a	820	CLA	C11-C12-C13-C15
23	a	829	CLA	C11-C10-C8-C7
23	b	813	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	824	CLA	C6-C7-C8-C10
23	b	832	CLA	C12-C13-C15-C16
23	4	310	CLA	C15-C16-C17-C18
23	b	838	CLA	C13-C15-C16-C17
21	6	302	XAT	C7-C8-C9-C10
22	7	302	A1L1G	C32-C33-C34-C35
23	b	827	CLA	C16-C17-C18-C20
26	b	847	LHG	O9-C7-O7-C5
23	a	807	CLA	C4-C3-C5-C6
23	b	810	CLA	CAA-CBA-CGA-O2A
23	3	314	CLA	O1A-CGA-O2A-C1
27	b	848	DGD	O1A-C1A-O1G-C1G
23	1	310	CLA	C2-C3-C5-C6
23	a	840	CLA	C2-C3-C5-C6
28	a	853	LMG	C12-C13-C14-C15
23	9	313	CLA	O1D-CGD-O2D-CED
23	b	807	CLA	C5-C6-C7-C8
23	b	828	CLA	C5-C6-C7-C8
28	a	853	LMG	C9-C8-O7-C10
23	1	306	CLA	O1A-CGA-O2A-C1
23	a	831	CLA	O1A-CGA-O2A-C1
23	b	828	CLA	O1A-CGA-O2A-C1
26	9	307	LHG	C32-C33-C34-C35
23	9	308	CLA	C16-C17-C18-C20
23	1	306	CLA	C16-C17-C18-C20
23	1	310	CLA	C16-C17-C18-C19
23	9	314	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	O1A-CGA-O2A-C1
23	9	318	CLA	CBA-CGA-O2A-C1
24	1	315	SQD	C9-C10-C11-C12
23	a	842	CLA	C8-C10-C11-C12
27	8	315	DGD	C1G-C2G-C3G-O3G
23	2	310	CLA	C16-C17-C18-C20
23	b	805	CLA	C16-C17-C18-C19
23	a	827	CLA	C5-C6-C7-C8
23	2	314	CLA	C2A-CAA-CBA-CGA
23	b	834	CLA	C2-C3-C5-C6
22	7	302	A1L1G	C45-C2-C44-C43
25	8	304	A1L1F	C57-C2-C44-C43
23	1	306	CLA	C3-C5-C6-C7
28	2	317	LMG	C31-C32-C33-C34
27	8	315	DGD	O2G-C2G-C3G-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	9	308	CLA	C11-C10-C8-C9
23	9	308	CLA	C11-C12-C13-C14
23	8	309	CLA	C11-C10-C8-C9
23	1	306	CLA	C11-C10-C8-C9
23	a	801	CLA	C6-C7-C8-C9
23	a	802	CLA	C6-C7-C8-C9
23	a	820	CLA	C11-C12-C13-C14
23	a	840	CLA	C11-C10-C8-C9
23	b	802	CLA	C6-C7-C8-C9
23	b	802	CLA	C11-C12-C13-C14
23	b	804	CLA	C6-C7-C8-C9
23	b	806	CLA	C6-C7-C8-C9
23	b	813	CLA	C11-C10-C8-C9
23	b	838	CLA	C11-C12-C13-C14
23	b	838	CLA	C14-C13-C15-C16
23	4	313	CLA	O1A-CGA-O2A-C1
26	a	845	LHG	C9-C10-C11-C12
23	a	841	CLA	C13-C15-C16-C17
23	a	808	CLA	O1D-CGD-O2D-CED
23	2	310	CLA	C16-C17-C18-C19
23	b	808	CLA	C16-C17-C18-C20
23	2	314	CLA	C4-C3-C5-C6
23	6	310	CLA	C2A-CAA-CBA-CGA
23	2	307	CLA	C2A-CAA-CBA-CGA
23	b	810	CLA	C16-C17-C18-C19
23	b	817	CLA	C10-C11-C12-C13
28	2	317	LMG	C33-C34-C35-C36
23	8	311	CLA	C3-C5-C6-C7
23	5	305	CLA	C4B-C3B-CAB-CBB
23	5	306	CLA	C4B-C3B-CAB-CBB
23	5	310	CLA	C4B-C3B-CAB-CBB
23	9	311	CLA	C4B-C3B-CAB-CBB
23	9	318	CLA	C4B-C3B-CAB-CBB
23	8	313	CLA	C4B-C3B-CAB-CBB
23	4	306	CLA	C4B-C3B-CAB-CBB
23	4	307	CLA	C4B-C3B-CAB-CBB
23	4	315	CLA	C4B-C3B-CAB-CBB
23	4	317	CLA	C4B-C3B-CAB-CBB
23	3	311	CLA	C1A-C2A-CAA-CBA
23	3	312	CLA	C4B-C3B-CAB-CBB
23	6	307	CLA	C4B-C3B-CAB-CBB
23	2	306	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	311	CLA	C4B-C3B-CAB-CBB
23	2	314	CLA	C1A-C2A-CAA-CBA
23	2	314	CLA	C4B-C3B-CAB-CBB
23	2	315	CLA	C4B-C3B-CAB-CBB
23	2	316	CLA	C4B-C3B-CAB-CBB
23	a	807	CLA	C4B-C3B-CAB-CBB
23	a	813	CLA	C4B-C3B-CAB-CBB
23	a	817	CLA	C4B-C3B-CAB-CBB
23	a	819	CLA	C4B-C3B-CAB-CBB
23	a	824	CLA	C1A-C2A-CAA-CBA
23	a	824	CLA	C4B-C3B-CAB-CBB
23	b	801	CLA	C4B-C3B-CAB-CBB
23	b	809	CLA	C4B-C3B-CAB-CBB
23	b	813	CLA	C1A-C2A-CAA-CBA
23	b	823	CLA	C1A-C2A-CAA-CBA
23	b	828	CLA	C4B-C3B-CAB-CBB
23	b	834	CLA	C4B-C3B-CAB-CBB
23	b	837	CLA	C4B-C3B-CAB-CBB
23	f	803	CLA	C4B-C3B-CAB-CBB
23	j	103	CLA	C4B-C3B-CAB-CBB
25	6	304	A1L1F	O13-C26-C30-C31
23	j	102	CLA	O1D-CGD-O2D-CED
21	5	301	XAT	C7-C8-C9-C10
25	h	203	A1L1F	C38-C39-C40-C41
23	b	802	CLA	C2A-CAA-CBA-CGA
23	b	808	CLA	C2A-CAA-CBA-CGA
23	b	818	CLA	C8-C10-C11-C12
23	7	313	CLA	CBD-CGD-O2D-CED
23	5	311	CLA	C2-C3-C5-C6
23	6	312	CLA	C2-C3-C5-C6
23	5	307	CLA	C11-C10-C8-C7
23	8	307	CLA	C6-C7-C8-C10
23	2	310	CLA	C11-C12-C13-C15
23	a	842	CLA	C12-C13-C15-C16
23	b	801	CLA	C11-C10-C8-C7
23	b	801	CLA	C12-C13-C15-C16
23	b	806	CLA	C11-C12-C13-C15
23	b	810	CLA	C11-C10-C8-C7
23	b	827	CLA	C11-C10-C8-C7
23	b	829	CLA	C11-C12-C13-C15
29	a	843	PQN	C22-C23-C25-C26
28	a	853	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	307	CLA	C5-C6-C7-C8
23	9	316	CLA	C3A-C2A-CAA-CBA
23	6	316	CLA	C3A-C2A-CAA-CBA
26	9	317	LHG	O6-C4-C5-O7
23	3	311	CLA	C2A-CAA-CBA-CGA
23	4	308	CLA	C14-C13-C15-C16
23	a	809	CLA	C6-C7-C8-C9
23	a	814	CLA	C6-C7-C8-C9
23	a	830	CLA	C8-C10-C11-C12
24	1	315	SQD	C13-C14-C15-C16
21	4	301	XAT	C29-C30-C31-C32
22	3	302	A1L1G	C36-C37-C38-C39
30	m	101	BCR	C13-C14-C15-C16
23	8	314	CLA	O1D-CGD-O2D-CED
25	8	304	A1L1F	C47-C48-C49-C50
23	a	823	CLA	C1-C2-C3-C4
23	b	831	CLA	C1-C2-C3-C4
23	a	806	CLA	O1D-CGD-O2D-CED
23	b	814	CLA	C3-C5-C6-C7
23	9	318	CLA	O1A-CGA-O2A-C1
24	5	316	SQD	O47-C45-C46-O48
24	1	315	SQD	O6-C44-C45-O47
26	a	846	LHG	O7-C5-C6-O8
26	b	847	LHG	O7-C5-C6-O8
23	4	312	CLA	CBA-CGA-O2A-C1
23	3	315	CLA	O1A-CGA-O2A-C1
23	7	312	CLA	O2A-C1-C2-C3
23	9	308	CLA	C10-C11-C12-C13
23	a	809	CLA	C10-C11-C12-C13
23	b	840	CLA	C15-C16-C17-C18
24	5	316	SQD	C44-C45-C46-O48
23	8	310	CLA	O1A-CGA-O2A-C1
22	9	301	A1L1G	O13-C26-C30-C31
23	9	313	CLA	CAD-CBD-CGD-O2D
23	8	309	CLA	CAD-CBD-CGD-O2D
23	8	314	CLA	CAD-CBD-CGD-O2D
23	1	313	CLA	CAD-CBD-CGD-O2D
23	a	814	CLA	CAD-CBD-CGD-O2D
23	a	839	CLA	CAD-CBD-CGD-O2D
23	a	844	CLA	CAD-CBD-CGD-O2D
23	b	832	CLA	CAD-CBD-CGD-O2D
23	b	836	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	311	CLA	CBA-CGA-O2A-C1
23	1	308	CLA	CBD-CGD-O2D-CED
23	8	309	CLA	C2A-CAA-CBA-CGA
23	b	824	CLA	C2A-CAA-CBA-CGA
26	a	846	LHG	C10-C11-C12-C13
21	6	306	XAT	C29-C30-C31-C32
21	7	301	XAT	C29-C30-C31-C32
21	j	101	XAT	C9-C10-C11-C12
22	3	302	A1L1G	C40-C41-C42-C44
22	1	301	A1L1G	C37-C38-C39-C28
23	5	313	CLA	CHA-CBD-CGD-O1D
23	5	313	CLA	CHA-CBD-CGD-O2D
23	9	313	CLA	CAD-CBD-CGD-O1D
23	9	315	CLA	CAD-CBD-CGD-O1D
23	8	309	CLA	CAD-CBD-CGD-O1D
23	8	314	CLA	CAD-CBD-CGD-O1D
23	4	314	CLA	CHA-CBD-CGD-O1D
23	4	314	CLA	CHA-CBD-CGD-O2D
23	4	315	CLA	CAD-CBD-CGD-O1D
23	6	310	CLA	CAD-CBD-CGD-O1D
23	6	311	CLA	CHA-CBD-CGD-O1D
23	2	307	CLA	CHA-CBD-CGD-O1D
23	7	309	CLA	CHA-CBD-CGD-O2D
23	7	309	CLA	CAD-CBD-CGD-O2D
23	1	313	CLA	CAD-CBD-CGD-O1D
23	a	806	CLA	CAD-CBD-CGD-O1D
23	a	814	CLA	CAD-CBD-CGD-O1D
23	a	828	CLA	CAD-CBD-CGD-O1D
23	a	839	CLA	CAD-CBD-CGD-O1D
23	a	844	CLA	CAD-CBD-CGD-O1D
23	b	821	CLA	CHA-CBD-CGD-O1D
23	b	832	CLA	CAD-CBD-CGD-O1D
23	b	835	CLA	CAD-CBD-CGD-O1D
23	b	836	CLA	CAD-CBD-CGD-O1D
23	f	802	CLA	CAD-CBD-CGD-O1D
23	f	803	CLA	CHA-CBD-CGD-O2D
23	j	102	CLA	CHA-CBD-CGD-O1D
23	j	102	CLA	CHA-CBD-CGD-O2D
26	9	317	LHG	C3-O3-P-O5
26	9	317	LHG	C3-O3-P-O6
26	9	317	LHG	C4-O6-P-O3
26	9	317	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	845	LHG	C3-O3-P-O5
26	a	846	LHG	C3-O3-P-O5
26	a	846	LHG	C4-O6-P-O3
26	a	846	LHG	C4-O6-P-O5
23	a	841	CLA	C4-C3-C5-C6
23	h	204	CLA	C4-C3-C5-C6
23	5	306	CLA	C2B-C3B-CAB-CBB
23	5	310	CLA	C2B-C3B-CAB-CBB
23	9	318	CLA	C2B-C3B-CAB-CBB
23	8	310	CLA	C2B-C3B-CAB-CBB
23	8	313	CLA	C2B-C3B-CAB-CBB
23	4	317	CLA	C2B-C3B-CAB-CBB
23	2	311	CLA	C2B-C3B-CAB-CBB
23	2	315	CLA	C2B-C3B-CAB-CBB
23	2	316	CLA	C2B-C3B-CAB-CBB
23	1	314	CLA	C2B-C3B-CAB-CBB
23	a	819	CLA	C2B-C3B-CAB-CBB
23	b	801	CLA	C2B-C3B-CAB-CBB
23	b	834	CLA	C2B-C3B-CAB-CBB
23	b	837	CLA	C2B-C3B-CAB-CBB
23	b	840	CLA	C2B-C3B-CAB-CBB
23	f	803	CLA	C2B-C3B-CAB-CBB
30	l	201	BCR	C1-C6-C7-C8
23	a	807	CLA	C2-C3-C5-C6
23	b	838	CLA	C2-C3-C5-C6
23	a	834	CLA	C5-C6-C7-C8
23	b	824	CLA	C8-C10-C11-C12
26	9	307	LHG	C2-C3-O3-P
23	1	308	CLA	C16-C17-C18-C19
23	b	808	CLA	C16-C17-C18-C19
23	b	839	CLA	C2C-C3C-CAC-CBC
23	2	308	CLA	C6-C7-C8-C9
23	b	803	CLA	C3-C5-C6-C7
23	b	822	CLA	C3-C5-C6-C7
26	9	317	LHG	C10-C11-C12-C13
24	1	315	SQD	C46-C45-O47-C7
23	a	830	CLA	C16-C17-C18-C19
23	b	805	CLA	CBA-CGA-O2A-C1
23	a	839	CLA	C15-C16-C17-C18
23	5	309	CLA	C6-C7-C8-C9
23	3	312	CLA	C6-C7-C8-C9
23	a	807	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	812	CLA	C6-C7-C8-C9
23	a	842	CLA	C14-C13-C15-C16
23	b	803	CLA	C14-C13-C15-C16
23	b	804	CLA	C11-C12-C13-C14
23	b	807	CLA	C11-C12-C13-C14
23	b	810	CLA	C11-C10-C8-C9
23	b	828	CLA	C14-C13-C15-C16
23	3	312	CLA	C6-C7-C8-C10
23	b	802	CLA	C11-C12-C13-C15
23	1	311	CLA	O1A-CGA-O2A-C1
23	b	805	CLA	O1A-CGA-O2A-C1
23	2	314	CLA	C2-C3-C5-C6
26	9	317	LHG	C13-C14-C15-C16
23	8	307	CLA	C16-C17-C18-C20
23	b	832	CLA	C2C-C3C-CAC-CBC
23	7	308	CLA	C8-C10-C11-C12
23	b	827	CLA	C10-C11-C12-C13
23	b	817	CLA	CBA-CGA-O2A-C1
22	3	306	A1L1G	C30-C31-C32-C33
23	3	308	CLA	CAA-CBA-CGA-O2A
23	1	305	CLA	C2A-CAA-CBA-CGA
23	1	308	CLA	C2A-CAA-CBA-CGA
23	a	821	CLA	C2A-CAA-CBA-CGA
23	b	817	CLA	O1A-CGA-O2A-C1
23	a	802	CLA	C4-C3-C5-C6
23	b	827	CLA	C16-C17-C18-C19
23	b	801	CLA	O1A-CGA-O2A-C1
23	a	801	CLA	CAA-CBA-CGA-O2A
23	1	311	CLA	O1D-CGD-O2D-CED
21	6	303	XAT	C11-C12-C13-C14
22	9	306	A1L1G	C32-C33-C34-C35
23	a	854	CLA	CBD-CGD-O2D-CED
26	b	847	LHG	C25-C26-C27-C28
23	4	317	CLA	C2A-CAA-CBA-CGA
23	a	813	CLA	C2A-CAA-CBA-CGA
23	b	827	CLA	C2A-CAA-CBA-CGA
22	1	301	A1L1G	C40-C41-C42-C44
24	5	316	SQD	C7-C8-C9-C10
23	a	841	CLA	C2-C3-C5-C6
23	b	801	CLA	CBA-CGA-O2A-C1
23	1	308	CLA	O1D-CGD-O2D-CED
23	a	801	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	826	CLA	C11-C10-C8-C9
23	b	827	CLA	C11-C10-C8-C9
29	a	843	PQN	C24-C23-C25-C26
23	9	309	CLA	C4B-C3B-CAB-CBB
23	3	314	CLA	C4B-C3B-CAB-CBB
23	a	832	CLA	C4B-C3B-CAB-CBB
23	b	830	CLA	C4B-C3B-CAB-CBB
23	a	830	CLA	C15-C16-C17-C18
23	b	803	CLA	C16-C17-C18-C20
23	a	813	CLA	CBA-CGA-O2A-C1
23	5	307	CLA	C8-C10-C11-C12
23	a	854	CLA	C15-C16-C17-C18
23	a	813	CLA	O1A-CGA-O2A-C1
23	2	309	CLA	C2A-CAA-CBA-CGA
23	5	315	CLA	CAA-CBA-CGA-O2A
23	a	802	CLA	C2-C3-C5-C6
23	b	802	CLA	C2-C3-C5-C6
23	6	317	CLA	C13-C15-C16-C17
22	9	301	A1L1G	C34-C35-C36-C37
22	7	302	A1L1G	C36-C37-C38-C39
23	a	830	CLA	C16-C17-C18-C20
23	a	826	CLA	C11-C10-C8-C7
23	a	831	CLA	C11-C10-C8-C7
23	b	802	CLA	C12-C13-C15-C16
23	b	807	CLA	C11-C12-C13-C15
23	f	802	CLA	C6-C7-C8-C10
23	3	312	CLA	CBA-CGA-O2A-C1
23	8	307	CLA	C16-C17-C18-C19
23	1	308	CLA	C16-C17-C18-C20
27	b	848	DGD	O2G-C2G-C3G-O3G
23	2	310	CLA	C3A-C2A-CAA-CBA
23	a	830	CLA	C4-C3-C5-C6
23	b	813	CLA	C3A-C2A-CAA-CBA
23	b	831	CLA	C3A-C2A-CAA-CBA
30	b	844	BCR	C11-C10-C9-C34
30	b	844	BCR	C20-C21-C22-C37
30	f	804	BCR	C35-C13-C14-C15
30	l	201	BCR	C11-C10-C9-C34
23	a	812	CLA	C3-C5-C6-C7
23	5	310	CLA	CAA-CBA-CGA-O1A
23	a	820	CLA	C13-C15-C16-C17
25	9	302	A1L1F	C3-C8-O7-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	5	306	CLA	CAA-CBA-CGA-O1A
23	7	308	CLA	C2-C1-O2A-CGA
25	h	203	A1L1F	C36-C37-C38-C39
23	b	839	CLA	C16-C17-C18-C20
21	7	303	XAT	C11-C12-C13-C20
23	8	312	CLA	CBD-CGD-O2D-CED
23	5	311	CLA	C4-C3-C5-C6
23	b	813	CLA	C10-C11-C12-C13
22	3	306	A1L1G	C32-C33-C34-C35
26	a	846	LHG	C1-C2-C3-O3
23	a	854	CLA	O1D-CGD-O2D-CED
23	9	314	CLA	C2A-CAA-CBA-CGA
26	a	845	LHG	C25-C26-C27-C28
23	5	307	CLA	C11-C10-C8-C9
23	1	310	CLA	C11-C12-C13-C14
23	a	822	CLA	C11-C10-C8-C9
23	a	829	CLA	C11-C12-C13-C14
23	a	831	CLA	C6-C7-C8-C9
23	a	831	CLA	C11-C10-C8-C9
23	a	844	CLA	C6-C7-C8-C9
23	a	854	CLA	C11-C10-C8-C9
23	b	808	CLA	C6-C7-C8-C9
23	a	839	CLA	C16-C17-C18-C20
23	8	305	CLA	CBD-CGD-O2D-CED
23	4	310	CLA	CBD-CGD-O2D-CED
23	a	832	CLA	CBD-CGD-O2D-CED
23	7	313	CLA	O1D-CGD-O2D-CED
23	3	312	CLA	O1A-CGA-O2A-C1
23	5	309	CLA	C2A-CAA-CBA-CGA
23	8	307	CLA	C2A-CAA-CBA-CGA
23	a	803	CLA	C2A-CAA-CBA-CGA
23	3	315	CLA	CAA-CBA-CGA-O1A
23	4	311	CLA	C1A-C2A-CAA-CBA
23	4	316	CLA	C1A-C2A-CAA-CBA
23	2	310	CLA	C1A-C2A-CAA-CBA
23	2	316	CLA	C1A-C2A-CAA-CBA
23	b	815	CLA	C1A-C2A-CAA-CBA
23	b	822	CLA	C1A-C2A-CAA-CBA
23	b	834	CLA	C1A-C2A-CAA-CBA
30	b	844	BCR	C11-C10-C9-C8
30	b	844	BCR	C20-C21-C22-C23
30	f	804	BCR	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	l	201	BCR	C11-C10-C9-C8
23	4	314	CLA	CAA-CBA-CGA-O1A
23	4	314	CLA	CAA-CBA-CGA-O2A
23	5	305	CLA	C2B-C3B-CAB-CBB
23	5	308	CLA	C2B-C3B-CAB-CBB
23	9	313	CLA	C2B-C3B-CAB-CBB
23	4	306	CLA	C2B-C3B-CAB-CBB
23	4	307	CLA	C2B-C3B-CAB-CBB
23	4	315	CLA	C2B-C3B-CAB-CBB
23	3	308	CLA	C2B-C3B-CAB-CBB
23	3	312	CLA	C2B-C3B-CAB-CBB
23	3	314	CLA	C2B-C3B-CAB-CBB
23	6	307	CLA	C2B-C3B-CAB-CBB
23	2	306	CLA	C2B-C3B-CAB-CBB
23	2	314	CLA	C2B-C3B-CAB-CBB
23	7	314	CLA	C2B-C3B-CAB-CBB
23	1	305	CLA	C2B-C3B-CAB-CBB
23	1	313	CLA	C2B-C3B-CAB-CBB
23	a	801	CLA	C2B-C3B-CAB-CBB
23	a	807	CLA	C2B-C3B-CAB-CBB
23	a	810	CLA	C2B-C3B-CAB-CBB
23	a	813	CLA	C2B-C3B-CAB-CBB
23	a	817	CLA	C2B-C3B-CAB-CBB
23	a	824	CLA	C2B-C3B-CAB-CBB
23	a	832	CLA	C2B-C3B-CAB-CBB
23	b	809	CLA	C2B-C3B-CAB-CBB
23	b	828	CLA	C2B-C3B-CAB-CBB
23	b	830	CLA	C2B-C3B-CAB-CBB
23	j	103	CLA	C2B-C3B-CAB-CBB
30	b	843	BCR	C5-C6-C7-C8
30	b	849	BCR	C23-C24-C25-C30
30	l	205	BCR	C1-C6-C7-C8
30	m	101	BCR	C5-C6-C7-C8
23	5	306	CLA	CAA-CBA-CGA-O2A
23	a	801	CLA	CBA-CGA-O2A-C1
23	b	840	CLA	CBA-CGA-O2A-C1
23	b	840	CLA	O1A-CGA-O2A-C1
23	b	808	CLA	C4-C3-C5-C6
23	a	801	CLA	O1A-CGA-O2A-C1
23	a	830	CLA	C2-C3-C5-C6
28	2	317	LMG	O9-C10-O7-C8
23	9	316	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	7	306	CLA	C2A-CAA-CBA-CGA
23	b	809	CLA	C2A-CAA-CBA-CGA
23	a	832	CLA	O1D-CGD-O2D-CED
23	5	313	CLA	CAA-CBA-CGA-O1A
23	a	817	CLA	CAA-CBA-CGA-O1A
23	8	312	CLA	O1D-CGD-O2D-CED
26	a	845	LHG	C14-C15-C16-C17
23	1	305	CLA	C3-C5-C6-C7
23	a	817	CLA	CAA-CBA-CGA-O2A
23	8	305	CLA	O1D-CGD-O2D-CED
26	9	317	LHG	C15-C16-C17-C18
23	2	314	CLA	C11-C10-C8-C7
23	6	317	CLA	C8-C10-C11-C12
21	6	302	XAT	C31-C32-C33-C40
21	7	301	XAT	C7-C8-C9-C19
23	1	307	CLA	C6-C7-C8-C9
23	7	307	CLA	CAA-CBA-CGA-O2A
23	b	808	CLA	C2-C3-C5-C6
28	2	317	LMG	C11-C10-O7-C8
23	b	839	CLA	C4C-C3C-CAC-CBC
23	6	310	CLA	C3-C5-C6-C7
23	5	313	CLA	CAA-CBA-CGA-O2A
23	7	317	CLA	CAA-CBA-CGA-O2A
23	b	837	CLA	C11-C12-C13-C14
28	a	853	LMG	C11-C12-C13-C14
23	b	817	CLA	CBD-CGD-O2D-CED
21	8	302	XAT	C9-C10-C11-C12
23	4	310	CLA	C13-C15-C16-C17
23	a	835	CLA	C4-C3-C5-C6
23	7	307	CLA	CAA-CBA-CGA-O1A
23	a	835	CLA	C2-C3-C5-C6
23	4	310	CLA	O1D-CGD-O2D-CED
23	5	307	CLA	C2A-CAA-CBA-CGA
23	5	314	CLA	C4-C3-C5-C6
23	b	833	CLA	C4-C3-C5-C6
24	1	315	SQD	C15-C16-C17-C18
23	a	826	CLA	C13-C15-C16-C17
23	9	313	CLA	C4B-C3B-CAB-CBB
23	8	306	CLA	C4B-C3B-CAB-CBB
23	4	310	CLA	C4B-C3B-CAB-CBB
23	a	810	CLA	C4B-C3B-CAB-CBB
23	a	842	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	819	CLA	CAA-CBA-CGA-O2A
23	a	804	CLA	O1A-CGA-O2A-C1
23	5	310	CLA	CBA-CGA-O2A-C1
23	1	314	CLA	CAA-CBA-CGA-O2A
23	1	306	CLA	C16-C17-C18-C19
25	6	304	A1L1F	C3-C8-O7-C54
23	a	830	CLA	O1A-CGA-O2A-C1
23	4	306	CLA	C2A-CAA-CBA-CGA
23	9	312	CLA	CAA-CBA-CGA-O2A
23	5	307	CLA	C11-C12-C13-C14
23	b	813	CLA	C16-C17-C18-C19
23	8	311	CLA	C6-C7-C8-C10
23	1	314	CLA	CAA-CBA-CGA-O1A
23	b	802	CLA	C10-C11-C12-C13
23	a	813	CLA	C6-C7-C8-C9
23	b	817	CLA	O1D-CGD-O2D-CED
23	7	317	CLA	CAA-CBA-CGA-O1A
23	a	828	CLA	C14-C13-C15-C16
23	a	839	CLA	C6-C7-C8-C9
23	a	840	CLA	C14-C13-C15-C16
23	b	806	CLA	C11-C12-C13-C14
23	b	829	CLA	C11-C12-C13-C14
23	2	314	CLA	O1A-CGA-O2A-C1
23	a	839	CLA	C2A-CAA-CBA-CGA
23	6	309	CLA	C2-C1-O2A-CGA
23	a	830	CLA	CBA-CGA-O2A-C1
23	a	842	CLA	CBA-CGA-O2A-C1
23	9	311	CLA	C3A-C2A-CAA-CBA
23	4	306	CLA	C3A-C2A-CAA-CBA
23	2	316	CLA	C3A-C2A-CAA-CBA
23	1	310	CLA	C3A-C2A-CAA-CBA
23	b	809	CLA	C3A-C2A-CAA-CBA
26	9	317	LHG	O1-C1-C2-C3
23	b	813	CLA	C13-C15-C16-C17
23	l	204	CLA	CAA-CBA-CGA-O2A
27	b	848	DGD	C1B-C2B-C3B-C4B
23	b	813	CLA	C5-C6-C7-C8
21	7	304	XAT	C9-C10-C11-C12
29	a	843	PQN	C18-C20-C21-C22
21	5	301	XAT	O4-C6-C7-C8
21	5	304	XAT	O24-C26-C27-C28
21	9	303	XAT	O24-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	8	301	XAT	O24-C26-C27-C28
21	4	301	XAT	O4-C6-C7-C8
21	4	305	XAT	O4-C6-C7-C8
21	3	303	XAT	O4-C6-C7-C8
21	6	305	XAT	O4-C6-C7-C8
21	6	306	XAT	O4-C6-C7-C8
21	2	301	XAT	O4-C6-C7-C8
21	2	305	XAT	O24-C26-C27-C28
21	7	305	XAT	O4-C6-C7-C8
21	7	305	XAT	O24-C26-C27-C28
22	3	302	A1L1G	C29-C14-C25-O15
28	j	105	LMG	C11-C12-C13-C14
23	b	833	CLA	C15-C16-C17-C18
23	9	316	CLA	C8-C10-C11-C12
23	a	804	CLA	CBA-CGA-O2A-C1
23	a	804	CLA	C6-C7-C8-C9
23	9	313	CLA	CAA-CBA-CGA-O2A
23	4	308	CLA	C3-C5-C6-C7
23	6	307	CLA	C2A-CAA-CBA-CGA
23	h	204	CLA	C2-C3-C5-C6
26	9	317	LHG	C35-C36-C37-C38
23	4	306	CLA	CAA-CBA-CGA-O2A
26	9	307	LHG	O7-C5-C6-O8
23	8	307	CLA	C6-C7-C8-C9
23	4	308	CLA	C6-C7-C8-C9
23	4	309	CLA	CAA-CBA-CGA-O2A
23	b	803	CLA	CAA-CBA-CGA-O2A
23	b	803	CLA	C10-C11-C12-C13
21	2	304	XAT	C7-C8-C9-C10
21	a	852	XAT	C31-C32-C33-C34
23	a	829	CLA	CAA-CBA-CGA-O2A
23	9	308	CLA	C2A-CAA-CBA-CGA
23	b	818	CLA	C2A-CAA-CBA-CGA
23	1	305	CLA	C11-C10-C8-C7
23	a	801	CLA	C11-C10-C8-C7
23	a	835	CLA	C11-C12-C13-C15
23	a	839	CLA	C6-C7-C8-C10
23	a	840	CLA	C12-C13-C15-C16
23	b	837	CLA	C11-C12-C13-C15
23	4	312	CLA	O1A-CGA-O2A-C1
23	9	309	CLA	C2B-C3B-CAB-CBB
23	8	306	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	6	308	CLA	C2B-C3B-CAB-CBB
23	6	316	CLA	C2B-C3B-CAB-CBB
23	b	818	CLA	C2B-C3B-CAB-CBB
30	b	846	BCR	C1-C6-C7-C8
30	b	846	BCR	C5-C6-C7-C8
30	b	849	BCR	C23-C24-C25-C26
30	f	804	BCR	C23-C24-C25-C26
30	f	804	BCR	C23-C24-C25-C30
30	l	201	BCR	C5-C6-C7-C8
30	l	205	BCR	C5-C6-C7-C8
23	b	837	CLA	CAA-CBA-CGA-O2A
23	5	311	CLA	C2-C1-O2A-CGA
23	7	306	CLA	C2-C1-O2A-CGA
23	a	814	CLA	C2-C1-O2A-CGA
23	a	822	CLA	C2-C1-O2A-CGA
23	b	810	CLA	C2-C1-O2A-CGA
23	b	824	CLA	C10-C11-C12-C13
23	1	306	CLA	CAA-CBA-CGA-O2A
23	1	309	CLA	CAA-CBA-CGA-O2A
23	a	818	CLA	CAA-CBA-CGA-O2A
23	b	835	CLA	C4C-C3C-CAC-CBC
25	9	302	A1L1F	O13-C26-C30-C29
25	6	304	A1L1F	O13-C26-C30-C29
23	a	827	CLA	C10-C11-C12-C13
23	3	313	CLA	C4-C3-C5-C6
23	b	801	CLA	CAA-CBA-CGA-O2A
25	9	302	A1L1F	C50-C51-C52-C53
23	4	308	CLA	C2A-CAA-CBA-CGA
23	2	308	CLA	C2A-CAA-CBA-CGA
23	j	102	CLA	C3-C5-C6-C7
24	1	315	SQD	O47-C7-C8-C9
24	5	316	SQD	C4-C5-C6-S
25	h	203	A1L1F	C14-C29-C30-C31
23	2	314	CLA	CBA-CGA-O2A-C1
23	b	807	CLA	CAA-CBA-CGA-O2A
23	6	309	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C12-C13-C14
23	b	803	CLA	C5-C6-C7-C8
28	j	105	LMG	C7-C8-C9-O8
23	9	311	CLA	C1A-C2A-CAA-CBA
23	4	316	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	3	315	CLA	C4B-C3B-CAB-CBB
23	a	803	CLA	C1A-C2A-CAA-CBA
23	a	814	CLA	C1A-C2A-CAA-CBA
23	a	840	CLA	C4B-C3B-CAB-CBB
23	b	803	CLA	C4B-C3B-CAB-CBB
23	b	825	CLA	C1A-C2A-CAA-CBA
23	4	306	CLA	CAA-CBA-CGA-O1A
23	b	838	CLA	C3-C5-C6-C7
23	8	308	CLA	C4-C3-C5-C6
27	8	315	DGD	O6D-C1D-O3G-C3G
30	m	101	BCR	C22-C23-C24-C25
23	a	810	CLA	CAA-CBA-CGA-O2A
25	6	304	A1L1F	O13-C45-C47-C48
30	f	801	BCR	C17-C18-C19-C20
23	b	807	CLA	C16-C17-C18-C19
23	b	810	CLA	CAA-CBA-CGA-O1A
25	8	304	A1L1F	C3-C8-O7-C54
23	a	836	CLA	CAA-CBA-CGA-O2A
23	h	204	CLA	CAA-CBA-CGA-O2A
23	a	829	CLA	C2A-CAA-CBA-CGA
23	a	841	CLA	C2A-CAA-CBA-CGA
26	9	317	LHG	C27-C28-C29-C30
23	b	819	CLA	C6-C7-C8-C9
23	b	809	CLA	CAA-CBA-CGA-O2A
23	b	817	CLA	CAA-CBA-CGA-O2A
23	7	316	CLA	C2-C3-C5-C6
23	6	312	CLA	C2-C1-O2A-CGA
23	a	810	CLA	C2-C1-O2A-CGA
23	1	312	CLA	CAA-CBA-CGA-O2A
23	b	832	CLA	CAA-CBA-CGA-O2A
23	6	308	CLA	C6-C7-C8-C10
23	1	310	CLA	C12-C13-C15-C16
23	a	801	CLA	C11-C12-C13-C15
23	a	834	CLA	C11-C12-C13-C15
23	b	805	CLA	C11-C12-C13-C15
23	b	818	CLA	C11-C10-C8-C7
23	l	203	CLA	C6-C7-C8-C10
23	a	826	CLA	C10-C11-C12-C13
23	b	810	CLA	C16-C17-C18-C20
26	9	307	LHG	C6-C5-O7-C7
23	9	315	CLA	C2C-C3C-CAC-CBC
23	a	834	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	9	317	LHG	C30-C31-C32-C33
23	j	102	CLA	CAA-CBA-CGA-O2A
26	a	845	LHG	O8-C23-C24-C25
23	b	837	CLA	CAA-CBA-CGA-O1A
23	j	102	CLA	C10-C11-C12-C13
23	5	309	CLA	C15-C16-C17-C18
23	4	310	CLA	C8-C10-C11-C12
23	a	801	CLA	C5-C6-C7-C8
23	9	312	CLA	C3A-C2A-CAA-CBA
23	1	306	CLA	C3A-C2A-CAA-CBA
23	a	814	CLA	C3A-C2A-CAA-CBA
23	a	810	CLA	C16-C17-C18-C20
23	a	814	CLA	C16-C17-C18-C19
22	3	306	A1L1G	C14-C29-C30-C31
25	6	301	A1L1F	O13-C45-C47-C48
23	b	817	CLA	CAA-CBA-CGA-O1A
23	a	818	CLA	CAA-CBA-CGA-O1A
23	b	801	CLA	CAA-CBA-CGA-O1A
23	6	308	CLA	C6-C7-C8-C9
23	a	834	CLA	C11-C12-C13-C14
23	f	802	CLA	C6-C7-C8-C9
23	3	312	CLA	CAA-CBA-CGA-O2A
23	4	309	CLA	CAA-CBA-CGA-O1A
24	1	315	SQD	O49-C7-C8-C9
23	9	314	CLA	C4-C3-C5-C6
24	5	316	SQD	O5-C5-C6-S
23	7	309	CLA	O1A-CGA-O2A-C1
25	9	302	A1L1F	O46-C45-O13-C26
23	b	824	CLA	C15-C16-C17-C18
21	6	302	XAT	C31-C32-C33-C34
21	7	301	XAT	C7-C8-C9-C10
30	i	101	BCR	C17-C18-C19-C20
23	b	807	CLA	CAA-CBA-CGA-O1A
23	b	832	CLA	CAA-CBA-CGA-O1A
23	3	309	CLA	C2A-CAA-CBA-CGA
23	7	308	CLA	C2A-CAA-CBA-CGA
24	5	316	SQD	C10-C11-C12-C13
23	b	809	CLA	CAA-CBA-CGA-O1A
25	6	304	A1L1F	O46-C45-C47-C48
23	b	824	CLA	C4-C3-C5-C6
23	9	314	CLA	CAA-CBA-CGA-O2A
23	6	316	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	813	CLA	CAA-CBA-CGA-O2A
23	1	312	CLA	CAA-CBA-CGA-O1A
23	h	204	CLA	CAA-CBA-CGA-O1A
22	3	306	A1L1G	O13-C26-C30-C31
23	5	314	CLA	CAD-CBD-CGD-O2D
23	9	309	CLA	CAD-CBD-CGD-O2D
23	8	313	CLA	CAD-CBD-CGD-O2D
23	4	310	CLA	CAD-CBD-CGD-O2D
23	3	310	CLA	CAD-CBD-CGD-O2D
23	6	315	CLA	CAD-CBD-CGD-O2D
23	7	306	CLA	CAD-CBD-CGD-O2D
23	a	810	CLA	CAD-CBD-CGD-O2D
23	a	816	CLA	CAD-CBD-CGD-O2D
23	a	828	CLA	CAD-CBD-CGD-O2D
23	a	832	CLA	CAD-CBD-CGD-O2D
23	a	854	CLA	CAD-CBD-CGD-O2D
23	b	835	CLA	CAD-CBD-CGD-O2D
23	a	836	CLA	CAA-CBA-CGA-O1A
23	a	816	CLA	C2-C1-O2A-CGA
23	a	839	CLA	C2-C1-O2A-CGA
23	7	308	CLA	CAA-CBA-CGA-O2A
23	7	316	CLA	CAA-CBA-CGA-O2A
23	a	826	CLA	C8-C10-C11-C12
23	b	829	CLA	O1A-CGA-O2A-C1
23	7	309	CLA	CBA-CGA-O2A-C1
23	b	804	CLA	CAA-CBA-CGA-O2A
23	a	813	CLA	CBD-CGD-O2D-CED
23	b	813	CLA	CBD-CGD-O2D-CED
23	j	102	CLA	CAA-CBA-CGA-O1A
23	7	308	CLA	C5-C6-C7-C8
24	1	315	SQD	C12-C13-C14-C15
23	7	310	CLA	CAA-CBA-CGA-O2A
23	a	835	CLA	CAA-CBA-CGA-O2A
25	9	302	A1L1F	C47-C45-O13-C26

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	h	203	A1L1F	C1-C11-C3-C4-C6-C8

232 monomers are involved in 691 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	303	A1L1G	1	0
26	a	846	LHG	3	0
23	a	801	CLA	6	0
23	8	313	CLA	3	0
23	a	805	CLA	1	0
23	5	310	CLA	2	0
25	9	302	A1L1F	2	0
26	b	847	LHG	1	0
24	1	315	SQD	3	0
30	l	201	BCR	3	0
21	3	301	XAT	7	0
23	a	833	CLA	2	0
25	6	301	A1L1F	2	0
23	b	829	CLA	4	0
21	5	301	XAT	3	0
23	9	311	CLA	2	0
23	b	812	CLA	4	0
23	9	316	CLA	7	0
30	b	846	BCR	2	0
23	b	821	CLA	2	0
23	a	807	CLA	4	0
23	3	308	CLA	2	0
23	9	312	CLA	4	0
23	b	804	CLA	4	0
23	5	314	CLA	2	0
23	b	817	CLA	8	0
28	j	105	LMG	7	0
29	a	843	PQN	3	0
23	a	803	CLA	4	0
23	4	306	CLA	2	0
23	5	309	CLA	3	0
23	a	804	CLA	4	0
23	a	806	CLA	8	0
23	b	818	CLA	3	0
24	5	316	SQD	1	0
23	b	830	CLA	5	0
23	a	814	CLA	3	0
21	7	304	XAT	9	0
23	a	816	CLA	2	0
30	b	842	BCR	5	0
23	7	307	CLA	2	0
27	b	848	DGD	6	0
30	f	804	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	845	LHG	3	0
23	6	313	CLA	2	0
23	6	314	CLA	1	0
22	9	306	A1L1G	1	0
23	1	311	CLA	2	0
30	i	101	BCR	3	0
23	f	802	CLA	2	0
23	a	838	CLA	1	0
23	a	828	CLA	4	0
31	c	102	SF4	3	0
23	3	312	CLA	2	0
30	h	202	BCR	4	0
23	b	808	CLA	1	0
23	2	308	CLA	4	0
23	b	824	CLA	6	0
23	a	809	CLA	3	0
23	b	831	CLA	2	0
23	4	314	CLA	1	0
23	3	310	CLA	1	0
23	6	317	CLA	4	0
23	a	837	CLA	1	0
30	m	101	BCR	1	0
23	4	309	CLA	3	0
23	4	315	CLA	1	0
21	3	303	XAT	2	0
30	a	848	BCR	4	0
23	8	311	CLA	3	0
21	2	305	XAT	3	0
21	9	303	XAT	8	0
21	a	852	XAT	4	0
23	a	830	CLA	5	0
21	6	302	XAT	4	0
23	b	801	CLA	3	0
26	9	317	LHG	4	0
21	9	305	XAT	3	0
21	3	304	XAT	5	0
23	1	306	CLA	6	0
23	b	803	CLA	3	0
23	b	823	CLA	6	0
23	j	103	CLA	2	0
30	b	844	BCR	6	0
23	b	805	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	837	CLA	4	0
23	a	822	CLA	5	0
30	f	801	BCR	8	0
23	8	314	CLA	1	0
30	b	843	BCR	2	0
21	1	303	XAT	2	0
23	7	314	CLA	3	0
23	2	307	CLA	1	0
23	a	840	CLA	6	0
30	b	849	BCR	5	0
23	9	315	CLA	1	0
30	a	849	BCR	3	0
21	8	303	XAT	7	0
23	a	819	CLA	5	0
23	4	307	CLA	1	0
27	8	315	DGD	2	0
21	2	304	XAT	2	0
23	a	826	CLA	7	0
23	5	307	CLA	7	0
21	6	306	XAT	3	0
23	9	310	CLA	2	0
23	8	305	CLA	5	0
23	b	825	CLA	3	0
23	a	820	CLA	7	0
21	4	303	XAT	9	0
29	b	841	PQN	2	0
23	b	833	CLA	4	0
23	7	306	CLA	2	0
25	h	203	A1L1F	4	0
23	a	802	CLA	5	0
23	9	309	CLA	1	0
21	4	305	XAT	4	0
23	a	839	CLA	5	0
23	h	204	CLA	3	0
23	8	312	CLA	2	0
21	3	305	XAT	4	0
23	4	310	CLA	5	0
23	3	309	CLA	1	0
21	5	304	XAT	5	0
23	a	841	CLA	7	0
23	4	308	CLA	7	0
23	b	826	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	l	205	BCR	9	0
23	b	806	CLA	2	0
23	a	842	CLA	3	0
23	6	315	CLA	3	0
23	b	802	CLA	3	0
23	9	308	CLA	6	0
22	7	302	A1L1G	2	0
21	7	301	XAT	5	0
23	b	822	CLA	6	0
23	5	311	CLA	1	0
23	5	315	CLA	1	0
23	b	813	CLA	6	0
25	1	304	A1L1F	2	0
23	7	312	CLA	1	0
21	1	302	XAT	3	0
23	b	820	CLA	3	0
23	9	318	CLA	6	0
21	4	301	XAT	5	0
23	a	810	CLA	4	0
23	2	316	CLA	2	0
23	2	310	CLA	2	0
23	a	829	CLA	5	0
25	8	304	A1L1F	2	0
23	4	317	CLA	6	0
22	1	301	A1L1G	1	0
23	b	836	CLA	6	0
23	b	839	CLA	2	0
30	a	847	BCR	4	0
21	2	301	XAT	2	0
23	1	305	CLA	1	0
21	4	304	XAT	3	0
21	7	303	XAT	13	0
23	7	315	CLA	2	0
22	9	301	A1L1G	2	0
23	5	308	CLA	1	0
28	a	853	LMG	11	0
23	7	316	CLA	2	0
23	9	314	CLA	8	0
21	j	101	XAT	5	0
21	8	301	XAT	3	0
21	7	305	XAT	2	0
23	5	312	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	823	CLA	3	0
23	a	813	CLA	1	0
30	h	201	BCR	2	0
23	9	313	CLA	3	0
21	4	302	XAT	6	0
23	a	808	CLA	1	0
23	a	824	CLA	1	0
23	a	825	CLA	5	0
23	b	811	CLA	3	0
23	4	316	CLA	1	0
23	b	832	CLA	3	0
23	b	840	CLA	5	0
23	7	313	CLA	4	0
23	6	308	CLA	4	0
23	a	831	CLA	5	0
23	a	827	CLA	3	0
23	8	308	CLA	2	0
23	4	311	CLA	1	0
26	9	307	LHG	2	0
23	8	309	CLA	1	0
23	b	827	CLA	4	0
21	6	303	XAT	7	0
30	b	845	BCR	8	0
23	a	854	CLA	2	0
23	b	828	CLA	4	0
25	6	304	A1L1F	4	0
28	2	317	LMG	3	0
23	1	312	CLA	2	0
23	a	818	CLA	11	0
23	b	816	CLA	6	0
23	b	819	CLA	2	0
21	5	302	XAT	8	0
21	6	305	XAT	6	0
23	1	203	CLA	2	0
23	4	313	CLA	3	0
21	9	304	XAT	6	0
23	7	308	CLA	7	0
23	b	809	CLA	3	0
23	b	838	CLA	4	0
30	j	104	BCR	10	0
23	3	311	CLA	1	0
21	8	302	XAT	7	0

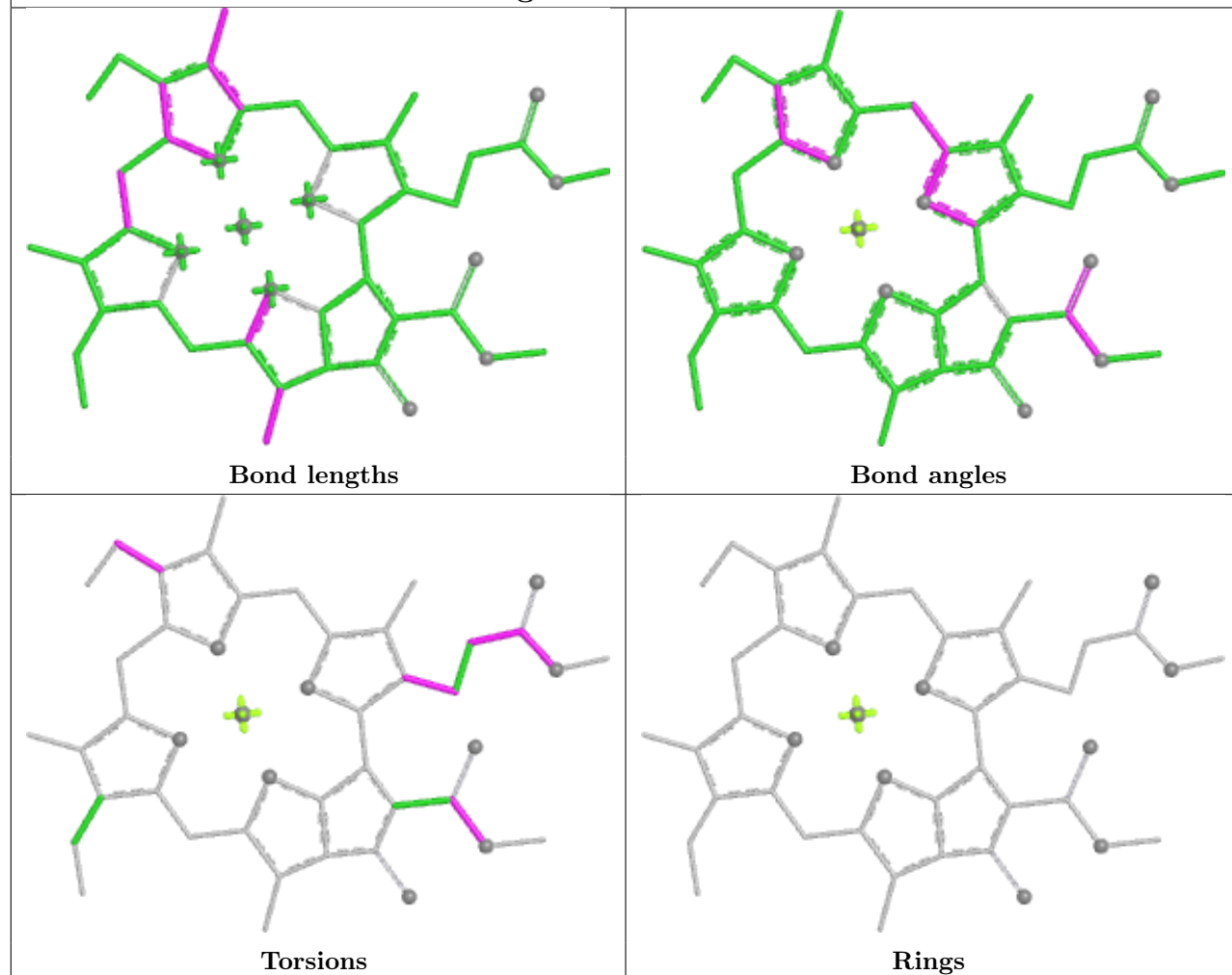
Continued on next page...

Continued from previous page...

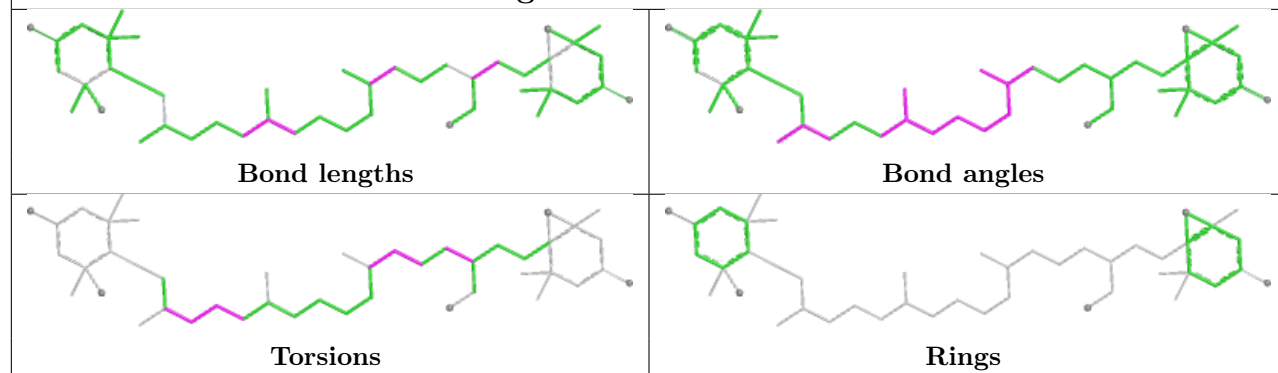
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1	308	CLA	4	0
23	8	307	CLA	6	0
23	2	314	CLA	1	0
23	a	832	CLA	2	0
23	b	835	CLA	5	0
23	j	102	CLA	7	0
23	l	202	CLA	1	0
23	8	306	CLA	1	0
23	b	807	CLA	6	0
23	a	844	CLA	5	0
23	4	312	CLA	1	0
30	a	850	BCR	3	0
23	a	835	CLA	5	0
21	2	303	XAT	11	0
23	b	814	CLA	3	0
27	4	318	DGD	11	0
23	3	313	CLA	3	0
23	5	305	CLA	3	0
23	a	834	CLA	6	0
21	2	302	XAT	1	0
23	7	311	CLA	3	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.

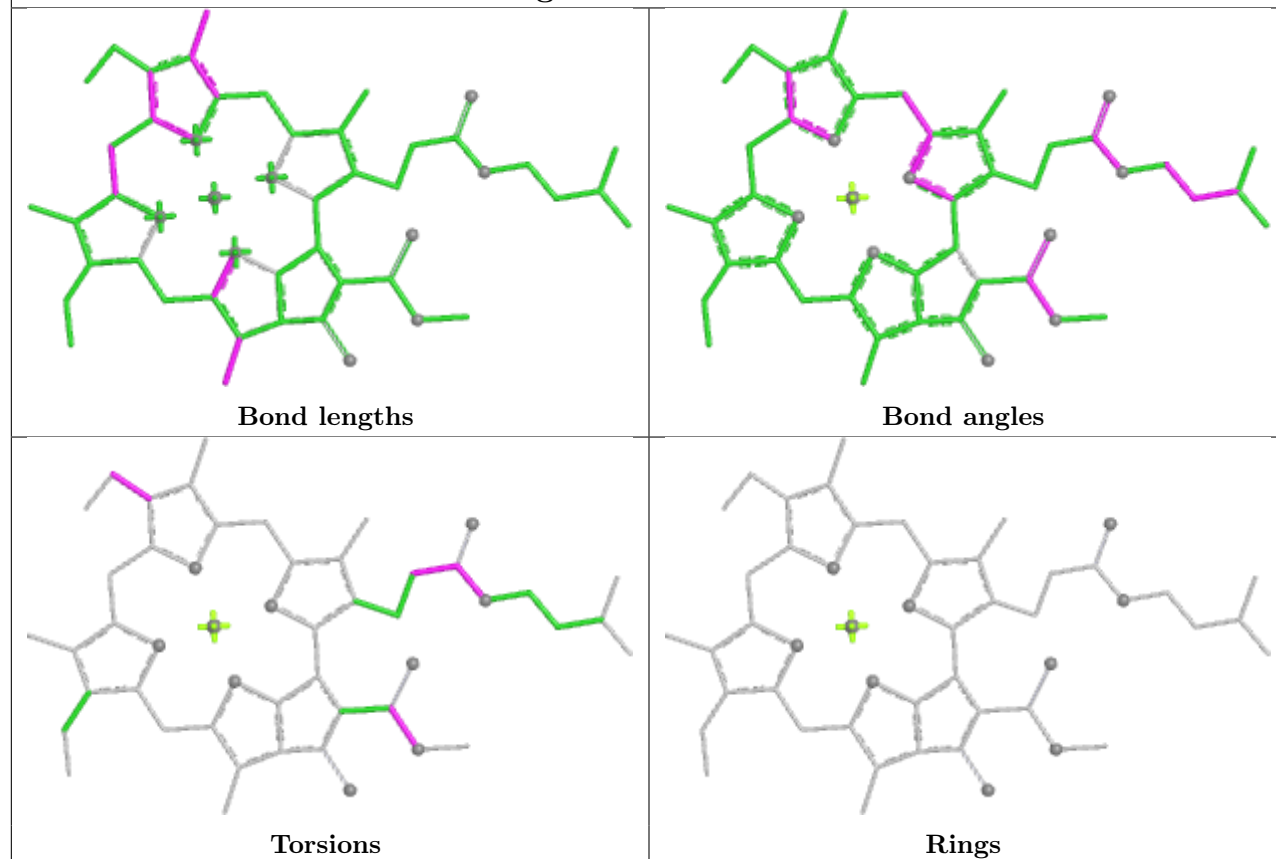
Ligand CLA 6 316



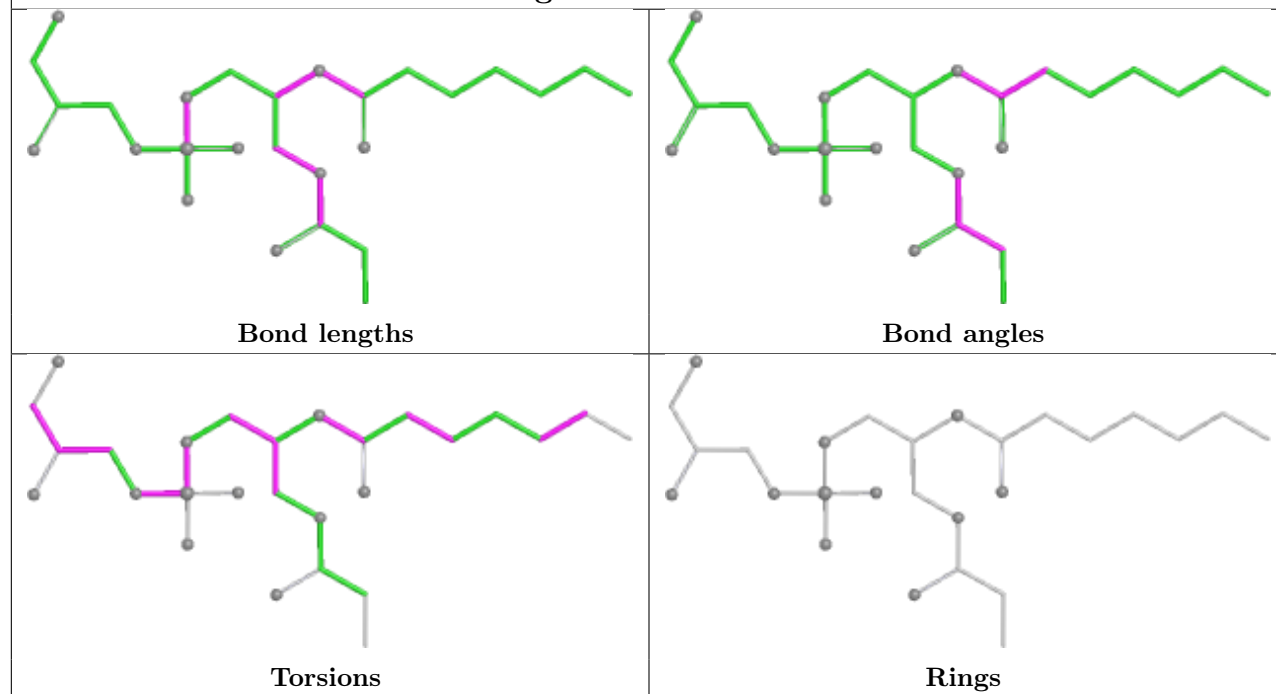
Ligand A1L1G 5 303



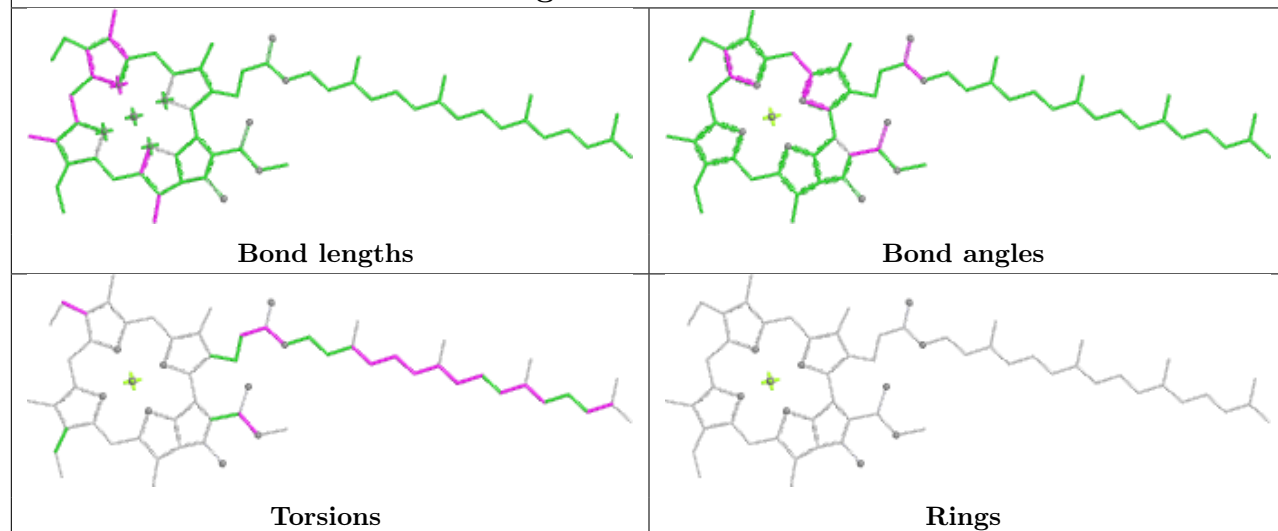
Ligand CLA a 836



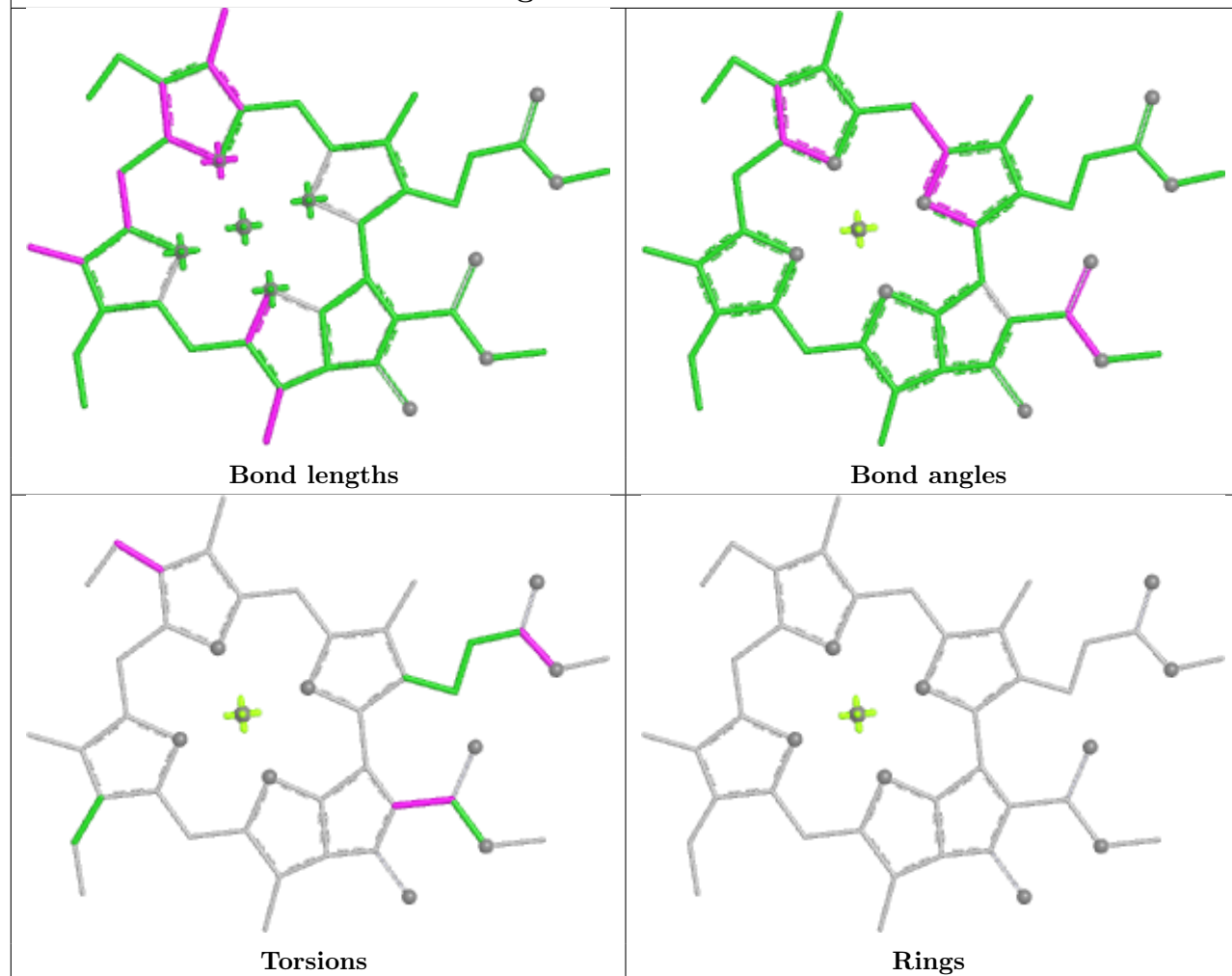
Ligand LHG a 846

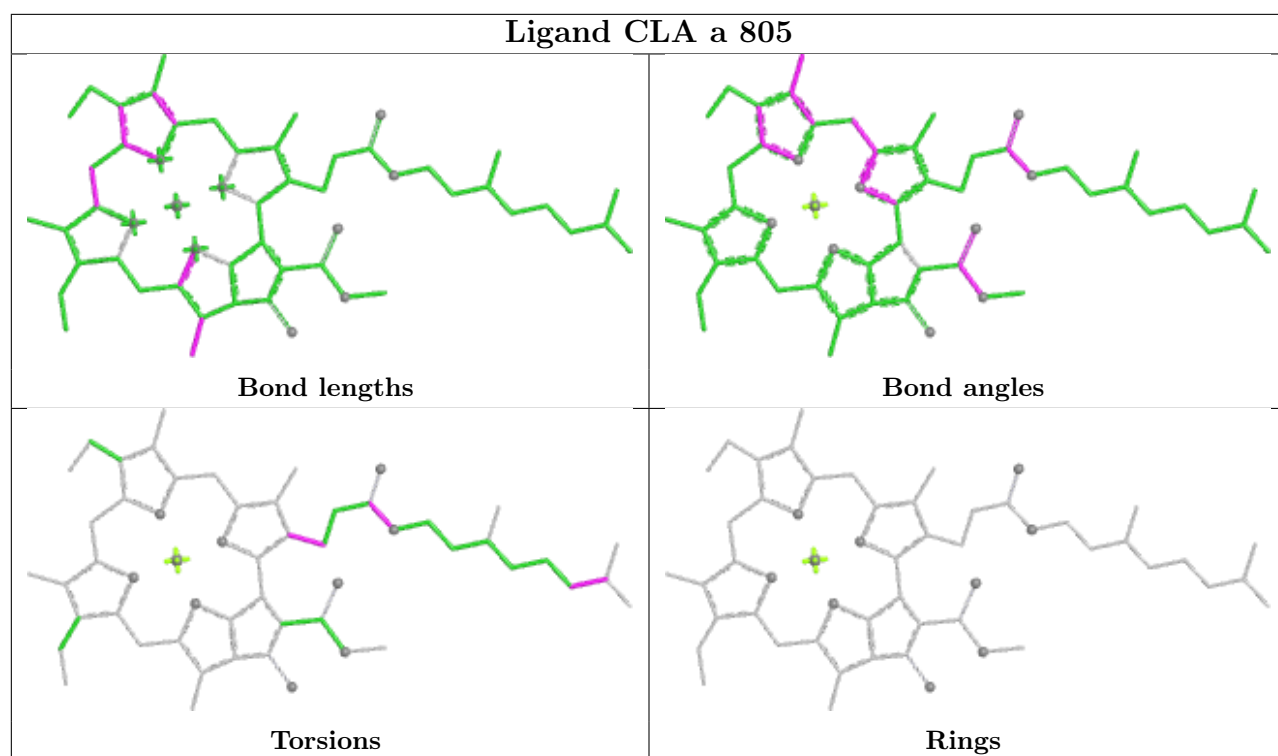


Ligand CLA a 801

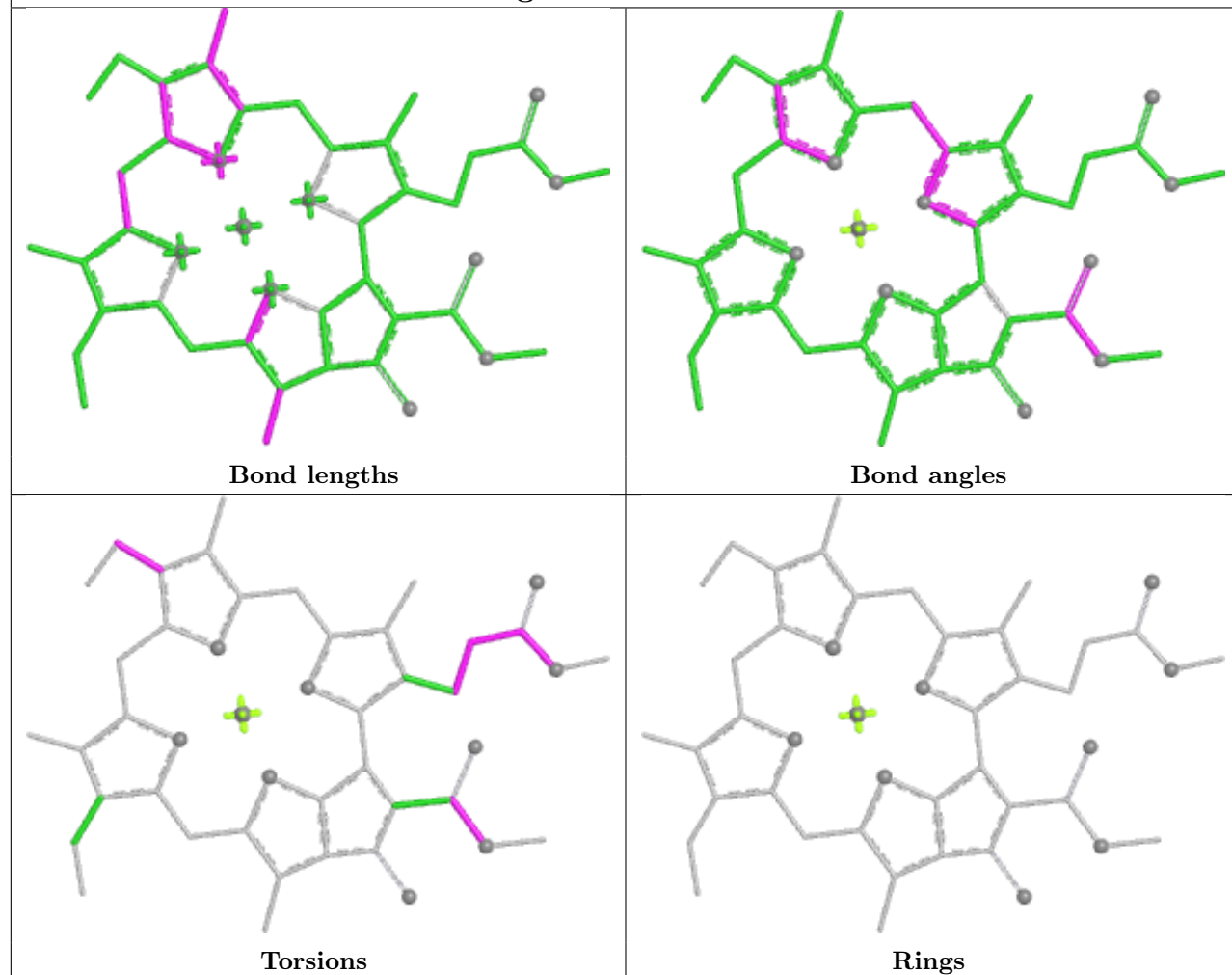


Ligand CLA 8 313

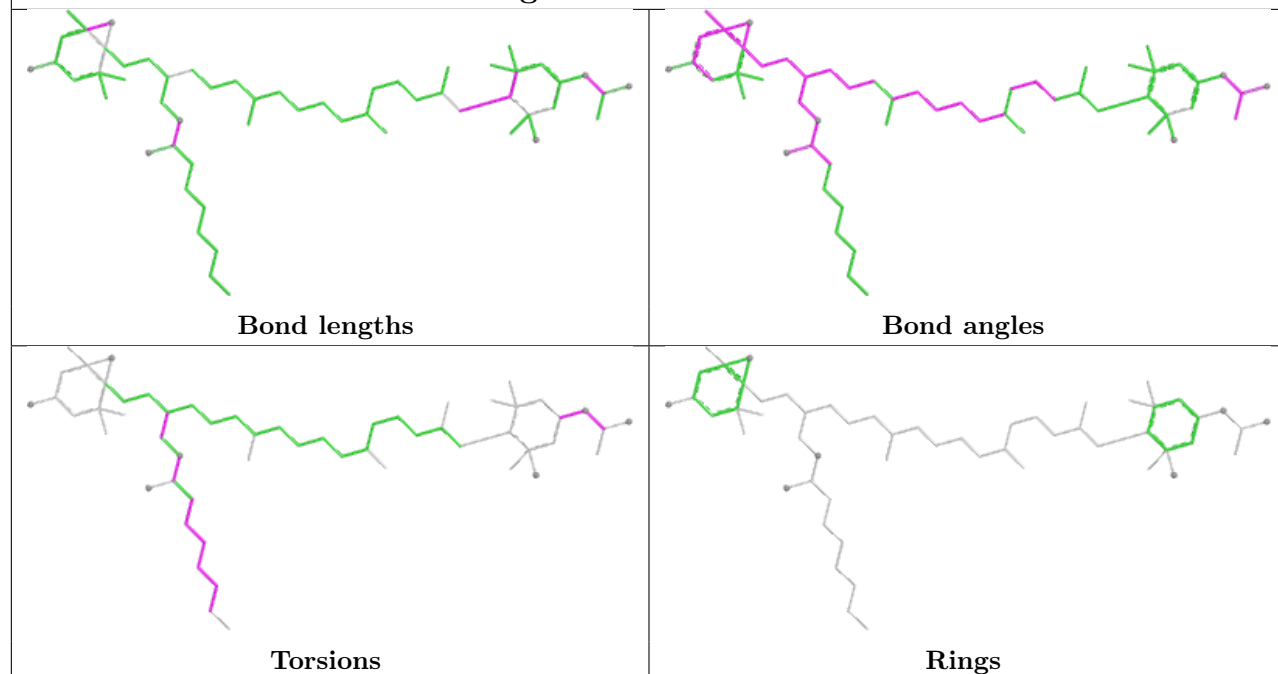


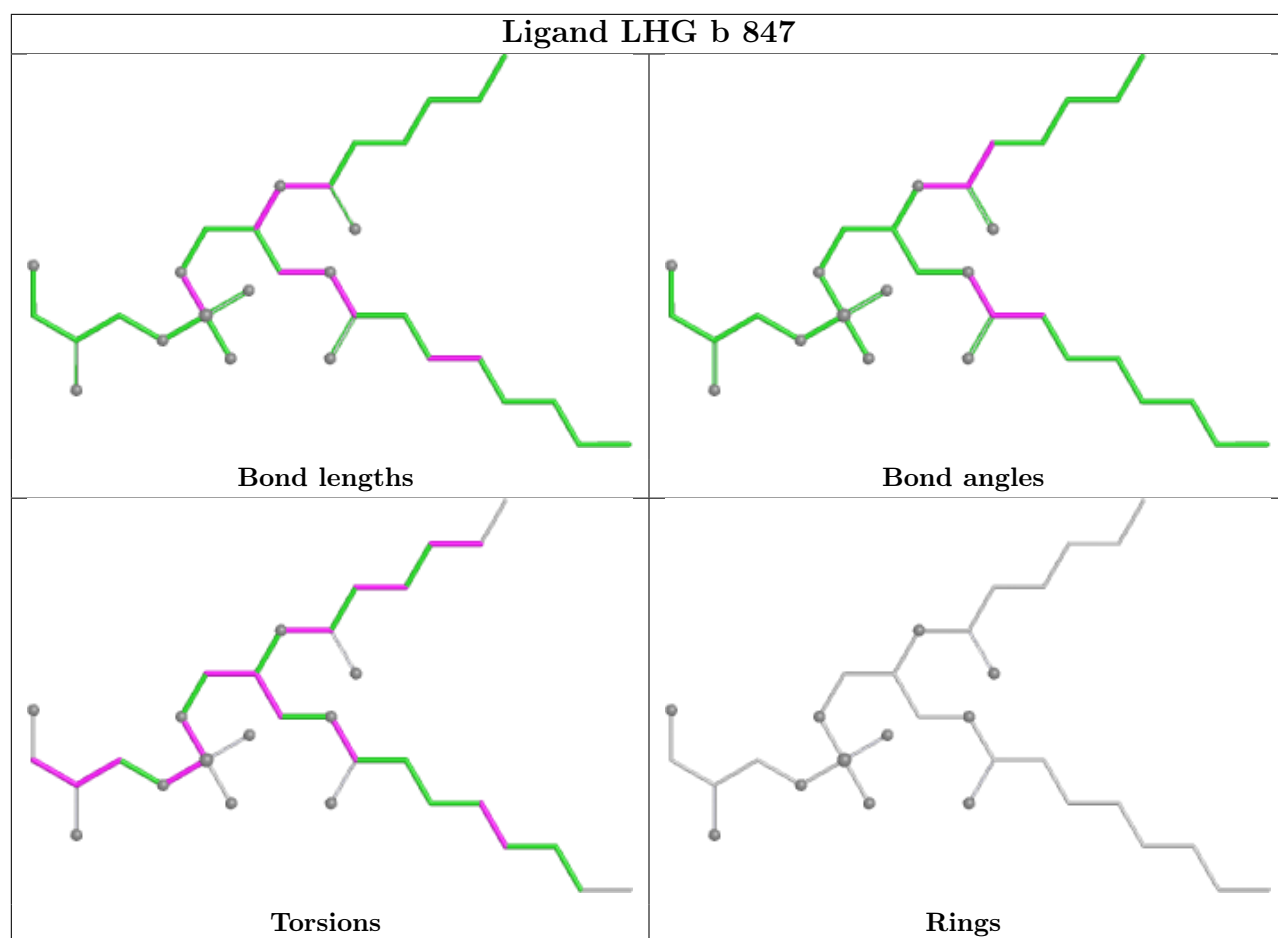


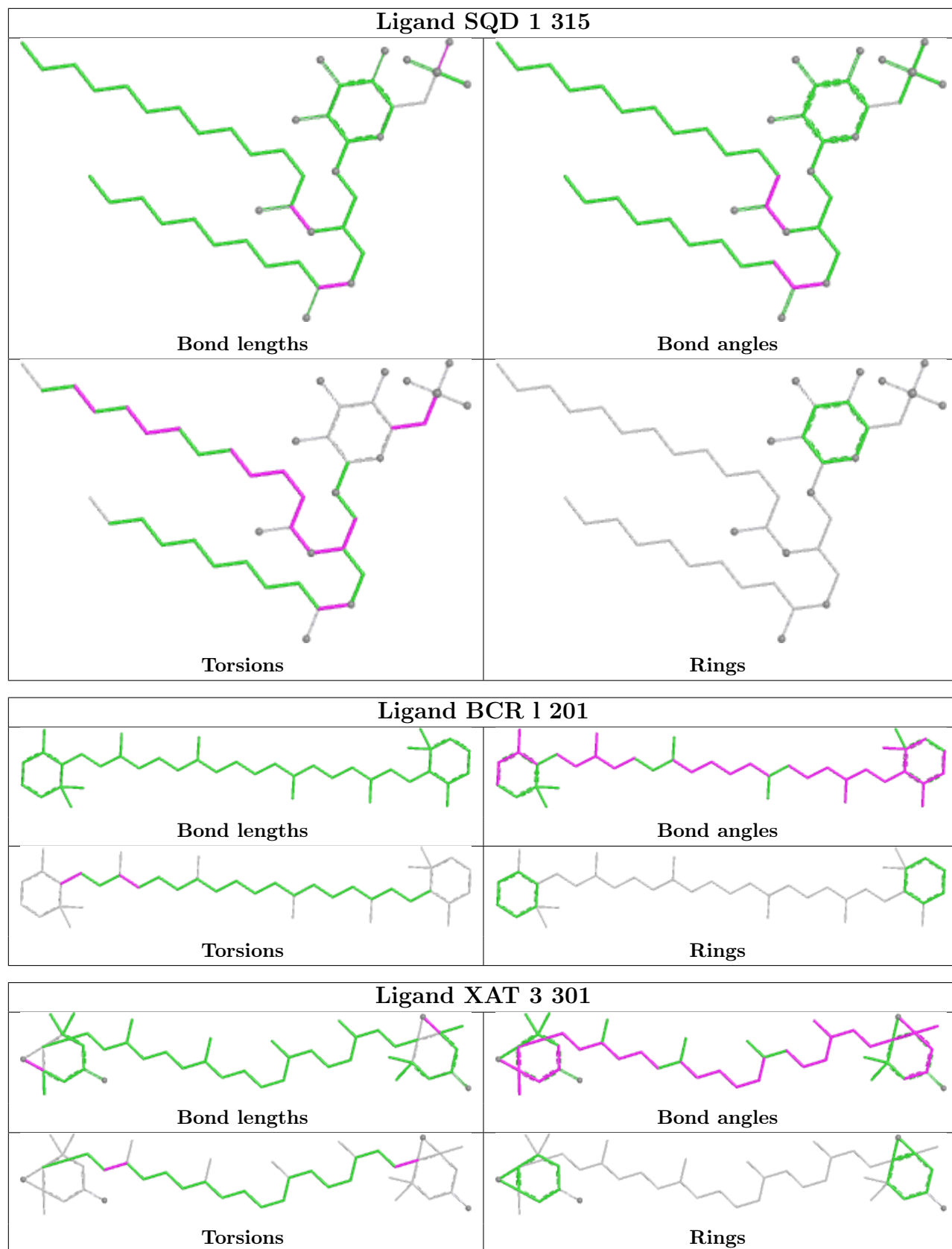
Ligand CLA 5 310



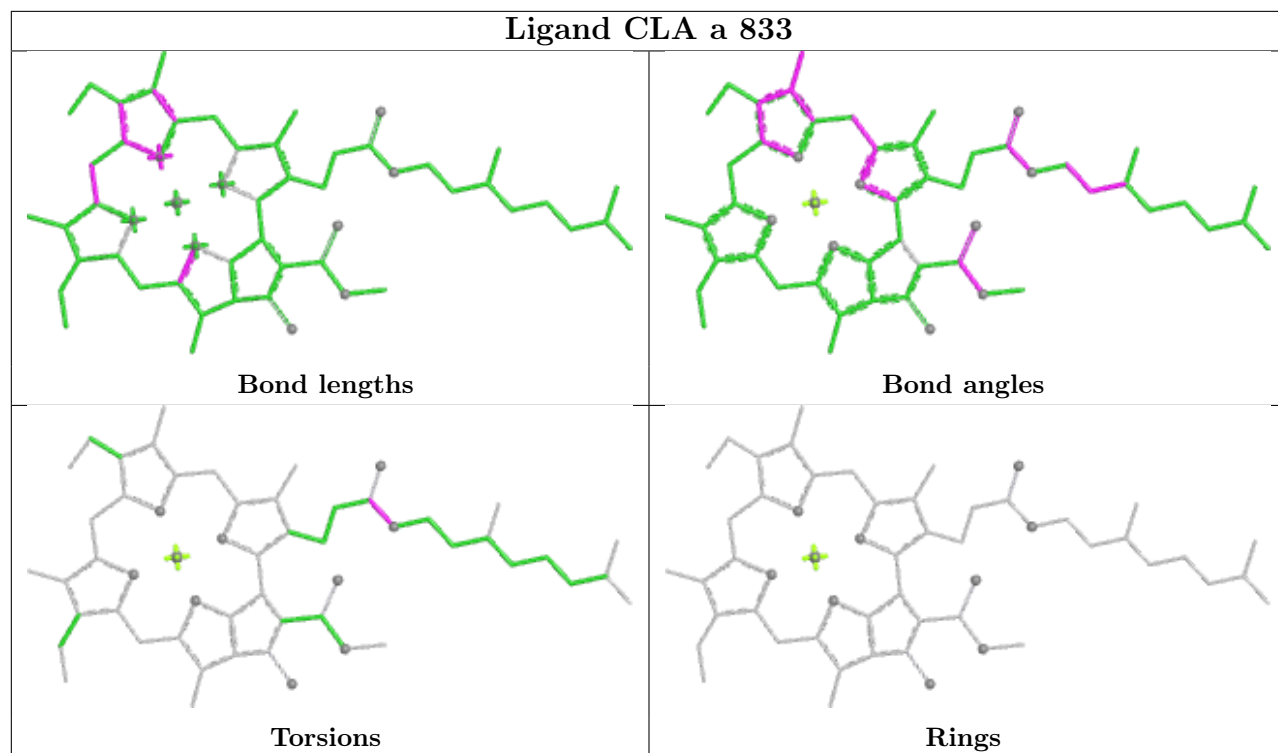
Ligand A1L1F 9 302



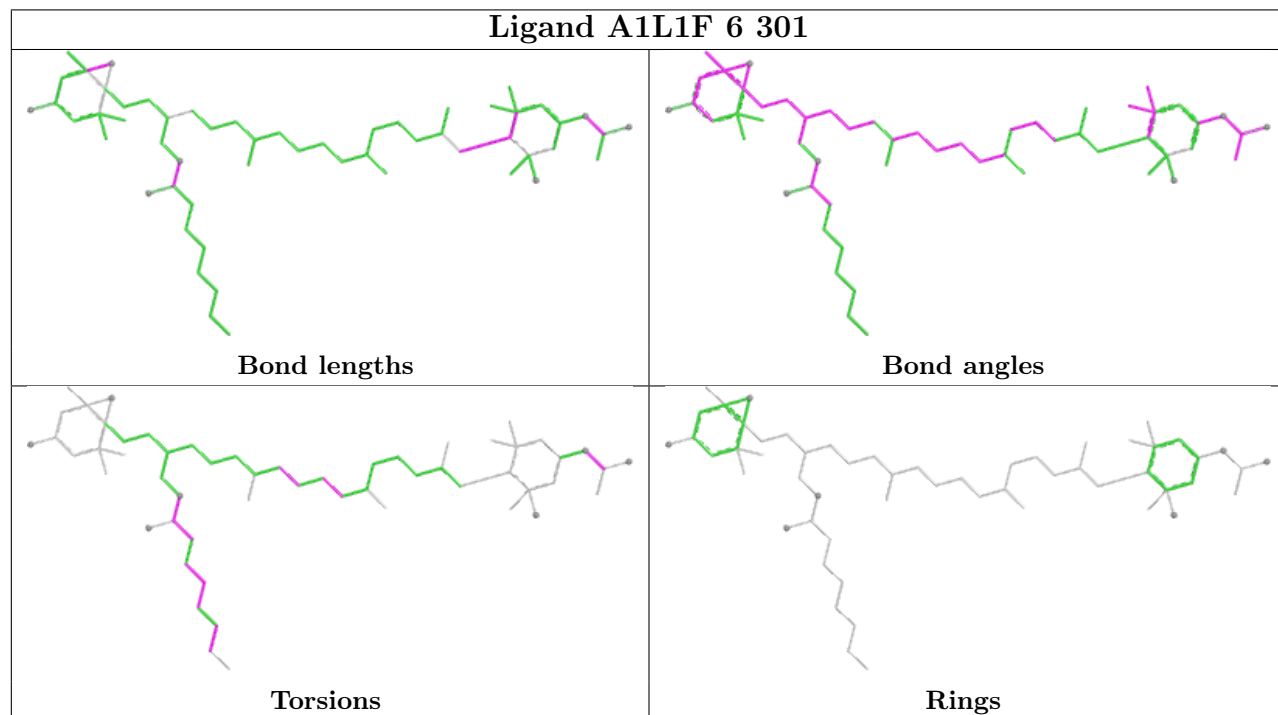


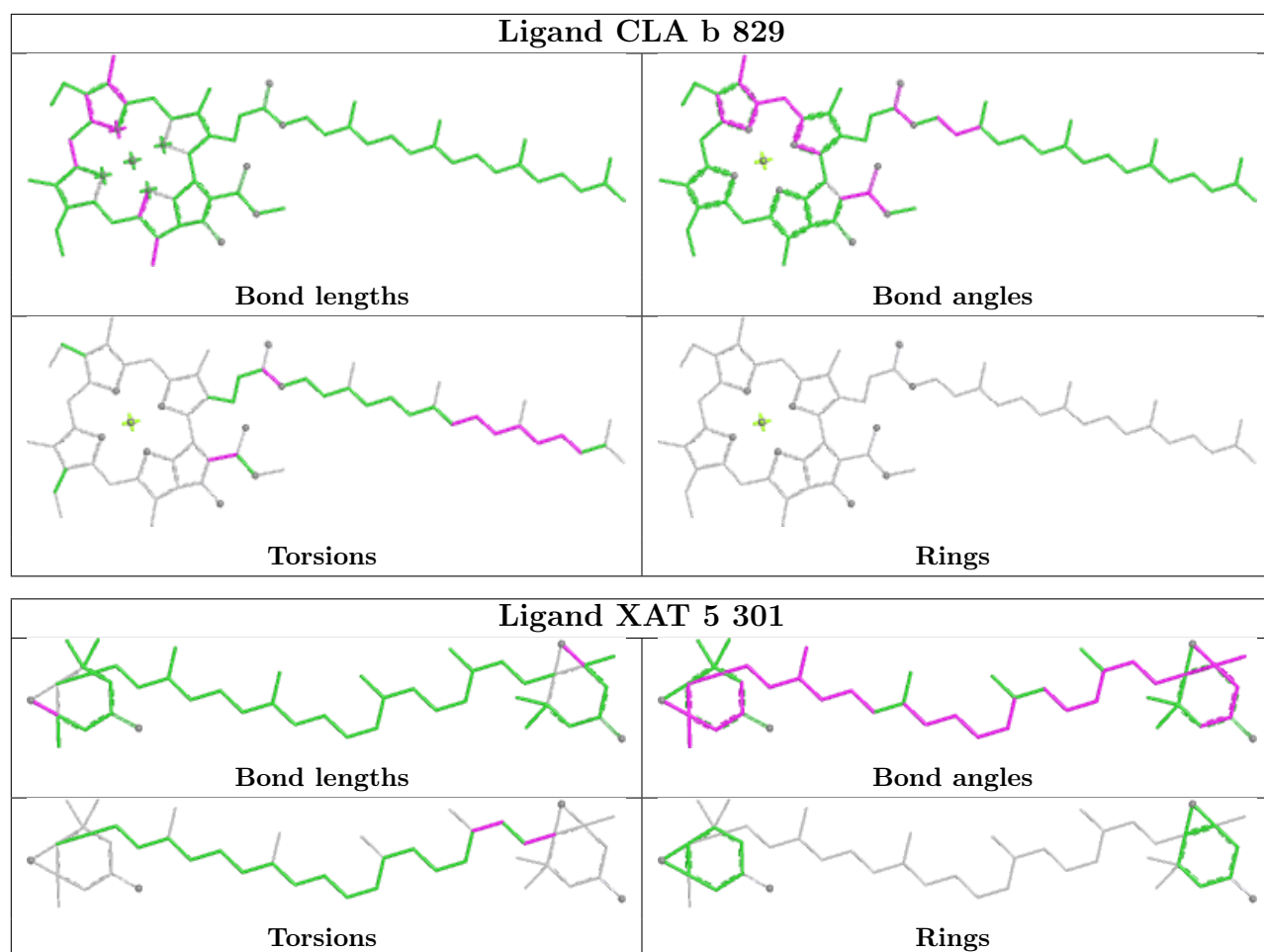


Ligand CLA a 833

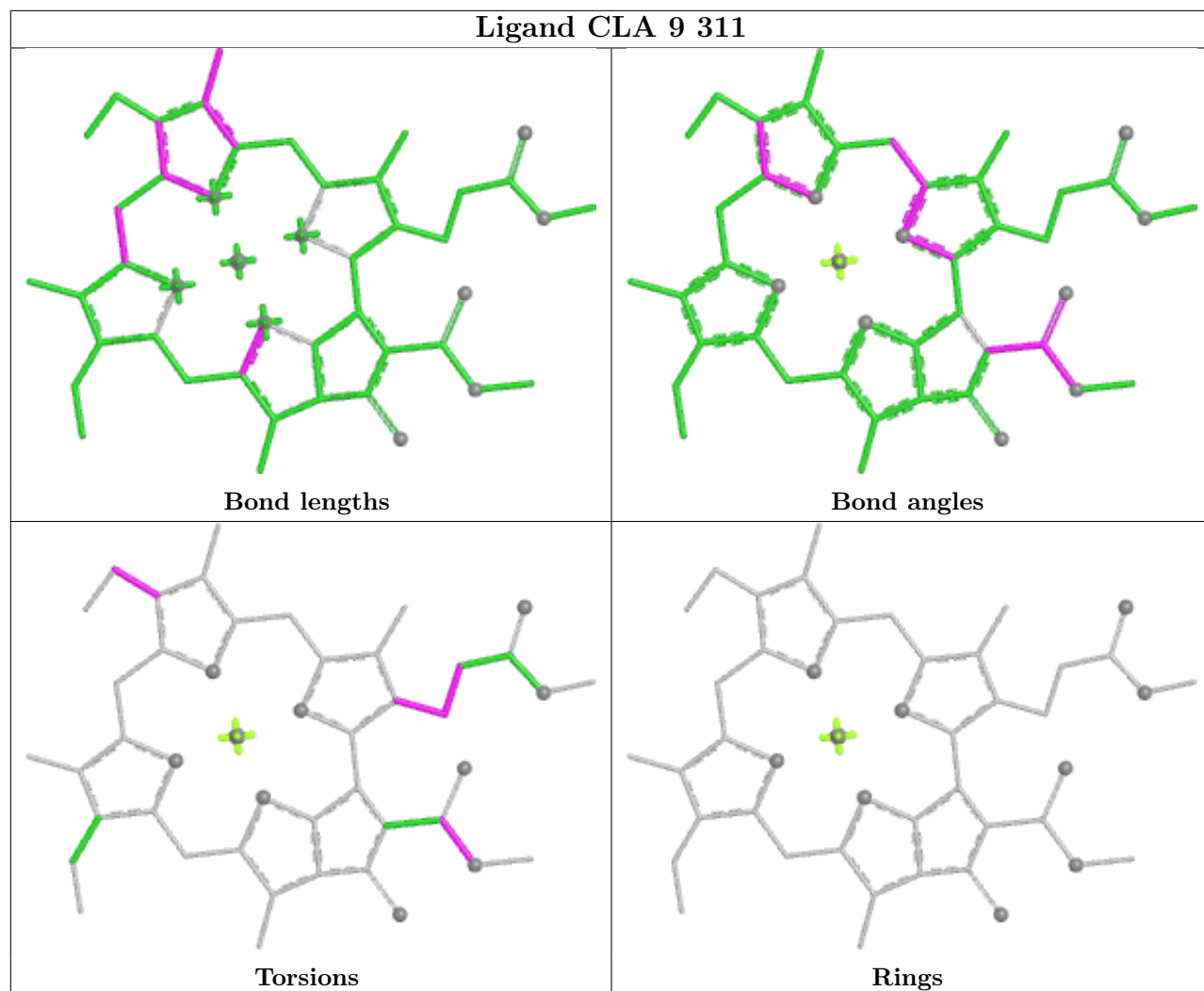


Ligand A1L1F 6 301

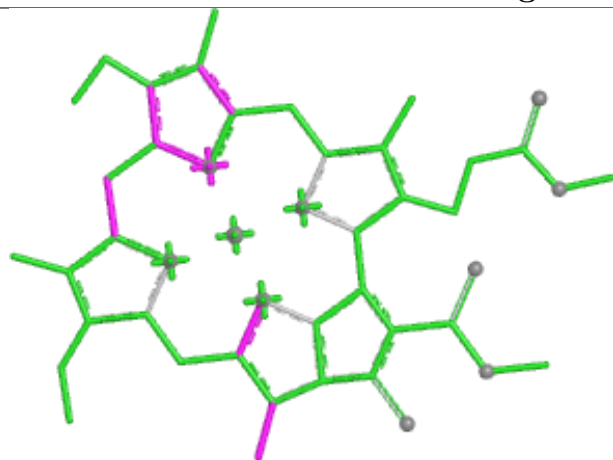




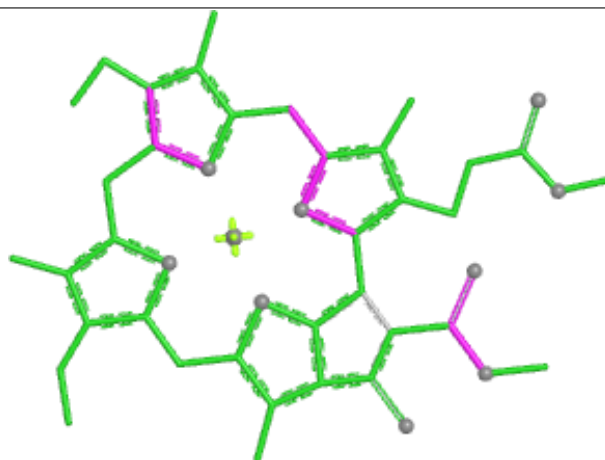
Ligand CLA 9 311



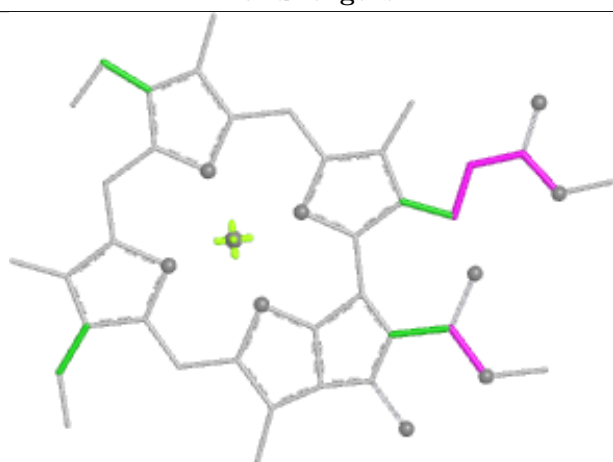
Ligand CLA 7 310



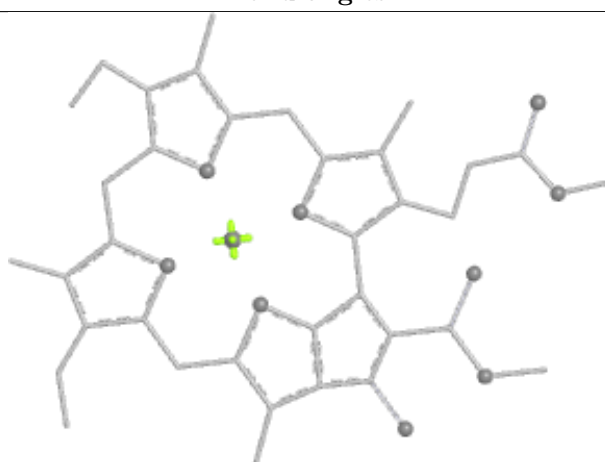
Bond lengths



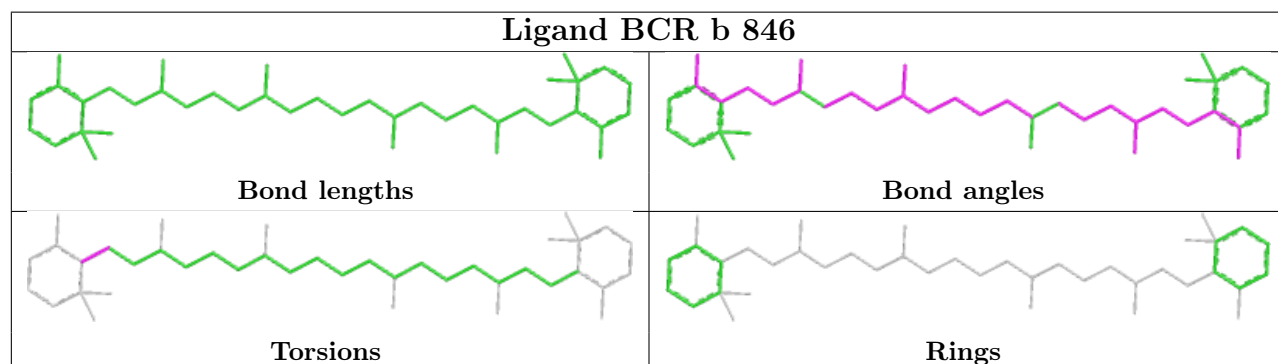
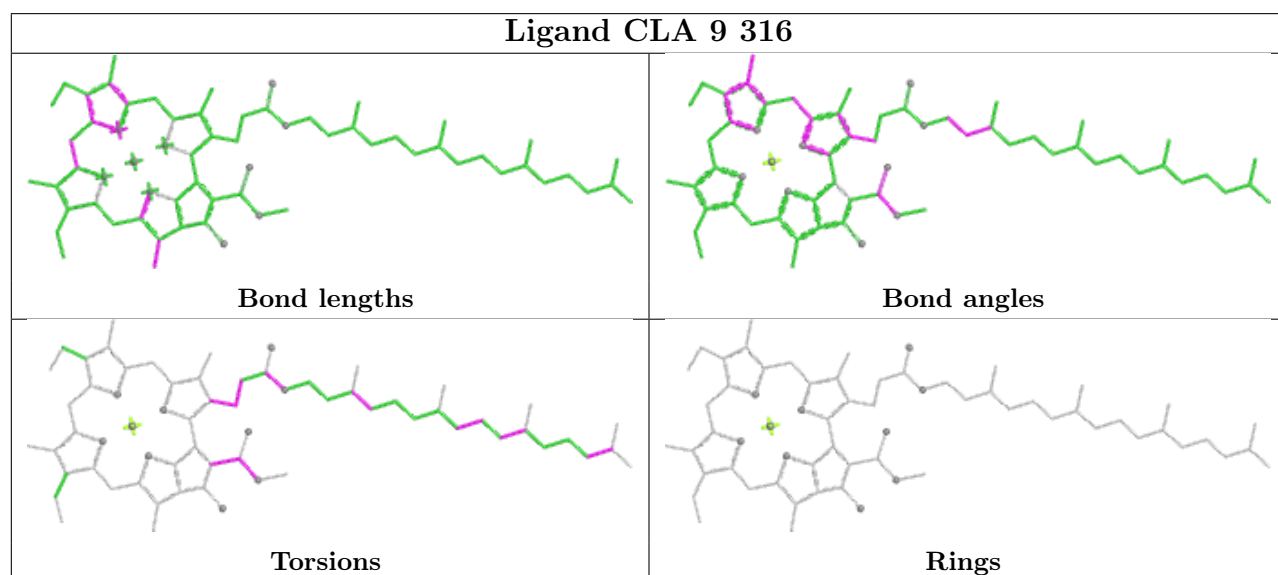
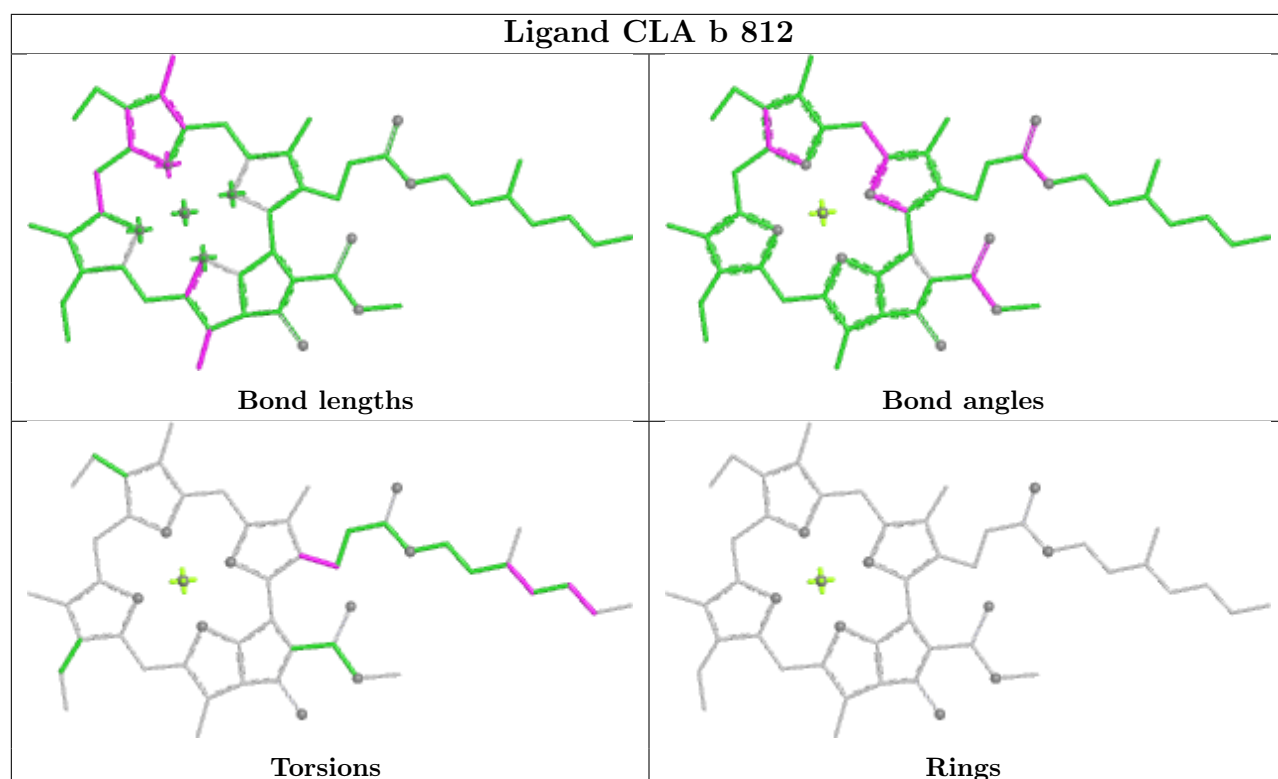
Bond angles



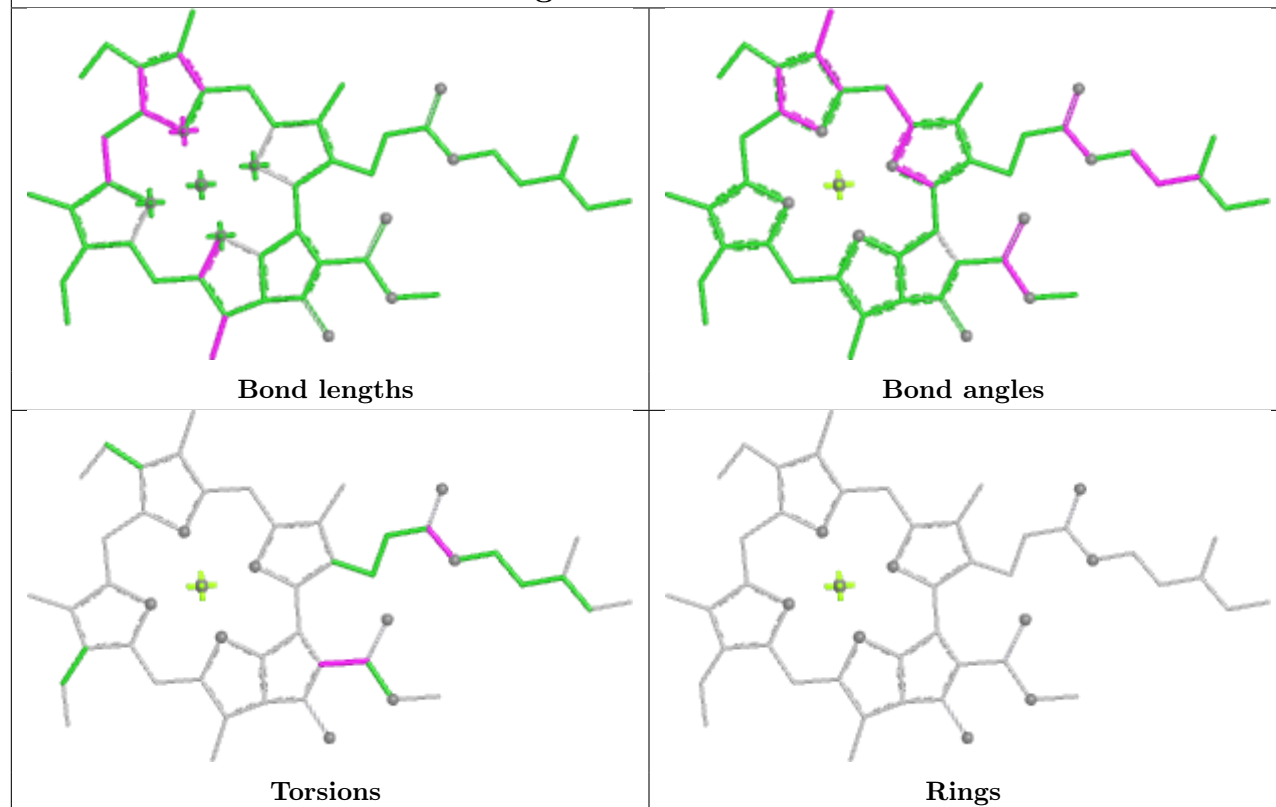
Torsions



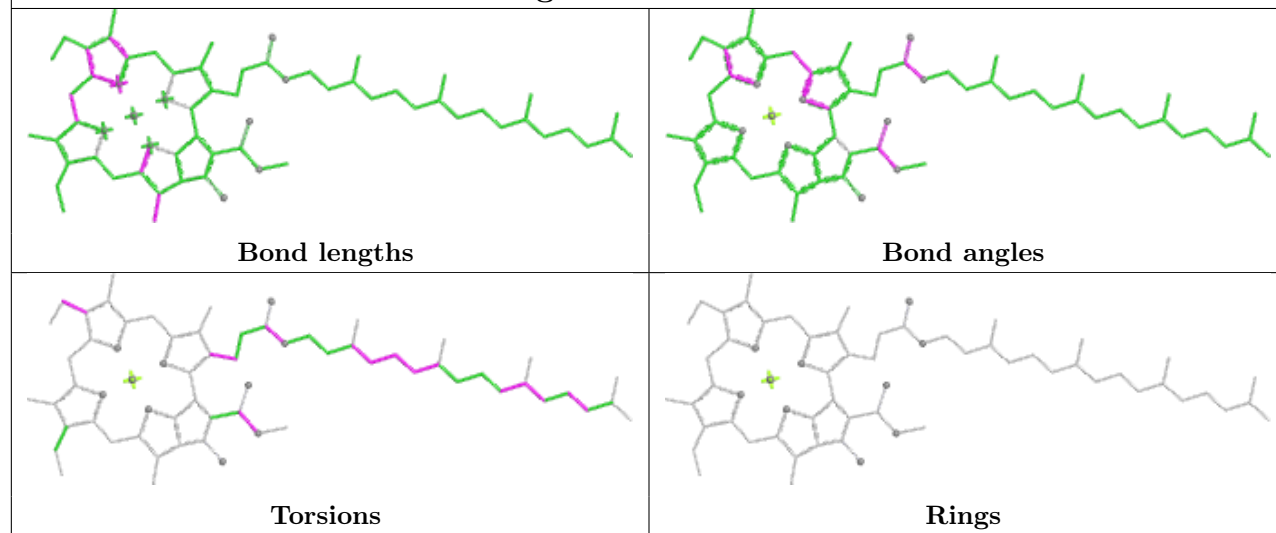
Rings



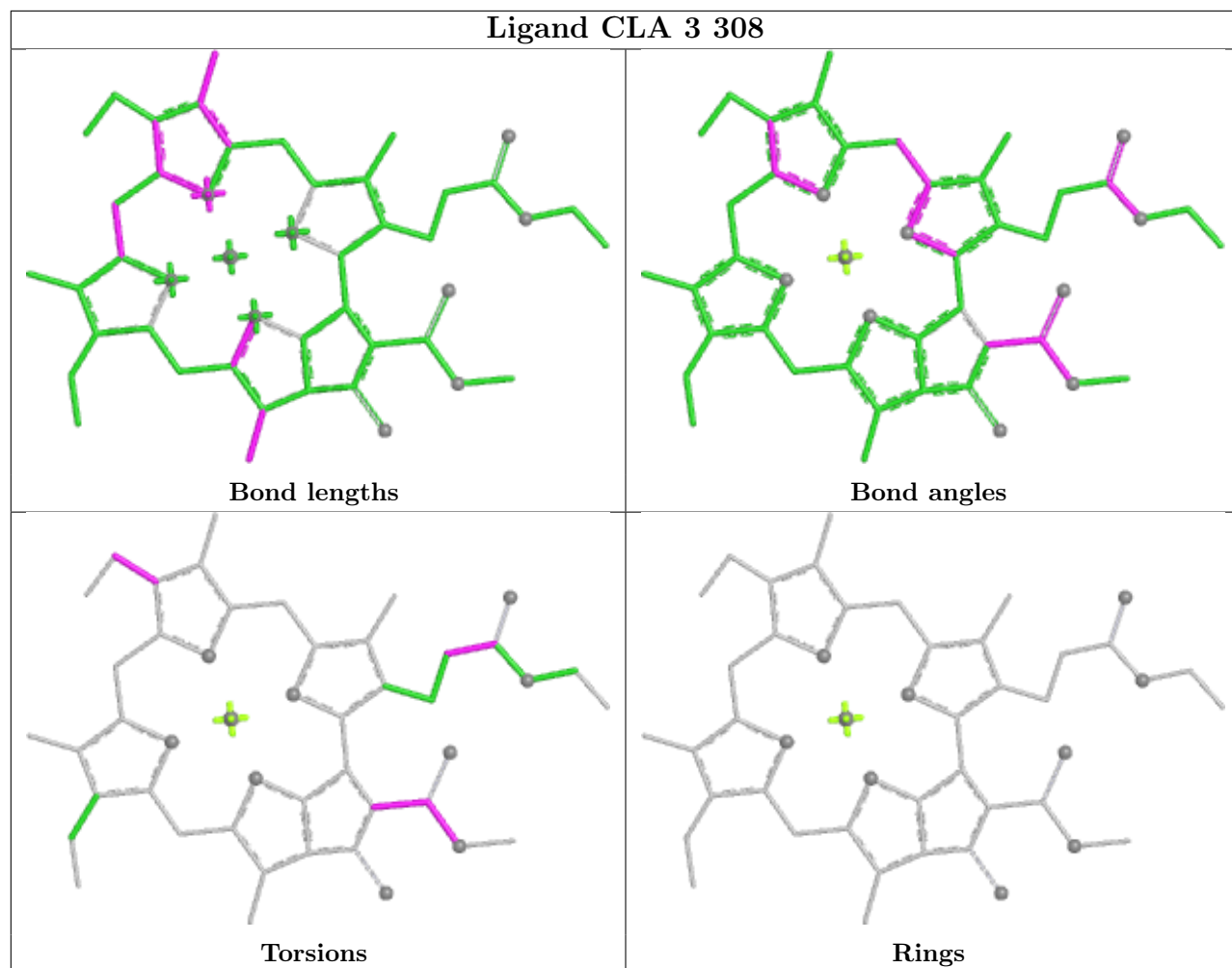
Ligand CLA b 821



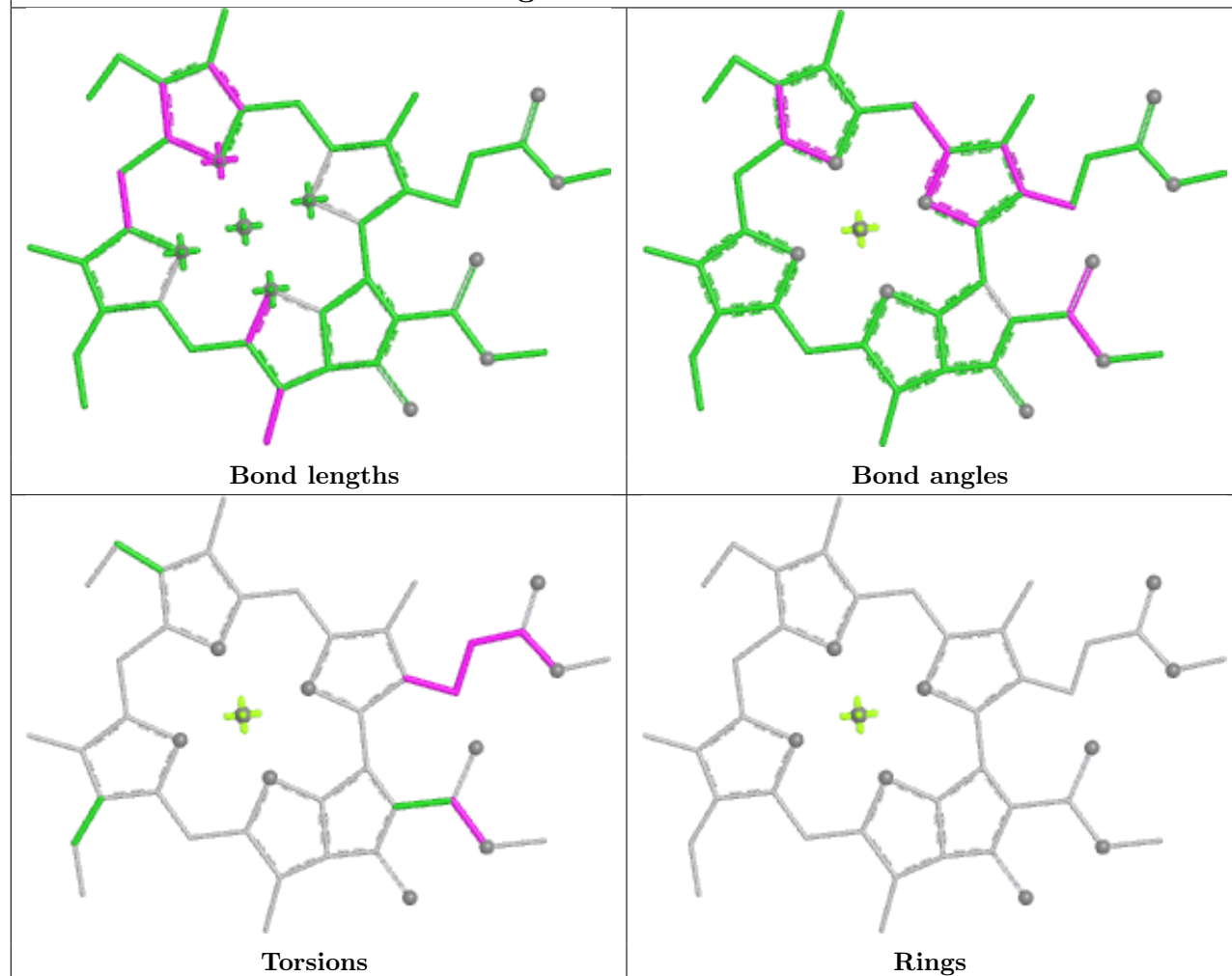
Ligand CLA a 807



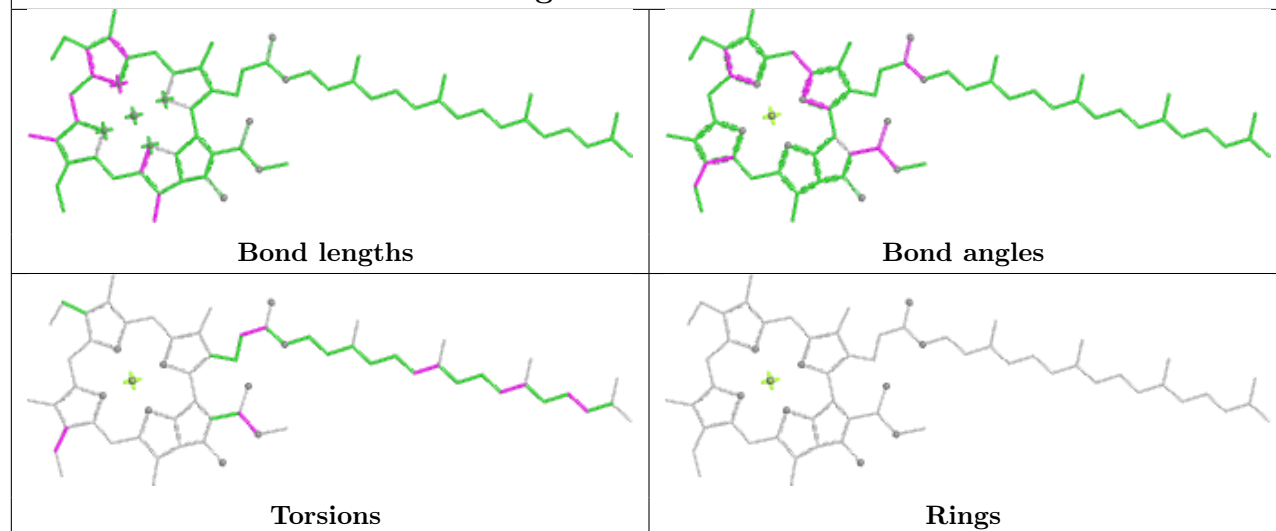
Ligand CLA 3 308



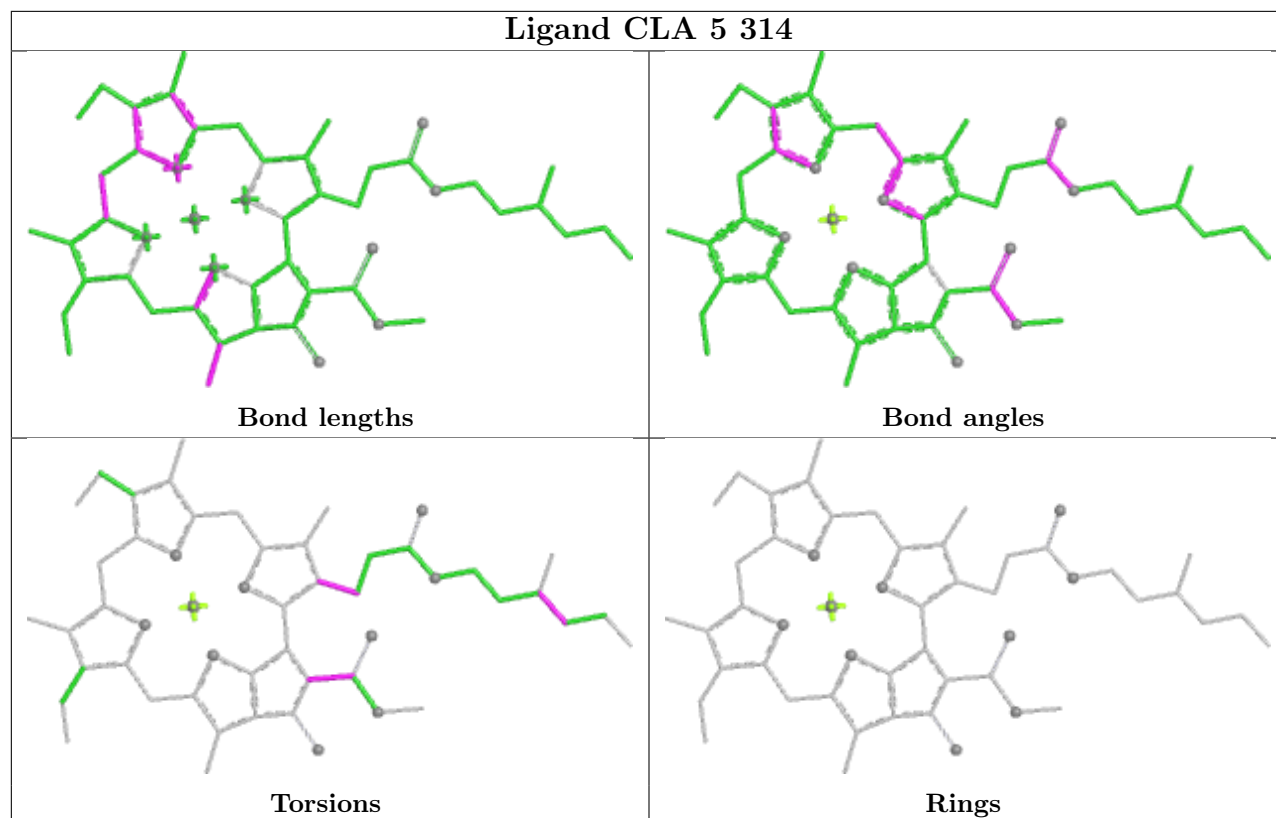
Ligand CLA 9 312



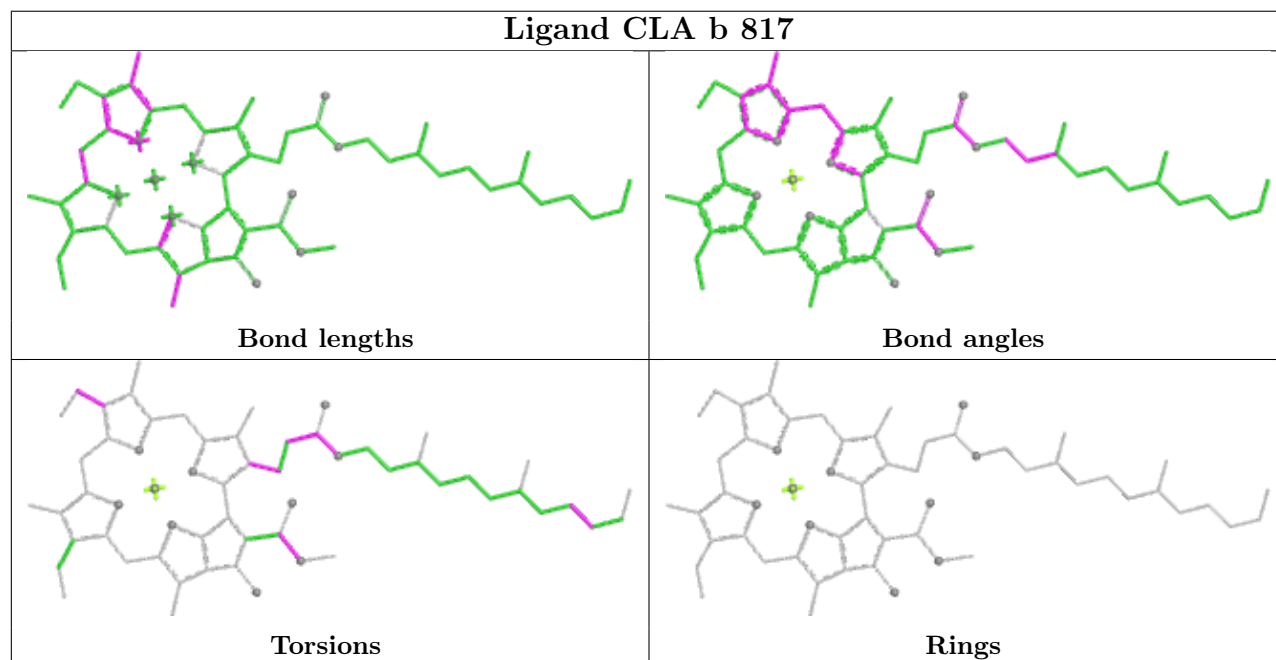
Ligand CLA b 804



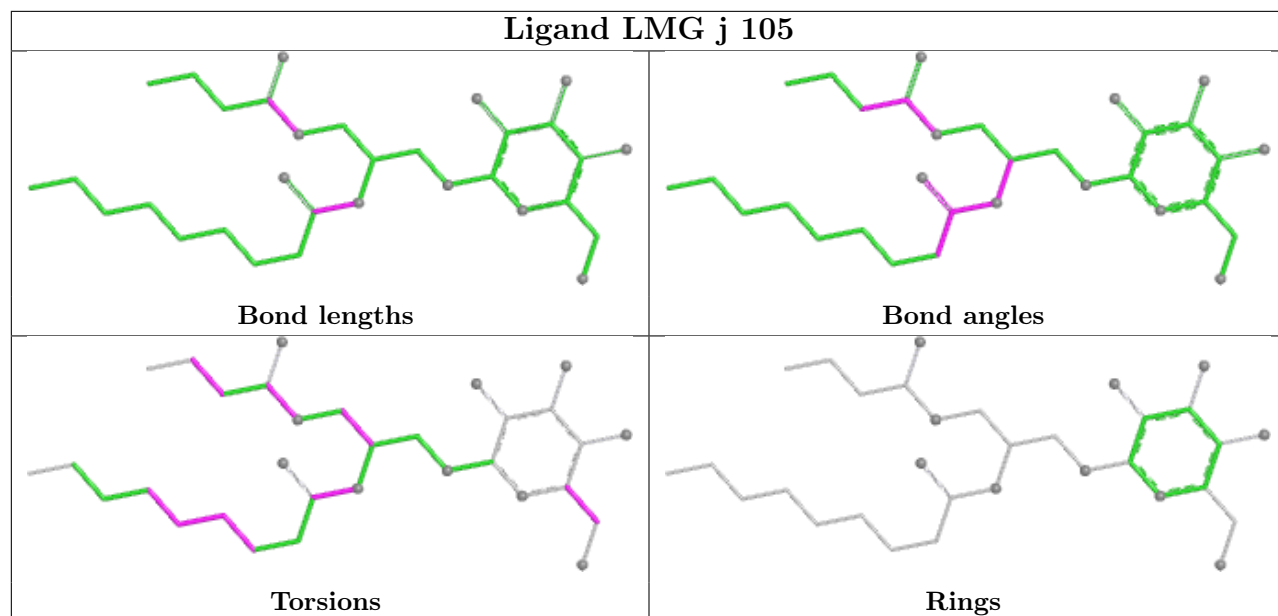
Ligand CLA 5 314



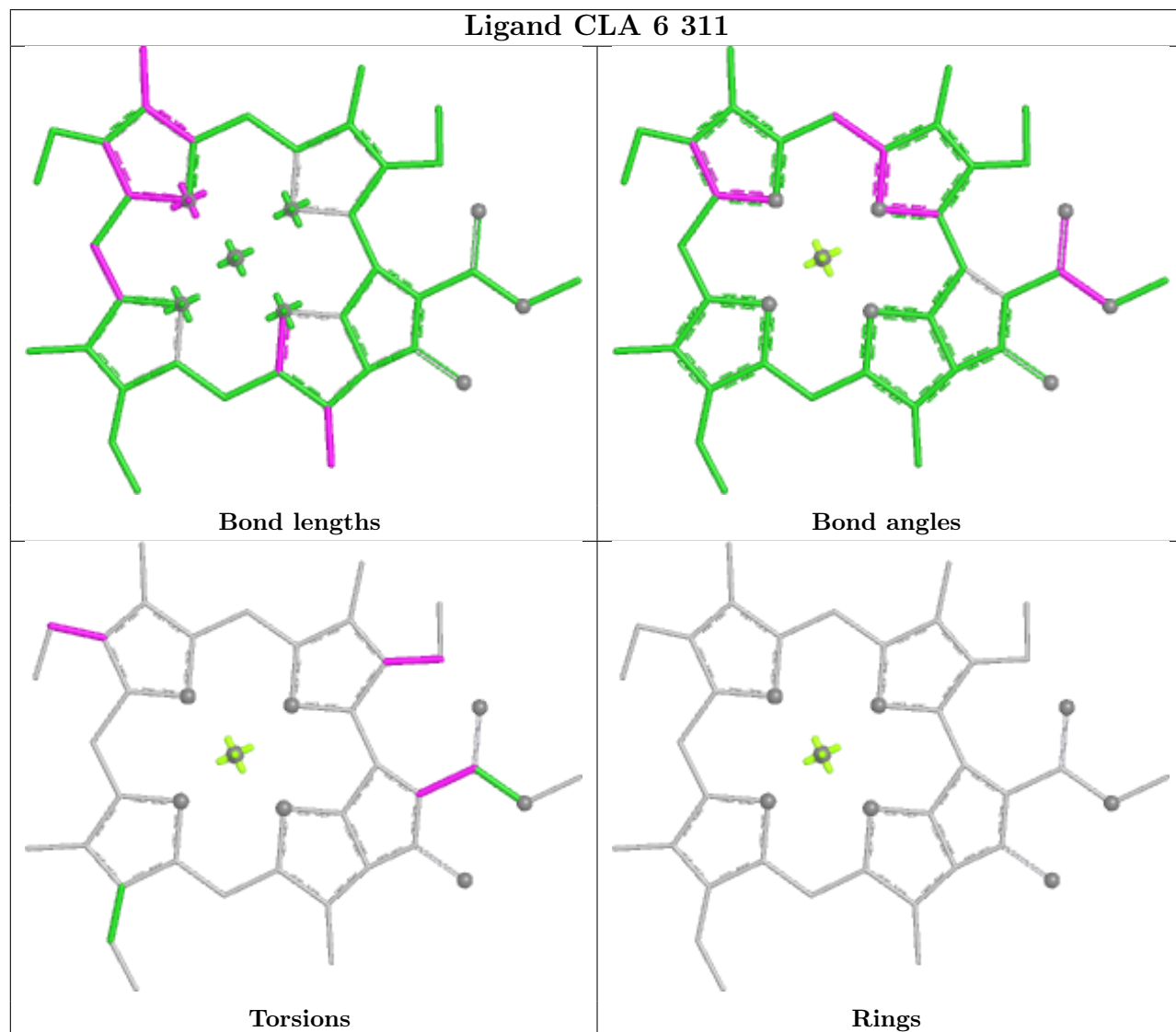
Ligand CLA b 817

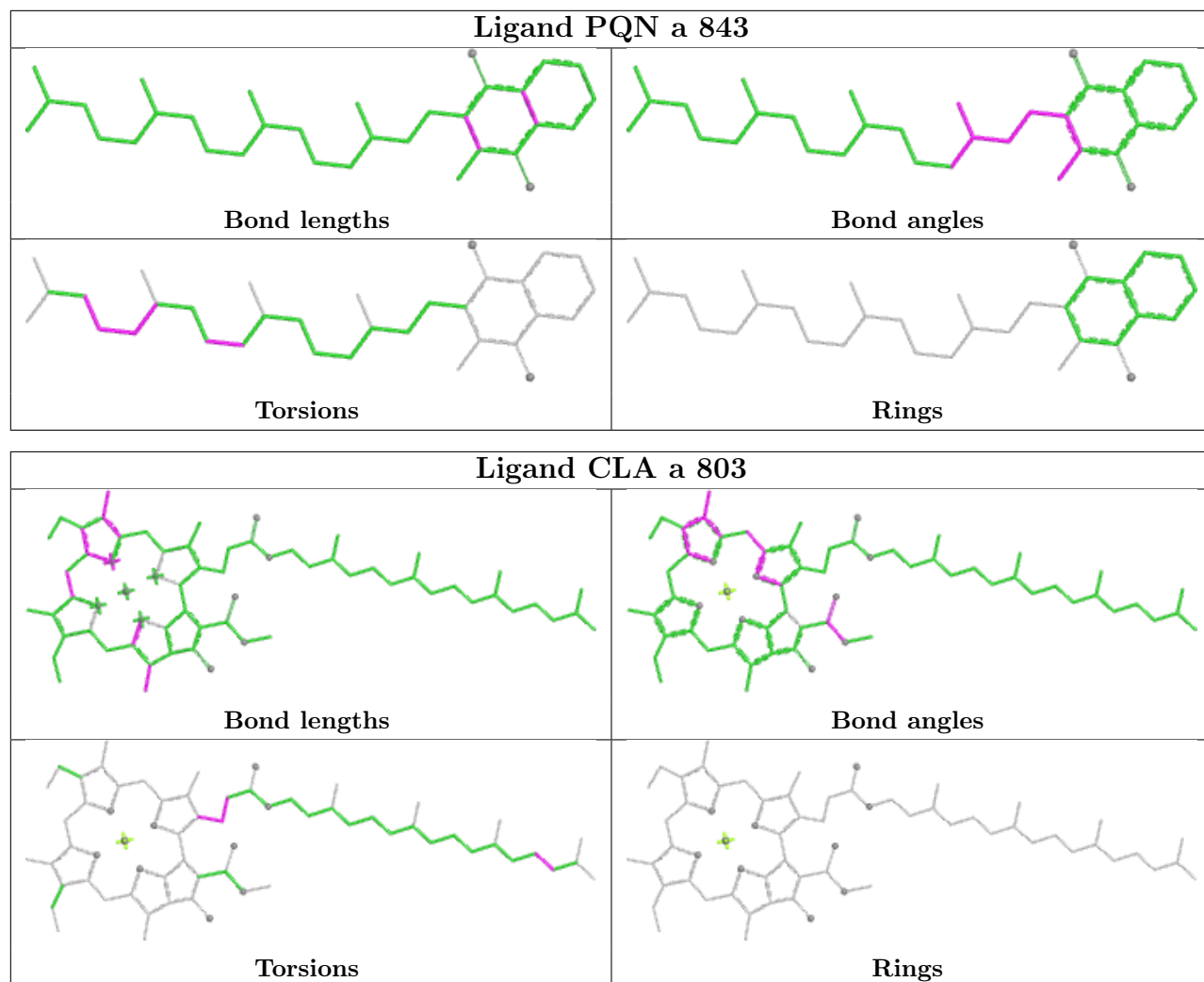


Ligand LMG j 105

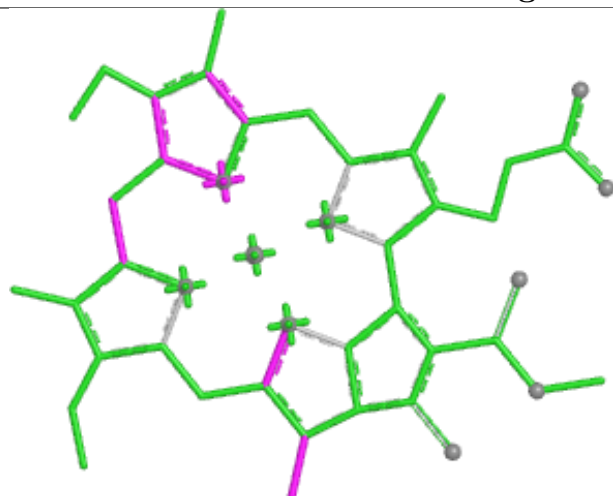


Ligand CLA 6 311

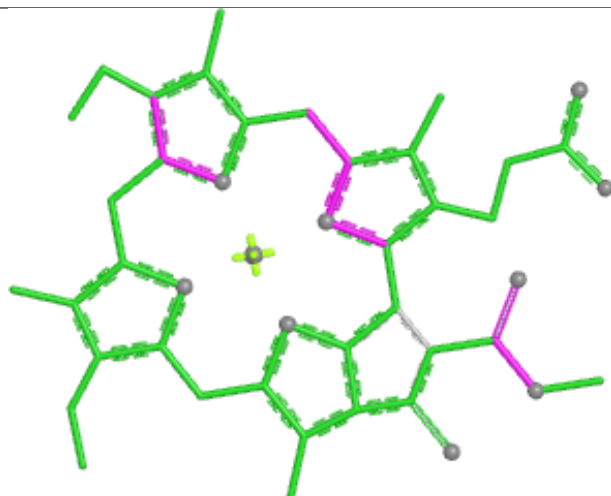




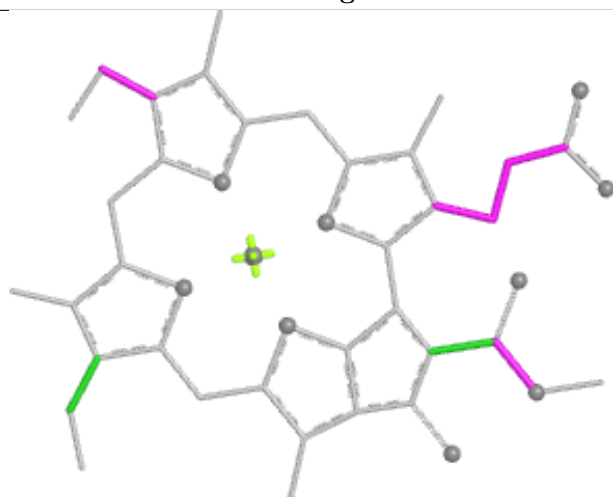
Ligand CLA 4 306



Bond lengths



Bond angles

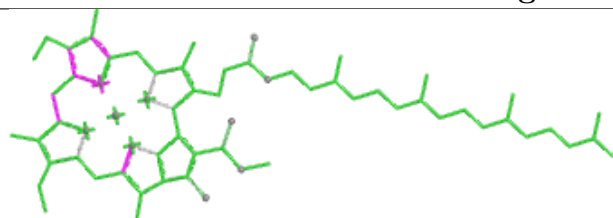


Torsions

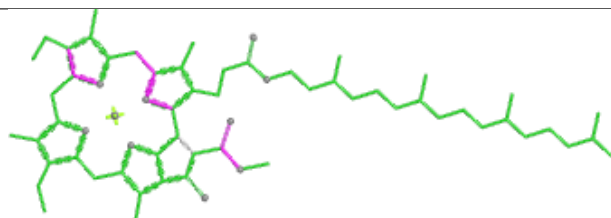


Rings

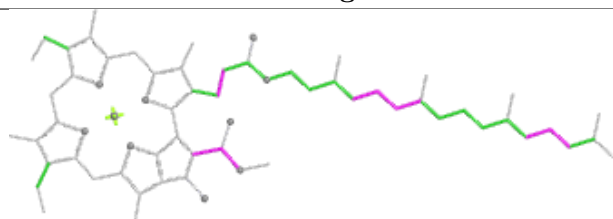
Ligand CLA 5 309



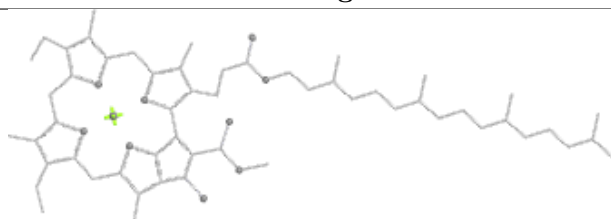
Bond lengths



Bond angles

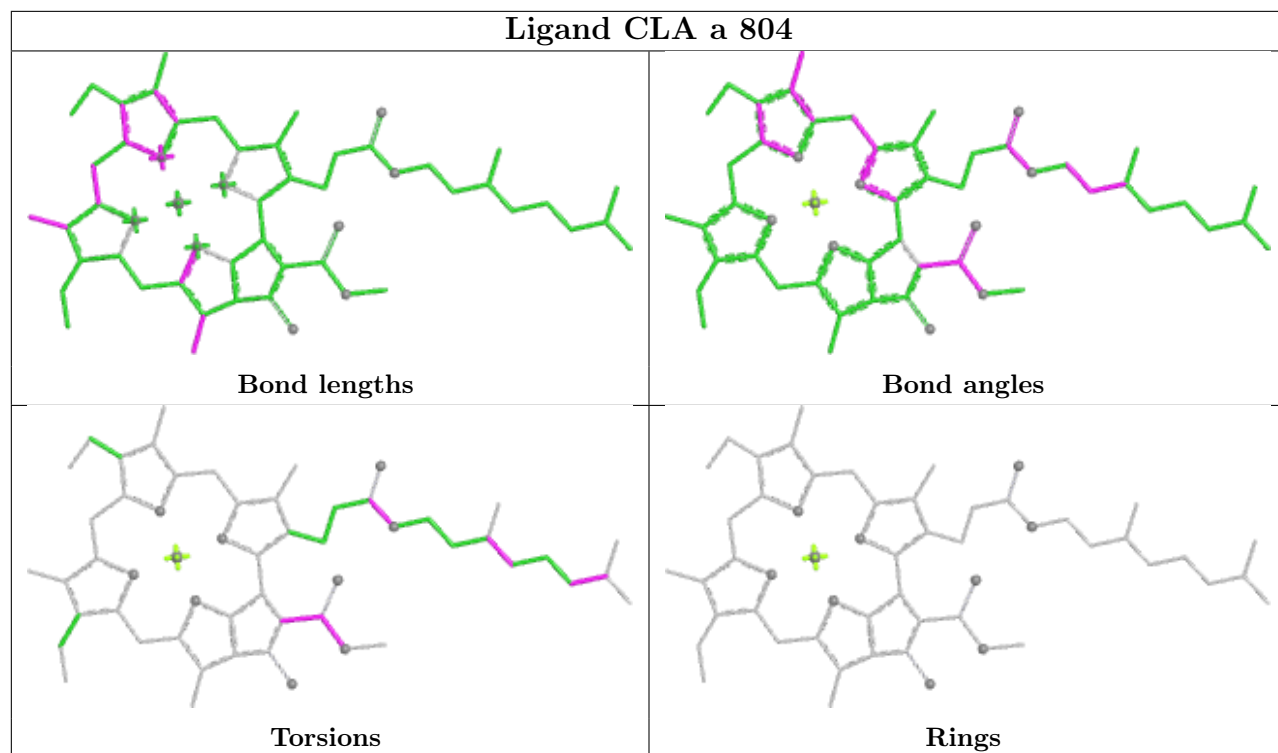


Torsions

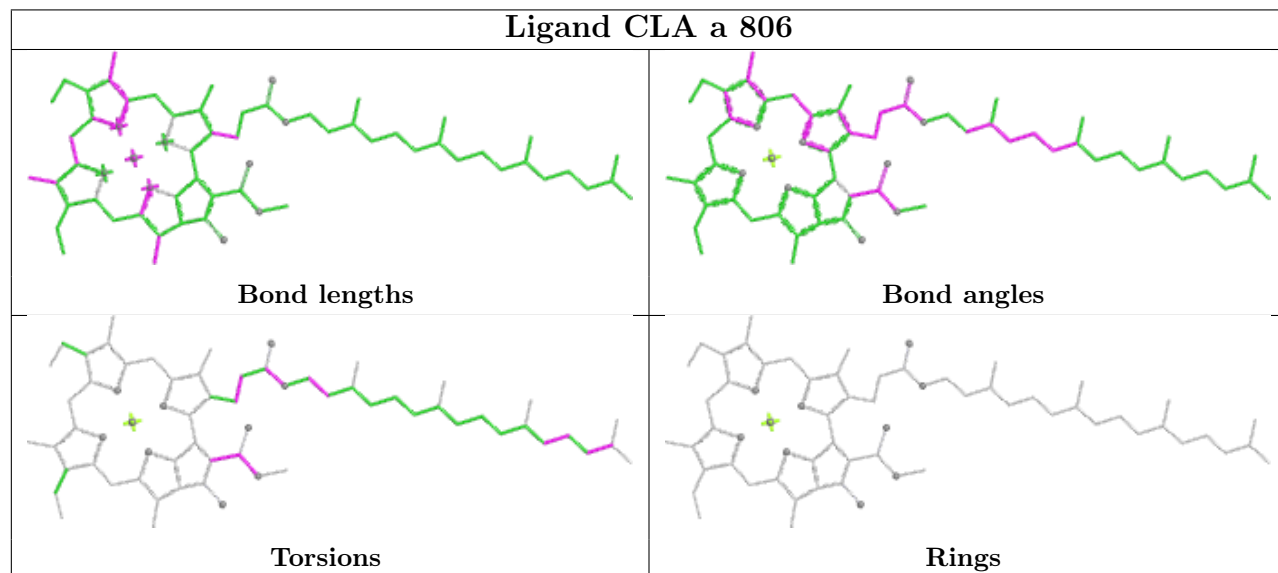


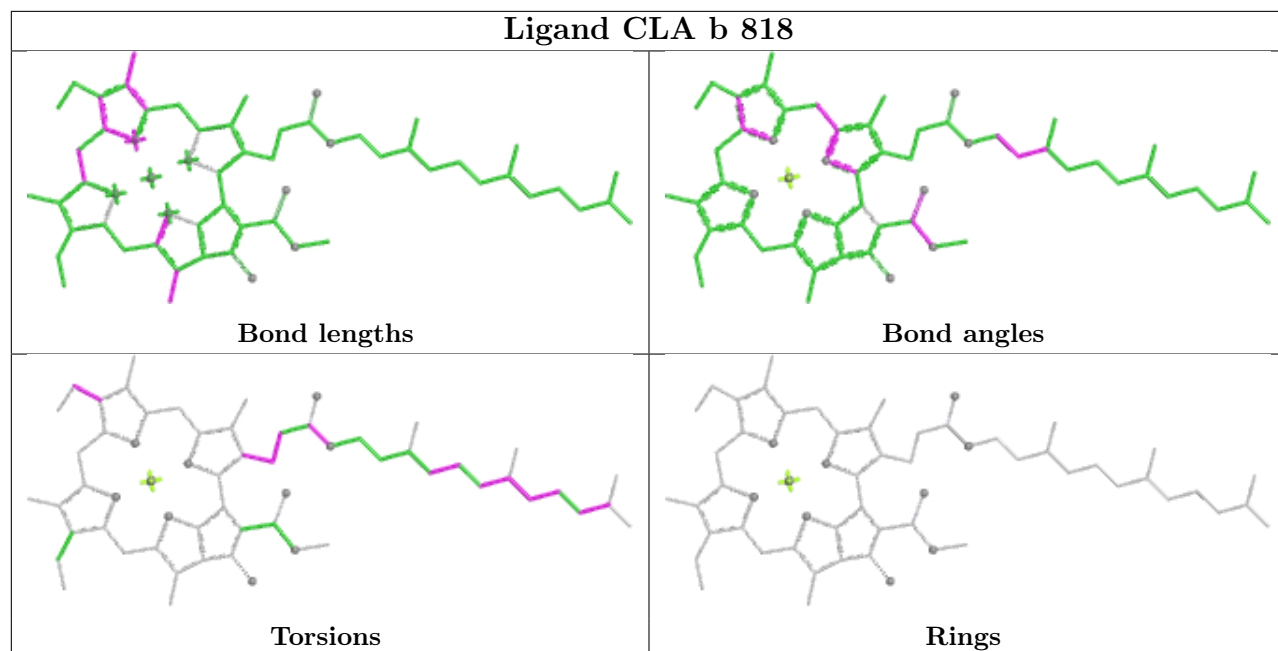
Rings

Ligand CLA a 804

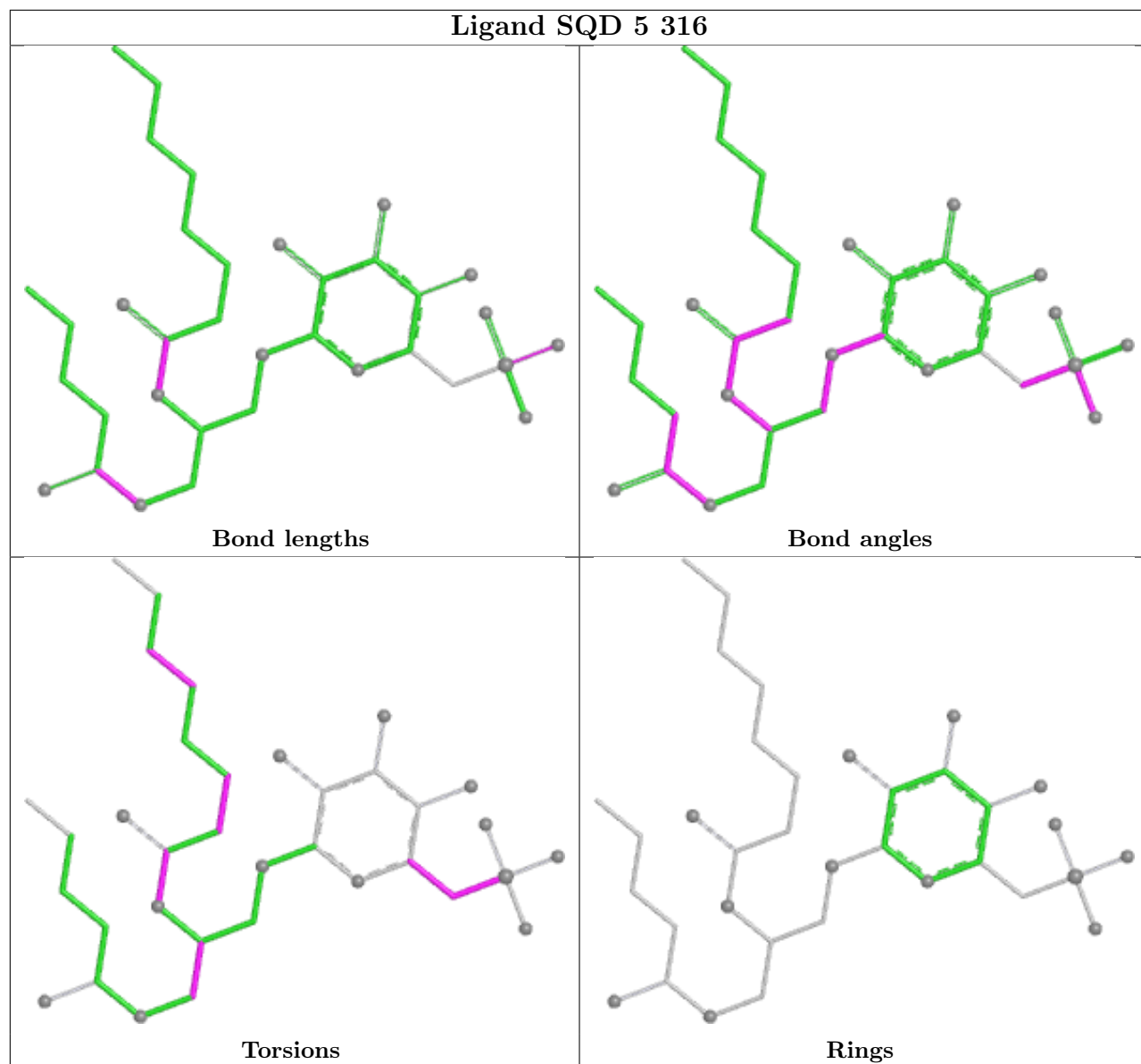


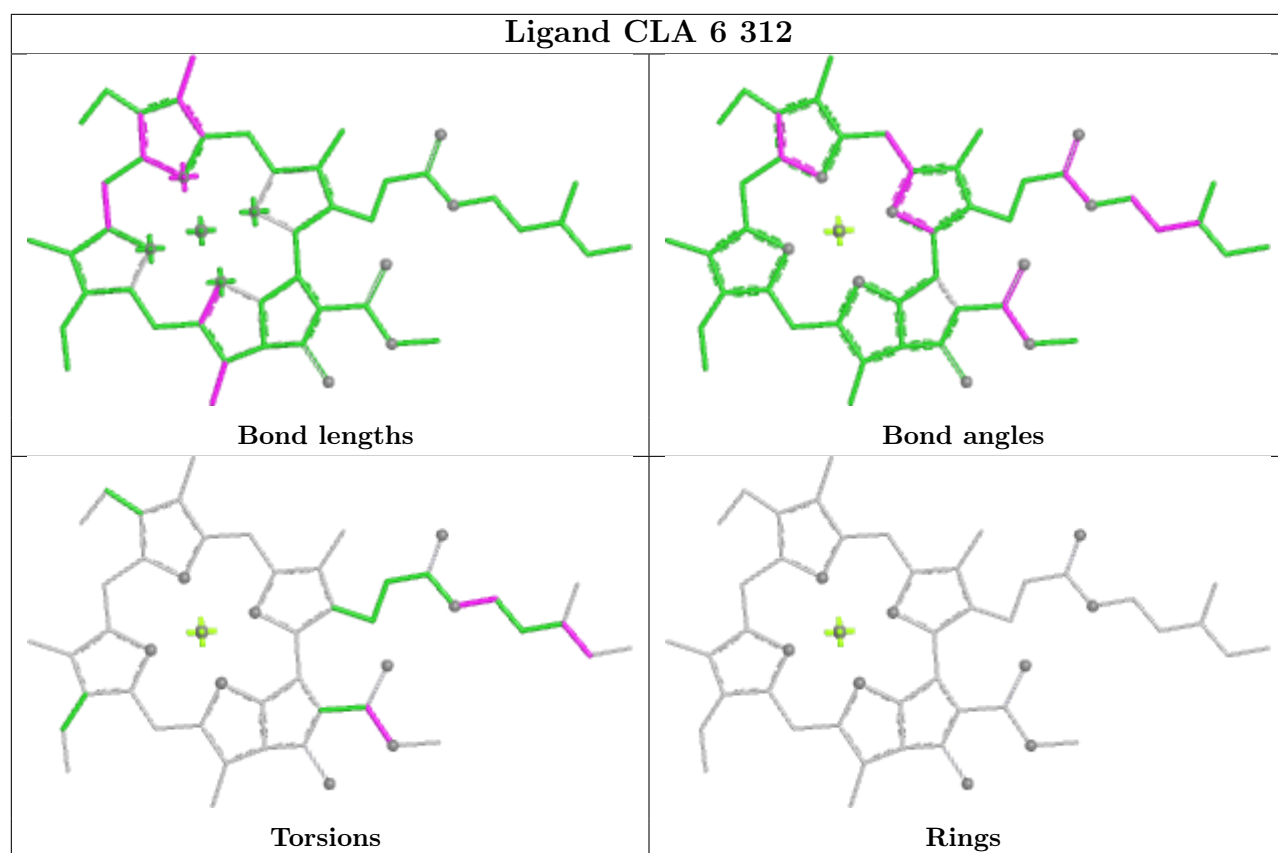
Ligand CLA a 806



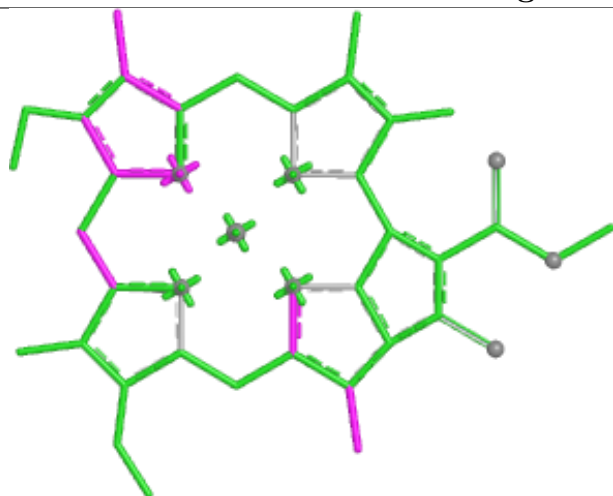


Ligand SQD 5 316

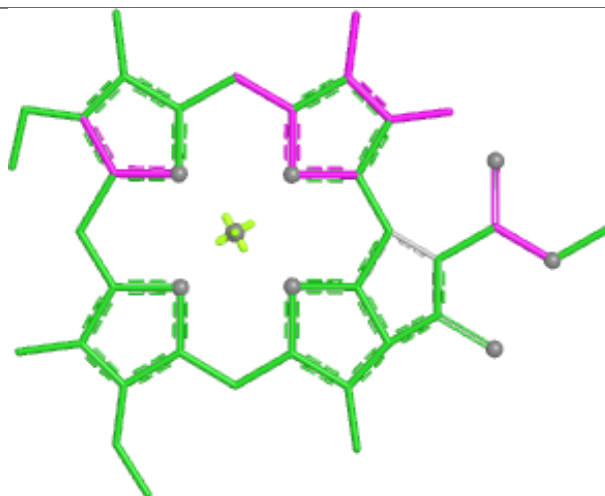




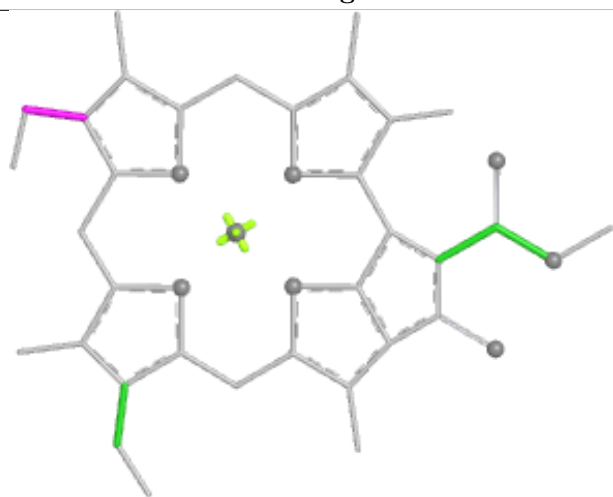
Ligand CLA b 830



Bond lengths



Bond angles

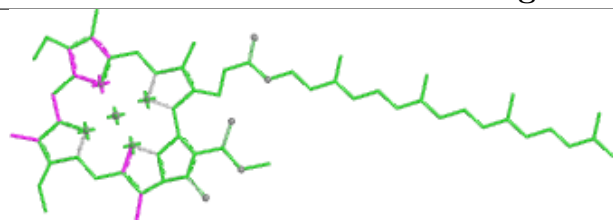


Torsions

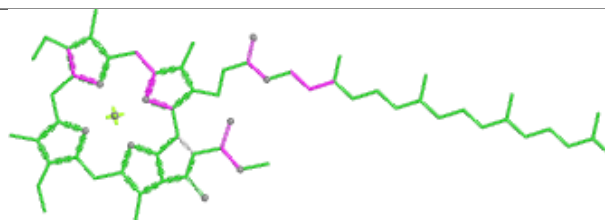


Rings

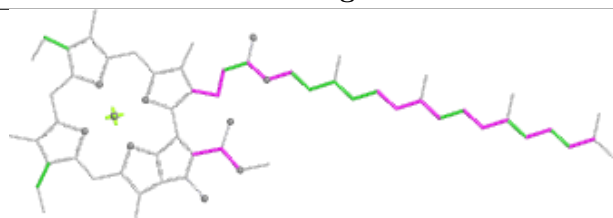
Ligand CLA a 814



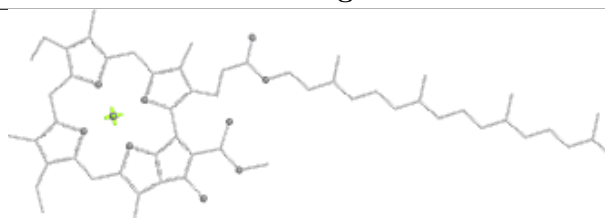
Bond lengths



Bond angles

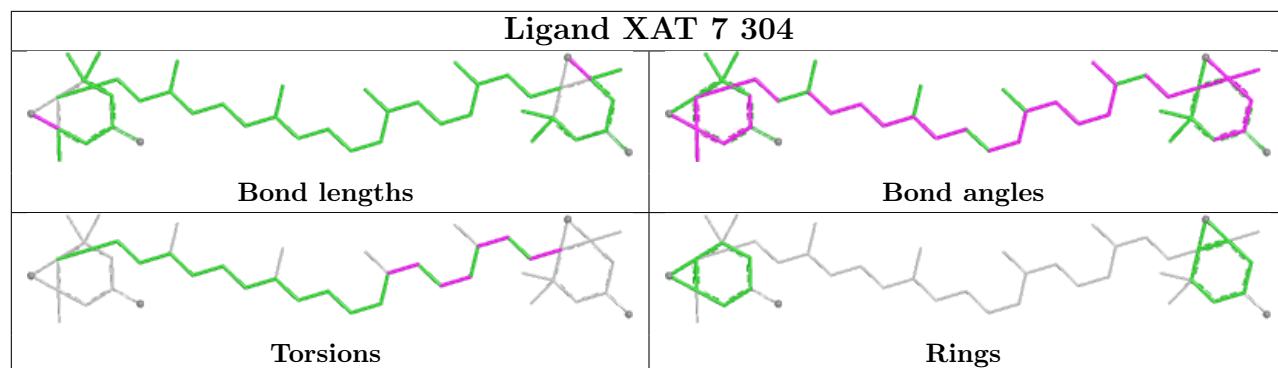


Torsions

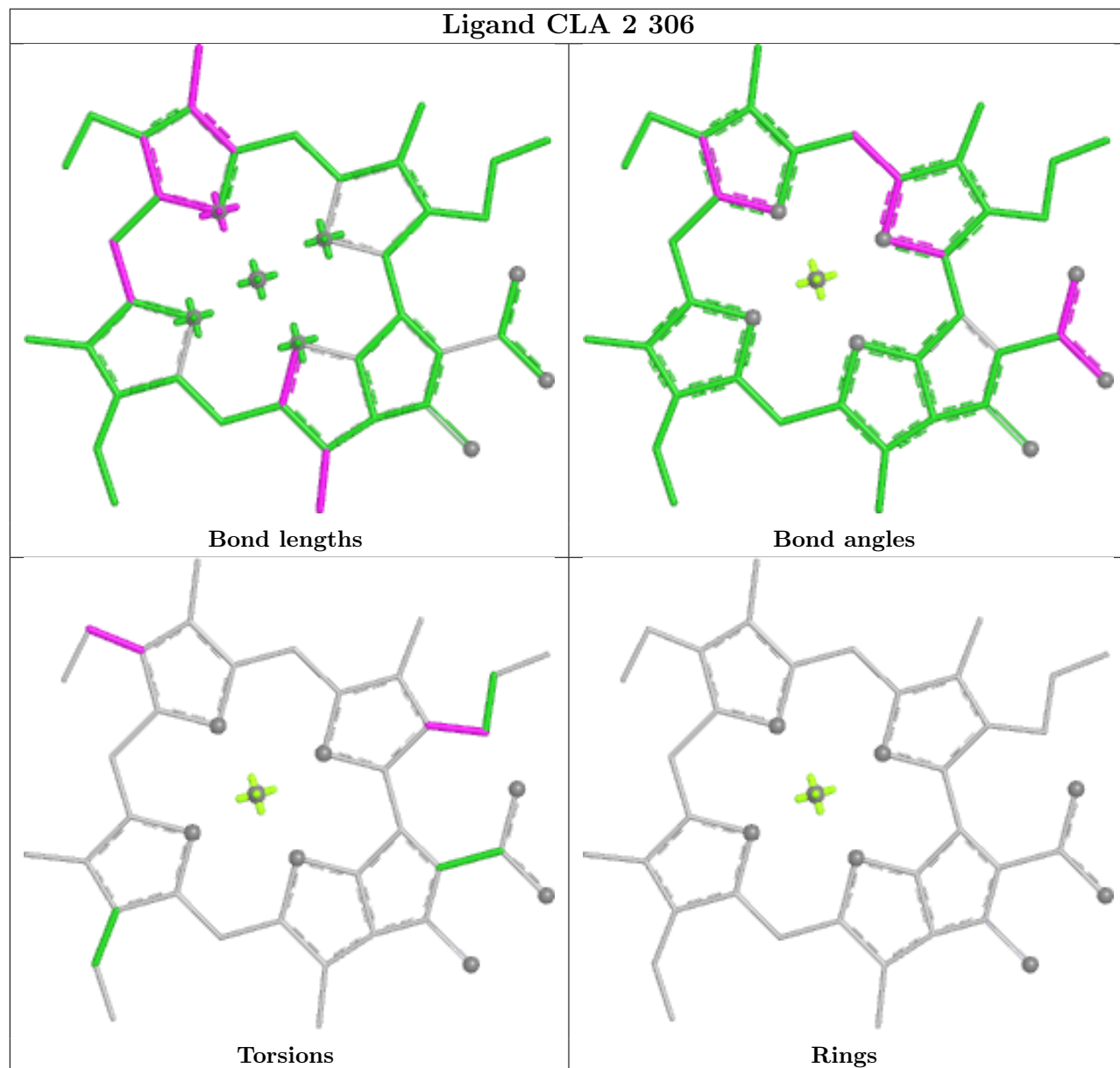


Rings

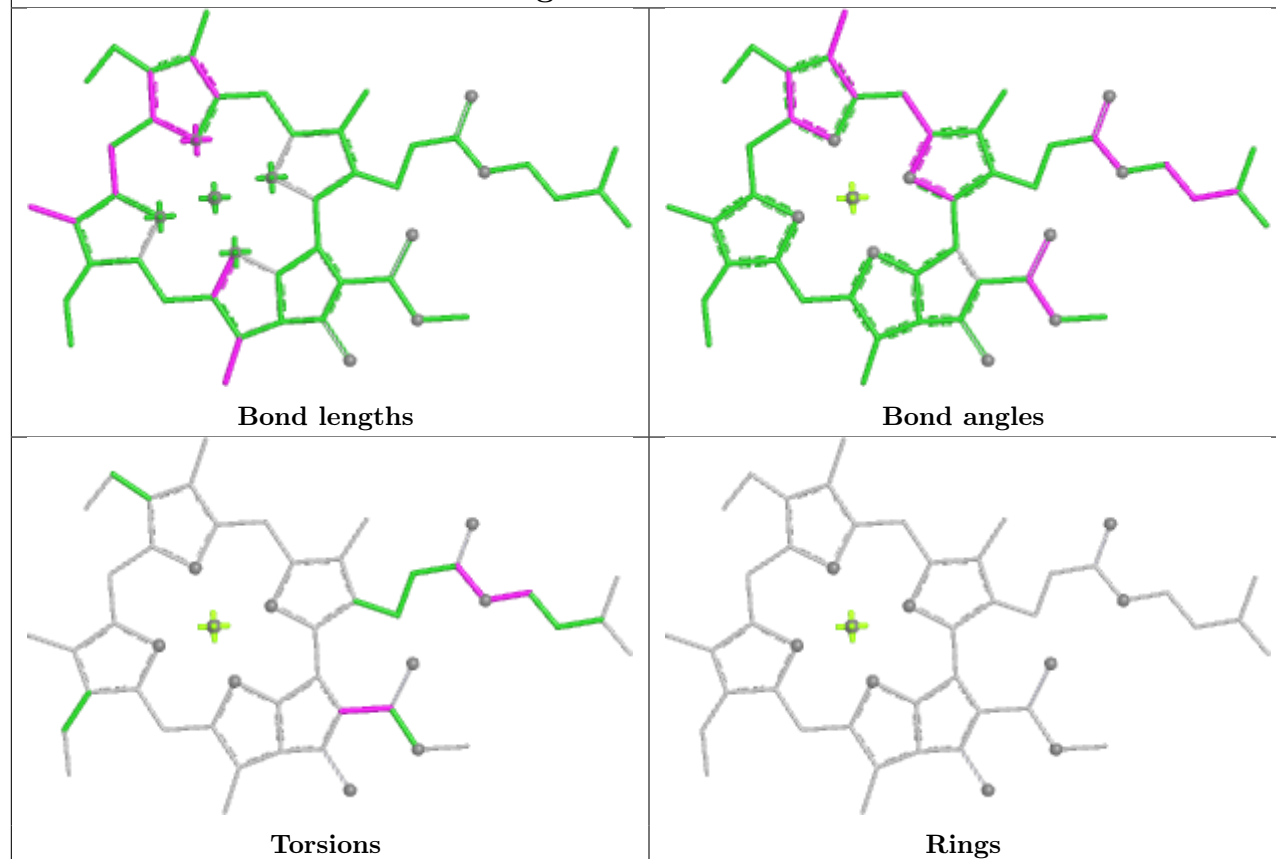
Ligand XAT 7 304



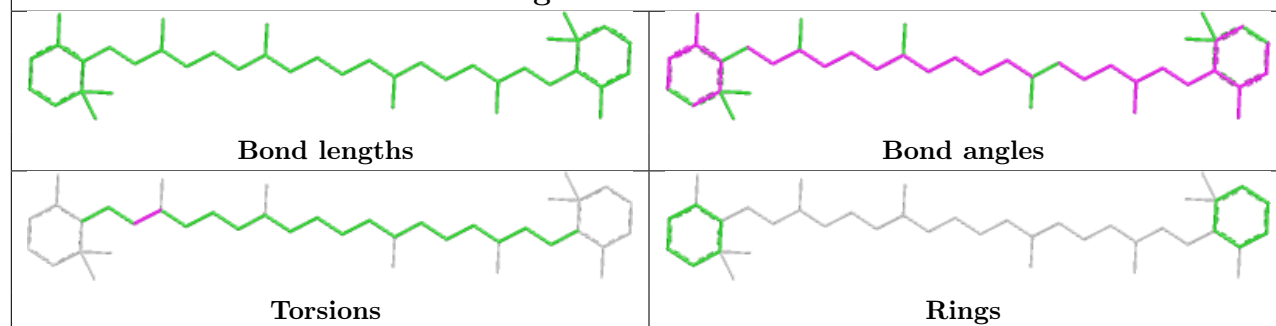
Ligand CLA 2 306



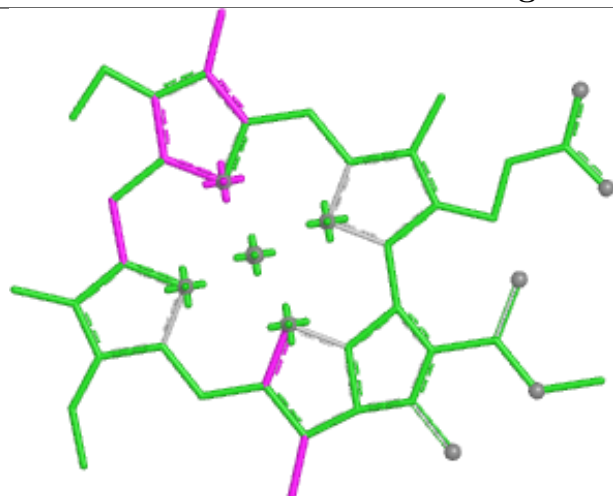
Ligand CLA a 816



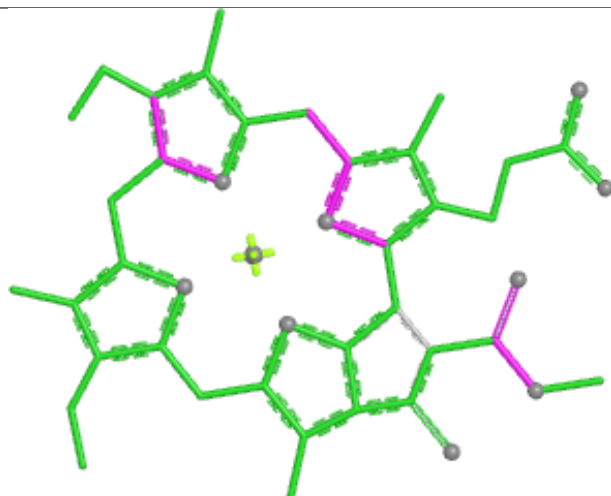
Ligand BCR b 842



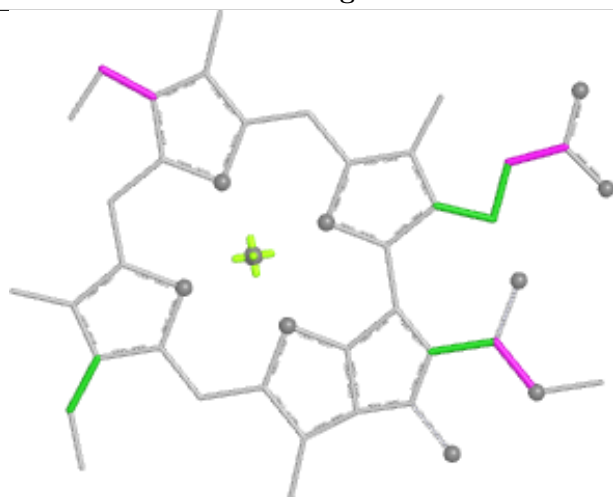
Ligand CLA 7 307



Bond lengths



Bond angles

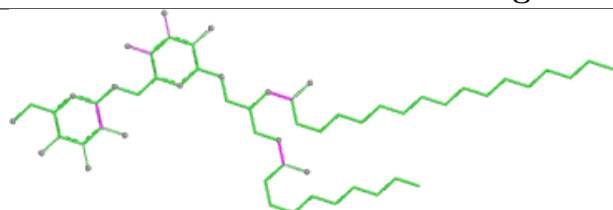


Torsions

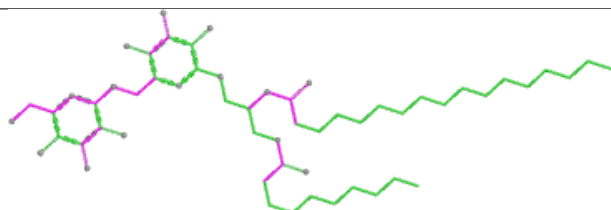


Rings

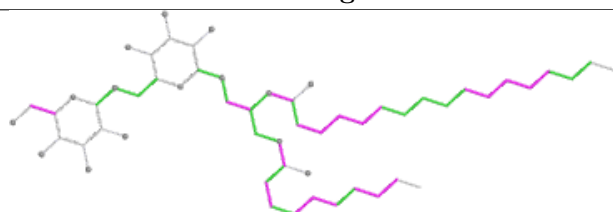
Ligand DGD b 848



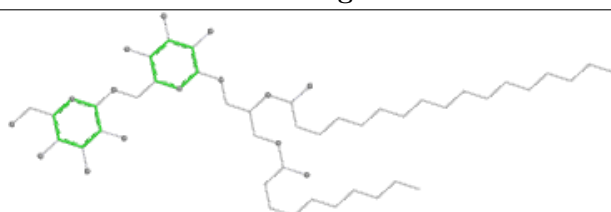
Bond lengths



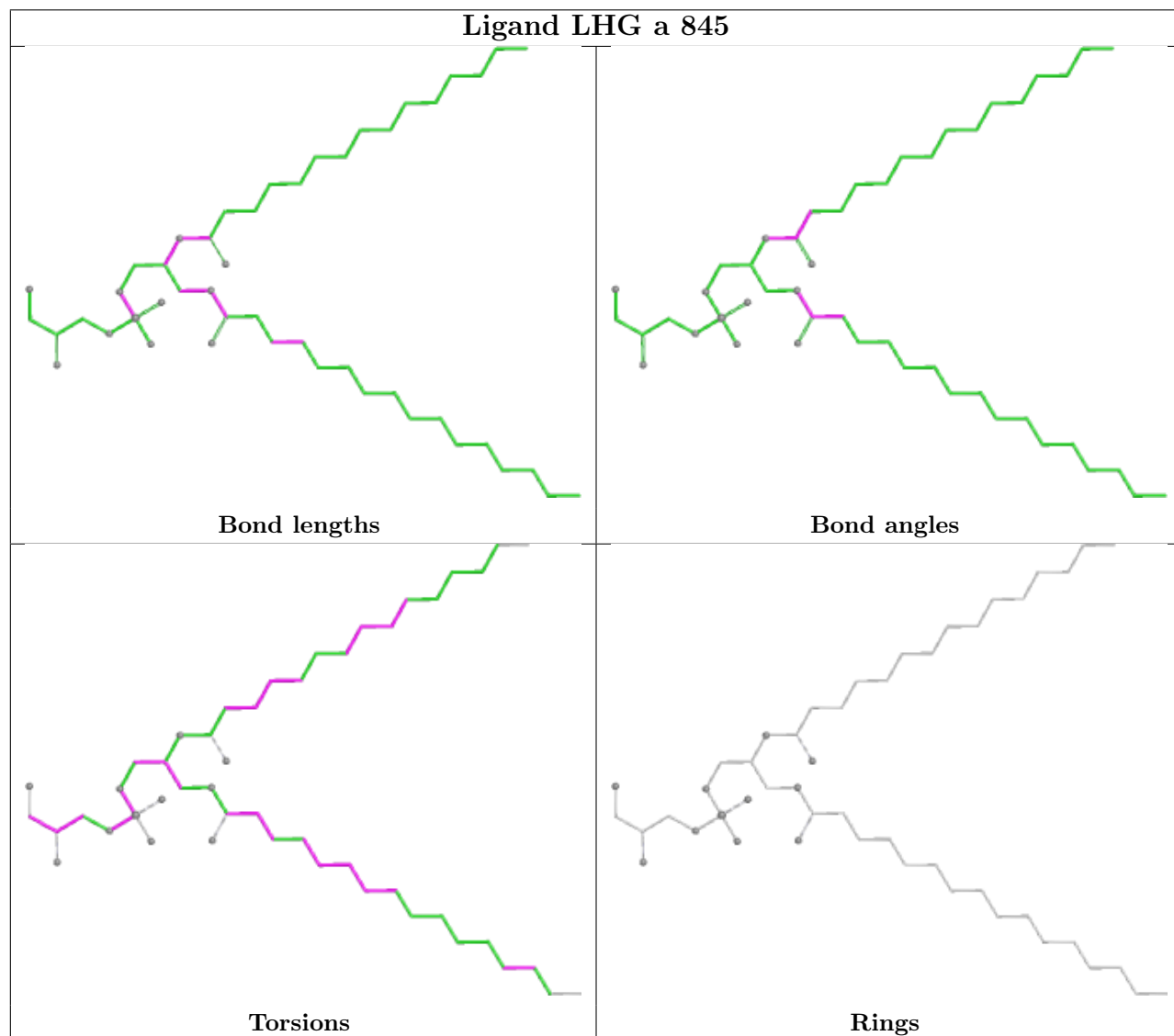
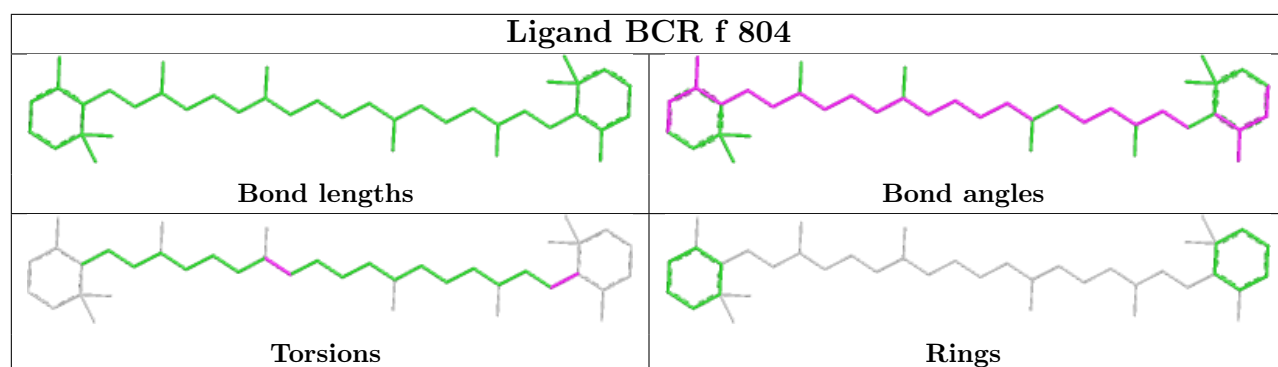
Bond angles

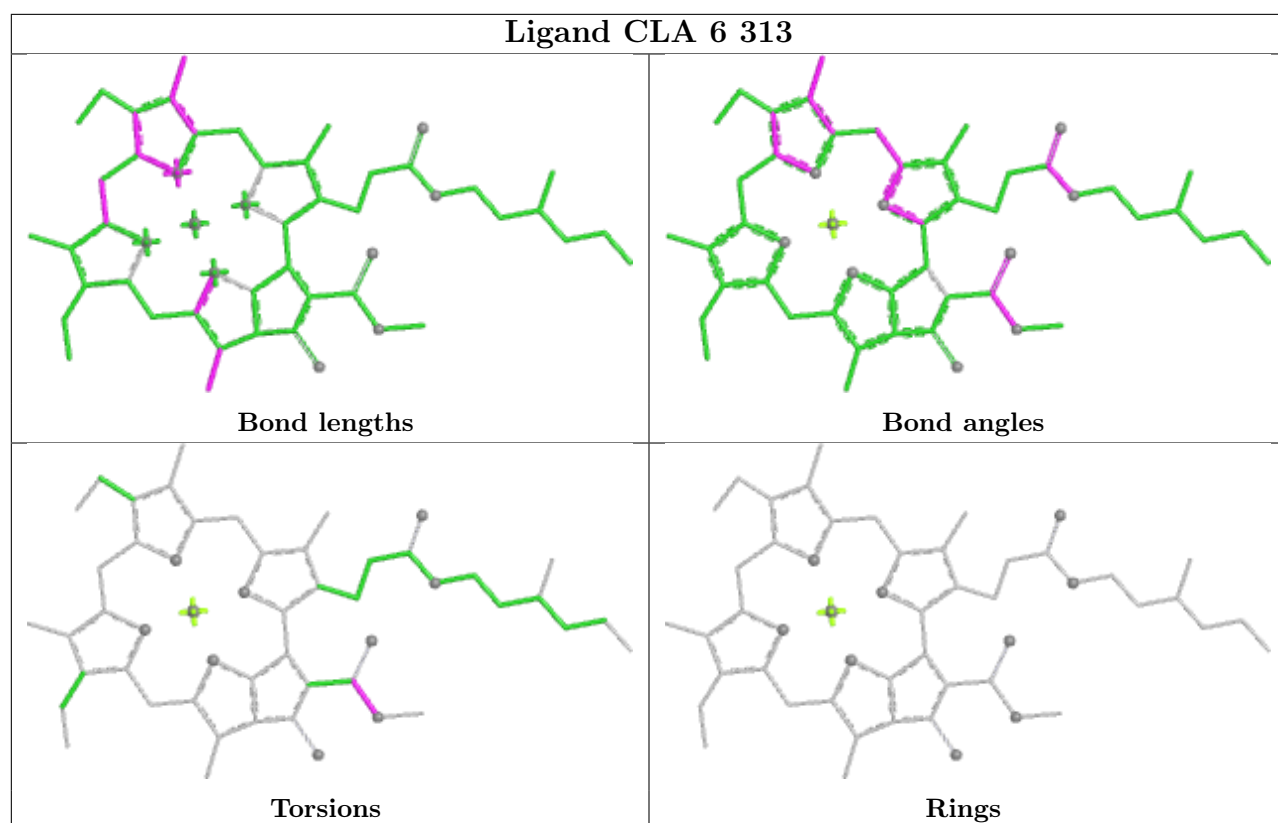


Torsions

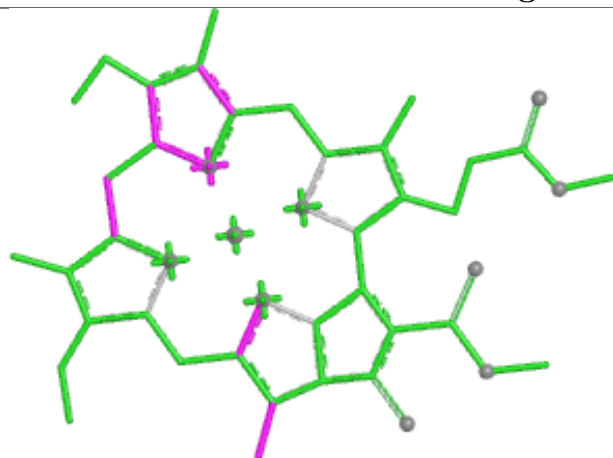


Rings

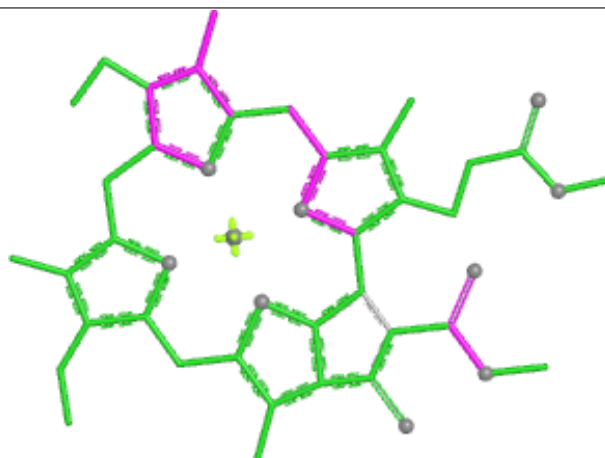




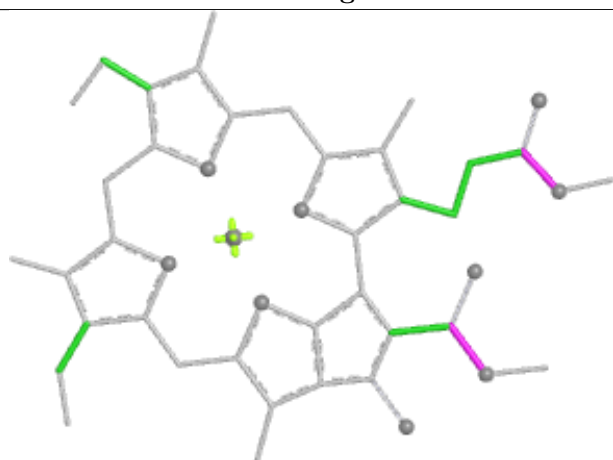
Ligand CLA 6 314



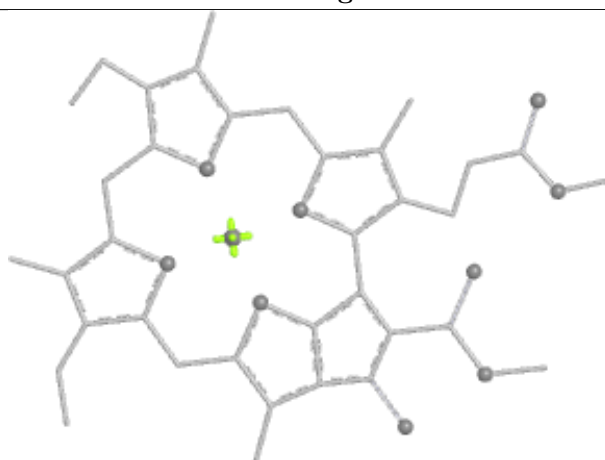
Bond lengths



Bond angles

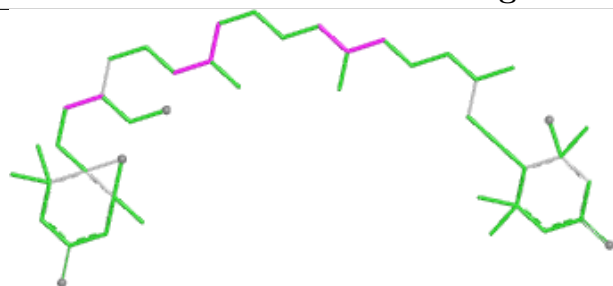


Torsions

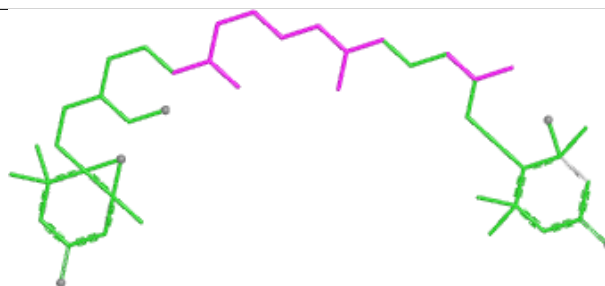


Rings

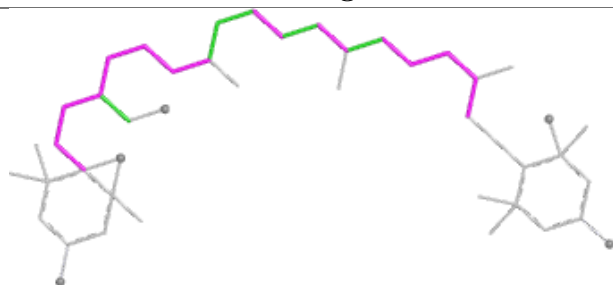
Ligand A1L1G 9 306



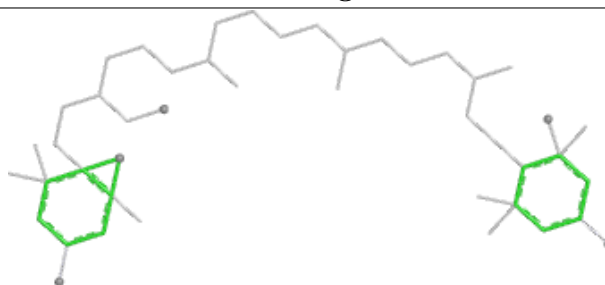
Bond lengths



Bond angles

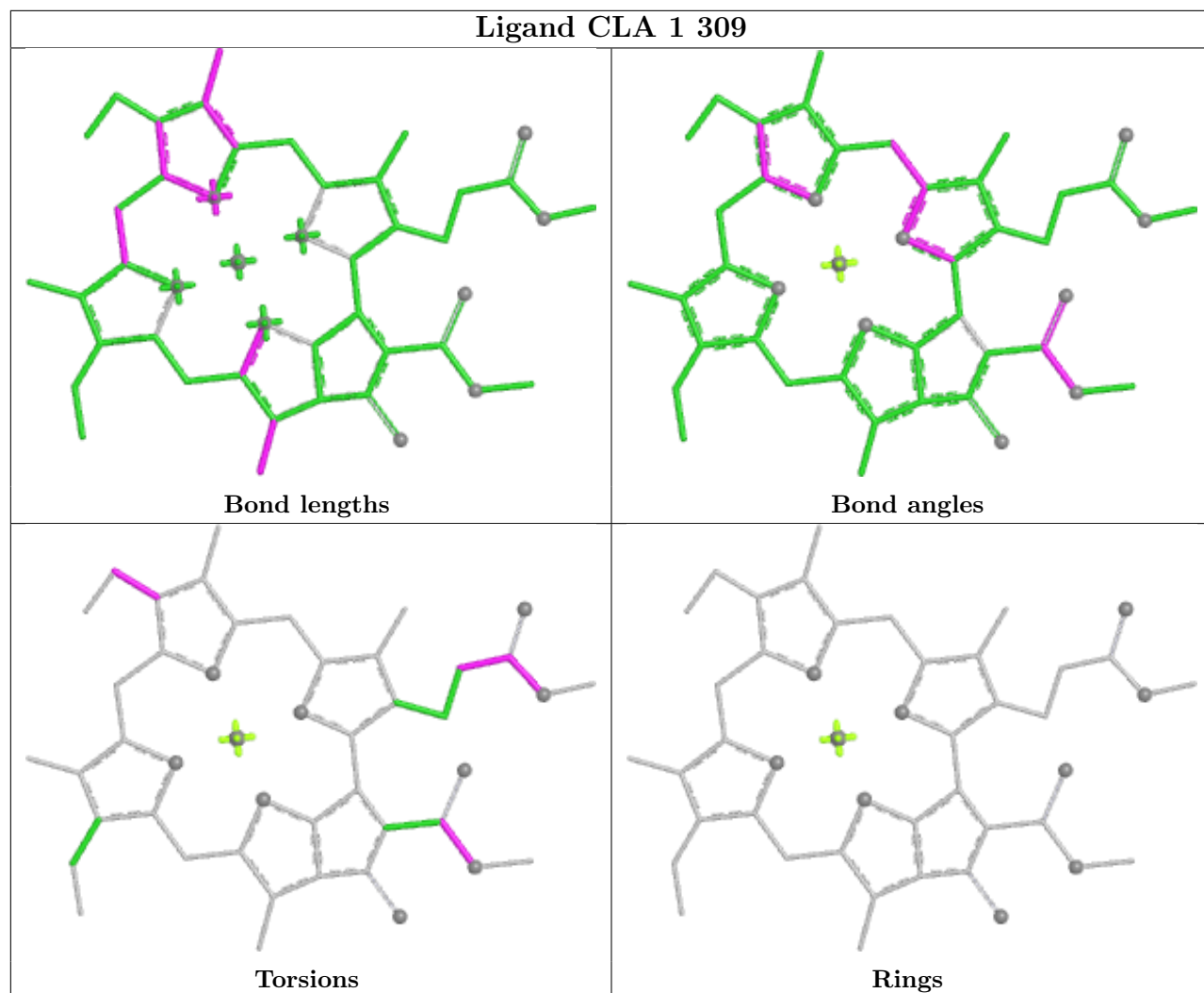


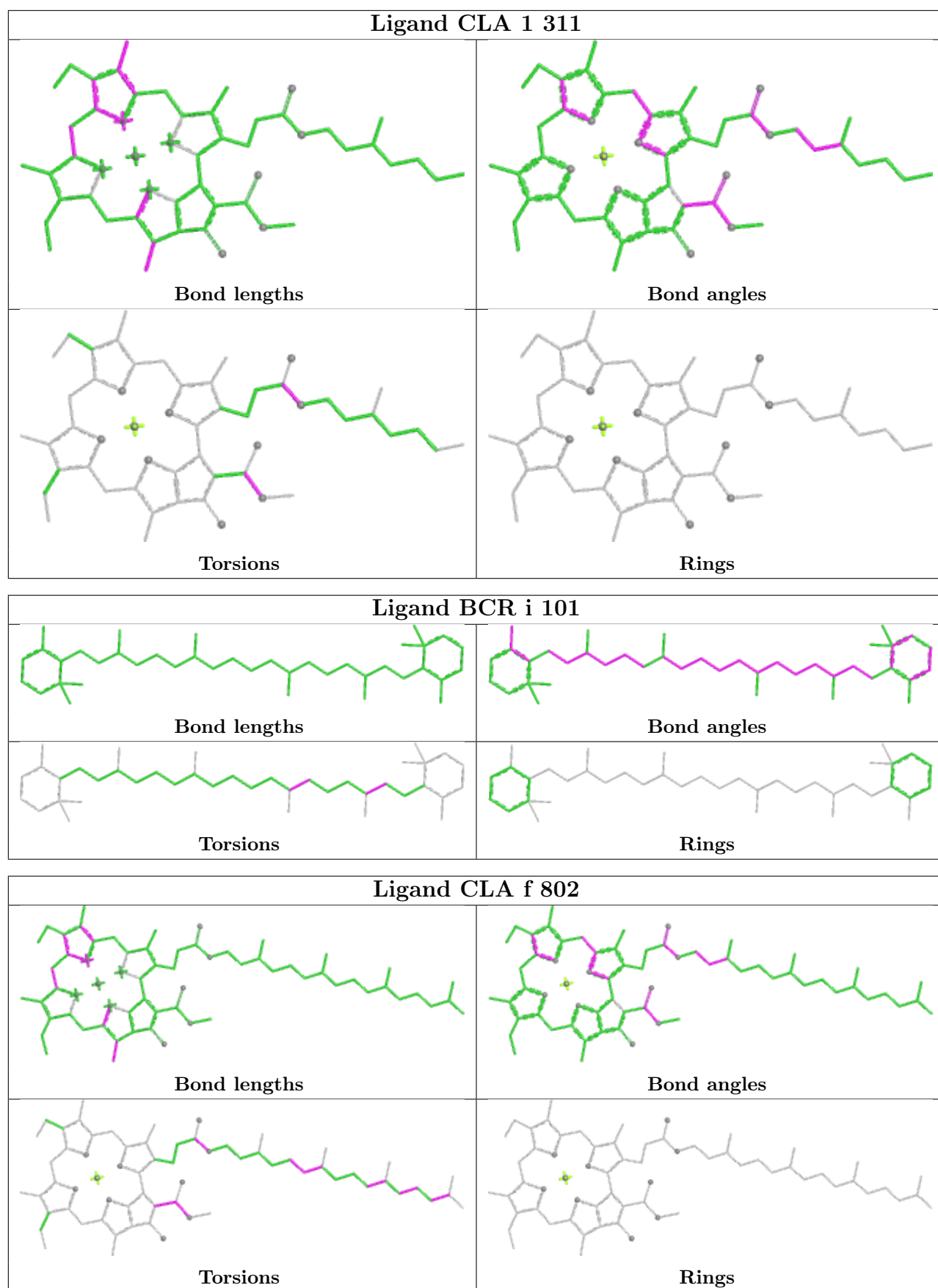
Torsions



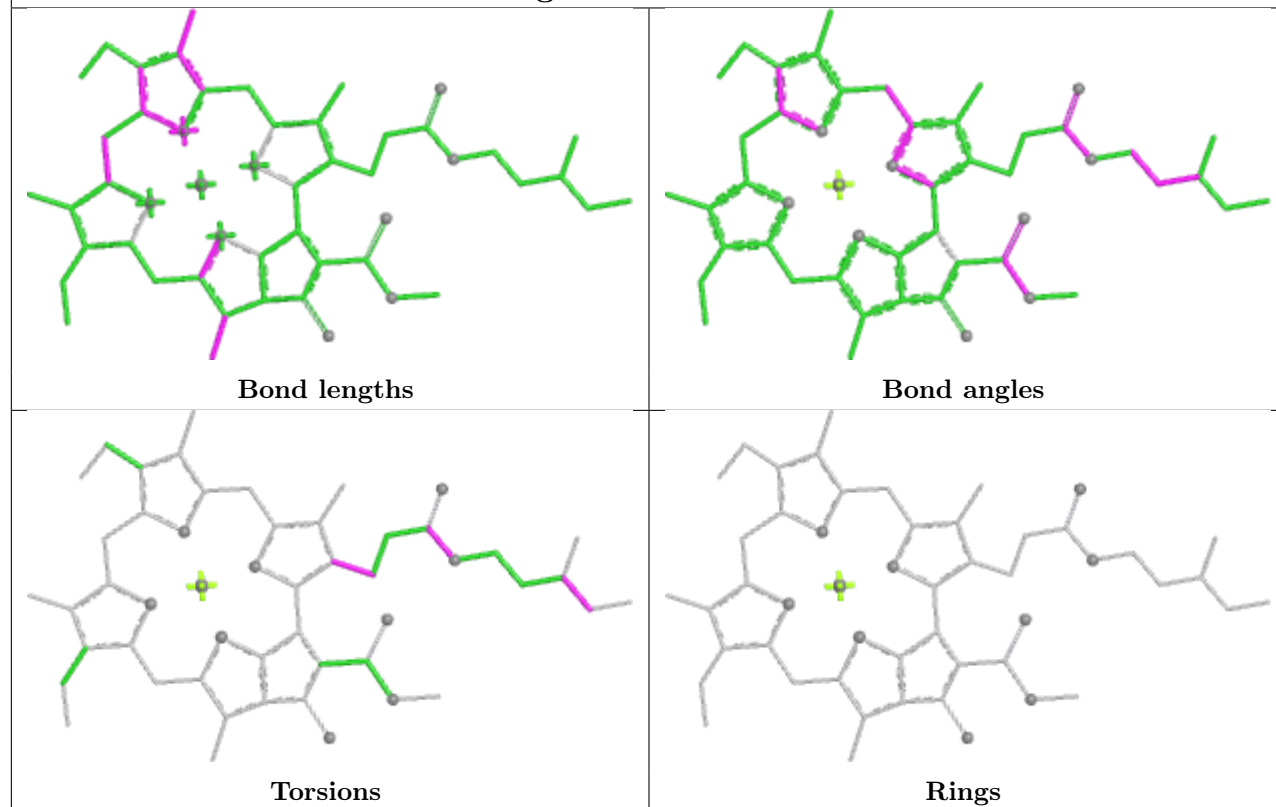
Rings

Ligand CLA 1 309

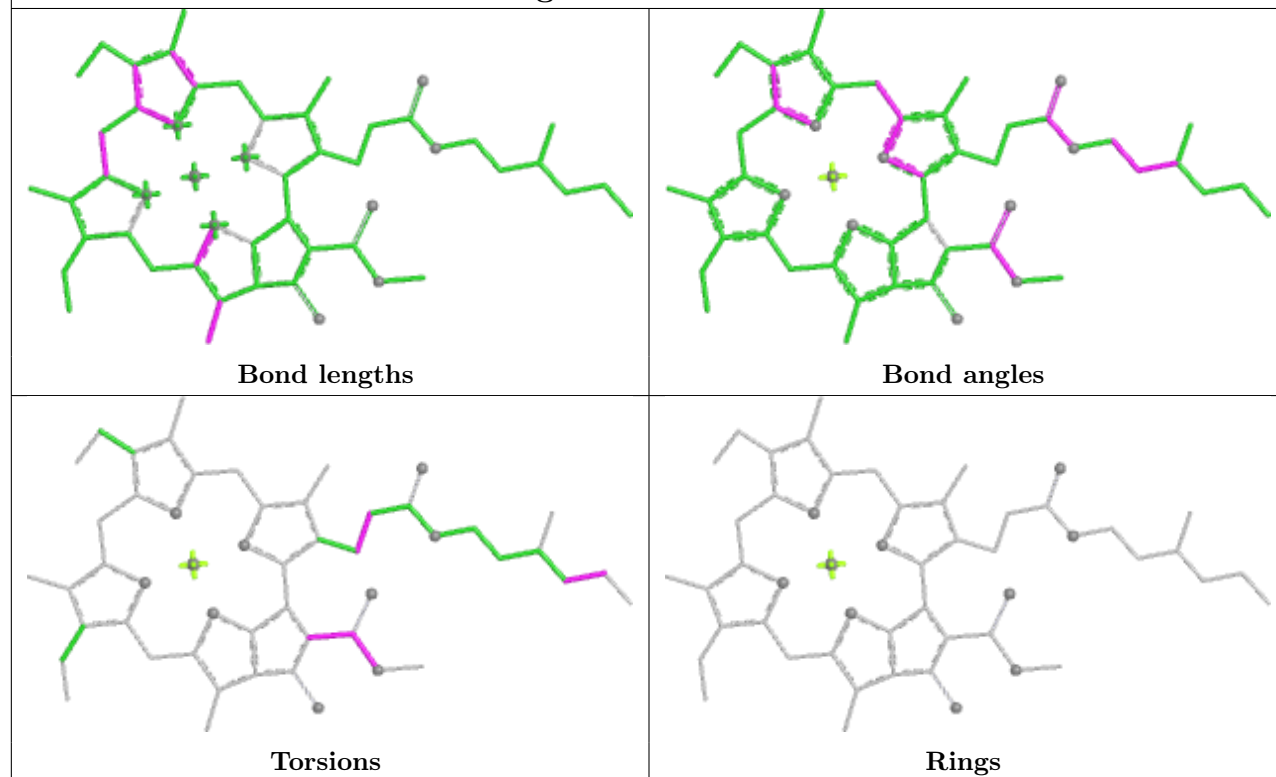




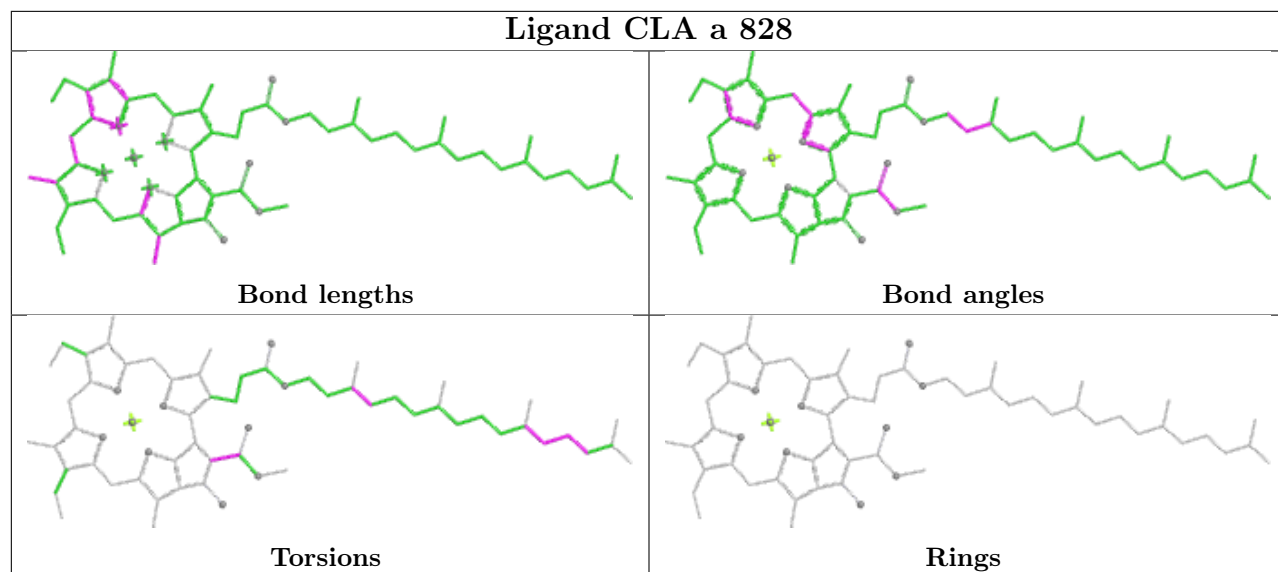
Ligand CLA a 838



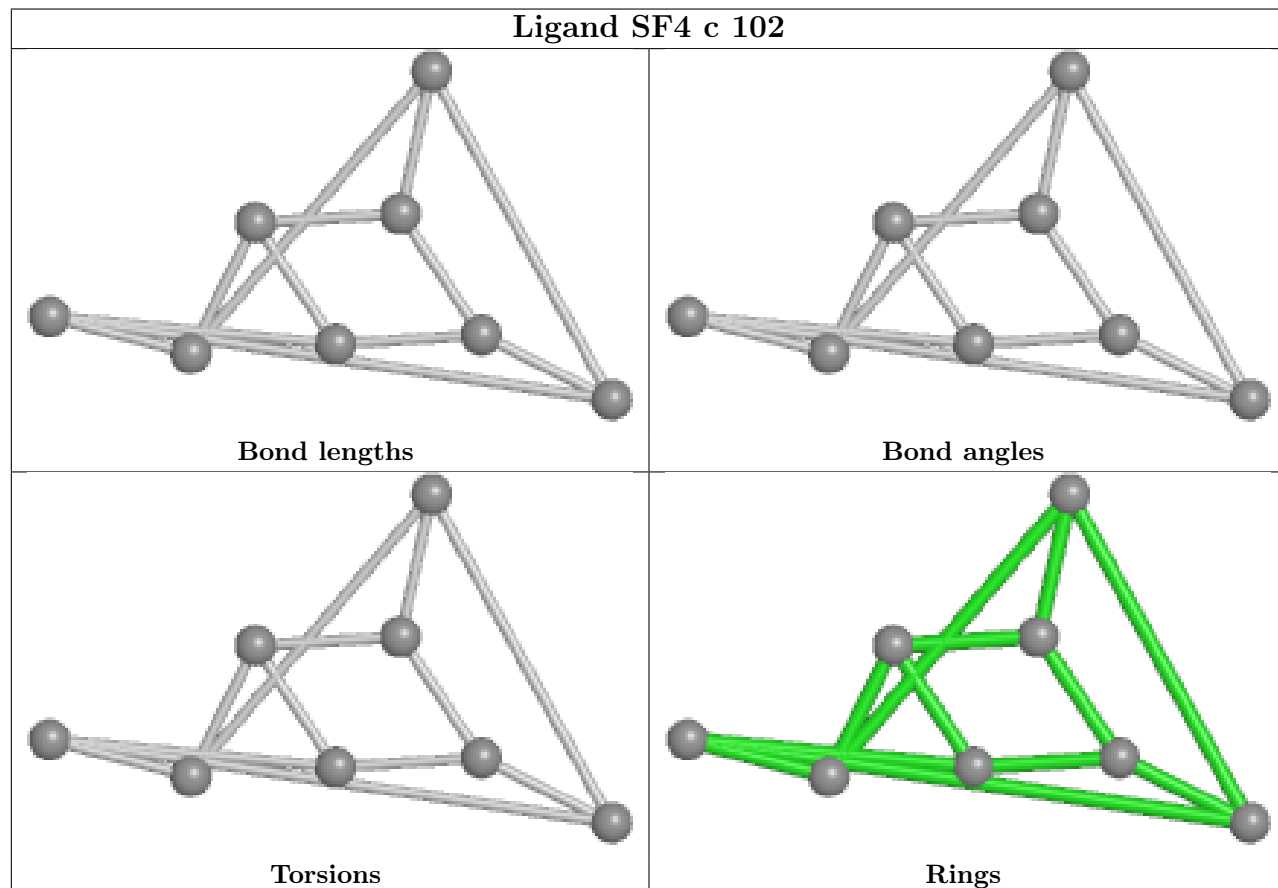
Ligand CLA 6 310



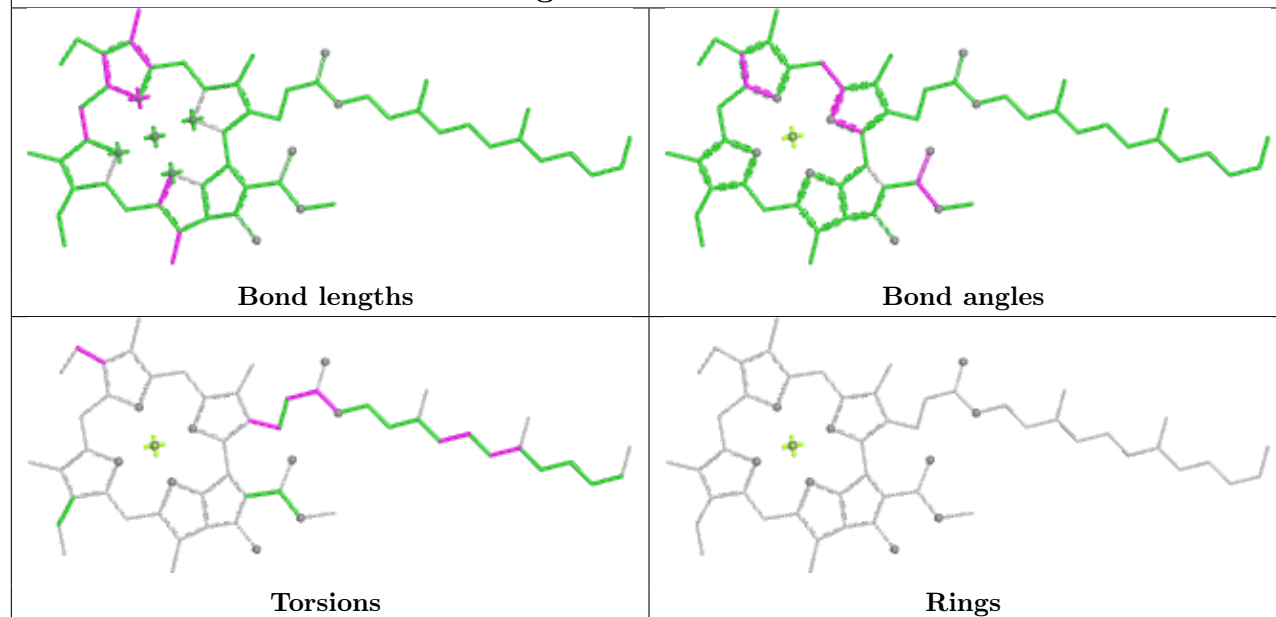
Ligand CLA a 828



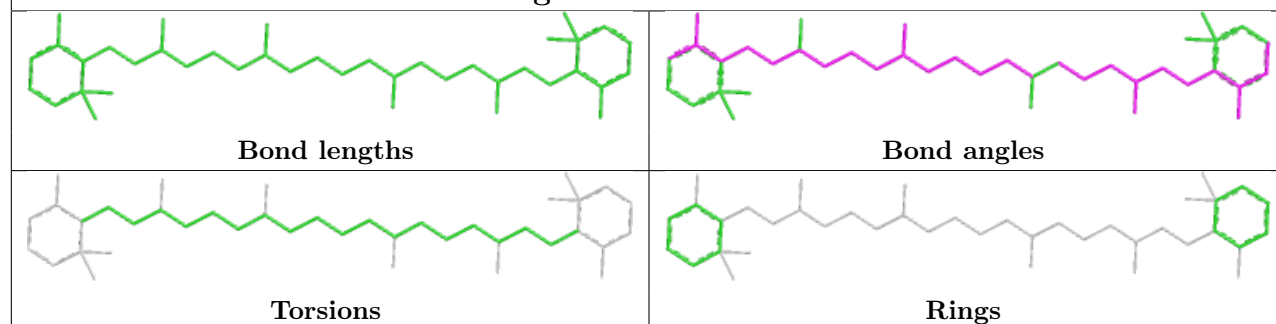
Ligand SF4 c 102



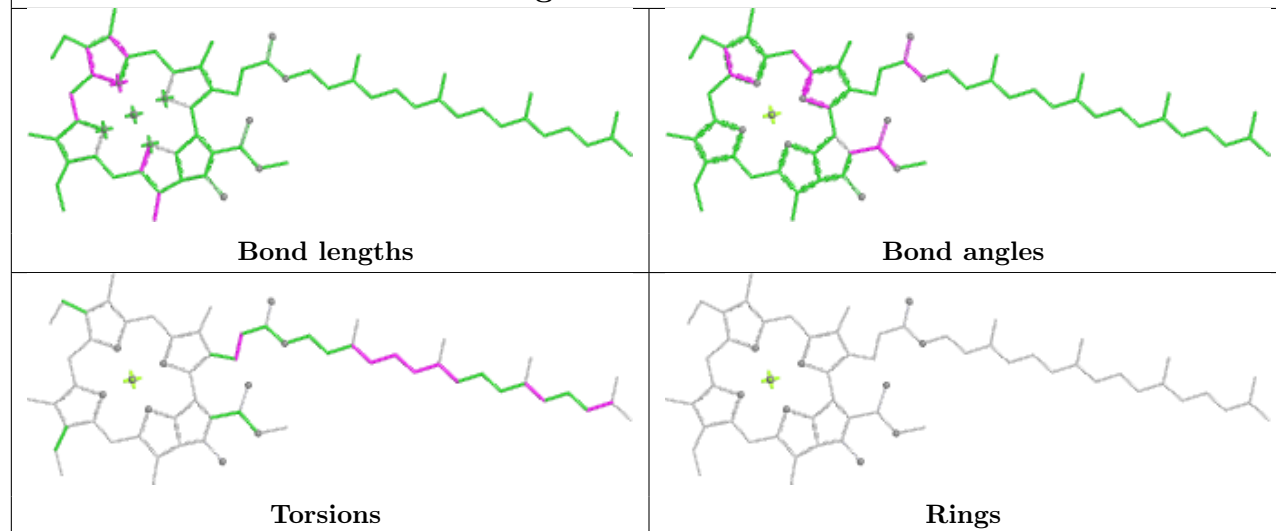
Ligand CLA 3 312



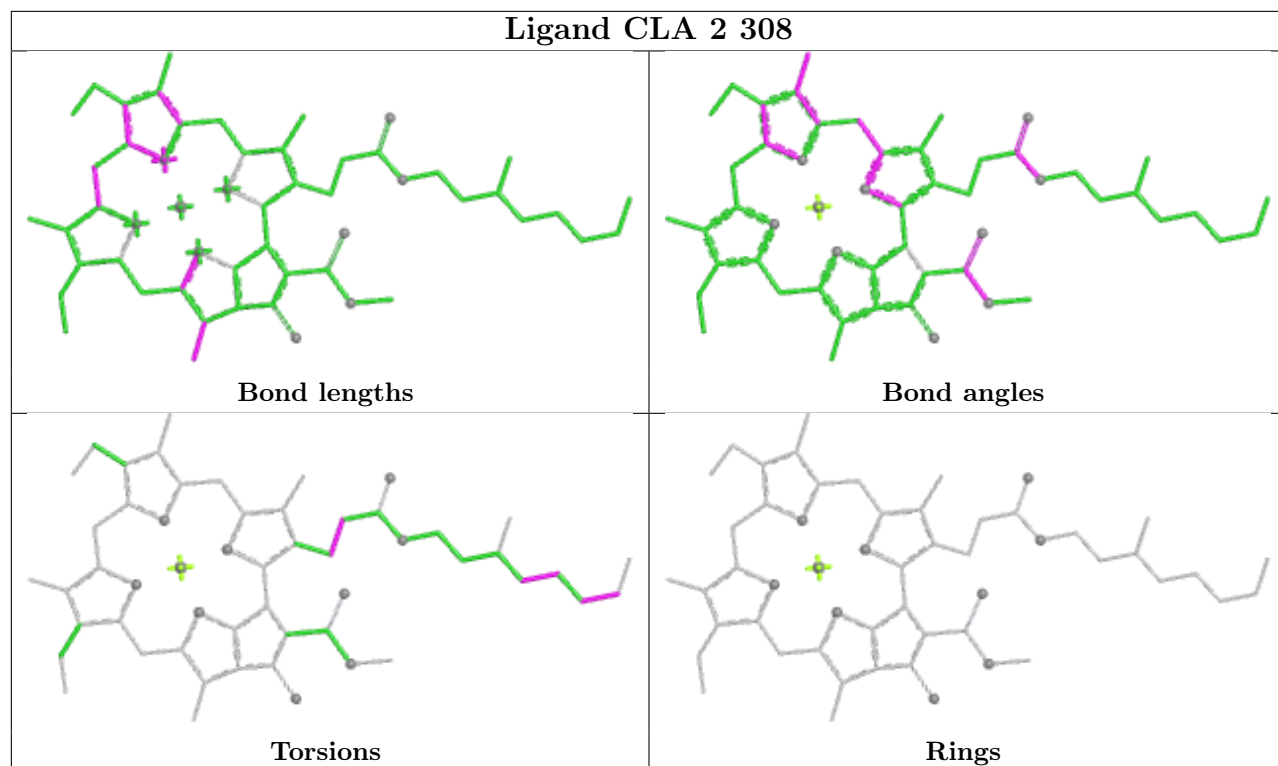
Ligand BCR h 202



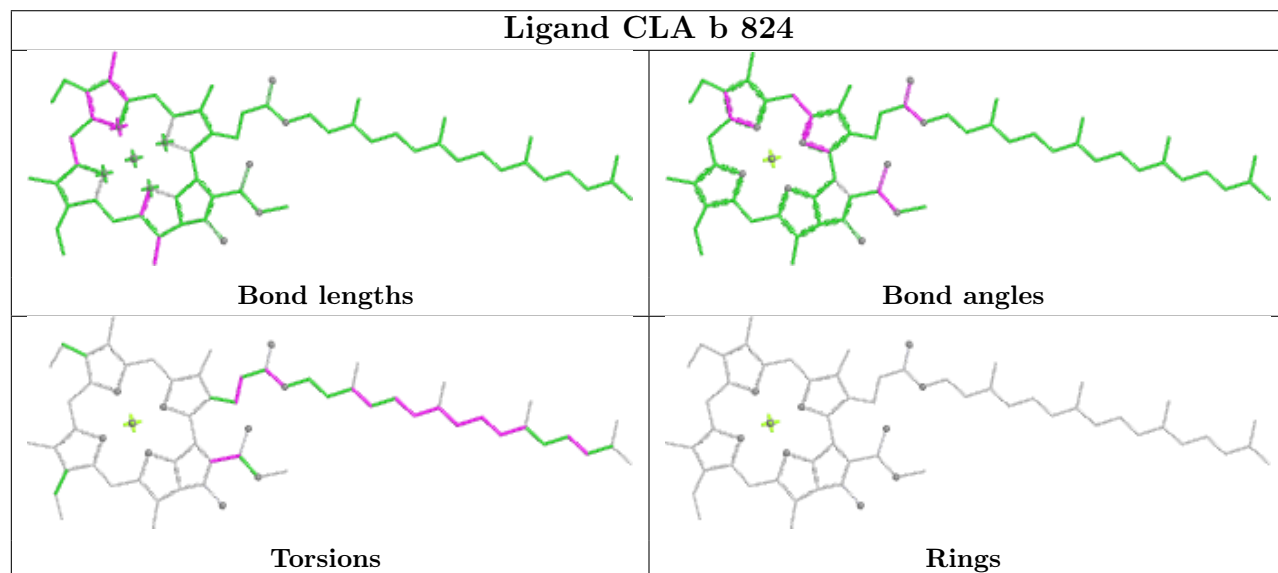
Ligand CLA b 808



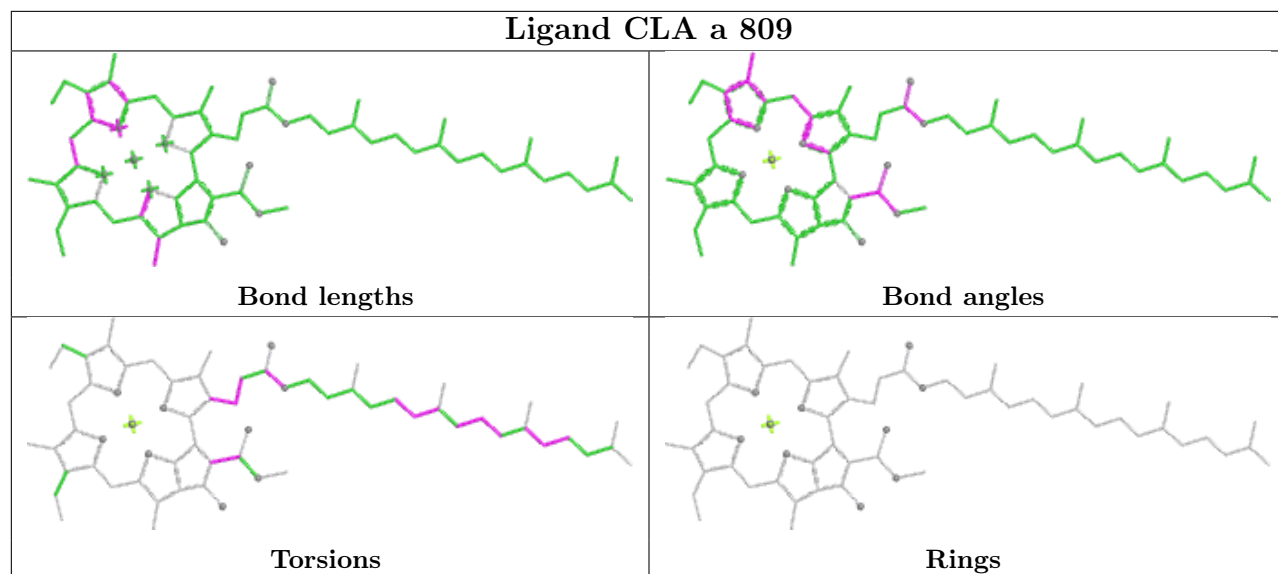
Ligand CLA 2 308



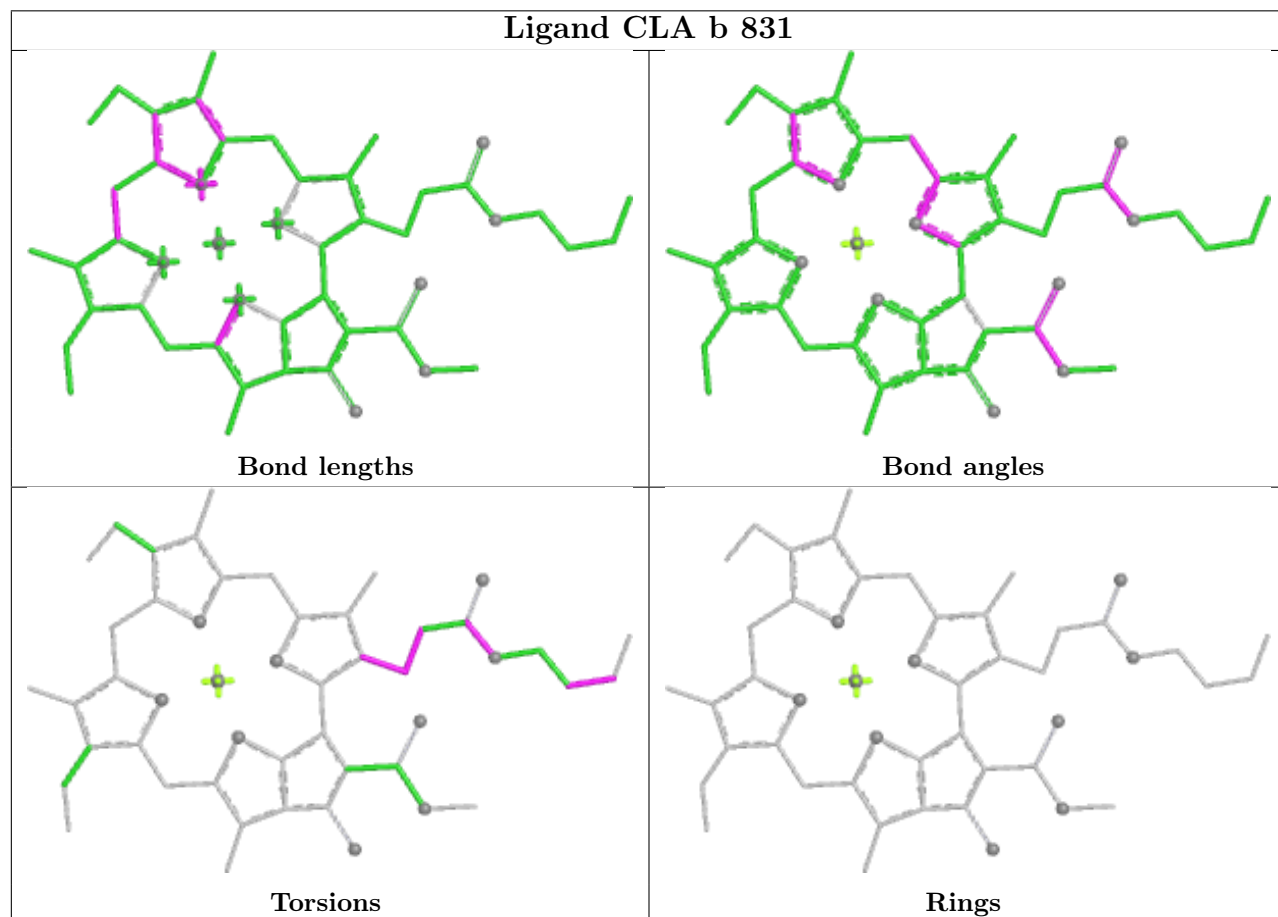
Ligand CLA b 824



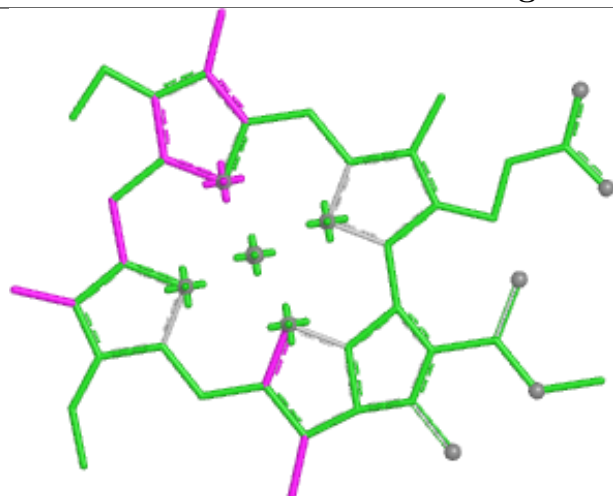
Ligand CLA a 809



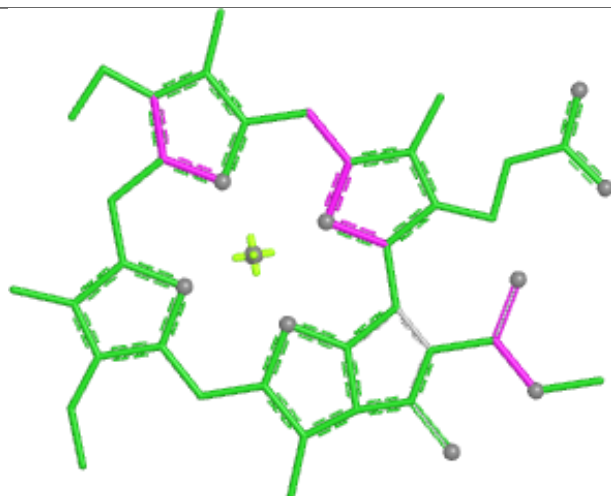
Ligand CLA b 831



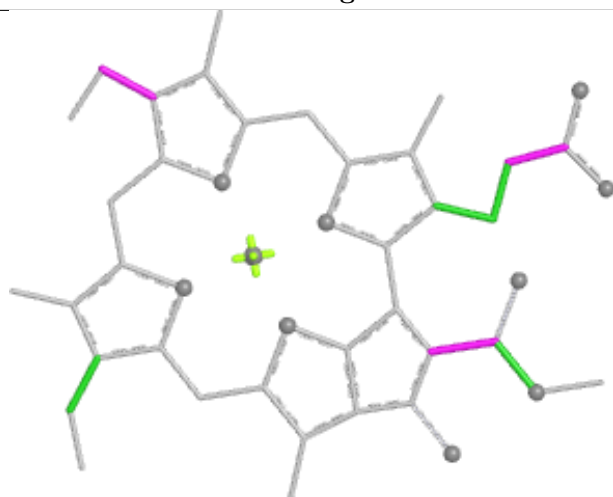
Ligand CLA 4 314



Bond lengths



Bond angles

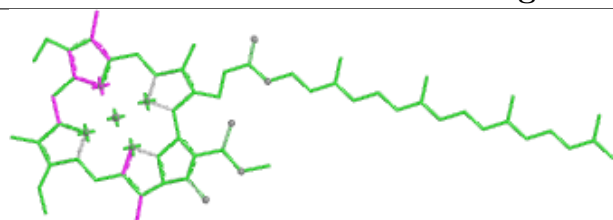


Torsions

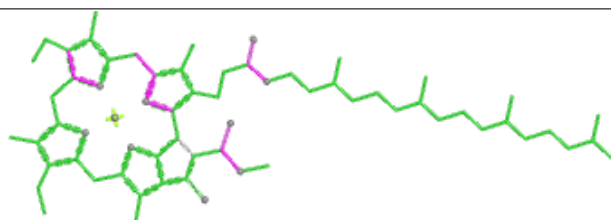


Rings

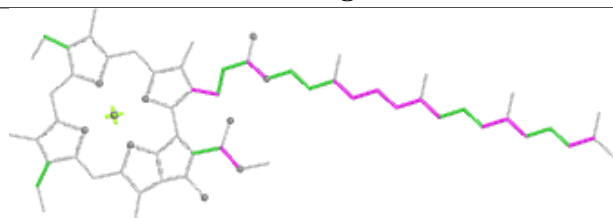
Ligand CLA 1 310



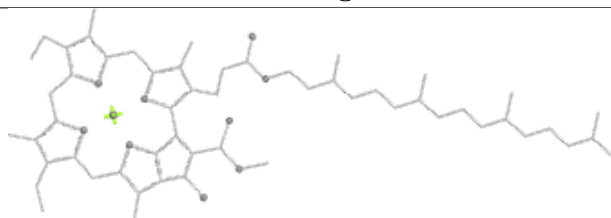
Bond lengths



Bond angles

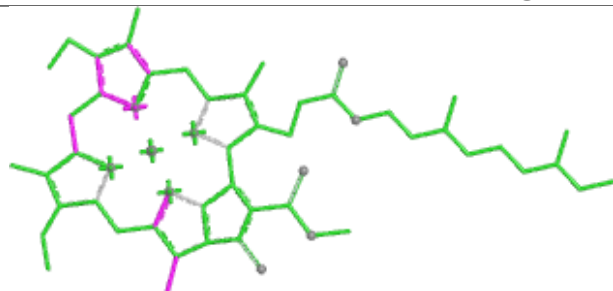


Torsions

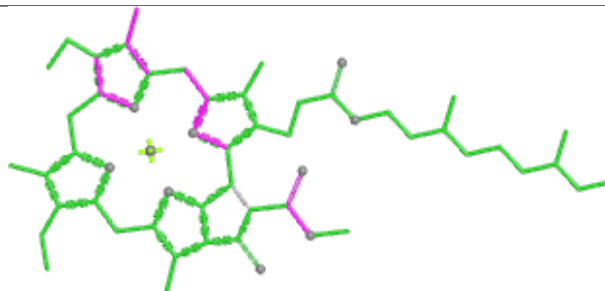


Rings

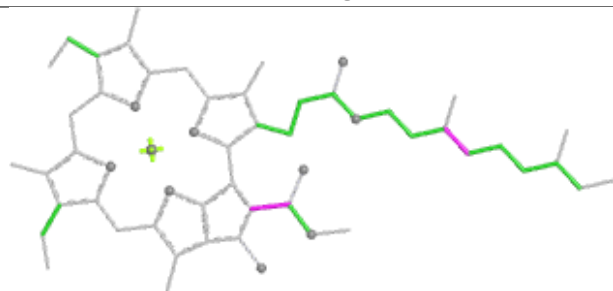
Ligand CLA 3 310



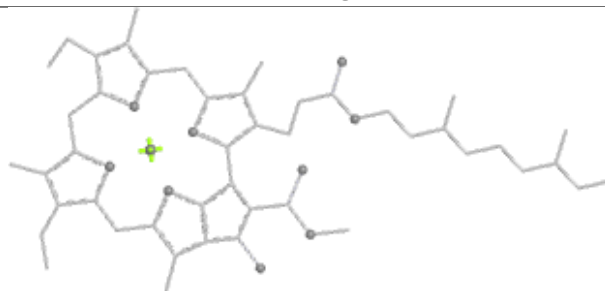
Bond lengths



Bond angles

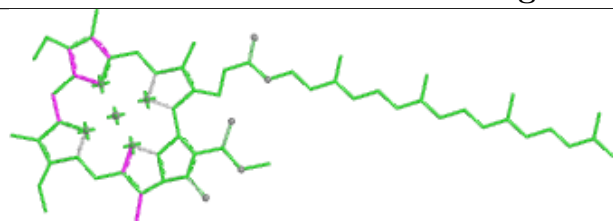


Torsions

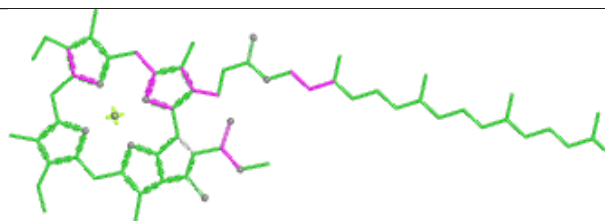


Rings

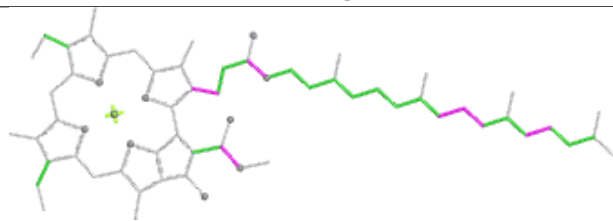
Ligand CLA 6 317



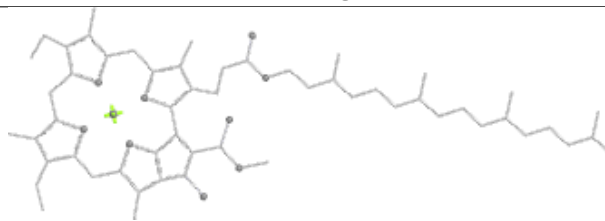
Bond lengths



Bond angles

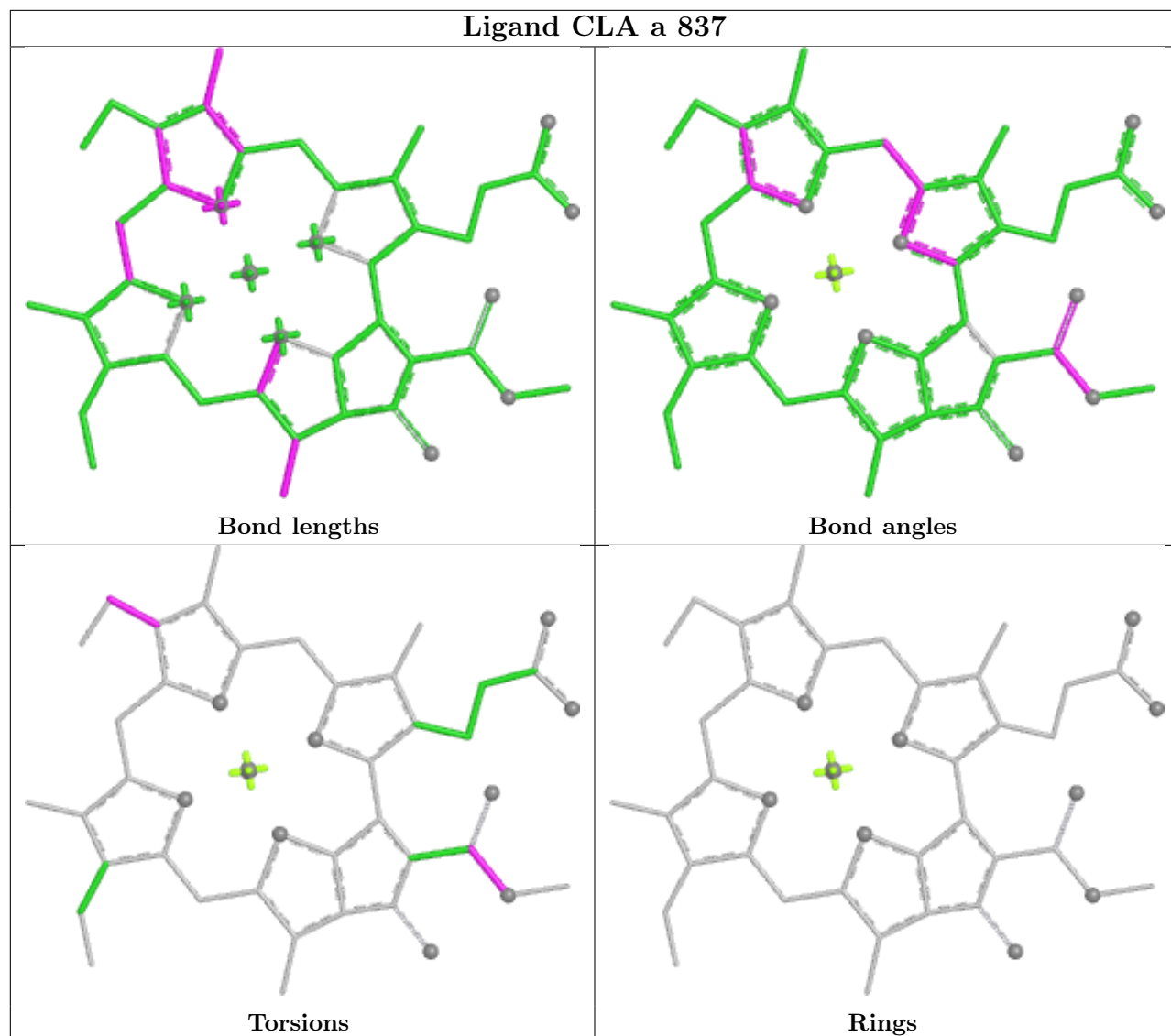


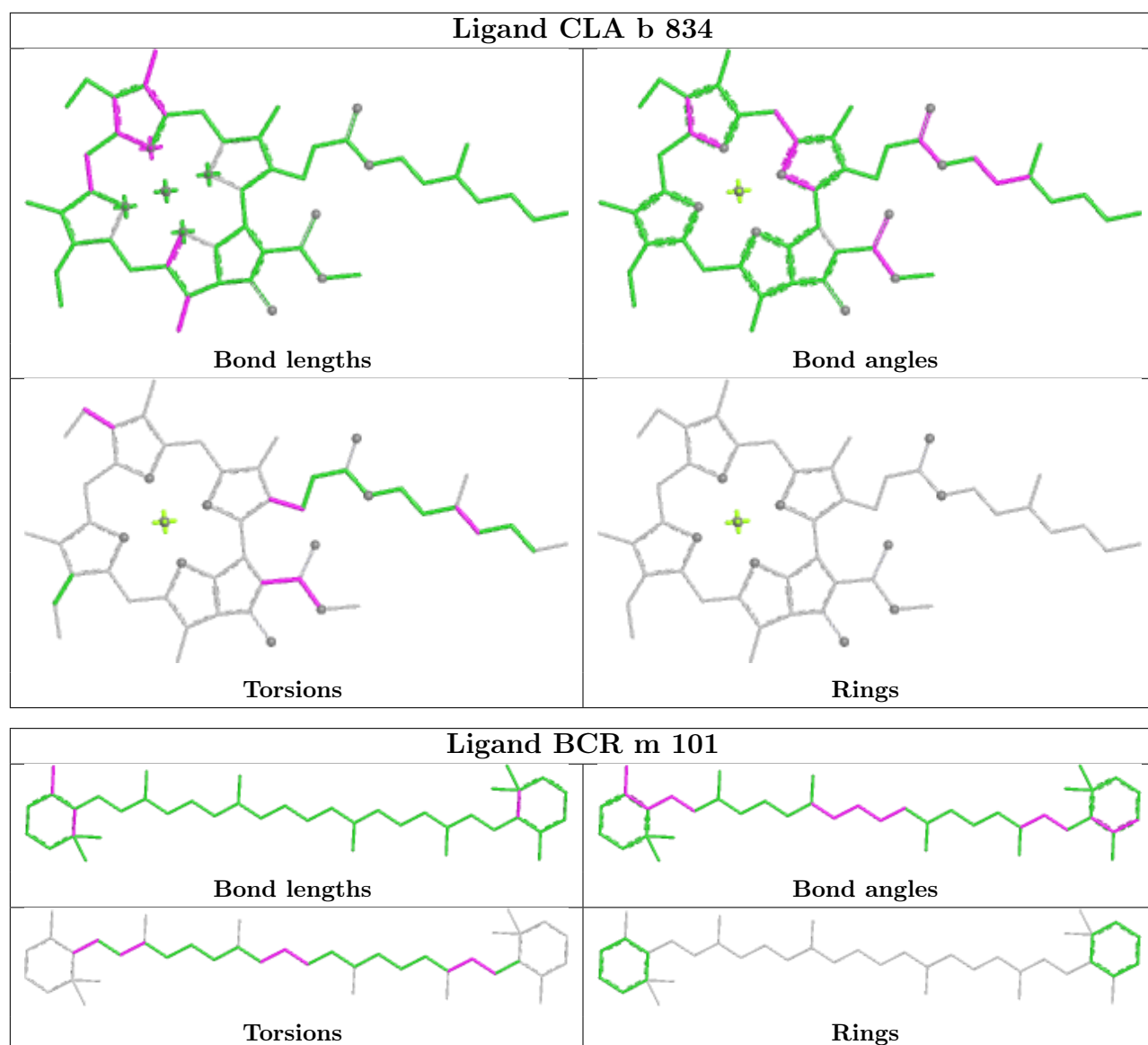
Torsions



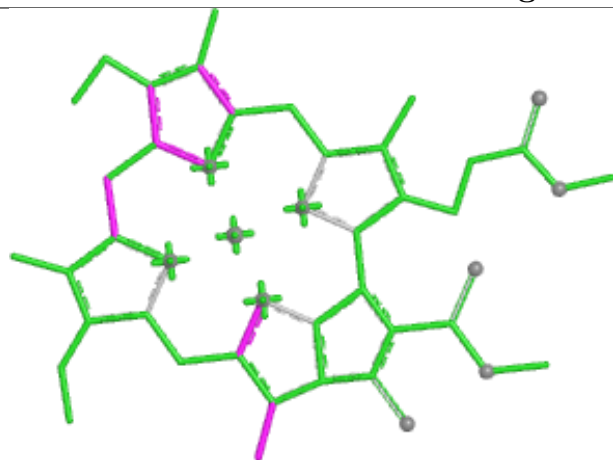
Rings

Ligand CLA a 837

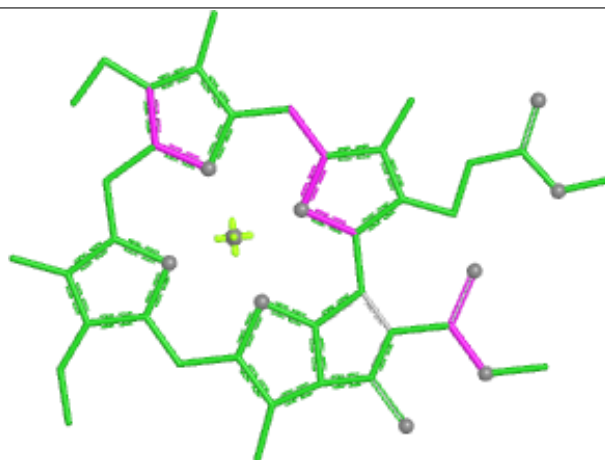




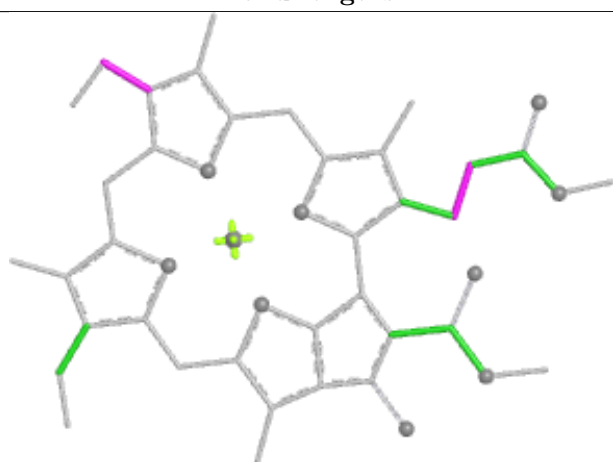
Ligand CLA 6 307



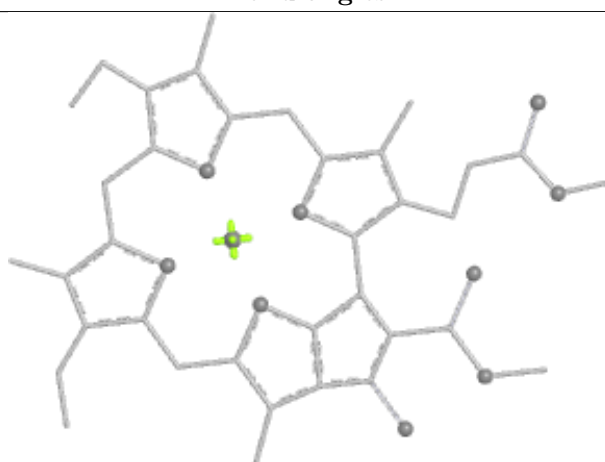
Bond lengths



Bond angles

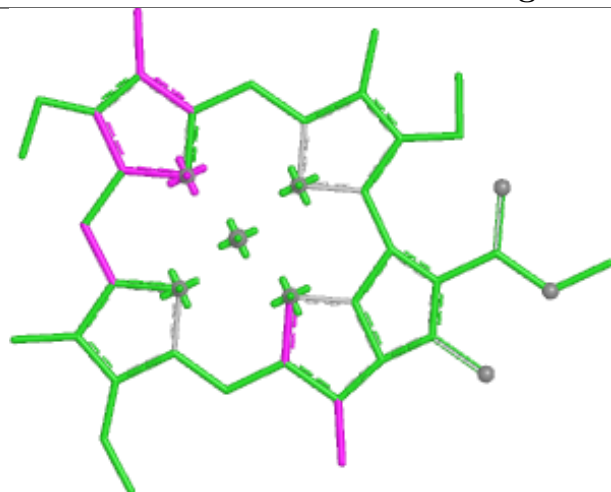


Torsions

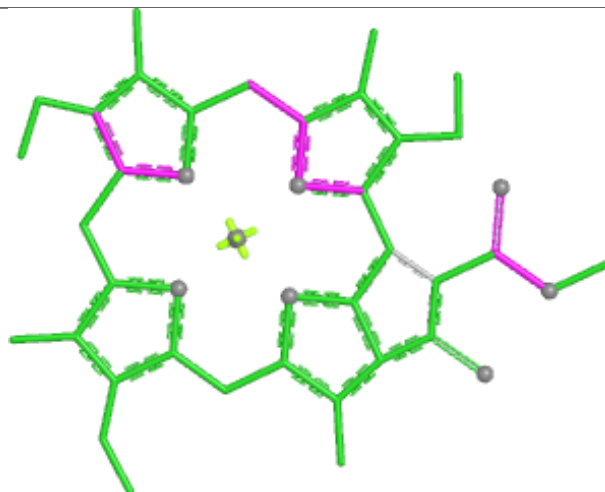


Rings

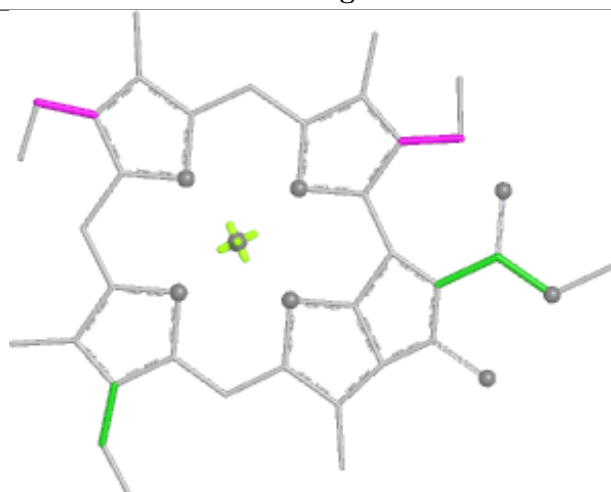
Ligand CLA 2 315



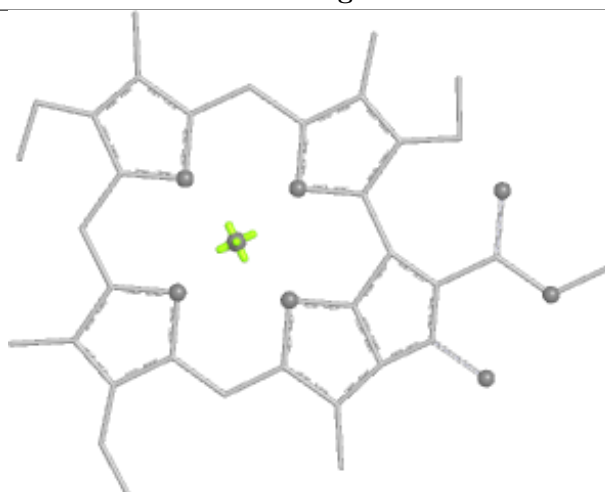
Bond lengths



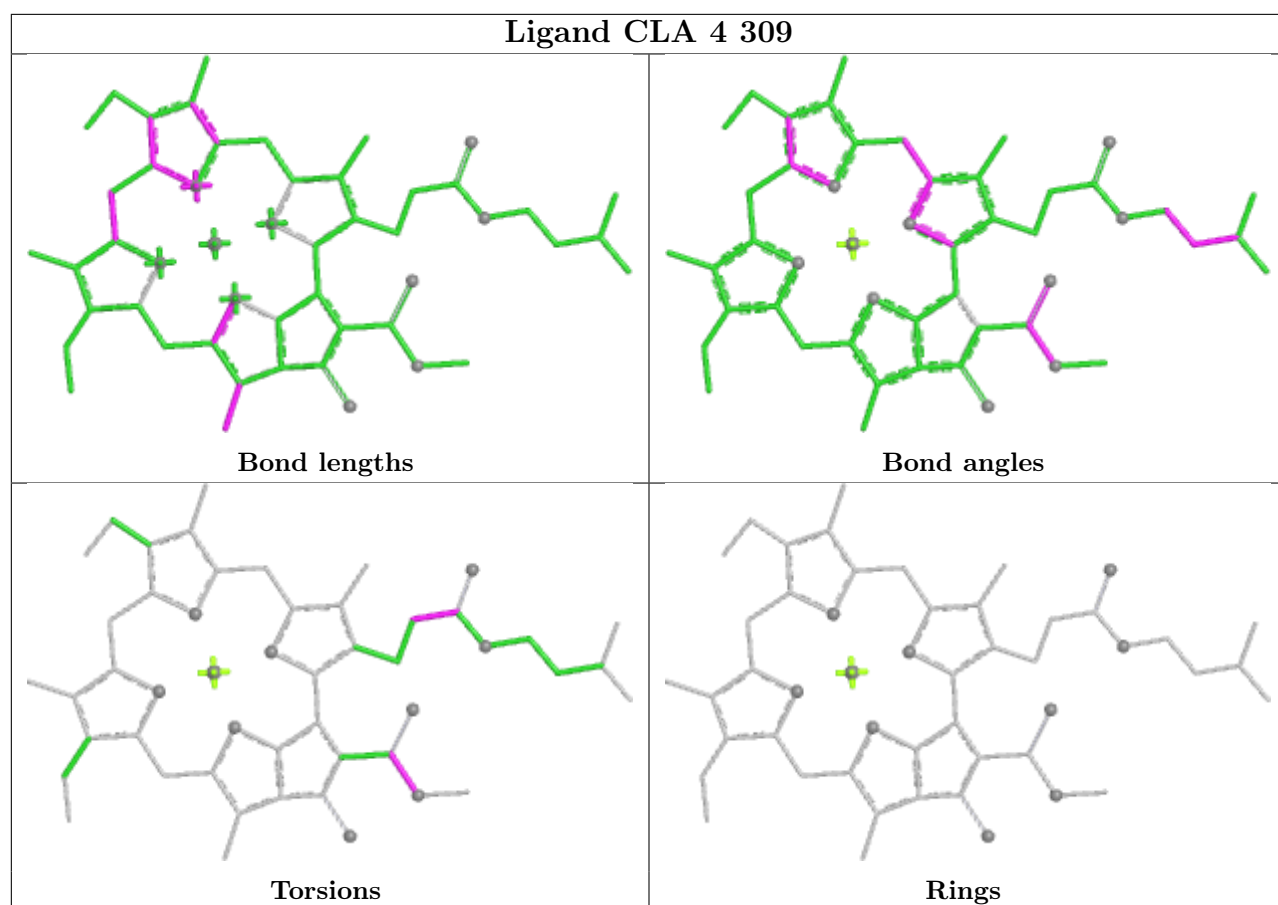
Bond angles



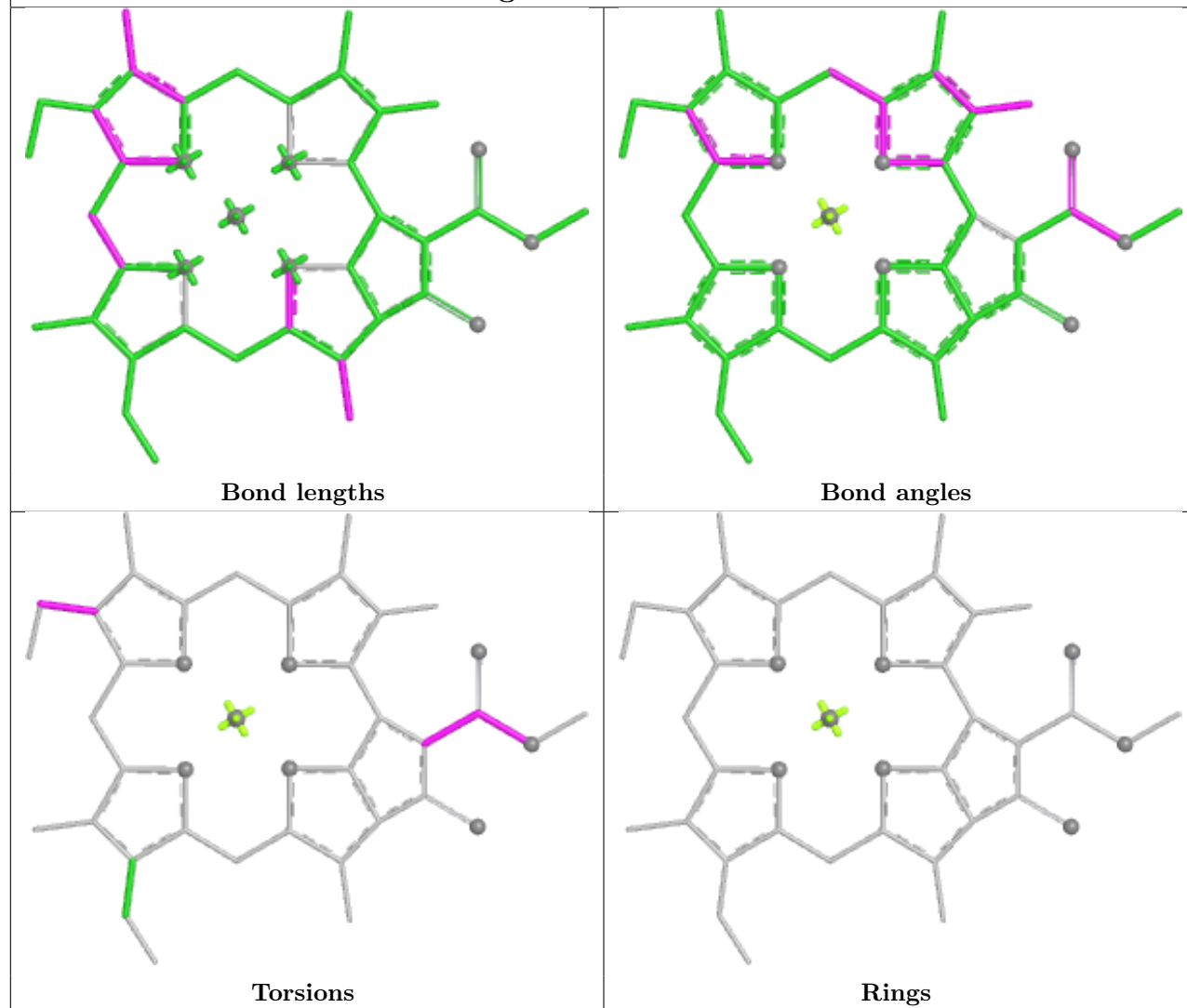
Torsions



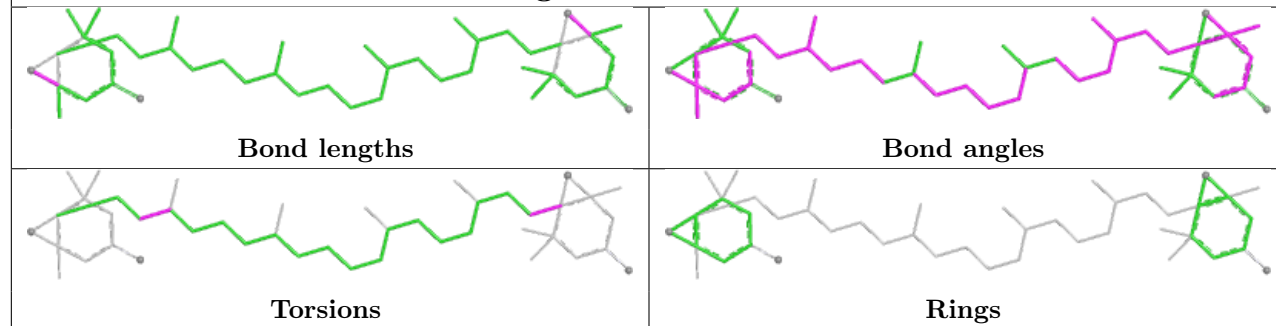
Rings

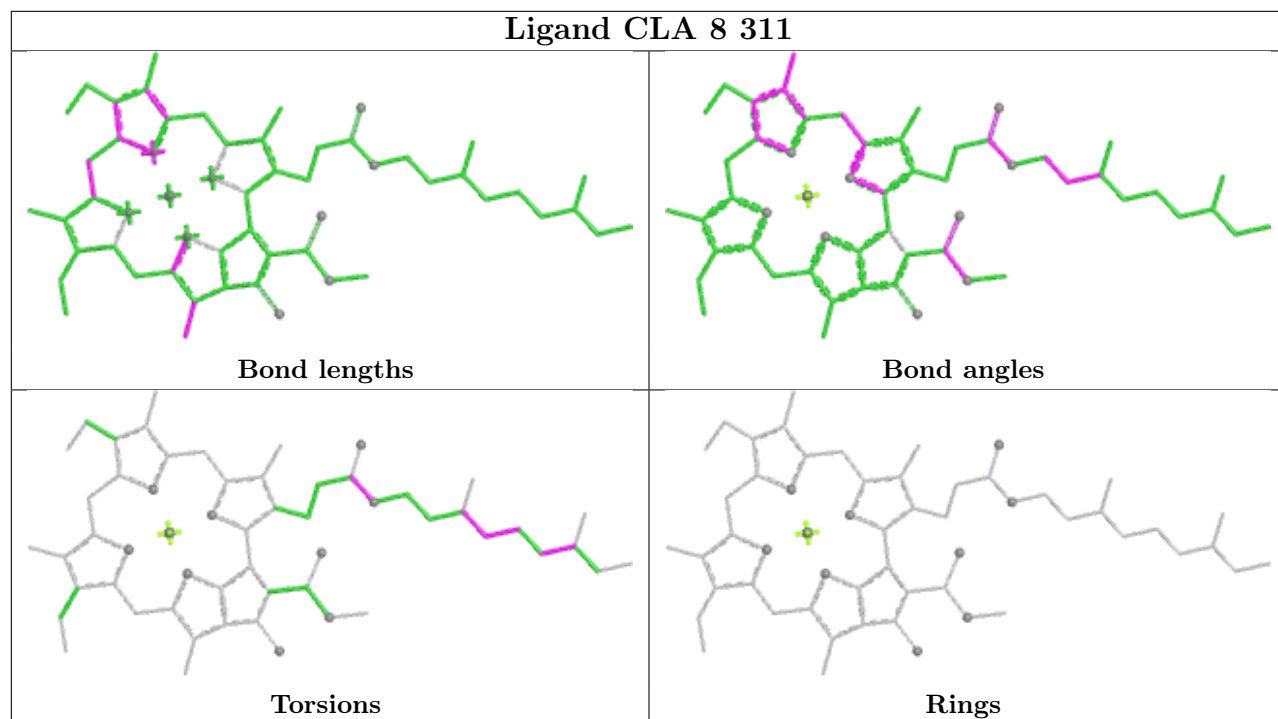
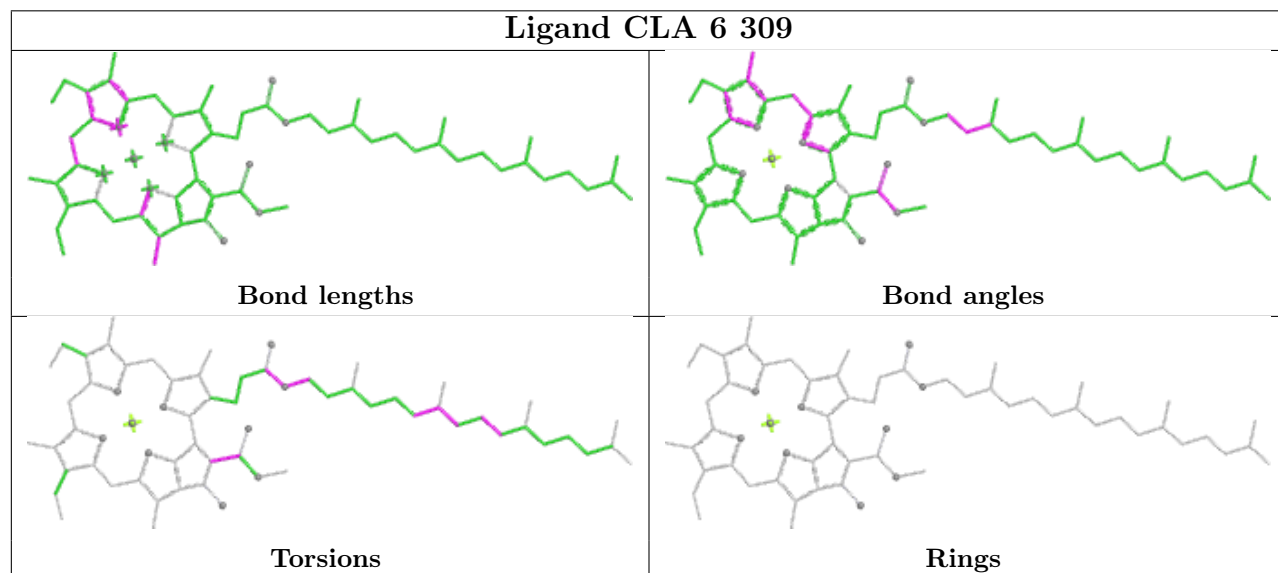
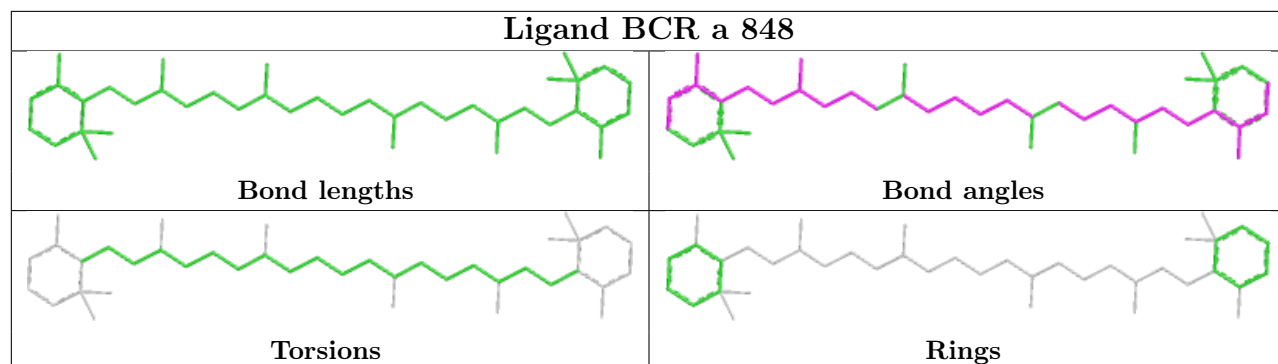


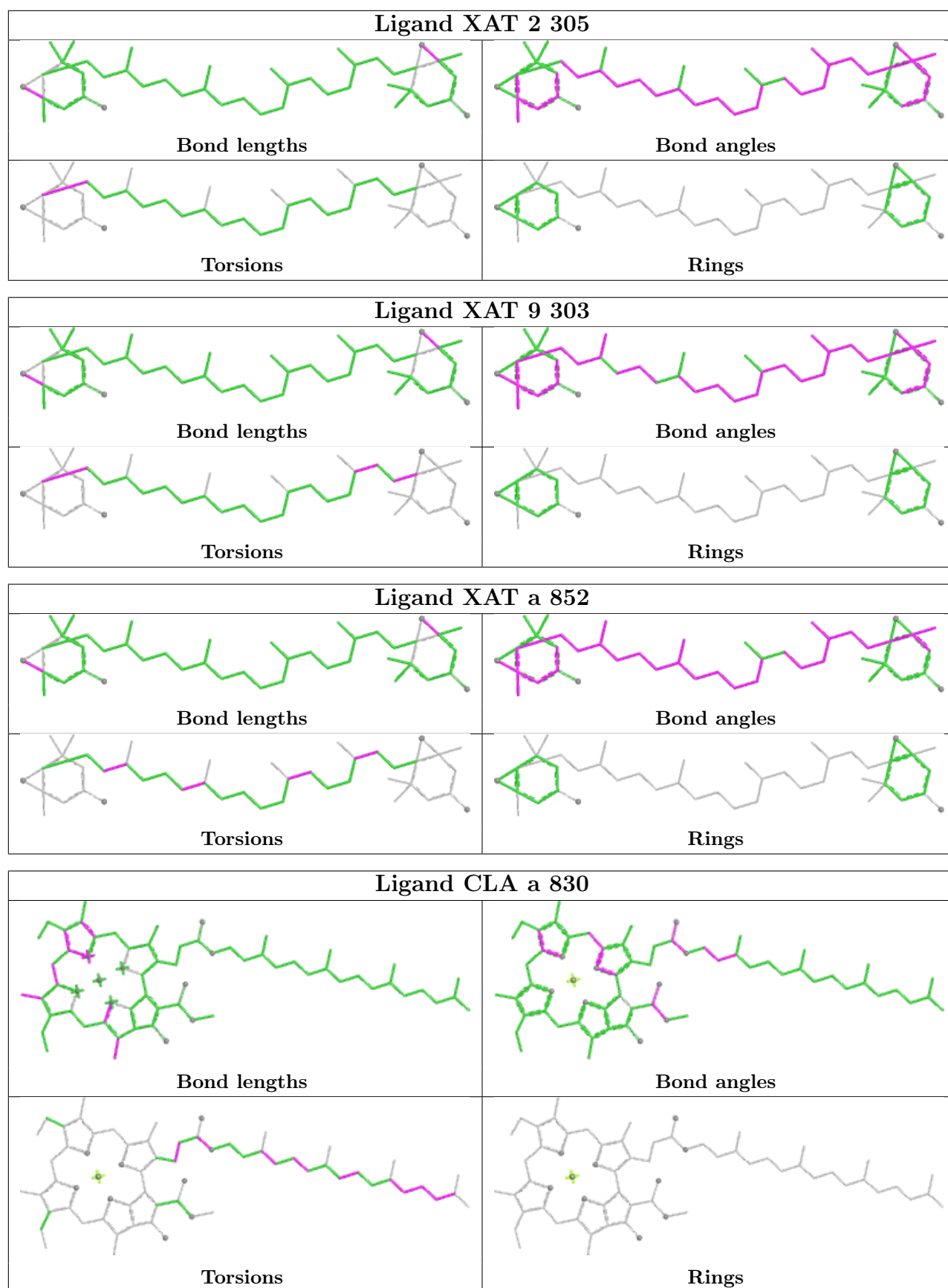
Ligand CLA 4 315



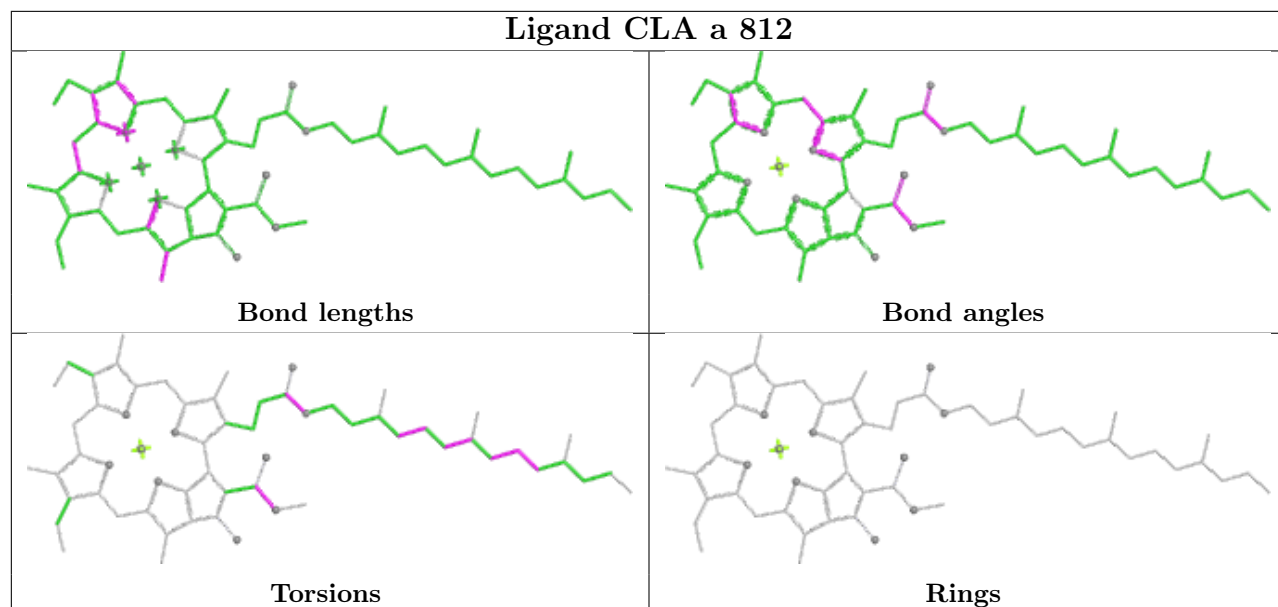
Ligand XAT 3 303



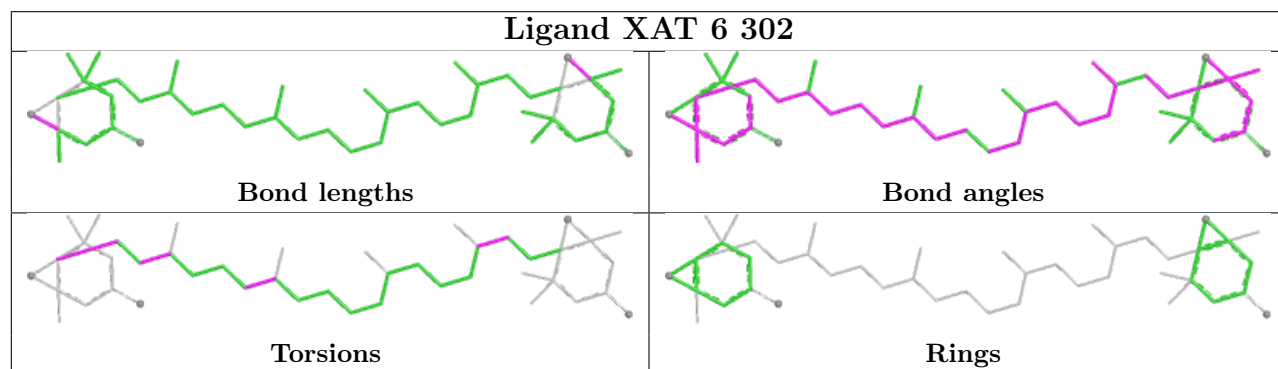




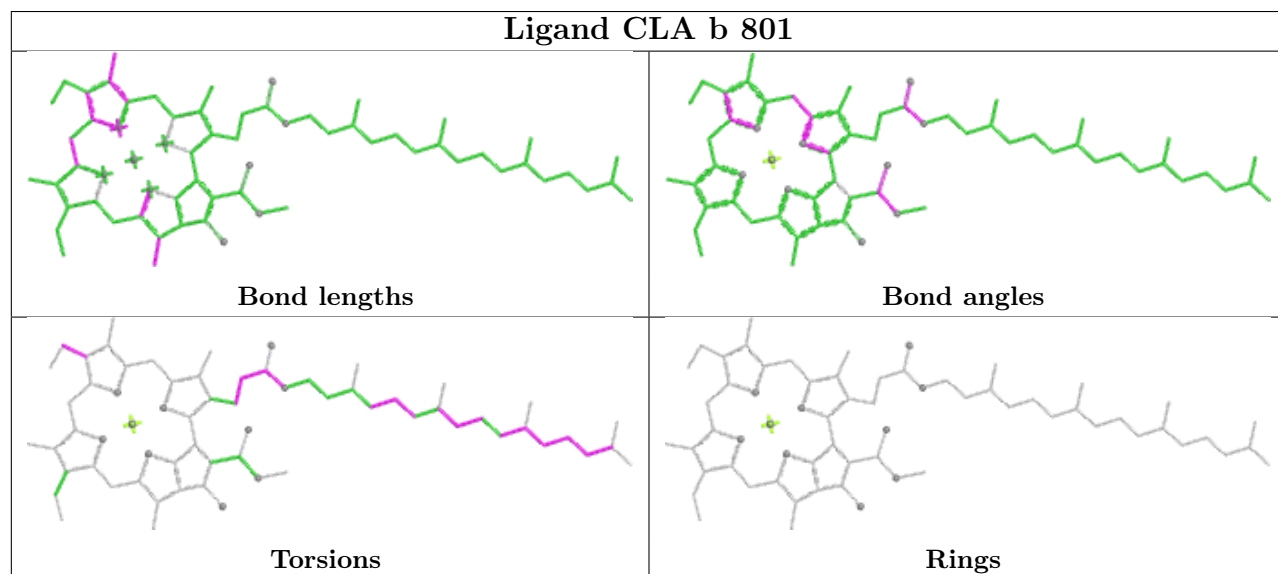
Ligand CLA a 812

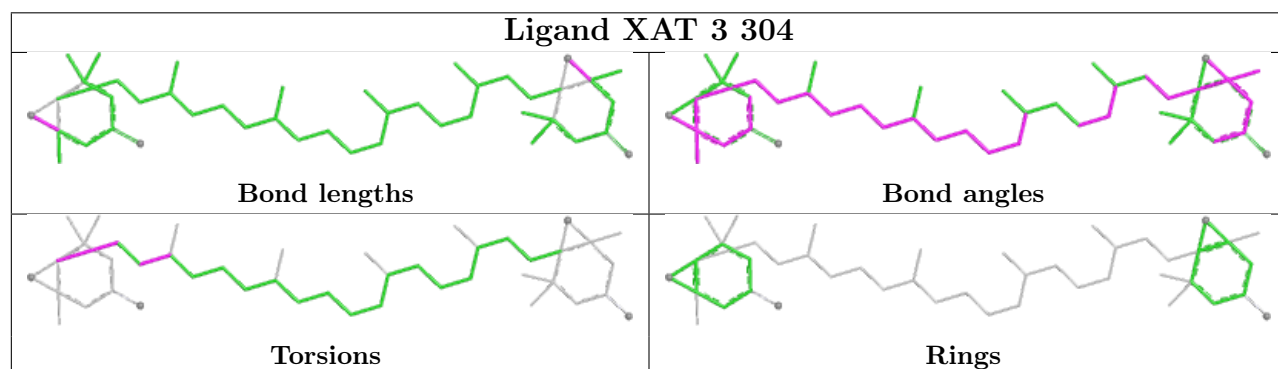
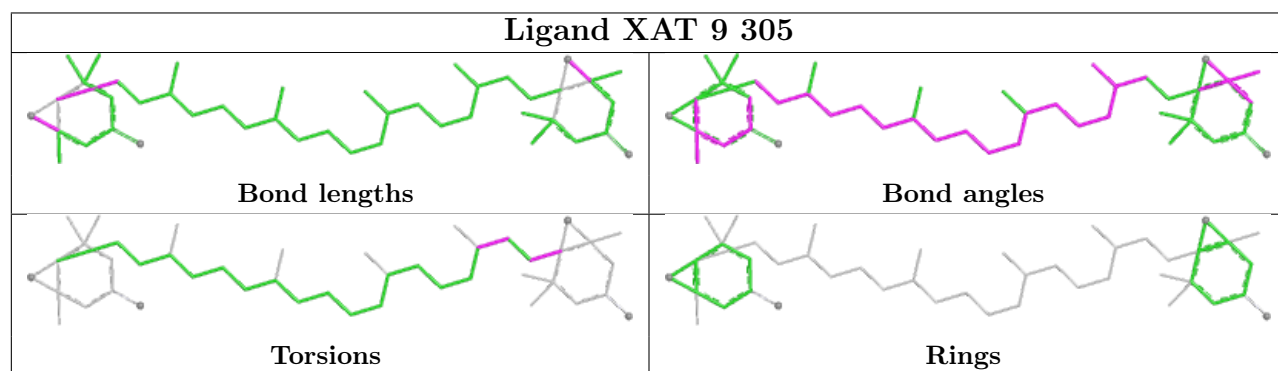
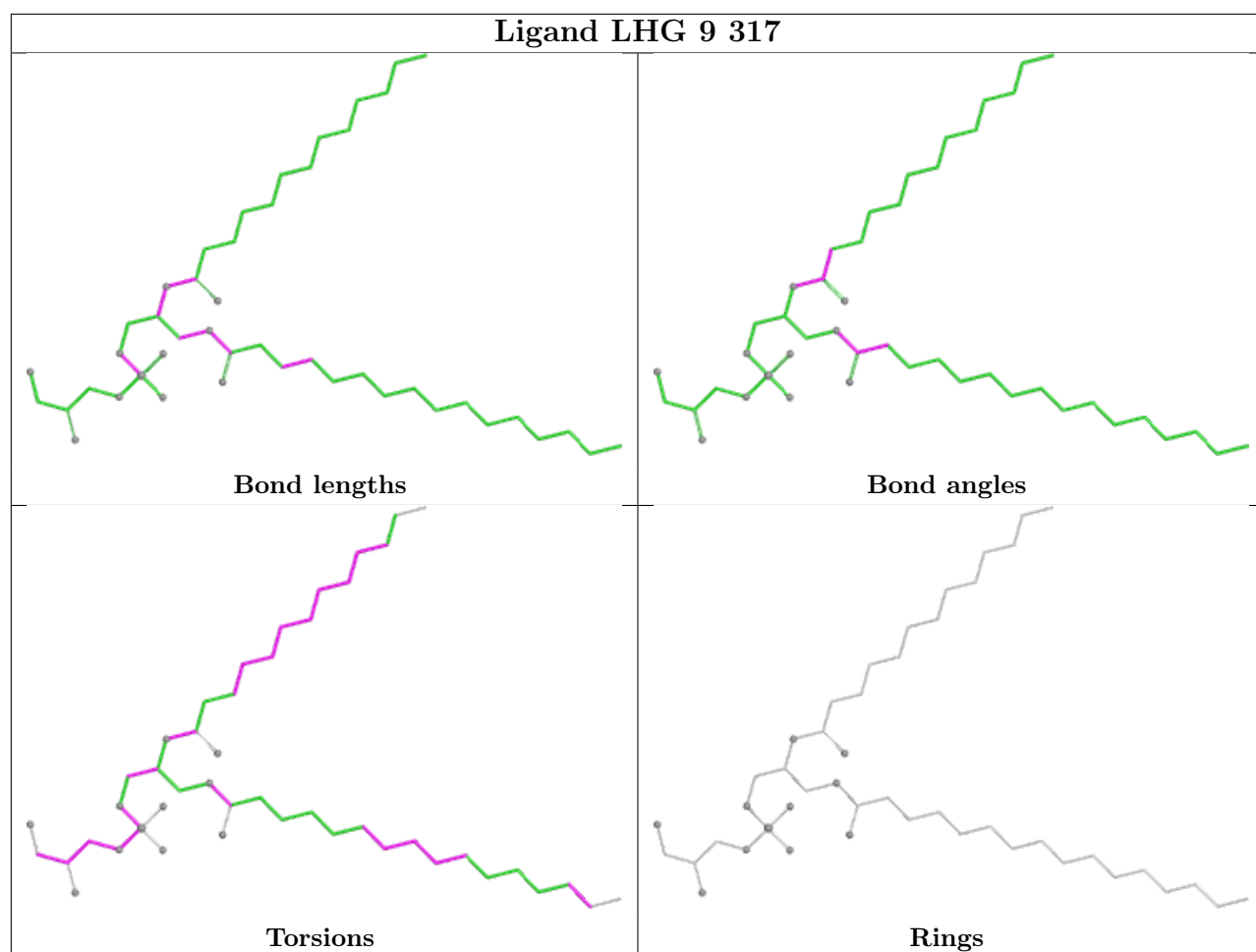


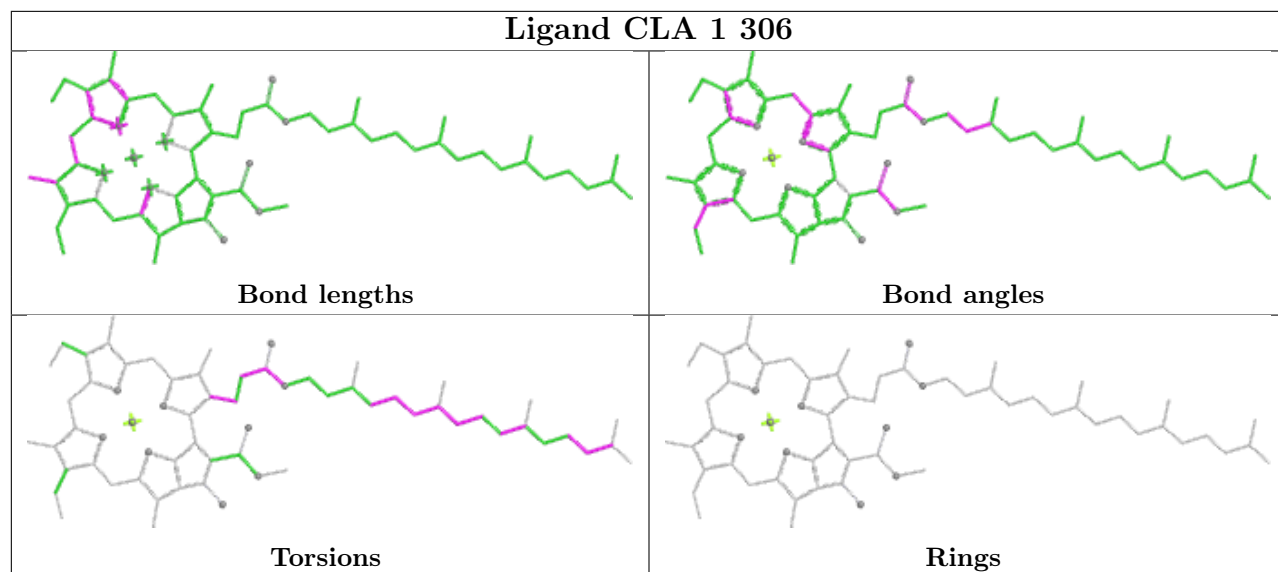
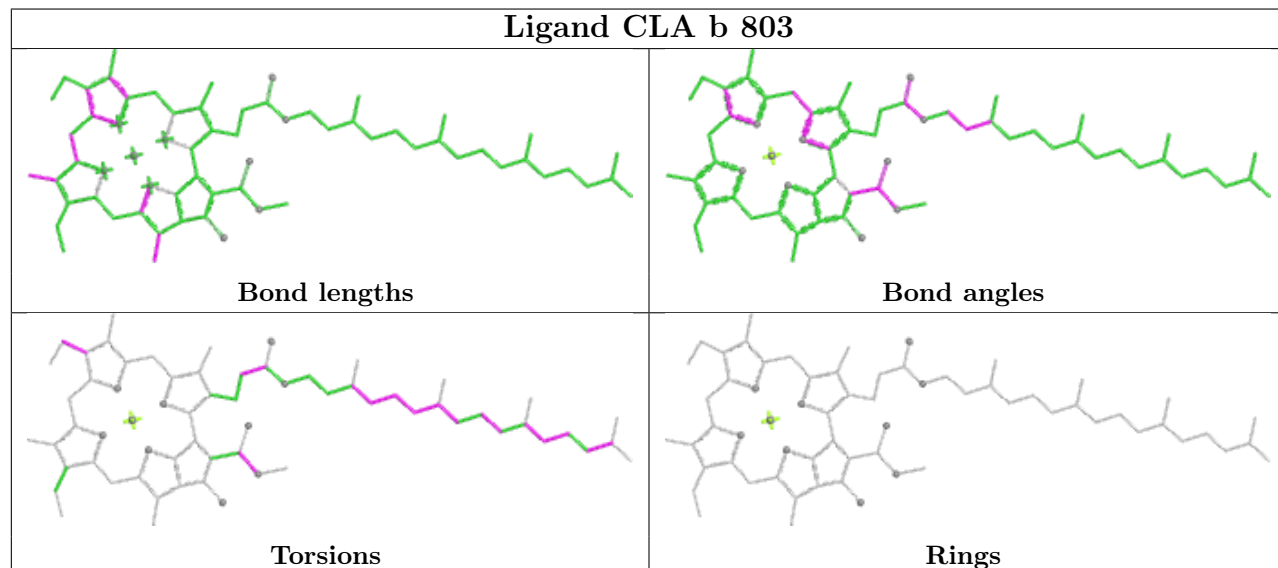
Ligand XAT 6 302



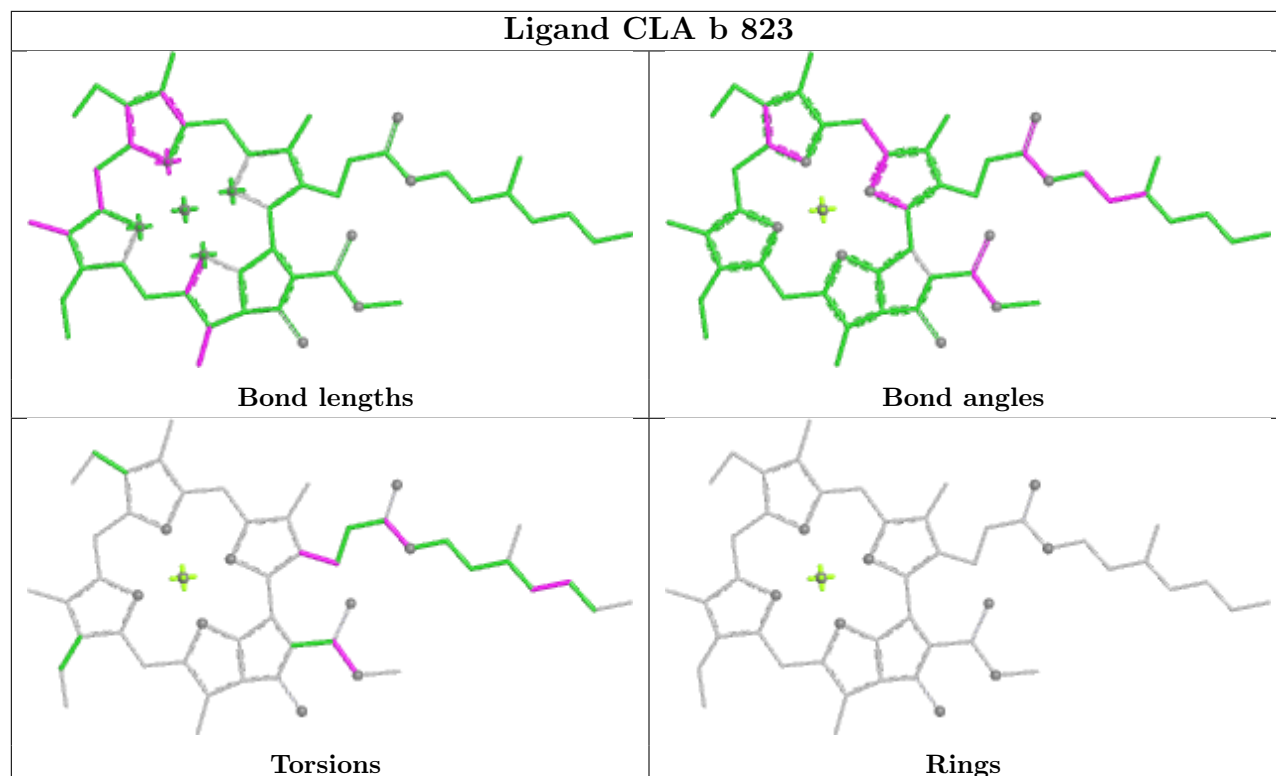
Ligand CLA b 801



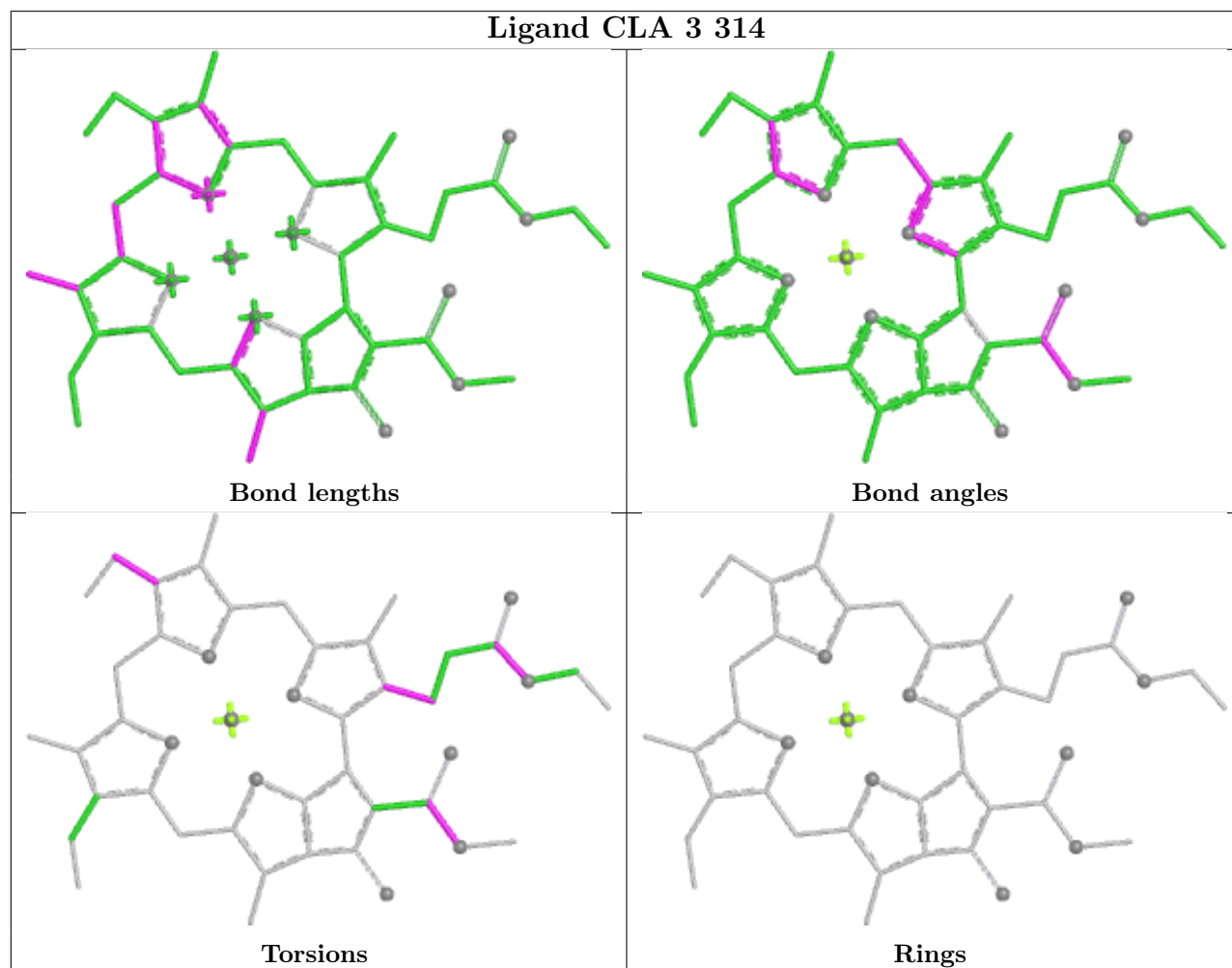


Ligand CLA 1 306**Ligand CLA b 803**

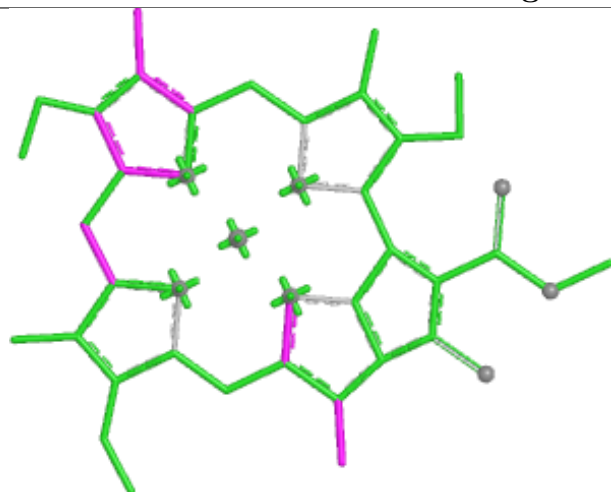
Ligand CLA b 823



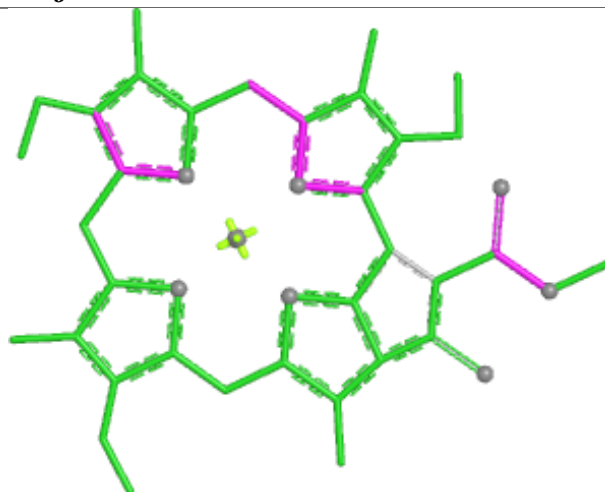
Ligand CLA 3 314



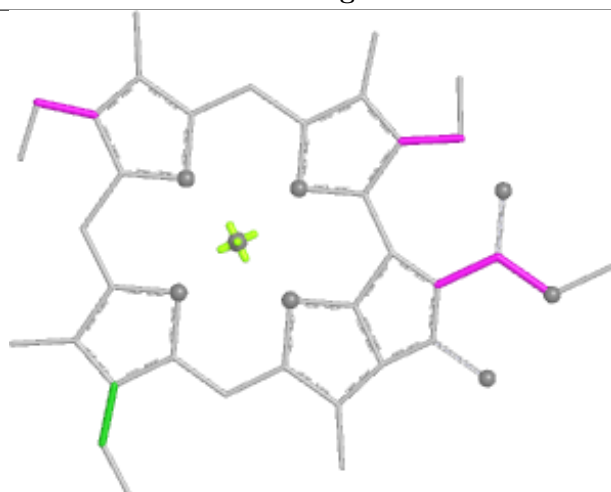
Ligand CLA j 103



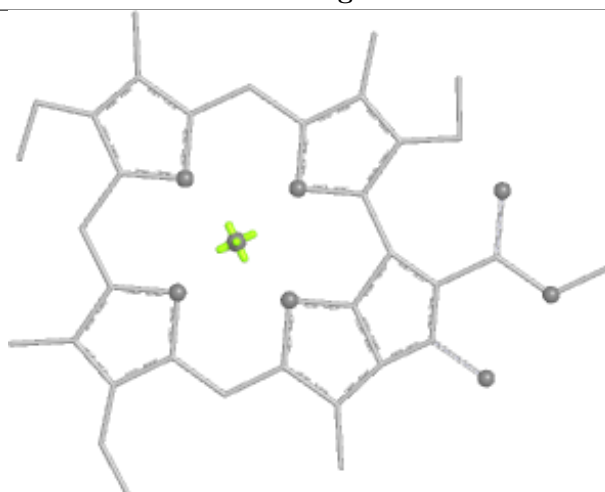
Bond lengths



Bond angles

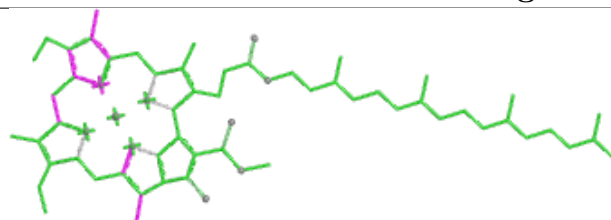


Torsions

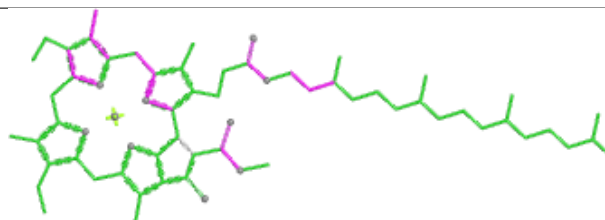


Rings

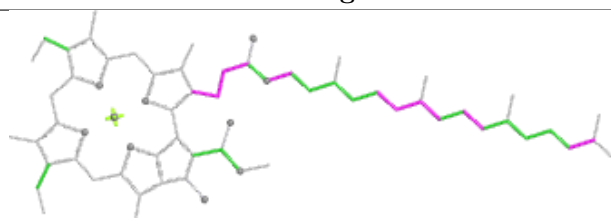
Ligand CLA b 810



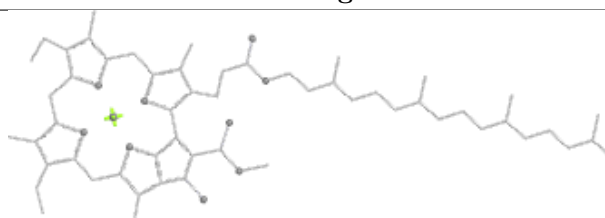
Bond lengths



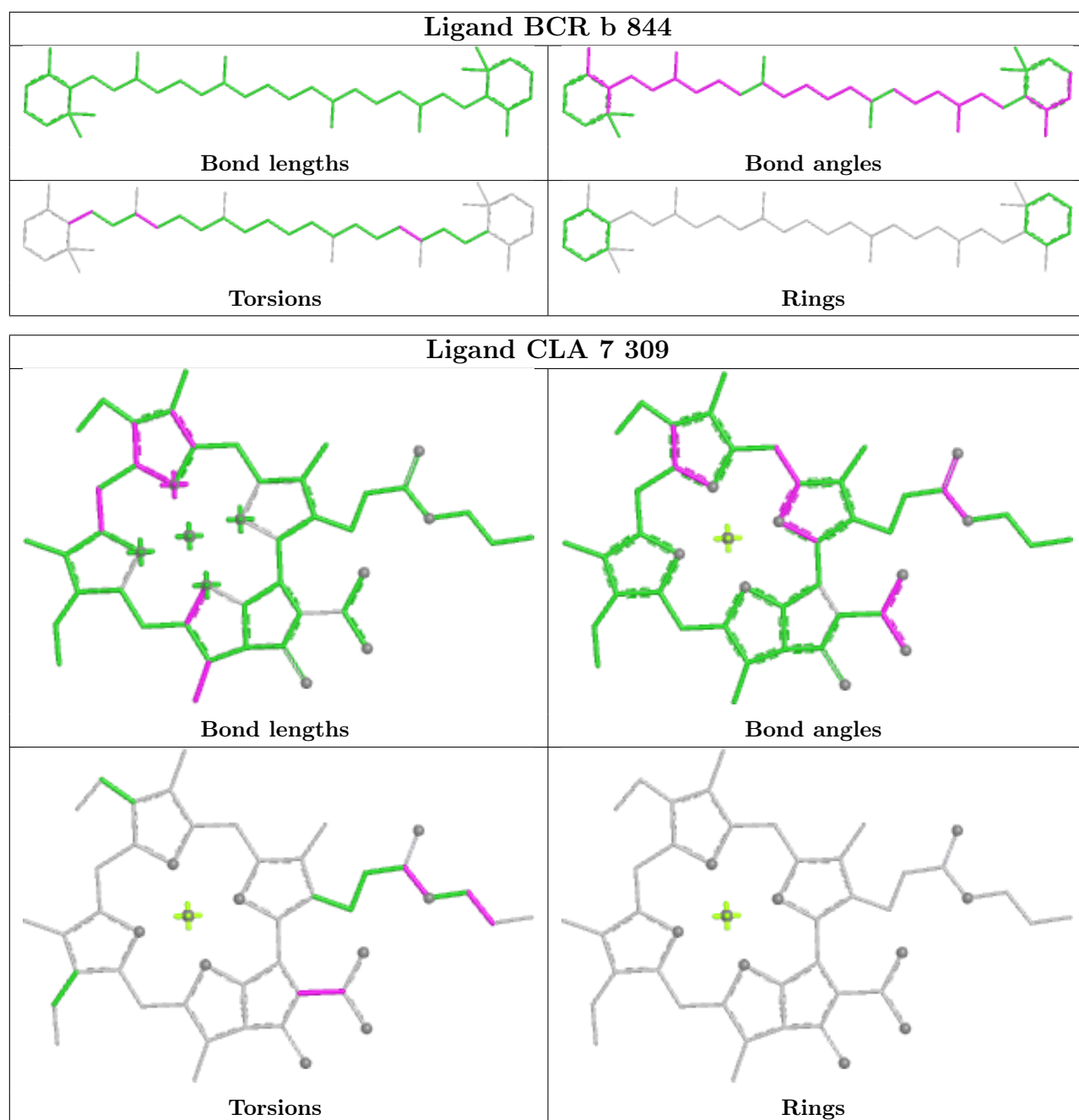
Bond angles



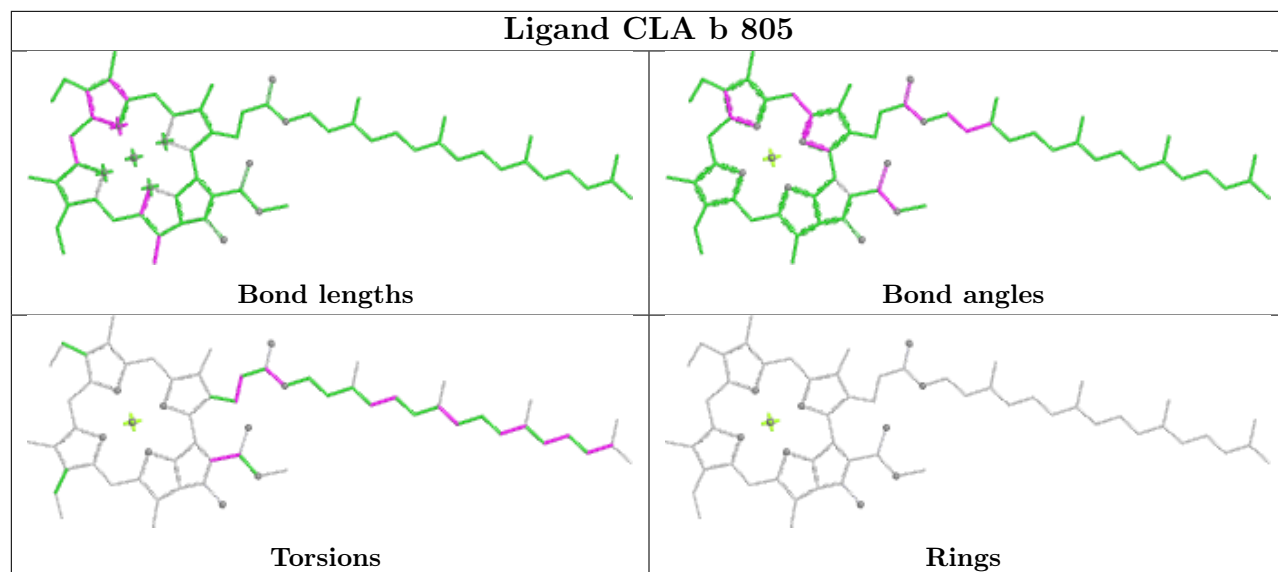
Torsions



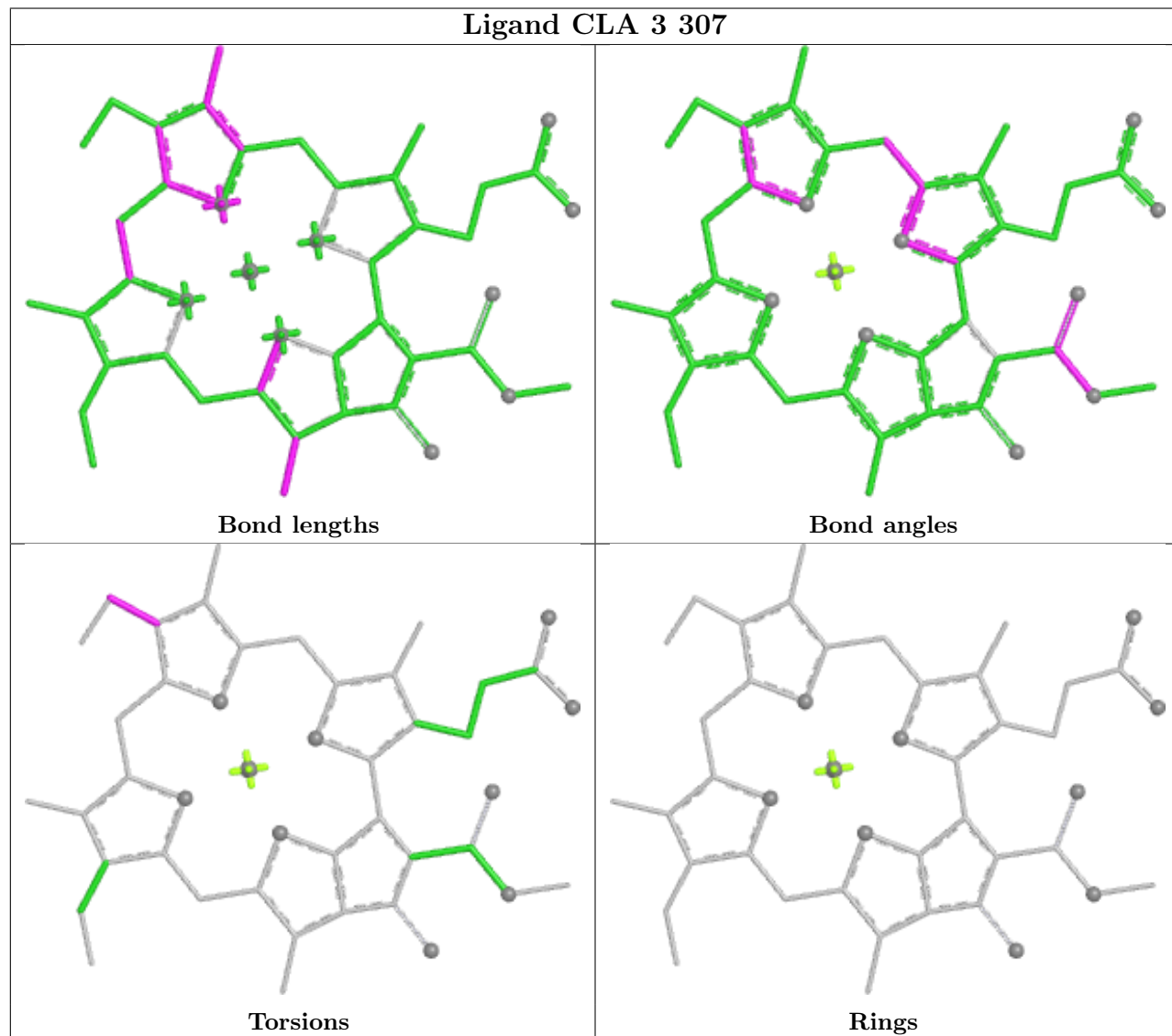
Rings

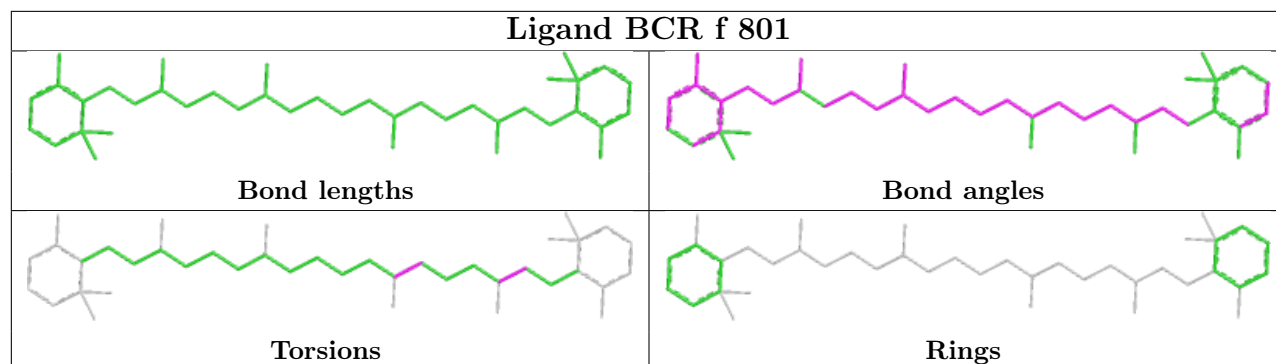
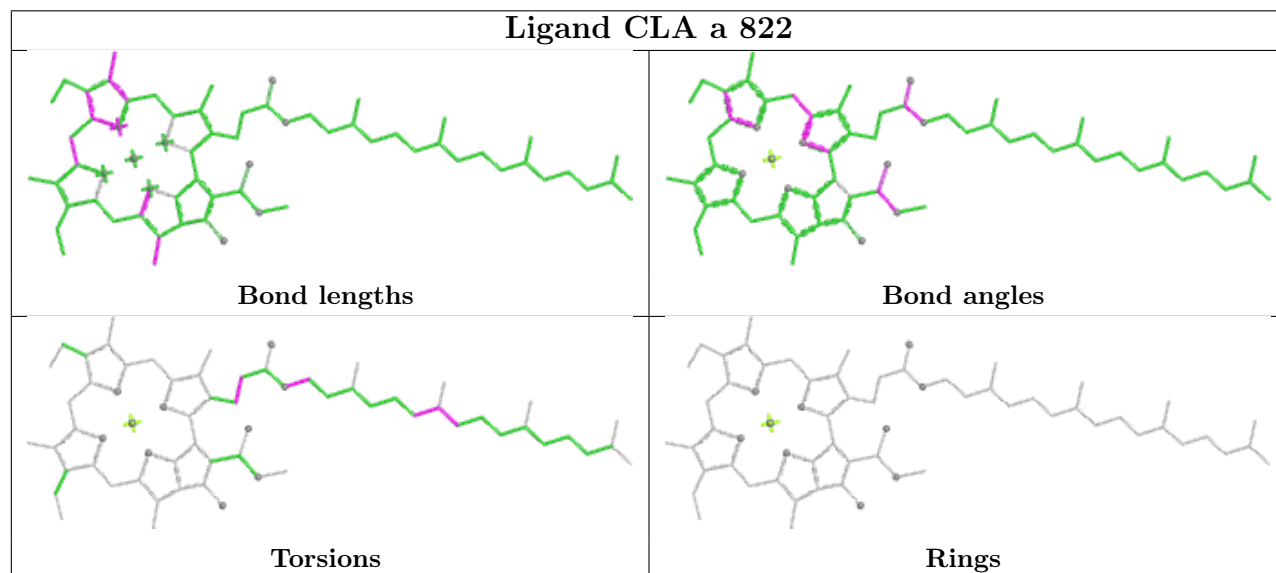
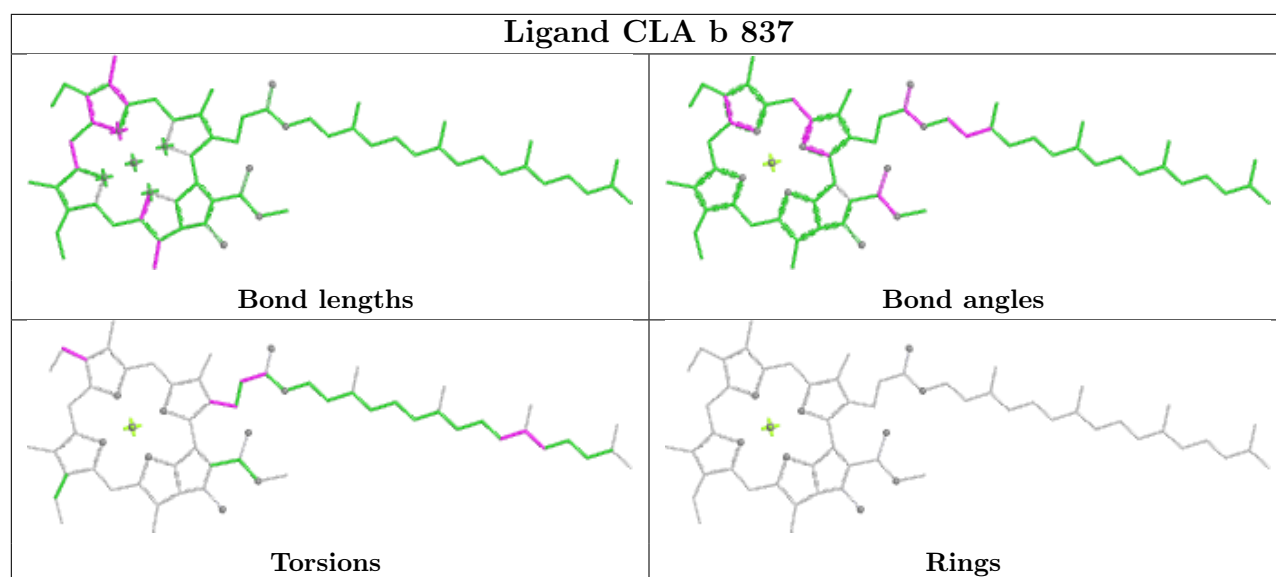


Ligand CLA b 805

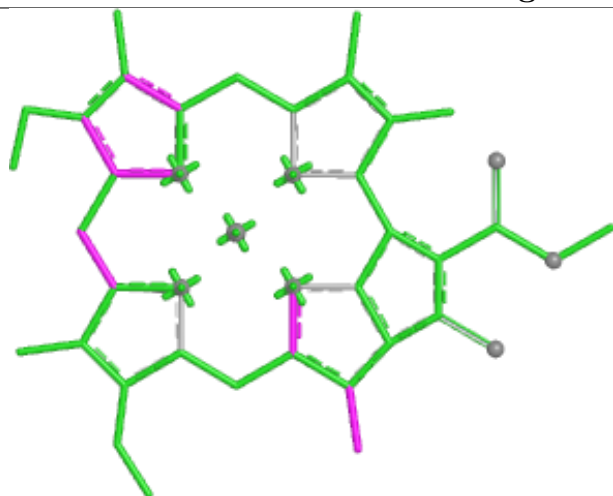


Ligand CLA 3 307

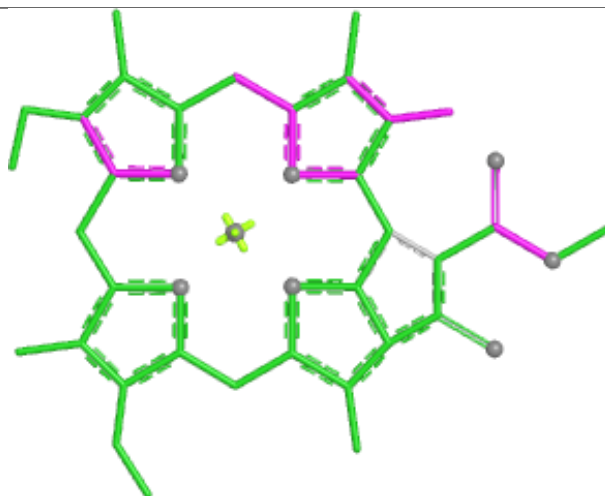




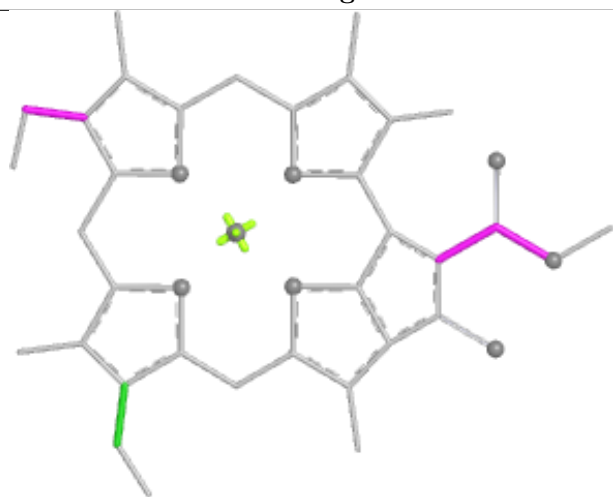
Ligand CLA 8 314



Bond lengths



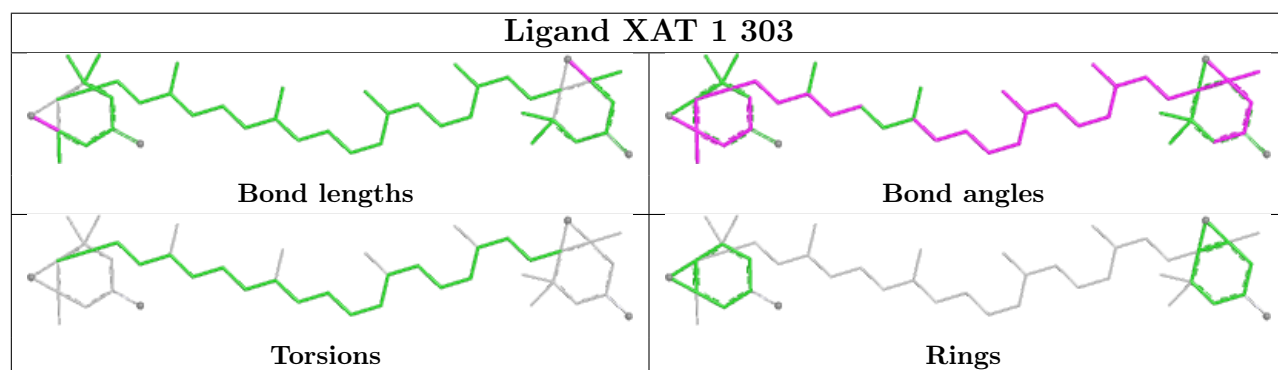
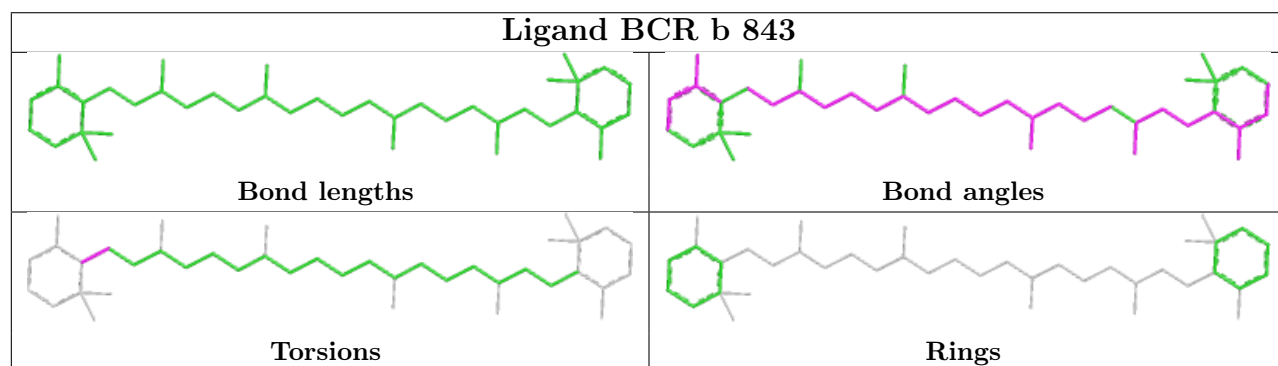
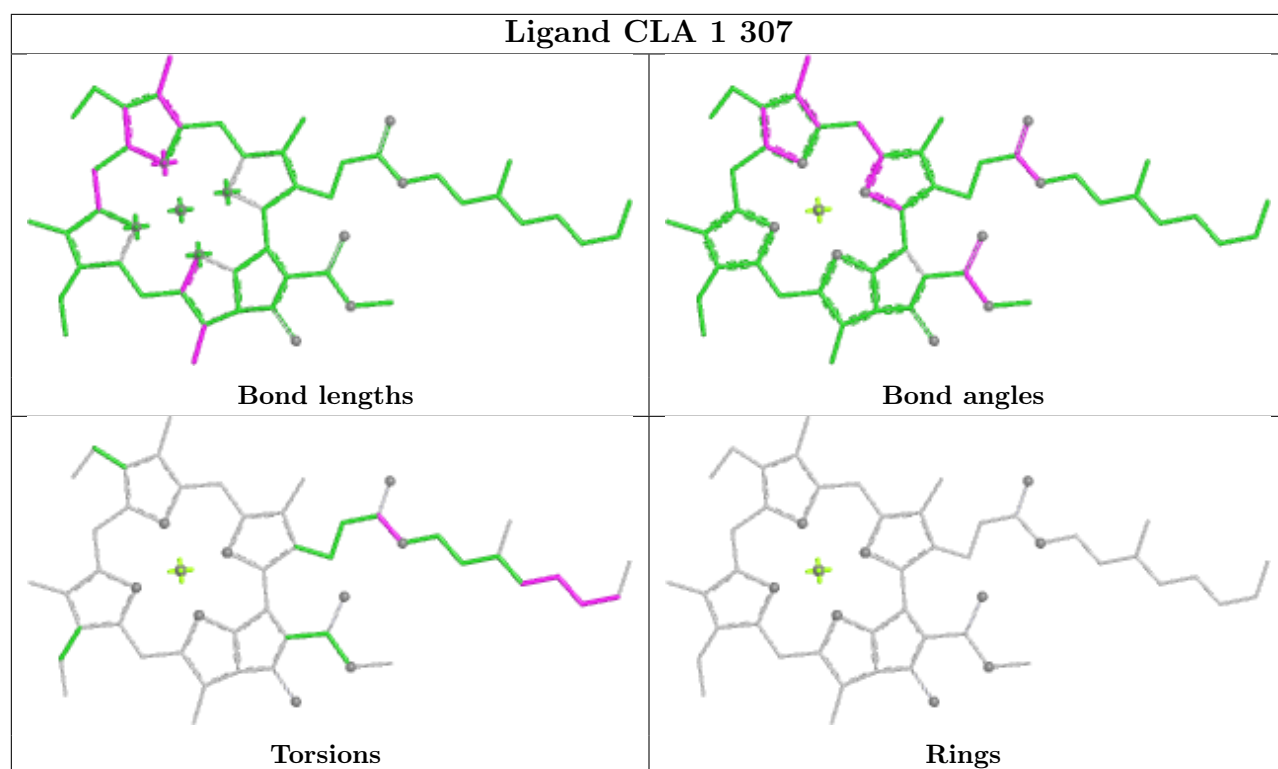
Bond angles



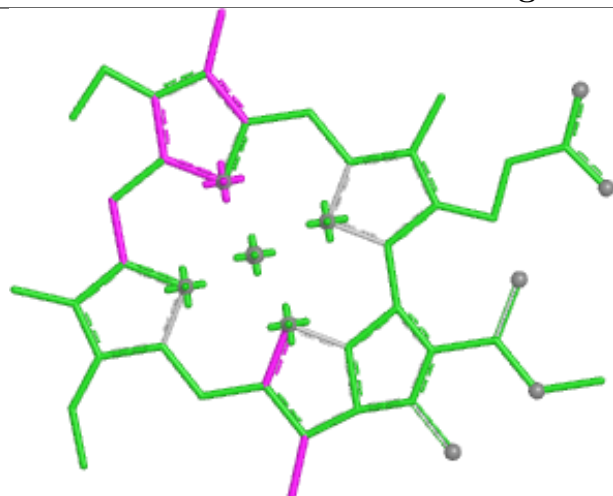
Torsions



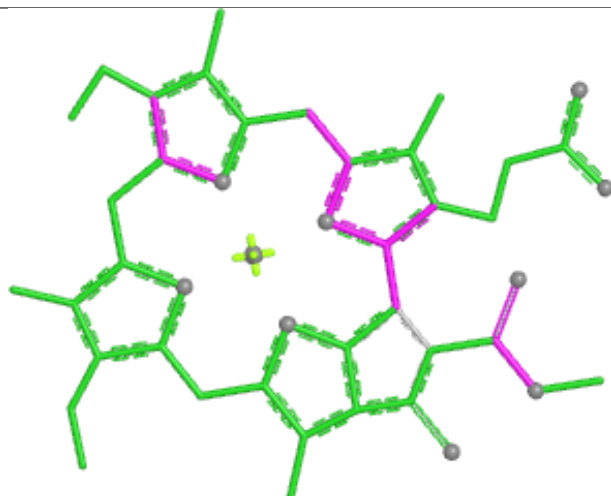
Rings



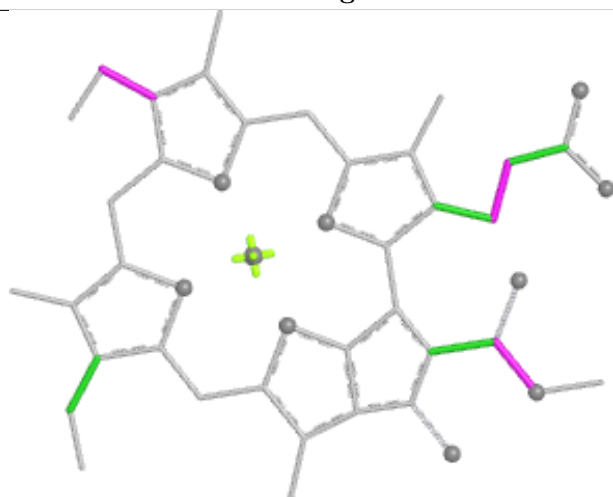
Ligand CLA 7 314



Bond lengths



Bond angles

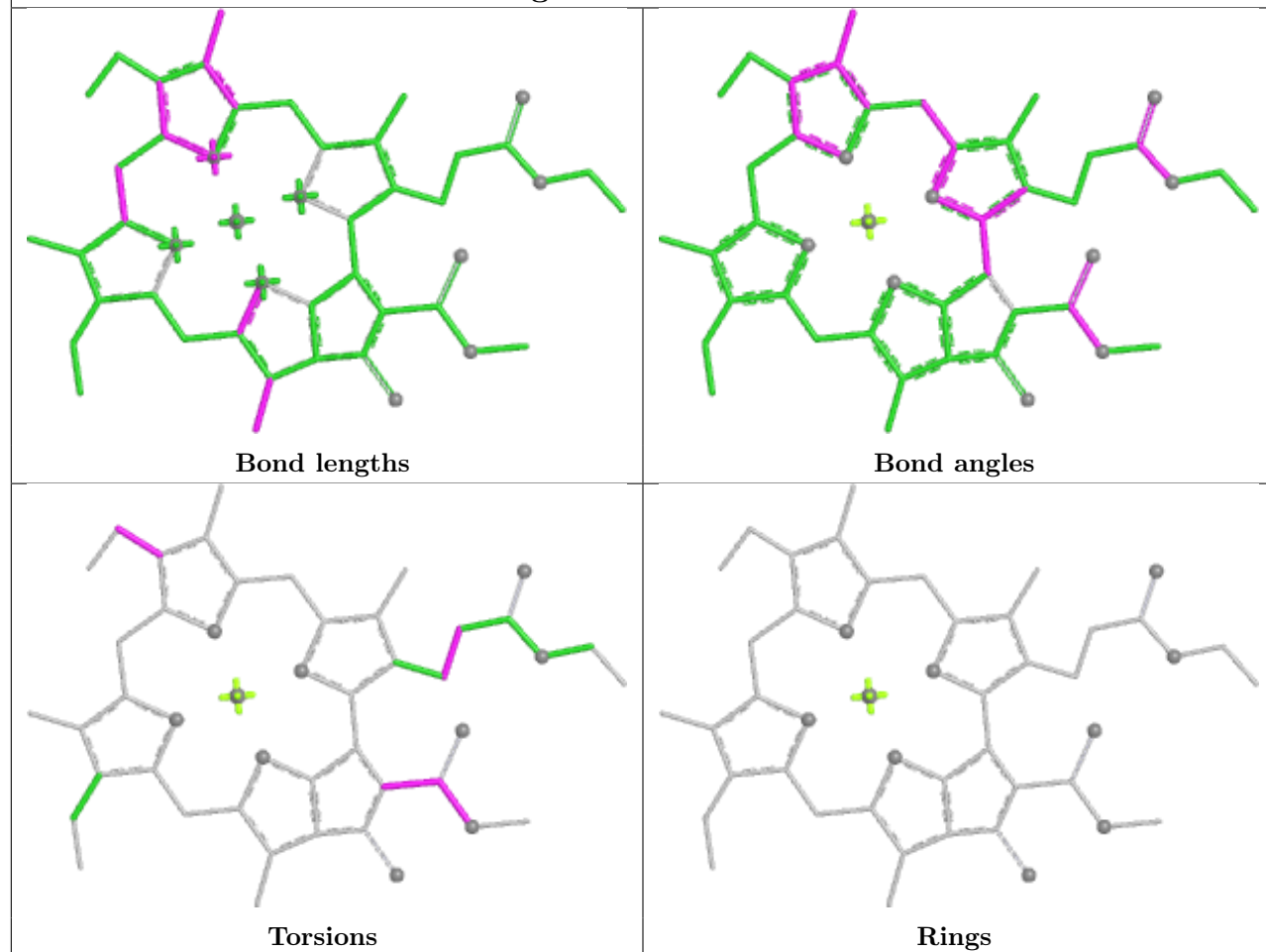


Torsions

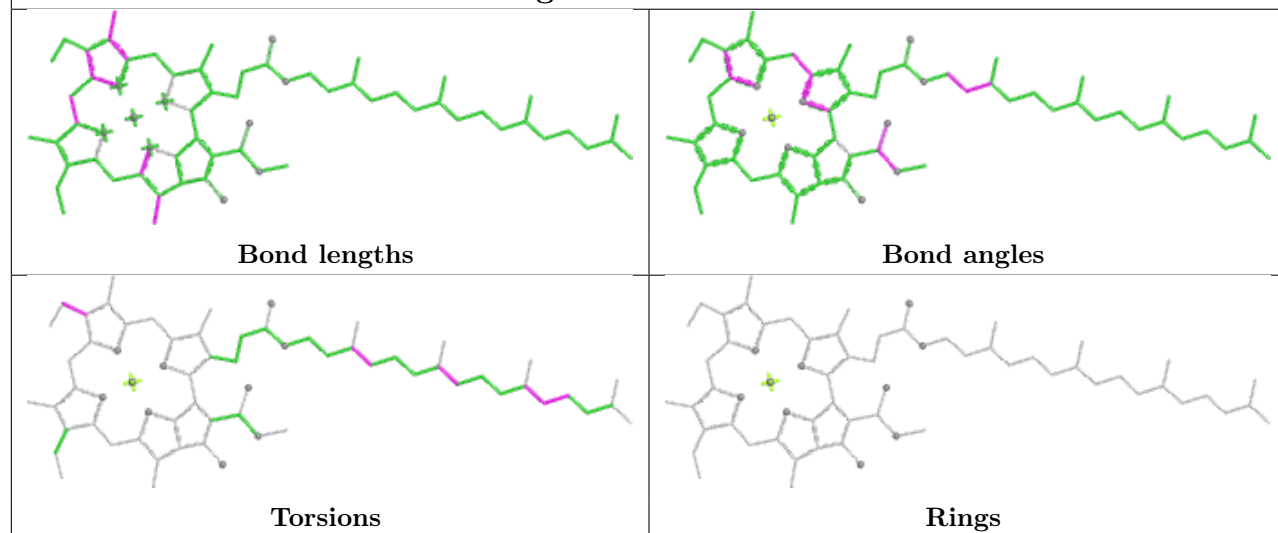


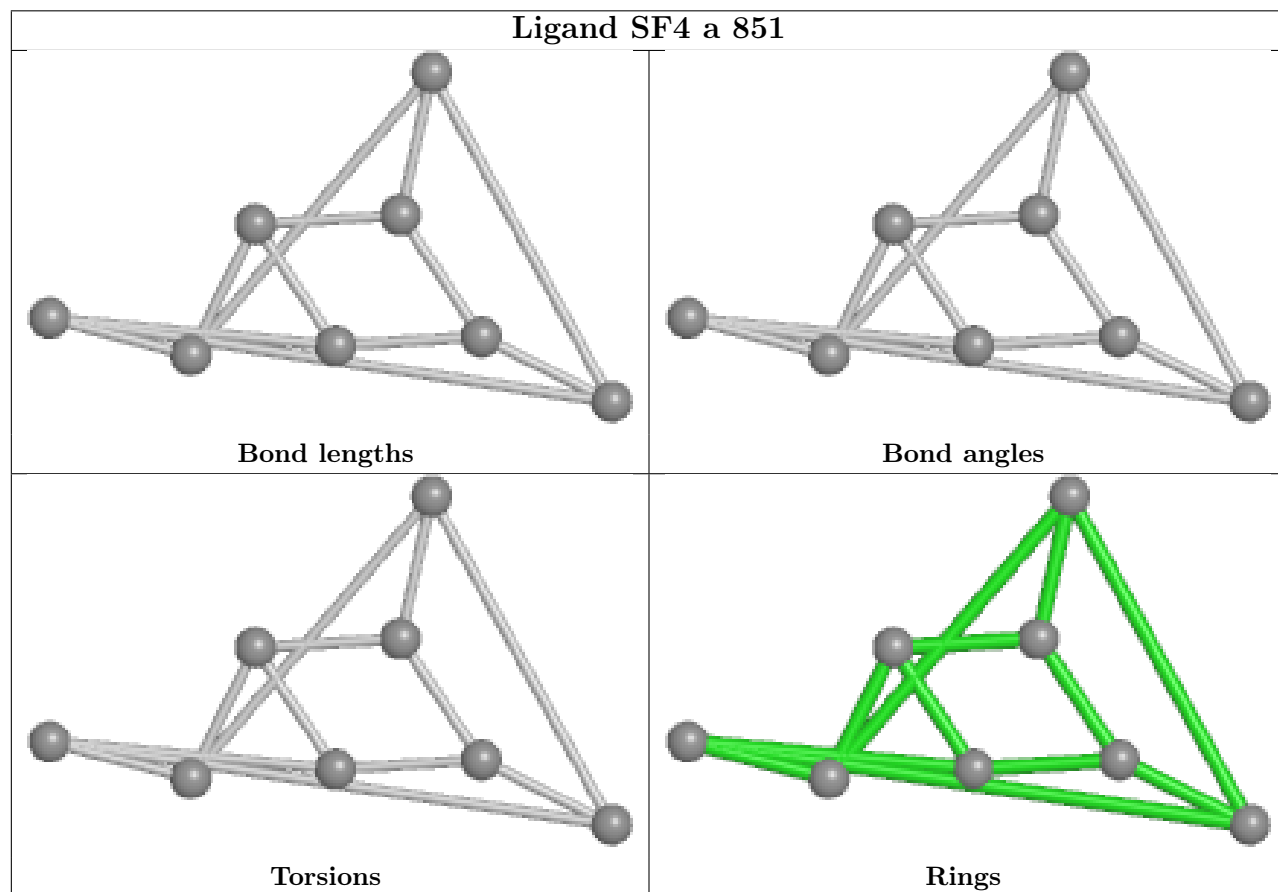
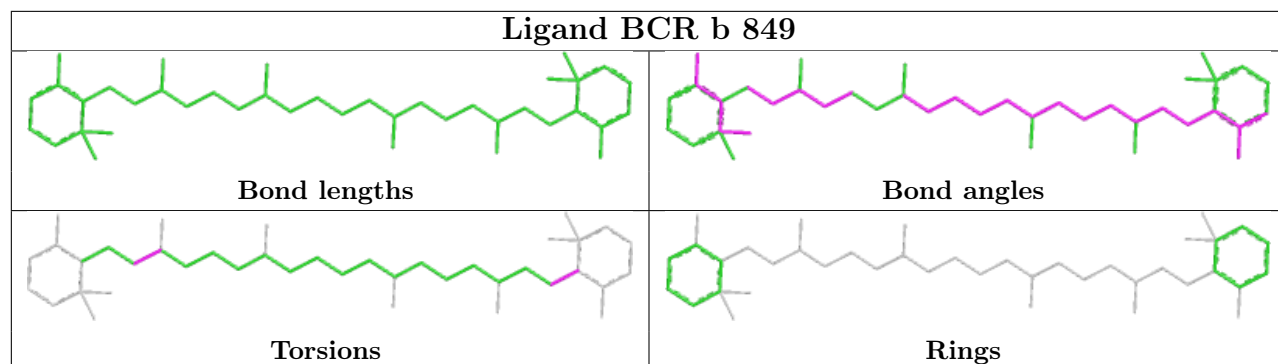
Rings

Ligand CLA 2 307

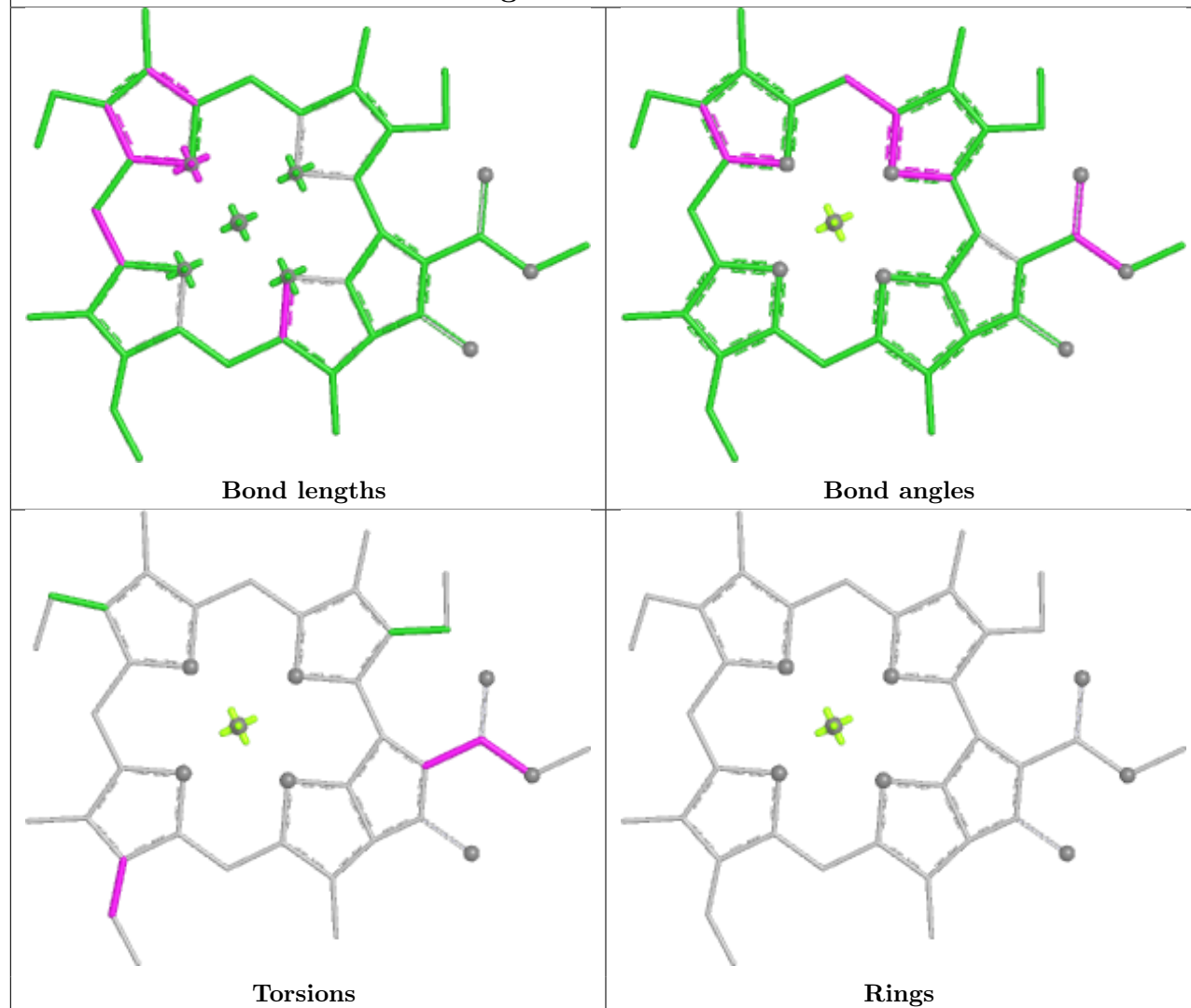


Ligand CLA a 840

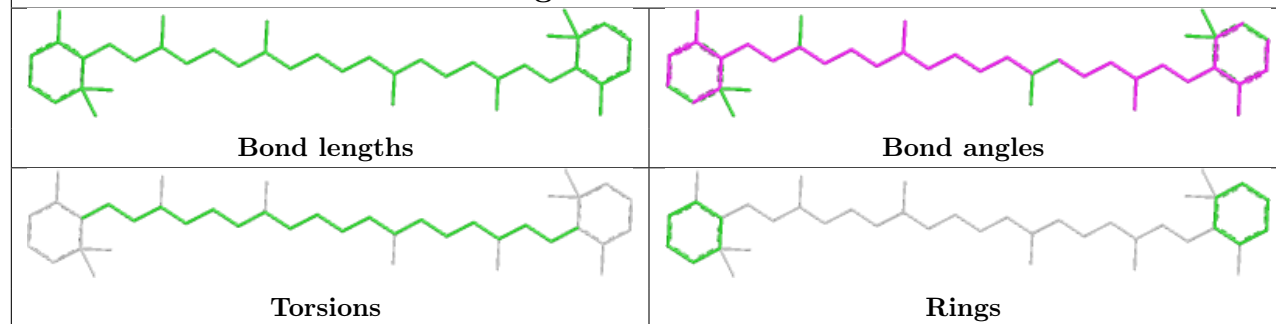


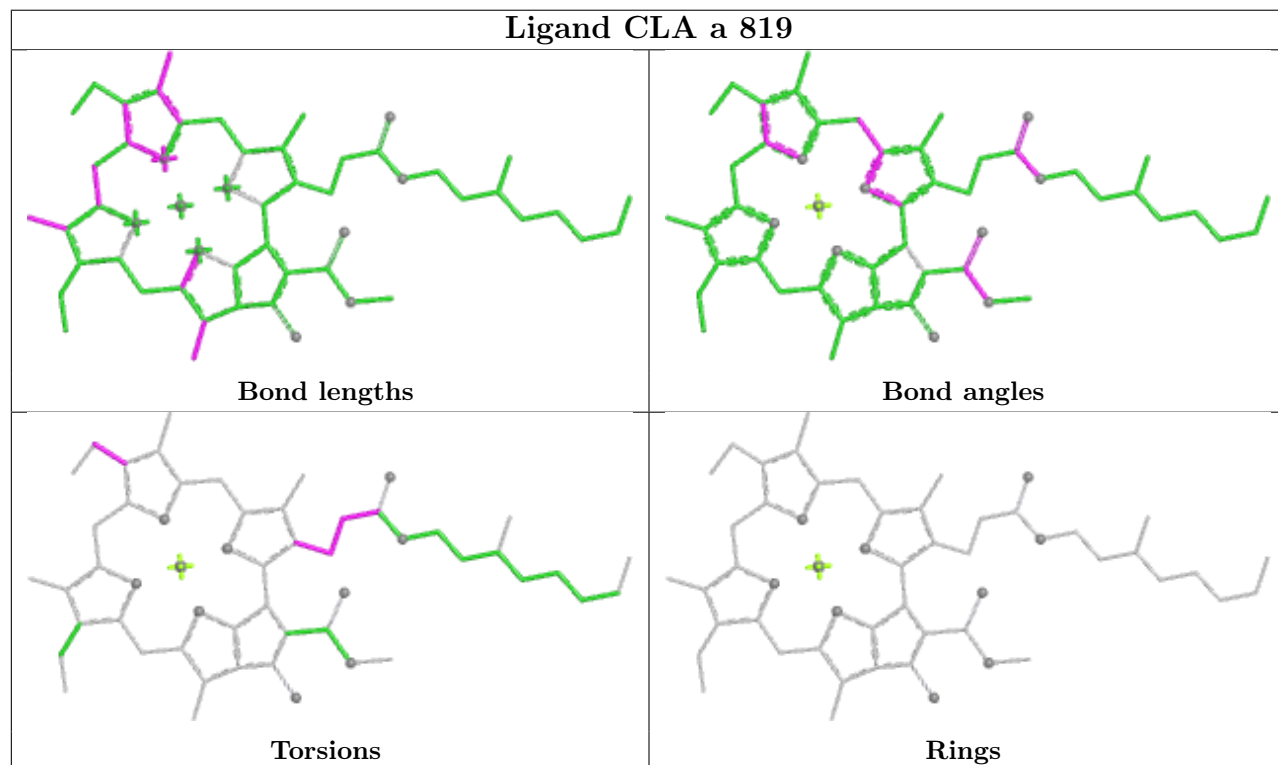
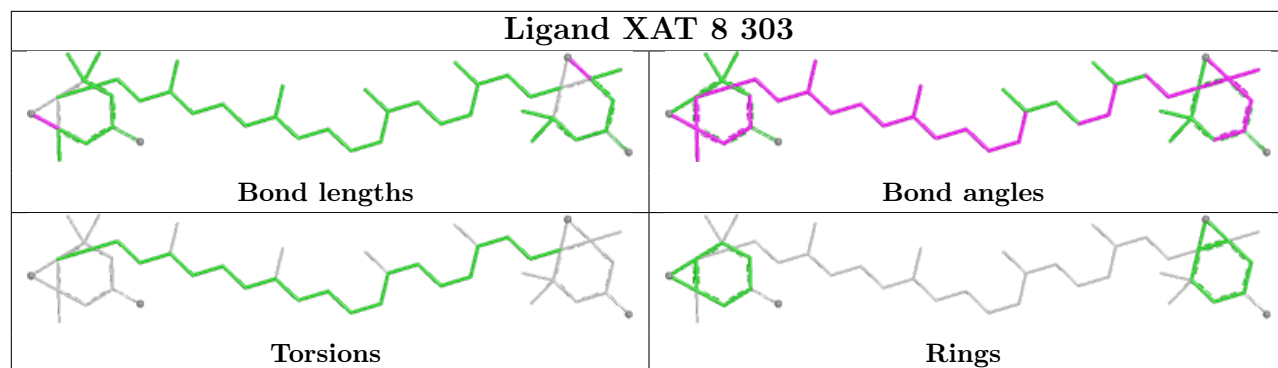


Ligand CLA 9 315

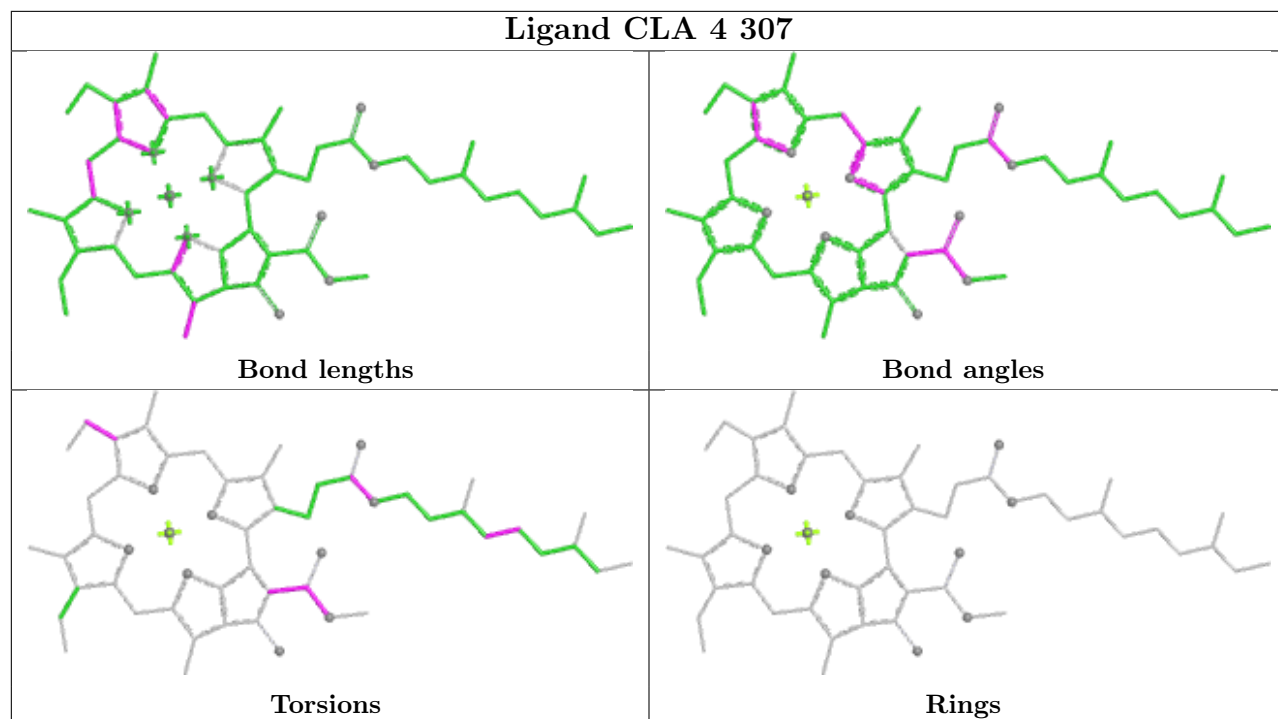


Ligand BCR a 849

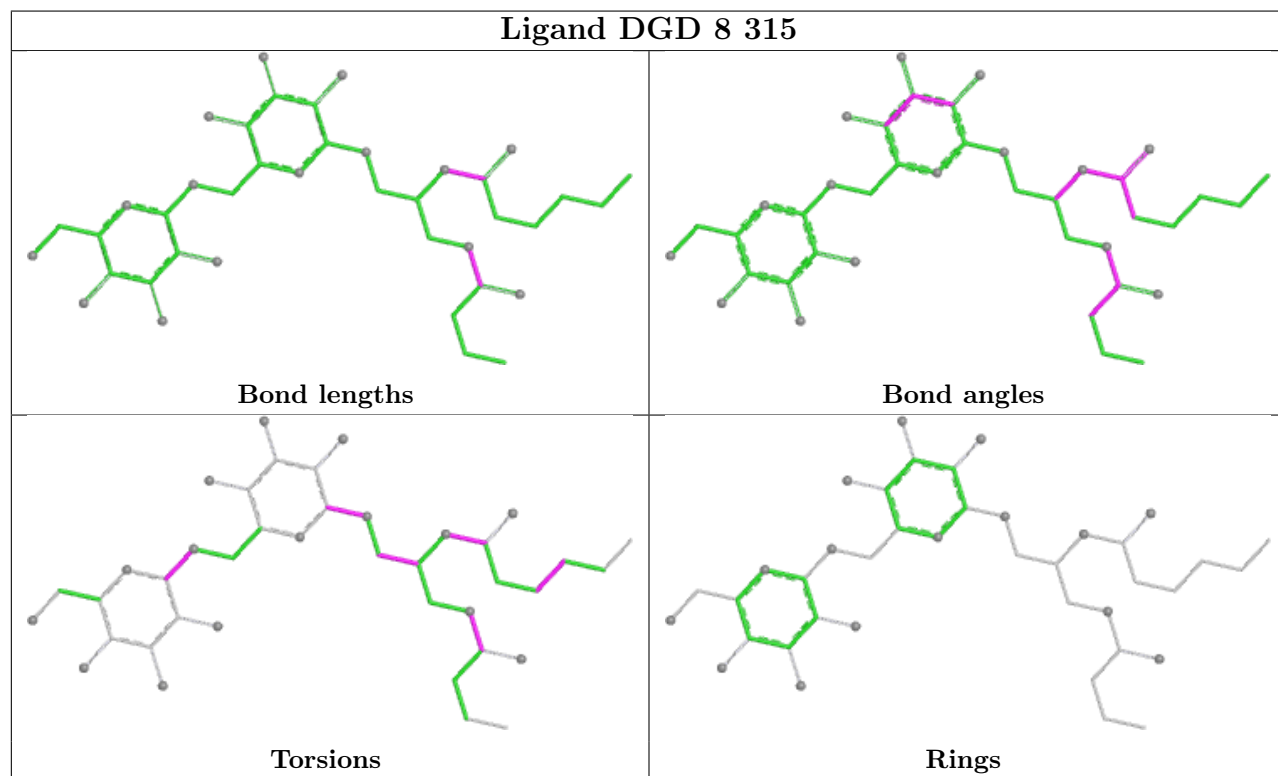


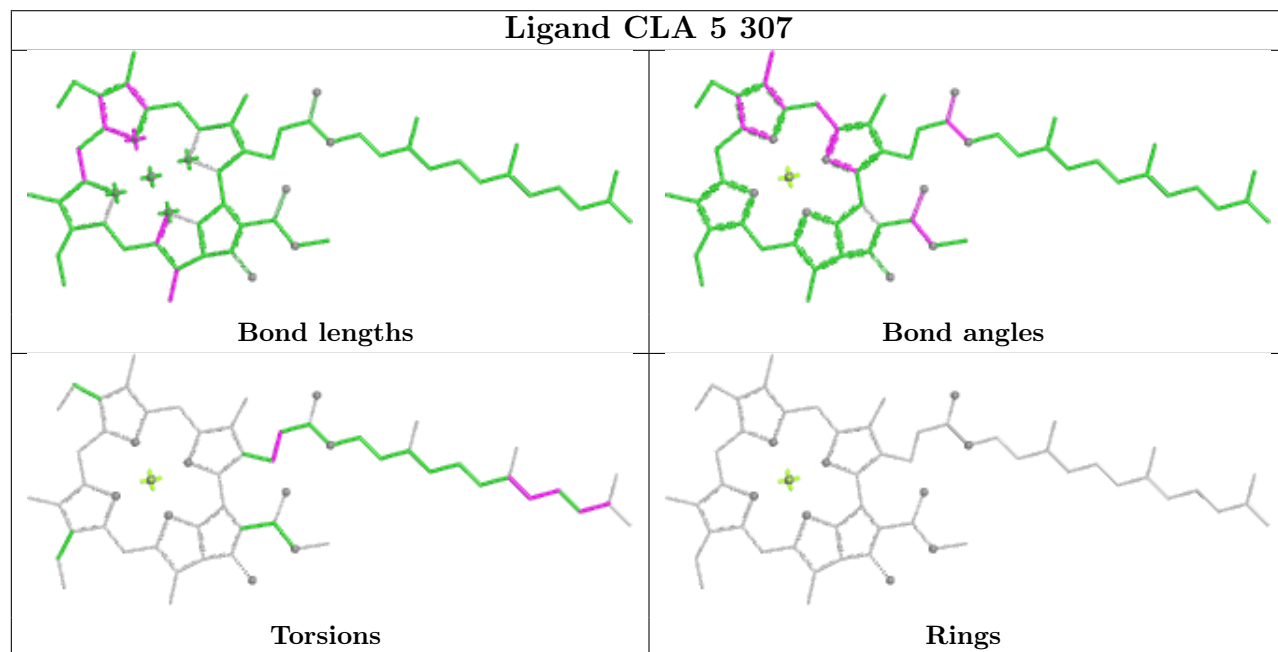
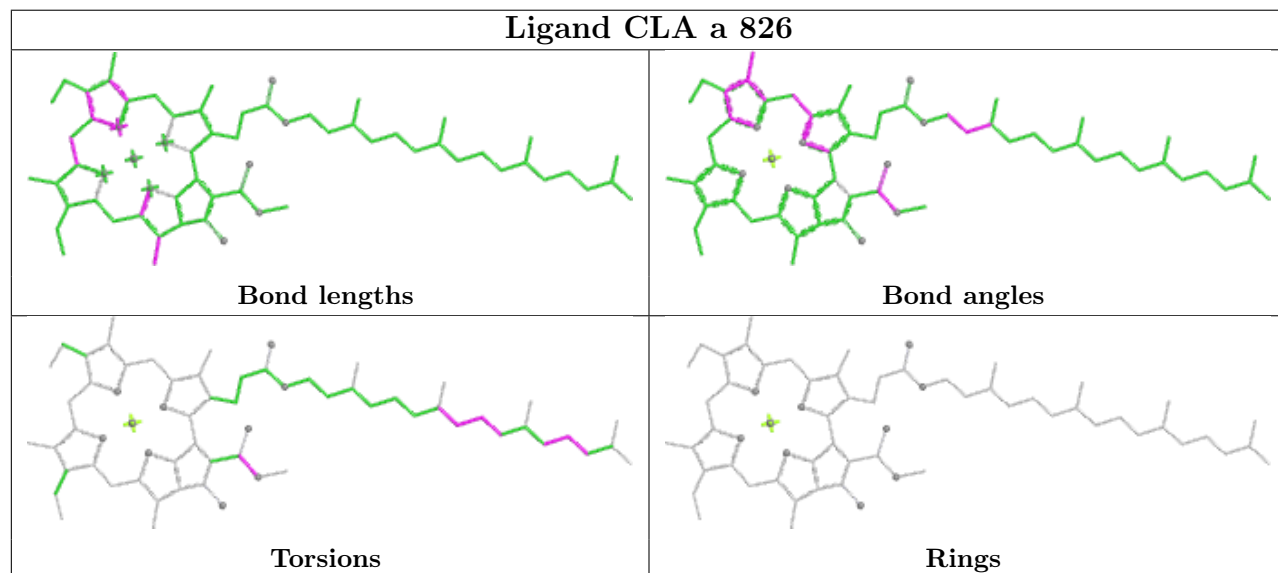
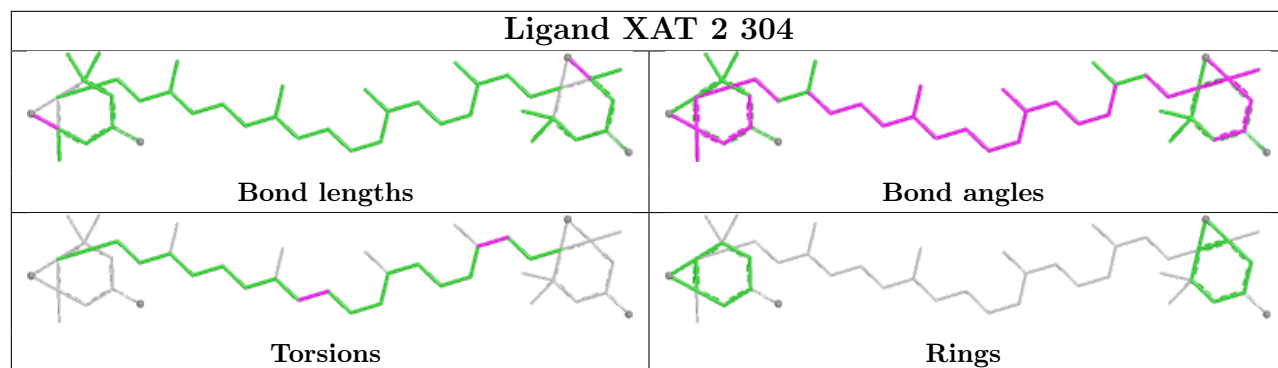


Ligand CLA 4 307

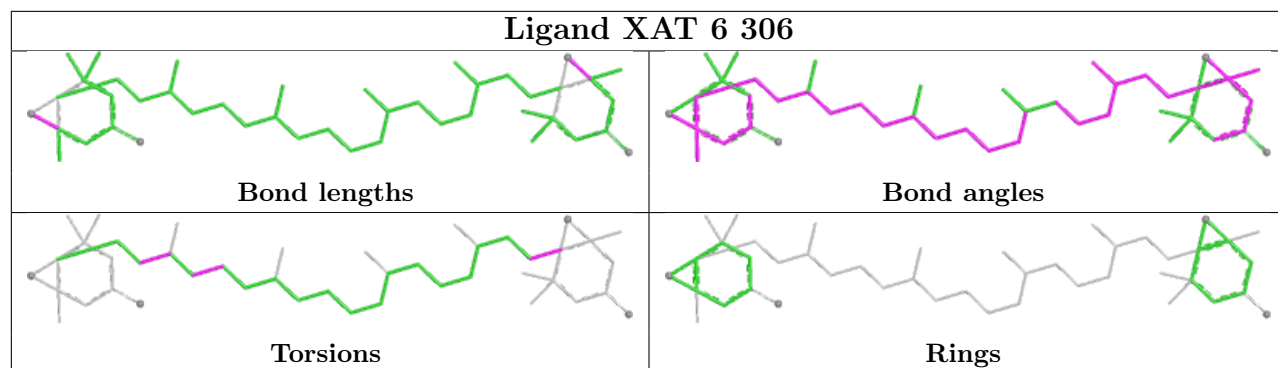


Ligand DGD 8 315

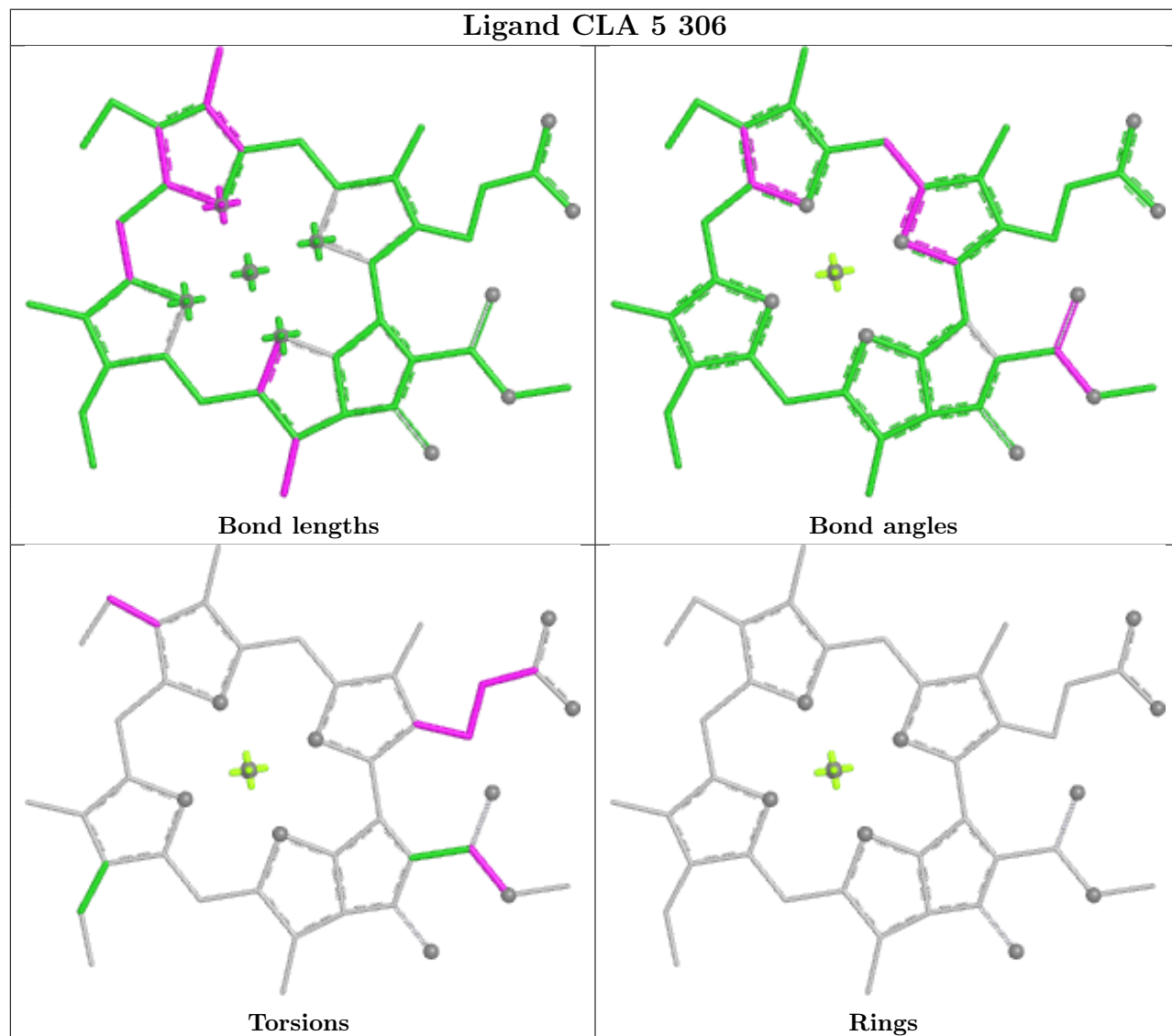




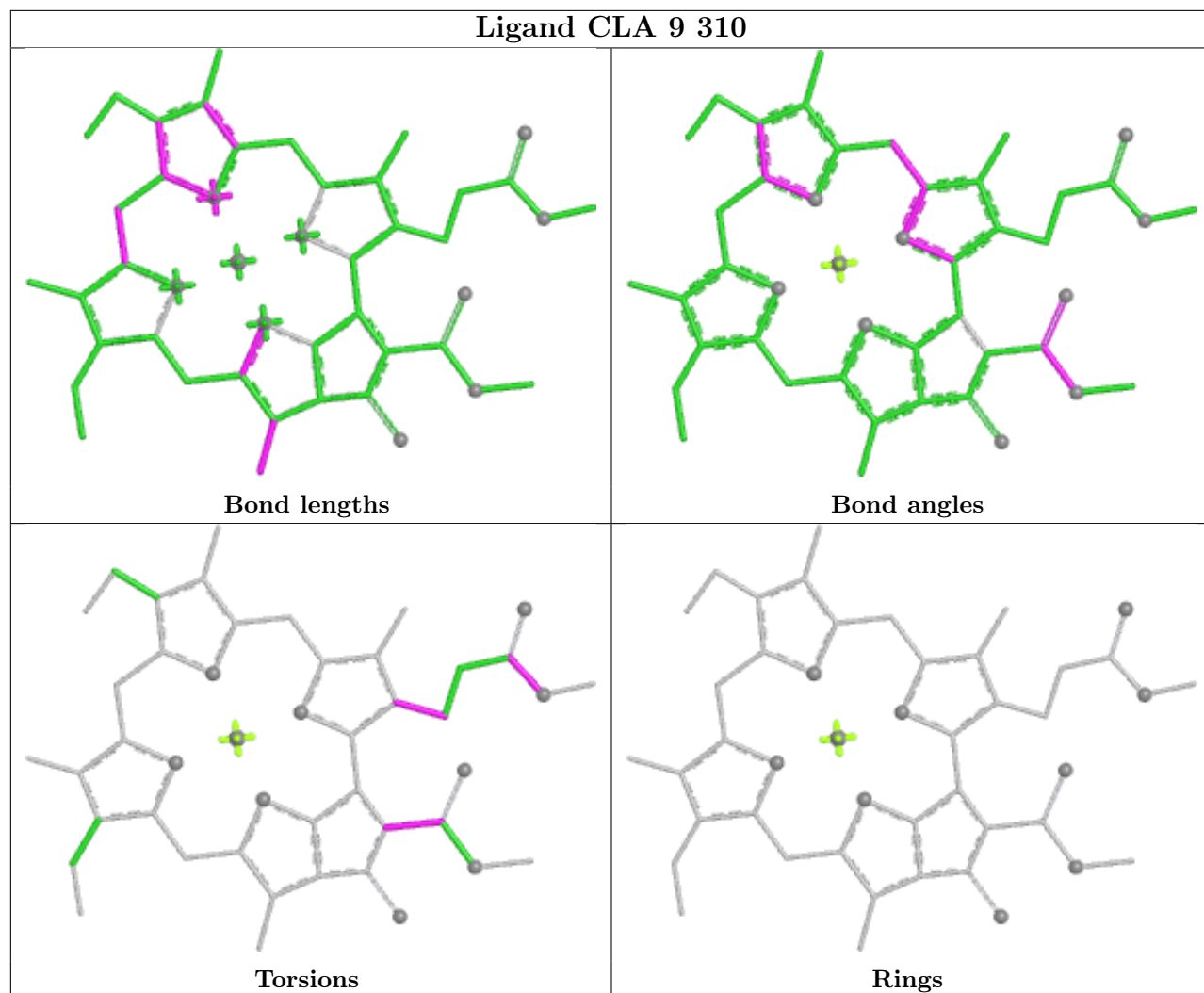
Ligand XAT 6 306



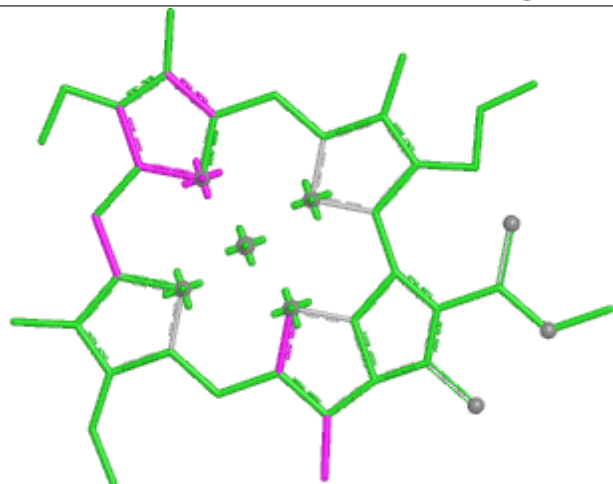
Ligand CLA 5 306



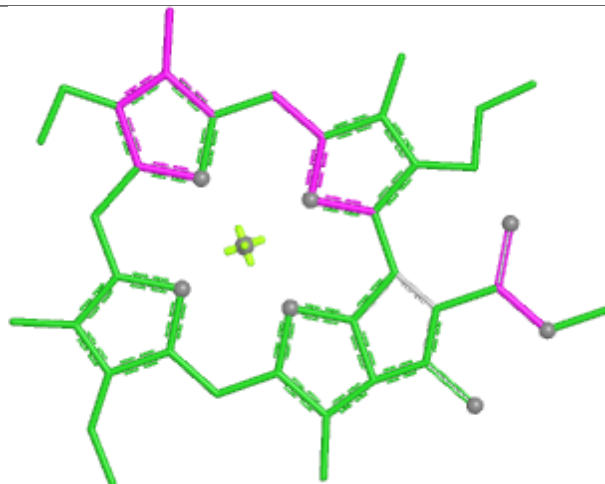
Ligand CLA 9 310



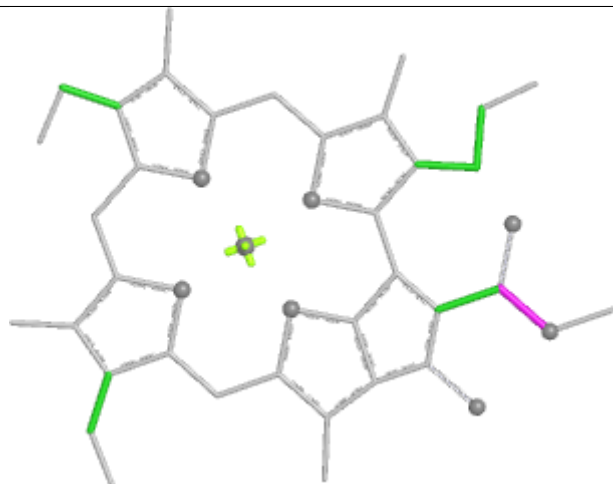
Ligand CLA 8 305



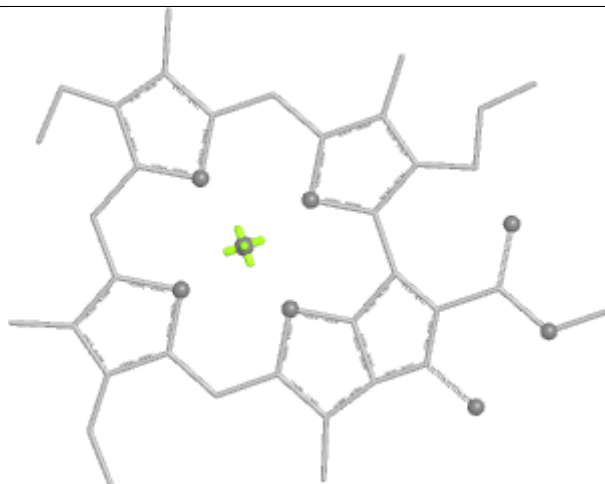
Bond lengths



Bond angles

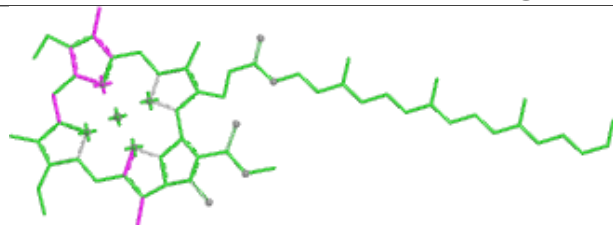


Torsions

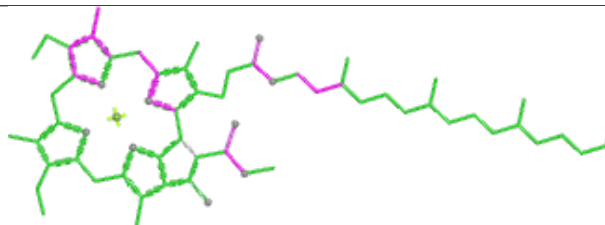


Rings

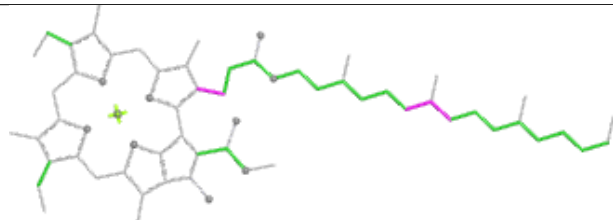
Ligand CLA b 825



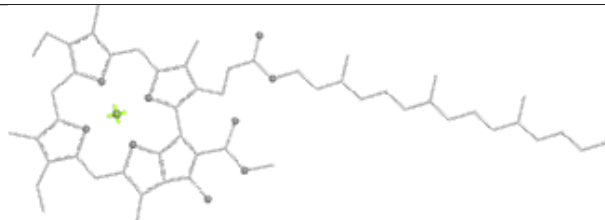
Bond lengths



Bond angles

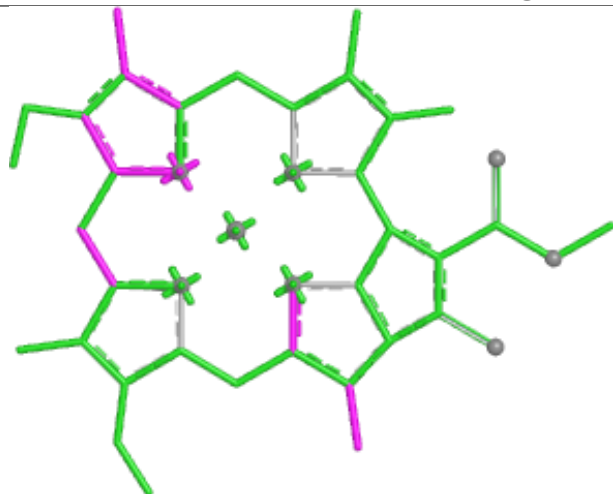


Torsions

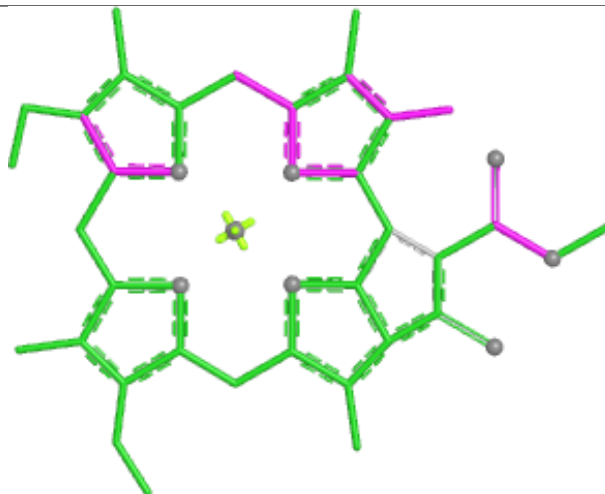


Rings

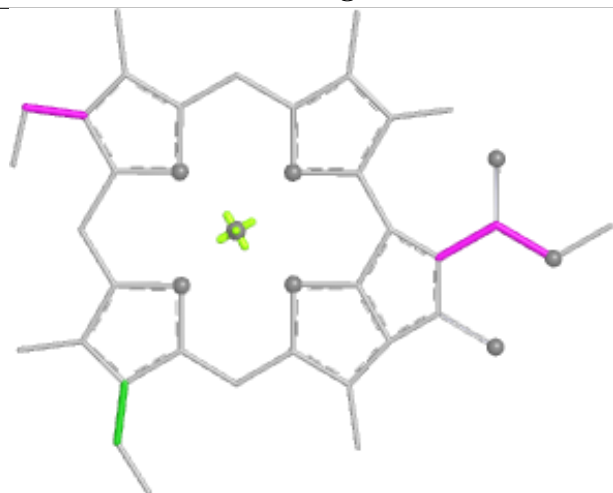
Ligand CLA 1 313



Bond lengths



Bond angles

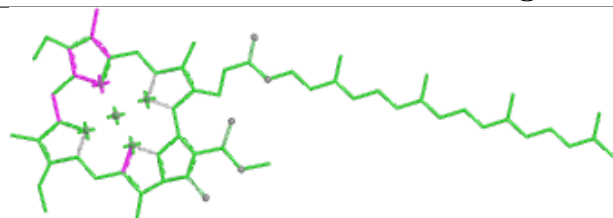


Torsions

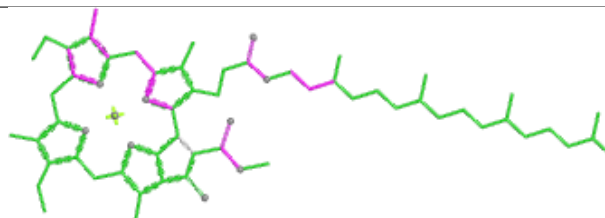


Rings

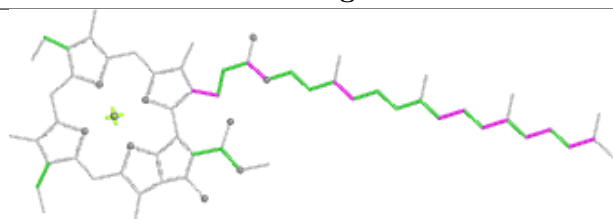
Ligand CLA a 820



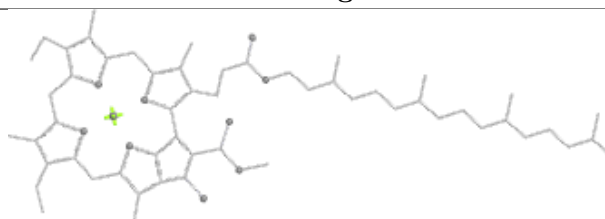
Bond lengths



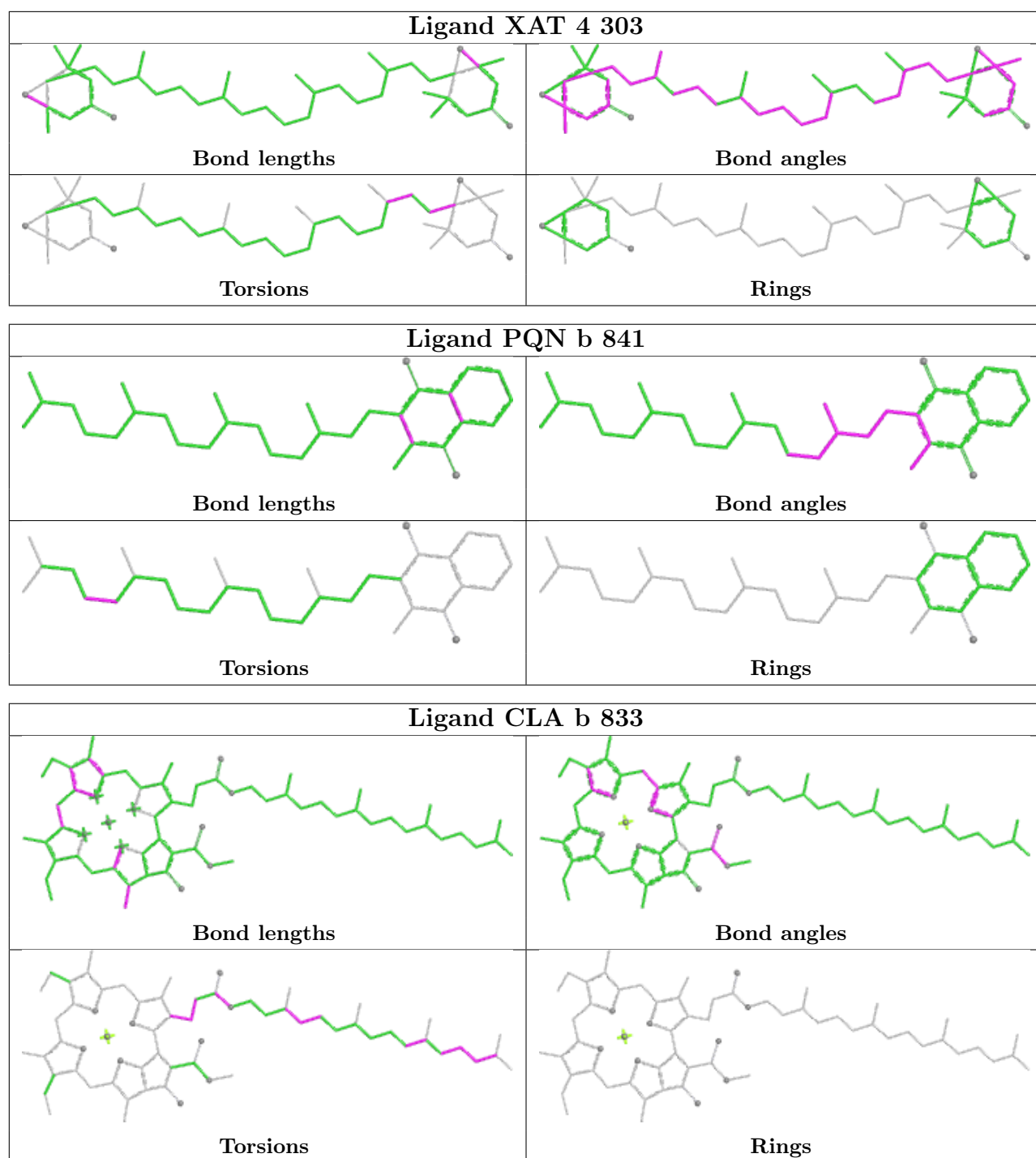
Bond angles



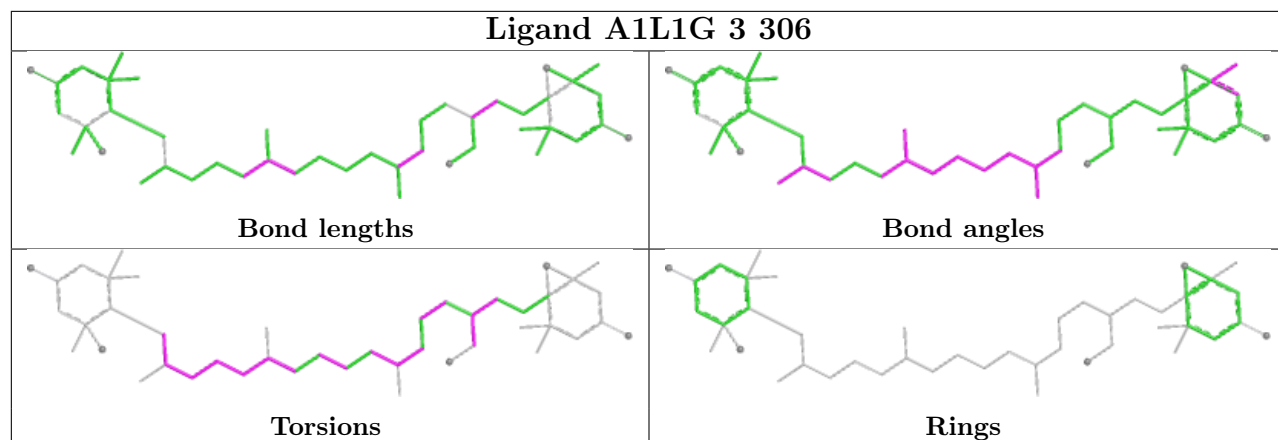
Torsions



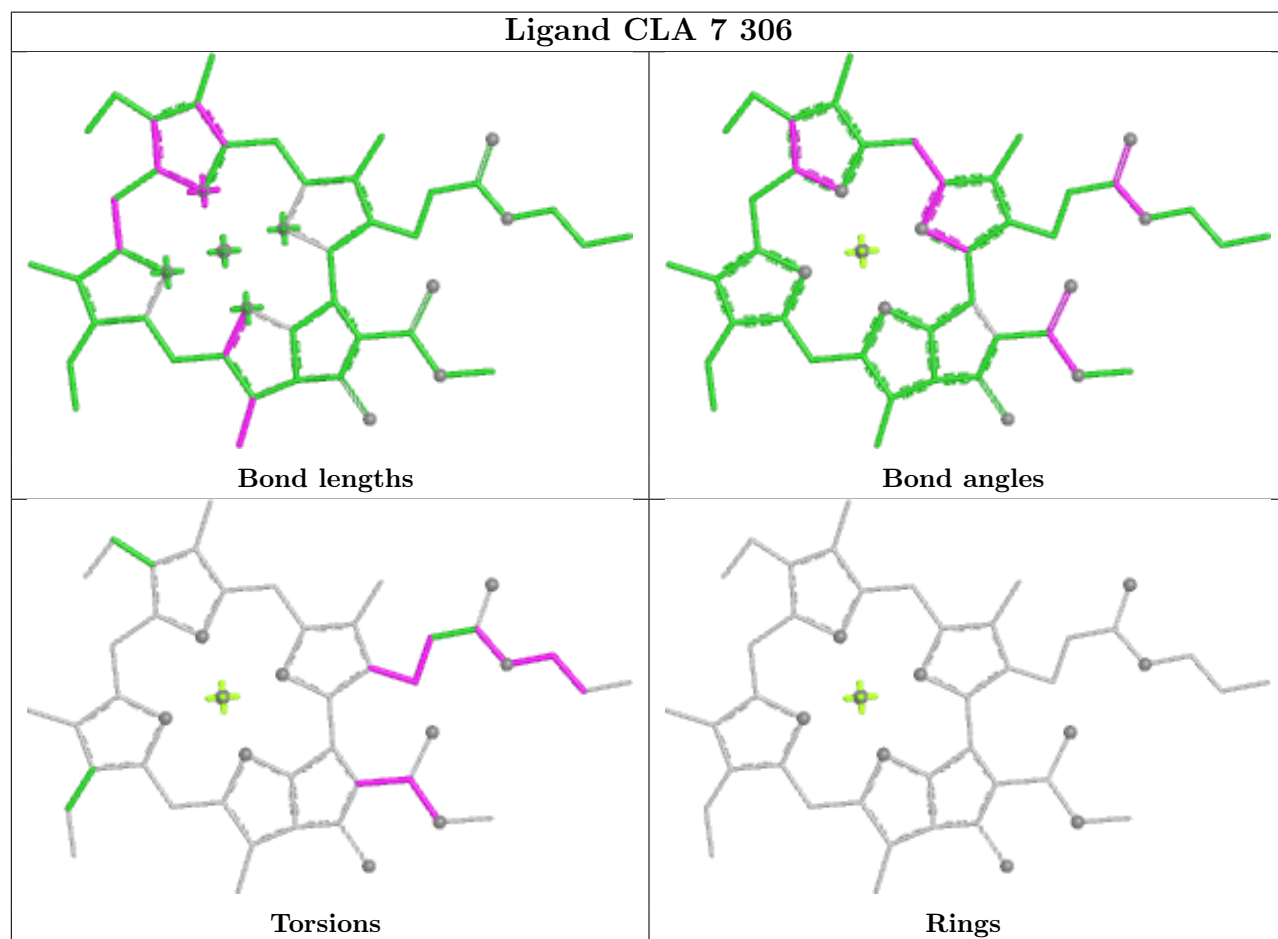
Rings

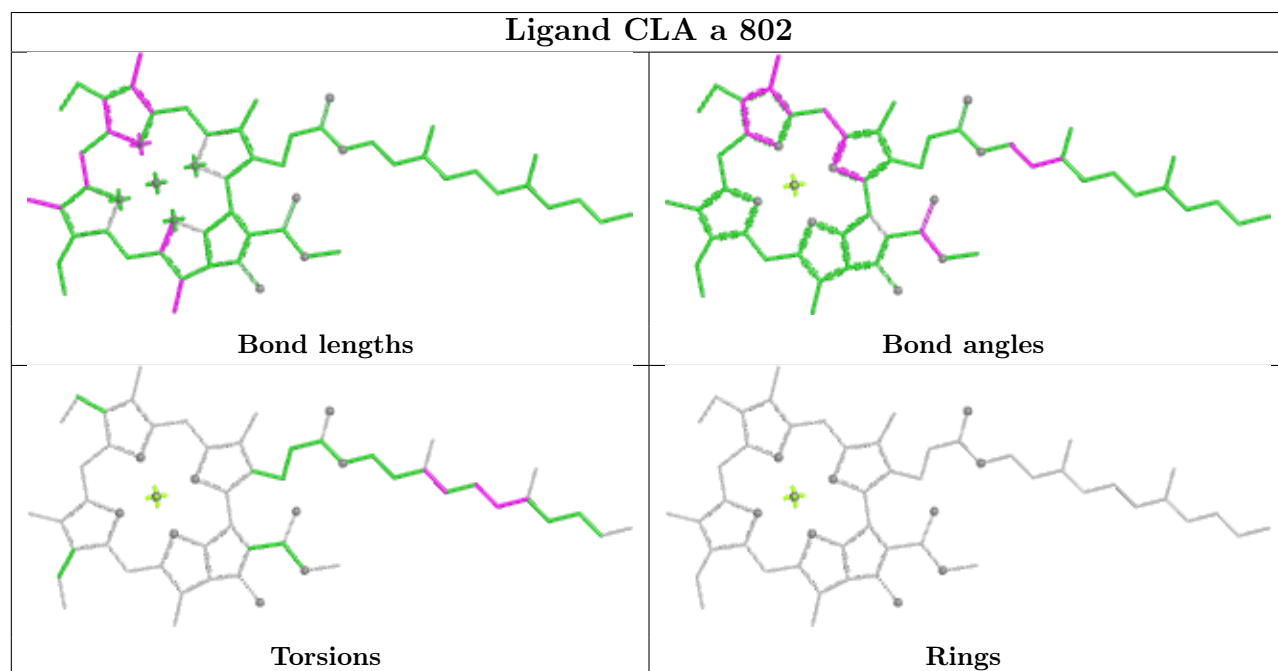
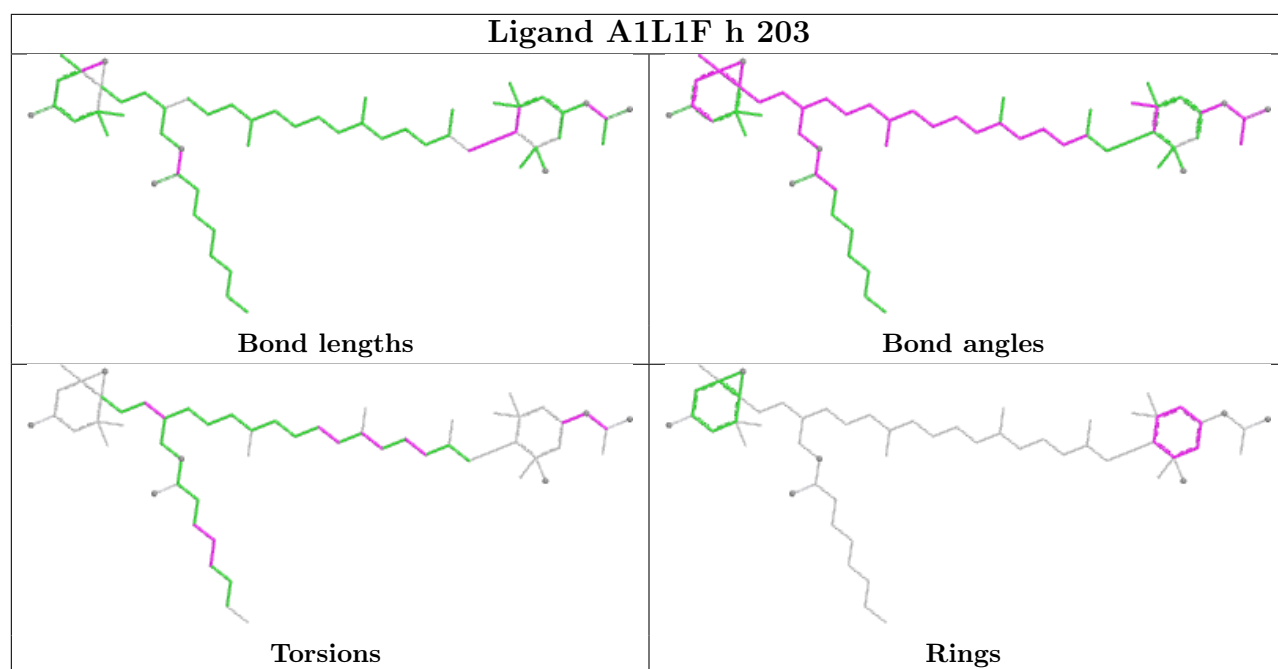


Ligand A1L1G 3 306

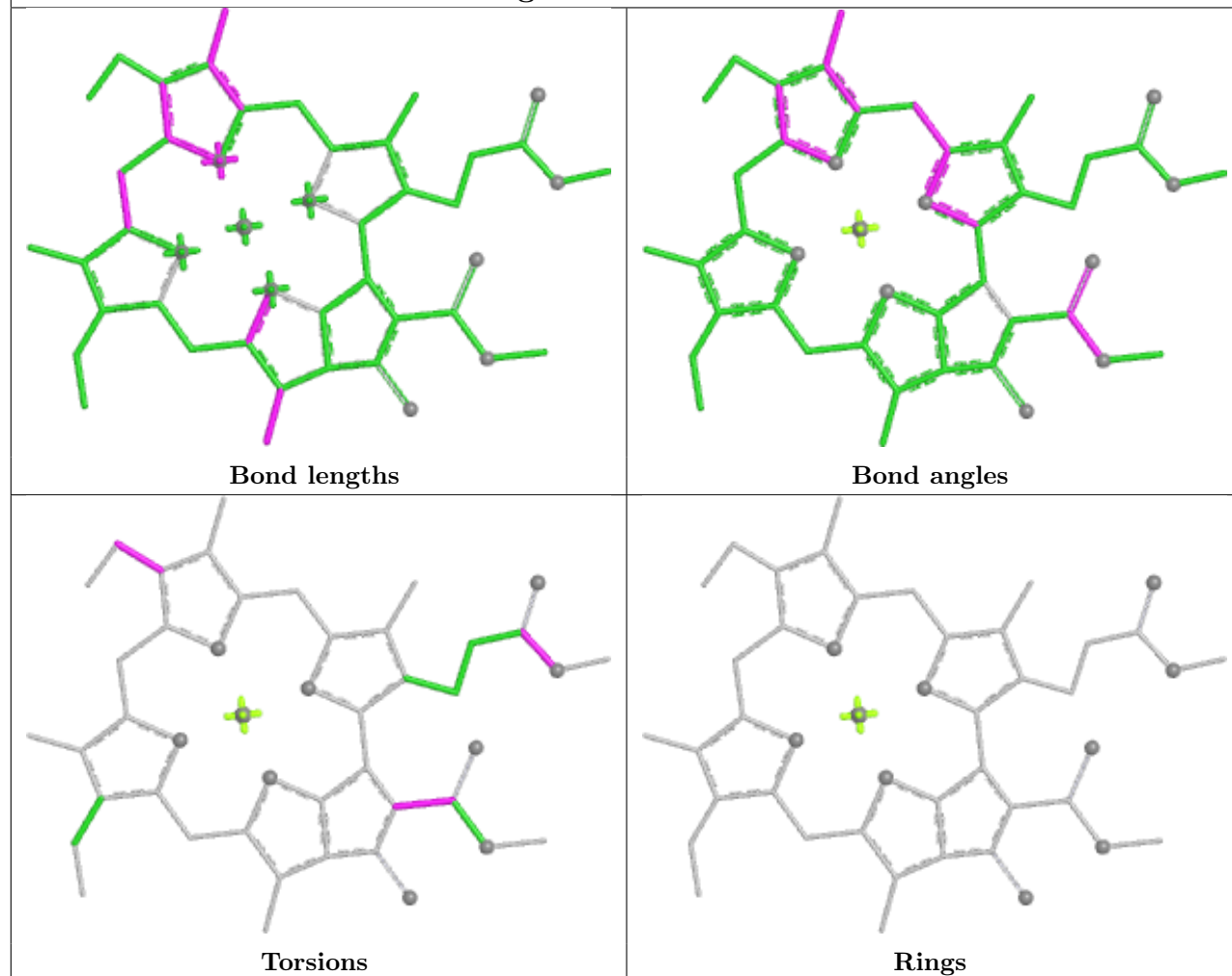


Ligand CLA 7 306

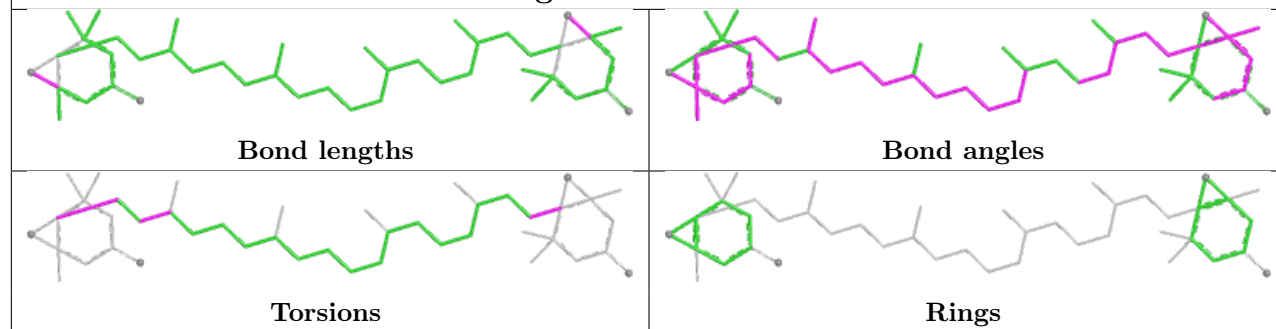




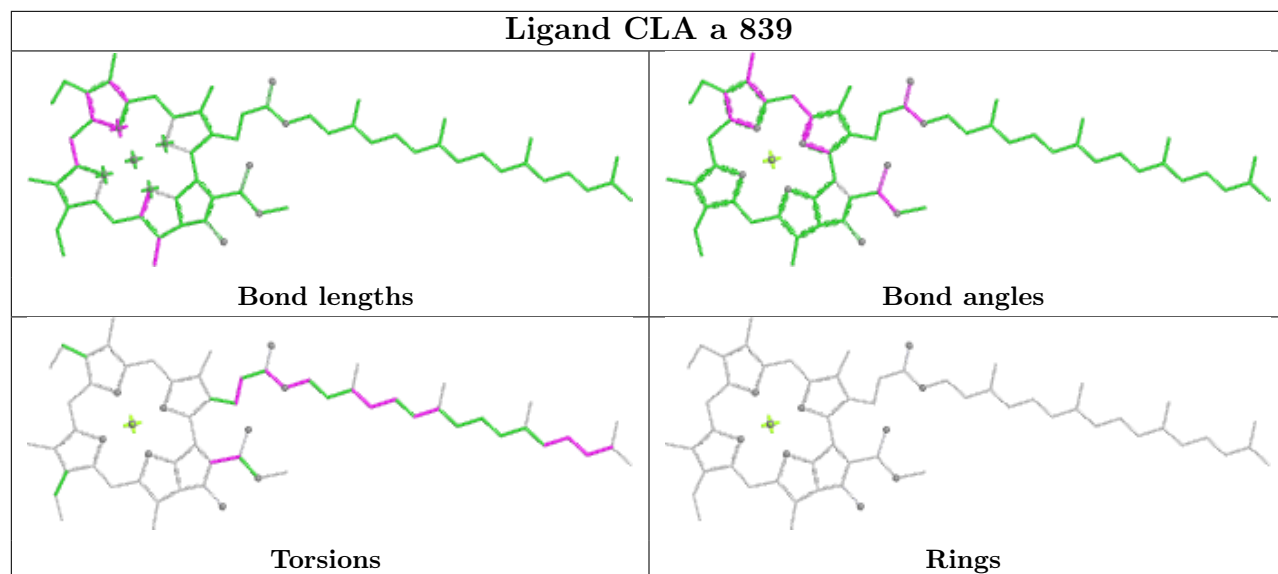
Ligand CLA 9 309



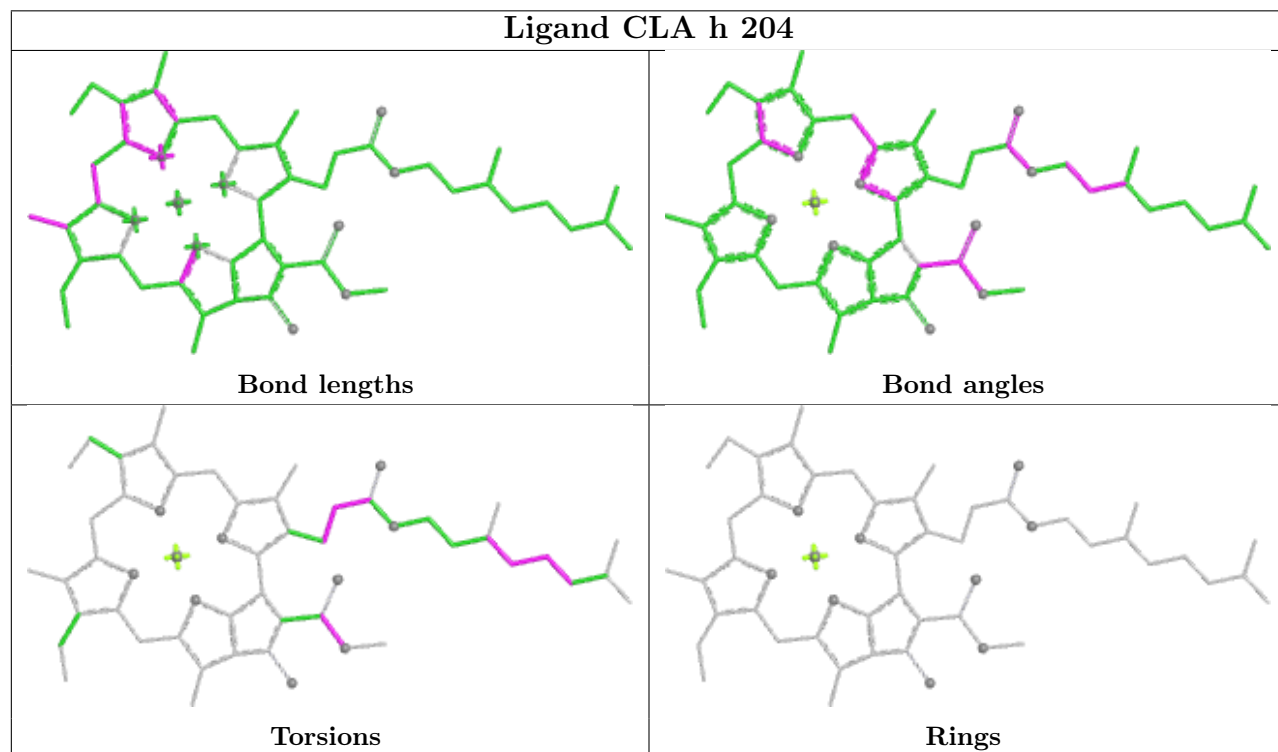
Ligand XAT 4 305



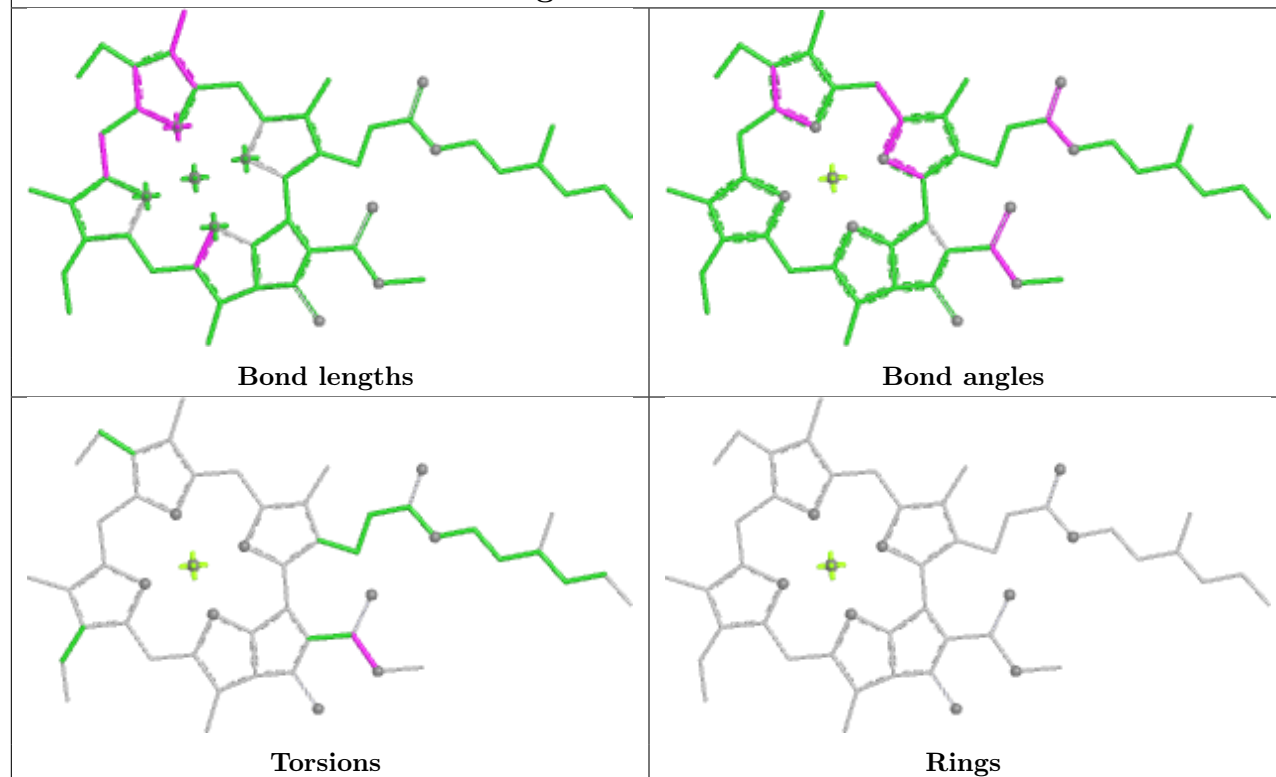
Ligand CLA a 839



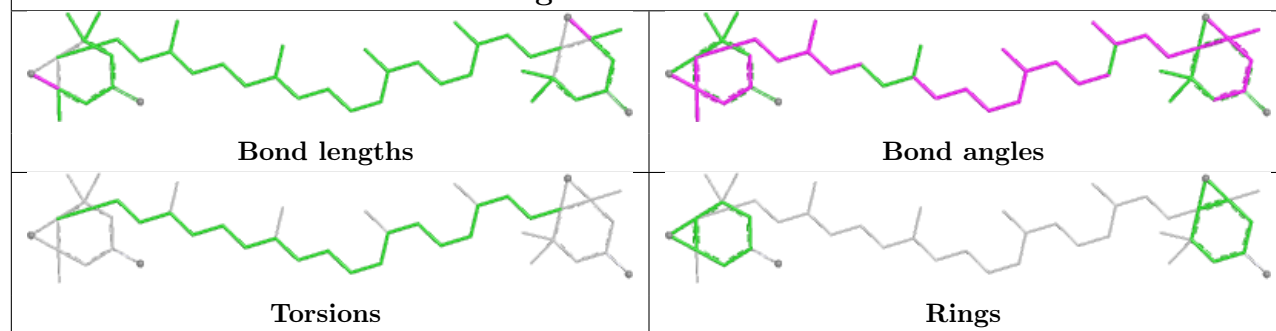
Ligand CLA h 204



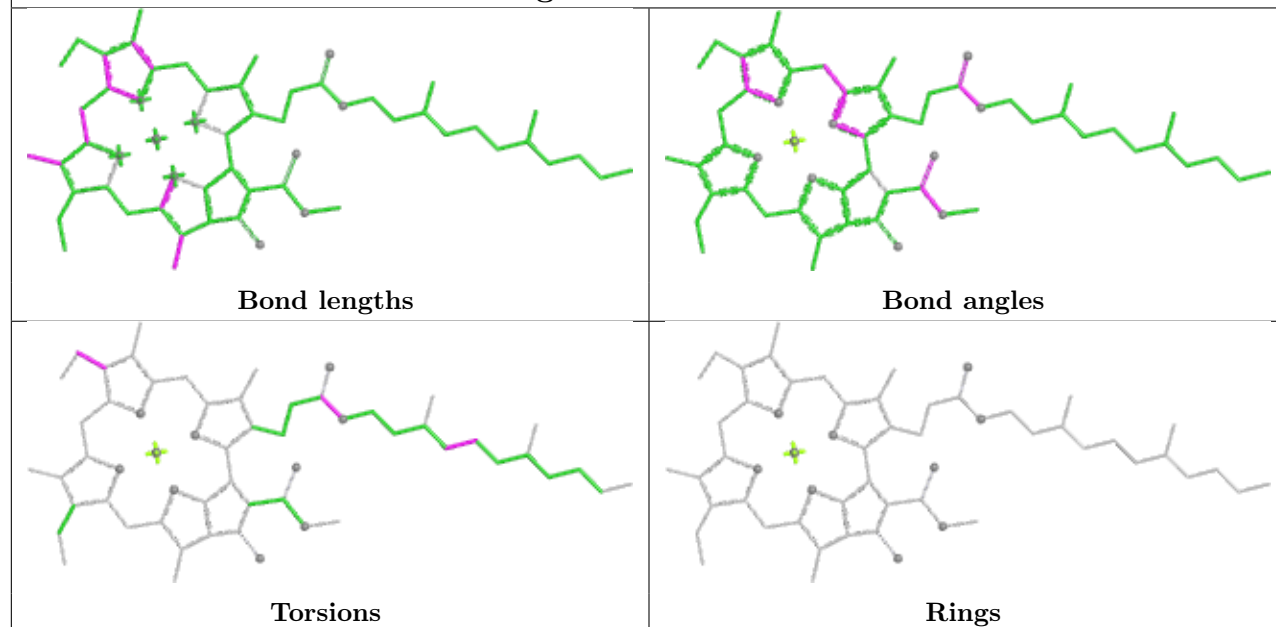
Ligand CLA 8 312



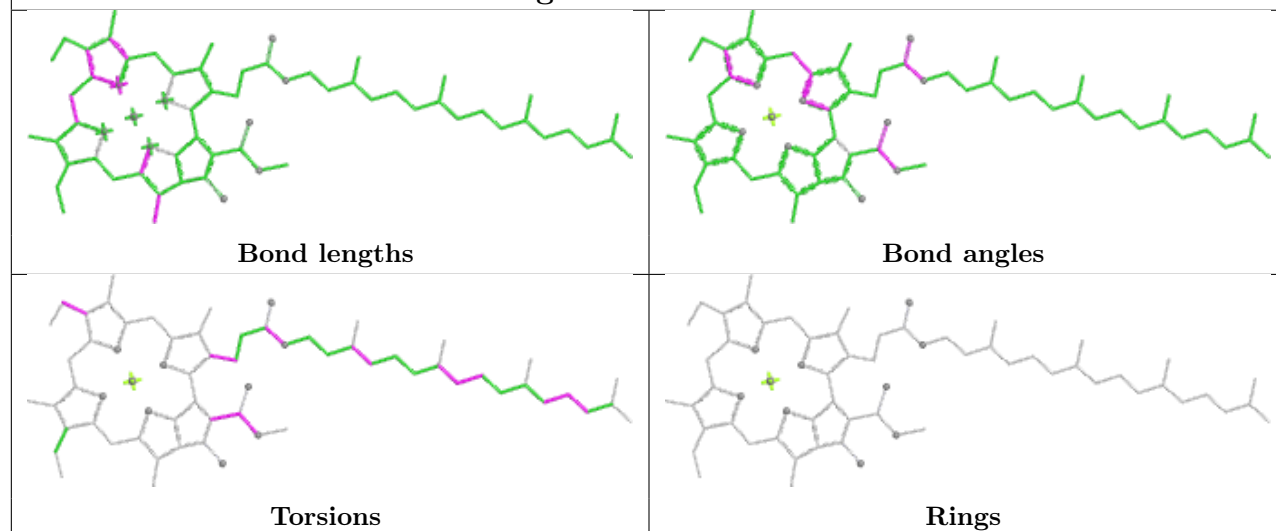
Ligand XAT 3 305



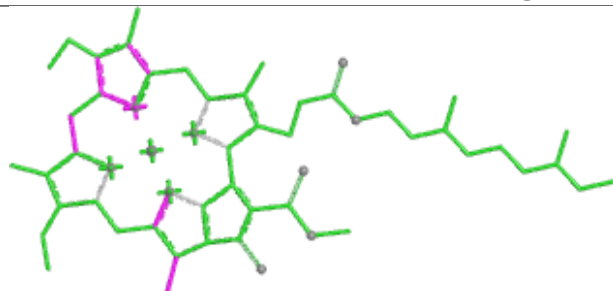
Ligand CLA 2 311



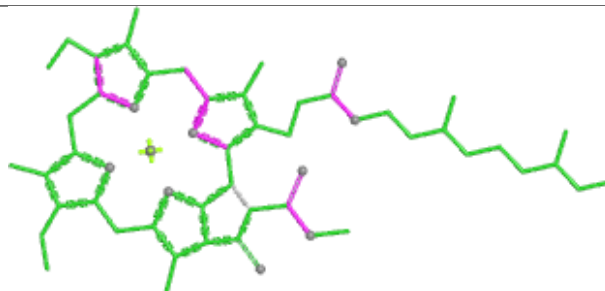
Ligand CLA 4 310



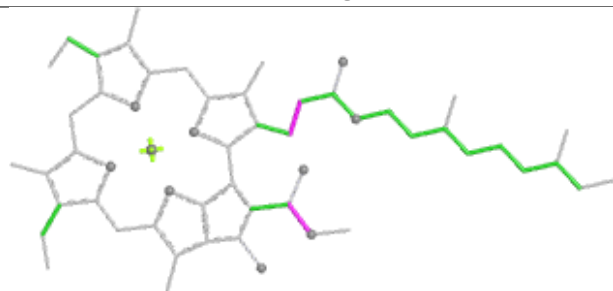
Ligand CLA 3 309



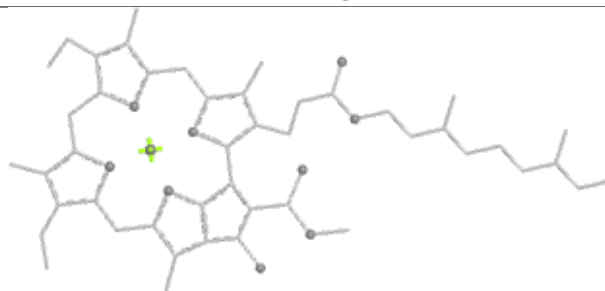
Bond lengths



Bond angles

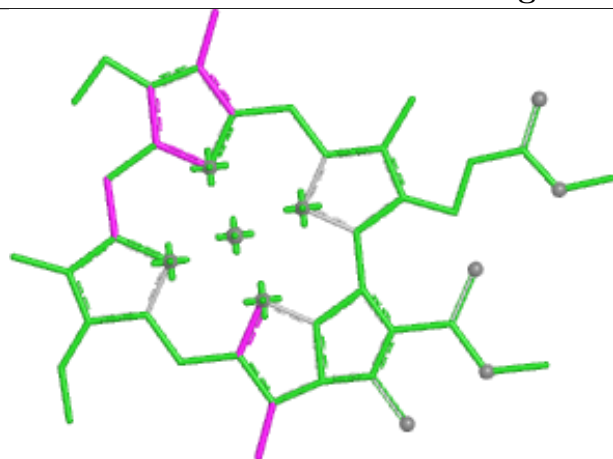


Torsions

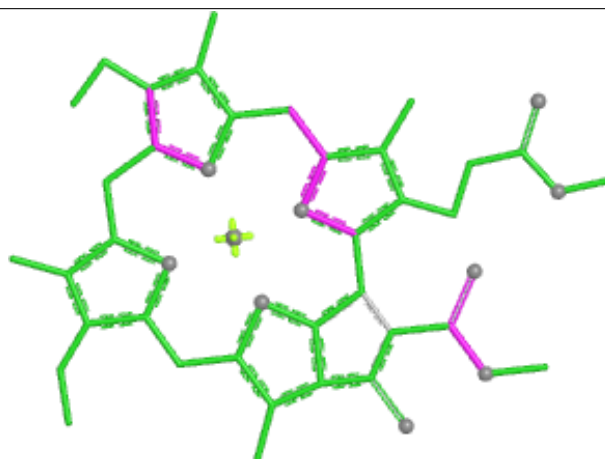


Rings

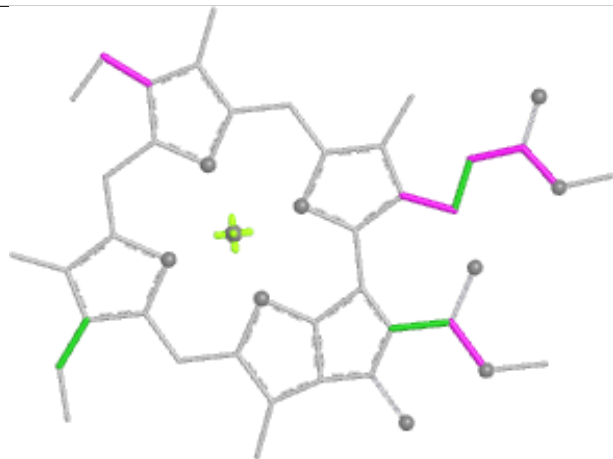
Ligand CLA 3 315



Bond lengths



Bond angles

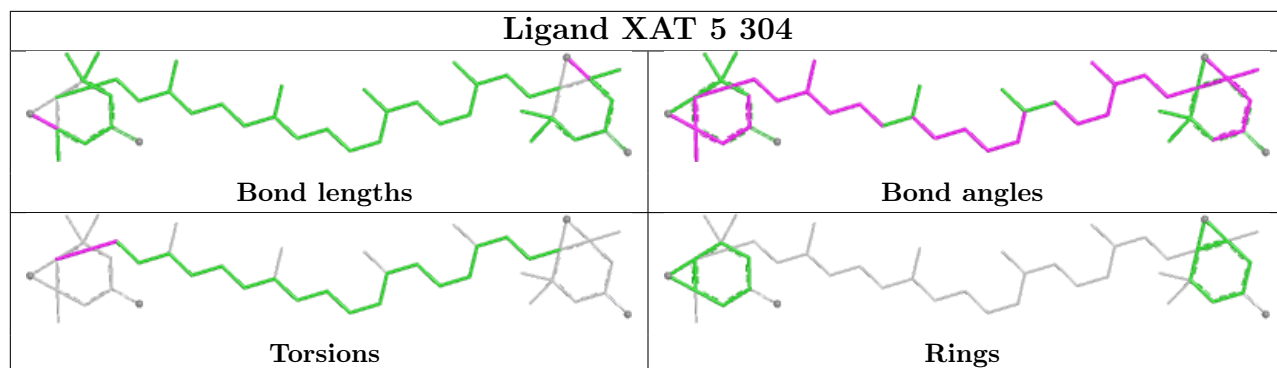


Torsions

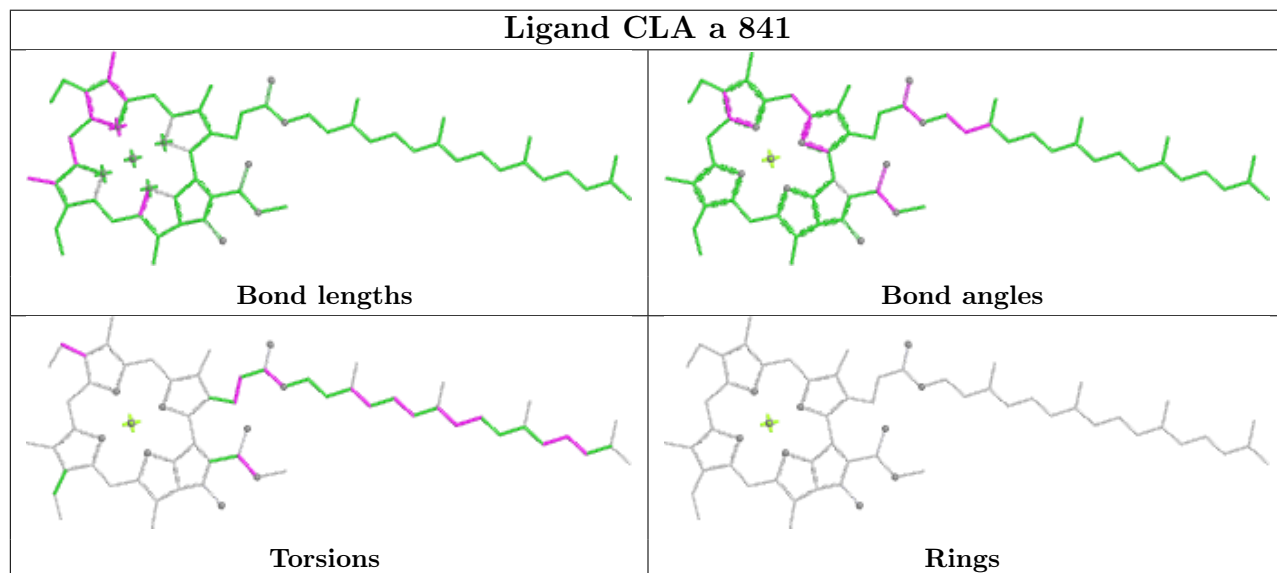


Rings

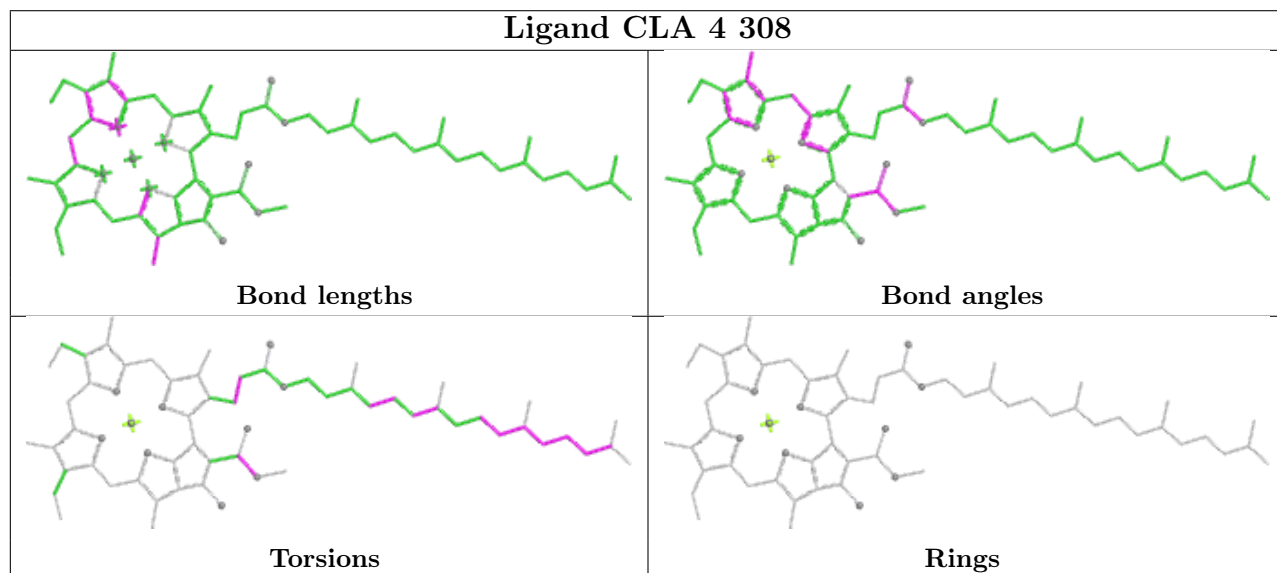
Ligand XAT 5 304

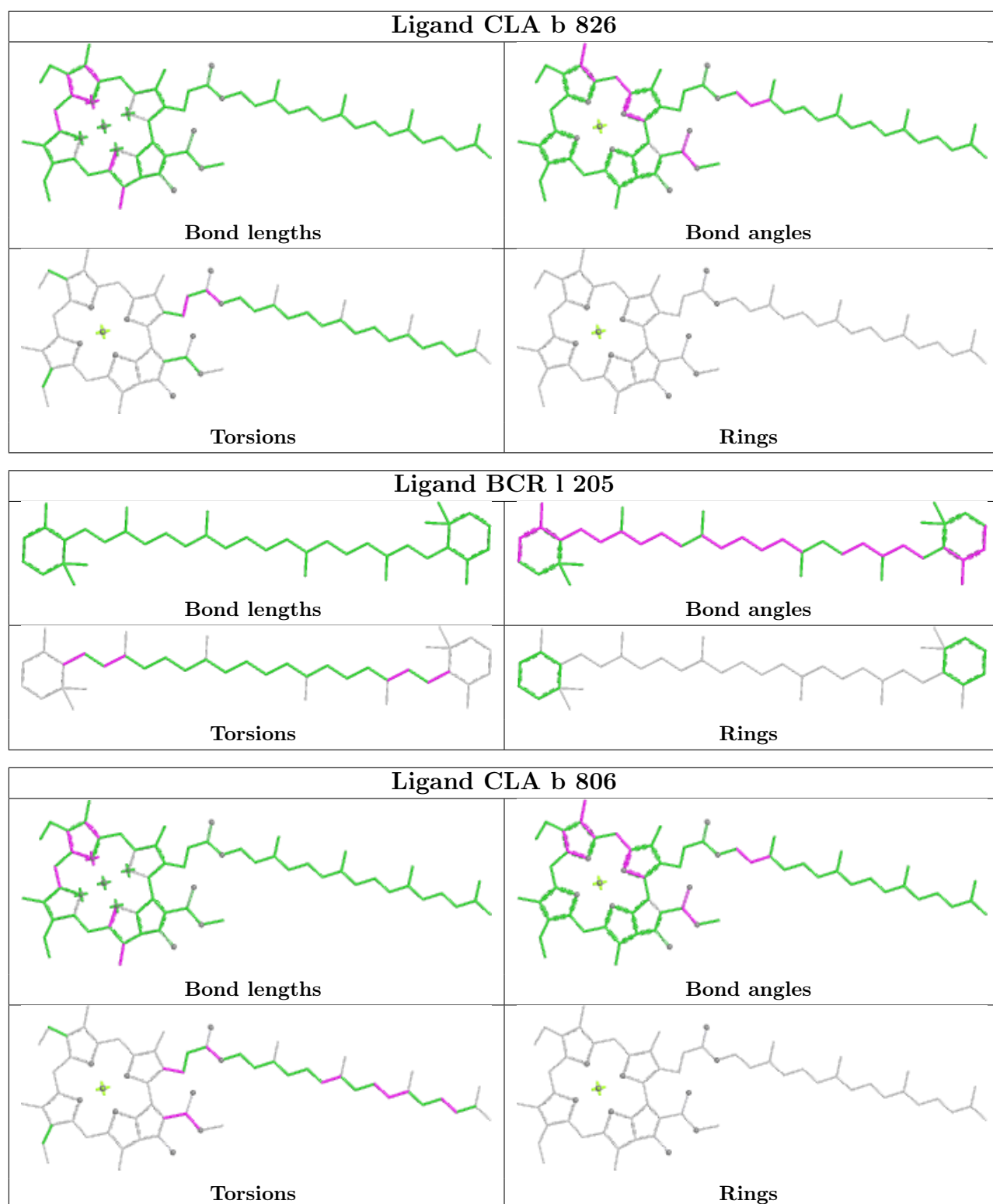


Ligand CLA a 841

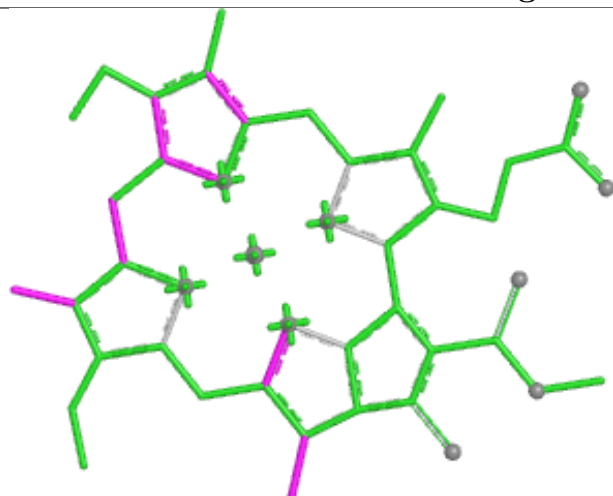


Ligand CLA 4 308

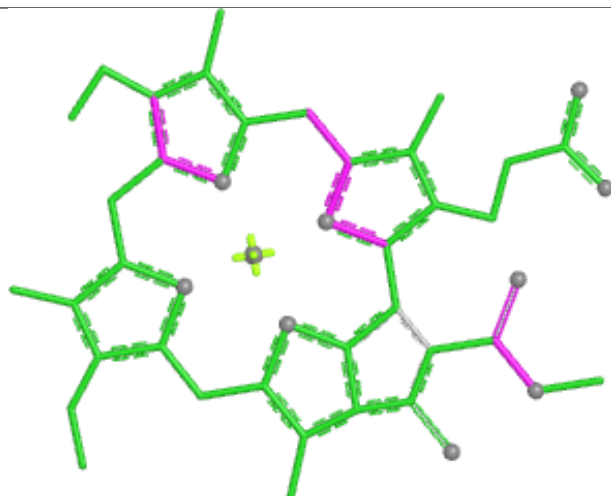




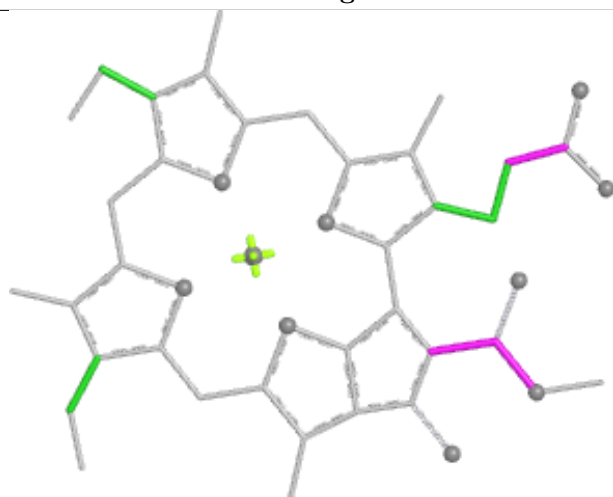
Ligand CLA 5 313



Bond lengths



Bond angles

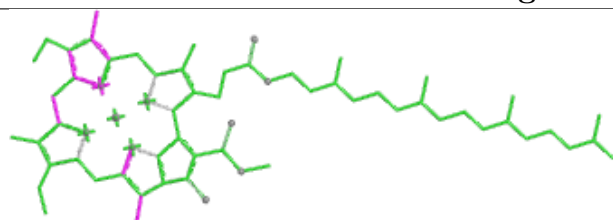


Torsions

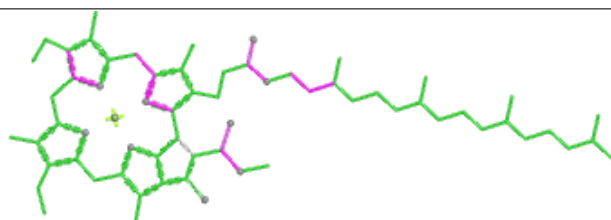


Rings

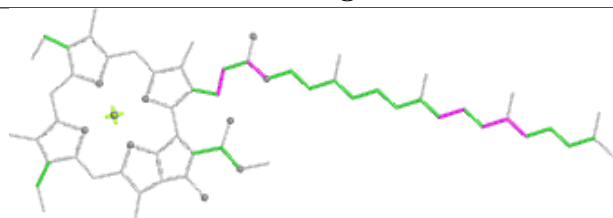
Ligand CLA a 842



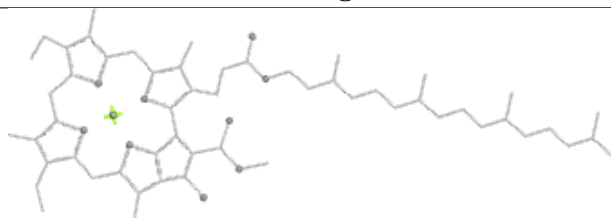
Bond lengths



Bond angles

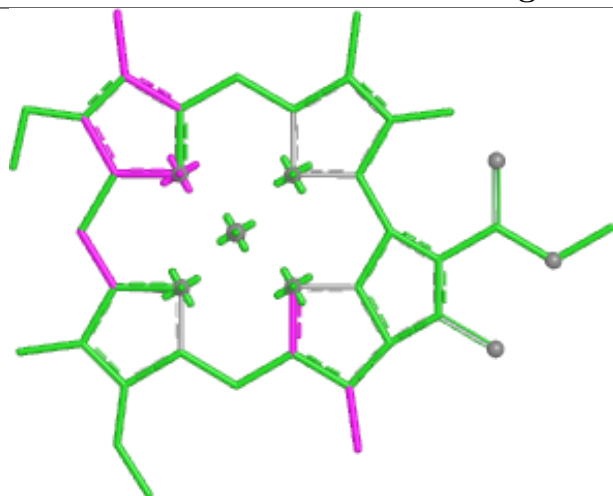


Torsions

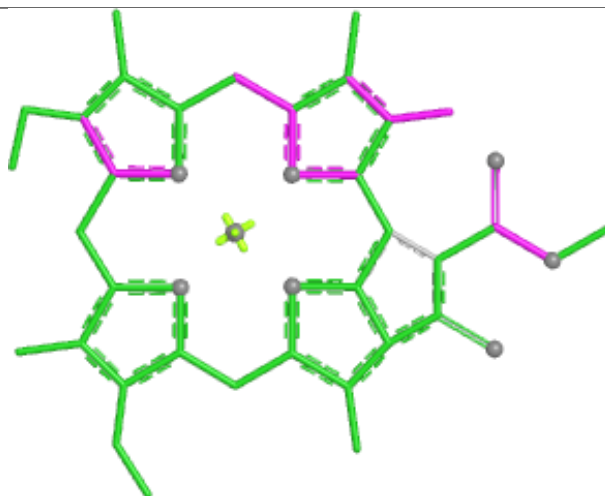


Rings

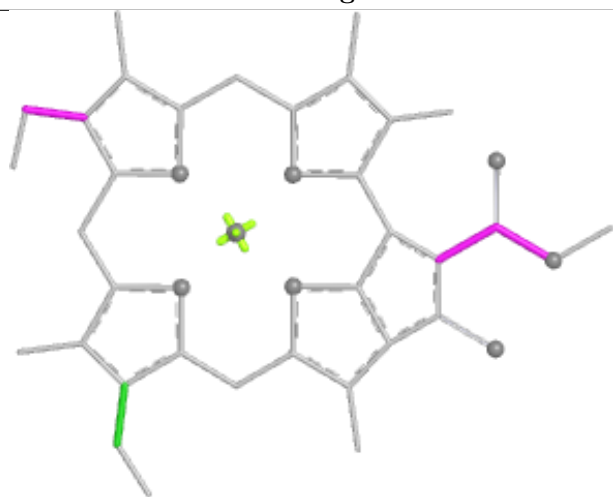
Ligand CLA 6 315



Bond lengths



Bond angles

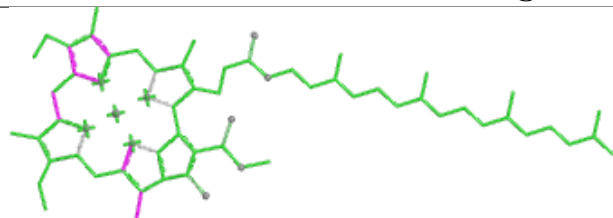


Torsions

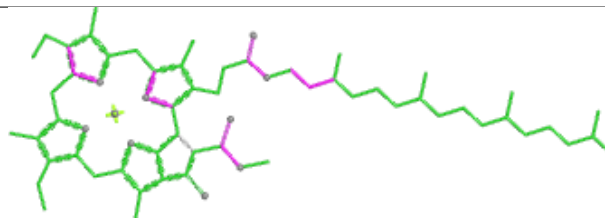


Rings

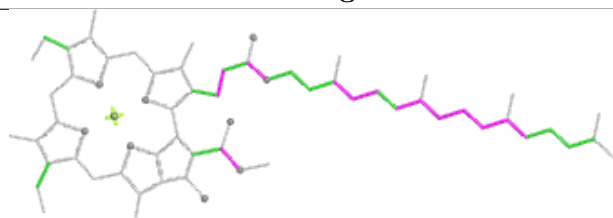
Ligand CLA b 802



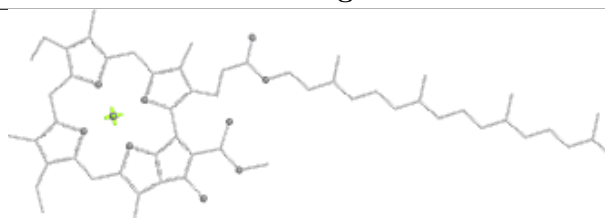
Bond lengths



Bond angles

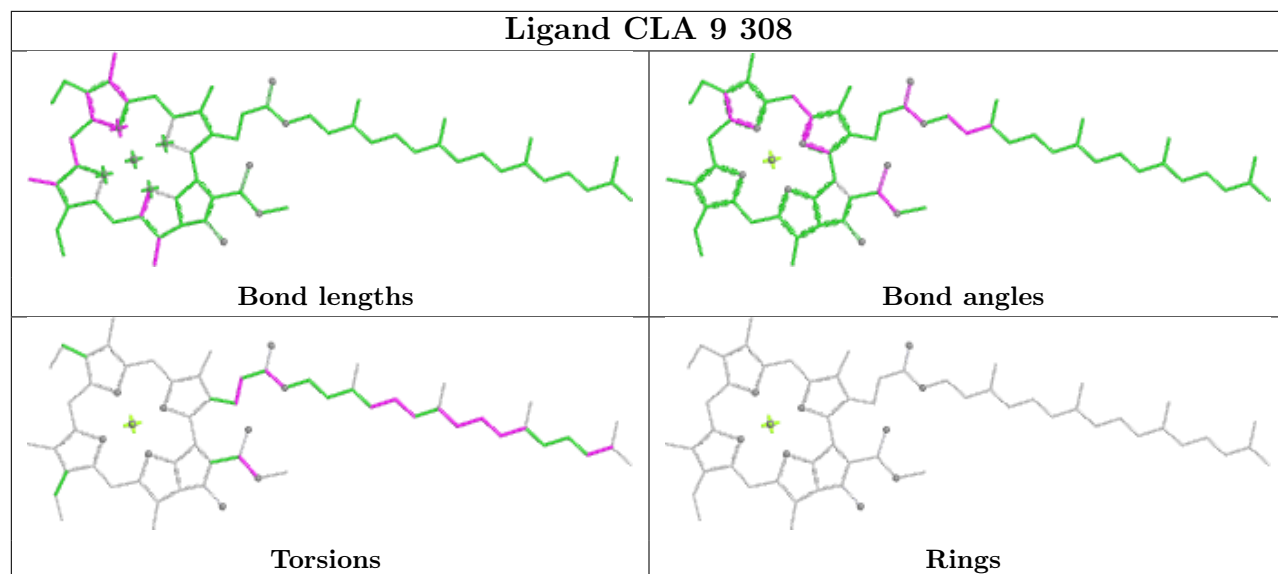


Torsions

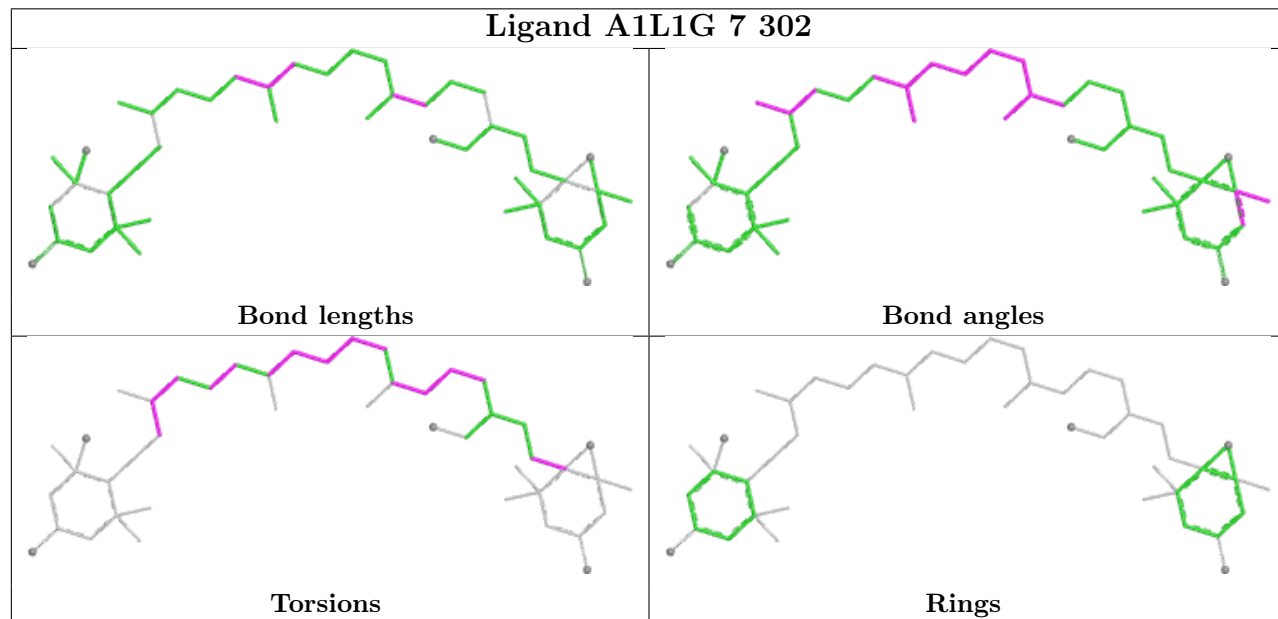


Rings

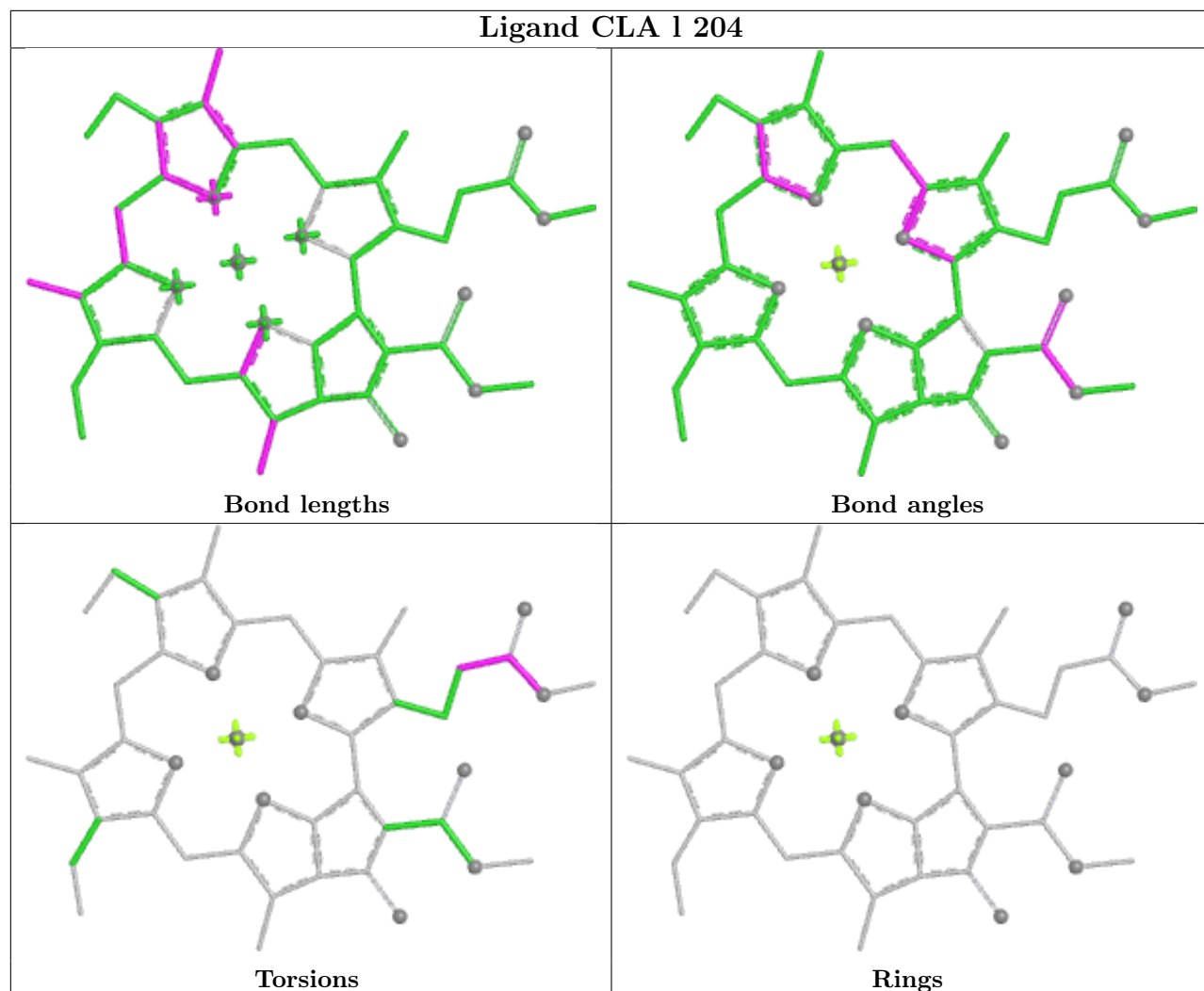
Ligand CLA 9 308



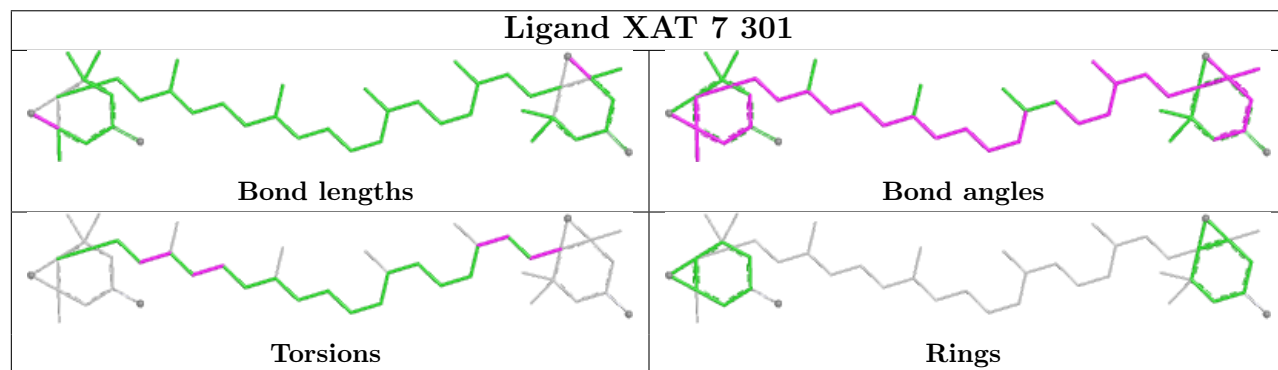
Ligand A1L1G 7 302



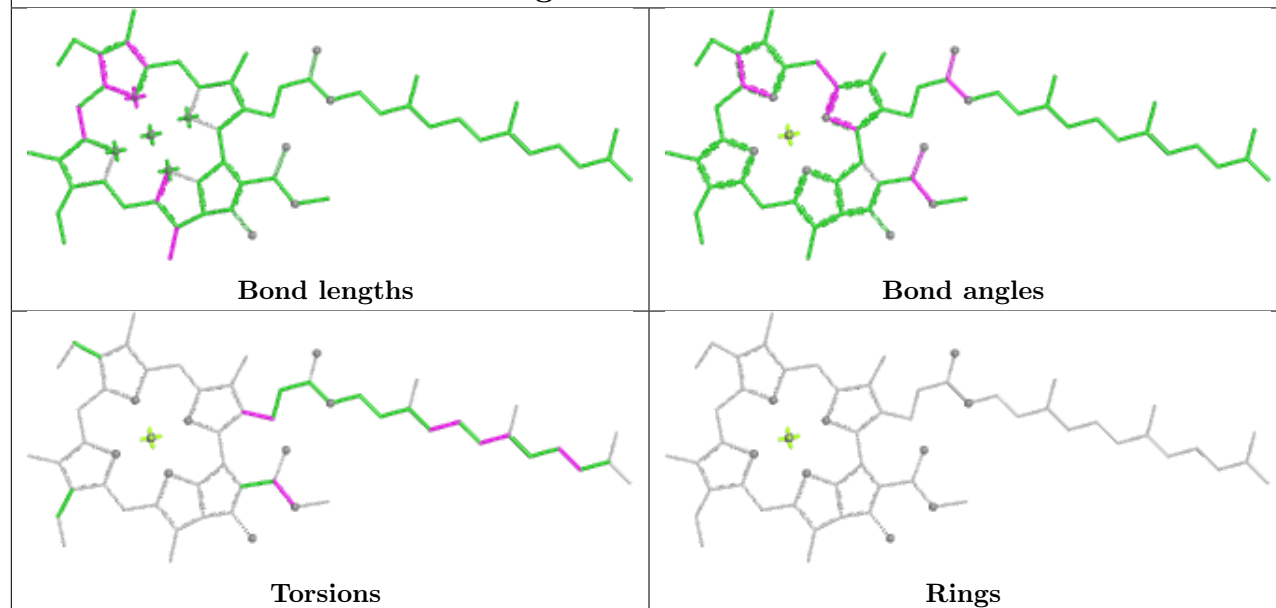
Ligand CLA 1 204



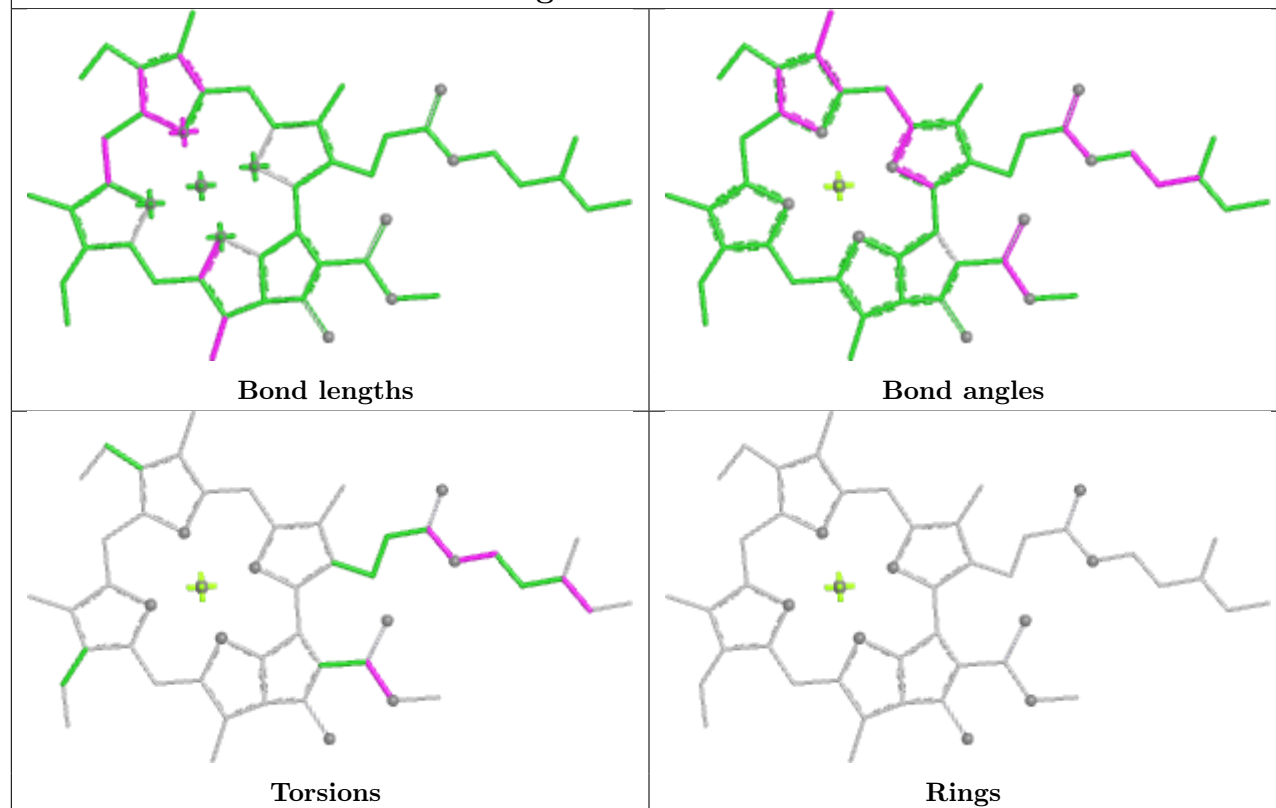
Ligand XAT 7 301



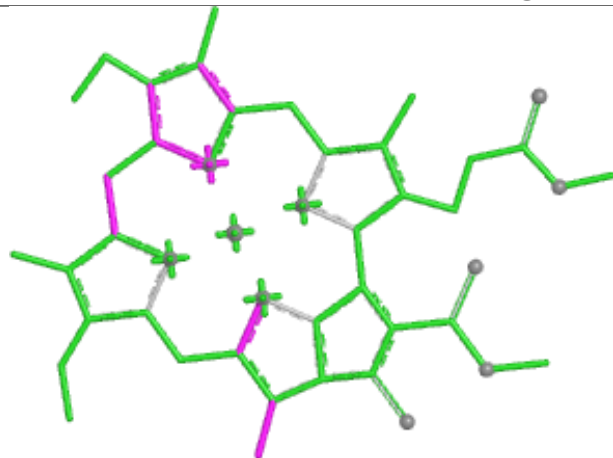
Ligand CLA b 822



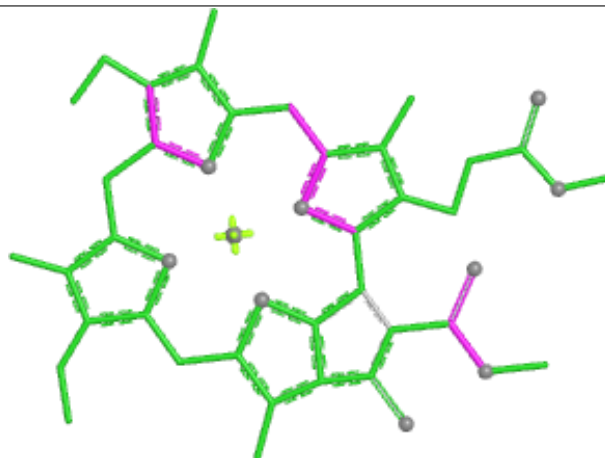
Ligand CLA 5 311



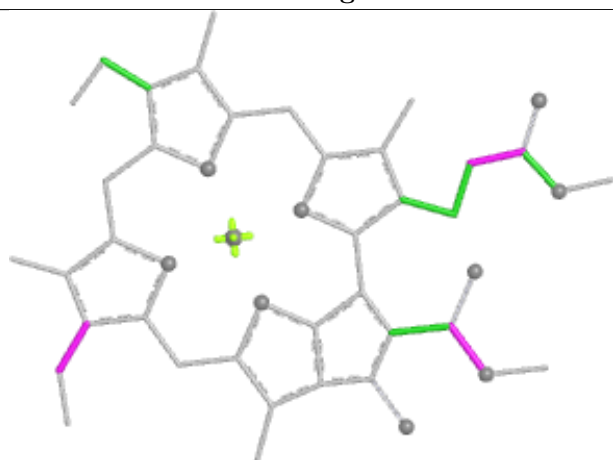
Ligand CLA 5 315



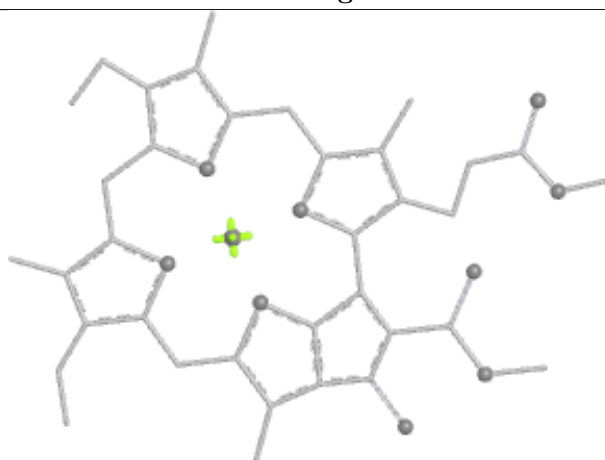
Bond lengths



Bond angles

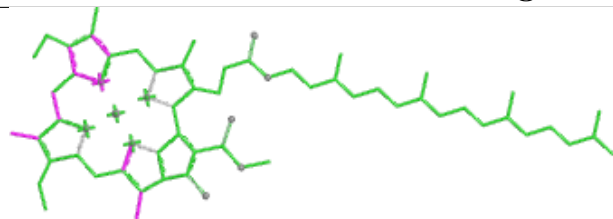


Torsions

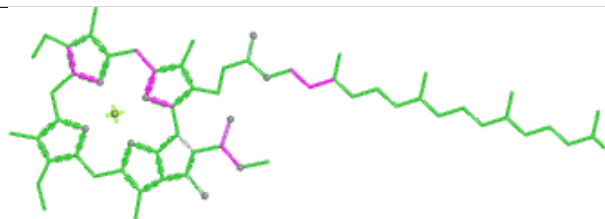


Rings

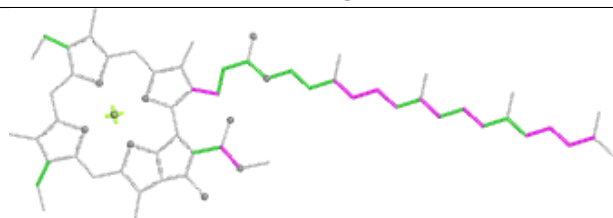
Ligand CLA b 813



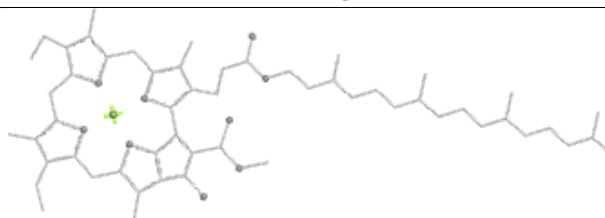
Bond lengths



Bond angles

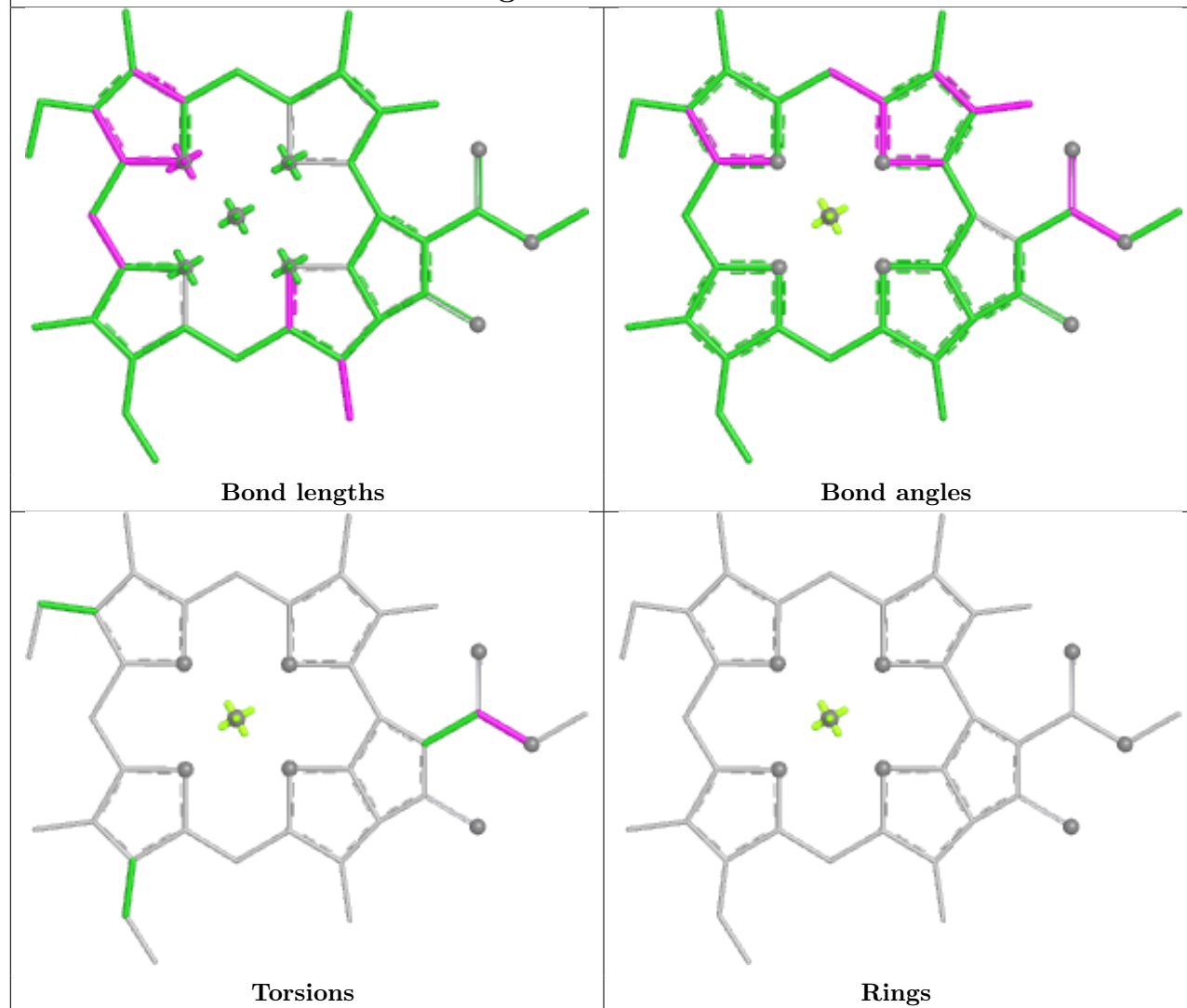


Torsions

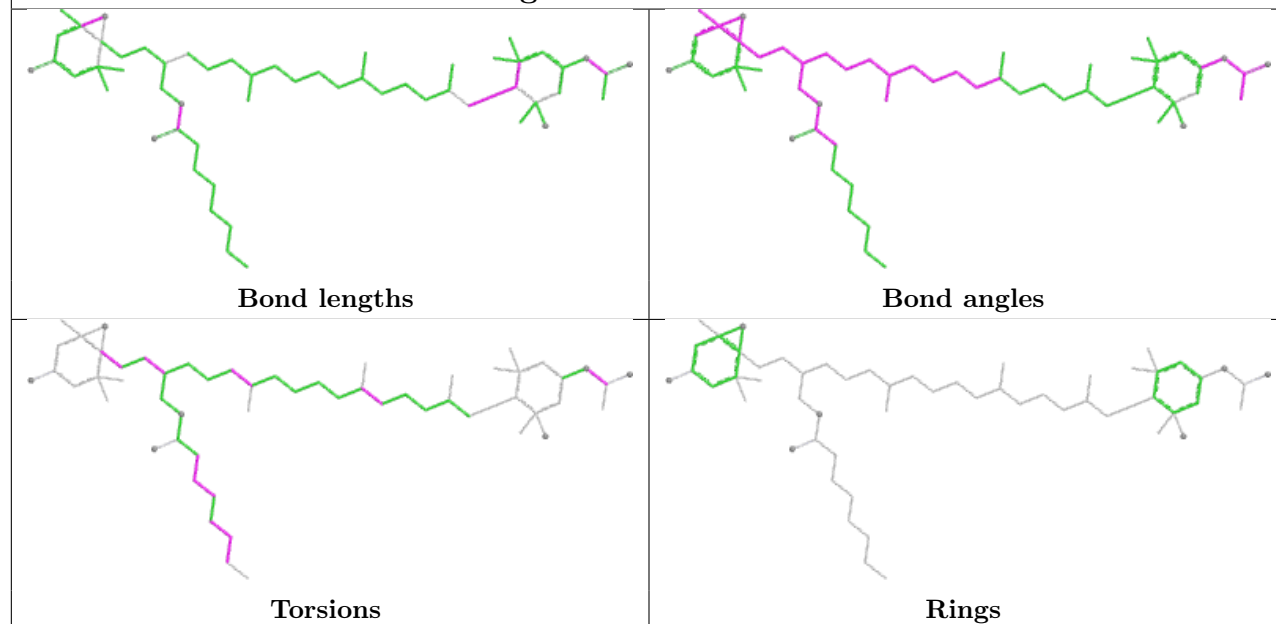


Rings

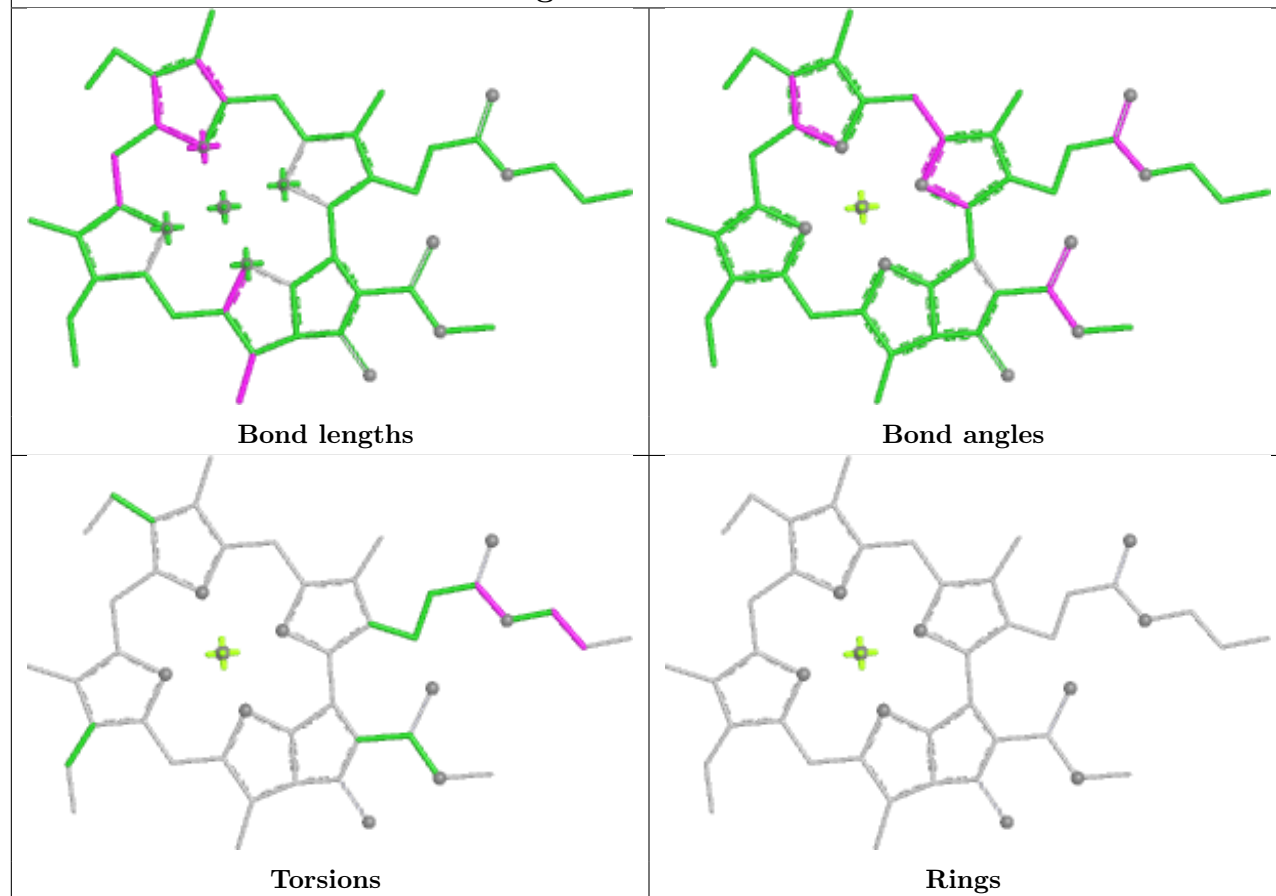
Ligand CLA 2 313



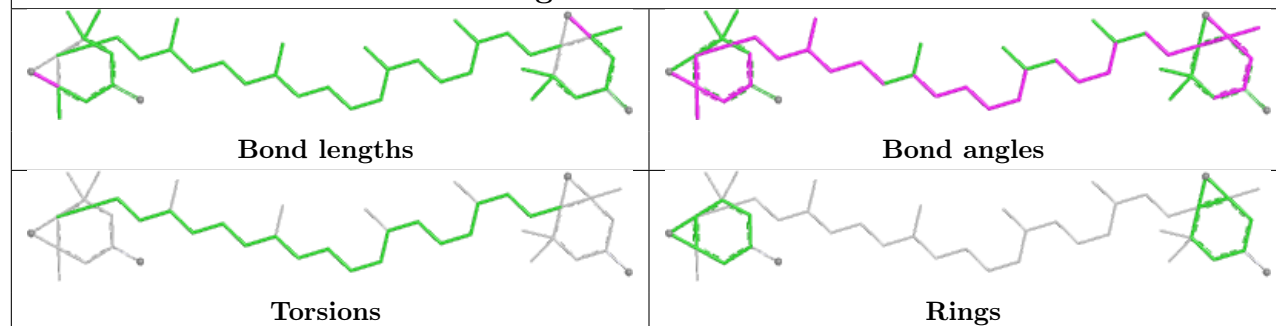
Ligand A1L1F 1 304



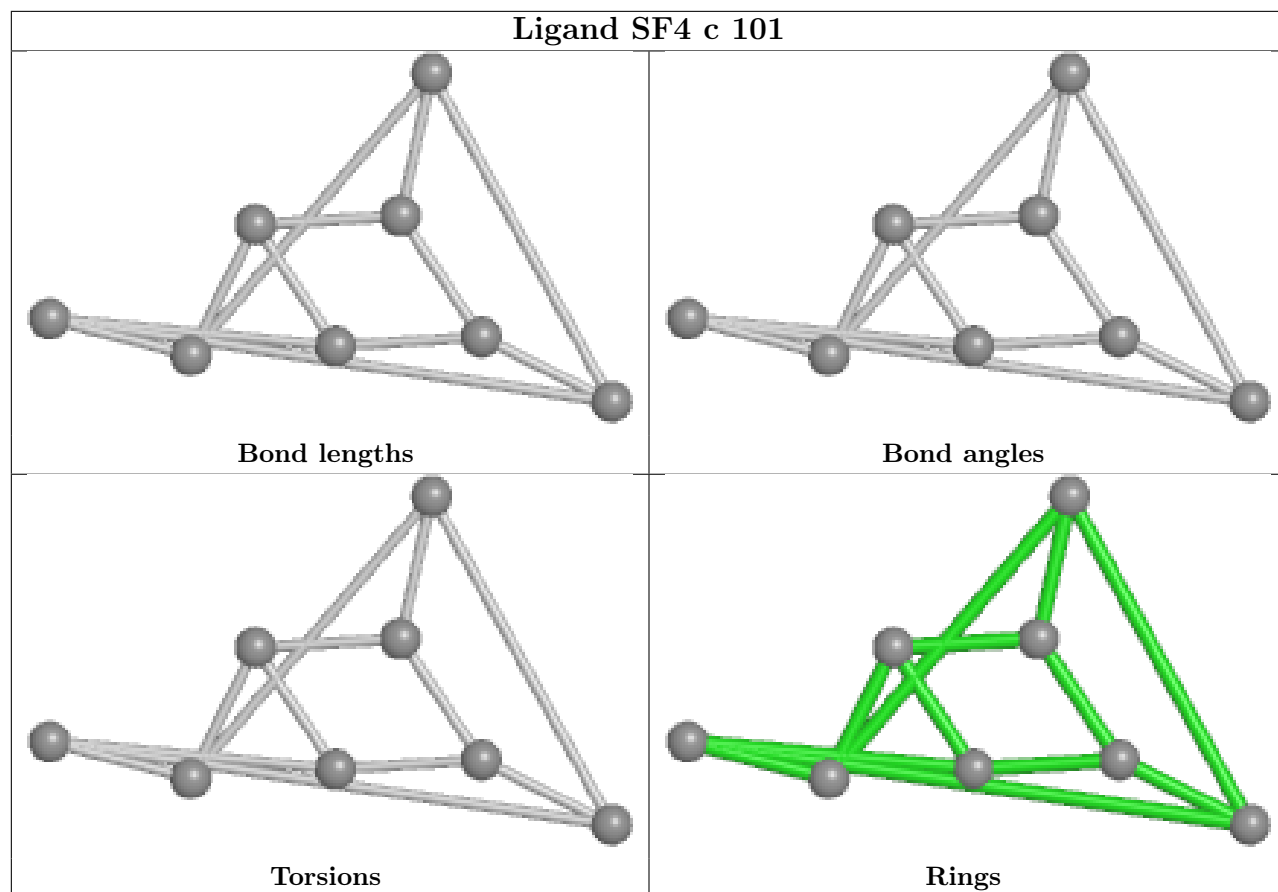
Ligand CLA 7 312



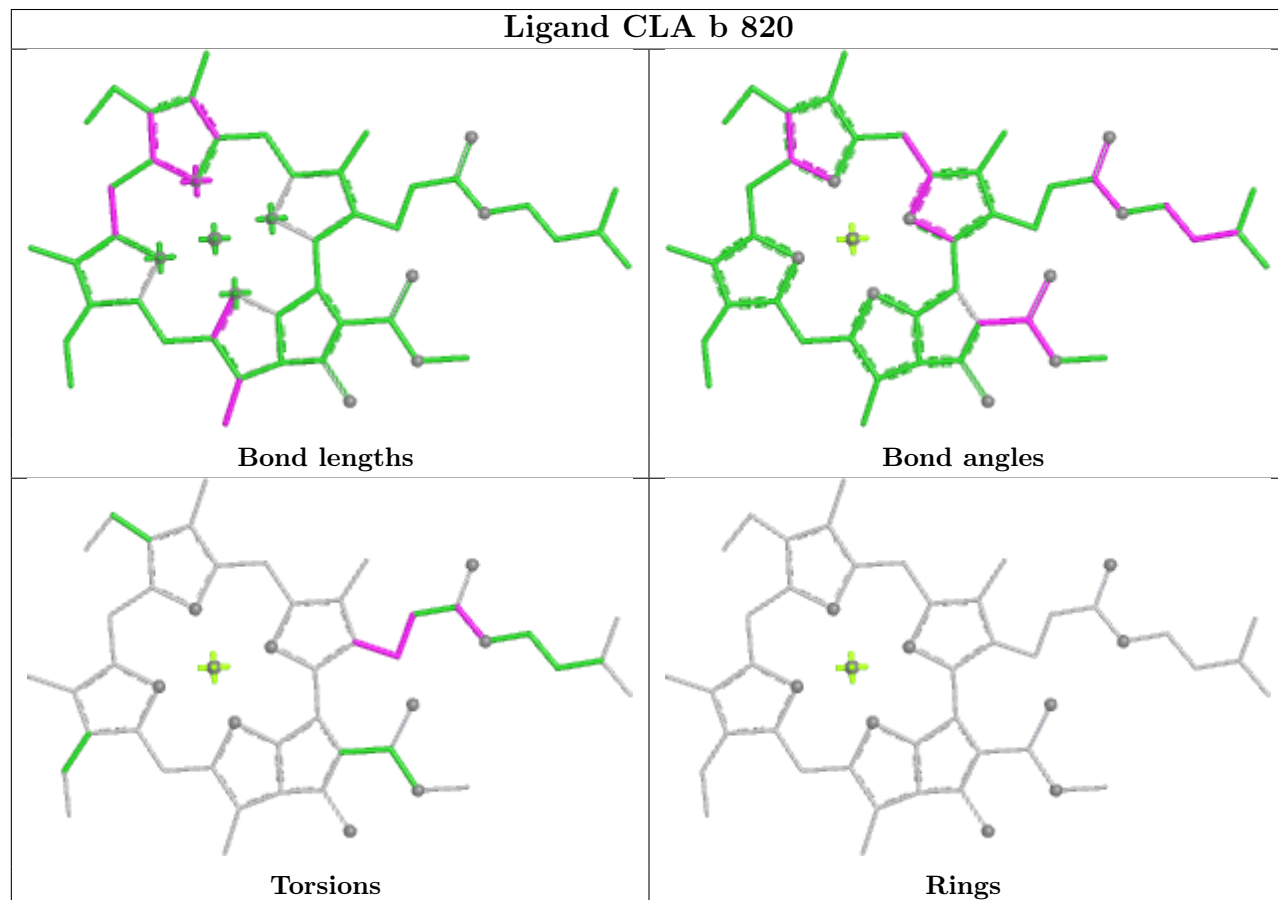
Ligand XAT 1 302



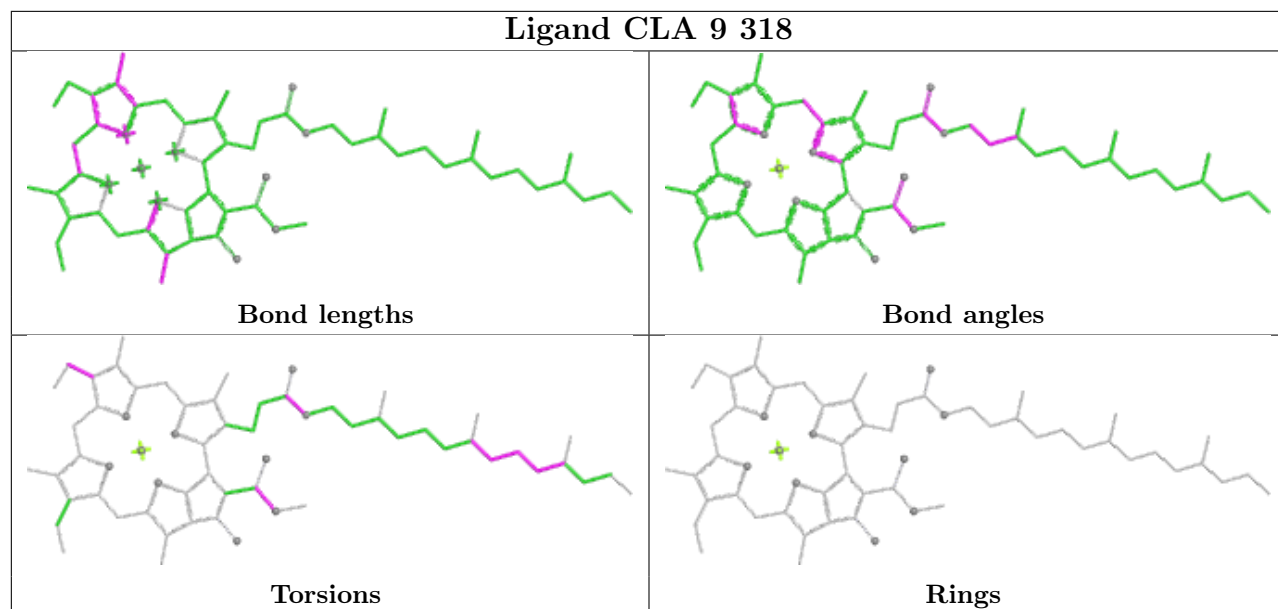
Ligand SF4 c 101



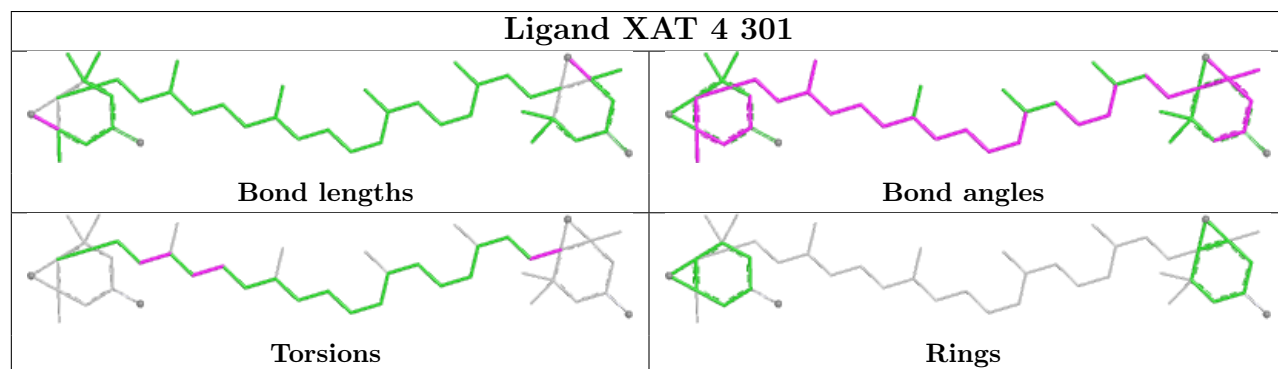
Ligand CLA b 820



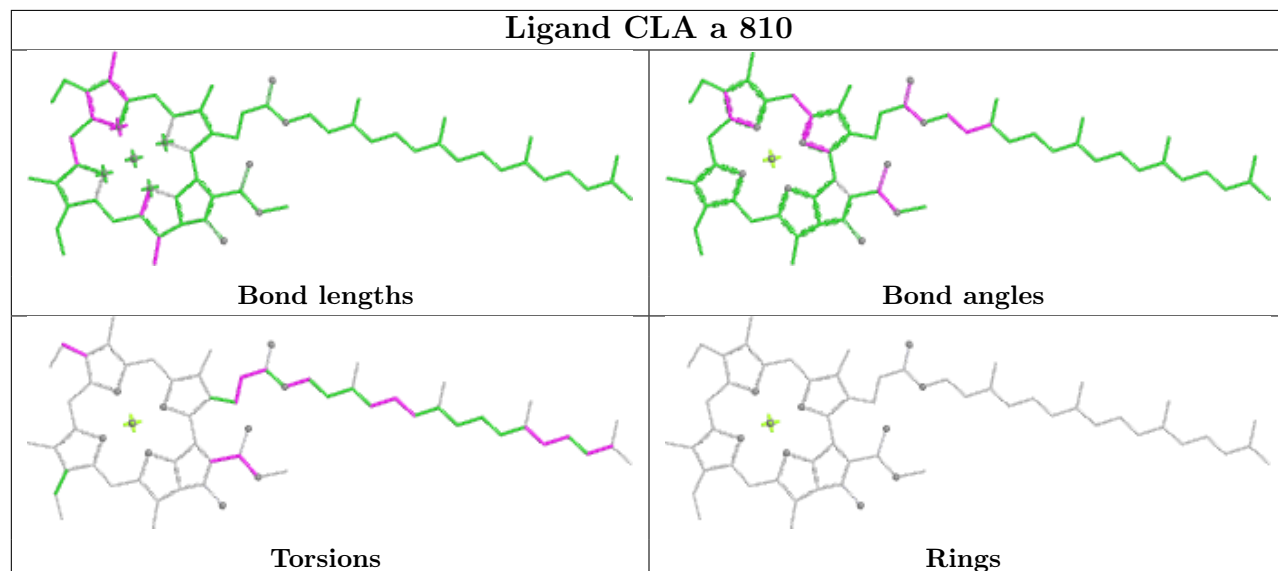
Ligand CLA 9 318



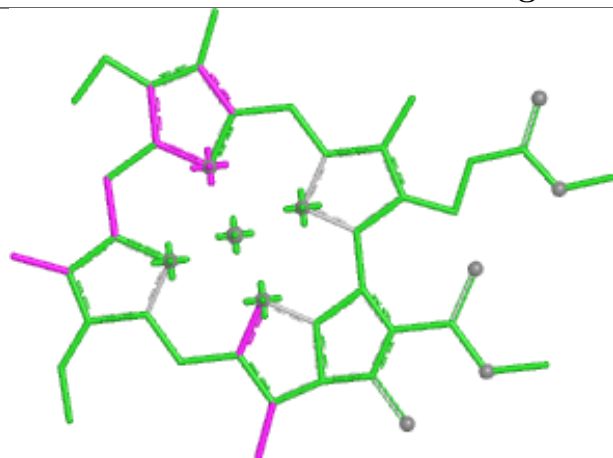
Ligand XAT 4 301



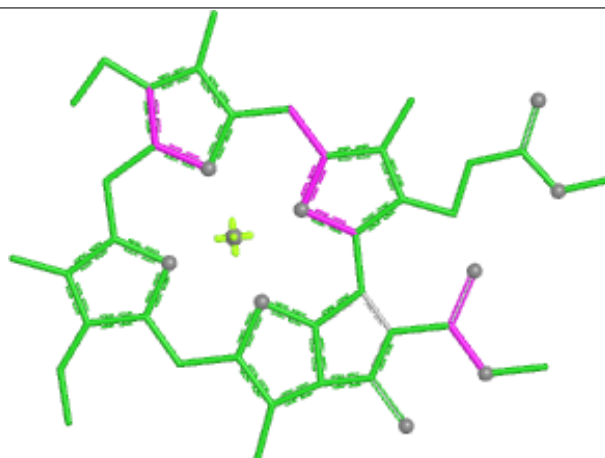
Ligand CLA a 810



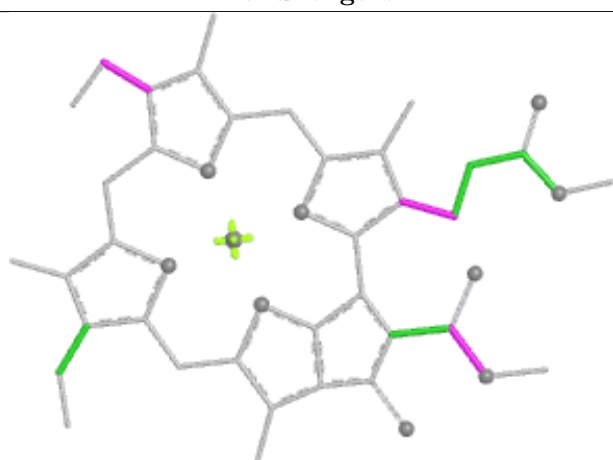
Ligand CLA 2 316



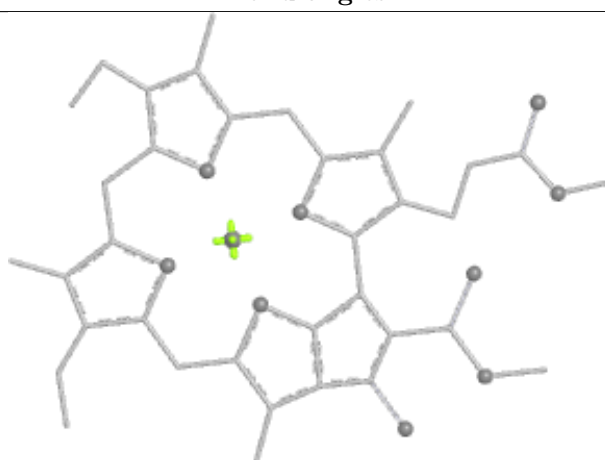
Bond lengths



Bond angles

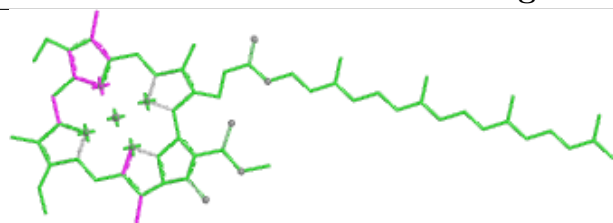


Torsions

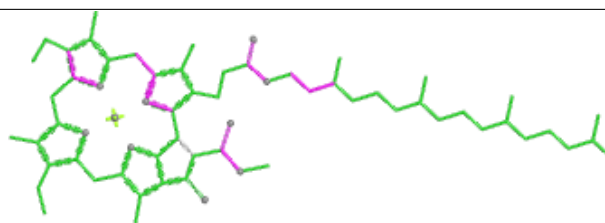


Rings

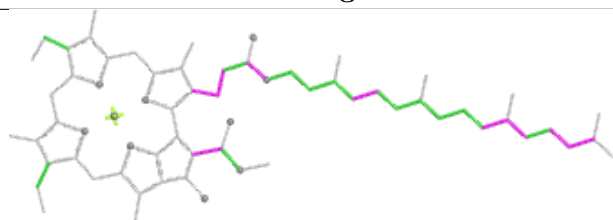
Ligand CLA 2 310



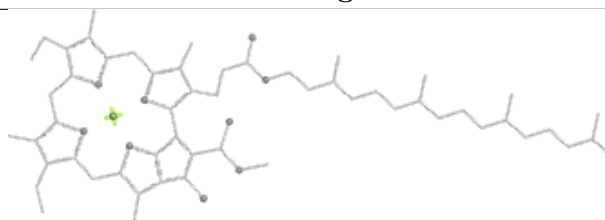
Bond lengths



Bond angles

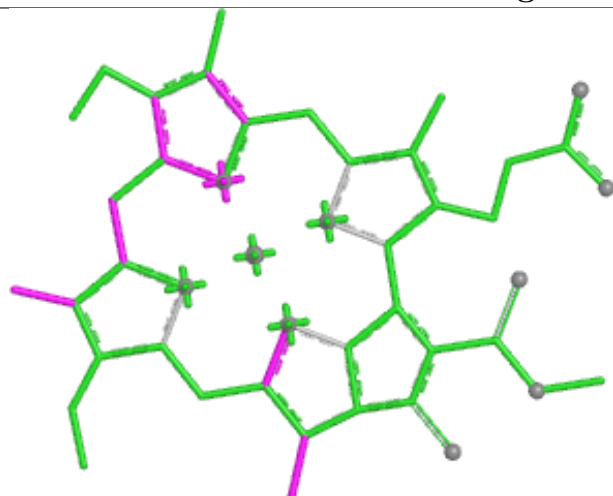


Torsions

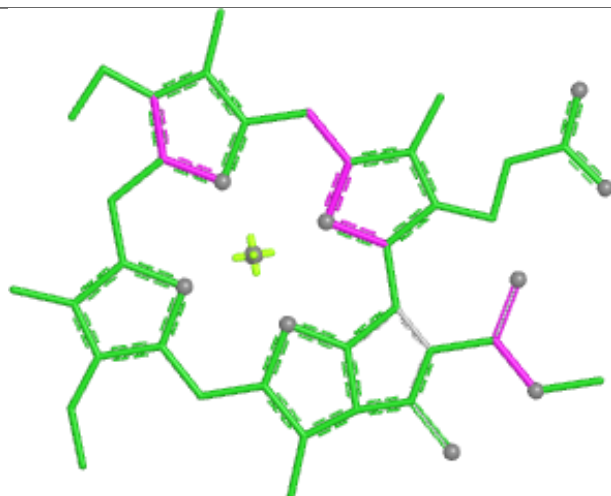


Rings

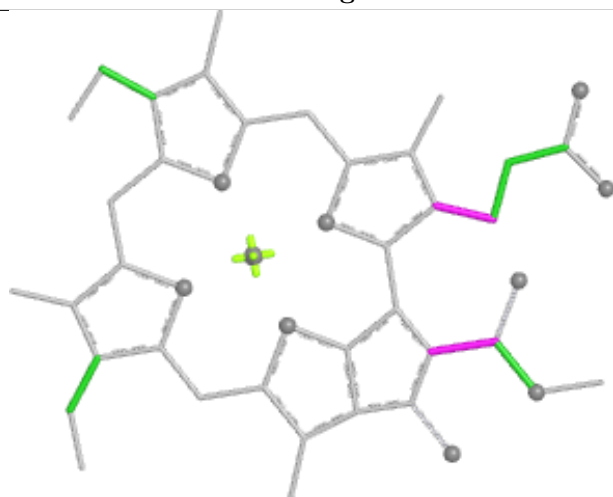
Ligand CLA b 815



Bond lengths



Bond angles

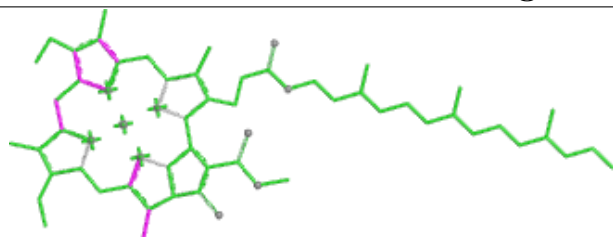


Torsions

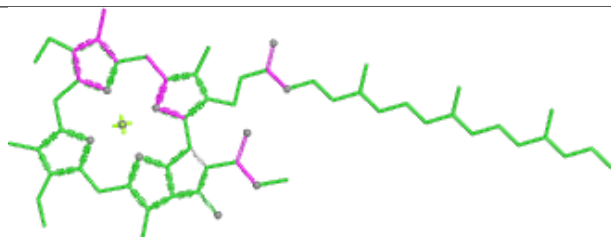


Rings

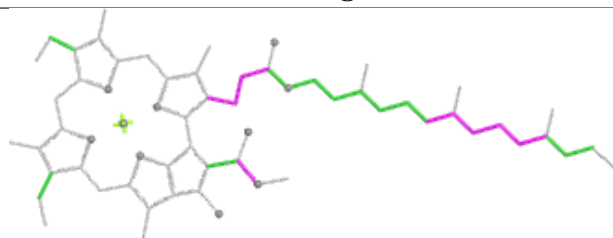
Ligand CLA a 829



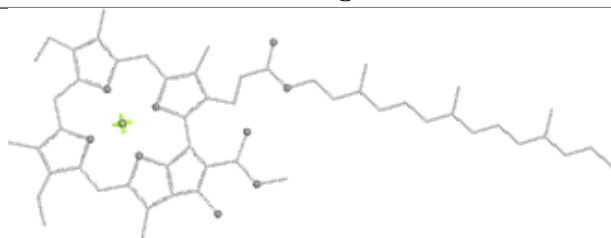
Bond lengths



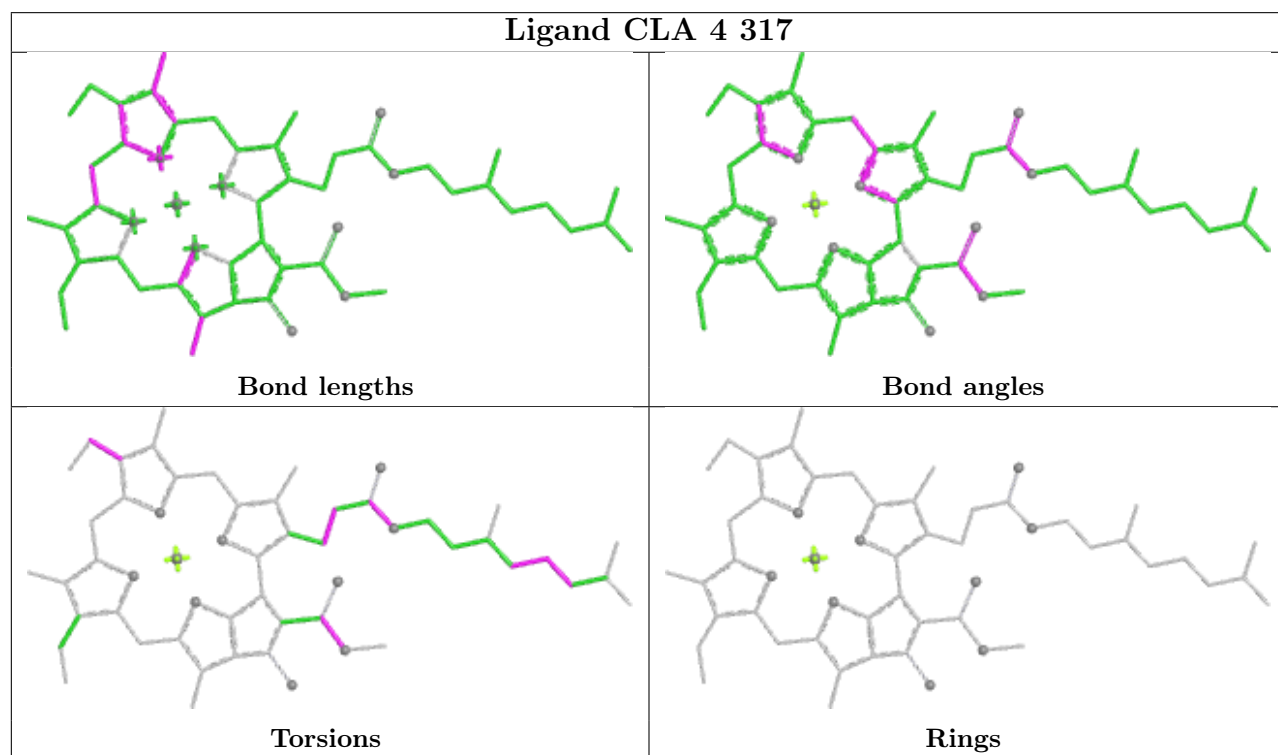
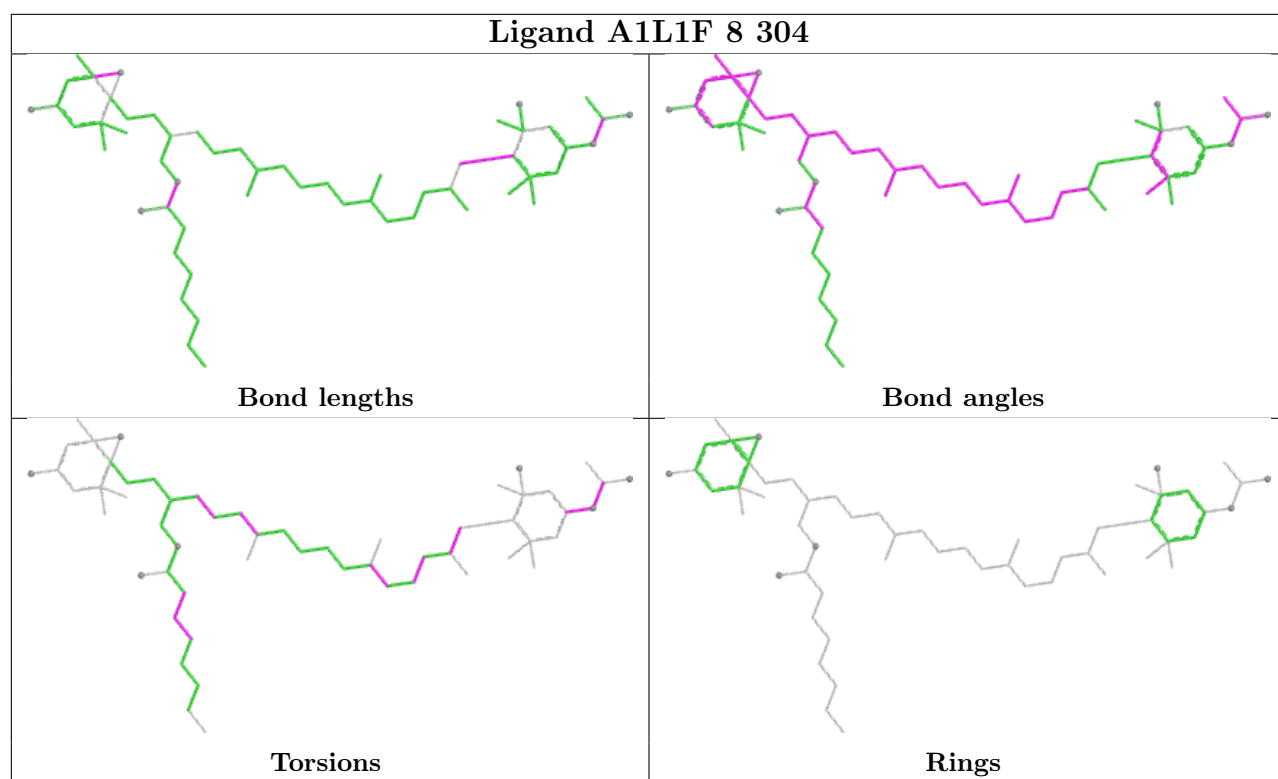
Bond angles



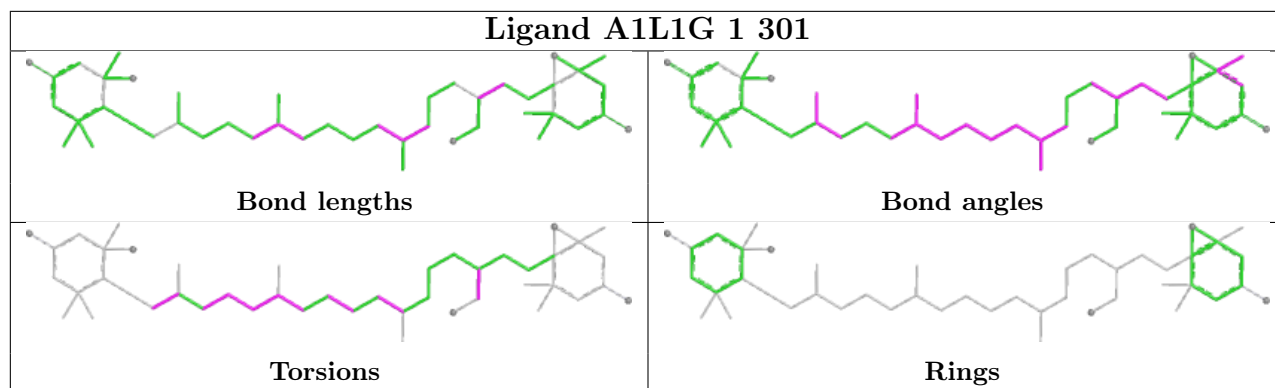
Torsions



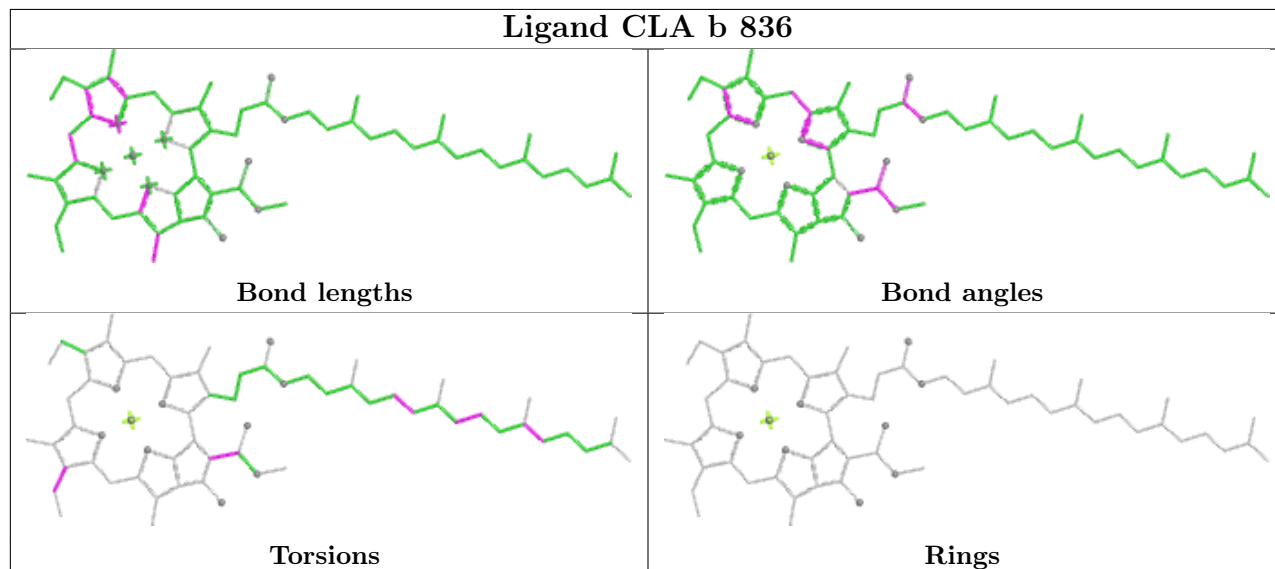
Rings



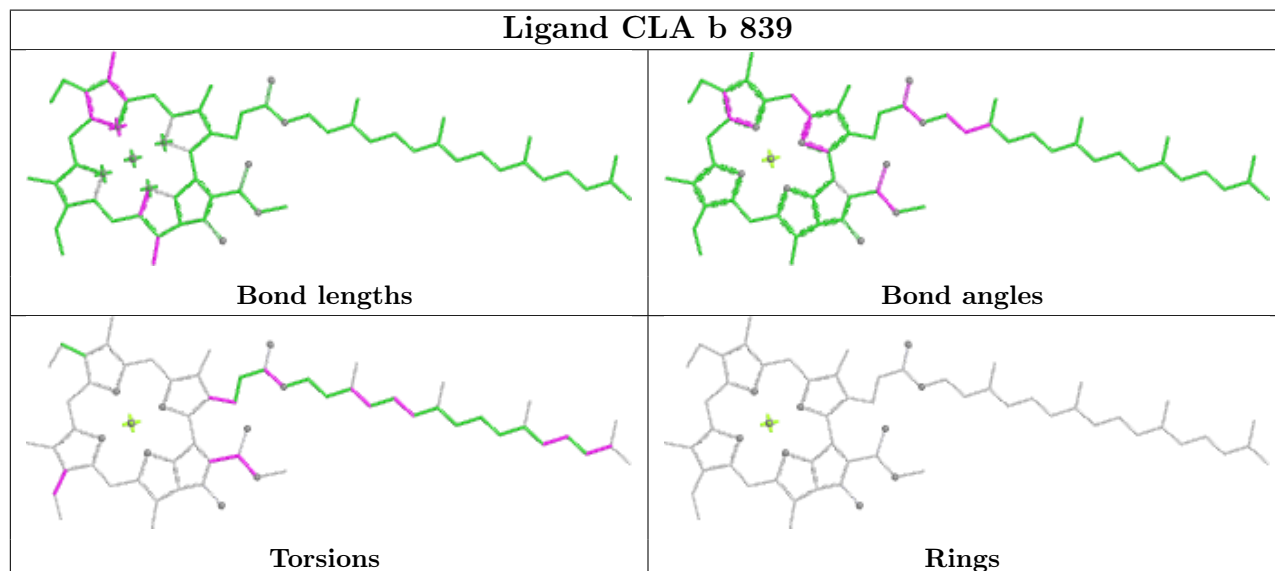
Ligand A1L1G 1 301

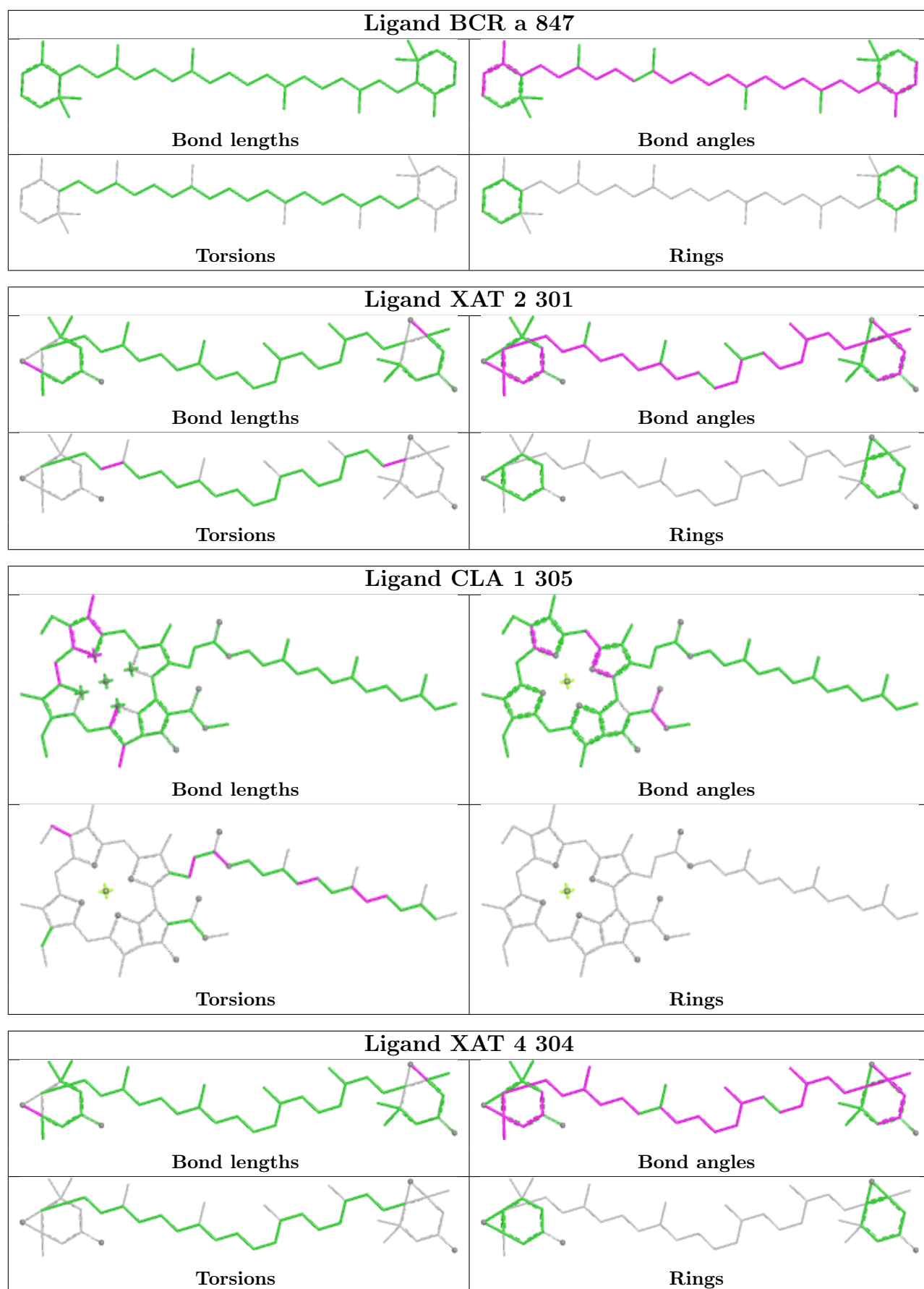


Ligand CLA b 836

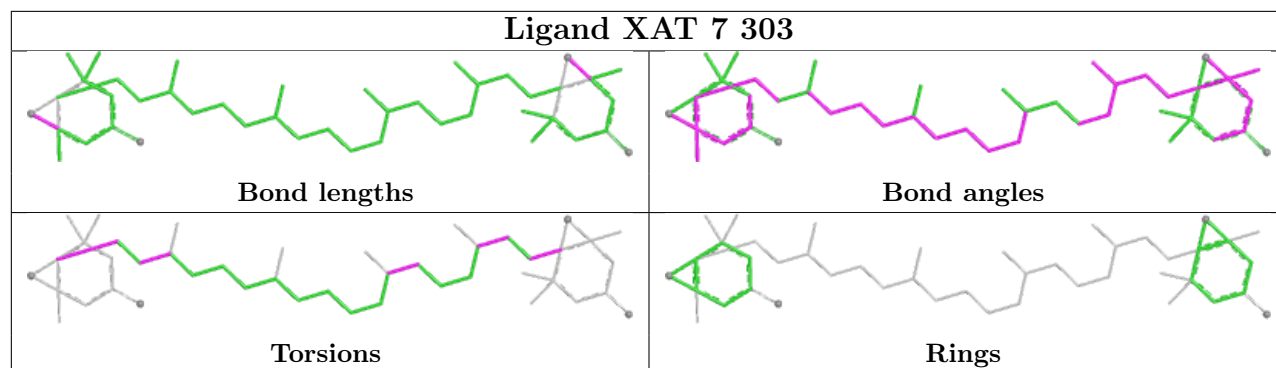


Ligand CLA b 839

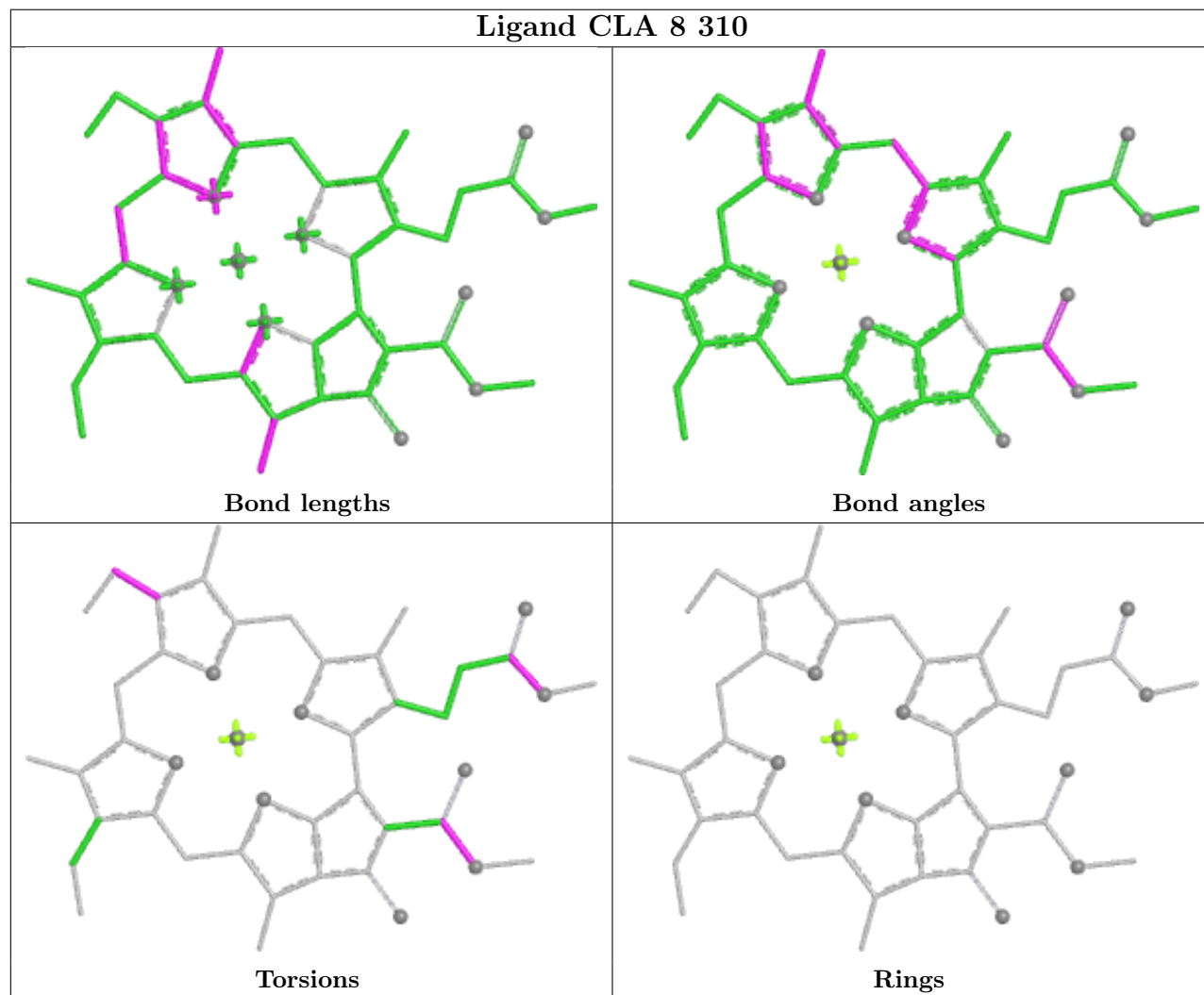




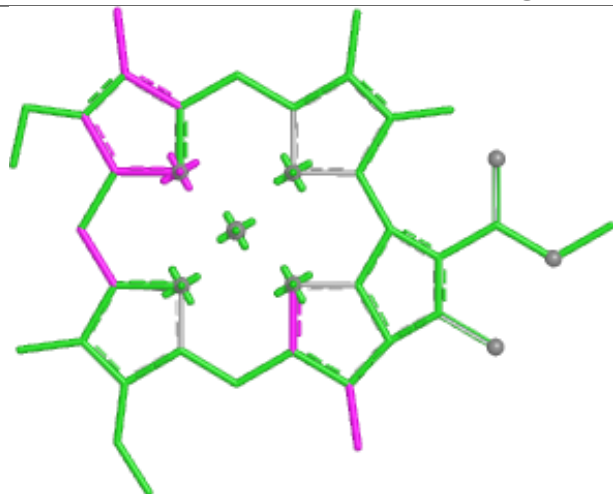
Ligand XAT 7 303



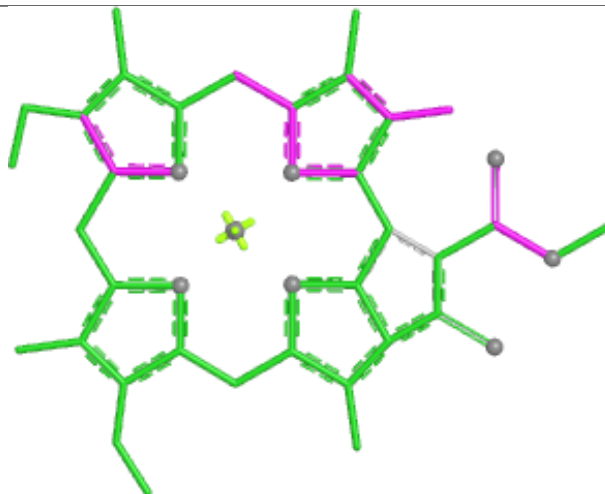
Ligand CLA 8 310



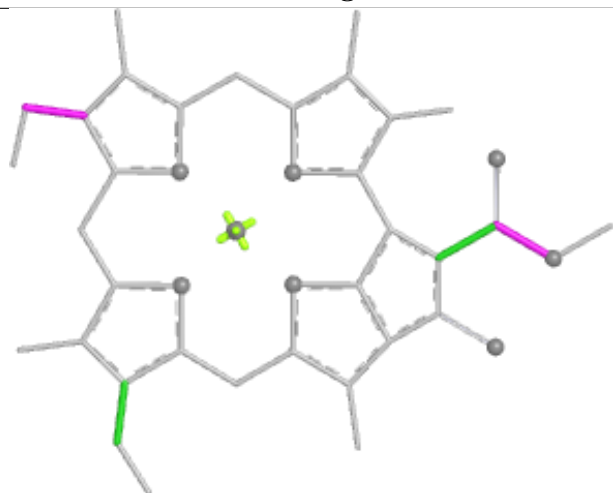
Ligand CLA 7 315



Bond lengths



Bond angles

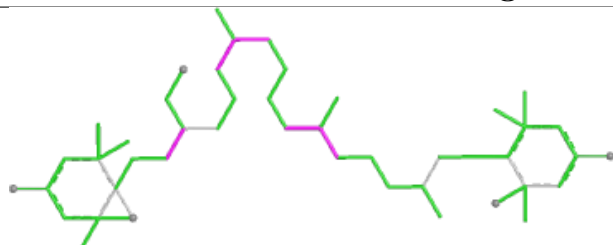


Torsions

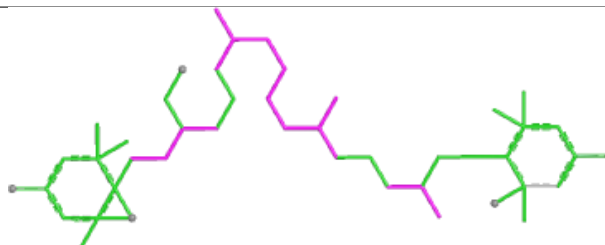


Rings

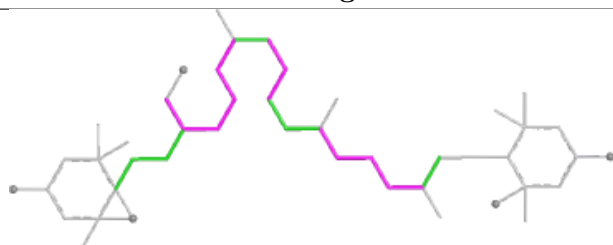
Ligand A1L1G 9 301



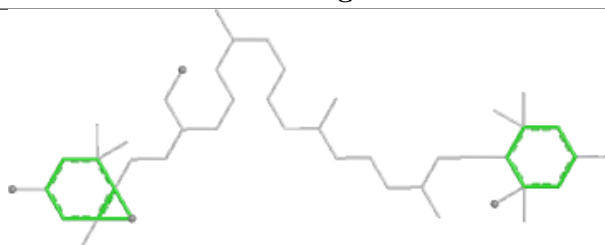
Bond lengths



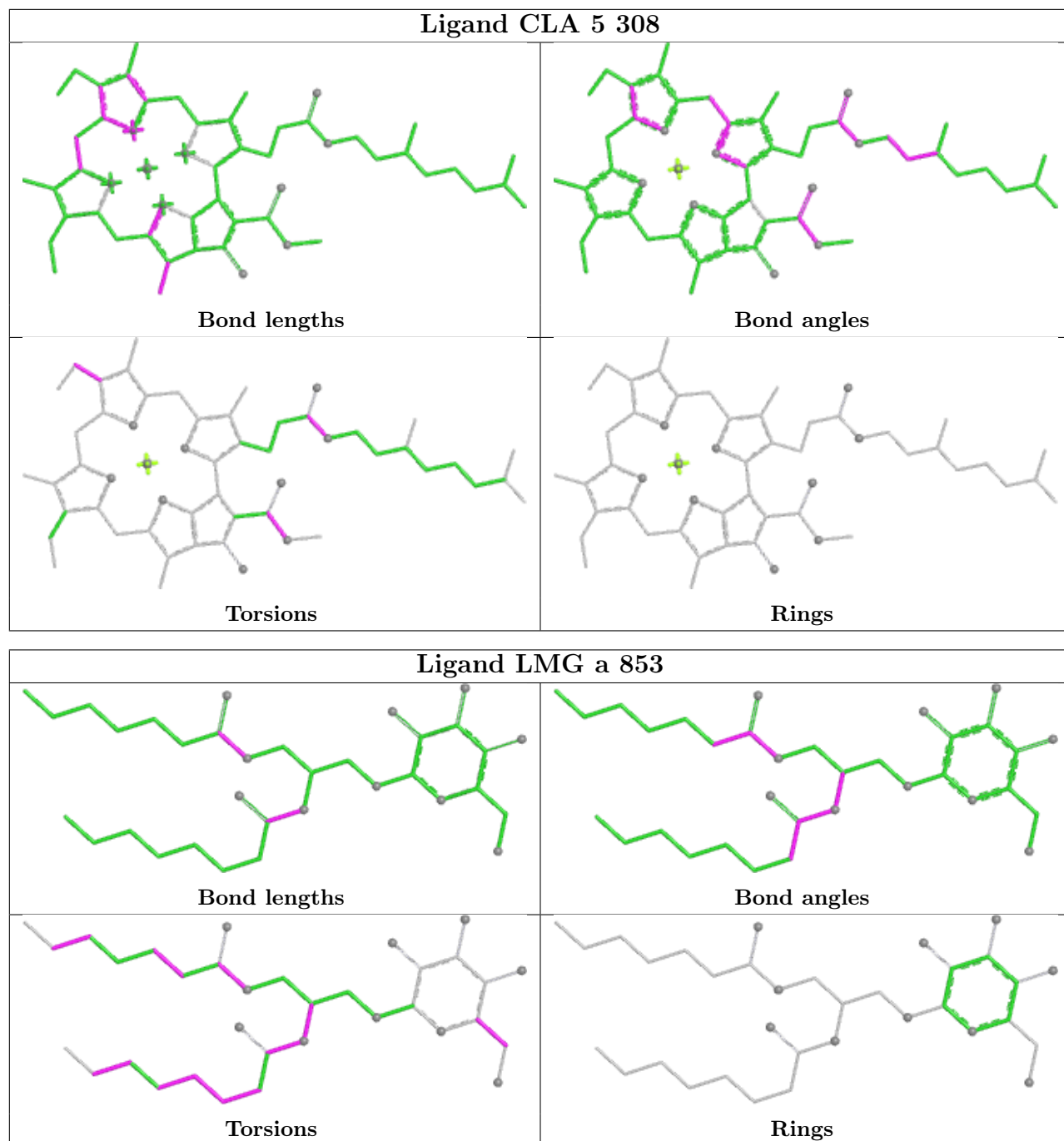
Bond angles



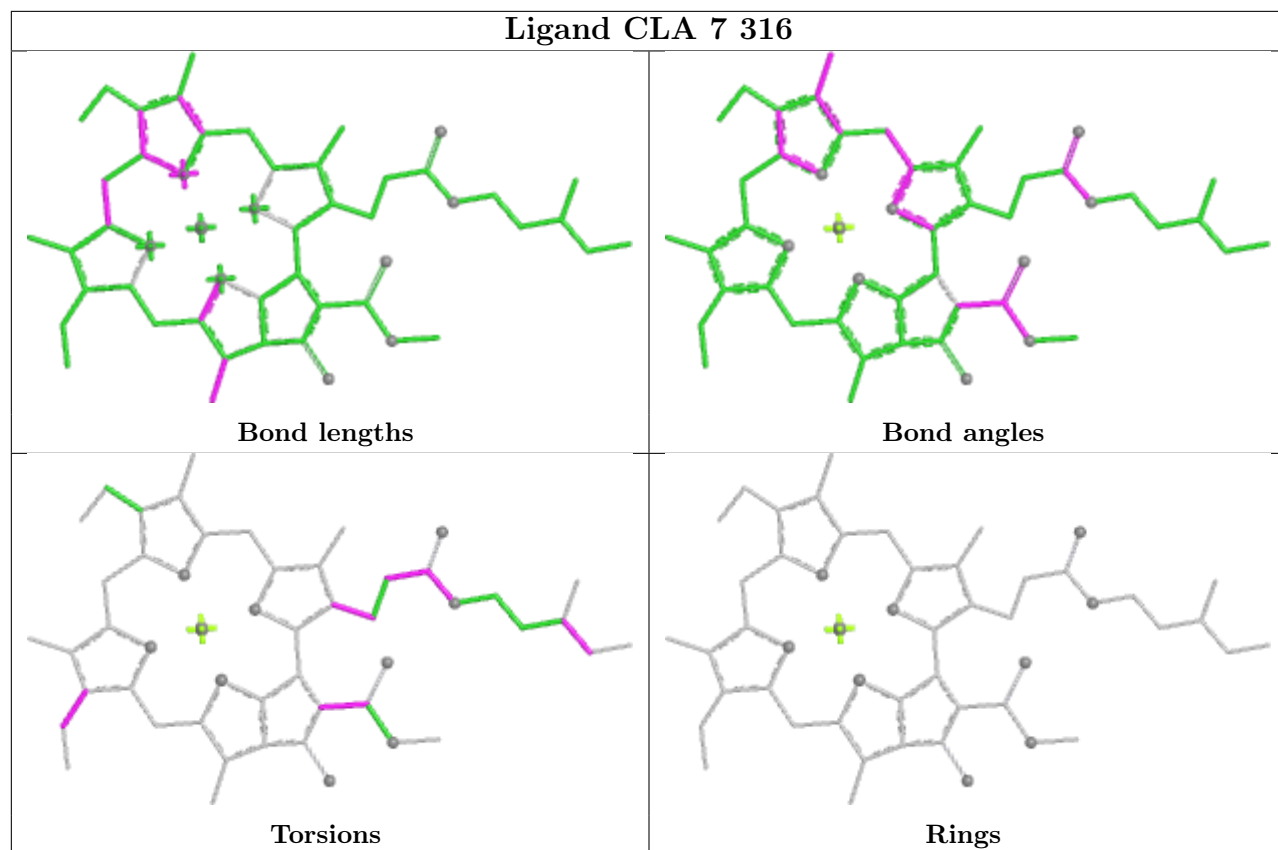
Torsions



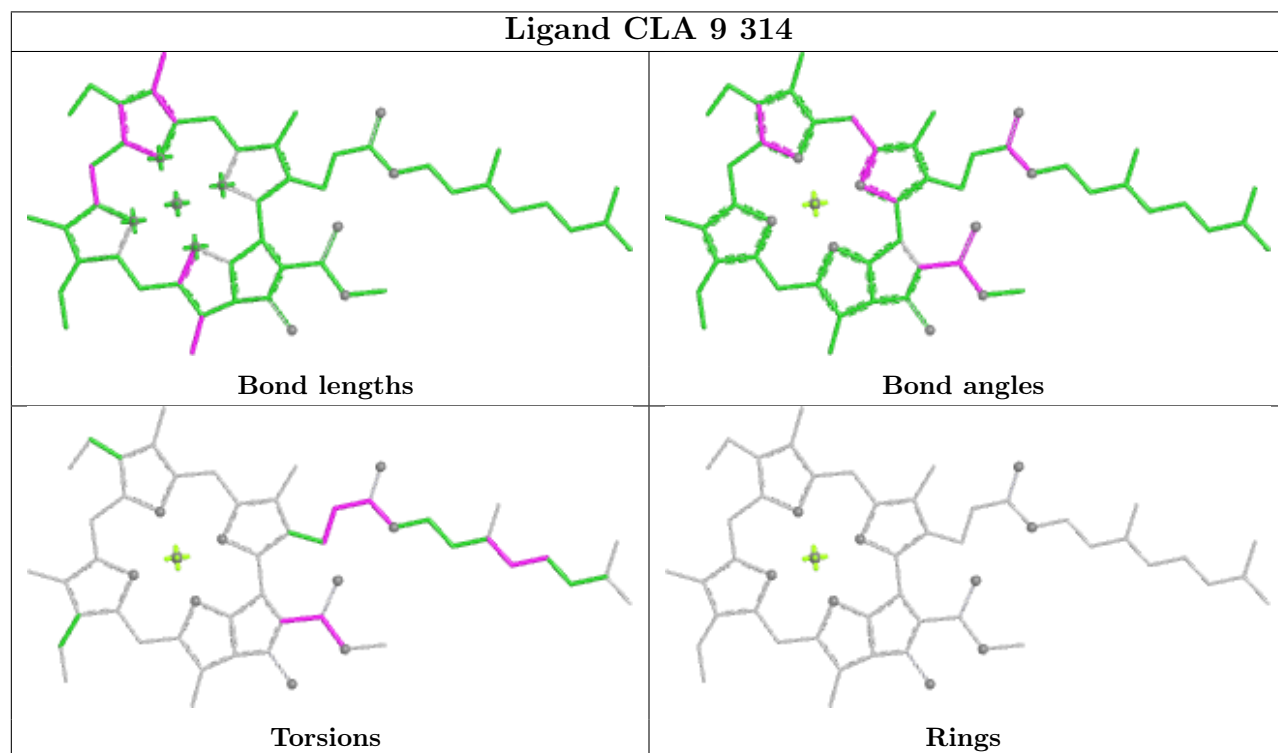
Rings

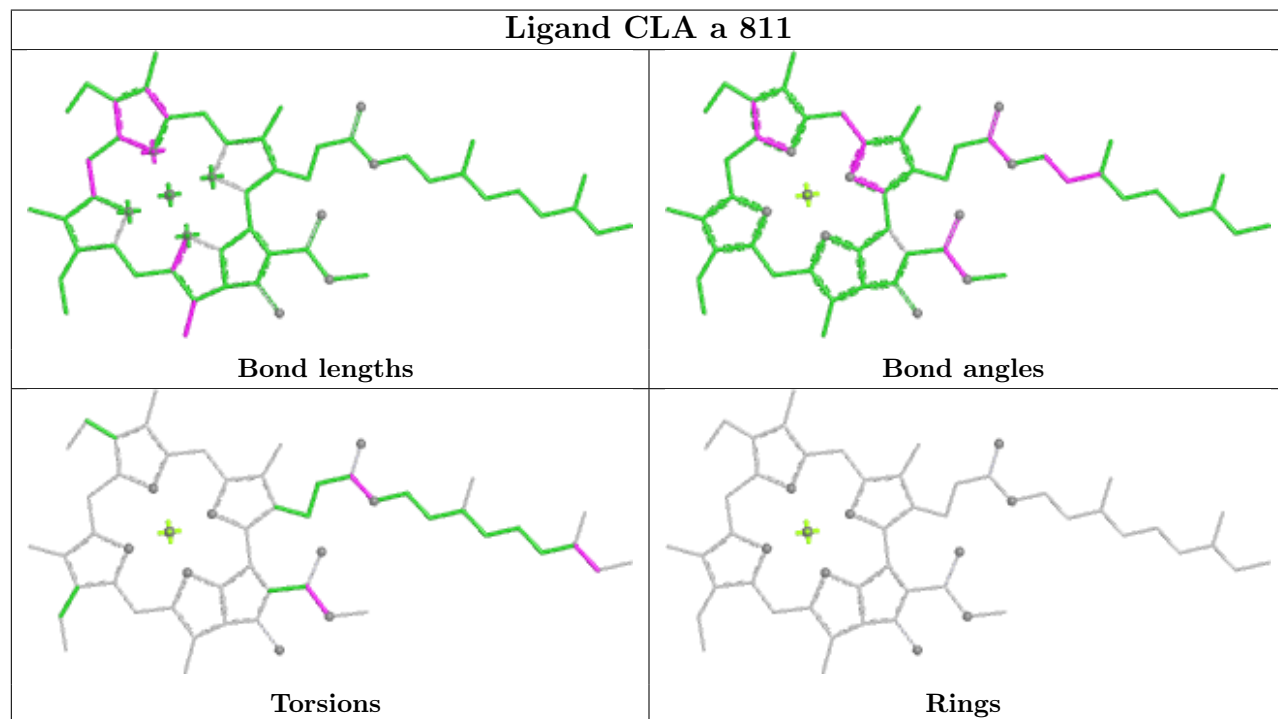
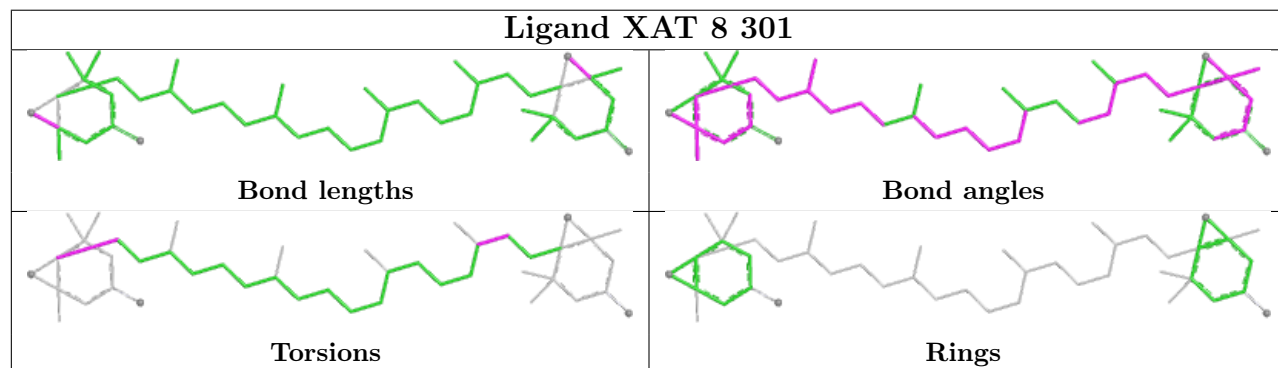
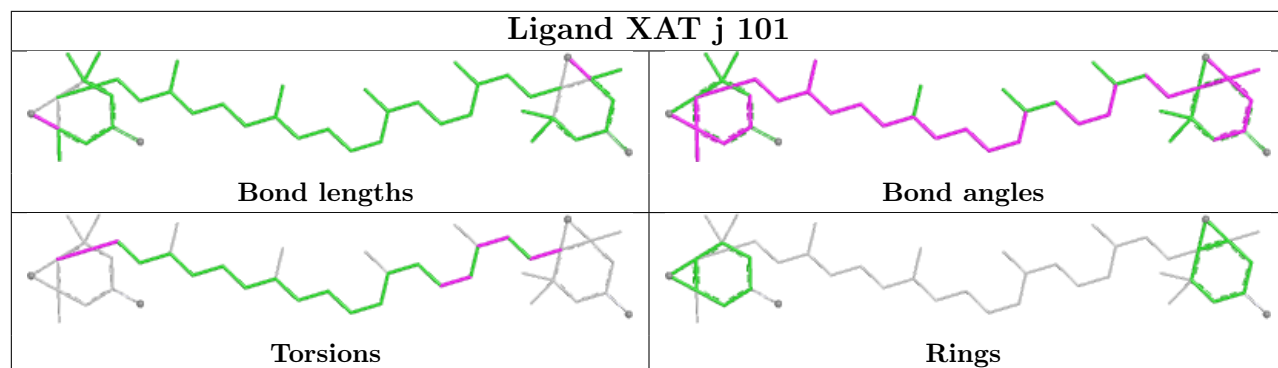


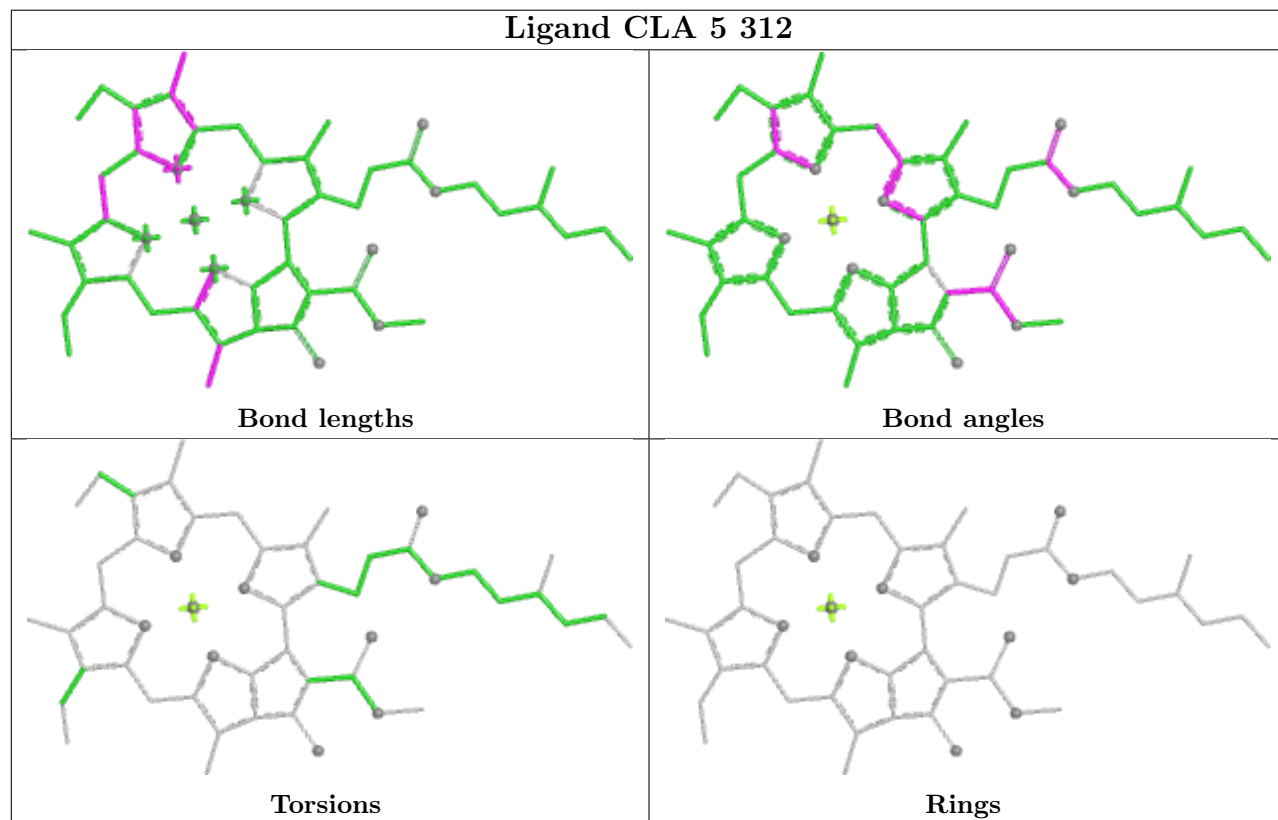
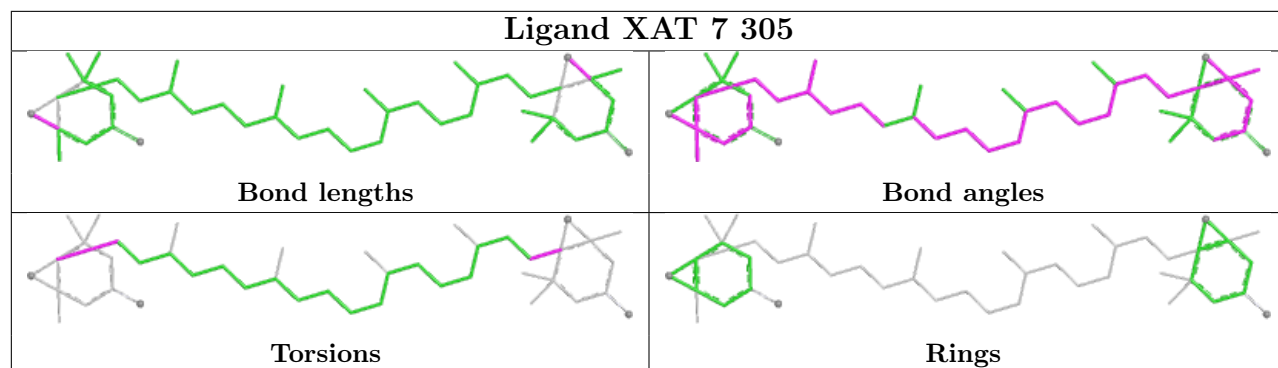
Ligand CLA 7 316



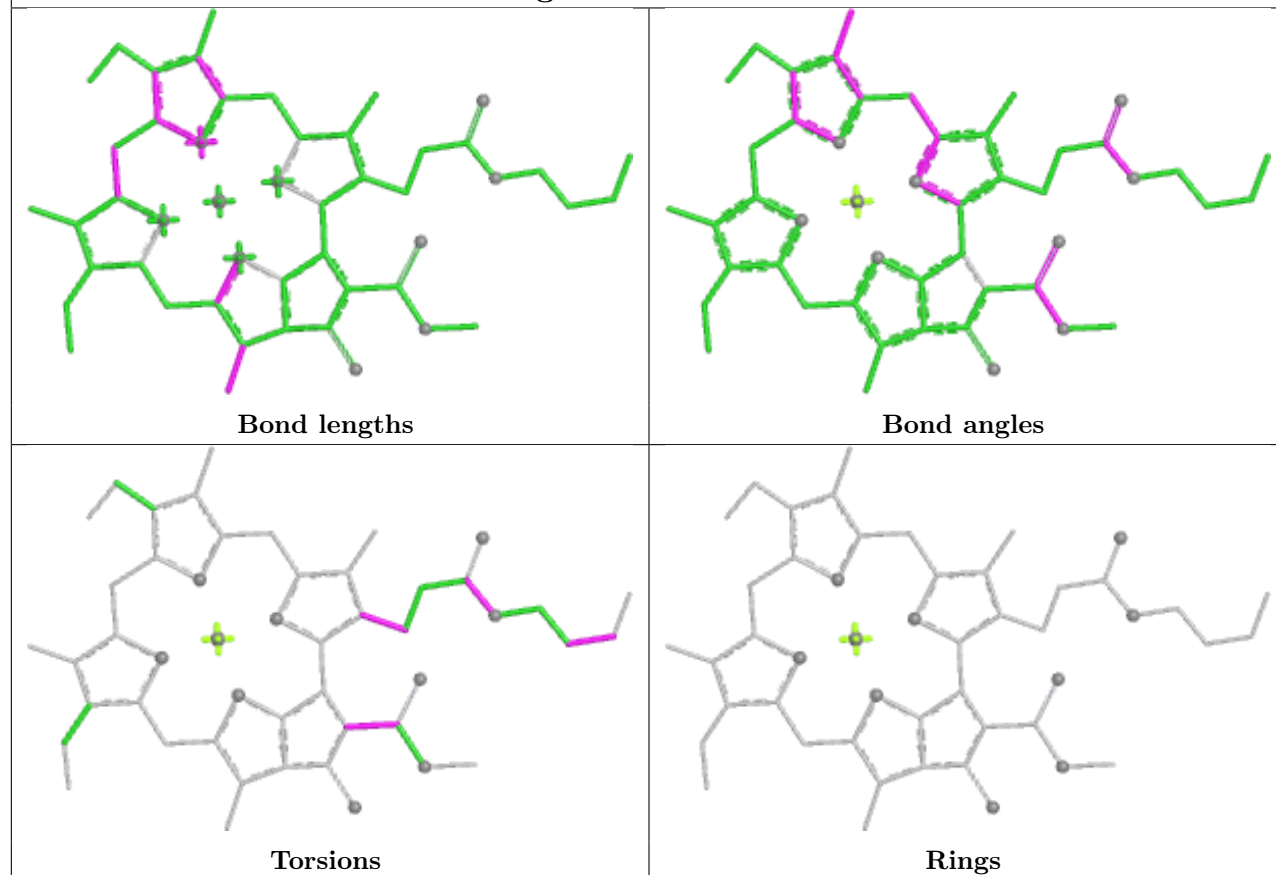
Ligand CLA 9 314



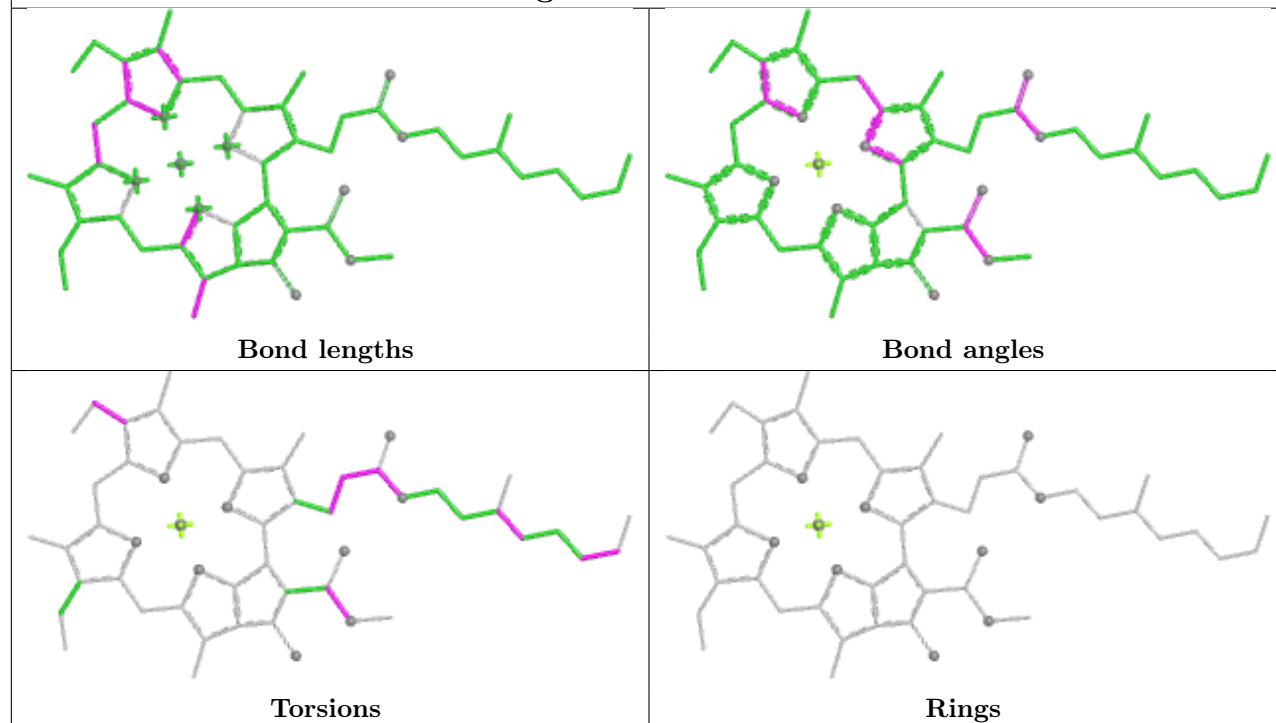


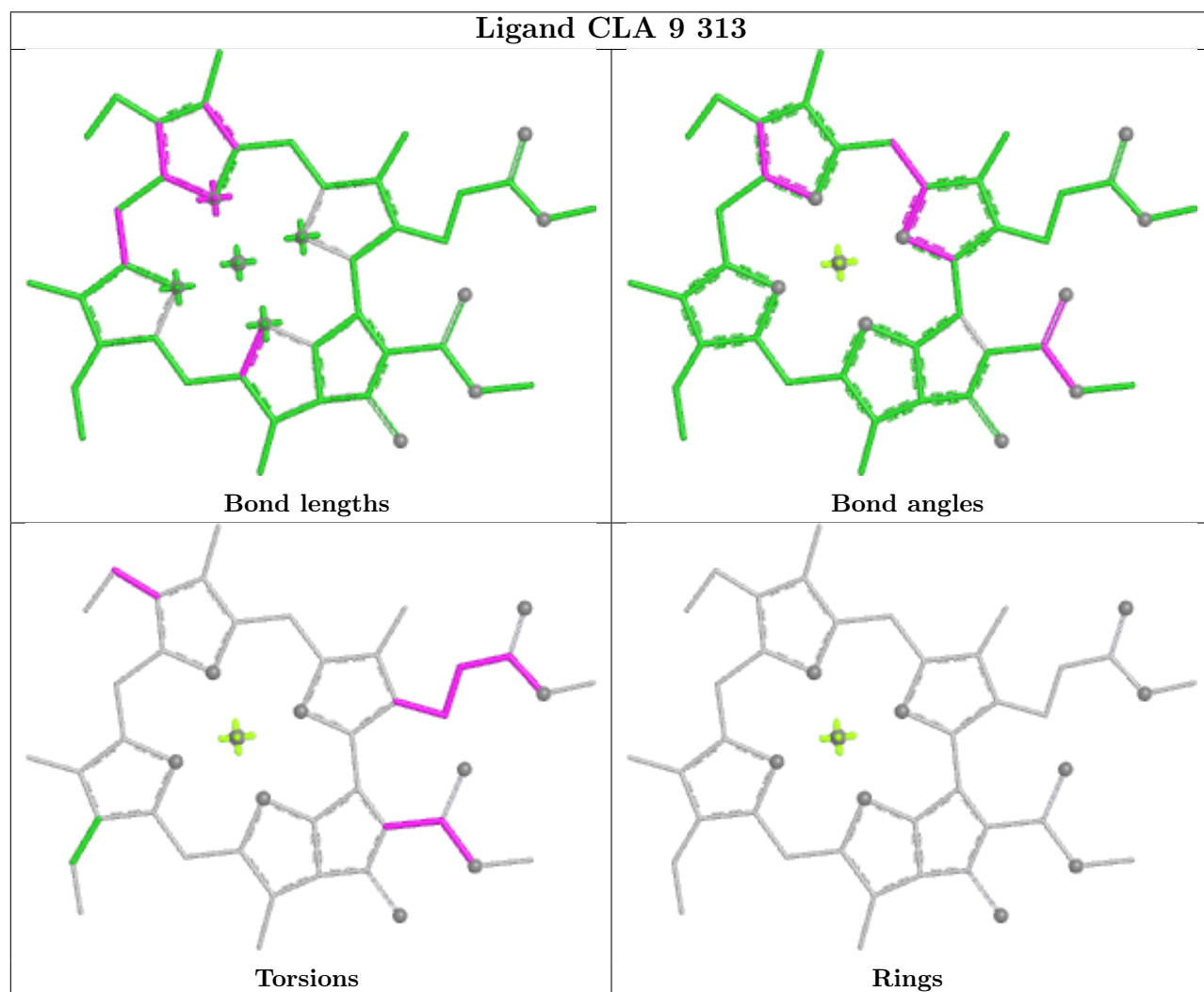
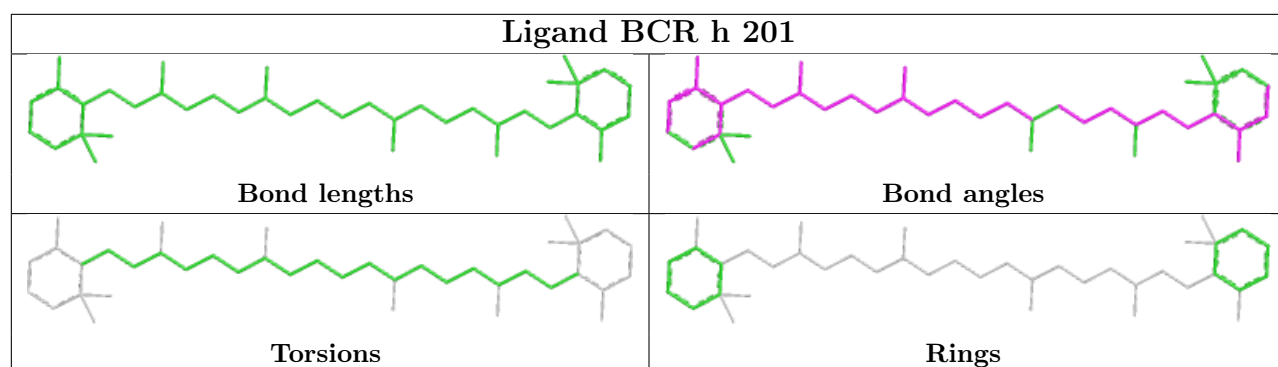


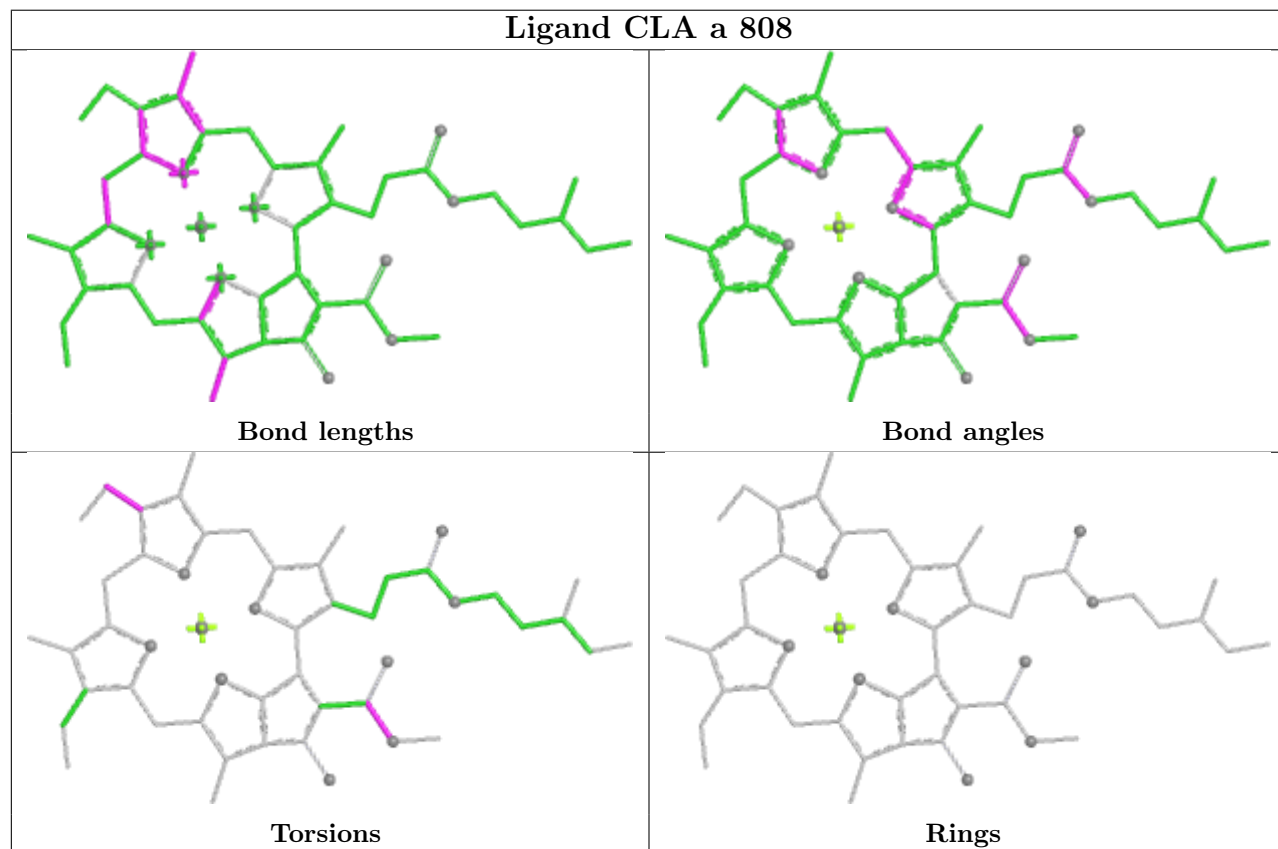
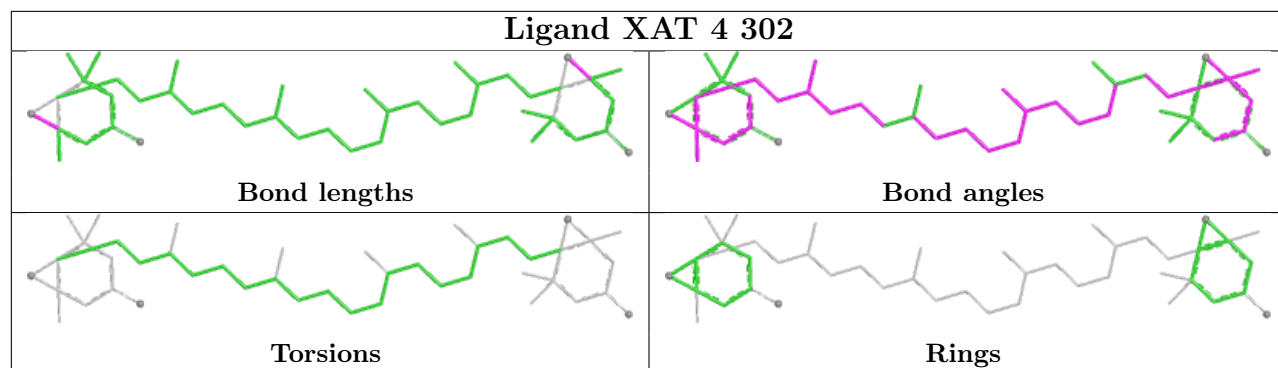
Ligand CLA a 823



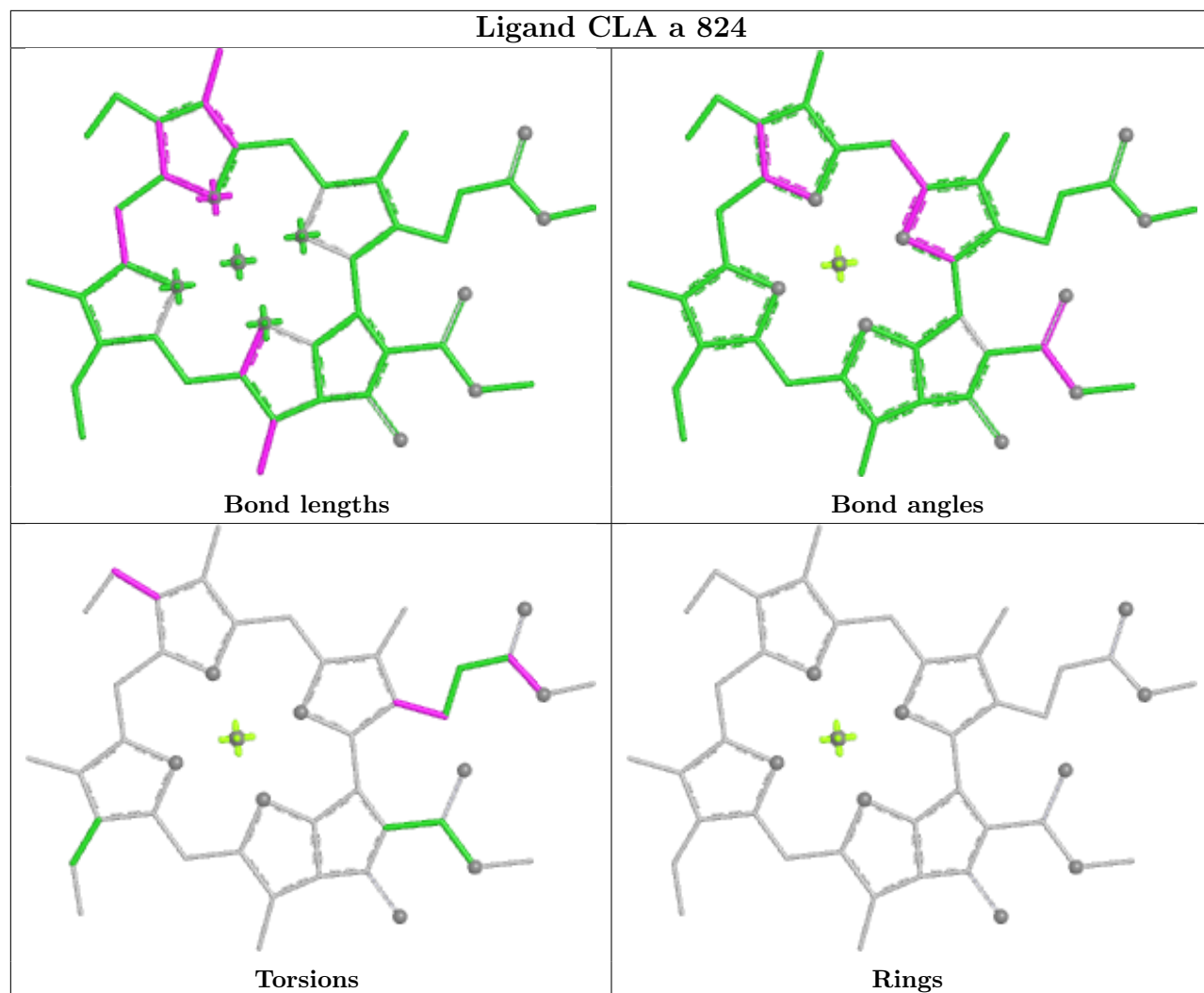
Ligand CLA a 813



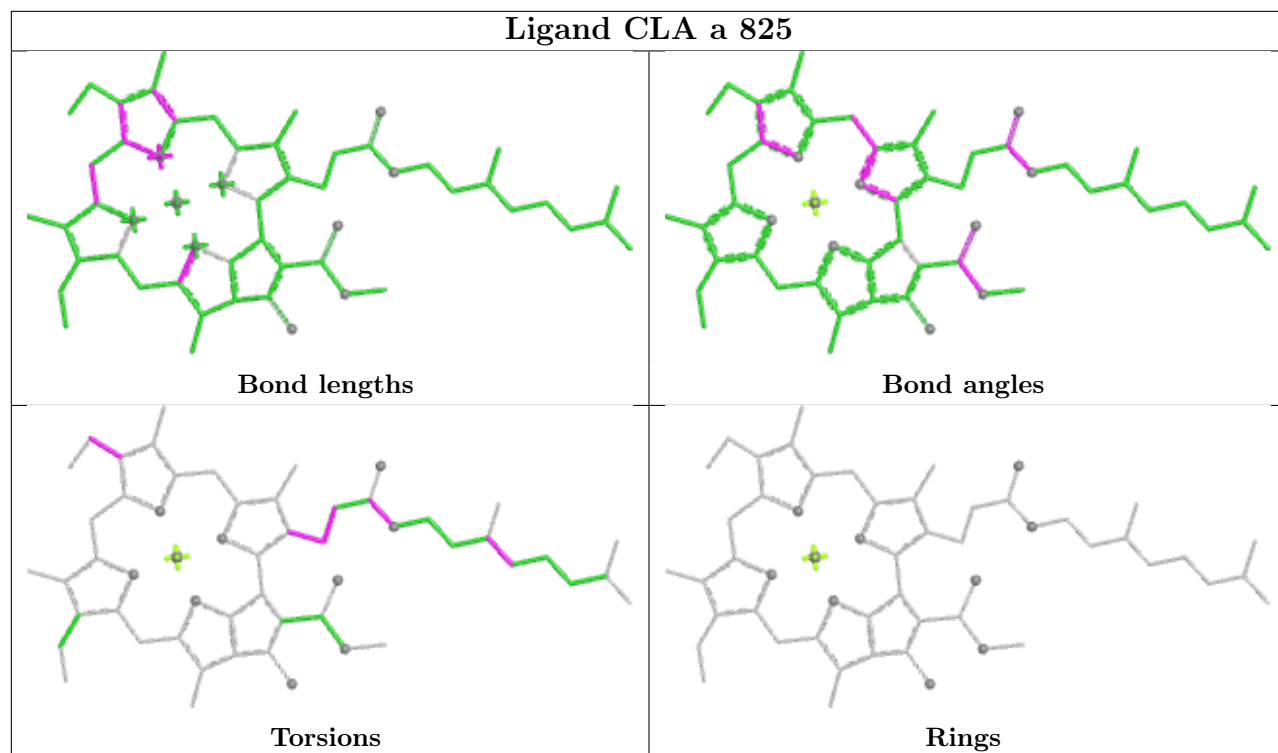




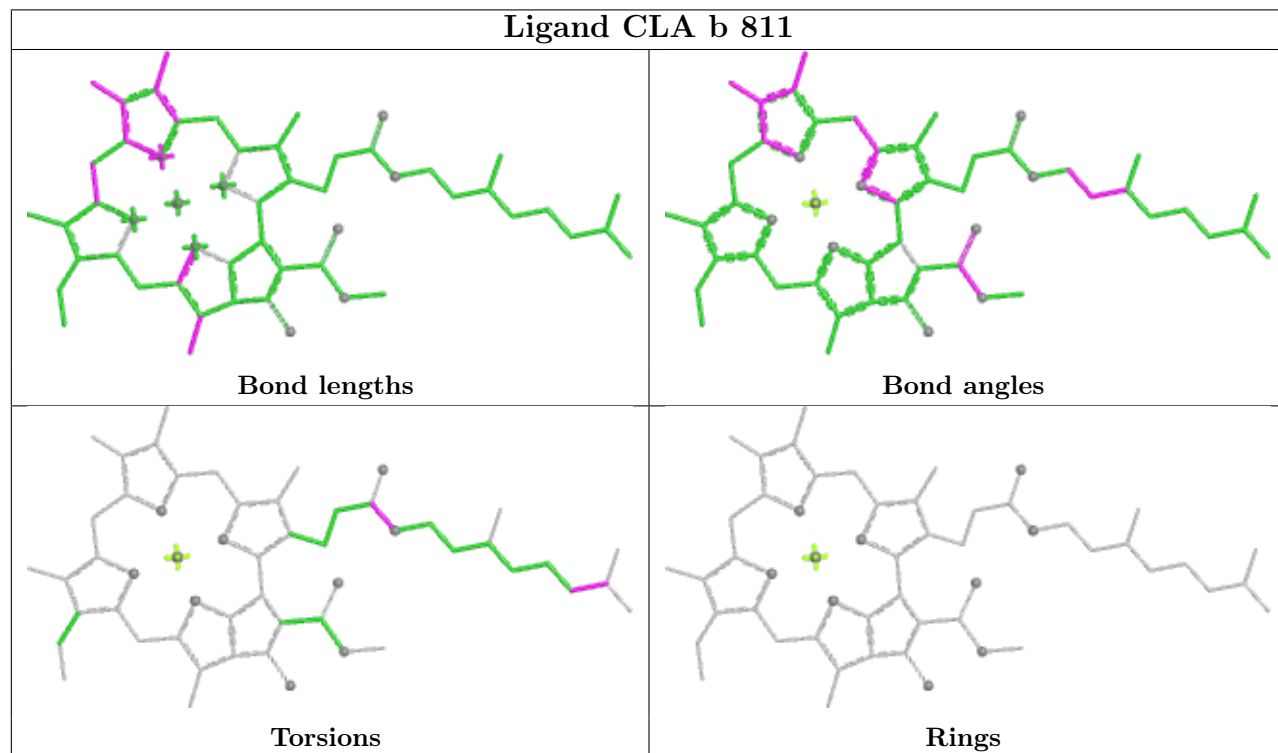
Ligand CLA a 824



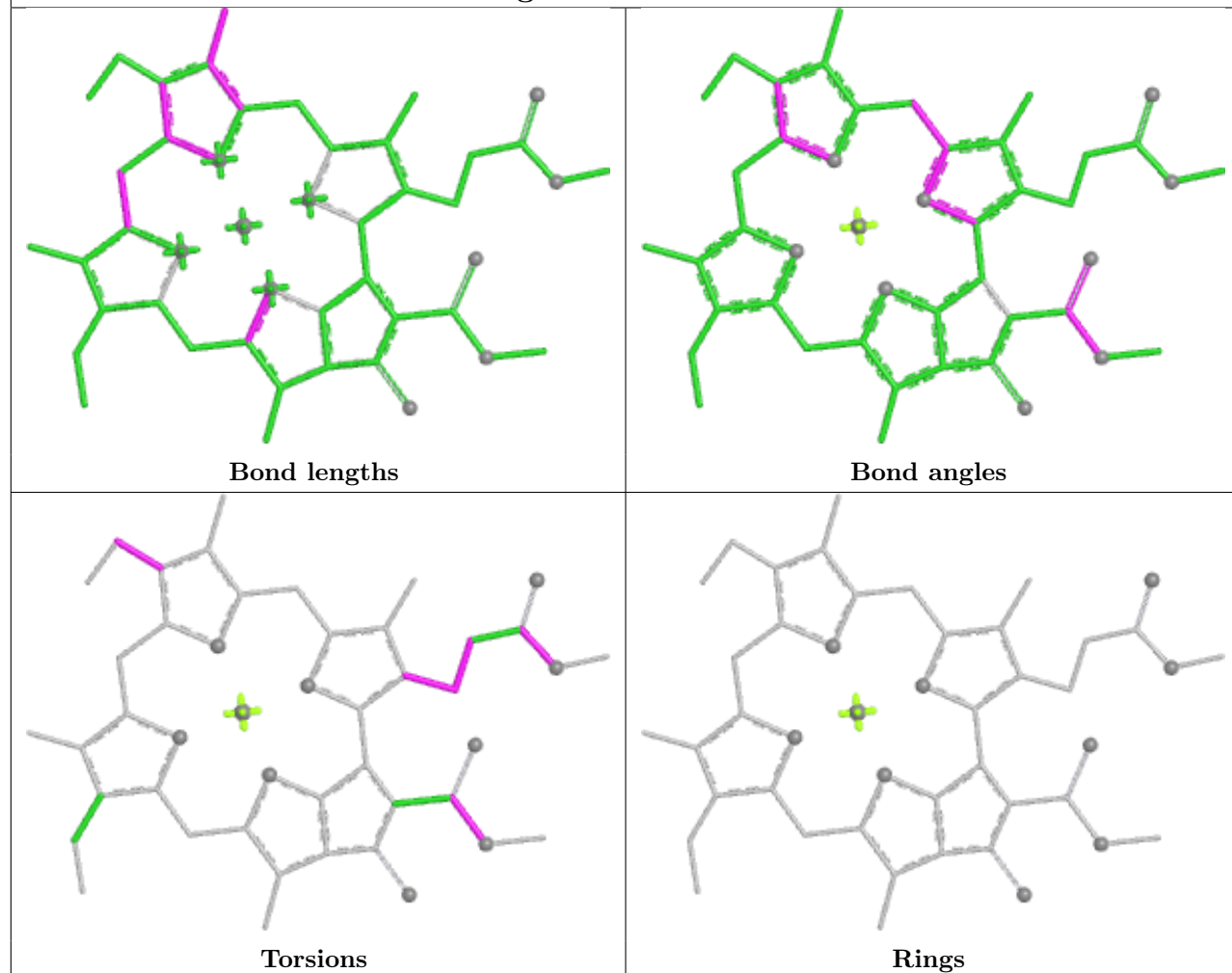
Ligand CLA a 825



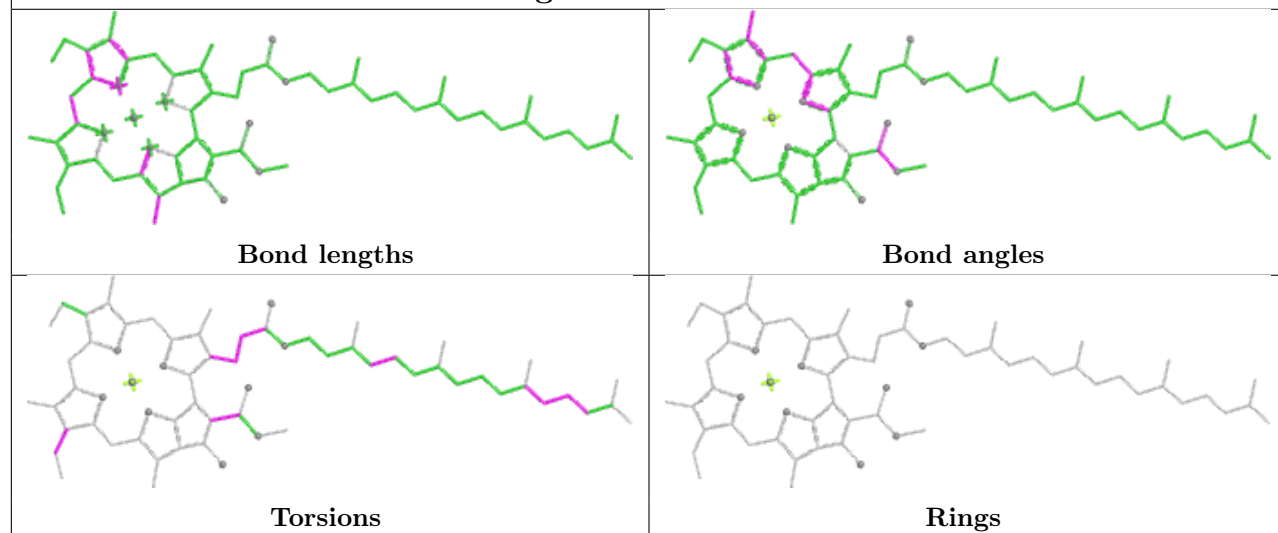
Ligand CLA b 811



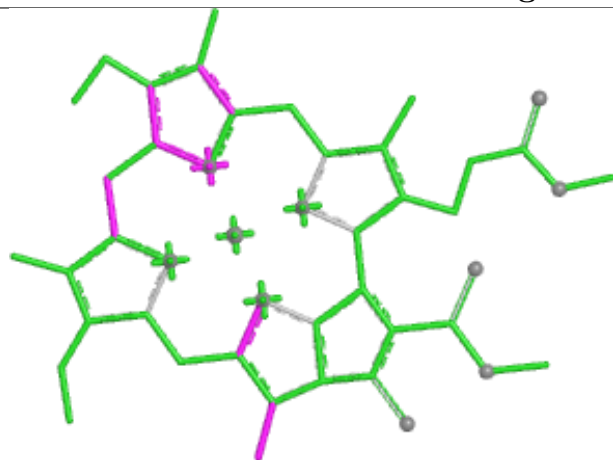
Ligand CLA 4 316



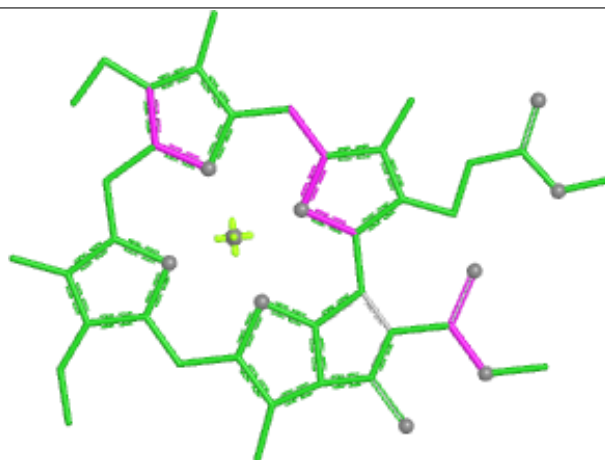
Ligand CLA b 832



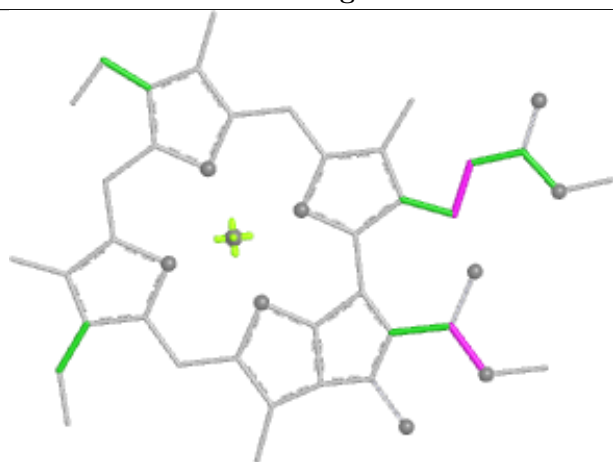
Ligand CLA 2 309



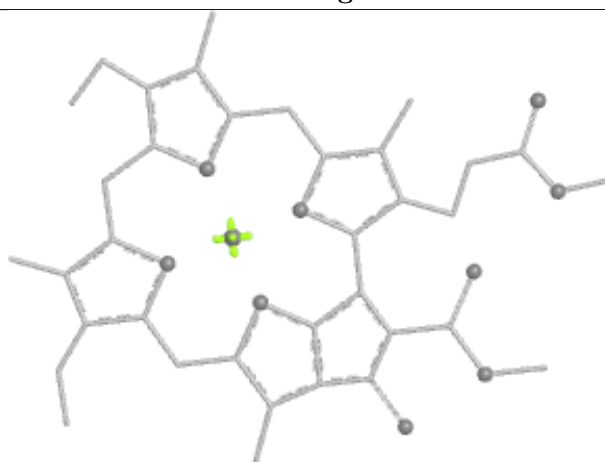
Bond lengths



Bond angles

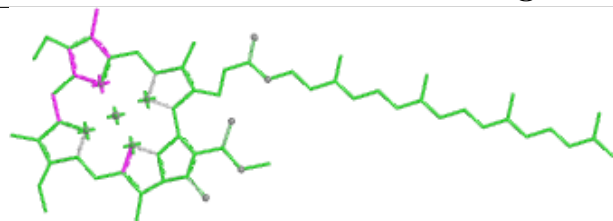


Torsions

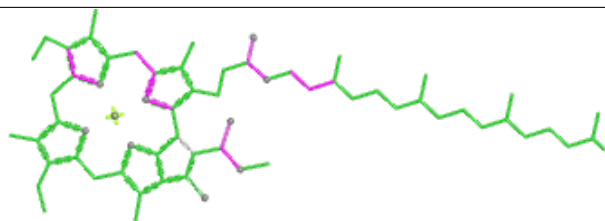


Rings

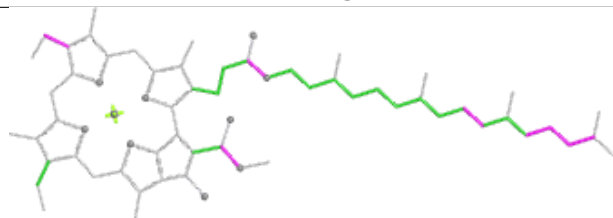
Ligand CLA b 840



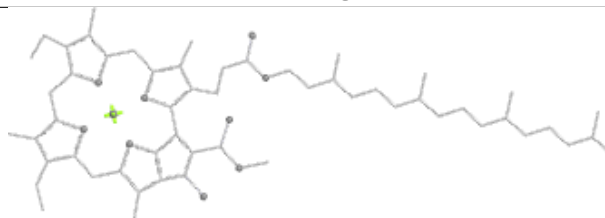
Bond lengths



Bond angles

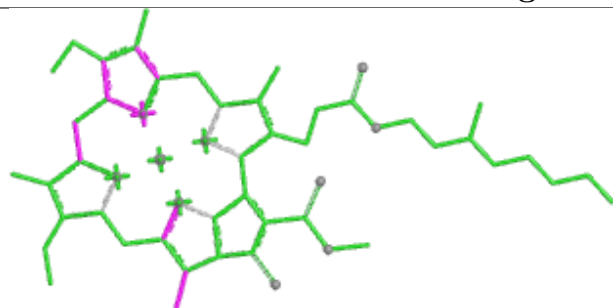


Torsions

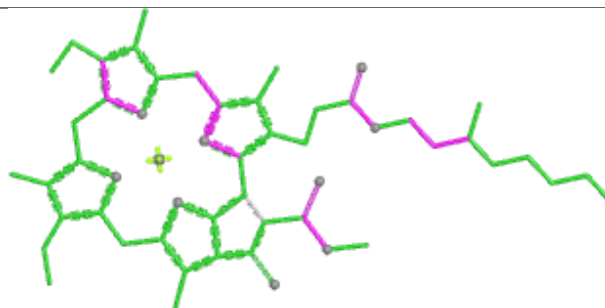


Rings

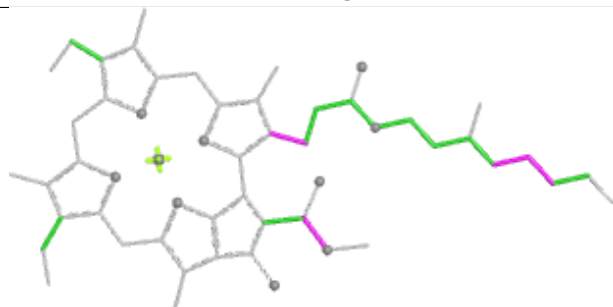
Ligand CLA 7 313



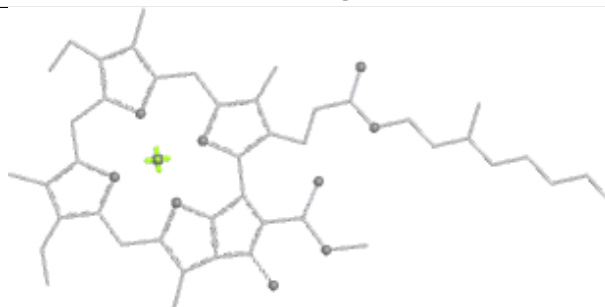
Bond lengths



Bond angles

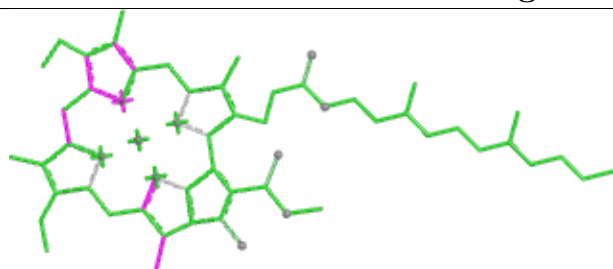


Torsions

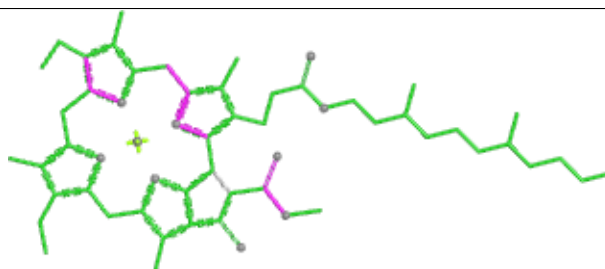


Rings

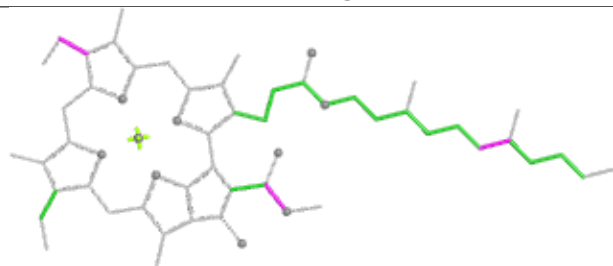
Ligand CLA 6 308



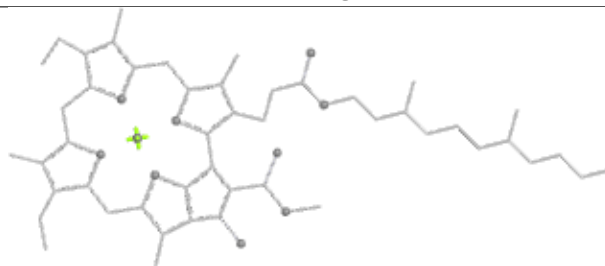
Bond lengths



Bond angles

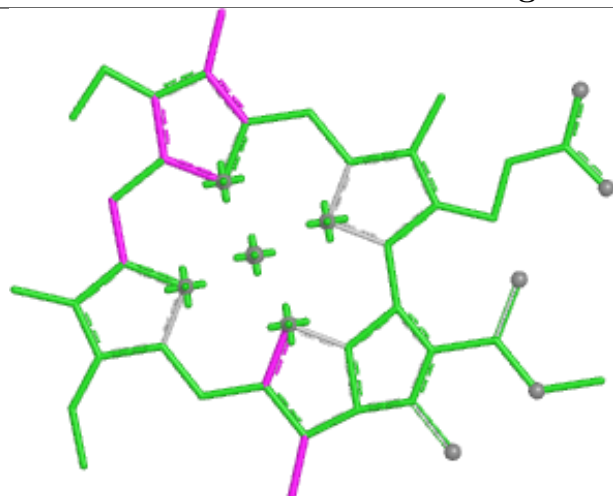


Torsions

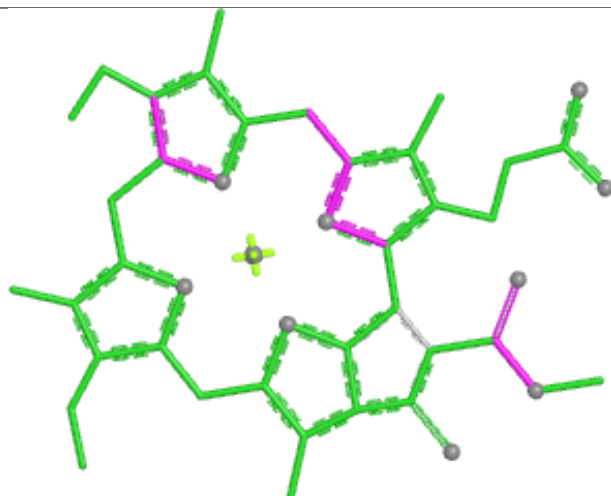


Rings

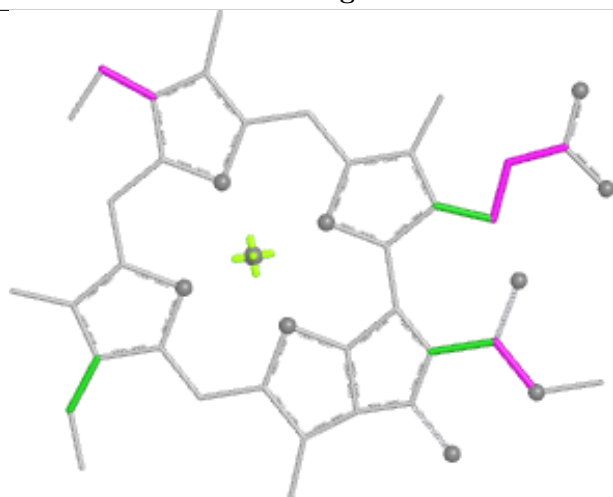
Ligand CLA 7 317



Bond lengths



Bond angles

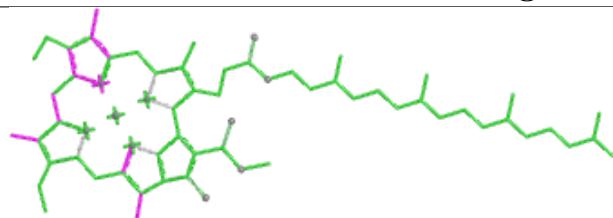


Torsions

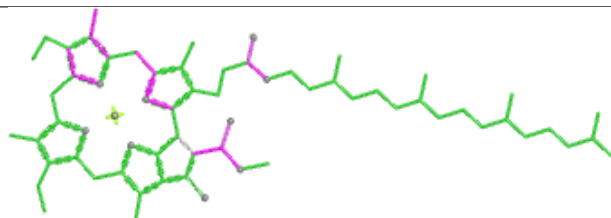


Rings

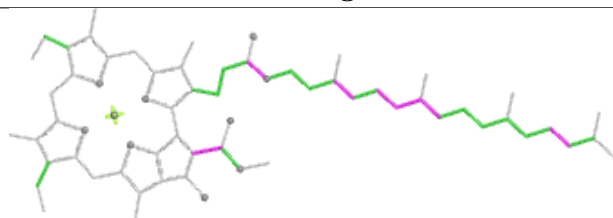
Ligand CLA a 831



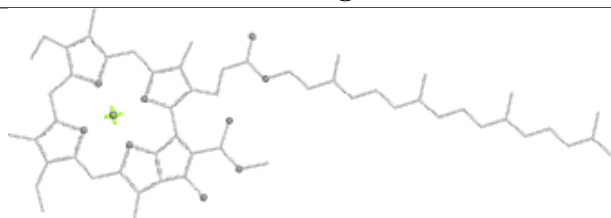
Bond lengths



Bond angles

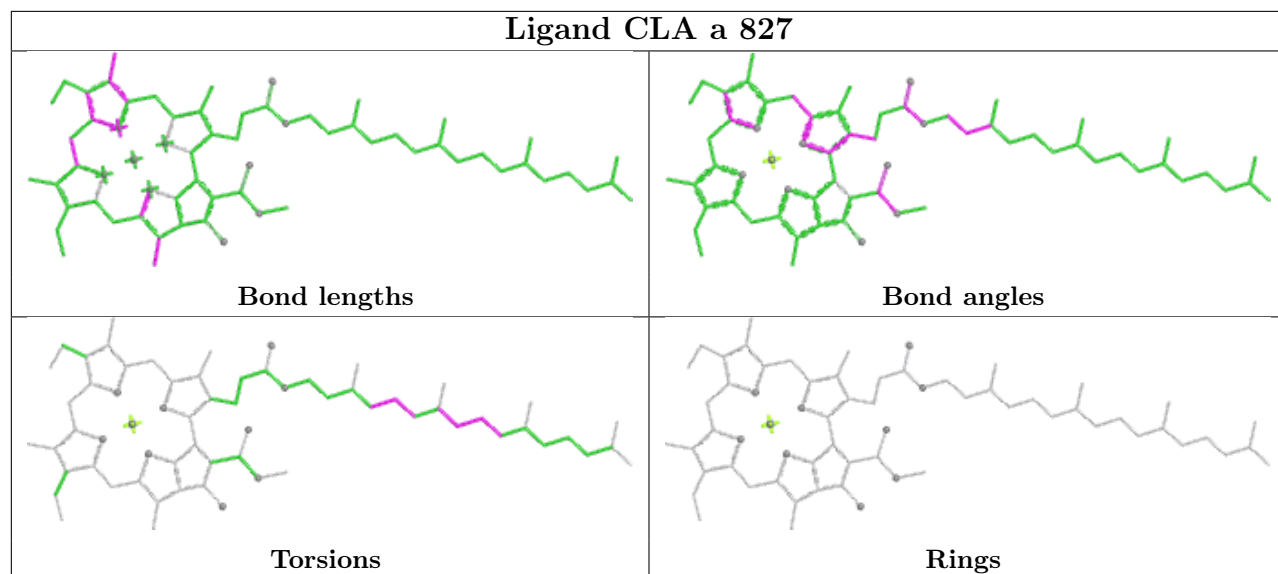


Torsions

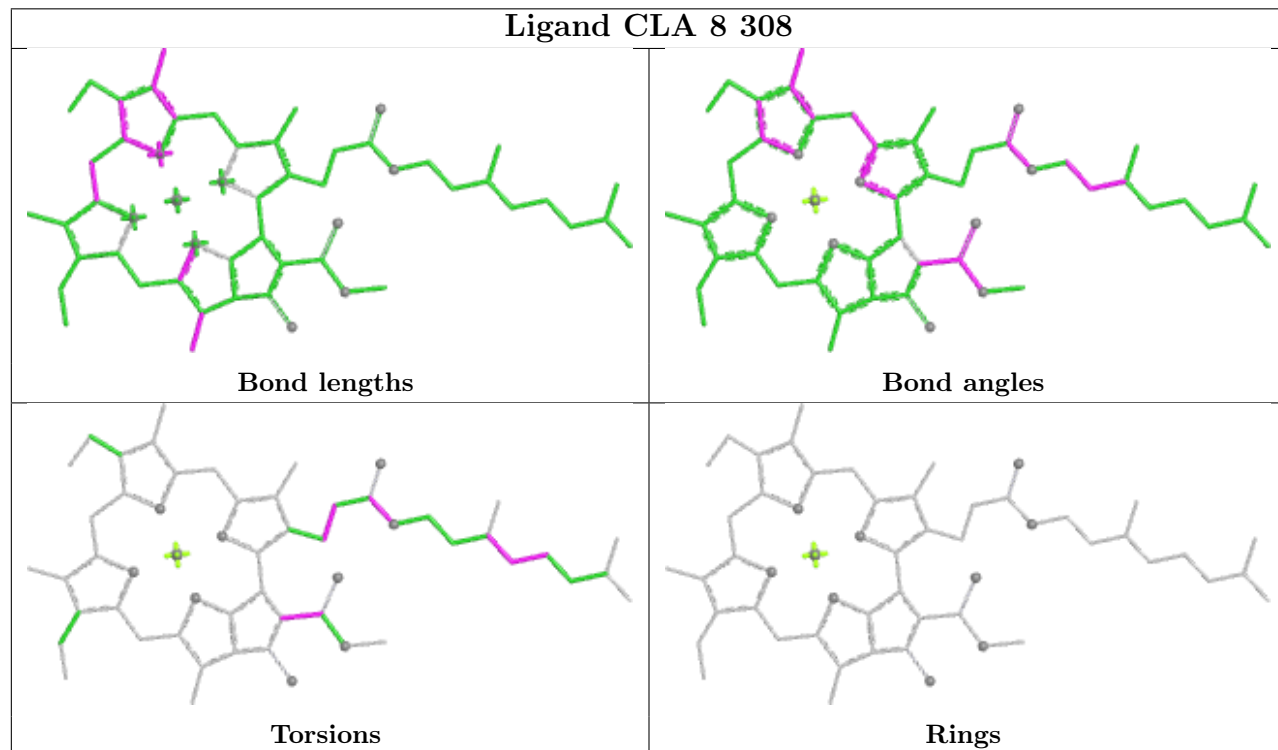


Rings

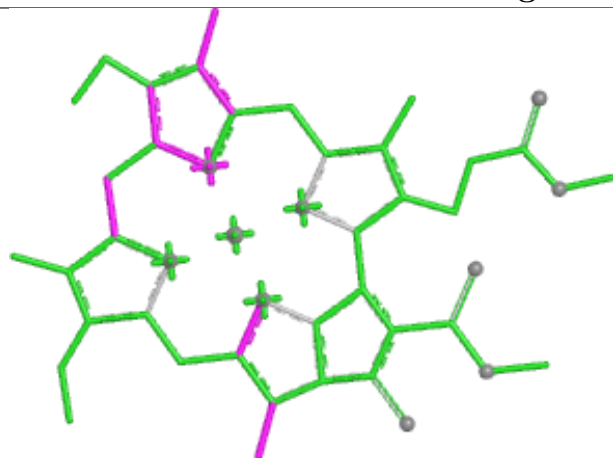
Ligand CLA a 827



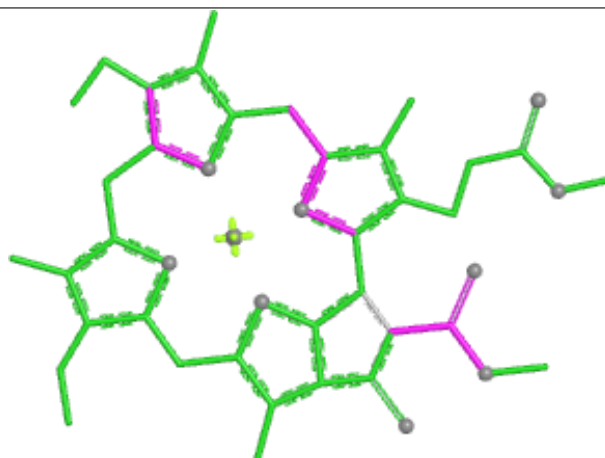
Ligand CLA 8 308



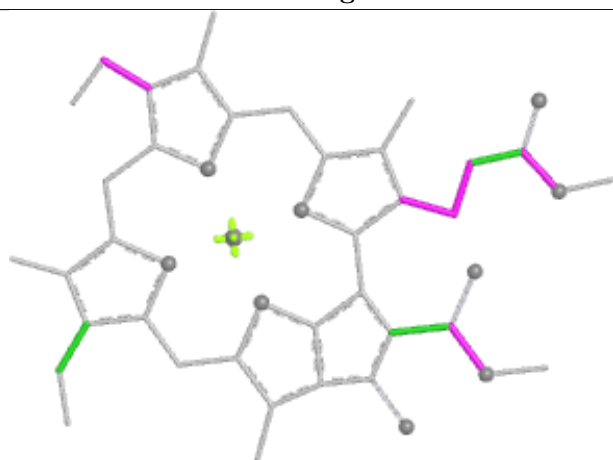
Ligand CLA 4 311



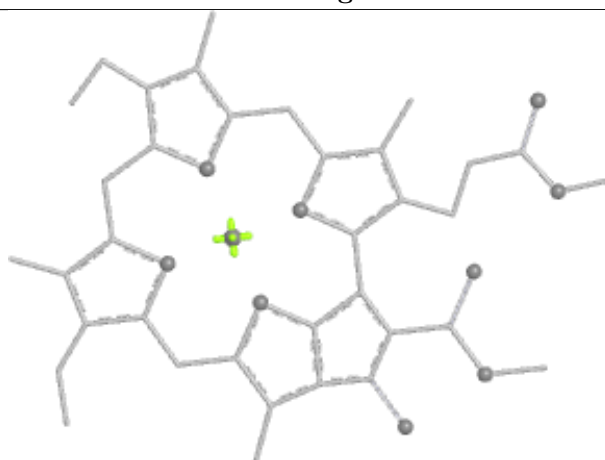
Bond lengths



Bond angles

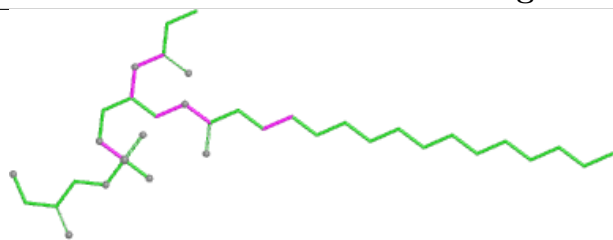


Torsions

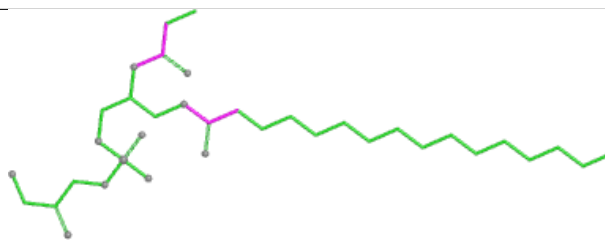


Rings

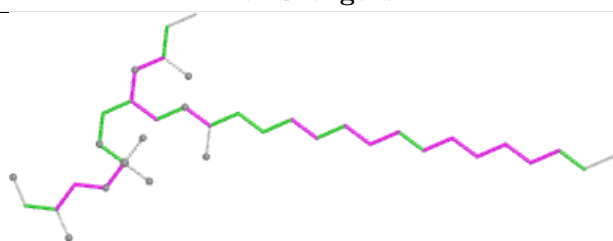
Ligand LHG 9 307



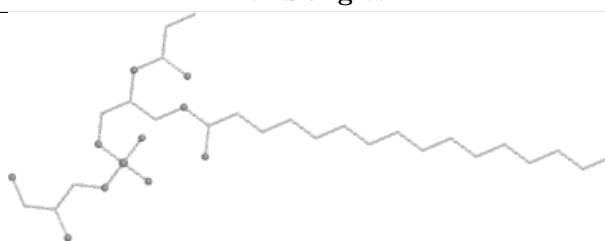
Bond lengths



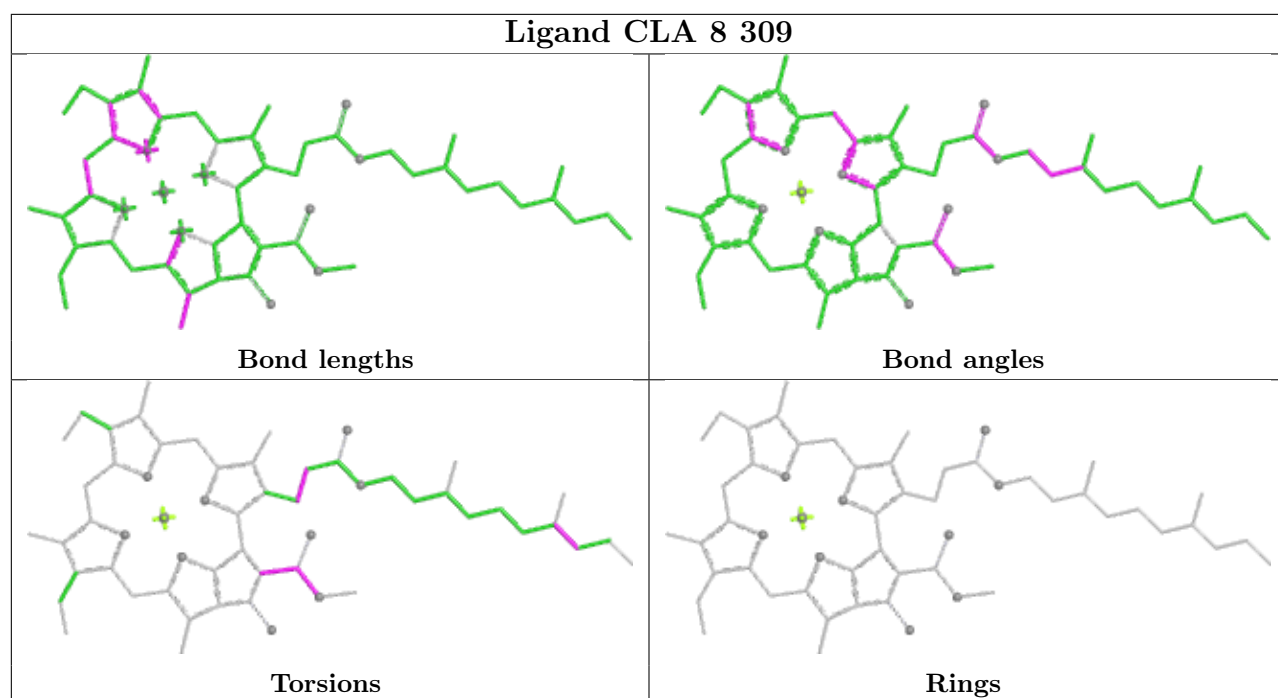
Bond angles



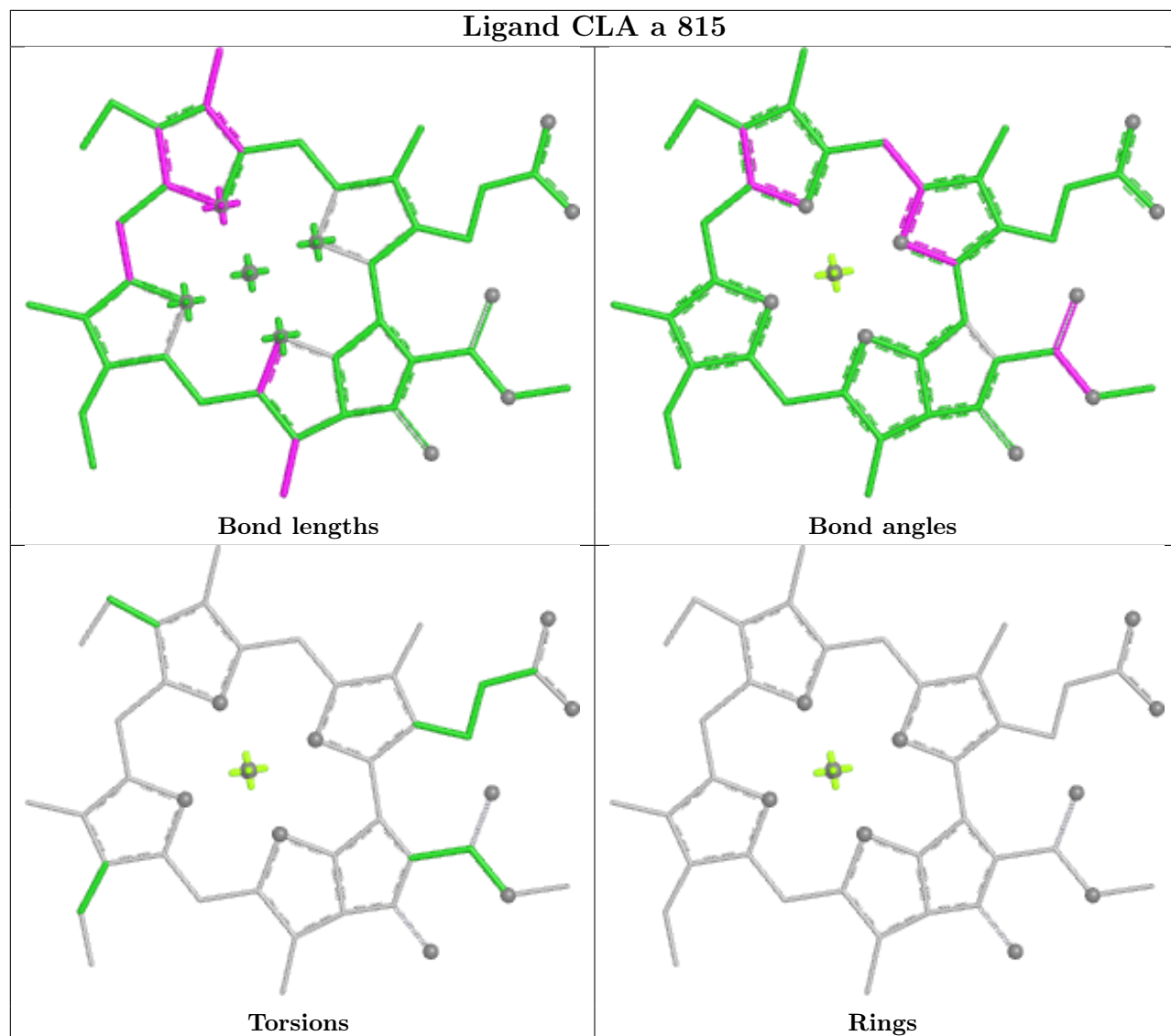
Torsions



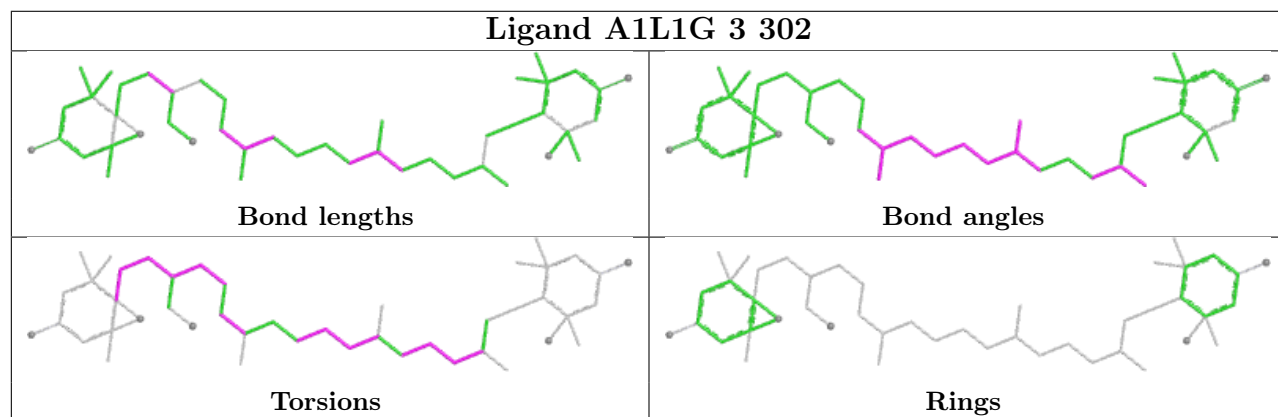
Rings

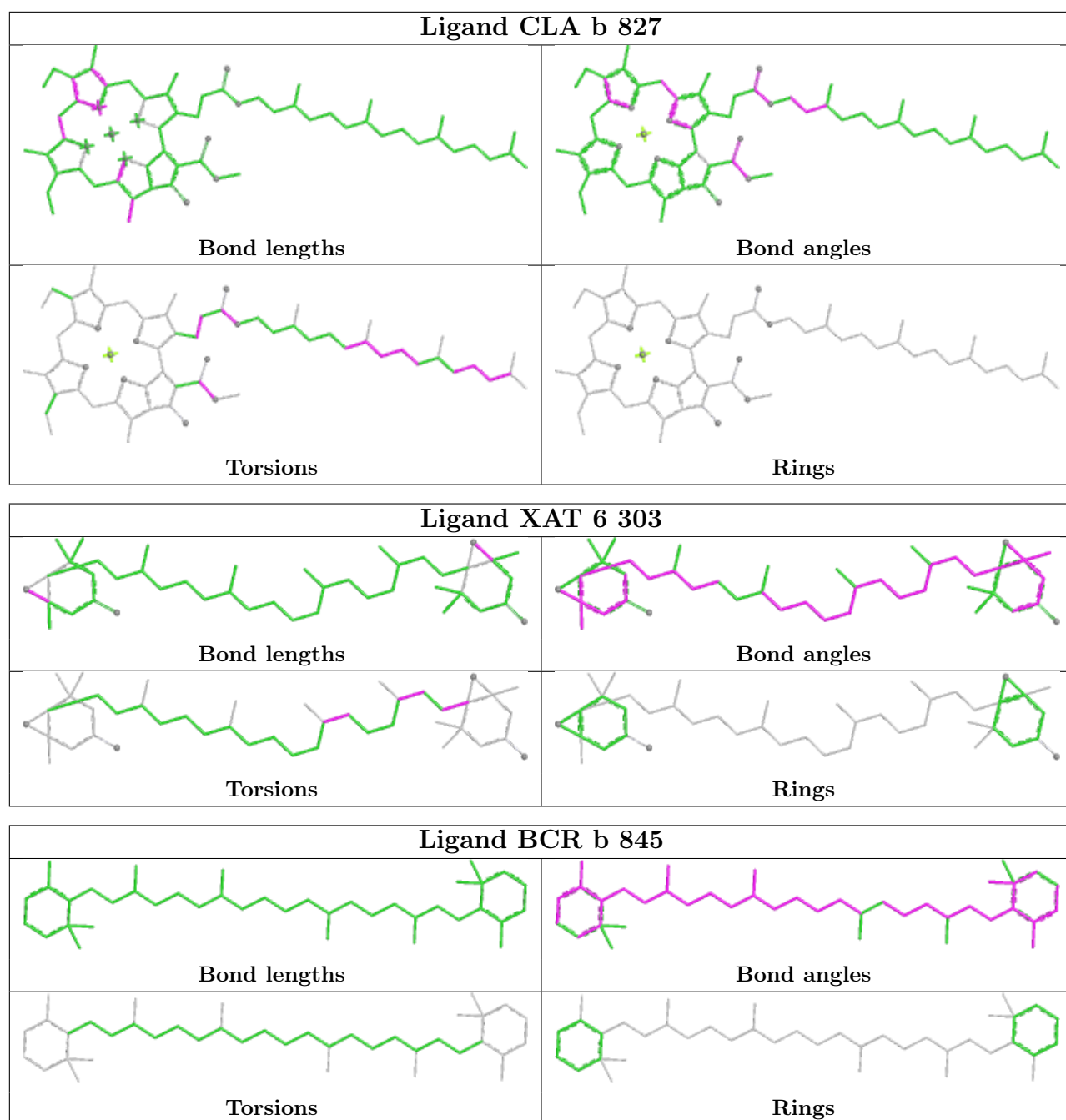


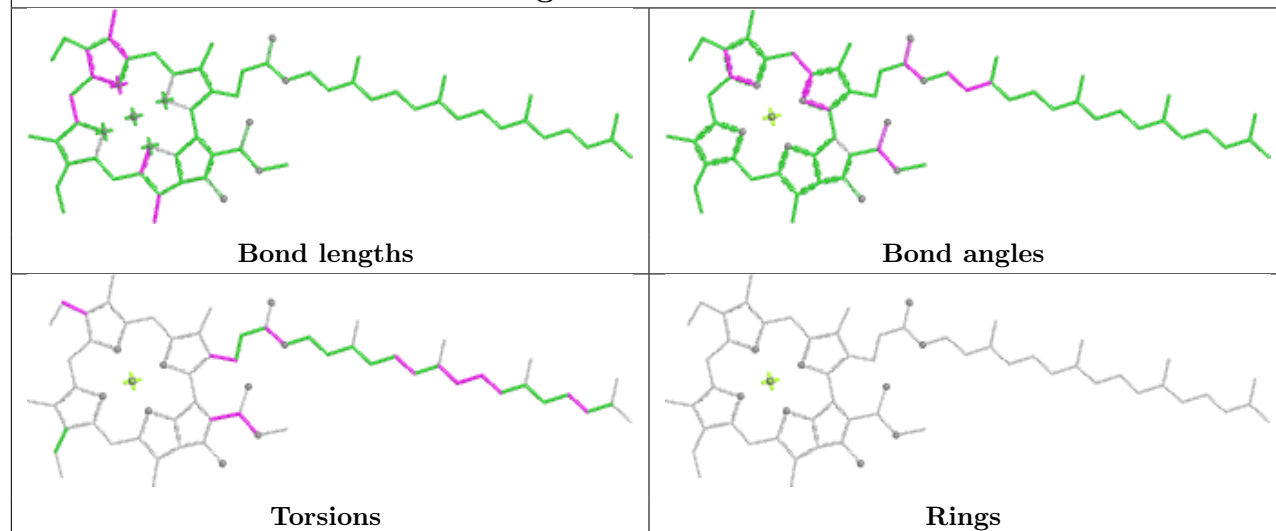
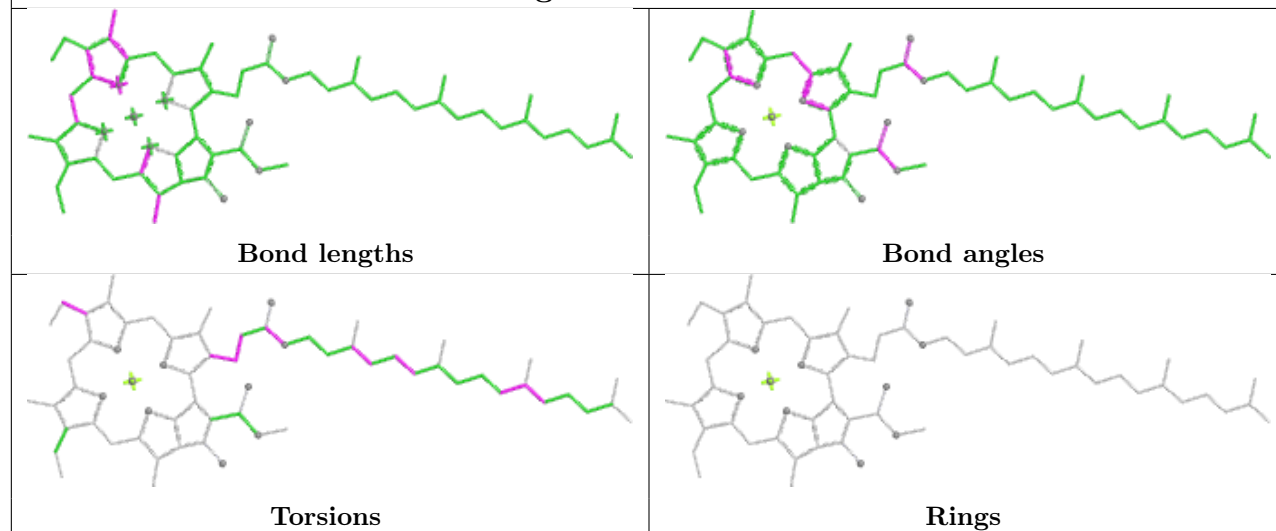
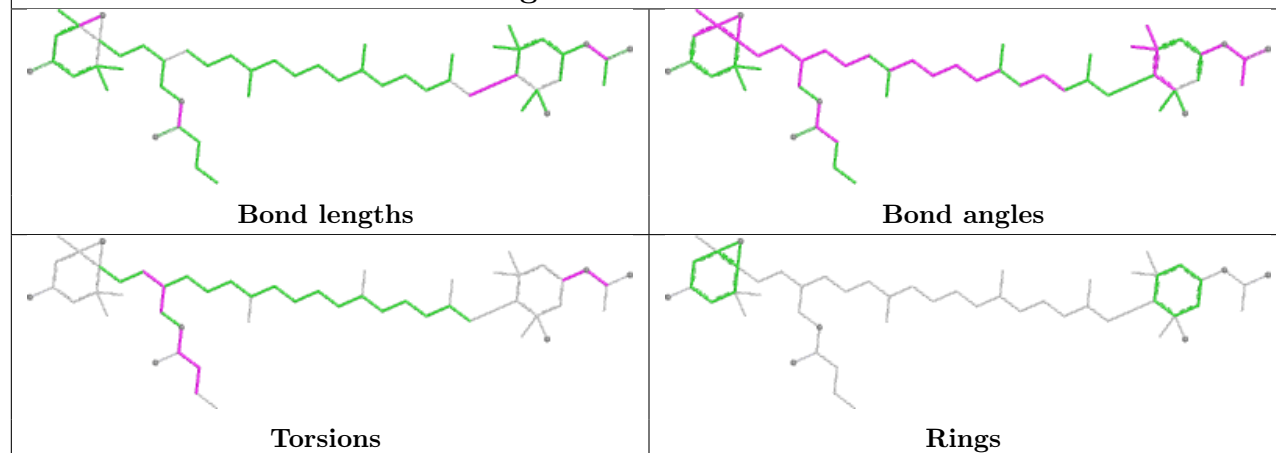
Ligand CLA a 815

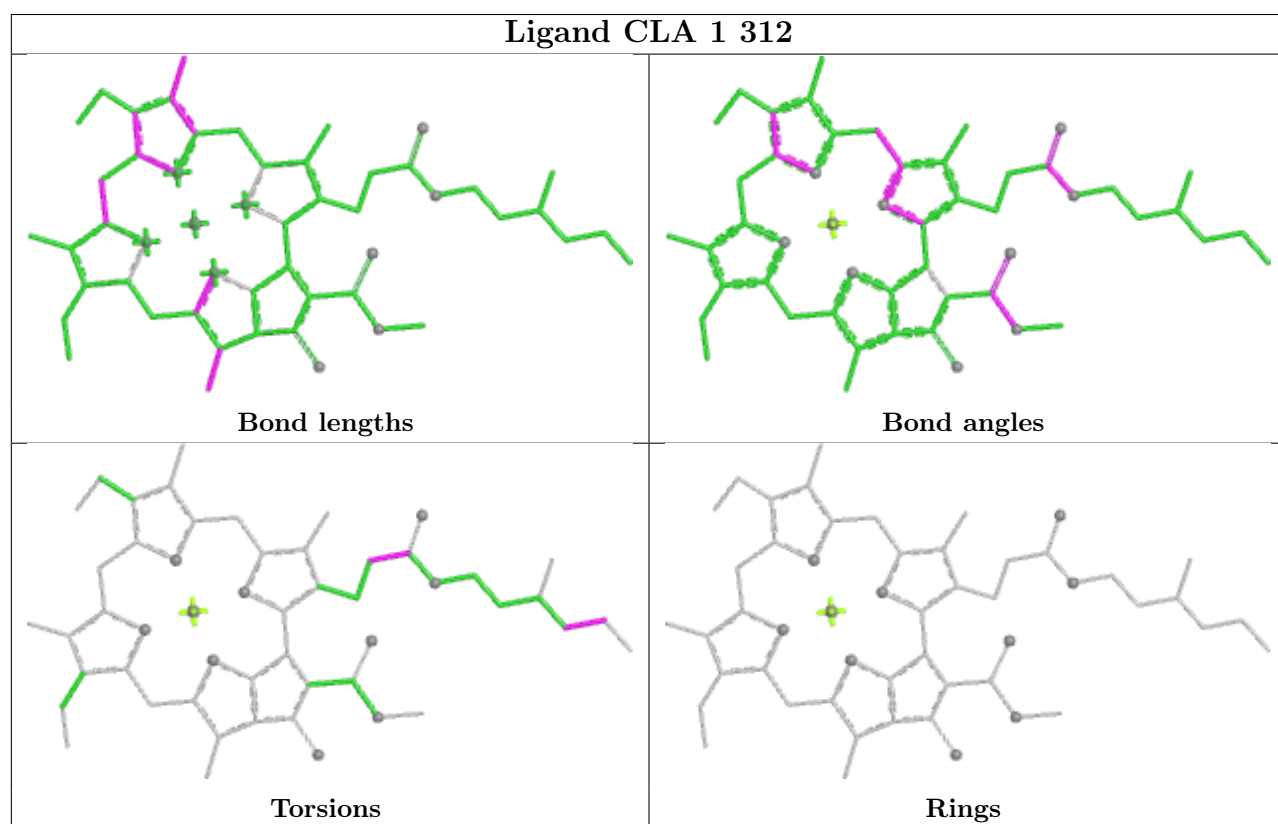
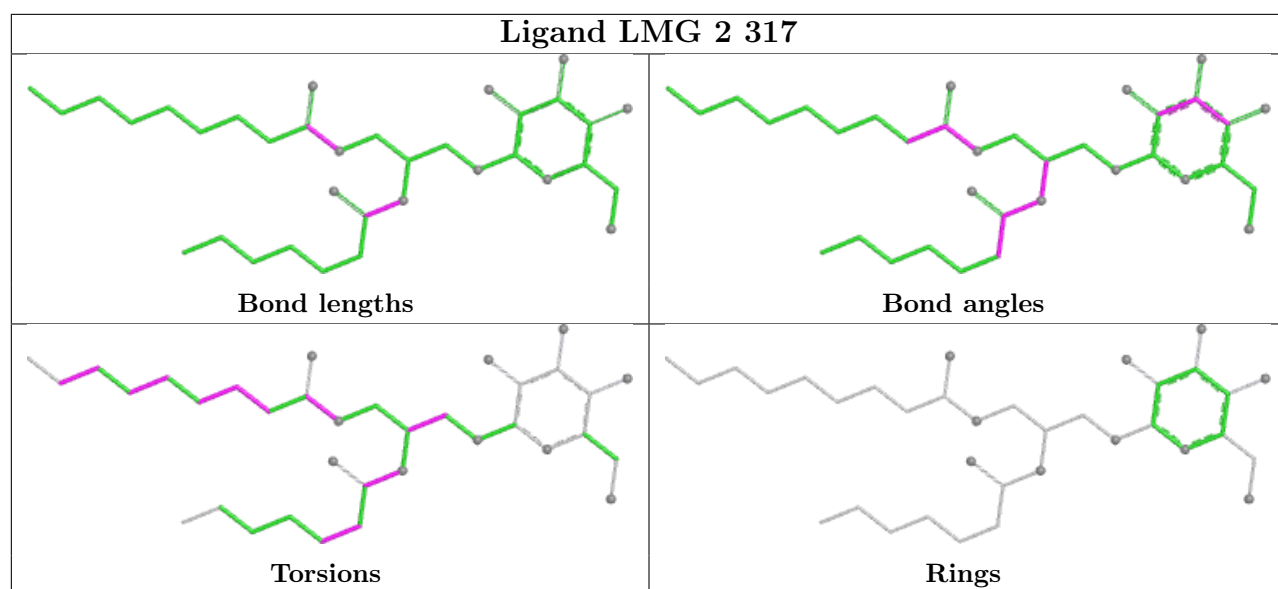


Ligand A1L1G 3 302

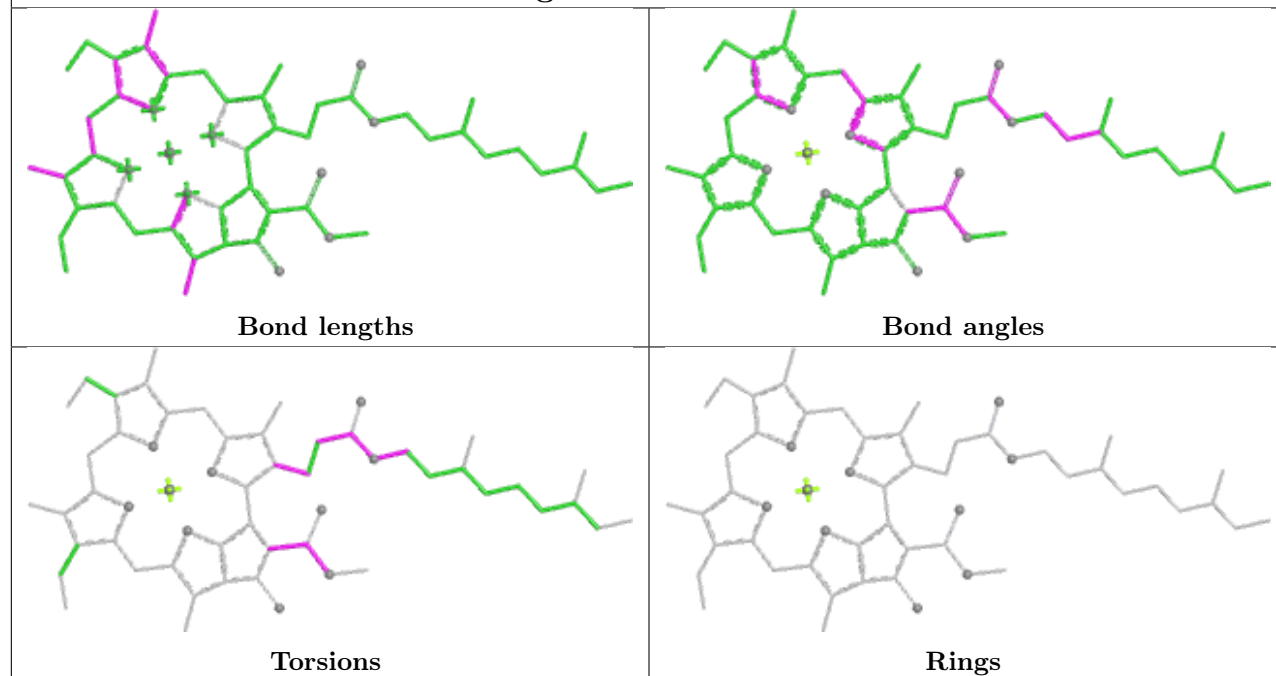




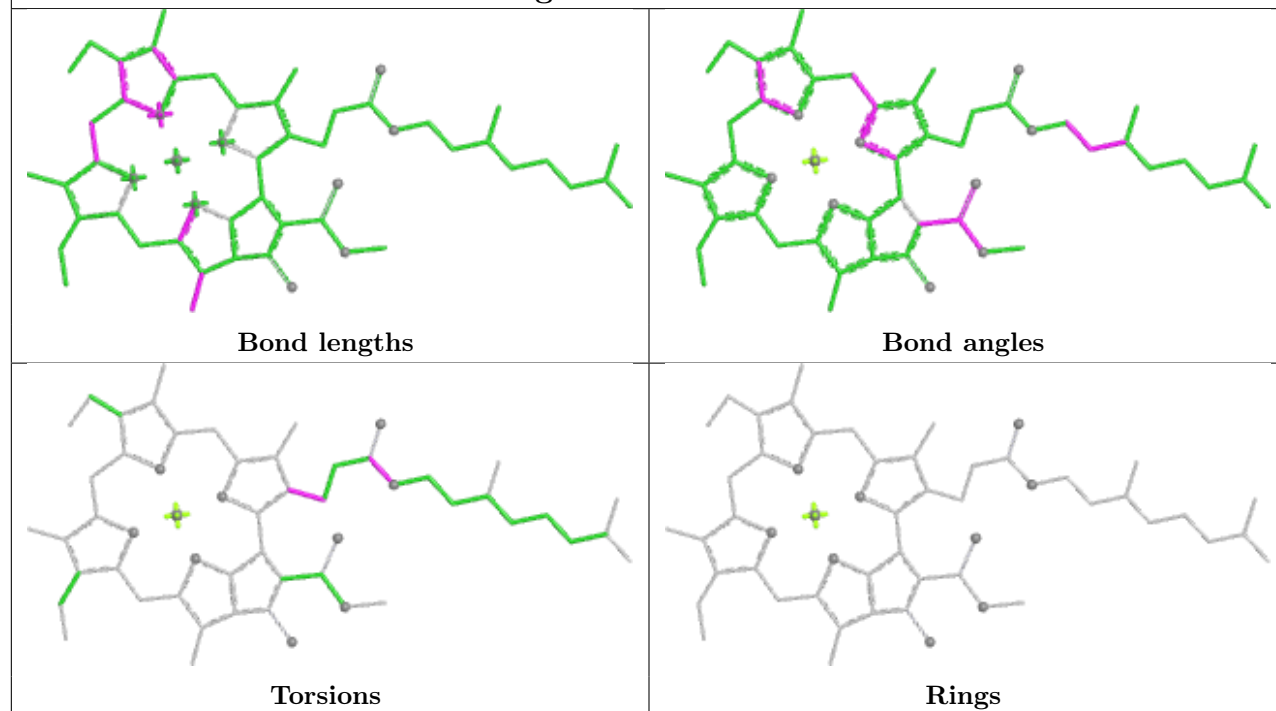
Ligand CLA a 854**Ligand CLA b 828****Ligand A1L1F 6 304**



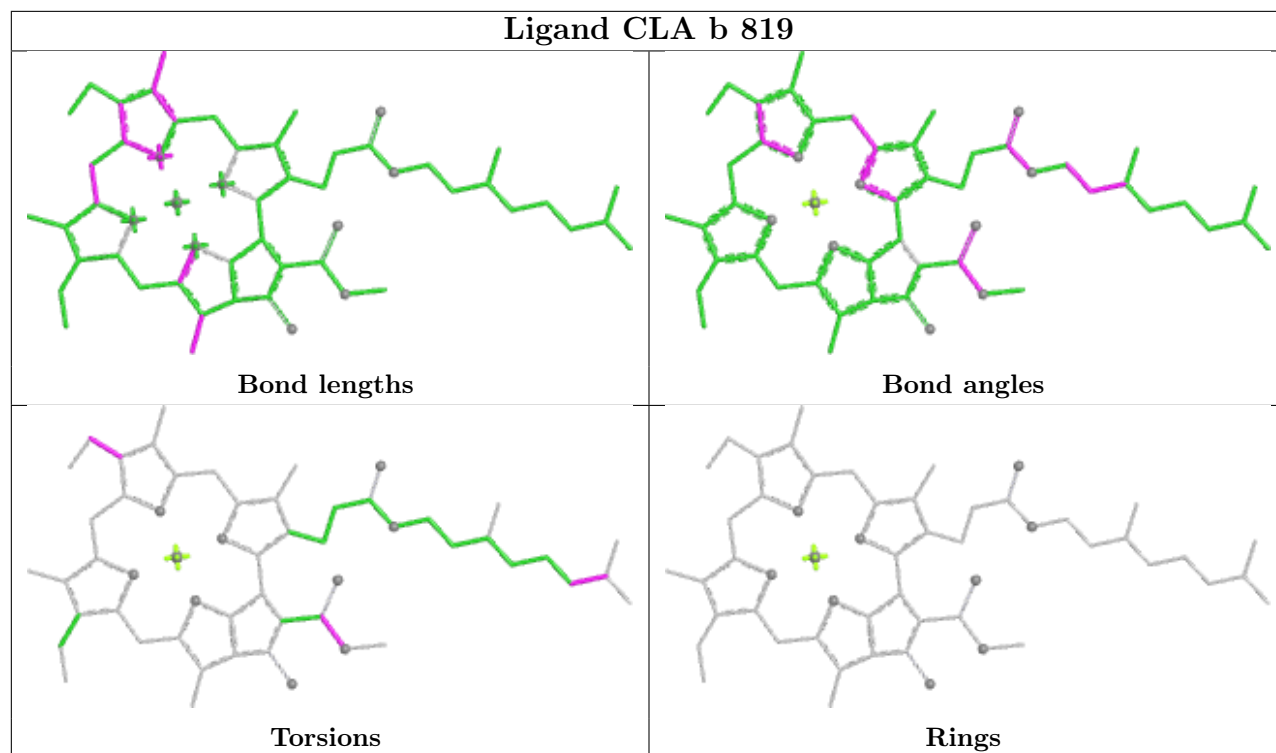
Ligand CLA a 818



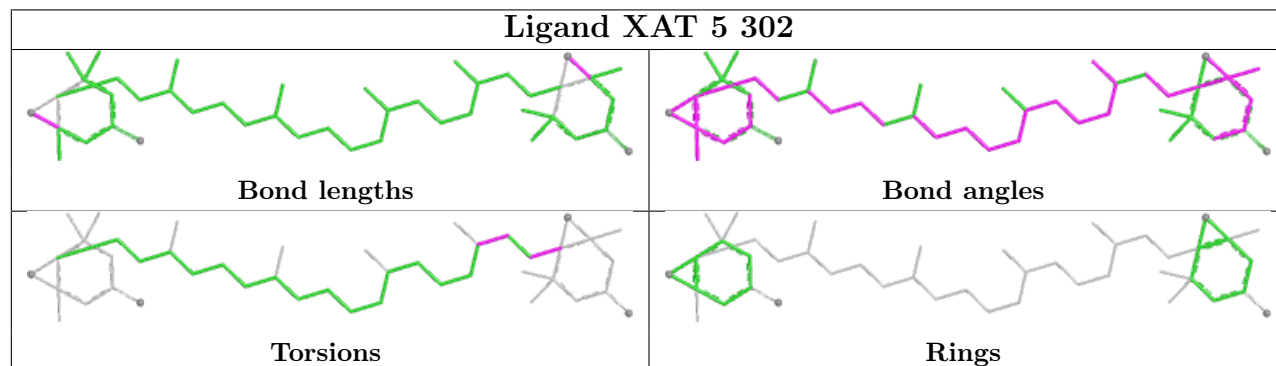
Ligand CLA b 816



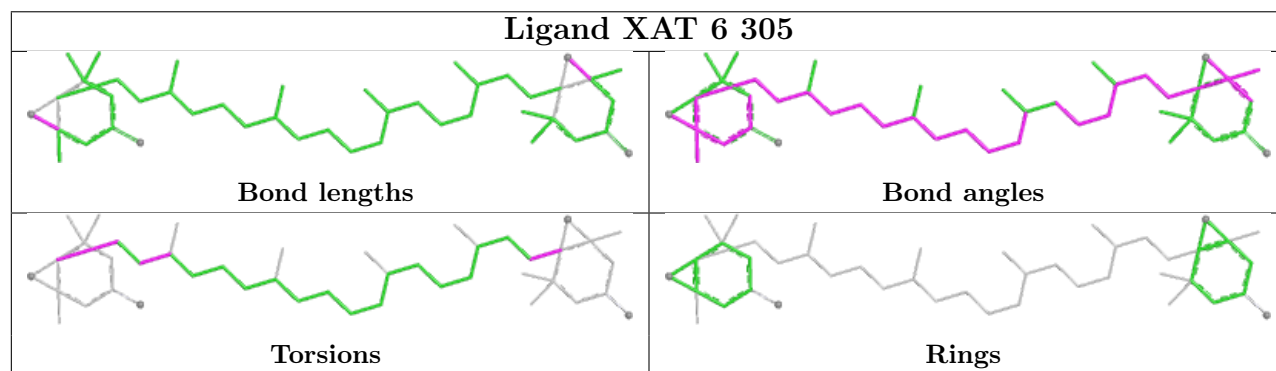
Ligand CLA b 819



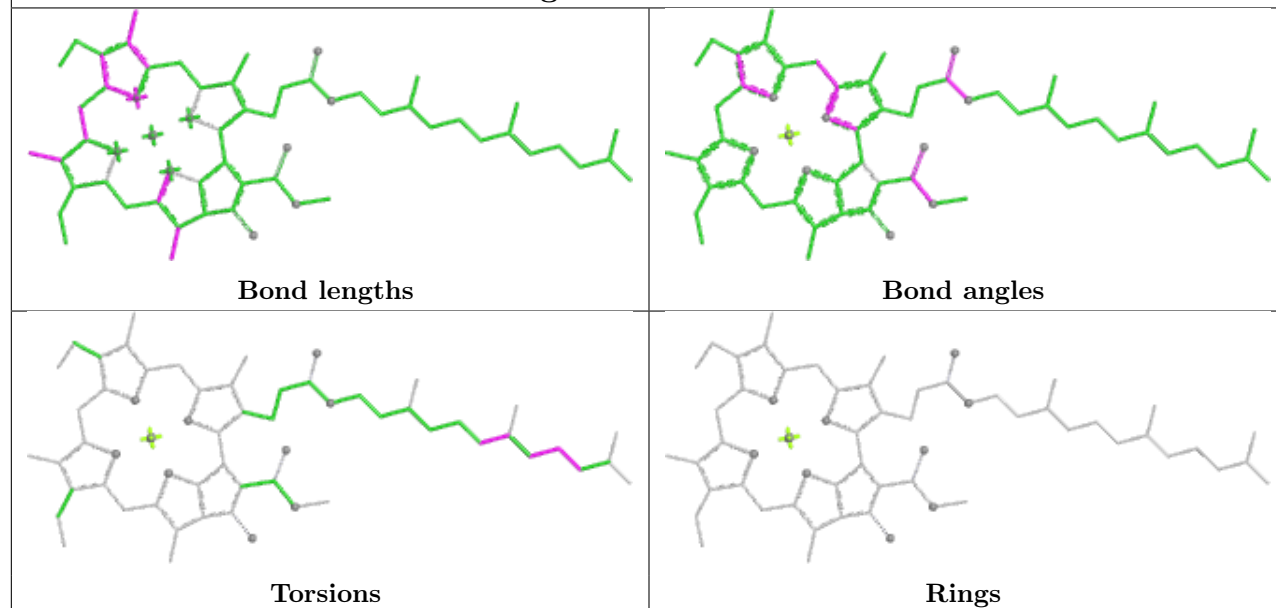
Ligand XAT 5 302



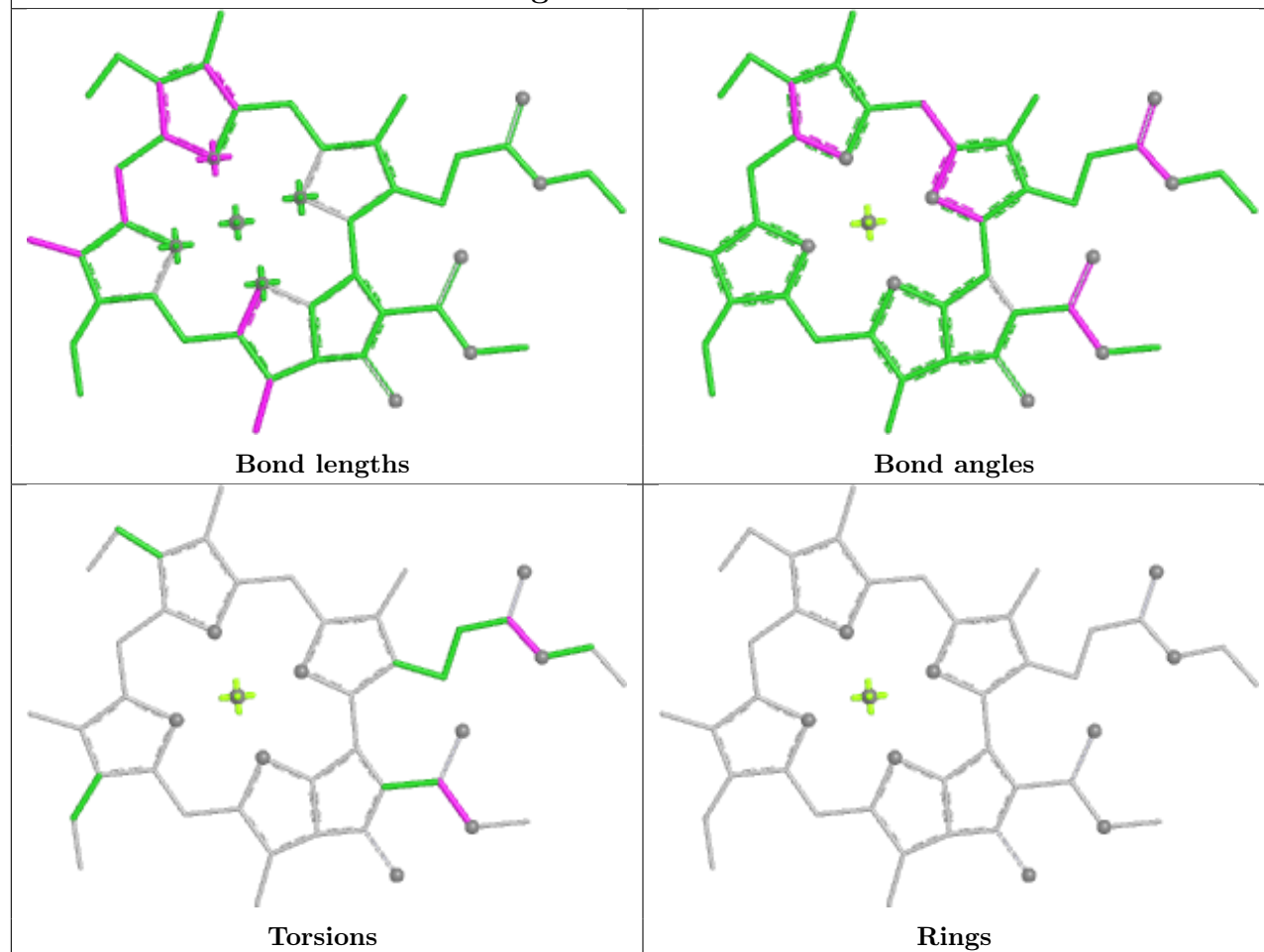
Ligand XAT 6 305



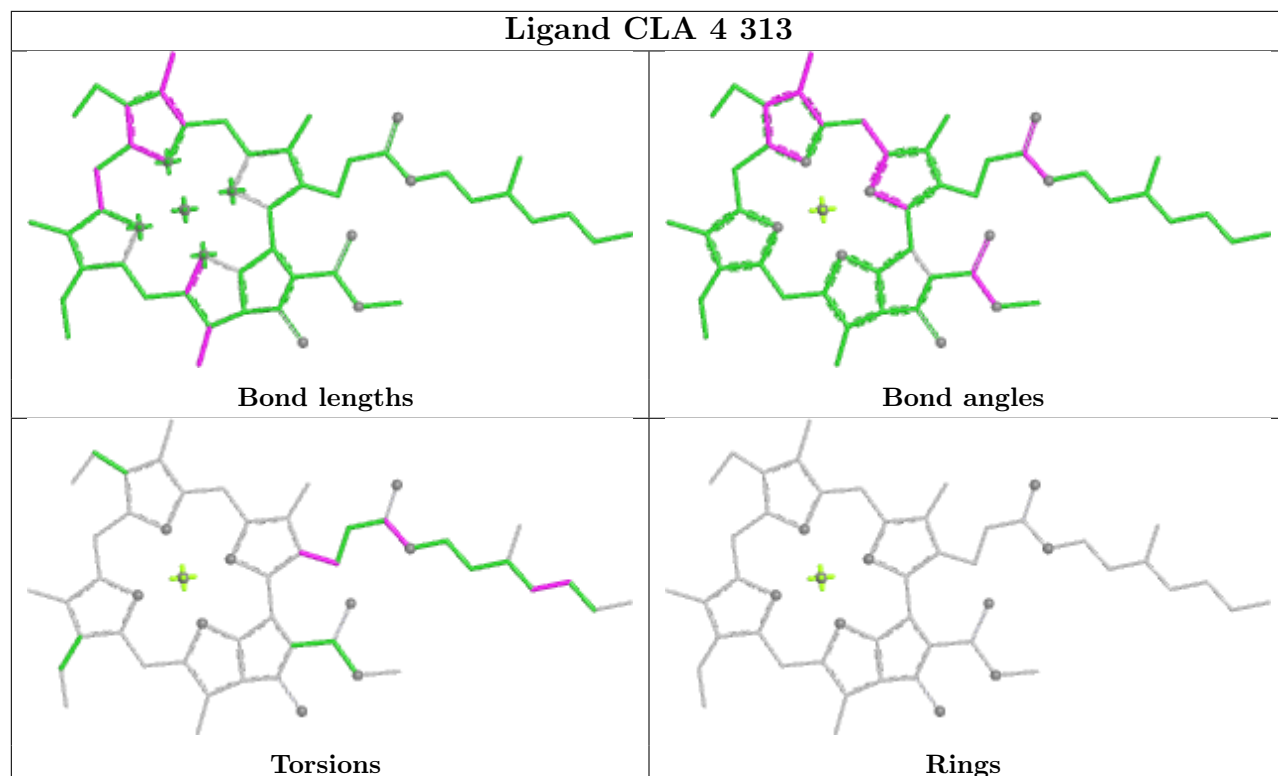
Ligand CLA 1 203



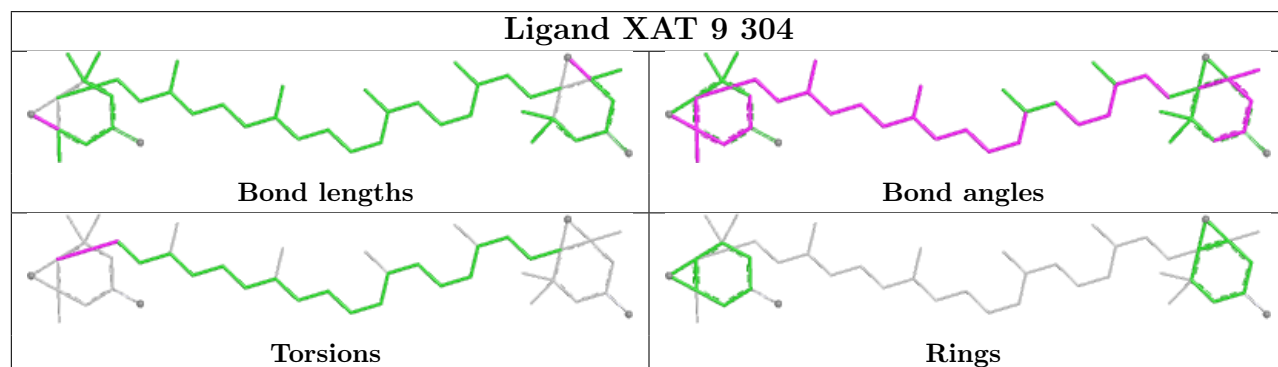
Ligand CLA 2 312

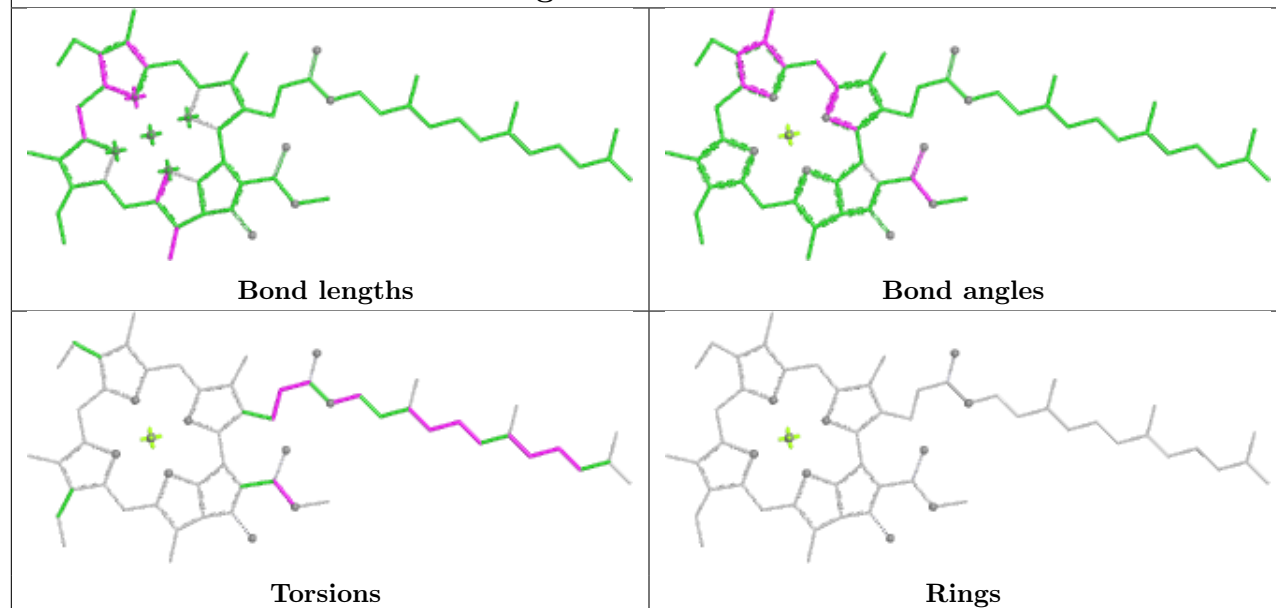
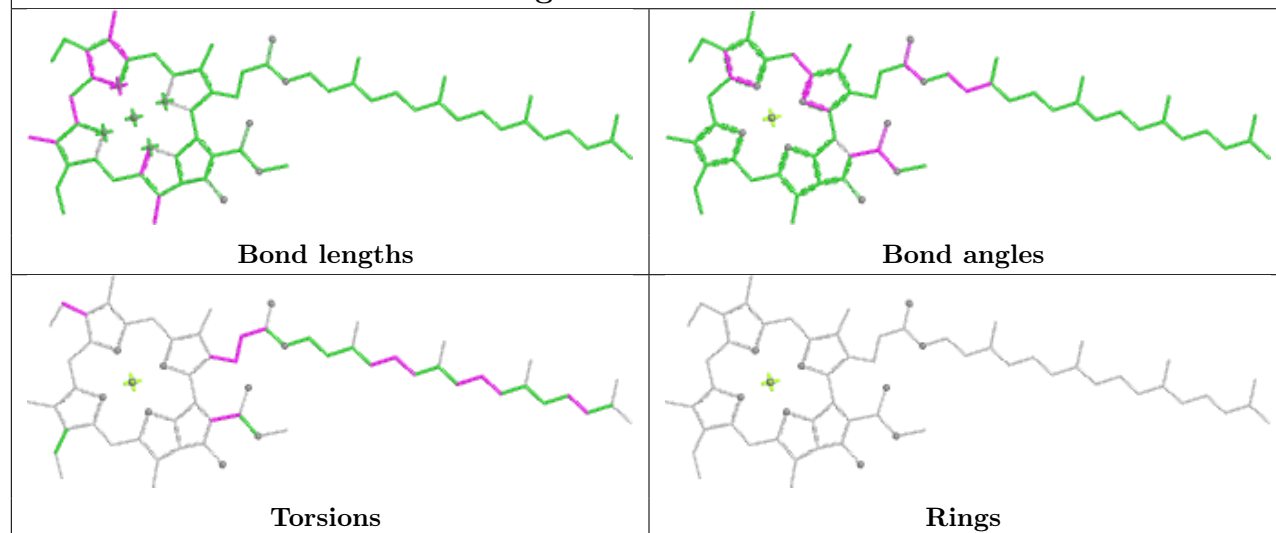


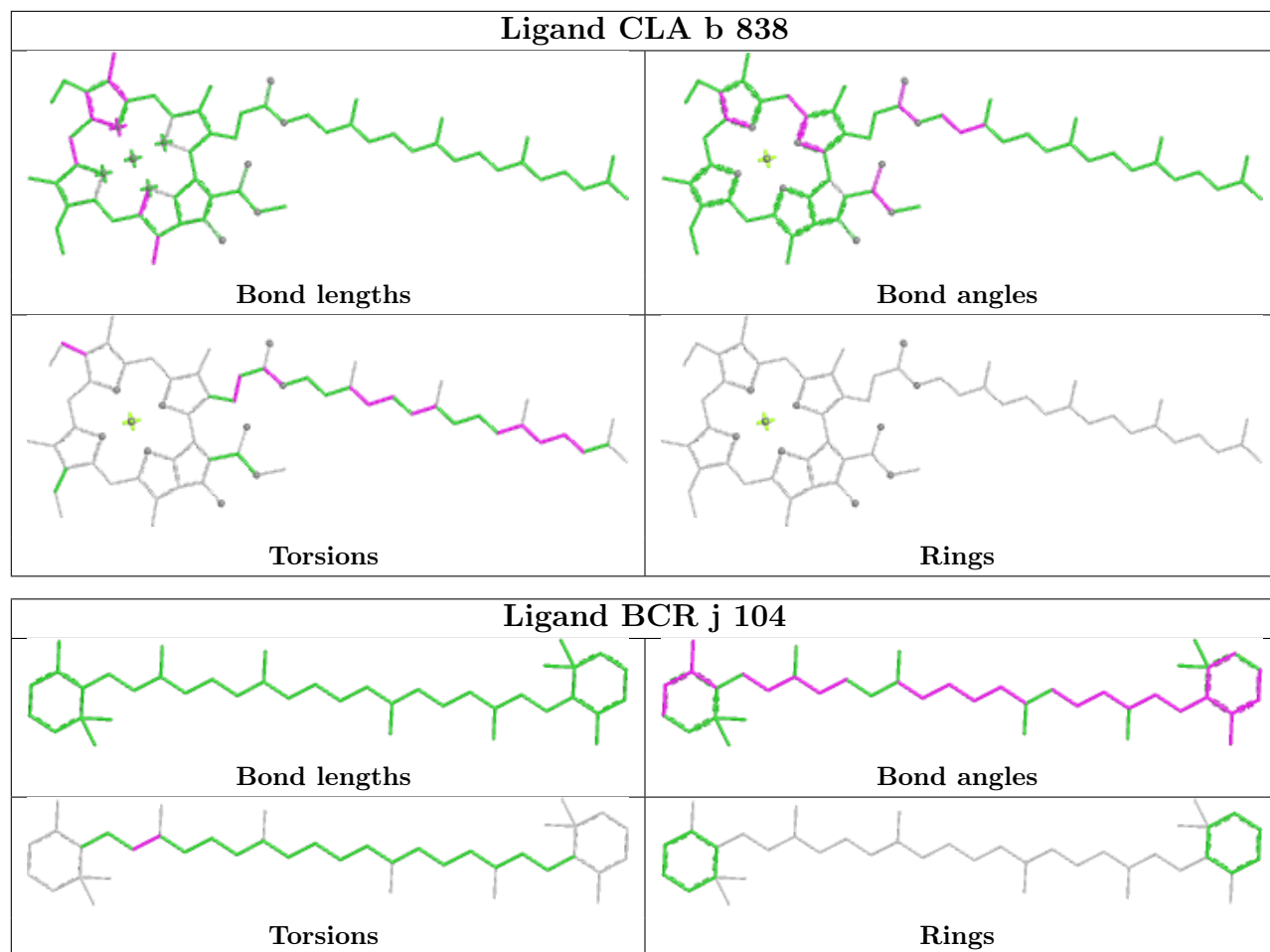
Ligand CLA 4 313



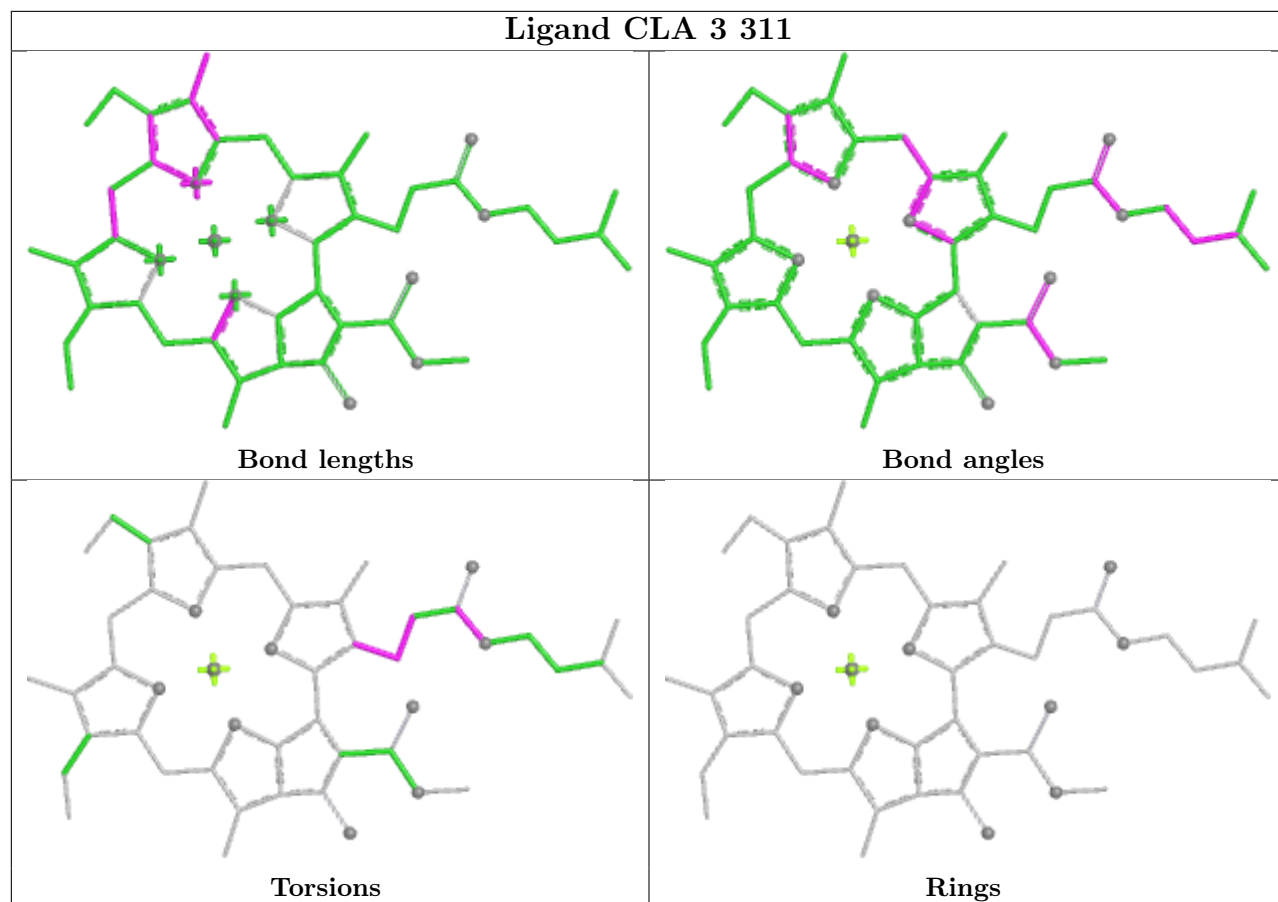
Ligand XAT 9 304



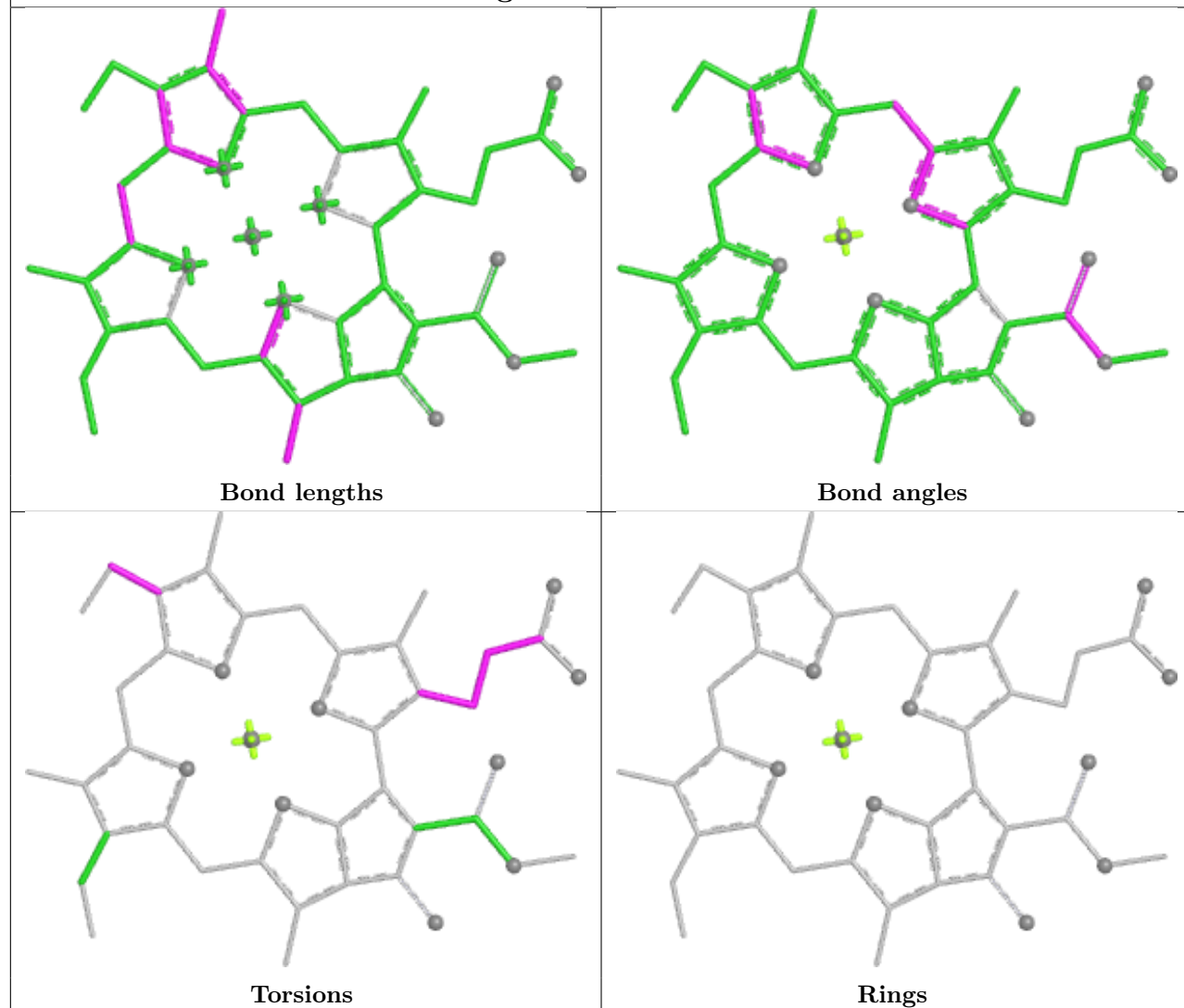
Ligand CLA 7 308**Ligand CLA b 809**



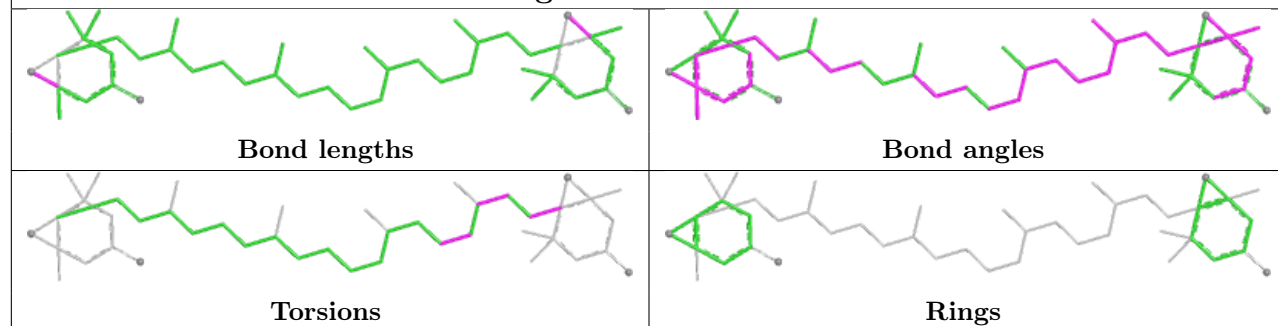
Ligand CLA 3 311



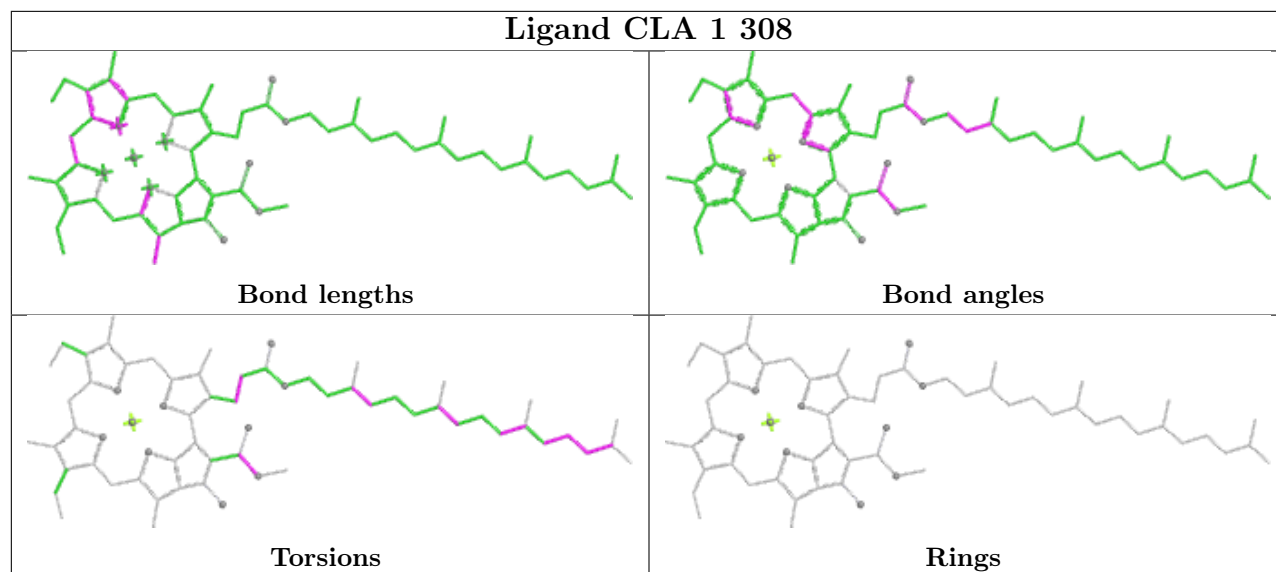
Ligand CLA 1 314



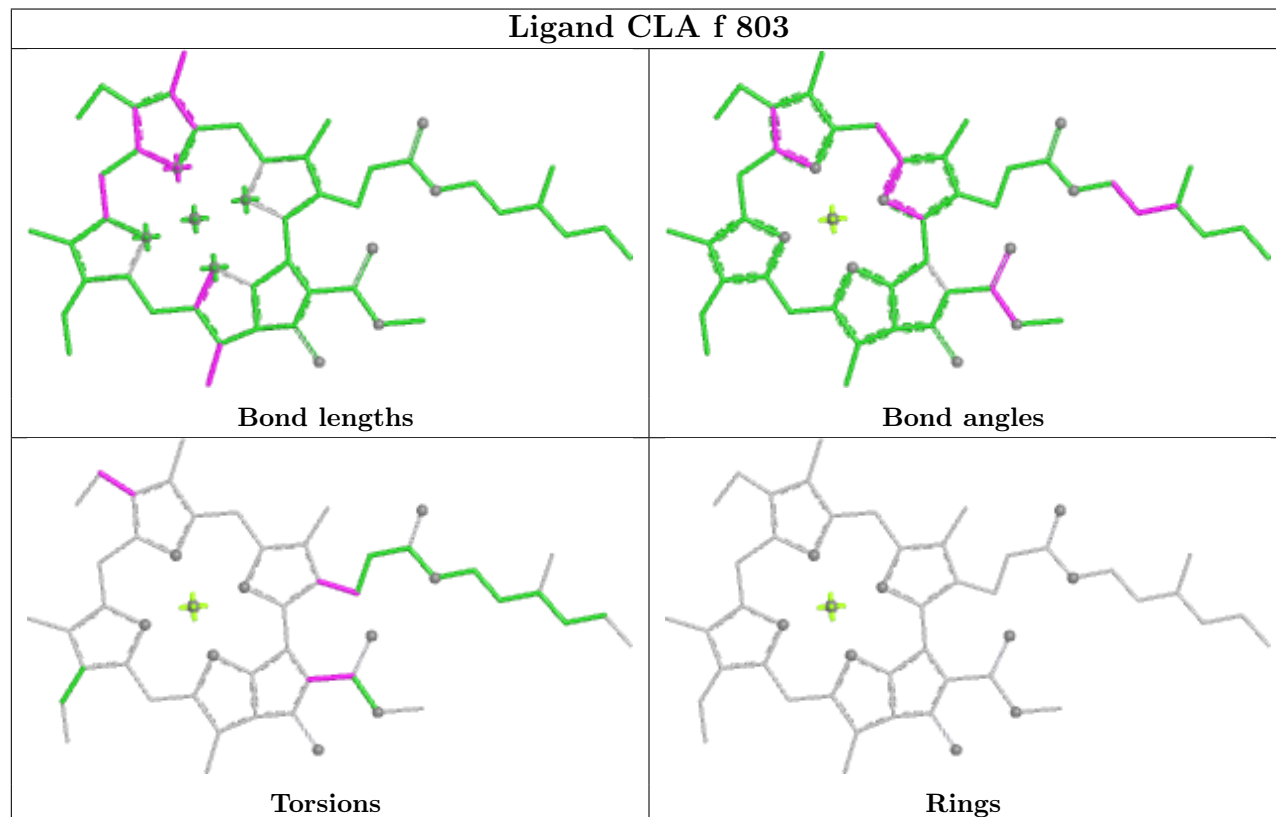
Ligand XAT 8 302

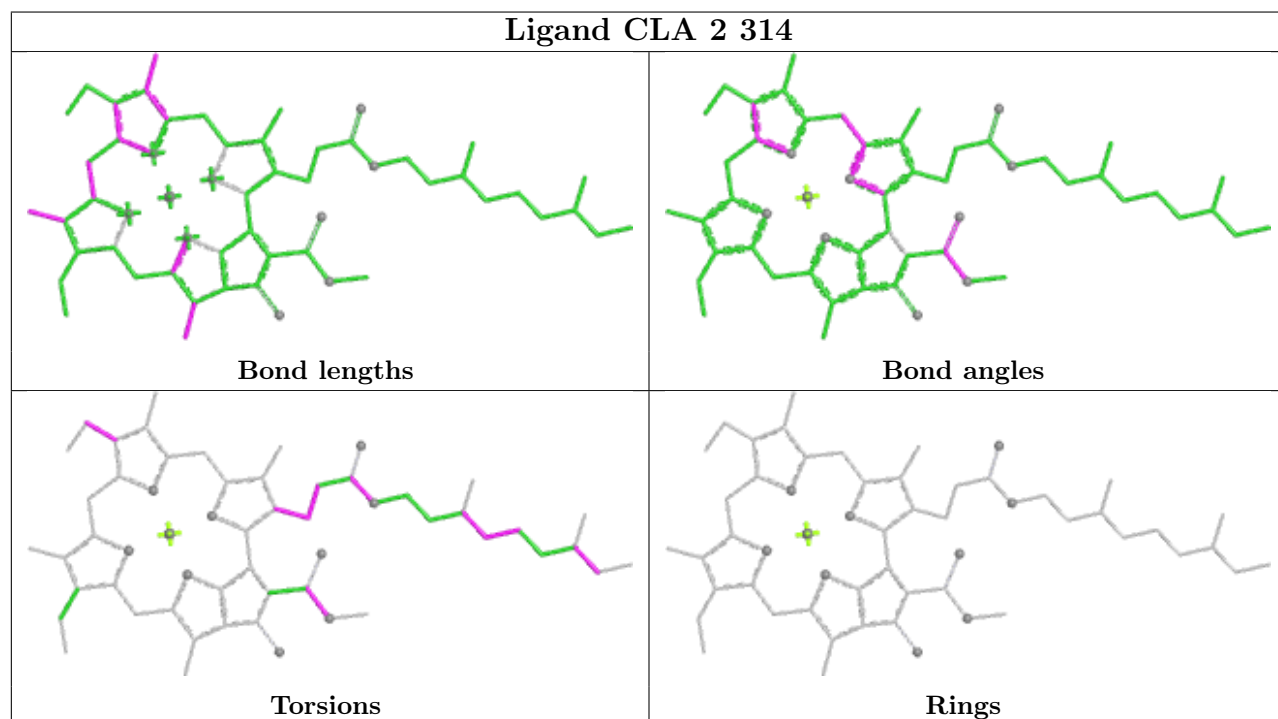
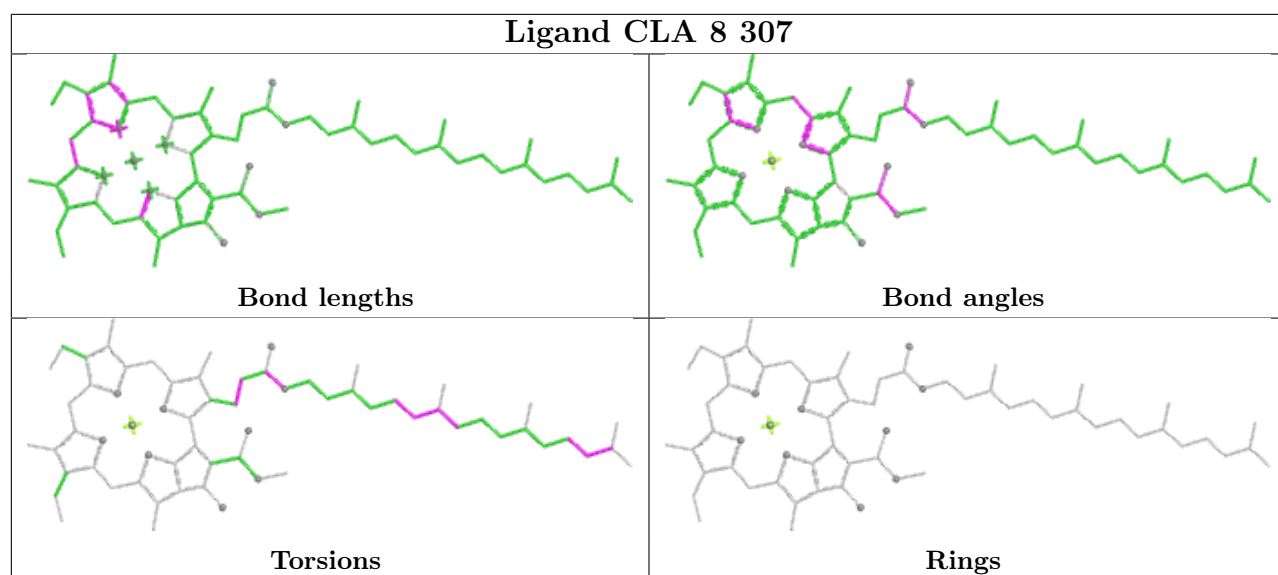


Ligand CLA 1 308

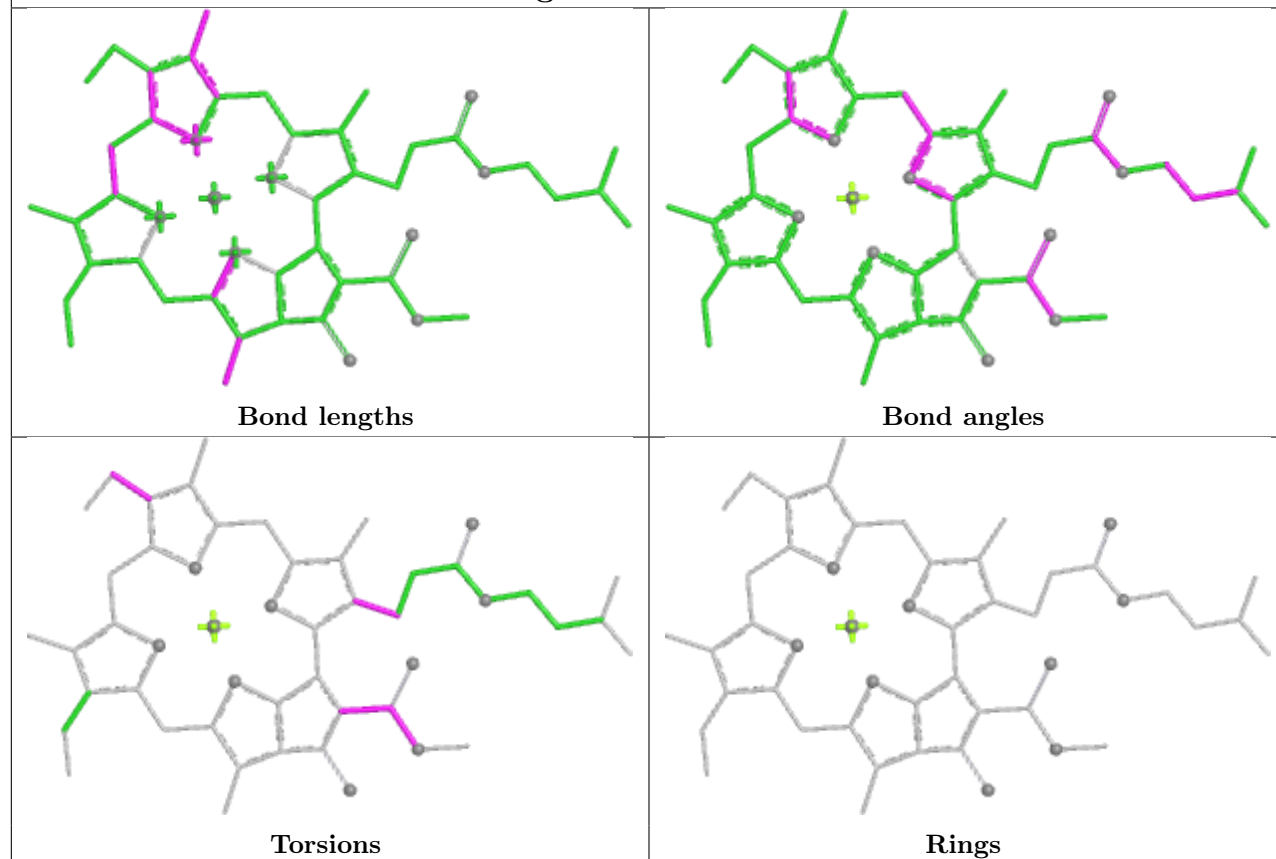


Ligand CLA f 803

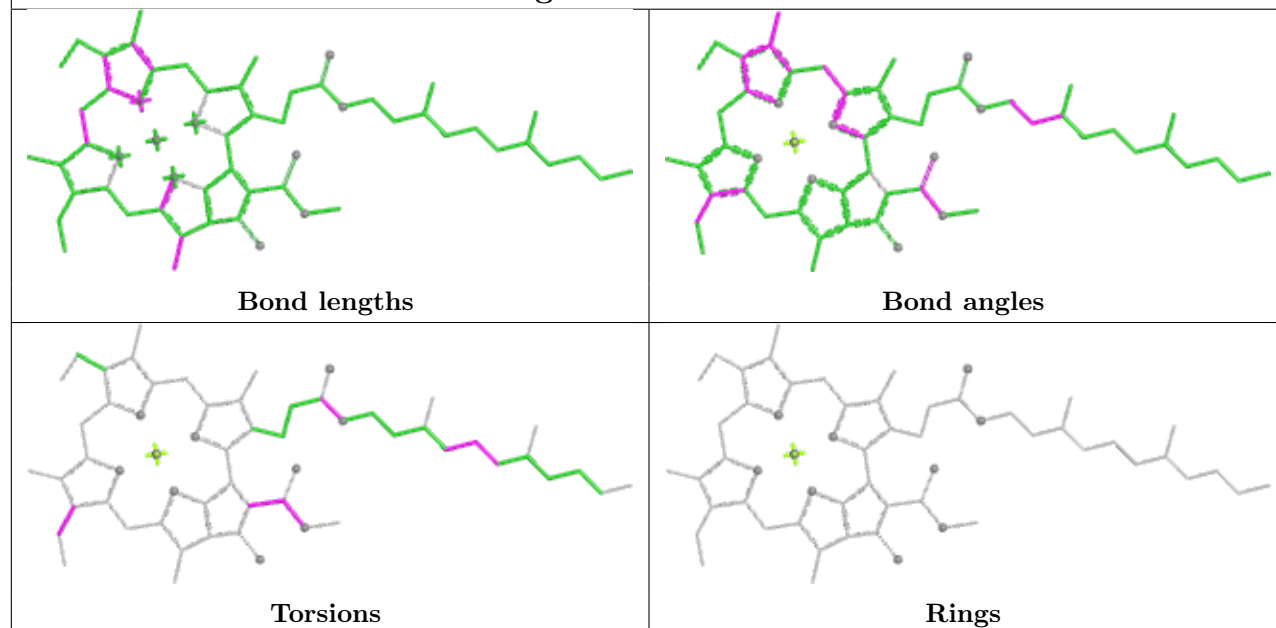




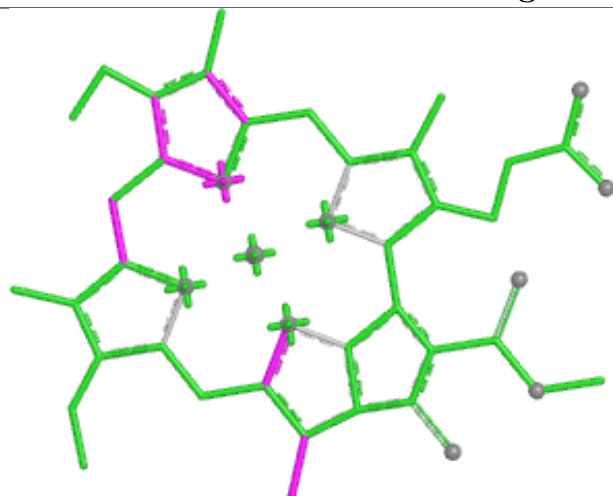
Ligand CLA a 832



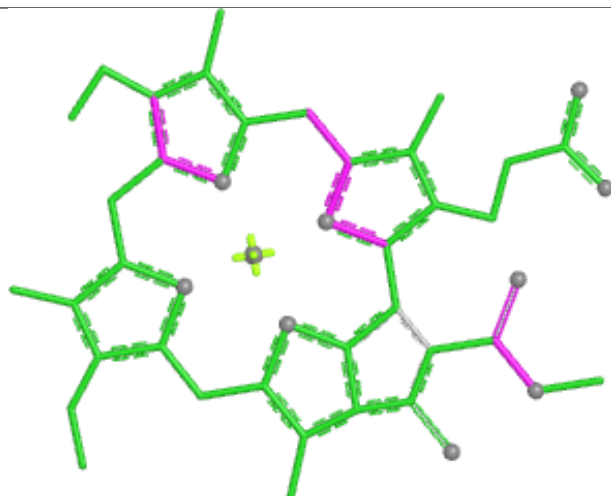
Ligand CLA b 835



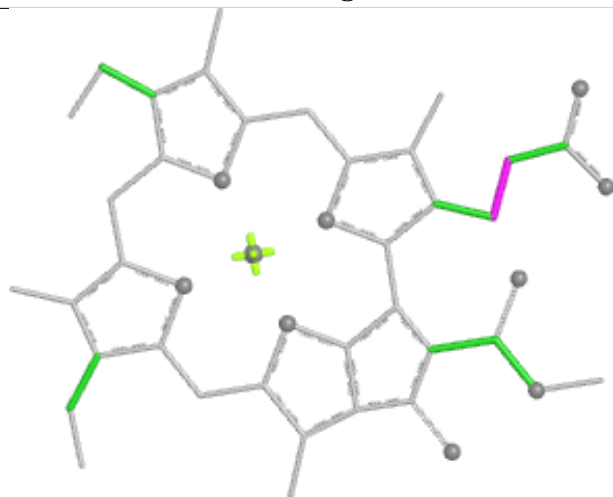
Ligand CLA a 821



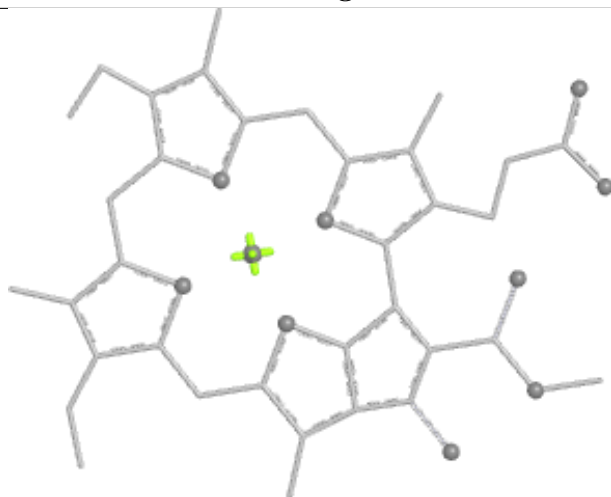
Bond lengths



Bond angles

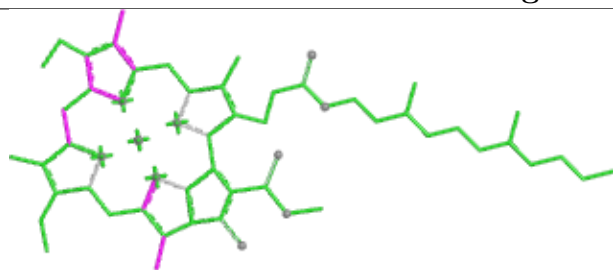


Torsions

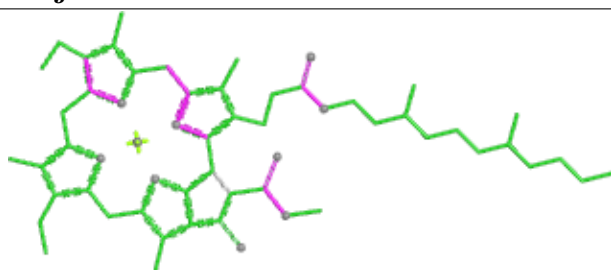


Rings

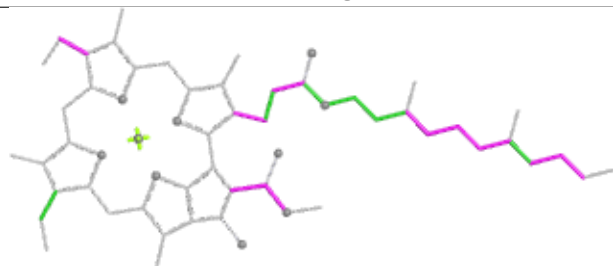
Ligand CLA j 102



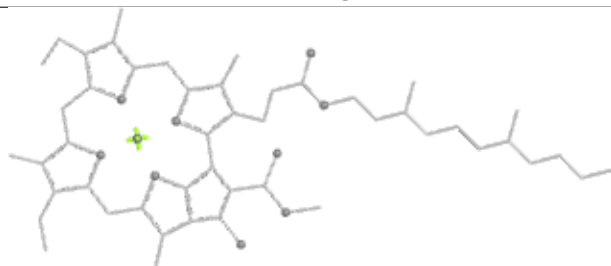
Bond lengths



Bond angles

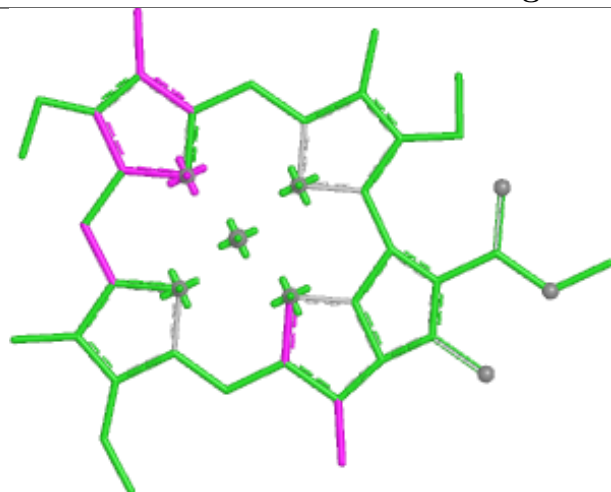


Torsions

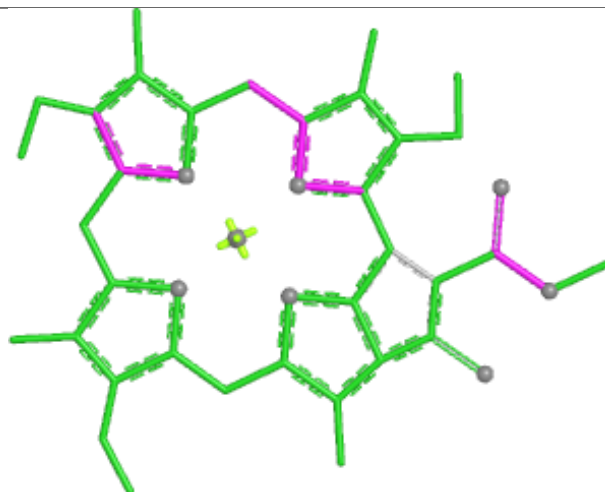


Rings

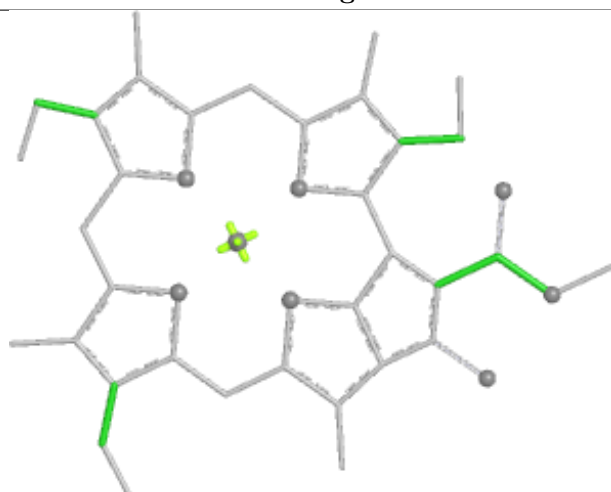
Ligand CLA 1 202



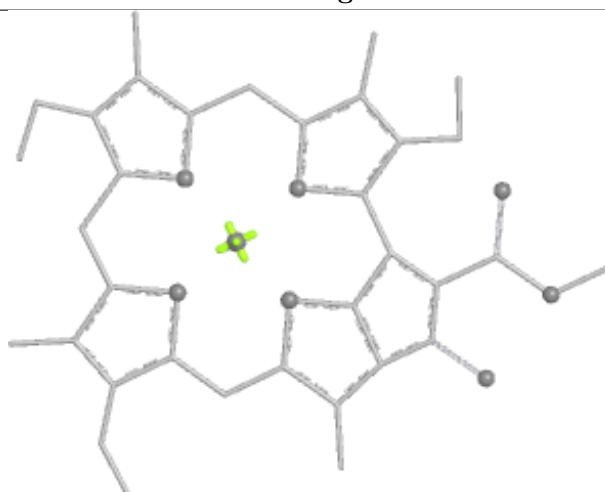
Bond lengths



Bond angles

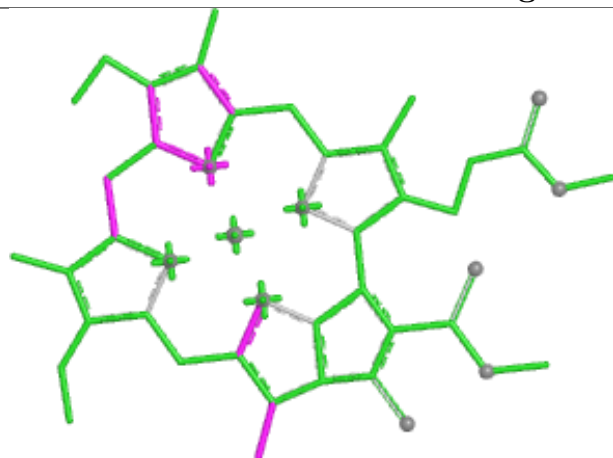


Torsions

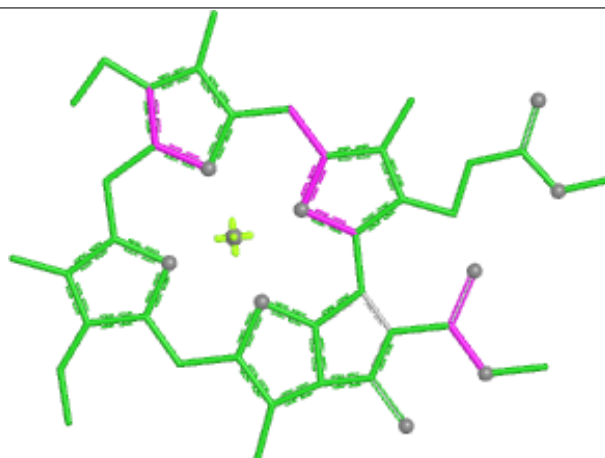


Rings

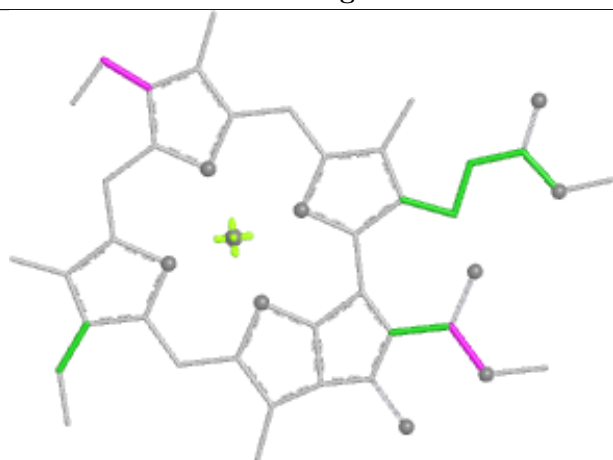
Ligand CLA 8 306



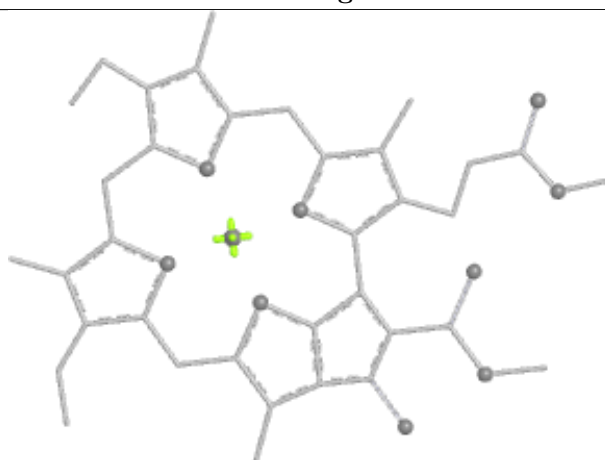
Bond lengths



Bond angles

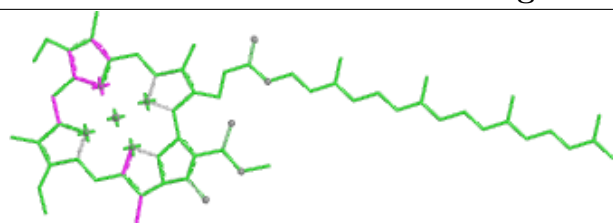


Torsions

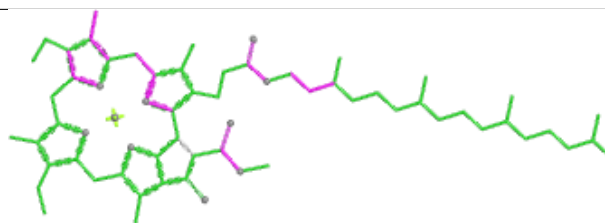


Rings

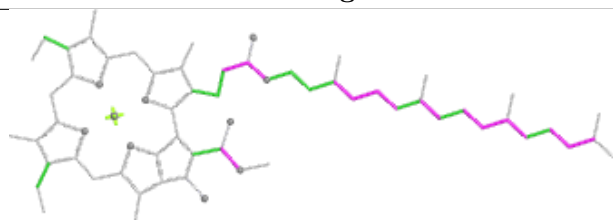
Ligand CLA b 807



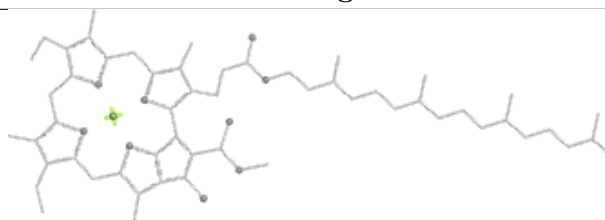
Bond lengths



Bond angles

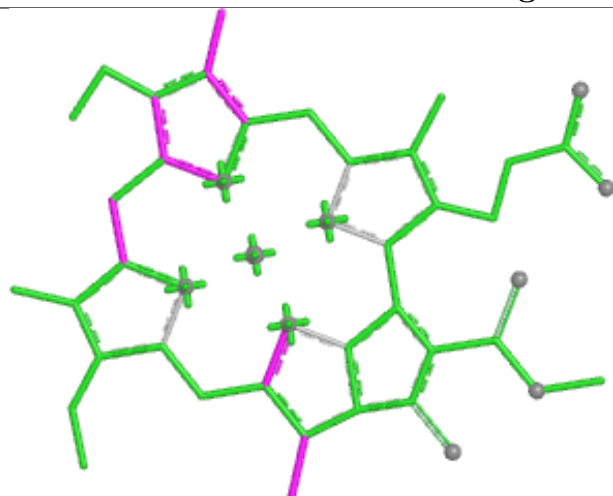


Torsions

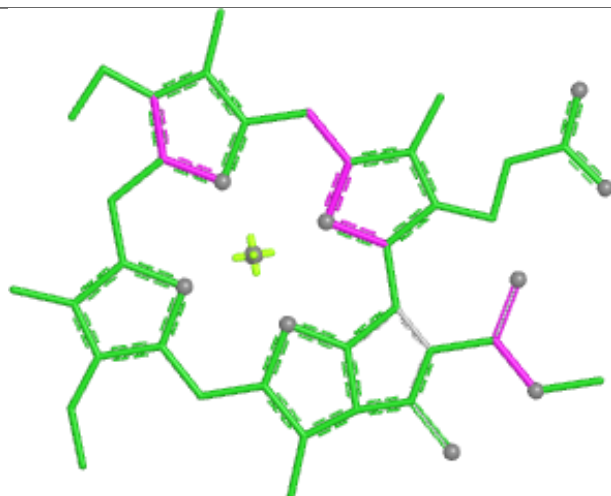


Rings

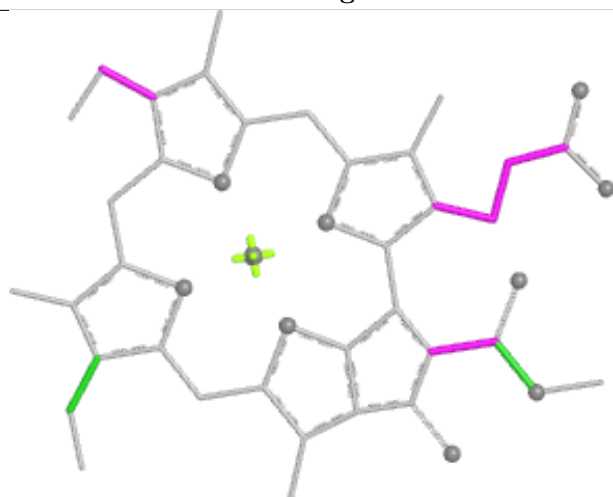
Ligand CLA a 817



Bond lengths



Bond angles

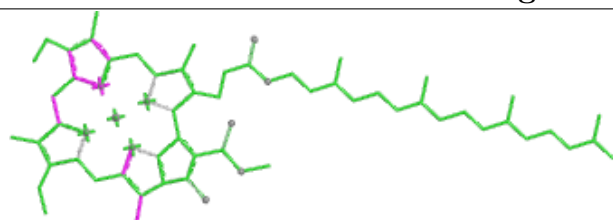


Torsions

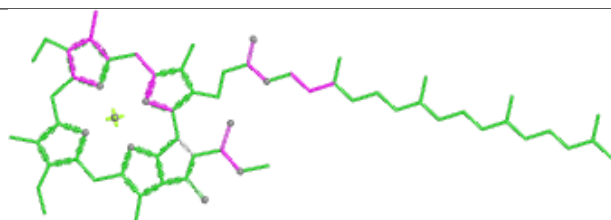


Rings

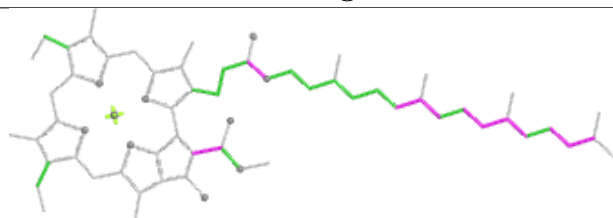
Ligand CLA a 844



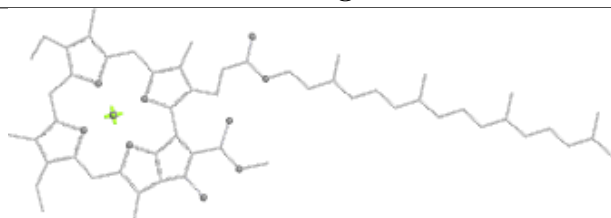
Bond lengths



Bond angles

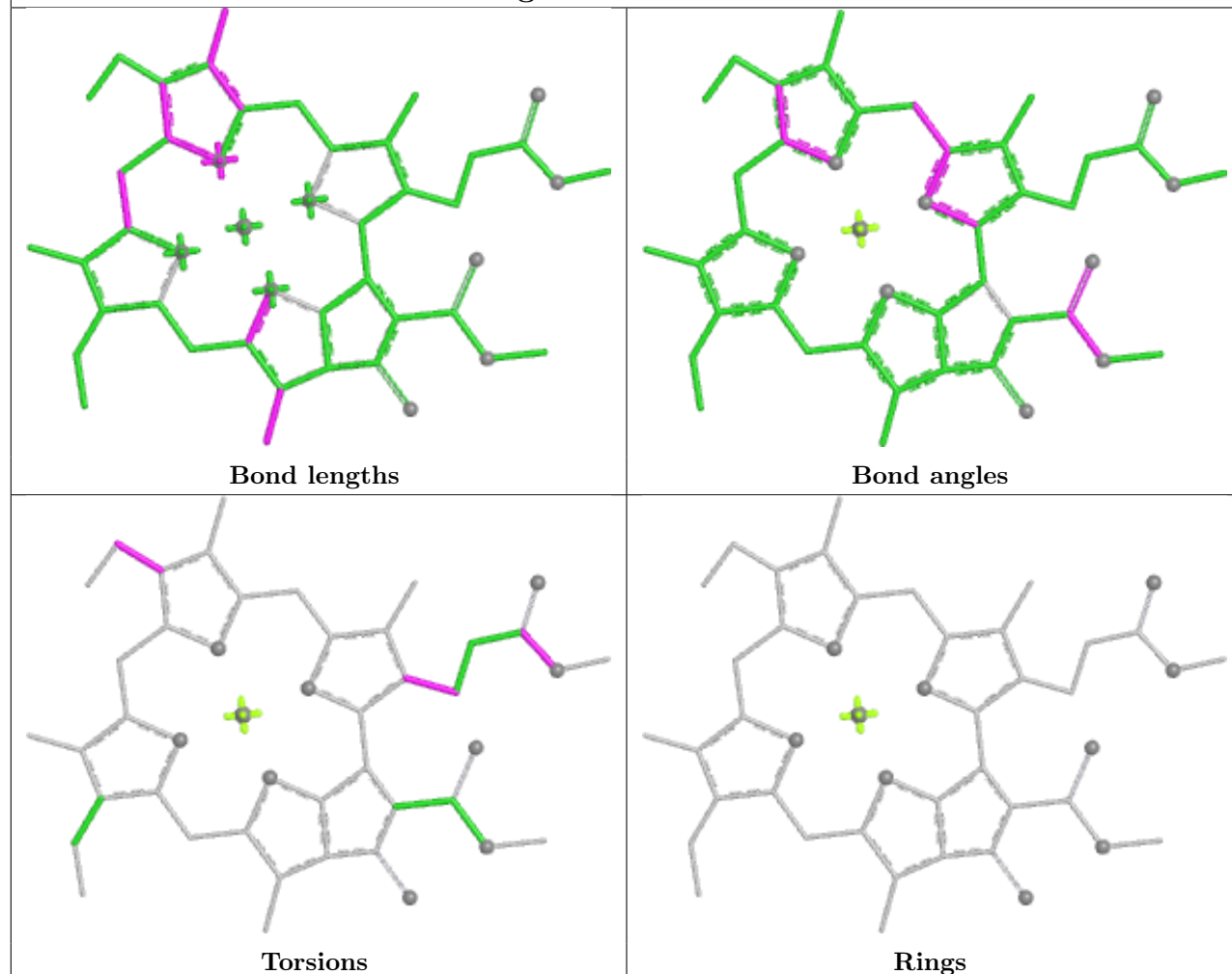


Torsions

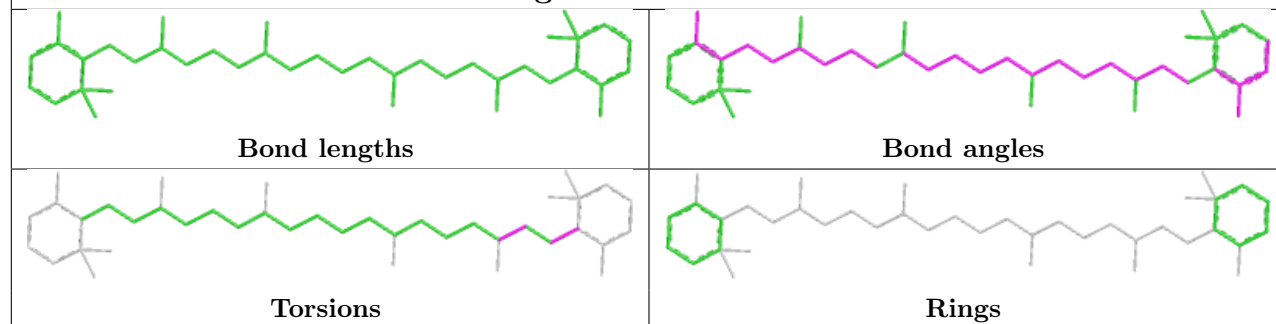


Rings

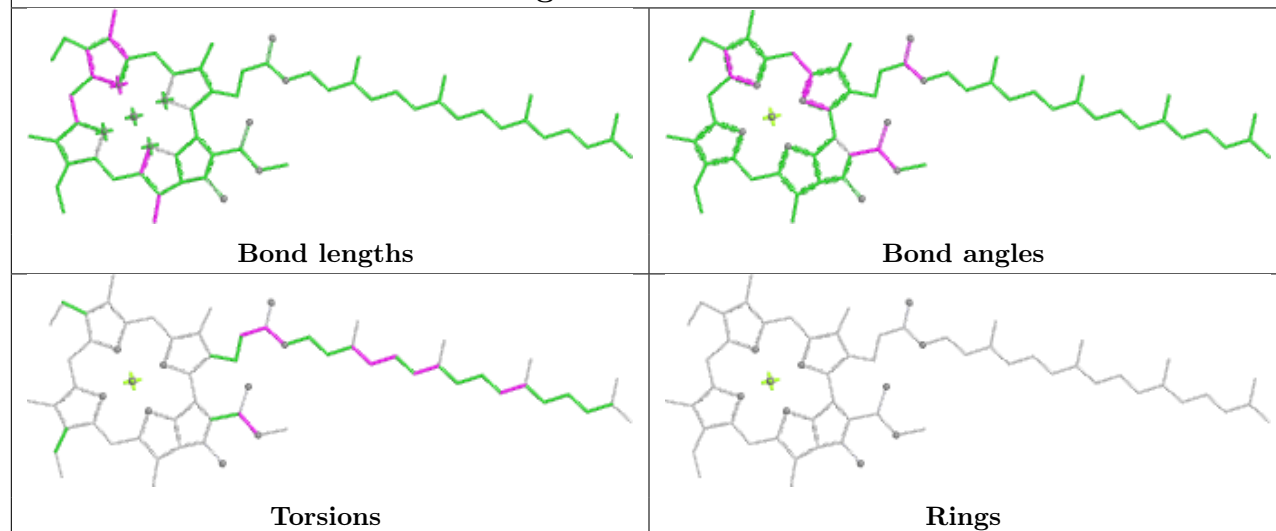
Ligand CLA 4 312



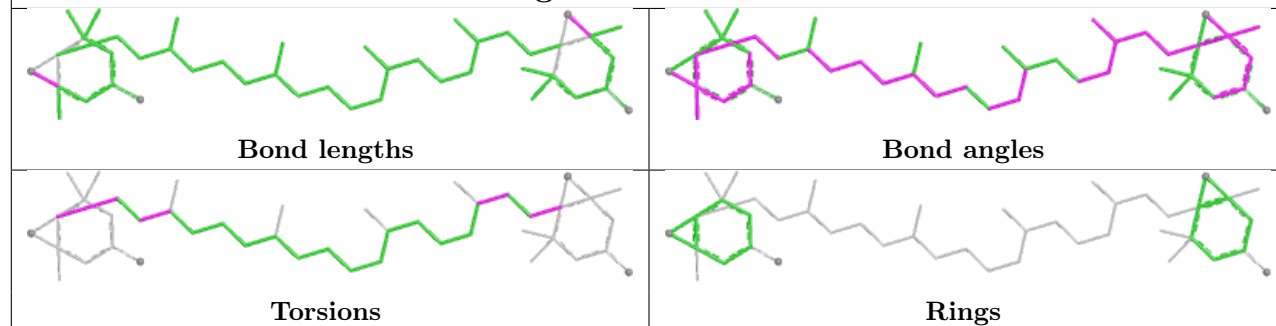
Ligand BCR a 850



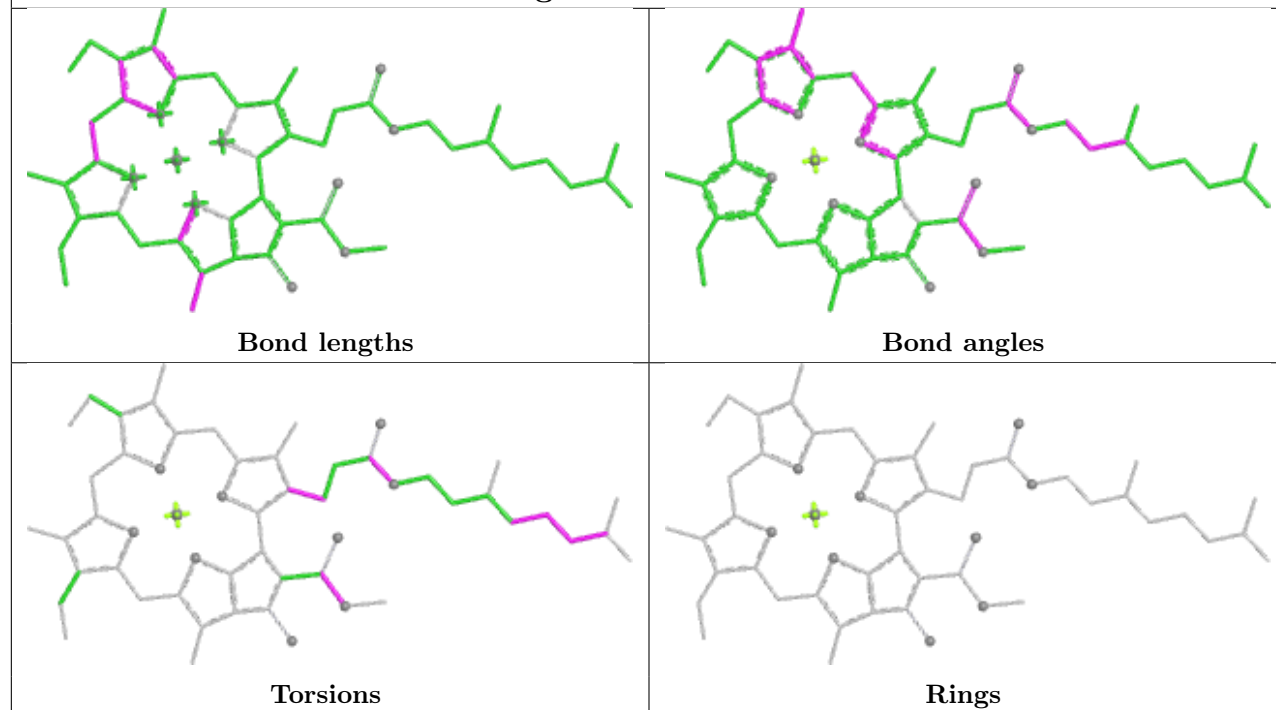
Ligand CLA a 835



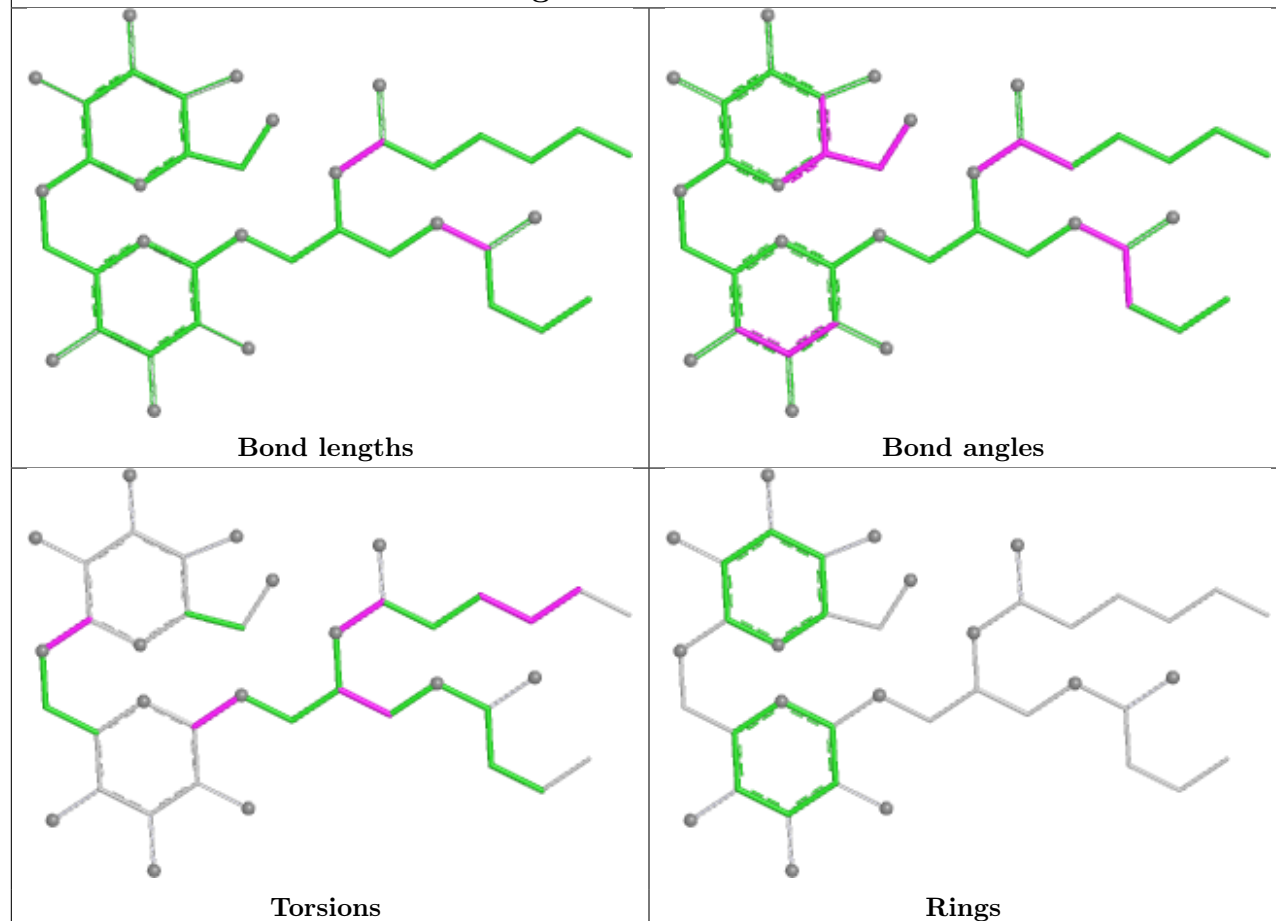
Ligand XAT 2 303



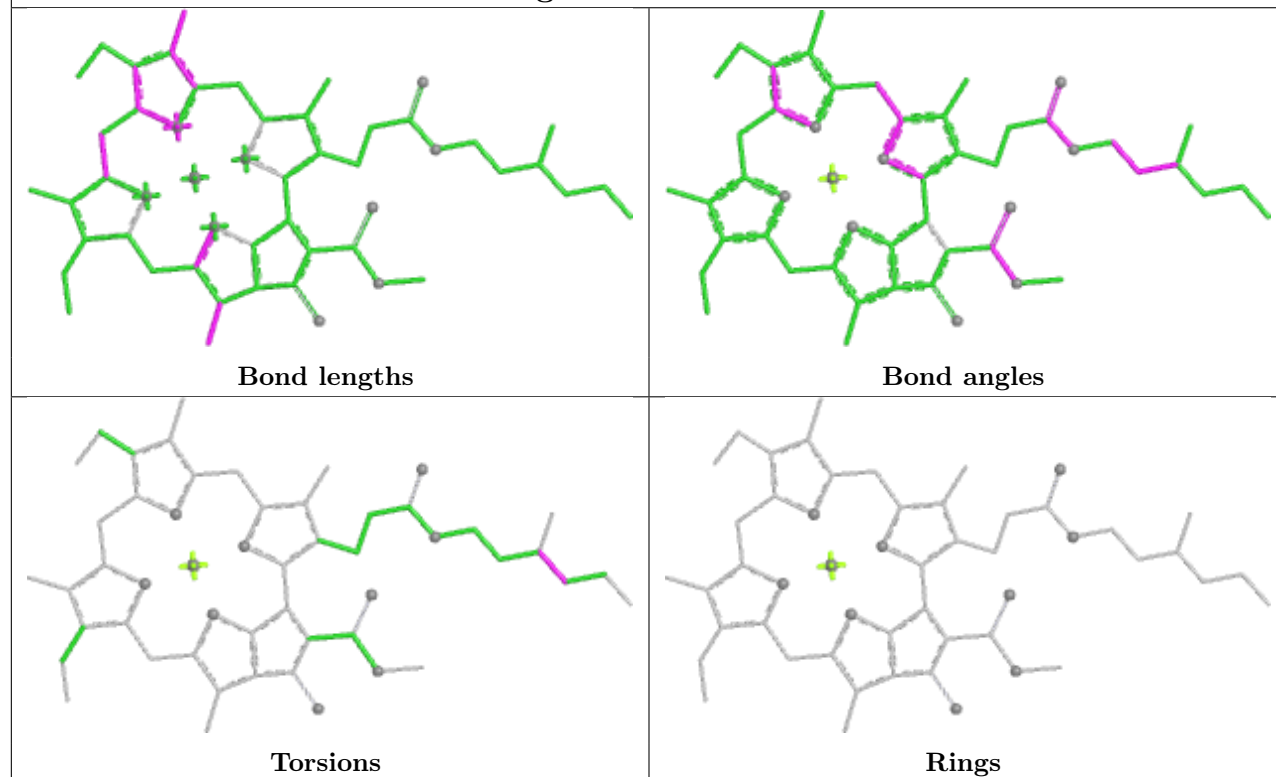
Ligand CLA b 814



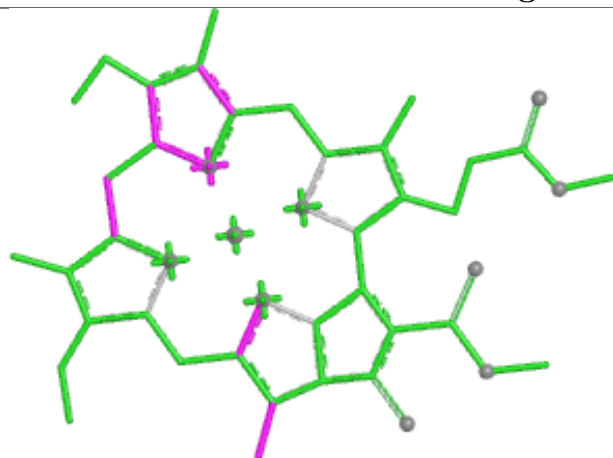
Ligand DGD 4 318



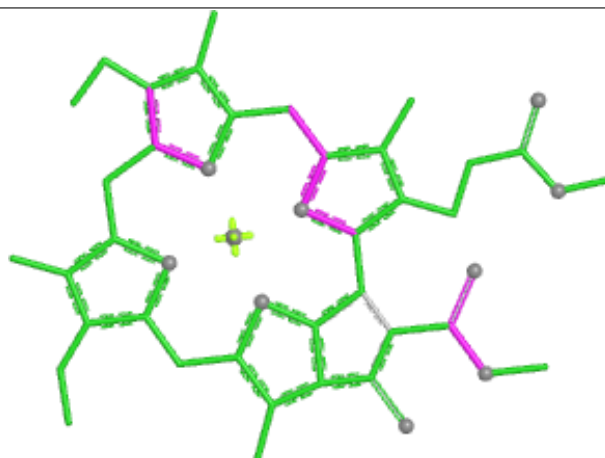
Ligand CLA 3 313



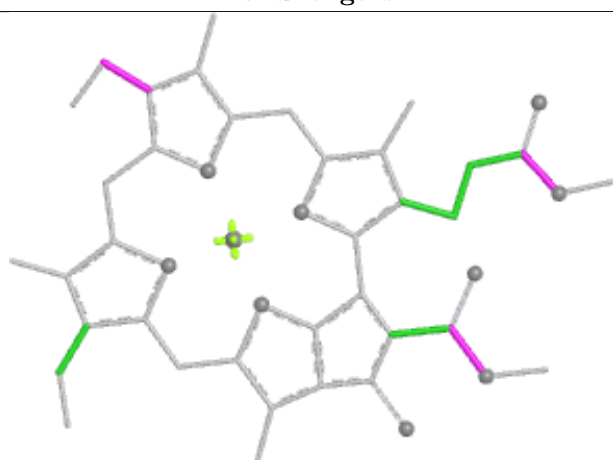
Ligand CLA 5 305



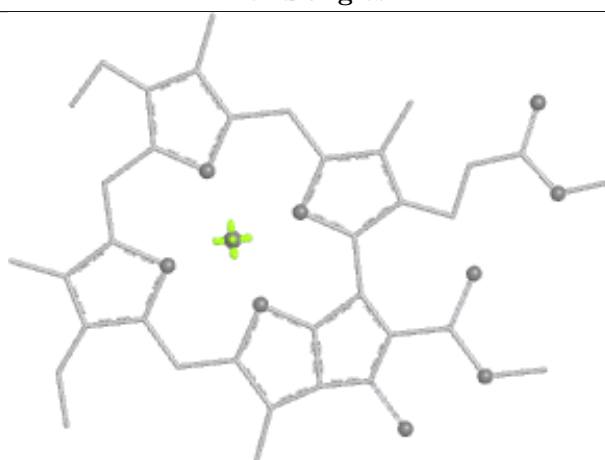
Bond lengths



Bond angles

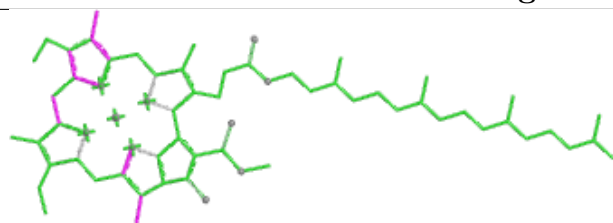


Torsions

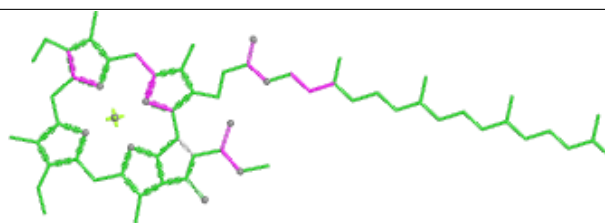


Rings

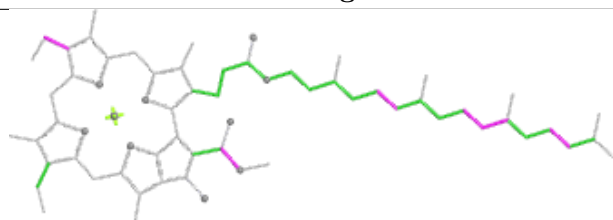
Ligand CLA a 834



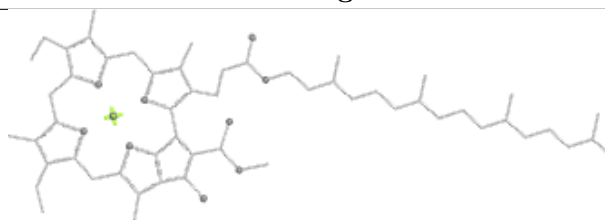
Bond lengths



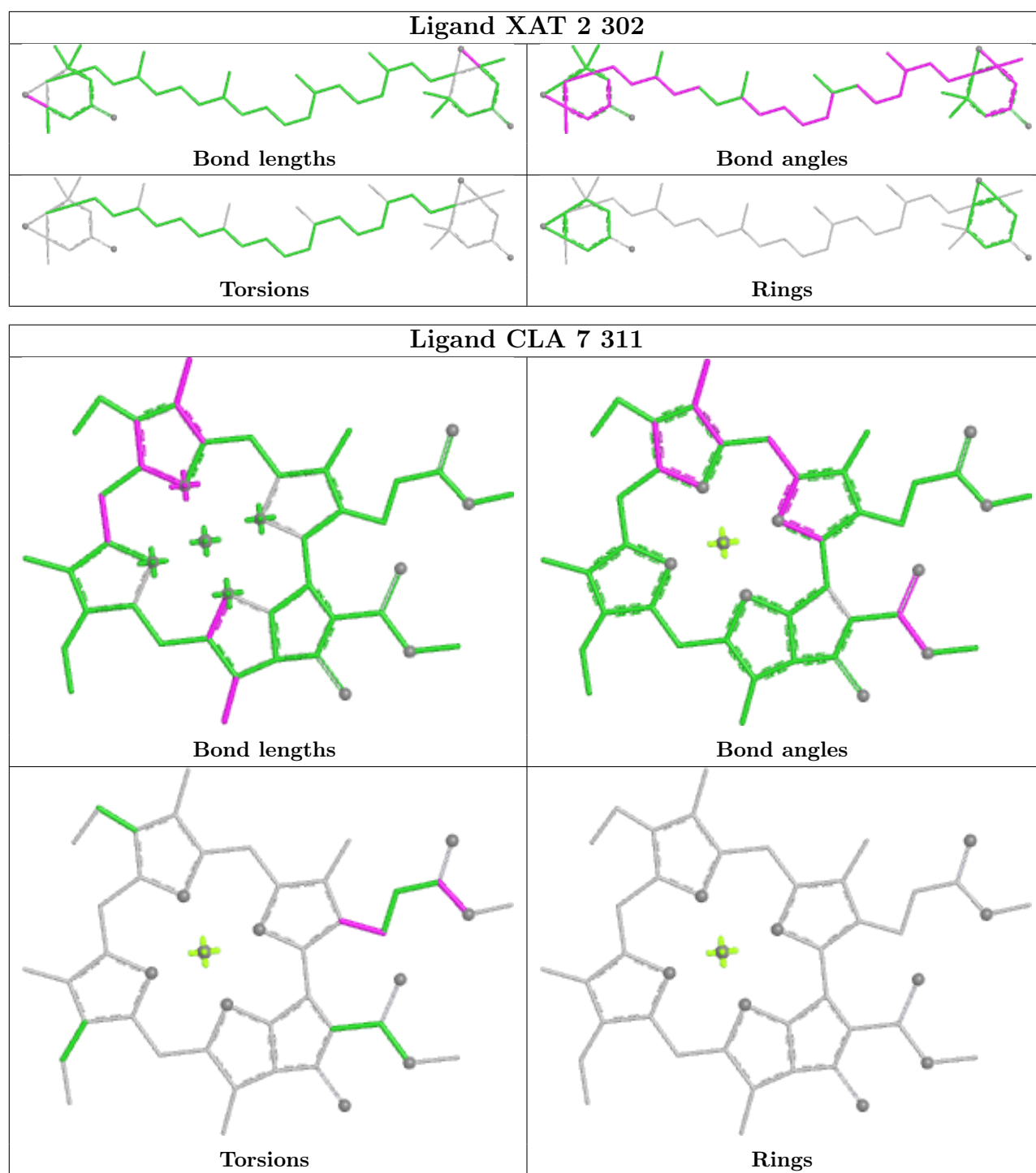
Bond angles



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.

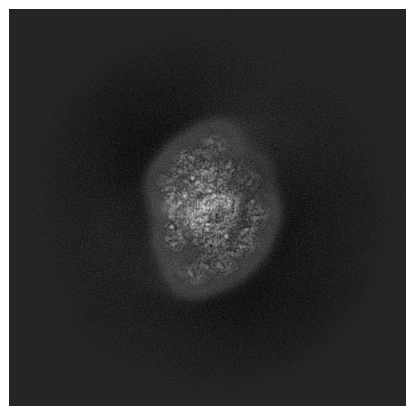
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60285. These allow visual inspection of the internal detail of the map and identification of artifacts.

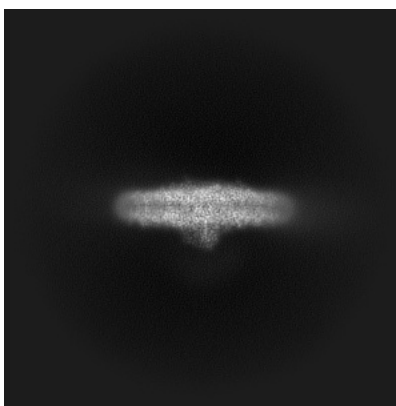
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

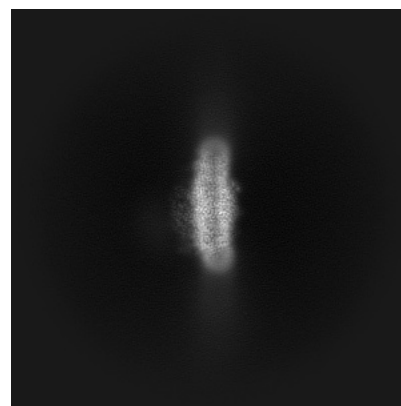
6.1.1 Primary map



X

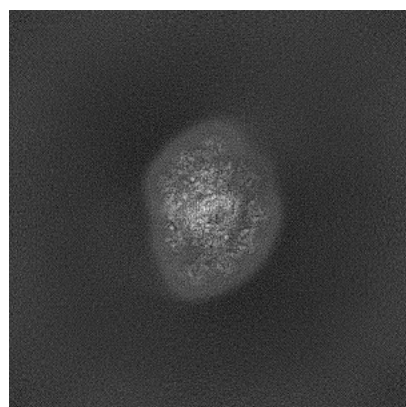


Y

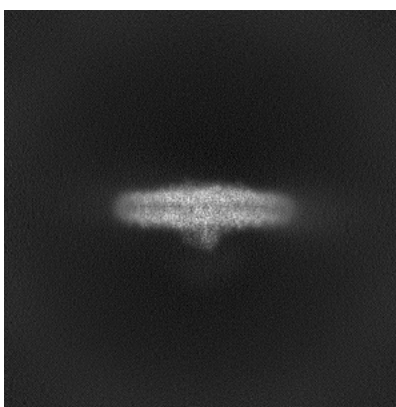


Z

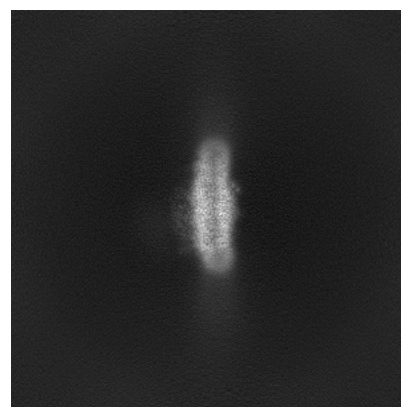
6.1.2 Raw map



X



Y

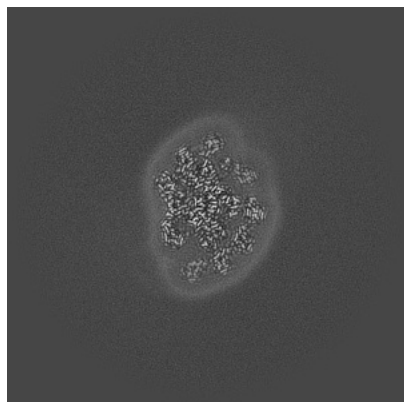


Z

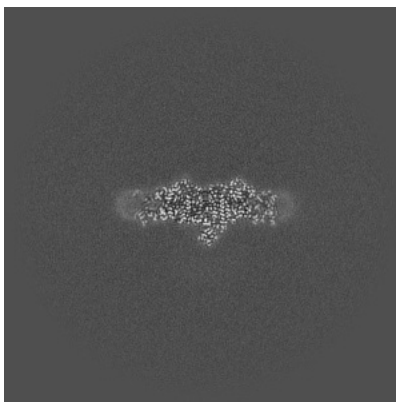
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

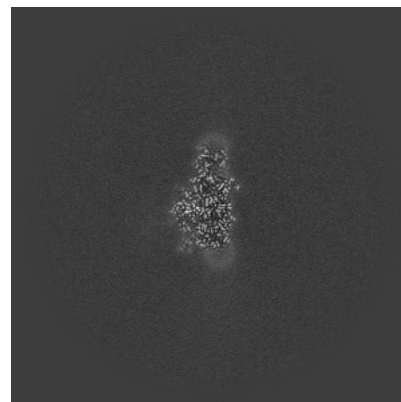
6.2.1 Primary map



X Index: 256

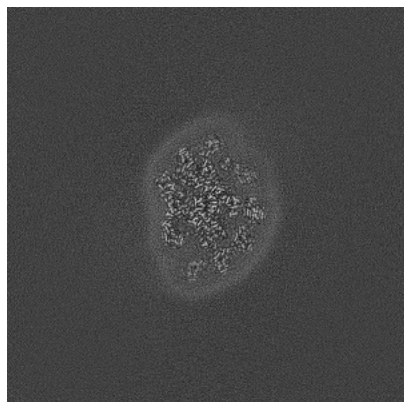


Y Index: 256

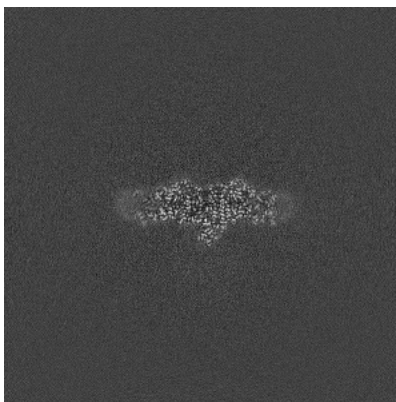


Z Index: 256

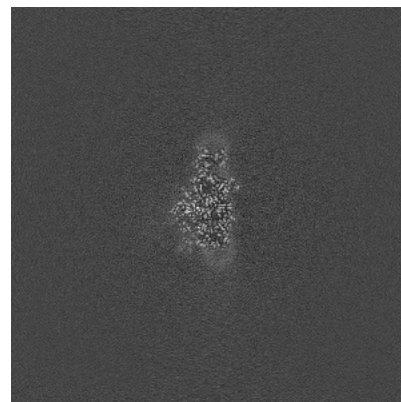
6.2.2 Raw map



X Index: 256



Y Index: 256

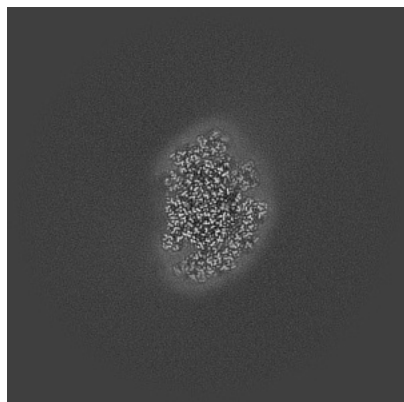


Z Index: 256

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

6.3 Largest variance slices [i](#)

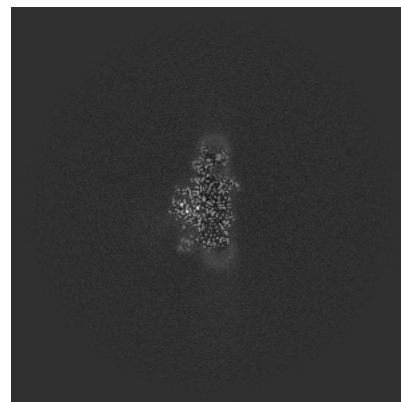
6.3.1 Primary map



X Index: 244

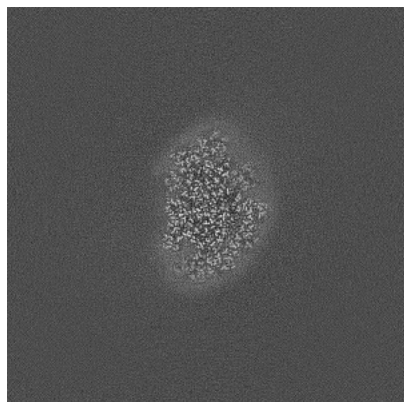


Y Index: 254



Z Index: 258

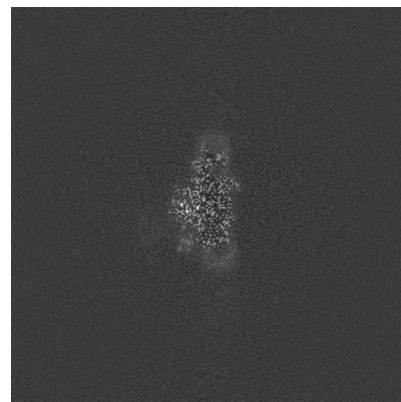
6.3.2 Raw map



X Index: 244



Y Index: 254

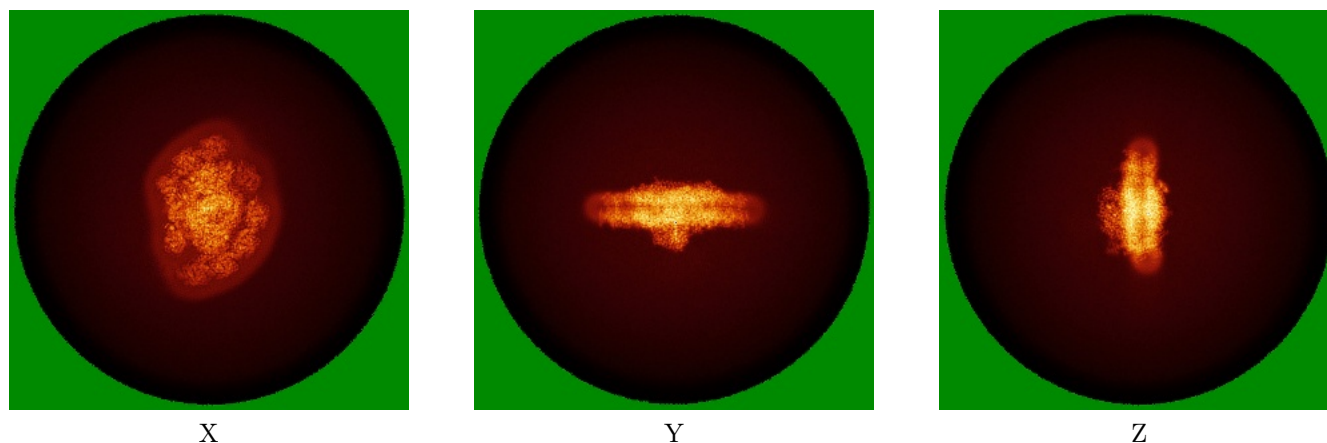


Z Index: 258

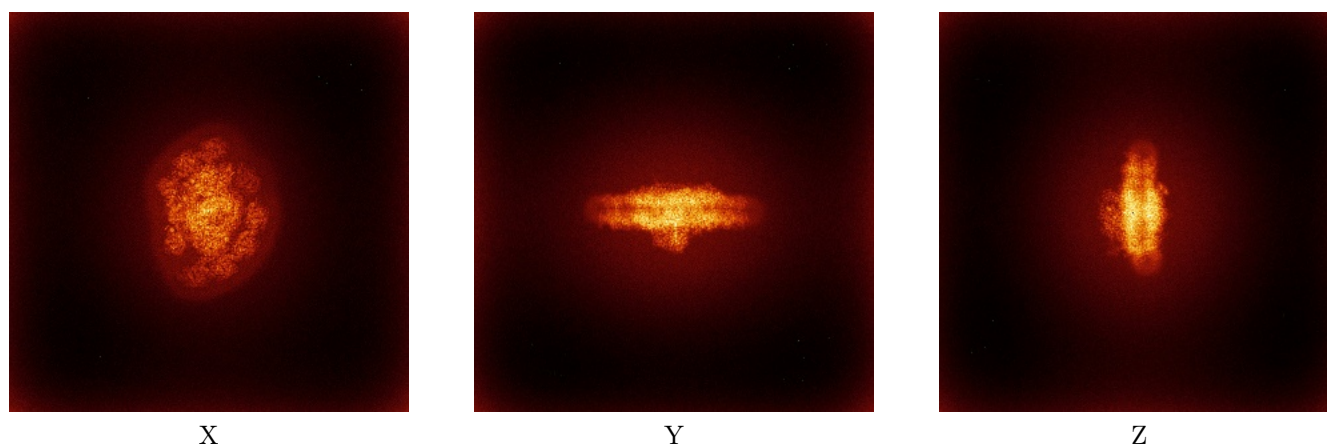
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

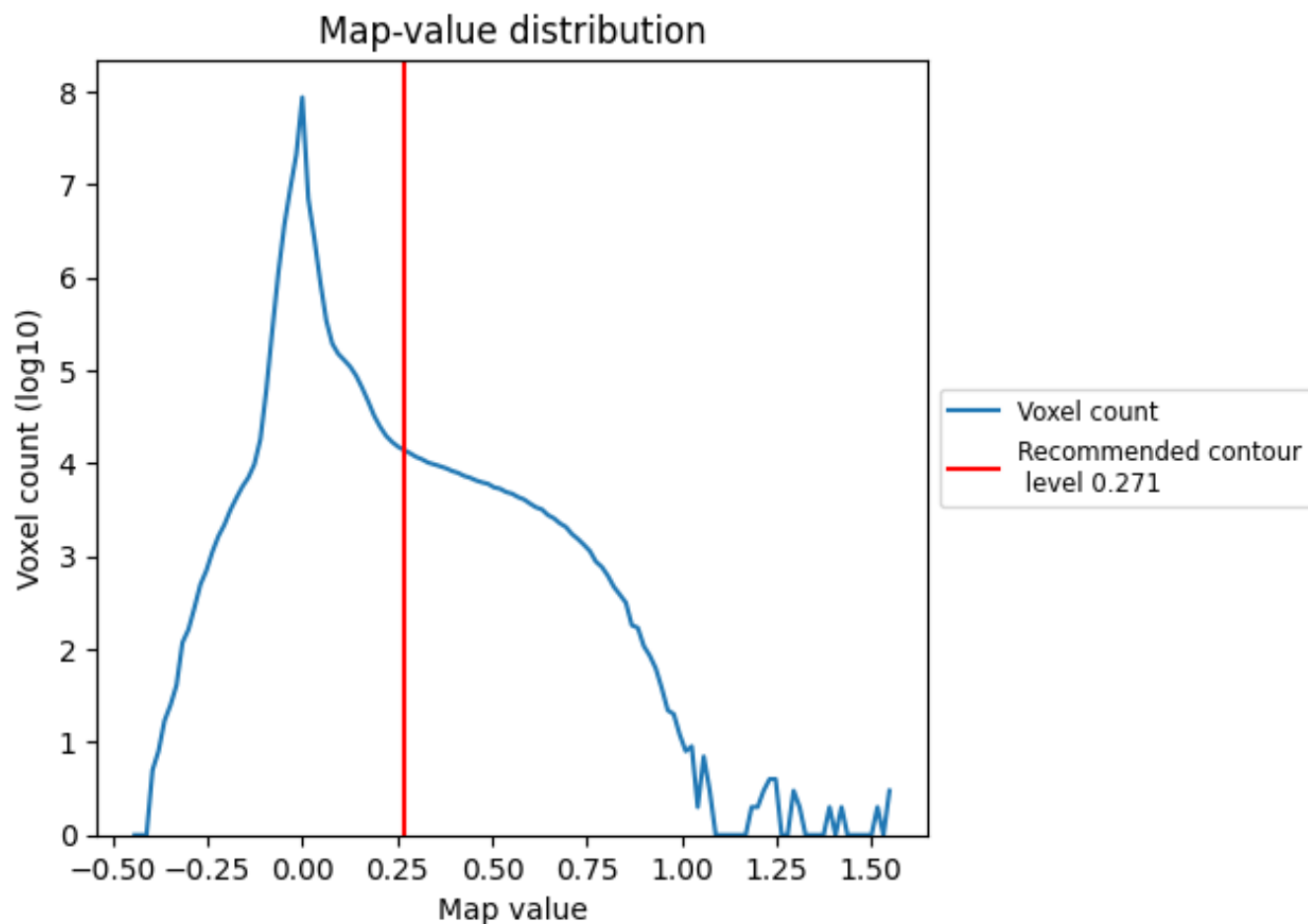
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

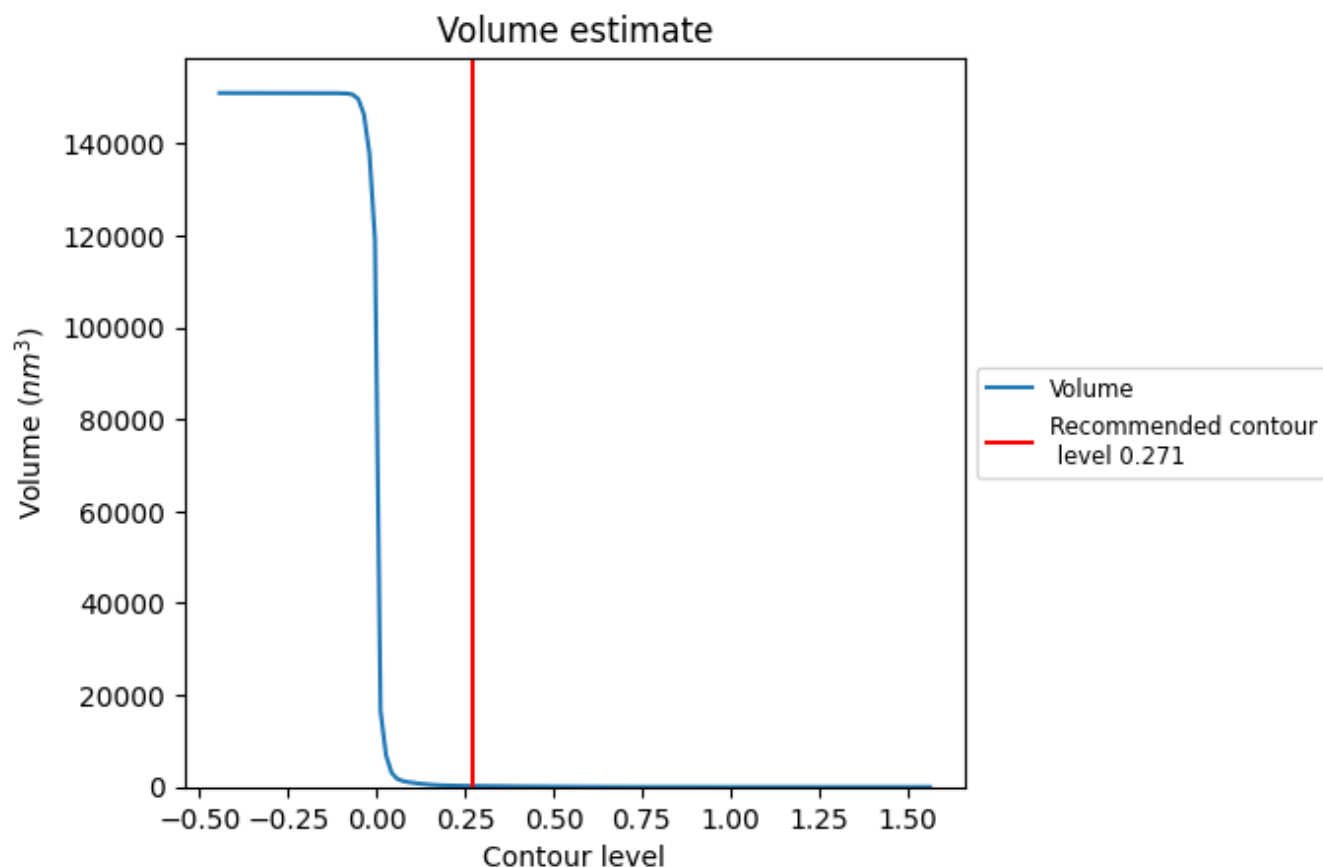
This section contains the results of statistical analysis of the map.

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.

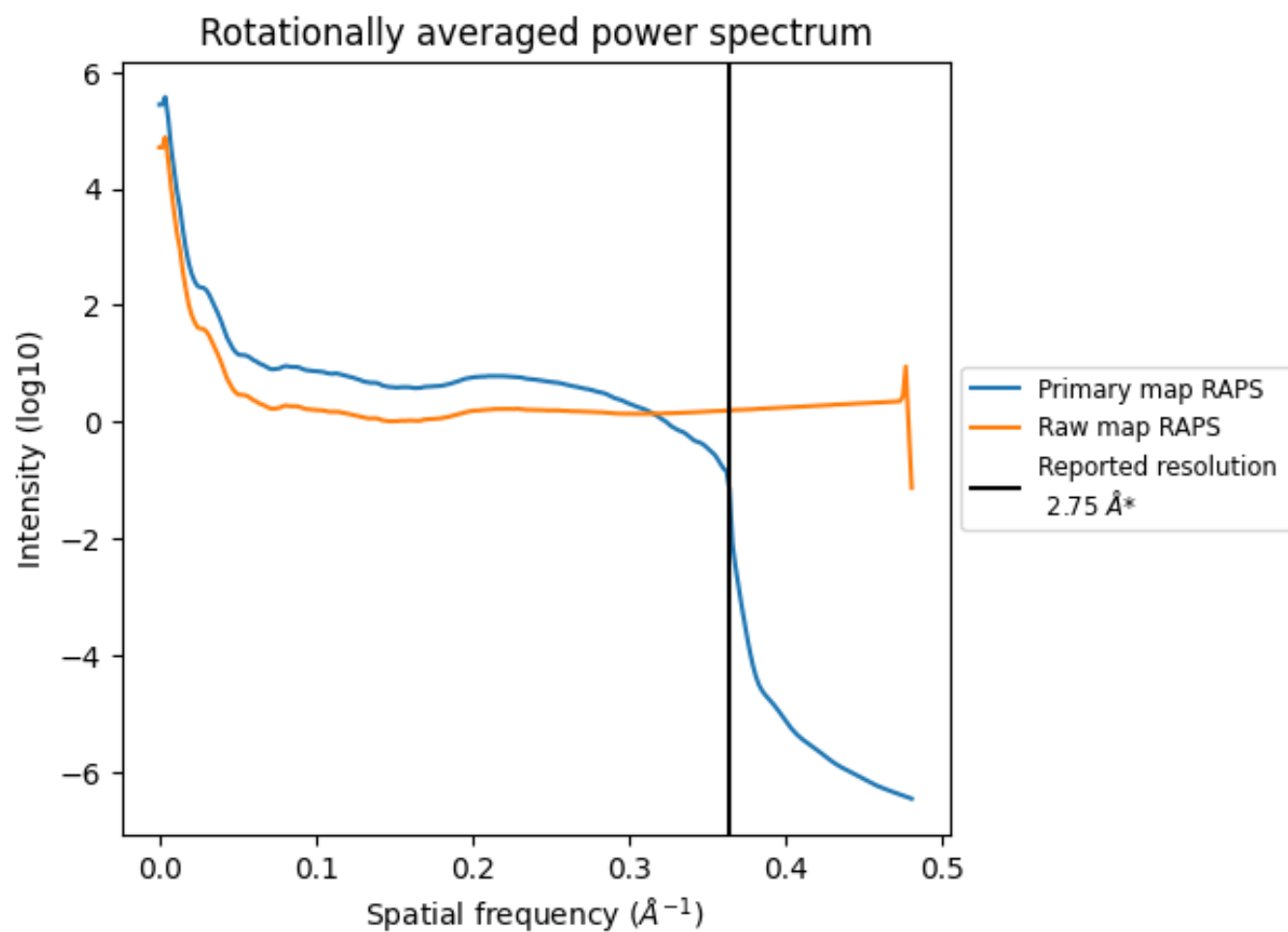
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217 nm³; this corresponds to an approximate mass of 196 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 ⓘ

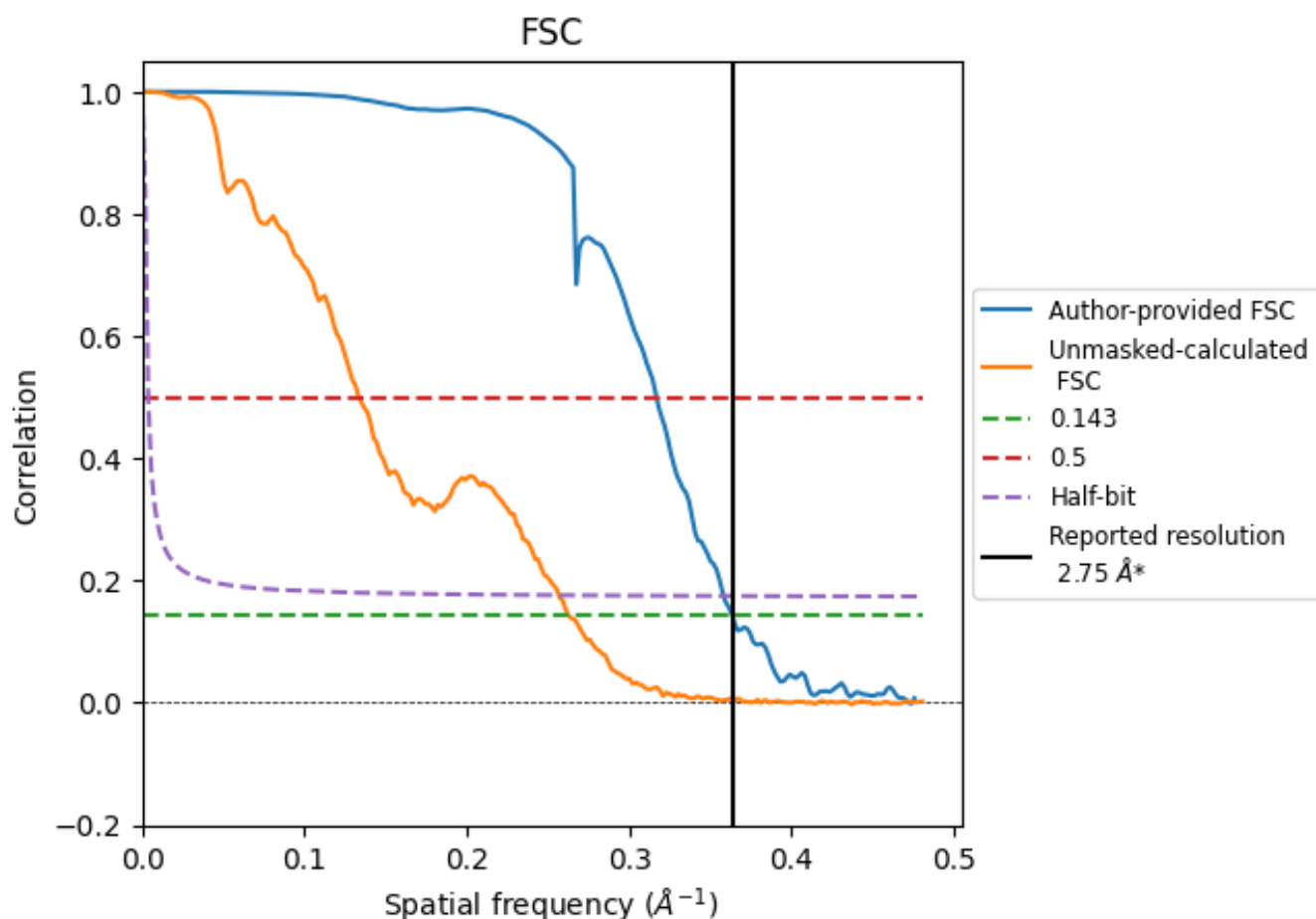


*Reported resolution corresponds to spatial frequency of 0.364 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.15	2.79
Unmasked-calculated*	3.81	7.49	3.89

*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 3.81 differs from the reported value 2.75 by more than 10 %

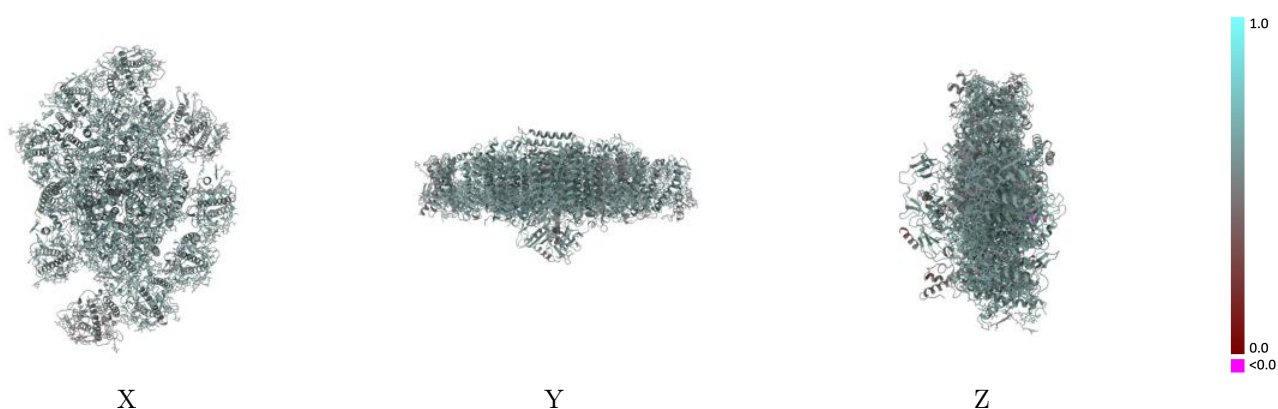
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60285 and PDB model 8ZO9. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)

This section was not generated.

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

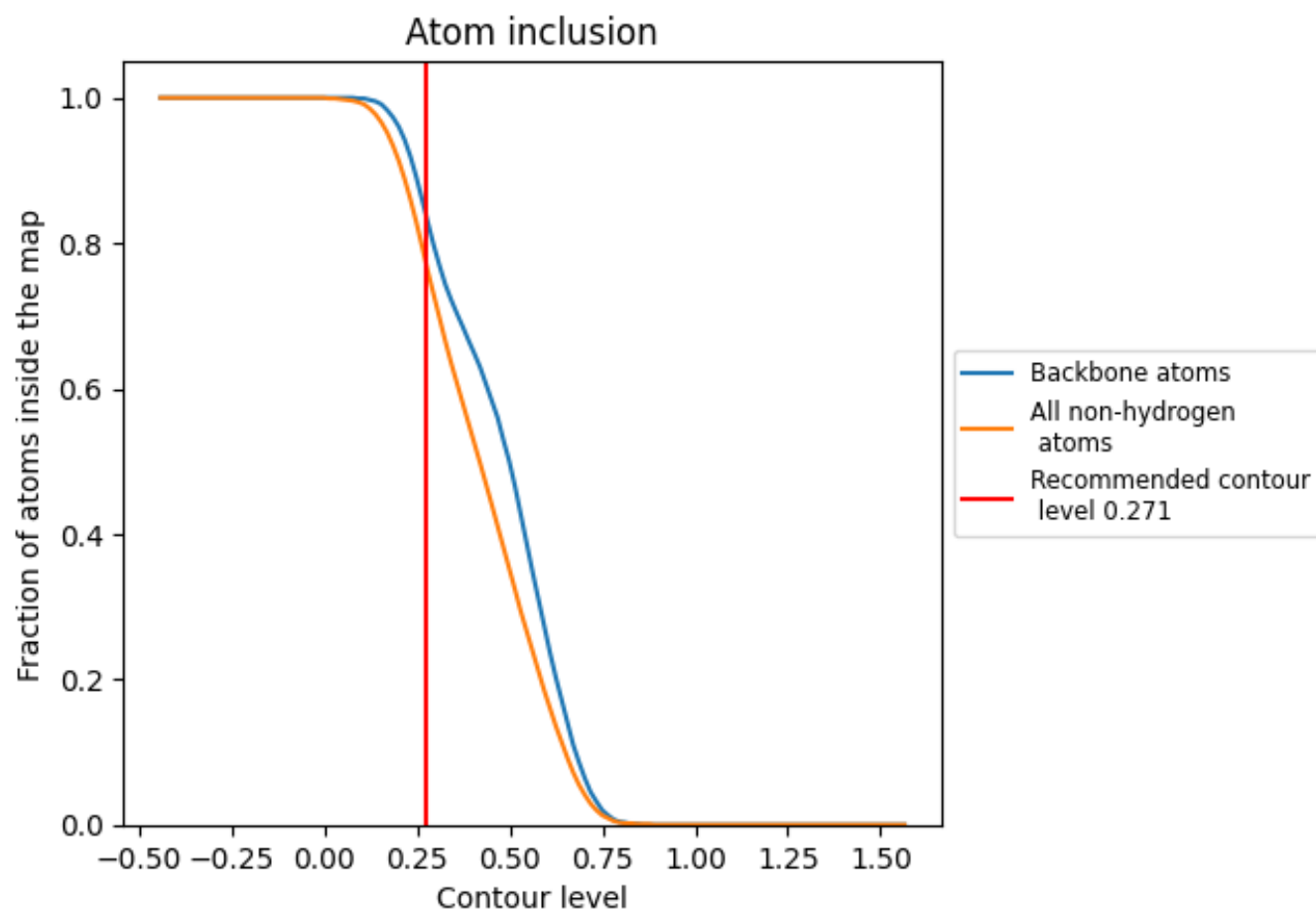


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.5770
1	 0.7560	 0.5730
2	 0.5750	 0.4970
3	 0.7540	 0.5700
4	 0.7690	 0.5720
5	 0.7580	 0.5640
6	 0.5310	 0.5320
7	 0.6370	 0.5430
8	 0.7790	 0.5750
9	 0.7560	 0.5710
a	 0.8550	 0.6030
b	 0.8580	 0.6030
c	 0.9110	 0.5870
d	 0.8270	 0.5880
e	 0.7670	 0.5820
f	 0.7830	 0.5720
g	 0.6150	 0.4920
h	 0.7180	 0.5680
i	 0.8390	 0.5860
j	 0.8190	 0.5860
l	 0.7720	 0.5630
m	 0.7770	 0.5600

