



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:10 AM JST

PDB ID : 6IJJ / pdb_00006ijj
EMDB ID : EMD-9678
Title : Photosystem I of Chlamydomonas reinhardtii
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.
Deposited on : 2018-10-10
Resolution : 2.89 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:

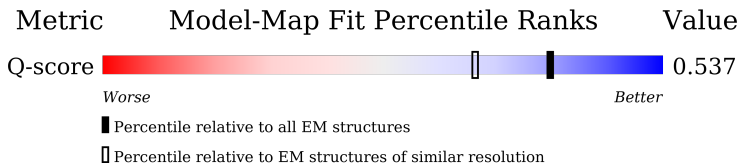
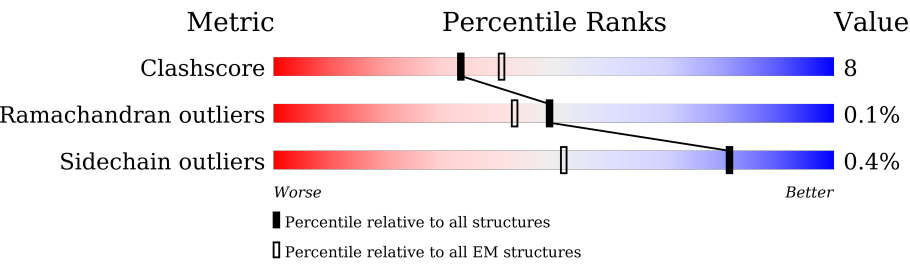
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.89 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	12148 (2.39 - 3.39)

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	A	751	 11% 82% 17% .
2	B	735	 11% 86% 13% .
3	C	81	 74% 25% .
4	D	196	 57% 15% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	143	
6	F	227	
7	I	106	
8	J	41	
9	K	160	
10	L	258	
11	1	248	
11	a	248	
12	3	298	
13	4	290	
14	5	274	
15	6	318	
16	7	241	
17	8	272	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 44968 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5812	3818	975	1001	18		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1129	722	200	200	7		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			505	322	89	94		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1254	811	209	231	3		

- Molecule 7 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 8 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	105	Total	C	N	O	S	0	0
			761	502	122	135	2		

- Molecule 11 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
11	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 12 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	221	Total	C	N	O	S	0	0
			1683	1099	271	305	8		

- Molecule 13 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 14 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	5	226	Total	C	N	O	S	0	0
			1765	1149	295	313	8		

- Molecule 15 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

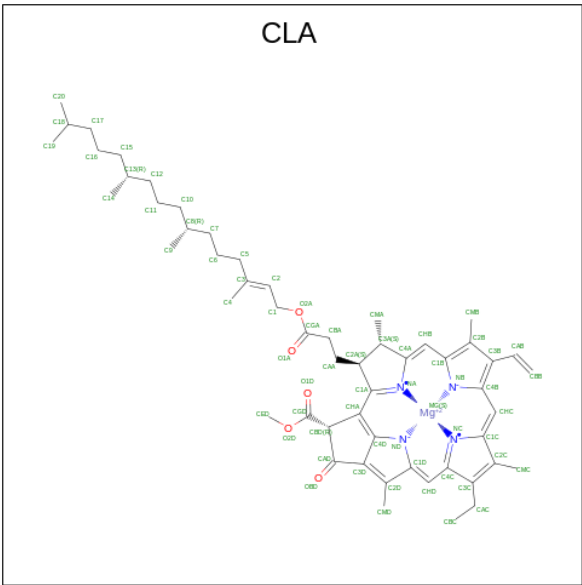
- Molecule 16 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 17 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	8	215	Total	C	N	O	S	0	0
			1630	1058	278	290	4		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	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
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
18	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	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
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

Continued on next page...

Continued from previous page...

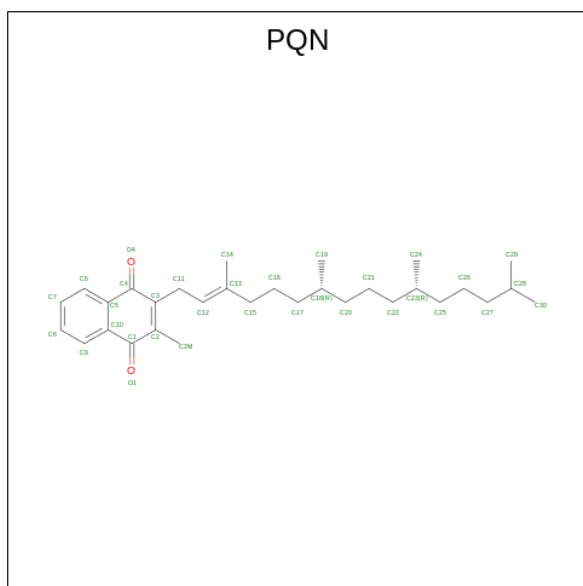
Mol	Chain	Residues	Atoms					AltConf
18	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
18	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

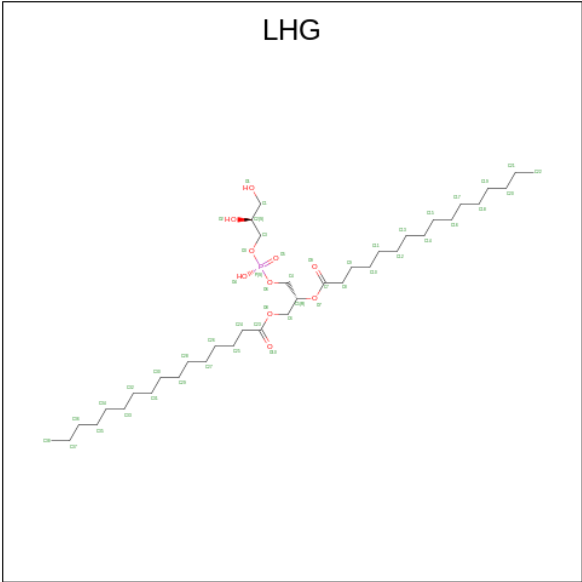
Mol	Chain	Residues	Atoms					AltConf
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



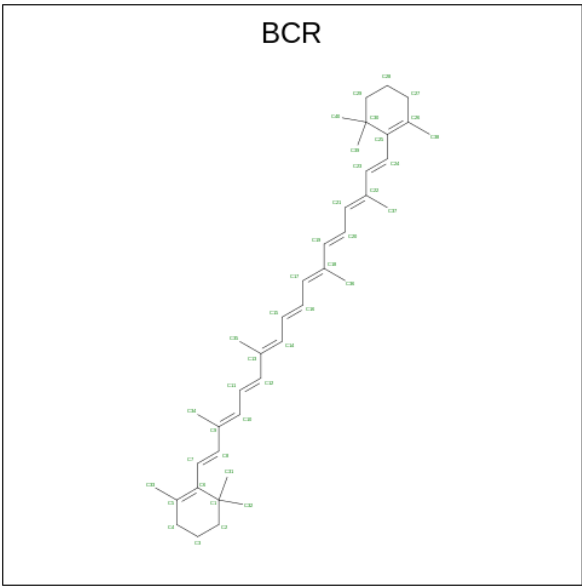
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	B	1	Total	C	O	P	0
			36	26	9	1	
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	a	1	Total	C	O	P	0
			49	38	10	1	
20	3	1	Total	C	O	P	0
			45	34	10	1	
20	3	1	Total	C	O	P	0
			49	38	10	1	
20	4	1	Total	C	O	P	0
			49	38	10	1	
20	5	1	Total	C	O	P	0
			49	38	10	1	
20	5	1	Total	C	O	P	0
			49	38	10	1	
20	6	1	Total	C	O	P	0
			48	37	10	1	
20	7	1	Total	C	O	P	0
			37	26	10	1	
20	8	1	Total	C	O	P	0
			49	38	10	1	
20	8	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



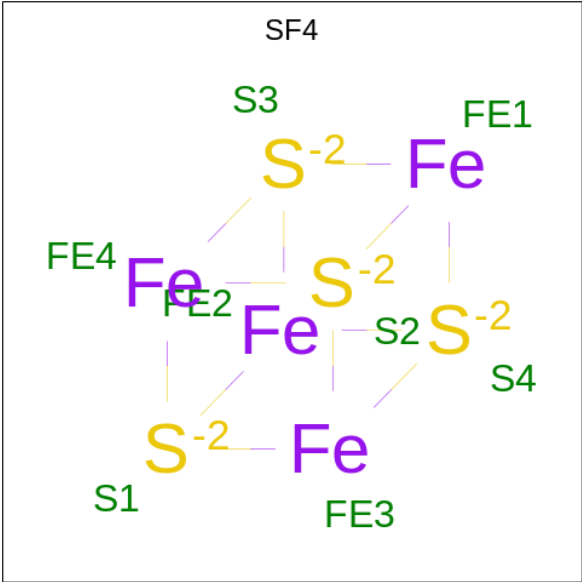
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

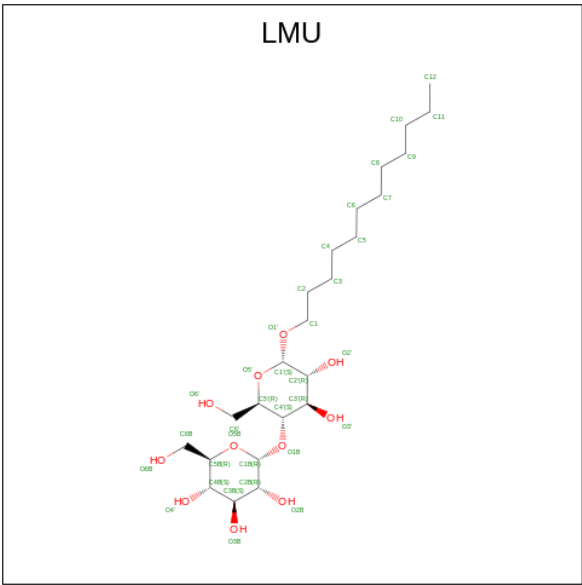
Mol	Chain	Residues	Atoms	AltConf
21	F	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	1	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0
21	5	1	Total C 40 40	0
21	6	1	Total C 40 40	0
21	7	1	Total C 40 40	0
21	7	1	Total C 40 40	0
21	8	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



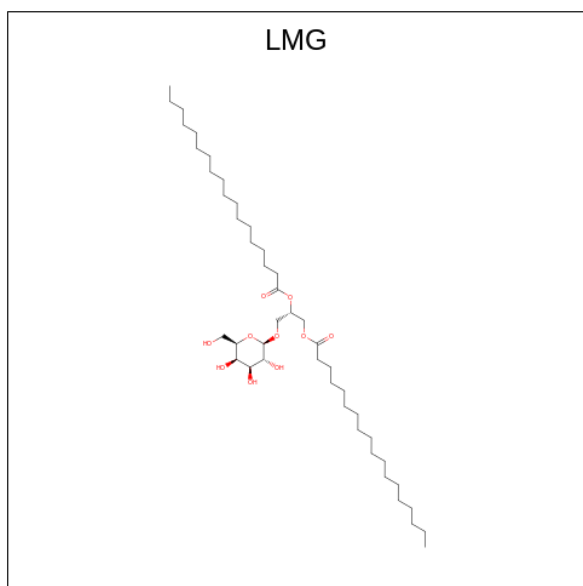
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	23	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			34	24	10	
23	A	1	Total	C	O	0
			34	24	10	
23	K	1	Total	C	O	0
			35	24	11	
23	5	1	Total	C	O	0
			33	22	11	
23	8	1	Total	C	O	0
			35	24	11	
23	8	1	Total	C	O	0
			35	24	11	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



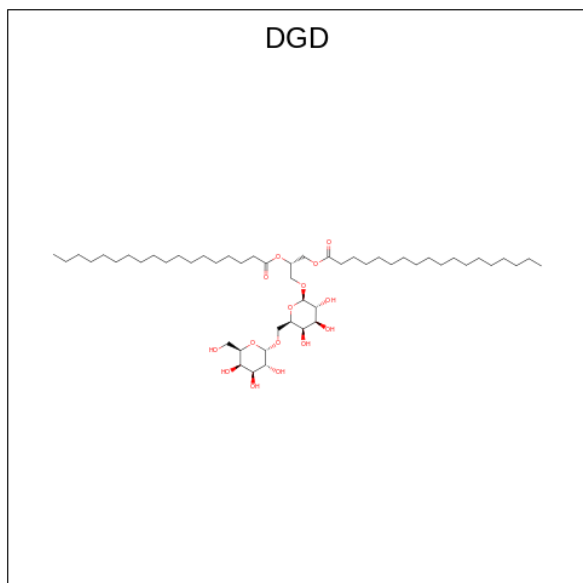
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			40	30	10	
24	J	1	Total	C	O	0
			40	30	10	
24	4	1	Total	C	O	0
			40	30	10	
24	4	1	Total	C	O	0
			40	30	10	
24	5	1	Total	C	O	0
			40	30	10	

Continued on next page...

Continued from previous page...

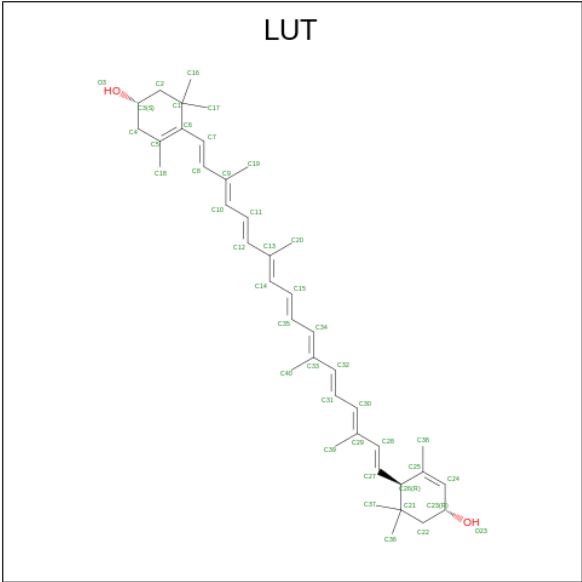
Mol	Chain	Residues	Atoms			AltConf
24	5	1	Total	C	O	0
			40	30	10	
24	7	1	Total	C	O	0
			44	34	10	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



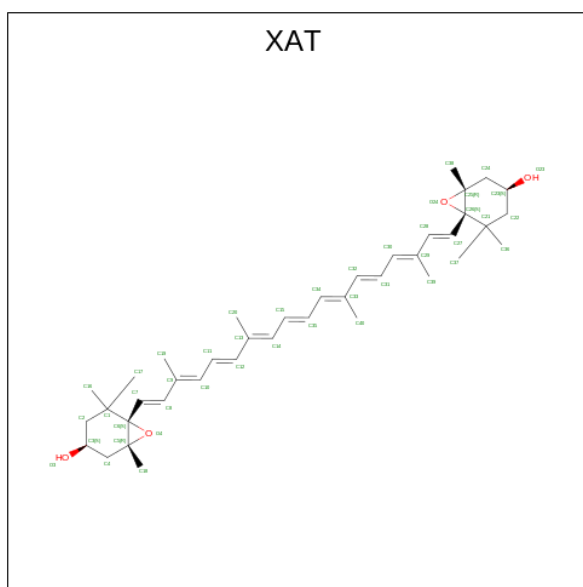
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			62	47	15	
25	J	1	Total	C	O	0
			58	43	15	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



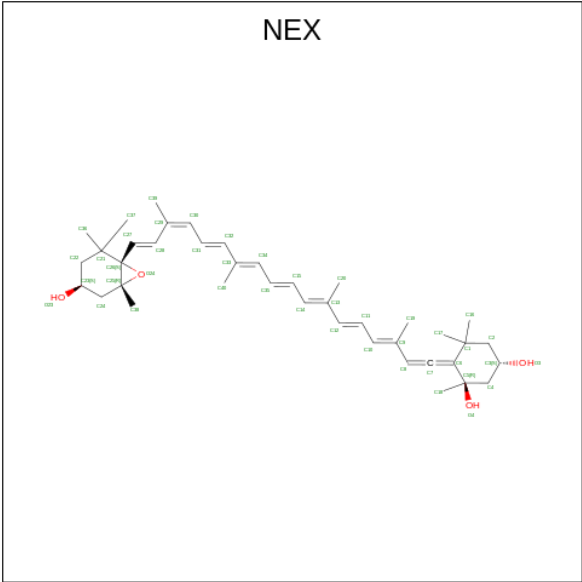
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	a	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	8	1	Total	C	O	0
			42	40	2	

- Molecule 27 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).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	a	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).

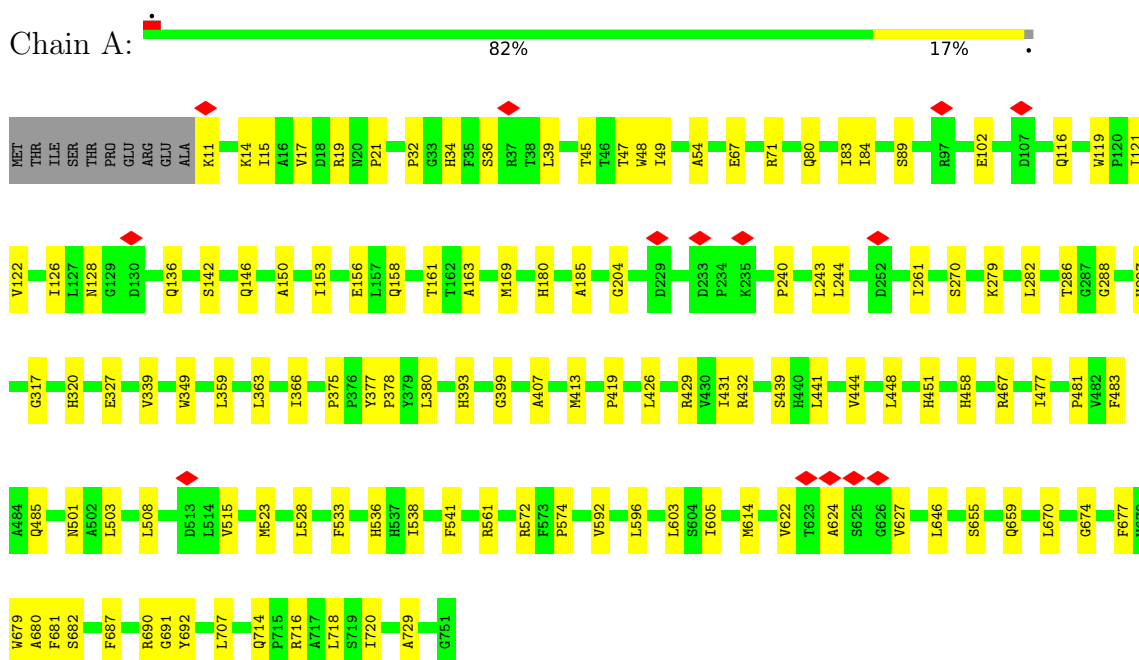


Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	

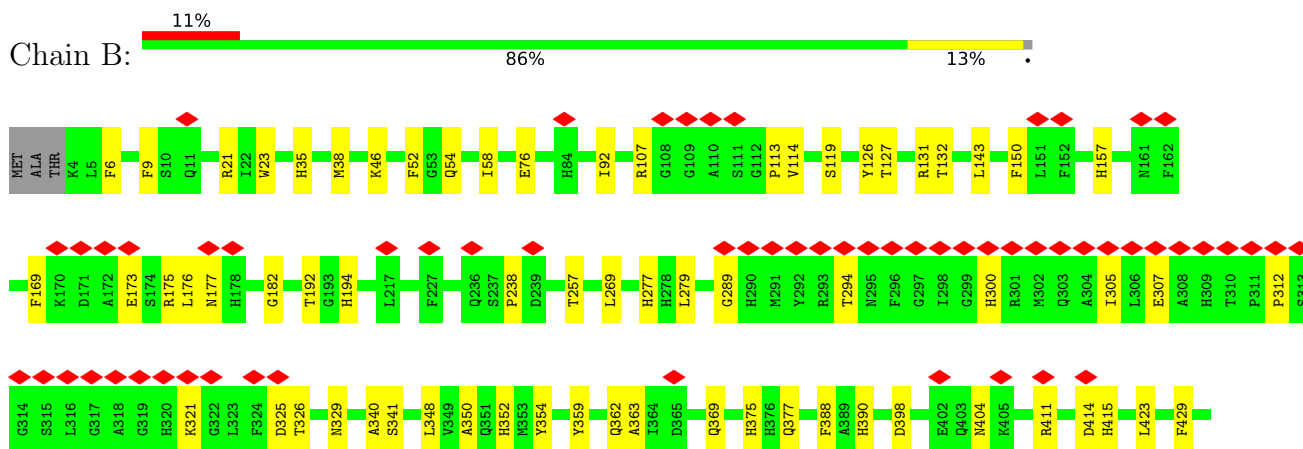
3 Residue-property plots [i](#)

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: PsaA



• Molecule 2: PsaB

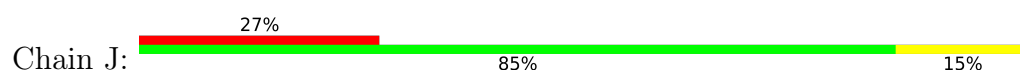




MET ALA LEU ALA ARG ALA GLY VAL SER ALA LYS SER ALA VAL ARG PRO THR VAL ALA ARG ALA SER VAL LYS PRO VAL VAL PRO THR VAL ALA ALA LEU LYS PRO ALA GLN LYS MET ALA LEU ALA GLY ALA SER VAL SER SER SER SER ALA GLU ALA SER GLN VAL ILE ALA THR VAL

ALA SER ALA ALA GLN TYR PRO PHE VAL PRO PRO S73 M74 A75 P76 F79 V80 P81 L82 T83 G84 L85 V86 L87 P88 A89 I90 A91 N92 A93 T94 L95 F96 V97 Y98 I99 E100 K101 E102 A103 P104 SER SER

• Molecule 8: PsaJ



M1 K2 T5 P12 F19 T20 E28 I29 N30 R31 D35 L37 V38 F39 S40 F41

• Molecule 9: PsaK

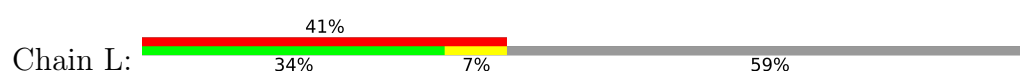


PRO ARG CYS ILE CYS LYS MET THR PRO ALA GLN ARG ARG ILE HIS CYS PRO PRO LEU ARG ALA PHE ALA SER SER CYS THR ASN LEU VAL HIS THR CYS PRO ARG LEU SER SER ILE THR ILE TYR GLN PRO ALA THR THR ARG PRO SER ALA ILE ARG PRO

THR LYS ALA ARG ARG SER VAL VAL ARG ASP GLY F76 I77 G78 S79 N82 L83 T84 R85 T92 L93 A94 A95 A96 A97 F98 G99 L100 T103 V104 K105 K106 N107 T108 T109 A110 G111 L112 K113 L114 V115 D116 S117 K118 N119 S120 A121 G122 V123 I124 S125 N126 D127

P128 A129 T132 I133 V134 D135 M139 G140 A141 A142 G143 H144 G145 L146 G149 V150 V151 L152 G156 I157 G158 A159 L160

• Molecule 10: PsaL



MET PRO THR LYS ALA GLY SER PRO LEU THR GLY VAL ILE THR TTP ARG LEU THR PHE ALA VAL SER ALA ALA HIS THR ARG THR VAL ASP THR ARG PRO ARG VAL THR ARG PRO ARG VAL GLY ILE TRP ARG ASP THR ALA LYS VAL ALA ARG VAL ARG ARG VAL THR ARG VAL GLY THR ASP THR LYS GLN ARG ILE PRO VAL GLU VAL GLU ARG ASN GLY ILE ALA THR PHE VAL GLY SER LEU ALA HIS THR TYR

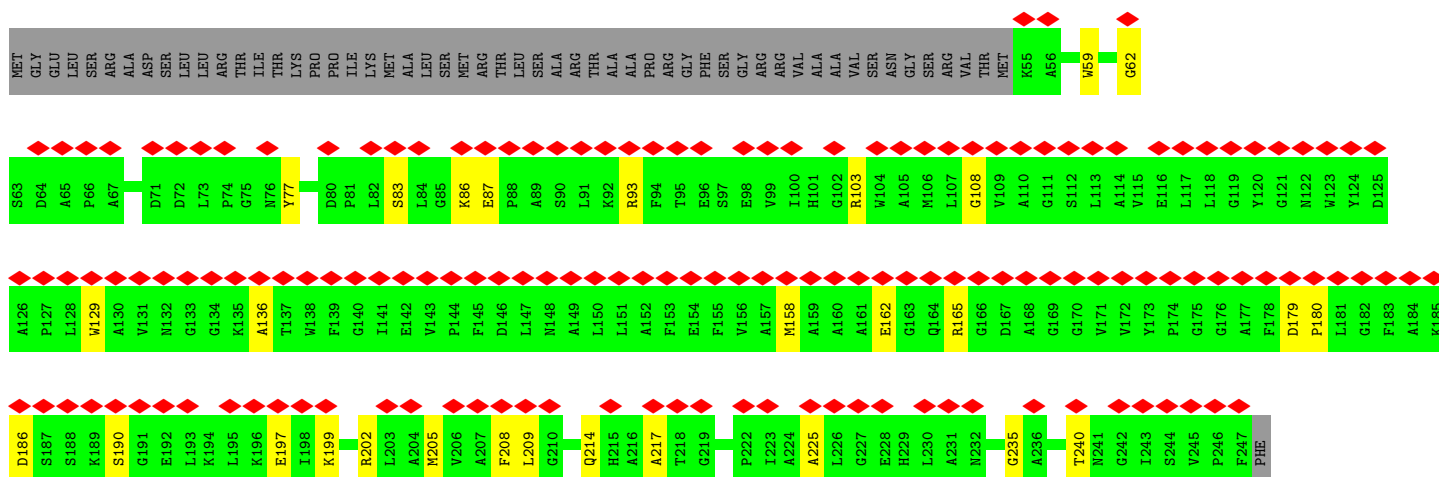
HIS LYS MET MET VAL ALA MET ARG SER THR THR GLY THR ARG THR ALA ALA ARG ARG GLN MET PRO LEU GLY LEU ARG THR THR ALA ARG ARG THR VAL THR VAL VAL VAL CYS ILE ALA ASP THR LYS VAL GLN VAL ILE SER PRO VAL VAL ASN GLY ASP PRO PHE VAL VAL GLY MET LEU GLU THR

VAL THR SER PRO ILE V127 A128 T129 Y130 L131 S132 M133 L134 P135 A136 Y137 R138 T139 G140 V141 P143 V144 L145 R146 G147 V148 E149 I150 G151 A152 A153 H154 G155 F156 L157 L158 A159 G160 P161 F162 I163 K164 L165 G166 P167 L168 R169 M170 V171 P172 E173 T174 A175 E176 I177 G179 S180

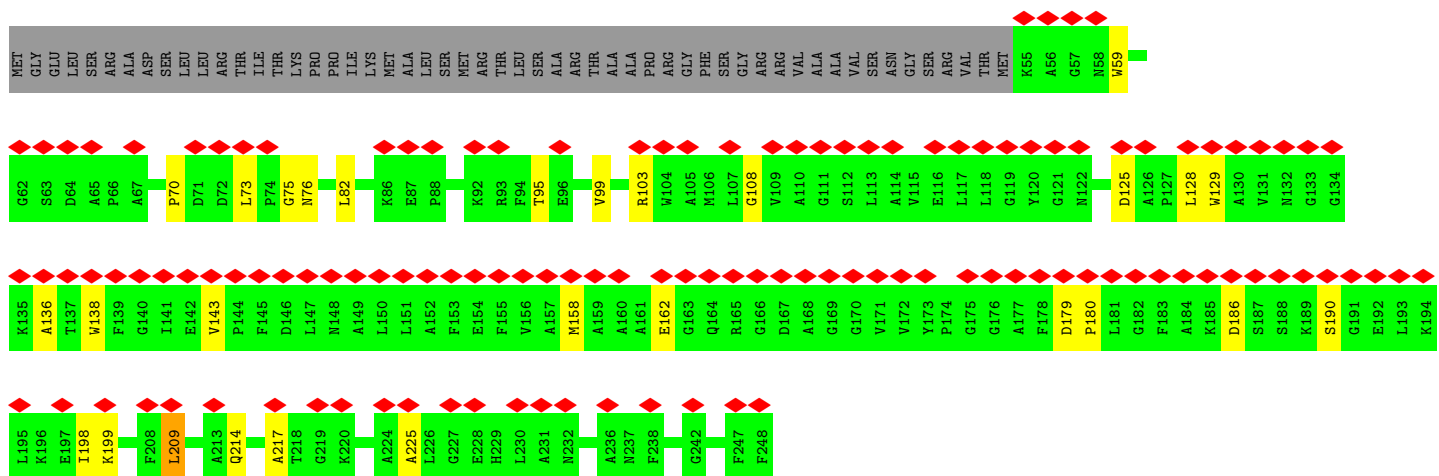
L181 S182 A183 A184 A185 L186 V187 L188 L189 L190 A191 L192 C193 L194 S195 I196 Y197 G198 S199 A200 Q201 F202 G197 G198 S199 A200 Q201 F202 G197 G198 S199 A200 Q201 F202

E241 A242 G243 V244 A245 A246 A247 Y248 C250 T251 G197 G198 S199 A200 Q201 F202 G197 G198 S199 A200 Q201 F202

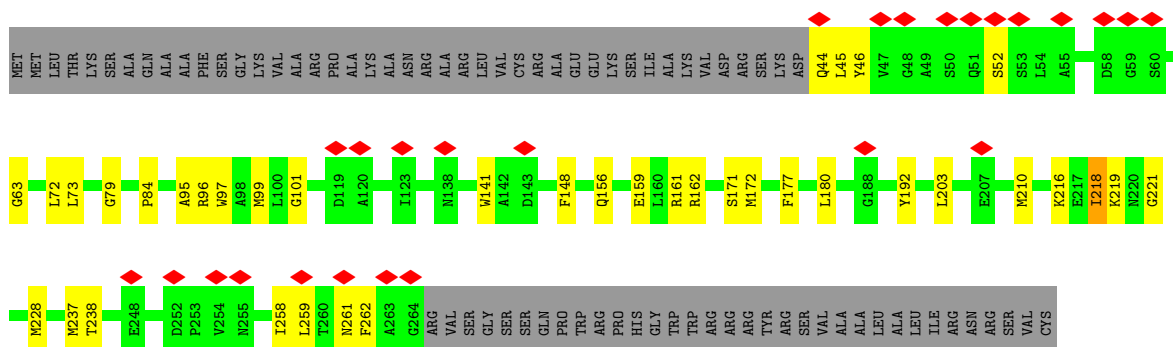
• Molecule 11: Lhca1



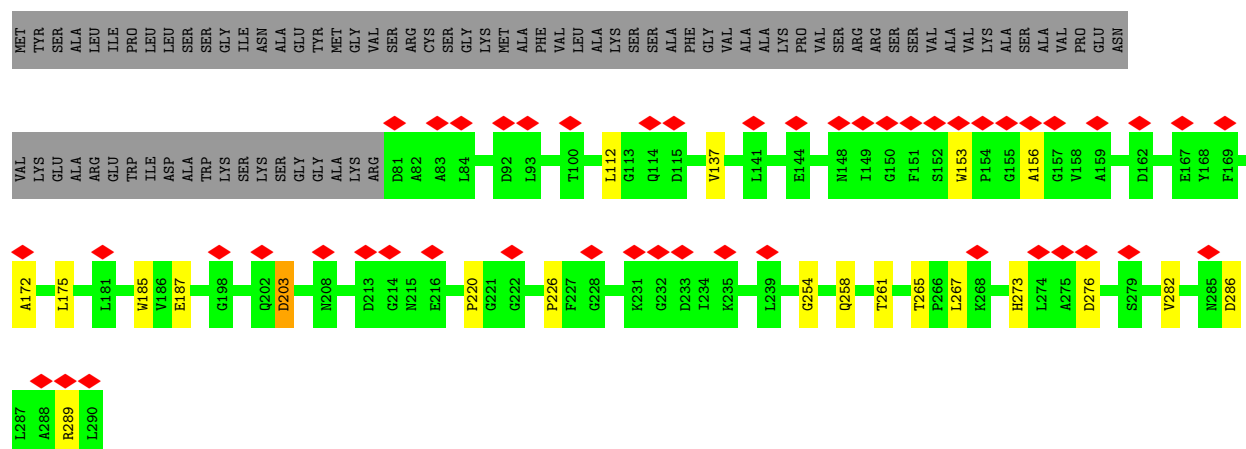
• Molecule 11: Lhca1



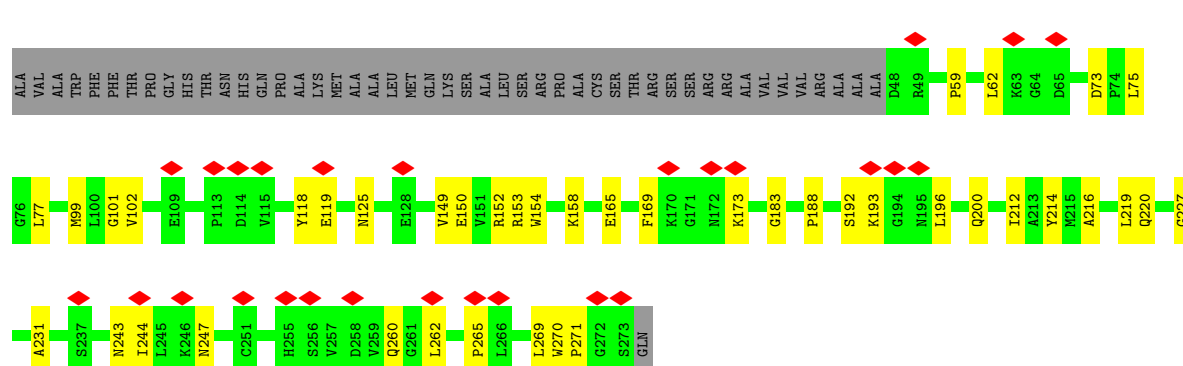
• Molecule 12: Lhca3



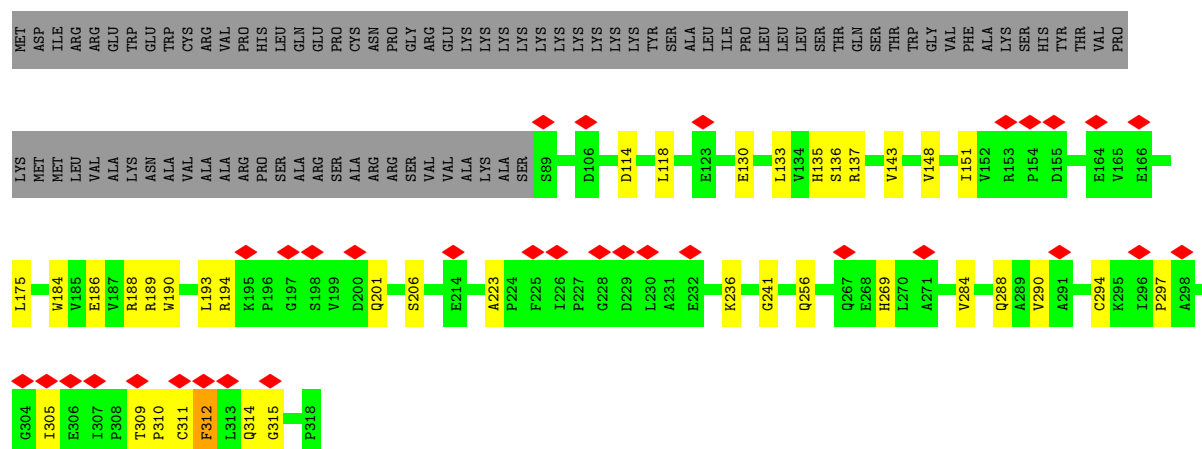
• Molecule 13: Lhca4



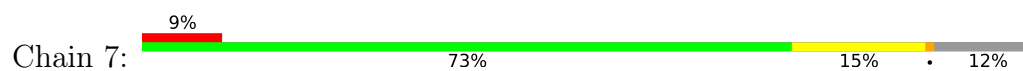
• Molecule 14: Lhca5

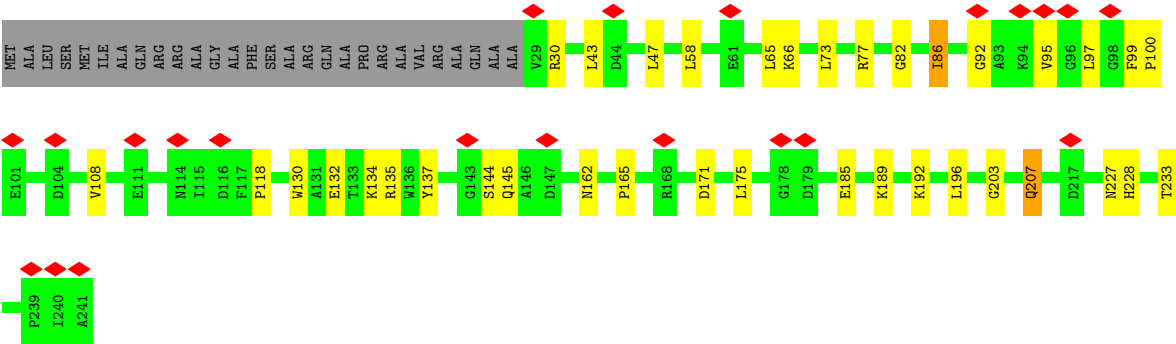


• Molecule 15: Lhca6

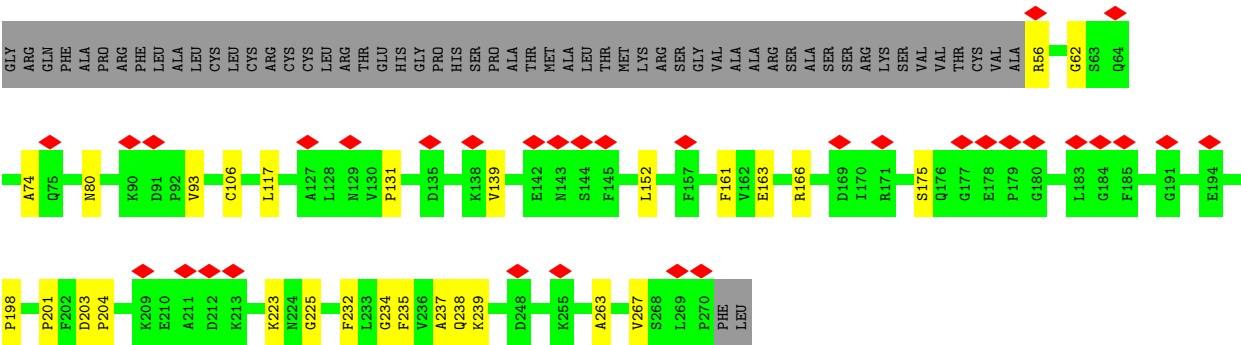


• Molecule 16: Lhca7





• Molecule 17: Lhca8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58955	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.37	0/6015	0.54	0/8201
2	B	0.34	0/6024	0.56	4/8225 (0.0%)
3	C	0.34	0/610	0.68	2/826 (0.2%)
4	D	0.32	0/1157	0.60	0/1563
5	E	0.25	0/515	0.51	0/700
6	F	0.27	0/1280	0.54	0/1733
7	I	0.27	0/250	0.53	0/345
8	J	0.27	0/349	0.54	0/478
9	K	0.24	0/583	0.57	0/790
10	L	0.22	0/779	0.50	0/1063
11	1	0.21	0/1478	0.50	0/2012
11	a	0.22	0/1490	0.51	0/2028
12	3	0.33	0/1731	0.64	0/2349
13	4	0.24	0/1686	0.49	0/2300
14	5	0.29	0/1820	0.57	0/2480
15	6	0.27	0/1833	0.54	0/2505
16	7	0.31	0/1701	0.59	0/2310
17	8	0.30	0/1680	0.59	0/2288
All	All	0.31	0/30981	0.56	6/42196 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	62	PHE	CA-C-N	5.50	132.05	121.54
3	C	62	PHE	C-N-CA	5.50	132.05	121.54
2	B	6	PHE	CA-C-N	-5.05	113.53	119.84
2	B	6	PHE	C-N-CA	-5.05	113.53	119.84
2	B	475	PHE	CA-C-N	5.03	131.14	121.54
2	B	475	PHE	C-N-CA	5.03	131.14	121.54

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	A	5819	0	5672	95	0
2	B	5812	0	5569	77	0
3	C	600	0	589	12	0
4	D	1129	0	1144	33	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	I	242	0	252	9	0
8	J	337	0	336	6	0
9	K	578	0	617	11	0
10	L	761	0	768	16	0
11	1	1433	0	1387	23	0
11	a	1444	0	1396	27	0
12	3	1683	0	1641	32	0
13	4	1631	0	1587	18	0
14	5	1765	0	1738	34	0
15	6	1771	0	1772	26	0
16	7	1649	0	1589	33	0
17	8	1630	0	1609	25	0
18	1	675	0	541	17	0
18	3	724	0	628	18	0
18	4	782	0	686	18	0
18	5	878	0	758	29	0
18	6	893	0	809	24	0
18	7	758	0	641	17	0
18	8	727	0	635	14	0
18	A	2625	0	2614	106	0
18	B	2277	0	2218	78	0
18	F	140	0	113	3	0
18	J	42	0	31	0	0
18	K	201	0	171	6	0
18	L	135	0	99	6	0
18	a	722	0	618	18	0
19	A	33	0	46	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	33	0	46	2	0
20	1	49	0	74	2	0
20	3	94	0	137	6	0
20	4	49	0	74	4	0
20	5	98	0	148	5	0
20	6	48	0	69	1	0
20	7	37	0	44	5	0
20	8	98	0	148	9	0
20	A	79	0	104	3	0
20	B	36	0	41	1	0
20	a	49	0	74	7	0
21	1	40	0	56	1	0
21	3	120	0	168	12	0
21	4	40	0	56	3	0
21	5	40	0	56	3	0
21	6	40	0	56	4	0
21	7	80	0	112	5	0
21	8	40	0	56	2	0
21	A	240	0	336	23	0
21	B	280	0	392	18	0
21	F	40	0	56	6	0
21	J	40	0	56	2	0
21	K	80	0	112	6	0
21	L	80	0	112	8	0
21	a	40	0	56	1	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	5	33	0	39	0	0
23	8	70	0	92	1	0
23	A	101	0	130	6	0
23	K	35	0	46	0	0
24	4	80	0	100	0	0
24	5	80	0	100	3	0
24	7	44	0	61	0	0
24	A	40	0	50	0	0
24	J	40	0	50	4	0
25	B	62	0	85	3	0
25	J	58	0	77	3	0
26	1	42	0	56	3	0
26	3	42	0	56	2	0
26	4	42	0	56	6	0
26	5	42	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	6	42	0	56	2	0
26	7	42	0	56	3	0
26	8	42	0	56	5	0
26	a	42	0	56	4	0
27	1	44	0	56	3	0
27	3	44	0	56	3	0
27	4	44	0	56	2	0
27	5	44	0	56	5	0
27	6	44	0	56	2	0
27	7	44	0	56	4	0
27	8	44	0	56	2	0
27	a	44	0	56	3	0
28	5	44	0	56	4	0
28	6	44	0	56	4	0
All	All	44968	0	44543	740	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 8.

All (740) 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:D:202:HIS:HB3	4:D:203:PRO:CD	1.63	1.28
4:D:202:HIS:CB	4:D:203:PRO:HD3	1.75	1.16
4:D:202:HIS:HB3	4:D:203:PRO:HD3	1.17	1.12
4:D:202:HIS:CG	4:D:203:PRO:HD3	1.95	1.01
12:3:46:TYR:OH	20:3:624:LHG:HC42	1.80	0.82
14:5:102:VAL:HG11	26:5:620:LUT:H12	1.62	0.82
4:D:104:TRP:CH2	4:D:204:ALA:O	2.34	0.81
11:a:199:LYS:HE2	20:a:620:LHG:O5	1.81	0.79
18:A:830:CLA:H2	21:A:849:BCR:HC7	1.67	0.76
4:D:202:HIS:HB3	4:D:203:PRO:HD2	1.62	0.76
18:3:609:CLA:HBB1	18:3:617:CLA:HBB1	1.66	0.76
18:8:611:CLA:HBC3	20:8:622:LHG:HC62	1.68	0.74
11:a:199:LYS:CE	20:a:620:LHG:O5	2.35	0.74
16:7:192:LYS:HD2	20:7:622:LHG:HC61	1.69	0.74
4:D:104:TRP:HH2	4:D:204:ALA:O	1.69	0.74
12:3:46:TYR:OH	20:3:624:LHG:C4	2.36	0.73
9:K:127:ASP:OD1	18:K:201:CLA:NA	2.23	0.71
15:6:135:HIS:HE1	18:6:603:CLA:NA	1.88	0.70
18:7:611:CLA:NB	20:7:622:LHG:O4	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:209:LEU:HD23	18:a:603:CLA:HBB2	1.74	0.70
11:a:199:LYS:NZ	20:a:620:LHG:O5	2.26	0.69
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.76	0.68
4:D:209:PRO:HA	4:D:216:ARG:HH22	1.59	0.68
11:1:77:TYR:OH	11:1:199:LYS:NZ	2.26	0.68
14:5:216:ALA:HB1	14:5:220:GLN:HE21	1.58	0.68
18:B:831:CLA:H2	21:F:305:BCR:H372	1.76	0.68
1:A:11:LYS:N	12:3:52:SER:HG	1.90	0.68
12:3:228:MET:HE2	27:3:619:XAT:H10	1.76	0.67
13:4:254:GLY:O	13:4:258:GLN:HB3	1.93	0.67
18:8:611:CLA:NB	20:8:622:LHG:O4	2.27	0.67
2:B:177:ASN:ND2	2:B:289:GLY:O	2.29	0.66
18:8:613:CLA:H102	20:8:622:LHG:H301	1.78	0.66
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.78	0.65
4:D:200:TYR:HE2	4:D:203:PRO:O	1.80	0.65
15:6:143:VAL:HG11	26:6:619:LUT:H12	1.77	0.65
1:A:17:VAL:HG11	18:A:811:CLA:HED3	1.78	0.64
1:A:153:ILE:O	1:A:158:GLN:NE2	2.30	0.64
1:A:707:LEU:O	6:F:168:ARG:NH1	2.31	0.64
3:C:2:ALA:N	3:C:71:SER:HG	1.96	0.64
4:D:200:TYR:CE2	4:D:203:PRO:O	2.50	0.64
14:5:220:GLN:OE1	18:5:613:CLA:NA	2.31	0.64
18:4:601:CLA:OBD	15:6:188:ARG:NH2	2.32	0.63
13:4:153:TRP:HB2	13:4:156:ALA:HB2	1.81	0.63
15:6:294:CYS:SG	15:6:314:GLN:NE2	2.71	0.63
18:B:825:CLA:HMA1	21:B:847:BCR:H14C	1.79	0.63
4:D:213:ASN:HB2	4:D:216:ARG:HH11	1.63	0.63
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.80	0.63
2:B:414:ASP:HA	6:F:226:PRO:HB3	1.82	0.62
2:B:398:ASP:OD1	4:D:236:LYS:NZ	2.29	0.62
12:3:219:LYS:NZ	20:3:624:LHG:O5	2.31	0.62
1:A:714:GLN:HE22	5:E:123:ASN:HA	1.65	0.62
18:A:811:CLA:HAB	18:A:814:CLA:H111	1.80	0.61
18:B:807:CLA:HHB	18:B:808:CLA:HHB	1.81	0.61
18:B:841:CLA:HBB2	18:1:602:CLA:H42	1.81	0.61
18:5:604:CLA:H2A	18:5:604:CLA:HED3	1.82	0.61
13:4:226:PRO:HD2	26:4:619:LUT:H23	1.81	0.61
1:A:441:LEU:HD22	18:A:840:CLA:HBB1	1.81	0.61
1:A:501:ASN:HB2	18:A:837:CLA:HED3	1.82	0.61
14:5:188:PRO:HD2	26:5:620:LUT:H23	1.83	0.61
1:A:467:ARG:NH2	18:A:835:CLA:O1D	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:ILE:HG12	4:D:156:ILE:HG22	1.83	0.61
18:B:808:CLA:H8	18:B:808:CLA:HBB1	1.83	0.61
16:7:118:PRO:HB2	17:8:263:ALA:HB1	1.83	0.61
18:A:807:CLA:H161	18:A:830:CLA:HBB2	1.81	0.60
3:C:58:CYS:HB3	3:C:63:LEU:HD12	1.83	0.60
10:L:138:ARG:O	10:L:146:ARG:NH2	2.34	0.60
11:a:99:VAL:HG22	11:a:198:ILE:HD11	1.84	0.60
18:A:827:CLA:H72	18:A:836:CLA:HAB	1.82	0.60
18:4:602:CLA:H2A	18:4:602:CLA:HED3	1.82	0.60
2:B:238:PRO:HB3	2:B:257:THR:HG21	1.83	0.60
11:a:214:GLN:HE21	11:a:225:ALA:HB3	1.67	0.60
18:B:813:CLA:H42	21:B:844:BCR:H21C	1.83	0.60
12:3:258:ILE:HG23	12:3:259:LEU:HD22	1.84	0.60
1:A:429:ARG:HG2	1:A:432:ARG:HH21	1.67	0.59
18:A:813:CLA:H43	12:3:72:LEU:HD21	1.84	0.59
18:B:808:CLA:HAB	18:B:809:CLA:HBA1	1.83	0.59
18:A:822:CLA:H101	21:A:851:BCR:H10C	1.84	0.59
11:1:103:ARG:NH1	11:1:197:GLU:OE2	2.34	0.59
1:A:614:MET:HE3	18:A:838:CLA:HBC1	1.84	0.59
11:1:93:ARG:NH1	18:1:603:CLA:O1A	2.35	0.59
18:A:824:CLA:HHB	18:A:845:CLA:HBC3	1.83	0.59
11:1:162:GLU:OE1	11:1:165:ARG:NH2	2.31	0.59
17:8:56:ARG:NH1	17:8:80:ASN:O	2.36	0.59
17:8:238:GLN:OE1	18:8:613:CLA:NA	2.36	0.58
16:7:100:PRO:HG3	16:7:108:VAL:HG11	1.84	0.58
18:B:819:CLA:HBB1	18:B:824:CLA:H61	1.85	0.58
18:A:804:CLA:HBB1	21:A:856:BCR:H281	1.85	0.58
2:B:169:PHE:O	2:B:175:ARG:NH2	2.37	0.58
2:B:388:PHE:HZ	18:B:825:CLA:HAB	1.69	0.58
2:B:300:HIS:HE1	18:B:821:CLA:NA	2.01	0.58
11:1:162:GLU:OE2	18:1:609:CLA:NC	2.38	0.57
17:8:239:LYS:HZ1	20:8:623:LHG:H201	1.69	0.57
4:D:148:GLU:O	4:D:178:GLN:NE2	2.35	0.57
1:A:622:VAL:HG22	1:A:624:ALA:H	1.70	0.57
9:K:82:ASN:ND2	18:K:204:CLA:OBD	2.38	0.57
9:K:150:ILE:HG12	18:K:203:CLA:HAB	1.86	0.57
18:4:610:CLA:H52	26:4:619:LUT:H30	1.86	0.57
11:a:108:GLY:HA2	27:a:618:XAT:H181	1.87	0.57
1:A:317:GLY:H	9:K:104:VAL:HG13	1.69	0.57
21:B:801:BCR:HC41	18:B:832:CLA:HBB2	1.87	0.57
16:7:66:LYS:O	16:7:162:ASN:ND2	2.33	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:GLU:HG3	2:B:321:LYS:HA	1.87	0.56
2:B:669:ARG:HB2	19:B:842:PQN:H7	1.86	0.56
18:B:812:CLA:H2A	18:B:812:CLA:HED3	1.87	0.56
6:F:171:LEU:HD11	18:F:301:CLA:HMD1	1.87	0.56
18:A:820:CLA:HAB	18:A:820:CLA:H8	1.87	0.56
2:B:157:HIS:HE1	18:B:811:CLA:NA	2.02	0.56
13:4:286:ASP:OD1	13:4:289:ARG:NH2	2.38	0.56
16:7:132:GLU:OE1	16:7:135:ARG:NH2	2.37	0.56
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.87	0.56
2:B:341:SER:HB3	18:B:824:CLA:H51	1.86	0.56
20:a:620:LHG:HC91	20:a:620:LHG:H281	1.86	0.56
1:A:45:THR:HG23	1:A:716:ARG:HG3	1.87	0.56
2:B:157:HIS:CE1	18:B:811:CLA:NA	2.74	0.56
18:B:817:CLA:H61	18:B:834:CLA:HAA1	1.86	0.56
5:E:101:GLN:NE2	5:E:123:ASN:OD1	2.35	0.56
2:B:126:TYR:O	2:B:131:ARG:NH1	2.38	0.56
2:B:423:LEU:HG	18:B:838:CLA:HBB1	1.87	0.56
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.87	0.56
18:B:837:CLA:H143	21:F:305:BCR:HC8	1.88	0.56
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.87	0.55
2:B:662:PHE:HA	2:B:665:LEU:HB2	1.88	0.55
1:A:34:HIS:NE2	18:A:812:CLA:O1A	2.39	0.55
18:B:827:CLA:HBC3	25:B:850:DGD:HBG3	1.88	0.55
18:B:828:CLA:H202	21:B:844:BCR:H352	1.88	0.55
15:6:118:LEU:HD23	16:7:175:LEU:HD21	1.88	0.55
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.39	0.55
11:1:186:ASP:HA	11:1:190:SER:HB3	1.86	0.55
3:C:27:GLU:HB2	4:D:216:ARG:HH21	1.72	0.55
16:7:30:ARG:NH2	16:7:43:LEU:O	2.38	0.55
18:4:601:CLA:H2	20:4:622:LHG:H131	1.88	0.55
14:5:101:GLY:HA2	27:5:621:XAT:H181	1.88	0.55
18:6:601:CLA:H2	20:6:623:LHG:H142	1.89	0.55
1:A:679:TRP:O	1:A:682:SER:OG	2.24	0.55
2:B:375:HIS:HE1	18:B:827:CLA:ND	2.05	0.55
18:A:811:CLA:H2	18:A:813:CLA:HBC2	1.88	0.54
18:B:808:CLA:H2	18:B:808:CLA:H102	1.89	0.54
10:L:135:PRO:HA	10:L:138:ARG:HE	1.72	0.54
11:1:214:GLN:HE21	11:1:225:ALA:HB3	1.70	0.54
11:a:199:LYS:NZ	20:a:620:LHG:P	2.80	0.54
21:7:621:BCR:HC31	20:8:622:LHG:HC81	1.89	0.54
1:A:605:ILE:HD12	18:A:801:CLA:H122	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:627:LMG:H131	27:6:621:XAT:H363	1.90	0.54
17:8:223:LYS:NZ	20:8:622:LHG:O6	2.32	0.54
18:A:818:CLA:H93	21:K:207:BCR:HC21	1.88	0.54
2:B:390:HIS:HE1	18:B:829:CLA:NA	2.06	0.54
1:A:128:ASN:O	6:F:90:ARG:NH2	2.40	0.54
2:B:325:ASP:O	2:B:329:ASN:ND2	2.41	0.54
11:1:217:ALA:HB2	18:1:616:CLA:HED2	1.89	0.54
15:6:256:GLN:NE2	28:6:624:NEX:O23	2.40	0.54
6:F:212:ARG:HH12	17:8:93:VAL:HB	1.72	0.54
11:1:62:GLY:HA3	17:8:175:SER:HB3	1.88	0.54
13:4:265:THR:HG22	13:4:267:LEU:H	1.72	0.54
7:I:88:PRO:O	7:I:92:MET:N	2.39	0.54
3:C:29:VAL:HG22	4:D:216:ARG:HG3	1.90	0.54
9:K:92:THR:HB	9:K:139:MET:HE3	1.90	0.54
11:1:108:GLY:HA2	27:1:618:XAT:H181	1.89	0.54
18:7:611:CLA:HBC1	20:7:622:LHG:H292	1.89	0.54
18:B:837:CLA:H111	18:B:837:CLA:H203	1.90	0.54
15:6:186:GLU:OE1	15:6:189:ARG:NH2	2.38	0.54
11:a:82:LEU:HD22	17:8:201:PRO:HA	1.90	0.53
20:5:625:LHG:HC91	24:5:627:LMG:H311	1.90	0.53
1:A:327:GLU:HG2	1:A:339:VAL:HG22	1.91	0.53
15:6:223:ALA:HB2	18:6:610:CLA:HBD	1.89	0.53
16:7:134:LYS:HG3	18:7:608:CLA:HBB1	1.90	0.53
1:A:279:LYS:HG2	1:A:503:LEU:HD12	1.89	0.53
14:5:260:GLN:HB2	28:5:624:NEX:H8	1.89	0.53
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.73	0.53
1:A:116:GLN:NE2	18:A:810:CLA:OBD	2.36	0.53
1:A:121:ILE:HG12	1:A:122:VAL:HG13	1.89	0.53
18:6:610:CLA:HBB1	18:6:612:CLA:H3A	1.90	0.53
1:A:121:ILE:HB	21:A:856:BCR:H322	1.91	0.53
2:B:312:PRO:HB2	11:1:87:GLU:HG3	1.90	0.53
3:C:40:ALA:O	4:D:221:GLN:NE2	2.40	0.53
1:A:359:LEU:HD12	18:A:828:CLA:H43	1.90	0.53
15:6:314:GLN:HG3	16:7:97:LEU:HD21	1.90	0.53
16:7:77:ARG:NH1	18:7:608:CLA:OBD	2.42	0.53
1:A:54:ALA:HB2	20:A:846:LHG:HC82	1.90	0.53
2:B:650:THR:HA	2:B:653:PHE:HB3	1.90	0.53
4:D:191:ARG:HB2	4:D:201:LEU:HD22	1.91	0.53
14:5:152:ARG:NH2	18:6:601:CLA:OBD	2.41	0.53
1:A:119:TRP:HB3	21:A:856:BCR:H323	1.91	0.52
21:A:852:BCR:H362	18:A:854:CLA:H42	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:28:GLU:OE1	8:J:31:ARG:NH2	2.42	0.52
1:A:670:LEU:HB3	18:A:854:CLA:H62	1.91	0.52
17:8:203:ASP:OD1	26:8:619:LUT:O23	2.26	0.52
18:B:803:CLA:H152	18:B:810:CLA:HBC1	1.91	0.52
18:B:841:CLA:H3A	20:B:851:LHG:H241	1.92	0.52
18:a:610:CLA:H2	26:a:617:LUT:H28	1.90	0.52
16:7:171:ASP:OD1	26:7:619:LUT:O23	2.26	0.52
18:A:828:CLA:H151	18:A:836:CLA:H112	1.91	0.52
2:B:546:LYS:NZ	5:E:96:SER:O	2.42	0.52
1:A:19:ARG:HE	12:3:79:GLY:HA2	1.74	0.52
2:B:352:HIS:ND1	18:B:817:CLA:OBD	2.41	0.52
12:3:96:ARG:HA	12:3:99:MET:HG2	1.91	0.52
11:a:179:ASP:OD1	26:a:617:LUT:O23	2.28	0.52
15:6:148:VAL:HA	15:6:151:ILE:HG12	1.90	0.52
1:A:89:SER:OG	1:A:163:ALA:O	2.26	0.52
13:4:172:ALA:HA	13:4:175:LEU:HD22	1.92	0.52
14:5:243:ASN:O	14:5:247:ASN:ND2	2.42	0.52
1:A:483:PHE:HB3	18:A:838:CLA:H11	1.90	0.51
2:B:119:SER:HA	18:B:827:CLA:HMA2	1.91	0.51
18:B:806:CLA:HBB	18:B:829:CLA:HAB	1.91	0.51
21:3:620:BCR:HC21	18:7:601:CLA:HMD1	1.90	0.51
14:5:158:LYS:NZ	18:5:619:CLA:O1D	2.40	0.51
11:a:199:LYS:HD3	18:a:611:CLA:C3D	2.40	0.51
18:4:601:CLA:HAB	20:4:622:LHG:H292	1.91	0.51
14:5:165:GLU:HG2	14:5:173:LYS:HG2	1.92	0.51
17:8:117:LEU:HD21	26:8:619:LUT:H10	1.92	0.51
11:a:217:ALA:HB2	18:a:616:CLA:HED2	1.92	0.51
1:A:180:HIS:CE1	18:A:811:CLA:NA	2.79	0.51
2:B:127:THR:HG21	2:B:359:TYR:HD1	1.75	0.51
18:4:602:CLA:HAB	27:4:620:XAT:H32	1.92	0.51
1:A:270:SER:HA	18:A:818:CLA:HAA2	1.93	0.51
10:L:134:LEU:HD12	18:L:303:CLA:HBD	1.92	0.51
11:a:103:ARG:NH2	18:a:608:CLA:OBD	2.44	0.51
11:a:180:PRO:HD2	26:a:617:LUT:H23	1.91	0.51
20:4:622:LHG:H172	18:6:617:CLA:HMA2	1.93	0.51
17:8:74:ALA:O	17:8:80:ASN:ND2	2.44	0.51
11:a:138:TRP:CD2	18:a:604:CLA:H2	2.45	0.51
12:3:63:GLY:HA3	12:3:218:ILE:HG21	1.93	0.51
13:4:261:THR:HA	18:4:616:CLA:HED1	1.93	0.51
1:A:161:THR:HG21	18:A:817:CLA:HAA2	1.92	0.51
18:5:610:CLA:H2	26:5:620:LUT:H373	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:125:ASP:HA	11:a:128:LEU:HD23	1.93	0.50
12:3:46:TYR:OH	20:3:624:LHG:HC41	2.11	0.50
18:A:802:CLA:H203	18:A:854:CLA:H172	1.92	0.50
2:B:458:PRO:HG3	2:B:518:PHE:HB2	1.92	0.50
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.93	0.50
8:J:36:PRO:HB3	25:J:103:DGD:HG2	1.93	0.50
12:3:210:MET:HE1	18:3:610:CLA:H2A	1.93	0.50
13:4:220:PRO:HB3	18:4:608:CLA:HBC2	1.92	0.50
18:A:806:CLA:H52	21:A:849:BCR:HC8	1.92	0.50
17:8:204:PRO:HD2	26:8:619:LUT:H23	1.92	0.50
1:A:142:SER:HA	18:A:829:CLA:HMA2	1.94	0.50
18:A:812:CLA:H192	18:A:812:CLA:H141	1.93	0.50
2:B:362:GLN:NE2	2:B:369:GLN:OE1	2.41	0.50
1:A:690:ARG:H	2:B:569:CYS:HB2	1.76	0.50
2:B:173:GLU:HG3	2:B:294:THR:HG22	1.92	0.50
2:B:445:GLN:OE1	2:B:453:GLN:NE2	2.45	0.50
18:B:825:CLA:HBB1	18:B:838:CLA:HHB	1.93	0.50
13:4:203:ASP:N	13:4:203:ASP:OD1	2.44	0.50
14:5:150:GLU:OE1	14:5:153:ARG:NH2	2.33	0.50
15:6:305:ILE:HG12	28:6:624:NEX:H161	1.93	0.50
20:5:625:LHG:H272	24:5:627:LMG:H352	1.93	0.50
18:3:617:CLA:HBB2	21:3:621:BCR:H312	1.94	0.50
2:B:620:TRP:HB3	18:B:802:CLA:H101	1.94	0.50
12:3:159:GLU:OE1	12:3:162:ARG:NH1	2.45	0.50
2:B:269:LEU:HD22	18:B:817:CLA:HBA1	1.94	0.49
21:A:848:BCR:H362	21:A:849:BCR:H21C	1.93	0.49
11:a:186:ASP:HA	11:a:190:SER:HB3	1.94	0.49
18:5:610:CLA:HBB1	18:5:612:CLA:H3A	1.95	0.49
18:B:837:CLA:HBC2	25:J:103:DGD:HAF1	1.92	0.49
4:D:136:VAL:HG12	4:D:165:LYS:HB3	1.93	0.49
15:6:184:TRP:CD1	21:6:622:BCR:H12C	2.48	0.49
17:8:117:LEU:HD23	17:8:235:PHE:HZ	1.77	0.49
1:A:282:LEU:HB2	1:A:515:VAL:HG21	1.94	0.49
10:L:190:LEU:HB3	21:L:305:BCR:H401	1.93	0.49
11:1:179:ASP:OD1	26:1:617:LUT:O23	2.31	0.49
21:3:620:BCR:HC42	20:7:622:LHG:HC92	1.93	0.49
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.95	0.49
1:A:204:GLY:HA3	18:A:814:CLA:HBB1	1.94	0.49
18:B:806:CLA:H92	18:B:829:CLA:H102	1.95	0.49
11:1:199:LYS:NZ	20:1:620:LHG:O5	2.40	0.49
2:B:194:HIS:CE1	18:B:814:CLA:NA	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:137:VAL:HG11	26:4:619:LUT:H10	1.93	0.49
18:7:610:CLA:HBB1	18:7:612:CLA:H3A	1.95	0.49
12:3:237:MET:HE2	12:3:261:ASN:HB3	1.94	0.49
16:7:196:LEU:HD21	18:7:611:CLA:HMD1	1.95	0.49
1:A:377:TYR:HD2	1:A:380:LEU:HD22	1.78	0.49
18:A:801:CLA:HED3	18:A:801:CLA:HBD	1.76	0.49
1:A:718:LEU:HG	19:A:844:PQN:H143	1.94	0.48
18:A:829:CLA:H171	21:J:102:BCR:H17C	1.95	0.48
21:B:846:BCR:H321	18:1:603:CLA:H43	1.94	0.48
6:F:162:TYR:HE2	6:F:200:ALA:HA	1.78	0.48
7:I:87:LEU:HD13	7:I:90:ILE:HD12	1.95	0.48
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.96	0.48
2:B:107:ARG:NH1	2:B:114:VAL:O	2.46	0.48
12:3:171:SER:OG	12:3:172:MET:N	2.46	0.48
18:5:606:CLA:HHC	18:5:606:CLA:HBB1	1.95	0.48
20:5:625:LHG:H181	18:6:620:CLA:HAB	1.95	0.48
1:A:407:ALA:HA	1:A:592:VAL:HG11	1.94	0.48
1:A:441:LEU:HA	1:A:444:VAL:HG12	1.95	0.48
1:A:596:LEU:HD21	18:A:831:CLA:HBC1	1.95	0.48
10:L:149:GLU:OE2	18:L:302:CLA:ND	2.47	0.48
12:3:161:ARG:HB3	18:3:608:CLA:HMC2	1.94	0.48
1:A:508:LEU:HD12	1:A:523:MET:HB3	1.95	0.48
4:D:179:LEU:HD22	4:D:185:LEU:HD12	1.95	0.48
12:3:101:GLY:HA2	27:3:619:XAT:H181	1.95	0.48
15:6:315:GLY:HA2	16:7:95:VAL:HG11	1.95	0.48
17:8:223:LYS:HZ1	20:8:622:LHG:P	2.36	0.48
18:A:836:CLA:H41	18:A:836:CLA:H62	1.55	0.48
1:A:21:PRO:HG2	1:A:185:ALA:HB3	1.95	0.48
10:L:193:CYS:SG	21:L:305:BCR:H19C	2.54	0.48
18:5:613:CLA:H111	20:5:623:LHG:H292	1.96	0.48
1:A:49:ILE:HD12	18:A:804:CLA:HBD	1.95	0.48
1:A:674:GLY:O	1:A:677:PHE:HB3	2.14	0.48
2:B:277:HIS:HE1	18:B:817:CLA:ND	2.09	0.48
18:a:613:CLA:H121	20:a:620:LHG:H282	1.96	0.48
18:3:609:CLA:HBA2	18:3:609:CLA:H3A	1.38	0.48
18:5:607:CLA:HBB2	18:5:609:CLA:HBC1	1.94	0.48
16:7:73:LEU:O	16:7:77:ARG:HG2	2.14	0.48
16:7:134:LYS:HB3	18:7:608:CLA:HMC2	1.95	0.48
1:A:419:PRO:HG3	4:D:148:GLU:HB2	1.95	0.48
12:3:161:ARG:NE	12:3:172:MET:SD	2.80	0.48
17:8:237:ALA:HB1	18:8:616:CLA:HBA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:807:CLA:H13	18:A:807:CLA:H101	1.69	0.48
18:A:835:CLA:HAA2	10:L:165:LEU:HD12	1.96	0.48
18:B:840:CLA:H201	10:L:196:ILE:HD13	1.96	0.48
11:a:75:GLY:HA3	11:a:198:ILE:HG21	1.95	0.48
12:3:238:THR:OG1	12:3:261:ASN:ND2	2.45	0.48
2:B:326:THR:HG21	2:B:404:ASN:HD21	1.79	0.47
2:B:517:ASP:HA	2:B:520:VAL:HG12	1.95	0.47
13:4:254:GLY:O	13:4:258:GLN:CB	2.61	0.47
14:5:219:LEU:HD22	14:5:270:TRP:HZ3	1.79	0.47
15:6:190:TRP:CE2	15:6:194:ARG:HD2	2.49	0.47
15:6:297:PRO:O	15:6:309:THR:OG1	2.32	0.47
1:A:244:LEU:O	23:A:857:LMU:O2'	2.31	0.47
1:A:320:HIS:CE1	18:A:823:CLA:NA	2.81	0.47
18:A:828:CLA:H152	18:A:828:CLA:H111	1.69	0.47
2:B:354:TYR:HA	2:B:369:GLN:HE22	1.79	0.47
18:1:610:CLA:HBB1	18:1:612:CLA:H3A	1.95	0.47
18:3:606:CLA:HBA1	21:3:620:BCR:H19C	1.95	0.47
2:B:182:GLY:HA3	18:B:813:CLA:HBB1	1.96	0.47
4:D:137:ILE:HD13	4:D:175:LEU:HD23	1.96	0.47
18:1:601:CLA:H11	17:8:161:PHE:HB2	1.96	0.47
18:6:607:CLA:HHB	28:6:624:NEX:H371	1.96	0.47
18:B:809:CLA:H101	18:B:829:CLA:H202	1.96	0.47
2:B:363:ALA:HA	2:B:369:GLN:HG3	1.97	0.47
6:F:189:VAL:H	24:J:104:LMG:HC61	1.79	0.47
2:B:671:TYR:OH	18:B:803:CLA:OBD	2.26	0.47
1:A:477:ILE:HG12	23:A:859:LMU:H1B	1.97	0.47
18:A:809:CLA:HAA1	18:A:829:CLA:HED2	1.97	0.47
10:L:161:PRO:HG3	18:L:304:CLA:HAB	1.95	0.47
14:5:244:ILE:HB	18:5:613:CLA:H2	1.95	0.47
18:B:813:CLA:H71	18:B:813:CLA:H142	1.97	0.47
18:B:824:CLA:H71	18:B:826:CLA:H42	1.97	0.47
18:B:831:CLA:HAC1	18:B:838:CLA:HBC3	1.97	0.47
12:3:203:LEU:HB2	18:3:610:CLA:HBA1	1.97	0.47
1:A:261:ILE:HG13	12:3:262:PHE:HD1	1.79	0.47
3:C:54:CYS:SG	3:C:55:GLU:N	2.88	0.47
6:F:162:TYR:OH	6:F:196:ALA:O	2.27	0.47
9:K:126:ASN:HB2	18:K:201:CLA:HBA2	1.97	0.47
1:A:572:ARG:HH21	20:A:846:LHG:HC32	1.80	0.46
21:A:856:BCR:H391	8:J:12:PRO:HB2	1.96	0.46
11:1:162:GLU:OE2	18:1:609:CLA:ND	2.48	0.46
18:4:610:CLA:HBB1	18:4:612:CLA:H3A	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7:47:LEU:HD11	16:7:65:LEU:HD11	1.97	0.46
11:a:73:LEU:HD11	11:a:95:THR:HG21	1.98	0.46
18:4:614:CLA:H62	18:4:614:CLA:H41	1.66	0.46
18:5:604:CLA:H92	18:5:604:CLA:H61	1.83	0.46
18:7:604:CLA:HBB1	27:7:620:XAT:H192	1.97	0.46
18:B:833:CLA:HMA1	25:J:103:DGD:HA71	1.97	0.46
4:D:104:TRP:HE3	4:D:104:TRP:O	1.98	0.46
13:4:112:LEU:HD13	18:4:602:CLA:H42	1.97	0.46
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.97	0.46
18:A:806:CLA:H203	18:A:814:CLA:H62	1.98	0.46
2:B:494:TRP:CH2	18:B:835:CLA:H2A	2.50	0.46
3:C:24:ASP:OD1	3:C:44:ARG:NH2	2.45	0.46
11:a:158:MET:HG2	18:a:609:CLA:HMC2	1.97	0.46
1:A:485:GLN:NE2	1:A:528:LEU:O	2.46	0.46
1:A:153:ILE:HD13	18:A:815:CLA:HED3	1.97	0.46
1:A:297:HIS:HE2	18:A:820:CLA:C2B	2.29	0.46
18:A:801:CLA:H62	18:A:801:CLA:H102	1.77	0.46
18:A:830:CLA:H91	18:A:830:CLA:H111	1.80	0.46
18:B:813:CLA:H203	21:B:844:BCR:H381	1.98	0.46
14:5:265:PRO:HB2	18:5:607:CLA:H42	1.97	0.46
21:8:621:BCR:H15C	21:8:621:BCR:H351	1.76	0.46
3:C:13:GLY:O	3:C:38:GLN:NE2	2.48	0.46
21:3:621:BCR:H20C	21:3:621:BCR:H361	1.65	0.46
17:8:198:PRO:HB3	18:8:608:CLA:HBC2	1.96	0.46
1:A:413:MET:HE1	1:A:431:ILE:HD11	1.97	0.46
18:A:814:CLA:H61	18:A:814:CLA:H41	1.64	0.46
19:A:844:PQN:H141	18:F:301:CLA:HBB2	1.97	0.46
18:B:829:CLA:HBC2	25:B:850:DGD:HB92	1.97	0.46
21:B:848:BCR:H20C	21:B:848:BCR:H361	1.77	0.46
25:B:850:DGD:O5D	25:B:850:DGD:O4D	2.32	0.46
9:K:85:MET:HG3	18:K:204:CLA:HMD3	1.98	0.46
13:4:137:VAL:HG11	26:4:619:LUT:H12	1.98	0.46
2:B:350:ALA:HB3	2:B:377:GLN:HE21	1.81	0.46
2:B:478:LEU:O	2:B:484:SER:OG	2.30	0.46
10:L:127:VAL:HG12	10:L:130:TYR:H	1.80	0.46
21:3:620:BCR:H11C	21:3:620:BCR:H341	1.76	0.46
15:6:269:HIS:CG	18:6:613:CLA:HAA2	2.51	0.46
1:A:102:GLU:OE2	1:A:156:GLU:N	2.48	0.46
18:A:802:CLA:CGA	18:A:802:CLA:H3A	2.46	0.46
18:A:818:CLA:H11	9:K:152:LEU:HD13	1.97	0.46
18:A:828:CLA:H2	18:A:836:CLA:H92	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:136:SER:HB2	15:6:241:GLY:HA3	1.97	0.46
16:7:185:GLU:HG2	16:7:189:LYS:HD2	1.98	0.46
18:A:814:CLA:H43	21:A:849:BCR:H14C	1.98	0.45
18:A:831:CLA:H102	18:A:842:CLA:HAA2	1.98	0.45
21:3:622:BCR:H20C	21:3:622:BCR:H361	1.55	0.45
14:5:77:LEU:HD13	18:5:602:CLA:H42	1.98	0.45
2:B:340:ALA:HB2	21:B:847:BCR:H372	1.97	0.45
12:3:141:TRP:HB3	14:5:271:PRO:HB3	1.99	0.45
16:7:192:LYS:NZ	20:7:622:LHG:O5	2.42	0.45
18:A:854:CLA:H41	18:A:854:CLA:H61	1.56	0.45
17:8:131:PRO:HG3	17:8:139:VAL:HG21	1.97	0.45
1:A:561:ARG:NH1	4:D:122:THR:O	2.50	0.45
1:A:45:THR:HG22	1:A:47:THR:H	1.81	0.45
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.81	0.45
21:B:846:BCR:H24C	21:B:847:BCR:H21C	1.98	0.45
4:D:191:ARG:HB3	4:D:199:GLN:HB3	1.98	0.45
10:L:189:ILE:HD11	21:L:301:BCR:H272	1.98	0.45
18:A:854:CLA:H11	2:B:617:LEU:HD12	1.96	0.45
2:B:143:LEU:HG	21:B:845:BCR:H382	1.99	0.45
2:B:359:TYR:OH	18:B:828:CLA:OBD	2.23	0.45
9:K:125:SER:HB2	9:K:132:THR:HG22	1.98	0.45
17:8:152:LEU:HD12	18:8:607:CLA:HBC3	1.97	0.45
21:B:801:BCR:H333	18:B:833:CLA:H11	1.99	0.45
4:D:137:ILE:HG21	4:D:175:LEU:HD23	1.98	0.45
18:a:610:CLA:H2	26:a:617:LUT:H26	1.99	0.45
26:4:619:LUT:H35	26:4:619:LUT:H401	1.81	0.45
18:7:602:CLA:H61	27:7:620:XAT:H28	1.97	0.45
2:B:494:TRP:HE1	18:B:834:CLA:HED1	1.82	0.45
18:B:807:CLA:O1A	7:I:83:THR:OG1	2.35	0.45
18:B:810:CLA:H172	10:L:188:LEU:HD23	1.99	0.45
11:1:209:LEU:HD23	18:1:603:CLA:HBB2	1.99	0.45
14:5:212:ILE:HD12	20:5:623:LHG:H261	1.98	0.45
4:D:104:TRP:O	4:D:104:TRP:CE3	2.70	0.45
6:F:195:LEU:HD13	6:F:195:LEU:HA	1.84	0.45
16:7:203:GLY:O	16:7:207:GLN:NE2	2.50	0.45
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.97	0.45
2:B:375:HIS:HE2	18:B:828:CLA:C1B	2.29	0.45
18:B:805:CLA:HBA1	18:B:805:CLA:H3A	1.72	0.45
27:5:621:XAT:H15	27:5:621:XAT:H201	1.82	0.45
16:7:82:GLY:HA2	27:7:620:XAT:H181	1.99	0.45
18:A:829:CLA:H141	18:A:829:CLA:H193	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:139:TRP:HB3	4:D:187:PRO:HB3	1.98	0.44
11:a:162:GLU:OE2	18:a:609:CLA:NC	2.50	0.44
12:3:177:PHE:CZ	18:3:608:CLA:HBB2	2.52	0.44
26:3:618:LUT:H15	26:3:618:LUT:H201	1.83	0.44
16:7:130:TRP:CD1	21:7:621:BCR:H12C	2.52	0.44
18:A:820:CLA:H203	18:A:828:CLA:H3A	1.98	0.44
18:A:820:CLA:HBA2	18:A:820:CLA:H3A	1.64	0.44
18:A:825:CLA:H193	18:A:825:CLA:H162	1.83	0.44
2:B:578:TYR:HE1	2:B:711:LEU:HB2	1.82	0.44
21:L:305:BCR:H11C	21:L:305:BCR:H341	1.84	0.44
12:3:156:GLN:OE1	18:3:617:CLA:ND	2.51	0.44
14:5:119:GLU:O	14:5:125:ASN:ND2	2.39	0.44
18:6:611:CLA:HAC2	18:6:613:CLA:H192	1.98	0.44
16:7:58:LEU:HD13	18:7:602:CLA:H42	1.99	0.44
18:A:806:CLA:H2	18:A:806:CLA:H62	1.71	0.44
2:B:21:ARG:HH22	7:I:99:ILE:HG22	1.82	0.44
11:a:199:LYS:HZ1	20:a:620:LHG:P	2.39	0.44
18:6:616:CLA:HBC3	18:6:620:CLA:HMC3	1.98	0.44
18:5:610:CLA:H61	18:5:612:CLA:HMA3	1.99	0.44
28:6:624:NEX:H15	28:6:624:NEX:H201	1.80	0.44
18:7:604:CLA:HAB	21:7:621:BCR:H393	1.98	0.44
1:A:36:SER:HB3	1:A:39:LEU:HB2	1.99	0.44
18:A:802:CLA:H171	18:A:842:CLA:H51	1.99	0.44
18:A:827:CLA:HAB	21:A:851:BCR:H311	2.00	0.44
2:B:54:GLN:HE21	2:B:58:ILE:HG13	1.83	0.44
2:B:175:ARG:HB2	18:B:813:CLA:HBC2	1.99	0.44
2:B:475:PHE:HE1	6:F:139:LEU:HD21	1.82	0.44
21:B:845:BCR:H24C	21:B:845:BCR:H371	1.71	0.44
4:D:109:LEU:HB2	4:D:190:TYR:CE2	2.53	0.44
18:3:617:CLA:O1D	18:7:601:CLA:H3A	2.17	0.44
27:3:619:XAT:H15	27:3:619:XAT:H201	1.81	0.44
17:8:234:GLY:O	17:8:238:GLN:HG3	2.18	0.44
1:A:622:VAL:HG23	1:A:627:VAL:HB	2.00	0.44
1:A:692:TYR:CE2	18:A:802:CLA:HMD1	2.52	0.44
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.35	0.44
7:I:81:PRO:O	7:I:85:LEU:HB2	2.18	0.44
18:4:613:CLA:H143	18:4:613:CLA:H111	1.82	0.44
14:5:183:GLY:N	18:5:610:CLA:OBD	2.51	0.44
16:7:144:SER:OG	16:7:145:GLN:N	2.50	0.44
18:8:610:CLA:H51	26:8:619:LUT:H373	2.00	0.44
1:A:363:LEU:HD11	18:A:830:CLA:H202	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:848:BCR:H20C	21:A:848:BCR:H361	1.78	0.44
4:D:202:HIS:CG	4:D:203:PRO:CD	2.83	0.44
18:1:613:CLA:H121	20:1:620:LHG:H282	2.00	0.44
21:1:619:BCR:H20C	21:1:619:BCR:H361	1.83	0.44
14:5:169:PHE:HE2	18:5:618:CLA:H3A	1.82	0.44
14:5:219:LEU:HD21	14:5:269:LEU:HD23	1.99	0.44
19:A:844:PQN:H142	19:A:844:PQN:H112	1.87	0.44
21:B:843:BCR:H11C	21:B:843:BCR:H341	1.83	0.44
14:5:196:LEU:O	14:5:200:GLN:HB2	2.18	0.44
27:8:620:XAT:H15	27:8:620:XAT:H201	1.79	0.44
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.99	0.44
18:A:842:CLA:H3A	18:A:842:CLA:HBA2	1.57	0.44
18:B:811:CLA:HBA1	18:B:812:CLA:HMD2	2.00	0.44
18:B:832:CLA:H2	18:B:832:CLA:H62	1.74	0.44
18:1:611:CLA:H52	18:1:611:CLA:H12	1.83	0.44
18:3:609:CLA:H2A	18:3:609:CLA:HED2	1.98	0.44
14:5:214:TYR:CZ	27:5:621:XAT:H8	2.53	0.44
18:B:818:CLA:H3A	18:B:818:CLA:HBA2	1.58	0.43
14:5:73:ASP:HB2	18:5:602:CLA:HBA2	2.00	0.43
28:5:624:NEX:H11	28:5:624:NEX:H191	1.88	0.43
15:6:284:VAL:HB	18:6:616:CLA:C1C	2.48	0.43
18:A:829:CLA:H143	18:A:829:CLA:H111	1.86	0.43
21:A:851:BCR:H20C	21:A:851:BCR:H361	1.85	0.43
12:3:192:TYR:HB3	18:3:610:CLA:HED2	1.99	0.43
20:4:622:LHG:H132	18:6:617:CLA:HED3	2.00	0.43
21:B:846:BCR:H11C	21:B:846:BCR:H341	1.84	0.43
17:8:161:PHE:CD2	21:8:621:BCR:H12C	2.53	0.43
1:A:146:GLN:HB3	1:A:377:TYR:HB3	1.99	0.43
18:A:804:CLA:H72	18:A:804:CLA:H111	1.83	0.43
18:A:819:CLA:HBC1	18:A:828:CLA:H18	2.00	0.43
6:F:137:PRO:HB2	18:F:304:CLA:HBC3	2.00	0.43
21:L:301:BCR:H24C	21:L:301:BCR:H371	1.76	0.43
18:3:603:CLA:HMD2	21:3:621:BCR:HC31	1.99	0.43
15:6:310:PRO:O	15:6:312:PHE:N	2.43	0.43
17:8:163:GLU:CD	17:8:166:ARG:HH21	2.26	0.43
18:8:606:CLA:H151	18:8:608:CLA:HED2	1.99	0.43
1:A:83:ILE:HD11	18:A:812:CLA:H122	2.00	0.43
1:A:240:PRO:HA	1:A:243:LEU:HD12	2.01	0.43
1:A:680:ALA:HB3	18:A:802:CLA:HBB2	2.00	0.43
18:B:818:CLA:H93	18:B:818:CLA:H61	1.89	0.43
3:C:7:ILE:HG22	3:C:65:VAL:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:624:LHG:HC61	20:3:624:LHG:H241	1.79	0.43
1:A:349:TRP:HB3	18:A:806:CLA:HAC1	2.00	0.43
11:1:180:PRO:HD2	26:1:617:LUT:H23	2.00	0.43
12:3:44:GLN:HB2	12:3:45:LEU:H	1.67	0.43
26:3:618:LUT:H35	26:3:618:LUT:H401	1.89	0.43
18:6:604:CLA:H93	18:6:604:CLA:H111	1.90	0.43
16:7:77:ARG:HD2	18:7:610:CLA:C4C	2.48	0.43
18:8:601:CLA:H93	18:8:613:CLA:H122	2.00	0.43
18:8:604:CLA:H3A	18:8:604:CLA:HBA2	1.73	0.43
5:E:84:LYS:HG2	5:E:87:SER:HB3	2.00	0.43
18:L:302:CLA:HBA2	18:L:302:CLA:H3A	1.43	0.43
18:a:609:CLA:H41	18:a:609:CLA:H62	1.81	0.43
21:4:621:BCR:H11C	21:4:621:BCR:H341	1.84	0.43
18:8:610:CLA:H41	18:8:610:CLA:H62	1.59	0.43
18:B:817:CLA:HBA2	18:B:817:CLA:H3A	1.38	0.43
14:5:214:TYR:CE2	27:5:621:XAT:H10	2.54	0.43
18:6:604:CLA:H161	18:6:604:CLA:H141	1.81	0.43
21:7:623:BCR:H371	21:7:623:BCR:H24C	1.77	0.43
1:A:393:HIS:HE1	18:A:829:CLA:ND	2.12	0.43
1:A:538:ILE:HG23	18:A:801:CLA:H193	2.00	0.43
18:A:819:CLA:HBA2	18:A:819:CLA:H3A	1.66	0.43
18:A:834:CLA:HBB1	23:A:859:LMU:H41	2.01	0.43
16:7:137:TYR:HB3	17:8:62:GLY:HA3	2.01	0.43
1:A:366:ILE:HG21	18:A:820:CLA:H201	1.99	0.43
1:A:439:SER:HB2	2:B:682:ALA:HB2	2.00	0.43
18:A:821:CLA:H3A	18:A:821:CLA:HBA2	1.62	0.43
18:A:828:CLA:H202	18:A:828:CLA:H162	1.89	0.43
21:A:850:BCR:H11C	21:A:850:BCR:H341	1.84	0.43
21:A:850:BCR:H24C	21:A:850:BCR:H371	1.79	0.43
2:B:411:ARG:O	2:B:415:HIS:ND1	2.52	0.43
21:F:305:BCR:H20C	21:F:305:BCR:H361	1.77	0.43
8:J:5:THR:HB	24:J:104:LMG:HC71	2.00	0.43
12:3:216:LYS:HE2	18:3:612:CLA:HAA2	2.00	0.43
20:3:623:LHG:HC41	16:7:227:ASN:HD21	1.83	0.43
13:4:185:TRP:CD1	21:4:621:BCR:H12C	2.54	0.43
18:8:613:CLA:H91	20:8:622:LHG:H321	2.00	0.43
1:A:14:LYS:NZ	1:A:15:ILE:O	2.42	0.42
18:A:835:CLA:H52	21:L:301:BCR:H363	2.01	0.42
2:B:76:GLU:HG2	2:B:132:THR:HA	2.01	0.42
11:1:208:PHE:CD2	27:1:618:XAT:H12	2.54	0.42
18:1:603:CLA:H41	18:1:603:CLA:H61	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:276:ASP:OD1	13:4:276:ASP:N	2.52	0.42
14:5:99:MET:SD	18:5:610:CLA:HAB	2.59	0.42
18:5:609:CLA:H3A	18:5:609:CLA:HBA2	1.73	0.42
15:6:236:LYS:HD3	18:6:612:CLA:HBD	1.99	0.42
18:6:604:CLA:H171	21:6:622:BCR:H392	2.01	0.42
16:7:92:GLY:HA3	16:7:99:PHE:HD2	1.83	0.42
16:7:189:LYS:HE3	18:7:612:CLA:HAA2	2.01	0.42
18:A:828:CLA:H203	18:A:836:CLA:H71	2.01	0.42
18:A:834:CLA:H141	18:A:834:CLA:H161	1.76	0.42
3:C:55:GLU:HB2	3:C:63:LEU:HG	2.01	0.42
6:F:188:ASP:HA	24:J:104:LMG:HC61	2.01	0.42
21:3:622:BCR:H341	21:3:622:BCR:H11C	1.59	0.42
14:5:192:SER:OG	14:5:193:LYS:N	2.50	0.42
18:5:602:CLA:H2	27:5:621:XAT:H382	2.01	0.42
15:6:130:GLU:HG2	15:6:193:LEU:HD12	2.01	0.42
13:4:273:HIS:CG	18:4:613:CLA:HAA2	2.54	0.42
18:4:603:CLA:HBC3	27:4:620:XAT:H11	2.02	0.42
14:5:154:TRP:CG	18:5:617:CLA:HBC1	2.54	0.42
2:B:588:ILE:HA	2:B:591:VAL:HG22	2.02	0.42
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.99	0.42
10:L:133:ASN:HB3	18:L:302:CLA:HAC1	2.01	0.42
21:L:305:BCR:H15C	21:L:305:BCR:H351	1.88	0.42
21:4:621:BCR:H15C	21:4:621:BCR:H351	1.82	0.42
14:5:149:VAL:HG21	21:5:622:BCR:H362	2.01	0.42
18:6:601:CLA:H111	18:6:601:CLA:H152	1.93	0.42
16:7:165:PRO:HB3	18:7:608:CLA:HBC2	2.02	0.42
2:B:429:PHE:CE2	18:B:837:CLA:HAB	2.55	0.42
14:5:59:PRO:HD2	14:5:62:LEU:HD12	2.02	0.42
15:6:133:LEU:HB3	15:6:137:ARG:NH2	2.34	0.42
1:A:655:SER:O	1:A:659:GLN:NE2	2.52	0.42
18:1:602:CLA:H2A	18:1:602:CLA:HED2	2.01	0.42
11:a:225:ALA:HB1	18:a:613:CLA:HED2	2.01	0.42
18:4:610:CLA:HBB2	26:4:619:LUT:H34	2.01	0.42
14:5:227:GLY:O	14:5:231:ALA:N	2.45	0.42
15:6:201:GLN:NE2	15:6:206:SER:OG	2.53	0.42
18:A:842:CLA:H101	18:A:842:CLA:H62	1.86	0.42
21:A:856:BCR:H15C	8:J:20:THR:HG22	2.00	0.42
18:B:827:CLA:HBA2	18:B:827:CLA:H3A	1.75	0.42
18:5:609:CLA:H13	18:5:609:CLA:H101	1.91	0.42
18:7:610:CLA:H93	18:7:612:CLA:HMA3	2.02	0.42
1:A:169:MET:HE2	18:A:814:CLA:H71	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:841:CLA:H111	18:A:841:CLA:HHC	2.02	0.42
18:B:839:CLA:HMA2	7:I:96:PHE:HE1	1.84	0.42
21:B:847:BCR:H351	21:B:847:BCR:H15C	1.79	0.42
24:J:104:LMG:H182	24:J:104:LMG:H152	1.84	0.42
11:a:70:PRO:O	11:a:76:ASN:ND2	2.53	0.42
18:B:807:CLA:HED2	7:I:76:PRO:HB3	2.02	0.42
7:I:82:LEU:HA	7:I:86:VAL:HB	2.02	0.42
21:3:620:BCR:H21C	21:3:620:BCR:H24C	1.86	0.42
21:5:622:BCR:H20C	21:5:622:BCR:H361	1.87	0.42
15:6:114:ASP:HB2	18:6:602:CLA:HBA2	2.02	0.42
18:8:610:CLA:H112	18:8:610:CLA:H91	1.76	0.42
1:A:691:GLY:N	2:B:569:CYS:O	2.48	0.42
2:B:490:GLY:HA3	2:B:495:LEU:HD13	2.00	0.42
4:D:136:VAL:HB	4:D:163:LEU:HD11	2.01	0.42
14:5:262:LEU:HA	15:6:288:GLN:HE21	1.84	0.42
27:6:621:XAT:H15	27:6:621:XAT:H201	1.86	0.42
21:7:621:BCR:H15C	21:7:621:BCR:H351	1.84	0.42
26:8:619:LUT:H35	26:8:619:LUT:H401	1.83	0.42
18:A:808:CLA:H11	23:A:858:LMU:H21	2.01	0.41
21:F:305:BCR:H24C	21:F:305:BCR:H371	1.70	0.41
21:K:207:BCR:H20C	21:K:207:BCR:H361	1.84	0.41
10:L:146:ARG:HH11	10:L:223:LEU:HD22	1.84	0.41
11:1:158:MET:HG2	18:1:609:CLA:HMC2	2.02	0.41
11:a:103:ARG:HG3	18:a:610:CLA:C3C	2.50	0.41
13:4:282:VAL:N	18:4:613:CLA:O1A	2.53	0.41
18:6:616:CLA:H192	18:6:620:CLA:HBC1	2.01	0.41
21:A:849:BCR:H15C	21:A:849:BCR:H351	1.81	0.41
18:B:803:CLA:H111	18:B:803:CLA:H142	1.78	0.41
11:1:103:ARG:NE	18:1:608:CLA:OBD	2.53	0.41
16:7:43:LEU:HD12	16:7:43:LEU:HA	1.88	0.41
16:7:82:GLY:O	16:7:86:ILE:HD12	2.20	0.41
16:7:228:HIS:HA	16:7:233:THR:HG21	2.01	0.41
26:7:619:LUT:H15	26:7:619:LUT:H201	1.82	0.41
27:7:620:XAT:H35	27:7:620:XAT:H401	1.85	0.41
18:A:811:CLA:H122	18:A:811:CLA:H162	1.88	0.41
18:A:812:CLA:H62	18:A:812:CLA:H41	1.96	0.41
18:A:839:CLA:HBB2	18:A:840:CLA:HBC3	2.02	0.41
2:B:478:LEU:HD23	2:B:478:LEU:HA	1.86	0.41
21:B:848:BCR:H351	21:B:848:BCR:H15C	1.82	0.41
18:1:603:CLA:HBB1	27:1:618:XAT:C35	2.50	0.41
11:a:129:TRP:CE2	11:a:136:ALA:HB2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:610:CLA:HBB1	18:3:610:CLA:H51	2.02	0.41
21:6:622:BCR:H24C	21:6:622:BCR:H371	1.94	0.41
18:A:822:CLA:H192	21:A:850:BCR:H272	2.01	0.41
18:A:830:CLA:HBD	18:A:830:CLA:H11	2.02	0.41
2:B:601:THR:HG21	2:B:610:PHE:HB2	2.02	0.41
21:B:843:BCR:H20C	21:B:843:BCR:H361	1.82	0.41
18:1:613:CLA:H3A	18:1:613:CLA:HBA2	1.84	0.41
12:3:95:ALA:HB1	12:3:221:GLY:HA3	2.02	0.41
13:4:187:GLU:OE2	18:4:609:CLA:ND	2.53	0.41
18:5:606:CLA:HBB2	18:5:607:CLA:CBB	2.50	0.41
20:8:623:LHG:H271	23:8:624:LMU:H81	2.02	0.41
1:A:126:ILE:HG21	2:B:447:PHE:HA	2.02	0.41
1:A:536:HIS:CG	18:A:839:CLA:HED3	2.55	0.41
11:1:235:GLY:HA2	11:1:240:THR:HG21	2.02	0.41
2:B:38:MET:HE1	2:B:46:LYS:HD2	2.02	0.41
2:B:348:LEU:HD23	18:B:818:CLA:H62	2.01	0.41
21:B:843:BCR:H24C	21:B:843:BCR:H371	1.92	0.41
4:D:128:LYS:HG2	4:D:132:GLU:HB2	2.02	0.41
12:3:73:LEU:HG	12:3:84:PRO:HB3	2.01	0.41
18:5:602:CLA:H162	18:5:602:CLA:H141	1.85	0.41
18:A:806:CLA:H112	18:A:806:CLA:H91	1.87	0.41
18:A:834:CLA:H152	19:B:842:PQN:H191	2.03	0.41
18:A:841:CLA:H162	18:A:841:CLA:H192	1.84	0.41
18:B:831:CLA:H13	18:B:831:CLA:H102	1.81	0.41
6:F:158:TYR:O	6:F:162:TYR:HB2	2.21	0.41
10:L:138:ARG:NH1	10:L:149:GLU:OE1	2.53	0.41
12:3:180:LEU:HD11	21:3:622:BCR:HC22	2.02	0.41
1:A:458:HIS:CE1	18:A:835:CLA:NA	2.89	0.41
1:A:681:PHE:HZ	18:A:842:CLA:HBC2	1.85	0.41
18:A:806:CLA:H161	18:A:806:CLA:H202	1.86	0.41
2:B:398:ASP:HA	4:D:233:ILE:HD13	2.02	0.41
18:B:829:CLA:H71	18:B:840:CLA:HED1	2.02	0.41
11:1:129:TRP:CE2	11:1:136:ALA:HB2	2.56	0.41
17:8:106:CYS:HB2	17:8:225:GLY:HA3	2.03	0.41
1:A:646:LEU:HD22	2:B:652:LEU:HD21	2.03	0.41
18:A:803:CLA:H141	18:A:803:CLA:H161	1.84	0.41
18:A:825:CLA:H93	18:A:825:CLA:H111	1.88	0.41
18:A:825:CLA:H43	21:A:851:BCR:H16C	2.02	0.41
21:A:852:BCR:H371	21:A:852:BCR:H24C	1.81	0.41
18:B:806:CLA:H93	18:B:806:CLA:H61	1.88	0.41
18:B:818:CLA:H62	18:B:818:CLA:H41	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:834:CLA:H61	18:B:834:CLA:H102	1.87	0.41
18:B:841:CLA:H3A	18:B:841:CLA:HBA1	1.82	0.41
10:L:145:LEU:HD21	18:L:302:CLA:HED3	2.03	0.41
18:a:613:CLA:HBA2	18:a:613:CLA:H3A	1.71	0.41
21:a:619:BCR:H24C	21:a:619:BCR:H371	1.86	0.41
12:3:97:TRP:CE2	18:3:608:CLA:HED2	2.55	0.41
18:5:607:CLA:H91	18:5:607:CLA:H111	1.93	0.41
28:5:624:NEX:H21	15:6:290:VAL:HG11	2.02	0.41
28:5:624:NEX:H30	18:6:616:CLA:H42	2.02	0.41
18:6:604:CLA:H71	21:6:622:BCR:H402	2.02	0.41
1:A:687:PHE:CG	2:B:665:LEU:HD22	2.56	0.41
18:A:818:CLA:CHD	18:A:819:CLA:HBB2	2.51	0.41
18:A:818:CLA:H91	18:A:818:CLA:H112	1.82	0.41
18:A:843:CLA:H202	18:A:843:CLA:H161	1.84	0.41
2:B:9:PHE:HB2	2:B:35:HIS:CG	2.56	0.41
18:B:831:CLA:H62	18:B:831:CLA:H41	1.97	0.41
6:F:137:PRO:HG2	21:F:305:BCR:H333	2.03	0.41
26:1:617:LUT:H35	26:1:617:LUT:H401	1.83	0.41
14:5:118:TYR:CD1	18:5:607:CLA:HMA2	2.56	0.41
18:5:602:CLA:H192	18:5:613:CLA:H162	2.02	0.41
18:5:608:CLA:HBB2	18:5:618:CLA:CHC	2.51	0.41
18:5:610:CLA:HMB3	18:5:612:CLA:HAA1	2.02	0.41
18:6:609:CLA:HBA1	18:6:609:CLA:H3A	1.93	0.41
18:A:841:CLA:H142	18:A:841:CLA:H112	1.87	0.40
21:A:848:BCR:H11C	21:A:848:BCR:H341	1.82	0.40
2:B:429:PHE:CD2	18:B:837:CLA:HAB	2.56	0.40
18:B:833:CLA:H41	18:B:833:CLA:H61	1.58	0.40
21:F:305:BCR:H16C	21:F:305:BCR:H19C	1.83	0.40
9:K:144:HIS:ND1	21:K:207:BCR:H12C	2.35	0.40
21:K:207:BCR:H11C	21:K:207:BCR:H341	1.94	0.40
11:1:83:SER:HB2	11:1:86:LYS:HE3	2.03	0.40
18:a:613:CLA:H152	18:a:613:CLA:H18	1.73	0.40
27:a:618:XAT:H15	27:a:618:XAT:H201	1.88	0.40
18:6:616:CLA:H91	18:6:616:CLA:H111	1.83	0.40
1:A:286:THR:HG23	1:A:288:GLY:H	1.86	0.40
1:A:729:ALA:HA	20:A:846:LHG:H341	2.03	0.40
21:A:850:BCR:H15C	21:A:850:BCR:H351	1.83	0.40
18:B:811:CLA:H41	18:B:811:CLA:H61	1.89	0.40
21:K:202:BCR:H11C	21:K:202:BCR:H341	1.86	0.40
11:a:143:VAL:HG11	18:a:606:CLA:HMD1	2.02	0.40
18:a:606:CLA:HBB2	18:a:607:CLA:CBB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:610:CLA:H43	18:3:612:CLA:HBA1	2.03	0.40
18:4:601:CLA:H3A	18:4:601:CLA:HBA2	1.48	0.40
1:A:48:TRP:HE3	1:A:49:ILE:HG22	1.86	0.40
18:A:815:CLA:HBD	18:A:817:CLA:HMA2	2.03	0.40
21:A:856:BCR:HC32	8:J:31:ARG:HH11	1.85	0.40
23:A:858:LMU:H122	23:A:858:LMU:H91	1.93	0.40
7:I:88:PRO:HA	7:I:91:ALA:HB3	2.04	0.40
11:1:202:ARG:HA	11:1:205:MET:HE3	2.03	0.40
21:3:621:BCR:H11C	21:3:621:BCR:H341	1.60	0.40
21:5:622:BCR:H24C	21:5:622:BCR:H371	1.92	0.40
26:6:619:LUT:H35	26:6:619:LUT:H401	1.86	0.40
16:7:196:LEU:HD12	26:7:619:LUT:H11	2.03	0.40
1:A:451:HIS:HB3	23:A:859:LMU:H92	2.03	0.40
18:B:810:CLA:HED1	21:L:301:BCR:H382	2.03	0.40
18:B:813:CLA:H141	18:B:813:CLA:H162	1.80	0.40
9:K:112:LEU:HG	18:K:206:CLA:HAA2	2.02	0.40
12:3:148:PHE:CG	18:3:607:CLA:HAA1	2.56	0.40
17:8:232:PHE:CD2	27:8:620:XAT:H12	2.57	0.40
18:A:829:CLA:H62	18:A:829:CLA:H101	1.88	0.40
2:B:52:PHE:HD1	2:B:150:PHE:HD1	1.69	0.40
21:J:102:BCR:H15C	21:J:102:BCR:H351	1.84	0.40
21:K:202:BCR:H15C	21:K:202:BCR:H351	1.80	0.40
18:a:603:CLA:HBB1	27:a:618:XAT:C35	2.51	0.40
14:5:192:SER:HB2	18:5:610:CLA:HAA1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	739/751 (98%)	708 (96%)	31 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	729/735 (99%)	699 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	142/196 (72%)	131 (92%)	9 (6%)	2 (1%)	9	30
5	E	62/143 (43%)	58 (94%)	4 (6%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	83/160 (52%)	73 (88%)	10 (12%)	0	100	100
10	L	101/258 (39%)	98 (97%)	3 (3%)	0	100	100
11	1	191/248 (77%)	171 (90%)	19 (10%)	1 (0%)	24	54
11	a	192/248 (77%)	175 (91%)	16 (8%)	1 (0%)	24	54
12	3	219/298 (74%)	202 (92%)	17 (8%)	0	100	100
13	4	208/290 (72%)	196 (94%)	12 (6%)	0	100	100
14	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
15	6	228/318 (72%)	206 (90%)	21 (9%)	1 (0%)	30	59
16	7	211/241 (88%)	193 (92%)	18 (8%)	0	100	100
17	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
All	All	3851/4887 (79%)	3594 (93%)	252 (6%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	202	HIS
4	D	203	PRO
15	6	312	PHE
11	1	59	TRP
11	a	59	TRP

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	A	601/610 (98%)	600 (100%)	1 (0%)	87	96
2	B	595/597 (100%)	594 (100%)	1 (0%)	87	96
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/152 (79%)	118 (98%)	2 (2%)	53	82
5	E	55/123 (45%)	55 (100%)	0	100	100
6	F	126/169 (75%)	126 (100%)	0	100	100
7	I	26/76 (34%)	26 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	K	59/123 (48%)	59 (100%)	0	100	100
10	L	74/198 (37%)	74 (100%)	0	100	100
11	1	136/180 (76%)	136 (100%)	0	100	100
11	a	137/180 (76%)	136 (99%)	1 (1%)	76	92
12	3	167/230 (73%)	166 (99%)	1 (1%)	78	93
13	4	165/226 (73%)	164 (99%)	1 (1%)	78	93
14	5	183/219 (84%)	182 (100%)	1 (0%)	81	93
15	6	184/260 (71%)	182 (99%)	2 (1%)	65	88
16	7	164/181 (91%)	162 (99%)	2 (1%)	63	86
17	8	161/207 (78%)	160 (99%)	1 (1%)	78	93
All	All	3059/3838 (80%)	3046 (100%)	13 (0%)	81	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	LEU
2	B	176	LEU
4	D	201	LEU
4	D	202	HIS
11	a	209	LEU
12	3	218	ILE
13	4	203	ASP
14	5	75	LEU
15	6	175	LEU
15	6	311	CYS
16	7	86	ILE
16	7	207	GLN
17	8	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	180	HIS
1	A	217	GLN
1	A	241	HIS
1	A	356	ASN
1	A	421	ASN
1	A	489	ASN
1	A	609	HIS
1	A	637	GLN
1	A	653	GLN
1	A	714	GLN
1	A	722	GLN
2	B	15	GLN
2	B	35	HIS
2	B	72	GLN
2	B	115	ASN
2	B	403	GLN
2	B	628	ASN
2	B	634	ASN
5	E	101	GLN
5	E	123	ASN
11	a	214	GLN
12	3	199	ASN
13	4	114	GLN
14	5	89	GLN
14	5	93	GLN
15	6	201	GLN
15	6	314	GLN
16	7	227	ASN
16	7	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

299 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
18	CLA	B	812	2	47,51,73	1.49	9 (19%)	56,86,113	1.48	4 (7%)
20	LHG	4	622	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	7 (13%)
18	CLA	A	817	-	49,53,73	1.46	9 (18%)	59,89,113	1.75	11 (18%)
18	CLA	A	814	1	69,73,73	1.23	9 (13%)	83,113,113	1.45	10 (12%)
18	CLA	1	608	-	47,52,73	1.53	7 (14%)	56,88,113	1.44	4 (7%)
21	BCR	A	850	-	41,41,41	0.75	0	56,56,56	1.95	15 (26%)
18	CLA	8	608	-	55,59,73	1.41	10 (18%)	66,96,113	1.53	6 (9%)
21	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
18	CLA	A	837	1	49,53,73	1.47	10 (20%)	59,89,113	1.59	8 (13%)
18	CLA	5	603	14	58,62,73	1.46	12 (20%)	73,100,113	1.44	8 (10%)
18	CLA	A	832	1	54,58,73	1.40	11 (20%)	65,95,113	1.45	9 (13%)
18	CLA	1	606	11	41,47,73	1.57	9 (21%)	48,80,113	1.52	6 (12%)
18	CLA	A	805	1	56,60,73	1.38	10 (17%)	67,97,113	1.49	9 (13%)
18	CLA	1	616	11	47,51,73	1.60	11 (23%)	60,87,113	1.49	7 (11%)
18	CLA	L	304	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	5 (8%)
22	SF4	A	853	-	0,12,12	-	-	-	-	-
18	CLA	B	832	2	64,68,73	1.27	9 (14%)	77,107,113	1.46	10 (12%)
18	CLA	B	827	2	66,70,73	1.24	9 (13%)	79,109,113	1.36	8 (10%)
20	LHG	3	624	18	48,48,48	0.63	0	51,54,54	1.22	6 (11%)
24	LMG	4	623	-	40,40,55	0.89	1 (2%)	48,48,63	1.23	4 (8%)
18	CLA	A	824	1	45,49,73	1.51	8 (17%)	54,84,113	1.59	9 (16%)
18	CLA	8	609	17	49,53,73	1.45	9 (18%)	59,89,113	1.52	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	J	102	-	41,41,41	0.70	0	56,56,56	1.99	18 (32%)
18	CLA	6	613	-	67,72,73	1.25	9 (13%)	80,112,113	1.40	8 (10%)
18	CLA	a	601	11	57,62,73	1.37	11 (19%)	68,100,113	1.37	6 (8%)
27	XAT	3	619	-	39,47,47	0.93	2 (5%)	54,74,74	2.63	21 (38%)
18	CLA	A	845	20	54,58,73	1.39	9 (16%)	65,95,113	1.46	4 (6%)
18	CLA	A	806	1	69,73,73	1.27	12 (17%)	83,113,113	1.53	9 (10%)
18	CLA	a	610	11	63,67,73	1.30	10 (15%)	76,106,113	1.32	7 (9%)
18	CLA	a	602	11	65,69,73	1.29	10 (15%)	78,108,113	1.34	6 (7%)
18	CLA	4	604	-	58,62,73	1.42	11 (18%)	73,100,113	1.40	8 (10%)
18	CLA	6	609	15	49,53,73	1.46	9 (18%)	59,89,113	1.55	8 (13%)
18	CLA	7	613	16	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
21	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
23	LMU	8	624	-	36,36,36	1.20	2 (5%)	47,47,47	0.96	2 (4%)
18	CLA	a	604	-	53,57,73	1.41	10 (18%)	62,93,113	1.57	10 (16%)
18	CLA	3	617	12	43,48,73	1.52	9 (20%)	51,83,113	1.53	6 (11%)
18	CLA	4	601	13	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
18	CLA	8	613	17	69,73,73	1.23	8 (11%)	83,113,113	1.47	5 (6%)
20	LHG	7	622	18	36,36,48	0.74	1 (2%)	39,42,54	1.28	4 (10%)
23	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.22	5 (11%)
18	CLA	5	610	14	58,62,73	1.35	10 (17%)	69,99,113	1.46	8 (11%)
18	CLA	B	829	2	69,73,73	1.32	10 (14%)	83,113,113	1.55	9 (10%)
18	CLA	B	835	-	49,53,73	1.48	9 (18%)	59,89,113	1.64	10 (16%)
18	CLA	3	612	12	47,51,73	1.49	9 (19%)	56,86,113	1.48	7 (12%)
18	CLA	a	616	11	49,53,73	1.46	8 (16%)	59,89,113	1.41	5 (8%)
18	CLA	7	610	16	69,73,73	1.22	10 (14%)	83,113,113	1.31	9 (10%)
20	LHG	8	622	18	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
21	BCR	a	619	-	41,41,41	0.69	0	56,56,56	1.93	16 (28%)
18	CLA	6	616	15	69,73,73	1.24	9 (13%)	83,113,113	1.43	12 (14%)
21	BCR	B	848	-	41,41,41	0.79	0	56,56,56	1.78	11 (19%)
18	CLA	4	603	13	48,52,73	1.55	10 (20%)	61,88,113	1.61	8 (13%)
18	CLA	6	610	15	69,73,73	1.23	10 (14%)	83,113,113	1.29	7 (8%)
18	CLA	3	614	12	43,48,73	1.54	10 (23%)	51,83,113	1.50	5 (9%)
18	CLA	3	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
18	CLA	7	612	16	48,52,73	1.53	9 (18%)	58,88,113	1.42	8 (13%)
18	CLA	5	616	14	45,50,73	1.59	11 (24%)	56,85,113	1.49	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	L	301	-	41,41,41	0.75	0	56,56,56	1.84	15 (26%)
18	CLA	8	607	-	45,49,73	1.58	10 (22%)	57,84,113	1.61	7 (12%)
26	LUT	6	619	-	42,43,43	0.76	0	51,60,60	1.57	12 (23%)
21	BCR	A	851	-	41,41,41	0.79	0	56,56,56	2.14	14 (25%)
21	BCR	3	621	-	41,41,41	0.70	0	56,56,56	2.46	20 (35%)
18	CLA	B	833	2	69,73,73	1.25	10 (14%)	83,113,113	1.41	9 (10%)
18	CLA	5	604	-	67,71,73	1.32	11 (16%)	84,111,113	1.37	8 (9%)
18	CLA	F	303	-	46,50,73	1.53	10 (21%)	55,85,113	1.50	5 (9%)
18	CLA	3	615	-	43,48,73	1.56	9 (20%)	51,83,113	1.64	6 (11%)
18	CLA	7	604	-	58,62,73	1.35	11 (18%)	70,100,113	1.45	9 (12%)
18	CLA	1	604	-	53,57,73	1.43	9 (16%)	62,93,113	1.58	9 (14%)
18	CLA	B	815	2	47,51,73	1.46	9 (19%)	56,86,113	1.54	5 (8%)
24	LMG	A	860	-	40,40,55	0.93	2 (5%)	48,48,63	1.27	5 (10%)
21	BCR	6	622	-	41,41,41	0.72	0	56,56,56	1.95	17 (30%)
18	CLA	1	601	11	57,62,73	1.38	10 (17%)	68,100,113	1.35	8 (11%)
18	CLA	A	803	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	8 (9%)
21	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.02	22 (39%)
25	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.47	10 (13%)
27	XAT	6	621	-	39,47,47	0.92	2 (5%)	54,74,74	2.72	20 (37%)
18	CLA	5	606	-	43,48,73	1.56	8 (18%)	51,83,113	1.46	6 (11%)
18	CLA	7	615	-	42,47,73	1.61	9 (21%)	52,81,113	1.57	6 (11%)
18	CLA	5	608	-	54,58,73	1.40	10 (18%)	65,95,113	1.54	10 (15%)
18	CLA	A	842	1	69,73,73	1.23	10 (14%)	83,113,113	1.35	4 (4%)
18	CLA	4	613	13	69,73,73	1.25	10 (14%)	83,113,113	1.36	7 (8%)
18	CLA	7	603	16	47,52,73	1.49	9 (19%)	56,88,113	1.53	6 (10%)
18	CLA	5	607	-	69,73,73	1.26	9 (13%)	83,113,113	1.57	14 (16%)
18	CLA	1	603	11	57,62,73	1.37	7 (12%)	68,100,113	1.48	5 (7%)
23	LMU	K	208	-	36,36,36	1.21	2 (5%)	47,47,47	1.33	5 (10%)
18	CLA	A	825	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
18	CLA	5	612	14	44,49,73	1.51	10 (22%)	52,84,113	1.54	9 (17%)
18	CLA	6	617	15	49,53,73	1.47	10 (20%)	59,89,113	1.41	4 (6%)
18	CLA	8	603	17	48,52,73	1.52	10 (20%)	61,88,113	1.64	9 (14%)
18	CLA	A	840	1	56,60,73	1.37	8 (14%)	67,97,113	1.54	10 (14%)
18	CLA	A	827	-	63,67,73	1.30	12 (19%)	75,105,113	1.45	11 (14%)
18	CLA	6	602	15	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	L	302	10	49,53,73	1.49	6 (12%)	59,89,113	1.57	6 (10%)
18	CLA	B	825	-	66,70,73	1.29	11 (16%)	79,109,113	1.28	7 (8%)
18	CLA	4	618	13	43,48,73	1.61	10 (23%)	54,83,113	1.61	8 (14%)
18	CLA	5	609	14	69,73,73	1.24	9 (13%)	83,113,113	1.35	10 (12%)
18	CLA	5	618	14	43,48,73	1.61	11 (25%)	54,83,113	1.65	9 (16%)
18	CLA	8	614	17	60,64,73	1.31	10 (16%)	72,102,113	1.47	7 (9%)
21	BCR	A	849	-	41,41,41	0.83	0	56,56,56	2.03	18 (32%)
21	BCR	3	622	-	41,41,41	0.71	0	56,56,56	2.61	21 (37%)
26	LUT	5	620	-	42,43,43	0.77	0	51,60,60	1.64	13 (25%)
18	CLA	5	602	14	69,73,73	1.26	9 (13%)	83,113,113	1.40	8 (9%)
18	CLA	6	612	15	44,49,73	1.51	10 (22%)	52,84,113	1.56	8 (15%)
18	CLA	4	610	13	65,69,73	1.26	9 (13%)	78,108,113	1.41	6 (7%)
21	BCR	B	843	-	41,41,41	0.70	0	56,56,56	1.94	15 (26%)
27	XAT	a	618	-	39,47,47	0.87	1 (2%)	54,74,74	2.61	20 (37%)
18	CLA	B	810	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	5 (6%)
18	CLA	3	609	12	64,68,73	1.29	9 (14%)	77,107,113	1.49	12 (15%)
18	CLA	6	604	-	69,73,73	1.24	11 (15%)	83,113,113	1.31	7 (8%)
21	BCR	K	202	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
21	BCR	B	844	-	41,41,41	0.73	0	56,56,56	2.03	18 (32%)
18	CLA	B	826	2	59,63,73	1.35	9 (15%)	71,101,113	1.52	6 (8%)
18	CLA	J	101	8	46,50,73	1.49	7 (15%)	55,85,113	1.58	6 (10%)
18	CLA	A	829	1	69,73,73	1.21	9 (13%)	83,113,113	1.37	7 (8%)
18	CLA	6	620	-	49,53,73	1.46	11 (22%)	59,89,113	1.71	9 (15%)
18	CLA	A	801	1	69,73,73	1.26	9 (13%)	83,113,113	1.37	8 (9%)
18	CLA	K	204	9	50,54,73	1.43	9 (18%)	60,90,113	1.51	4 (6%)
18	CLA	3	608	-	59,63,73	1.42	11 (18%)	71,101,113	1.45	7 (9%)
18	CLA	8	610	17	64,68,73	1.25	9 (14%)	77,107,113	1.34	8 (10%)
18	CLA	4	602	13	64,68,73	1.28	8 (12%)	77,107,113	1.46	9 (11%)
20	LHG	1	620	18	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
26	LUT	4	619	-	42,43,43	0.79	0	51,60,60	1.62	11 (21%)
27	XAT	7	620	-	39,47,47	0.91	2 (5%)	54,74,74	2.67	20 (37%)
18	CLA	A	810	1	54,58,73	1.41	11 (20%)	65,95,113	1.43	9 (13%)
27	XAT	4	620	-	39,47,47	0.89	1 (2%)	54,74,74	2.61	18 (33%)
26	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.66	14 (27%)
18	CLA	a	606	11	47,52,73	1.50	9 (19%)	55,87,113	1.47	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	8	612	17	44,49,73	1.49	9 (20%)	52,84,113	1.55	9 (17%)
21	BCR	B	801	-	41,41,41	0.71	0	56,56,56	2.01	13 (23%)
21	BCR	L	305	-	41,41,41	0.68	0	56,56,56	1.77	12 (21%)
18	CLA	A	822	-	69,73,73	1.25	9 (13%)	83,113,113	1.42	8 (9%)
18	CLA	A	808	1	54,58,73	1.37	9 (16%)	65,95,113	1.55	7 (10%)
18	CLA	a	607	-	49,53,73	1.47	8 (16%)	59,89,113	1.50	6 (10%)
18	CLA	a	614	11	58,62,73	1.35	9 (15%)	67,99,113	1.37	5 (7%)
18	CLA	4	606	-	43,48,73	1.54	9 (20%)	51,83,113	1.54	6 (11%)
18	CLA	B	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.52	8 (9%)
18	CLA	a	609	11	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
18	CLA	A	815	1	54,58,73	1.40	10 (18%)	65,95,113	1.44	8 (12%)
18	CLA	4	612	13	44,49,73	1.52	9 (20%)	52,84,113	1.50	8 (15%)
20	LHG	B	851	18	35,35,48	0.72	1 (2%)	38,40,54	1.33	5 (13%)
21	BCR	A	848	-	41,41,41	0.77	0	56,56,56	1.86	15 (26%)
18	CLA	A	811	1	69,73,73	1.21	9 (13%)	83,113,113	1.34	6 (7%)
18	CLA	4	607	-	49,53,73	1.48	10 (20%)	59,89,113	1.56	5 (8%)
27	XAT	1	618	-	39,47,47	0.86	1 (2%)	54,74,74	2.59	20 (37%)
26	LUT	3	618	-	42,43,43	0.79	0	51,60,60	1.55	9 (17%)
21	BCR	3	620	-	41,41,41	0.72	0	56,56,56	2.06	19 (33%)
18	CLA	B	828	2	69,73,73	1.26	11 (15%)	83,113,113	1.32	8 (9%)
18	CLA	B	811	2	58,62,73	1.40	10 (17%)	73,100,113	1.41	7 (9%)
18	CLA	A	807	1	69,73,73	1.27	10 (14%)	83,113,113	1.35	6 (7%)
18	CLA	3	613	12	56,61,73	1.35	10 (17%)	66,98,113	1.53	7 (10%)
18	CLA	4	609	13	65,69,73	1.27	7 (10%)	78,108,113	1.42	9 (11%)
24	LMG	5	626	-	40,40,55	0.88	0	48,48,63	1.20	5 (10%)
18	CLA	5	611	20	46,50,73	1.48	8 (17%)	55,85,113	1.48	5 (9%)
18	CLA	6	607	-	45,49,73	1.58	10 (22%)	57,84,113	1.67	8 (14%)
18	CLA	6	601	15	69,73,73	1.23	9 (13%)	83,113,113	1.44	8 (9%)
26	LUT	7	619	-	42,43,43	0.89	2 (4%)	51,60,60	1.85	14 (27%)
18	CLA	1	613	-	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
18	CLA	7	614	16	46,50,73	1.48	9 (19%)	55,85,113	1.51	6 (10%)
18	CLA	B	824	-	69,73,73	1.28	10 (14%)	83,113,113	1.35	9 (10%)
18	CLA	B	821	2	50,54,73	1.48	7 (14%)	60,90,113	1.46	6 (10%)
18	CLA	A	838	1	54,58,73	1.38	10 (18%)	65,95,113	1.59	8 (12%)
18	CLA	6	618	15	43,48,73	1.57	11 (25%)	54,83,113	1.69	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	804	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
21	BCR	7	623	-	41,41,41	0.71	0	56,56,56	1.81	13 (23%)
18	CLA	A	816	1	49,53,73	1.45	9 (18%)	59,89,113	1.62	8 (13%)
18	CLA	A	821	1	57,61,73	1.34	9 (15%)	68,98,113	1.48	5 (7%)
18	CLA	B	802	2	69,73,73	1.24	9 (13%)	83,113,113	1.31	8 (9%)
18	CLA	A	813	1	58,62,73	1.34	10 (17%)	69,99,113	1.52	6 (8%)
20	LHG	a	620	18	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
18	CLA	A	854	-	69,73,73	1.25	11 (15%)	83,113,113	1.41	11 (13%)
20	LHG	A	846	-	48,48,48	0.71	1 (2%)	51,54,54	1.27	6 (11%)
21	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)
18	CLA	B	804	2	45,49,73	1.49	10 (22%)	54,84,113	1.62	9 (16%)
21	BCR	5	622	-	41,41,41	0.69	0	56,56,56	2.11	20 (35%)
18	CLA	3	610	12	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)
23	LMU	A	859	-	35,35,36	1.27	3 (8%)	43,45,47	1.23	4 (9%)
23	LMU	8	625	-	36,36,36	1.19	2 (5%)	47,47,47	1.27	6 (12%)
18	CLA	B	813	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
18	CLA	8	616	17	47,51,73	1.59	7 (14%)	60,87,113	1.68	11 (18%)
21	BCR	1	619	-	41,41,41	0.66	0	56,56,56	1.93	16 (28%)
18	CLA	A	818	1	64,68,73	1.27	9 (14%)	77,107,113	1.49	9 (11%)
18	CLA	B	814	2	68,72,73	1.23	11 (16%)	81,111,113	1.38	7 (8%)
18	CLA	B	819	-	59,63,73	1.37	9 (15%)	71,101,113	1.43	5 (7%)
20	LHG	5	625	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
24	LMG	J	104	-	40,40,55	0.90	2 (5%)	48,48,63	1.22	4 (8%)
18	CLA	K	201	9	49,53,73	1.47	8 (16%)	59,89,113	1.72	10 (16%)
18	CLA	a	608	-	47,52,73	1.51	8 (17%)	56,88,113	1.47	8 (14%)
18	CLA	B	817	2	63,67,73	1.32	11 (17%)	75,105,113	1.44	9 (12%)
18	CLA	3	607	12	60,64,73	1.37	10 (16%)	75,102,113	1.41	10 (13%)
18	CLA	7	606	-	45,49,73	1.52	10 (22%)	54,84,113	1.52	7 (12%)
18	CLA	B	823	2	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
18	CLA	1	612	11	49,53,73	1.47	7 (14%)	59,89,113	1.46	5 (8%)
18	CLA	A	835	1	65,69,73	1.26	9 (13%)	78,108,113	1.55	9 (11%)
20	LHG	6	623	18	47,47,48	0.65	1 (2%)	50,53,54	1.27	6 (12%)
18	CLA	6	608	-	55,59,73	1.39	10 (18%)	66,96,113	1.44	7 (10%)
18	CLA	7	607	-	46,50,73	1.49	9 (19%)	55,85,113	1.58	7 (12%)
24	LMG	5	627	-	40,40,55	0.86	0	48,48,63	1.20	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	803	-	69,73,73	1.24	11 (15%)	83,113,113	1.76	13 (15%)
18	CLA	1	607	-	43,48,73	1.55	9 (20%)	51,83,113	1.54	5 (9%)
18	CLA	B	805	2	69,73,73	1.21	9 (13%)	83,113,113	1.39	9 (10%)
18	CLA	1	609	11	44,48,73	1.62	7 (15%)	56,83,113	1.62	9 (16%)
21	BCR	F	305	-	41,41,41	0.78	0	56,56,56	2.14	18 (32%)
18	CLA	5	614	14	48,52,73	1.50	9 (18%)	55,87,113	1.49	6 (10%)
24	LMG	7	624	-	44,44,55	0.83	0	52,52,63	1.25	5 (9%)
23	LMU	A	857	-	34,34,36	1.38	3 (8%)	44,44,47	1.26	4 (9%)
18	CLA	B	816	2	59,63,73	1.34	10 (16%)	71,101,113	1.46	7 (9%)
18	CLA	K	203	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	8 (9%)
18	CLA	A	802	2	69,73,73	1.21	9 (13%)	83,113,113	1.56	11 (13%)
18	CLA	L	303	10	49,53,73	1.46	8 (16%)	59,89,113	1.47	5 (8%)
18	CLA	1	602	11	65,69,73	1.27	10 (15%)	78,108,113	1.35	6 (7%)
18	CLA	8	602	17	64,68,73	1.29	9 (14%)	77,107,113	1.38	6 (7%)
23	LMU	5	628	-	34,34,36	1.26	2 (5%)	45,45,47	1.31	7 (15%)
28	NEX	5	624	-	38,46,46	1.00	1 (2%)	50,70,70	2.18	16 (32%)
18	CLA	A	836	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
20	LHG	3	623	-	44,44,48	0.60	0	47,50,54	1.26	6 (12%)
18	CLA	B	809	2	69,73,73	1.23	11 (15%)	83,113,113	1.39	6 (7%)
18	CLA	A	833	1	49,53,73	1.47	9 (18%)	59,89,113	1.56	7 (11%)
18	CLA	B	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.36	8 (9%)
18	CLA	6	614	15	64,68,73	1.29	10 (15%)	77,107,113	1.38	5 (6%)
18	CLA	a	611	20	41,46,73	1.64	10 (24%)	52,81,113	1.62	7 (13%)
18	CLA	B	818	2	64,68,73	1.28	11 (17%)	77,107,113	1.45	8 (10%)
18	CLA	B	836	2	54,58,73	1.40	11 (20%)	65,95,113	1.46	7 (10%)
18	CLA	3	603	12	59,63,73	1.38	10 (16%)	71,101,113	1.56	13 (18%)
18	CLA	F	301	-	61,65,73	1.35	10 (16%)	73,103,113	1.39	9 (12%)
22	SF4	C	101	-	0,12,12	-	-	-	-	-
18	CLA	A	823	1	46,50,73	1.46	9 (19%)	55,85,113	1.56	6 (10%)
18	CLA	4	611	20	46,50,73	1.48	10 (21%)	55,85,113	1.43	6 (10%)
18	CLA	8	604	-	54,58,73	1.39	9 (16%)	65,95,113	1.47	6 (9%)
18	CLA	B	837	2	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
18	CLA	5	619	-	47,51,73	1.57	10 (21%)	60,87,113	1.77	11 (18%)
20	LHG	A	847	18	29,29,48	0.83	1 (3%)	32,35,54	1.29	3 (9%)
18	CLA	B	838	2	51,55,73	1.40	8 (15%)	61,91,113	1.49	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	A	852	-	41,41,41	0.78	1 (2%)	56,56,56	2.10	16 (28%)
18	CLA	B	840	2	69,73,73	1.23	9 (13%)	83,113,113	1.42	4 (4%)
18	CLA	7	601	16	64,68,73	1.29	9 (14%)	77,107,113	1.46	8 (10%)
21	BCR	8	621	-	41,41,41	0.71	0	56,56,56	1.94	18 (32%)
18	CLA	3	602	12	64,68,73	1.27	10 (15%)	77,107,113	1.37	7 (9%)
18	CLA	a	613	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	7 (8%)
18	CLA	6	611	20	46,50,73	1.46	10 (21%)	55,85,113	1.46	5 (9%)
18	CLA	7	616	16	47,51,73	1.57	10 (21%)	60,87,113	1.53	6 (10%)
18	CLA	A	828	1	68,72,73	1.24	10 (14%)	81,111,113	1.41	6 (7%)
18	CLA	B	839	-	69,73,73	1.23	9 (13%)	83,113,113	1.37	9 (10%)
18	CLA	8	601	17	69,73,73	1.25	10 (14%)	83,113,113	1.36	10 (12%)
21	BCR	A	856	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
18	CLA	A	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	6 (7%)
18	CLA	4	614	13	60,64,73	1.33	9 (15%)	72,102,113	1.38	7 (9%)
18	CLA	8	606	-	68,72,73	1.28	10 (14%)	82,112,113	1.27	5 (6%)
18	CLA	B	807	2	56,60,73	1.37	10 (17%)	67,97,113	1.41	8 (11%)
18	CLA	A	831	1	69,73,73	1.34	11 (15%)	83,113,113	1.61	16 (19%)
26	LUT	8	619	-	42,43,43	0.77	0	51,60,60	1.58	10 (19%)
18	CLA	B	834	2	64,68,73	1.29	9 (14%)	77,107,113	1.35	7 (9%)
18	CLA	5	613	14	68,72,73	1.23	7 (10%)	81,111,113	1.44	5 (6%)
18	CLA	A	841	1	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
18	CLA	B	841	20	48,52,73	1.51	7 (14%)	57,87,113	1.48	9 (15%)
18	CLA	a	603	11	58,62,73	1.36	7 (12%)	69,99,113	1.46	7 (10%)
18	CLA	F	304	-	45,49,73	1.50	9 (20%)	54,84,113	1.53	7 (12%)
19	PQN	B	842	-	34,34,34	2.90	11 (32%)	42,45,45	2.04	5 (11%)
18	CLA	3	606	-	57,62,73	1.37	9 (15%)	68,100,113	1.39	5 (7%)
18	CLA	A	830	1	69,73,73	1.25	11 (15%)	83,113,113	1.40	9 (10%)
18	CLA	a	612	11	49,53,73	1.47	9 (18%)	59,89,113	1.45	7 (11%)
18	CLA	1	610	11	42,47,73	1.57	9 (21%)	51,81,113	1.56	9 (17%)
18	CLA	3	611	20	41,46,73	1.64	10 (24%)	52,81,113	1.68	8 (15%)
20	LHG	5	623	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
21	BCR	B	847	-	41,41,41	0.73	0	56,56,56	2.00	18 (32%)
26	LUT	a	617	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
18	CLA	4	608	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	5 (6%)
18	CLA	A	819	1	63,67,73	1.32	10 (15%)	75,105,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	B	850	-	63,63,67	0.98	1 (1%)	77,77,81	1.42	11 (14%)
18	CLA	B	830	2	47,51,73	1.52	9 (19%)	56,86,113	1.66	7 (12%)
18	CLA	7	611	20	63,67,73	1.25	9 (14%)	75,105,113	1.40	7 (9%)
20	LHG	8	623	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
18	CLA	1	611	20	69,73,73	1.23	8 (11%)	83,113,113	1.36	7 (8%)
18	CLA	A	809	1	69,73,73	1.21	10 (14%)	83,113,113	1.36	7 (8%)
18	CLA	5	601	14	60,64,73	1.35	9 (15%)	72,102,113	1.38	5 (6%)
18	CLA	A	826	-	68,72,73	1.25	11 (16%)	81,111,113	1.40	10 (12%)
22	SF4	C	102	-	0,12,12	-	-	-	-	-
18	CLA	8	611	20	46,50,73	1.48	10 (21%)	55,85,113	1.48	7 (12%)
18	CLA	4	616	13	47,51,73	1.56	11 (23%)	60,87,113	1.58	7 (11%)
19	PQN	A	844	-	34,34,34	2.87	11 (32%)	42,45,45	2.23	7 (16%)
27	XAT	5	621	-	39,47,47	0.93	0	54,74,74	2.78	21 (38%)
18	CLA	A	843	-	68,72,73	1.23	10 (14%)	81,111,113	1.35	6 (7%)
18	CLA	A	839	1	59,63,73	1.34	9 (15%)	71,101,113	1.42	6 (8%)
24	LMG	4	624	-	40,40,55	0.91	1 (2%)	48,48,63	1.22	4 (8%)
18	CLA	6	606	-	43,48,73	1.54	8 (18%)	51,83,113	1.54	8 (15%)
18	CLA	6	603	15	58,62,73	1.41	10 (17%)	73,100,113	1.43	8 (10%)
18	CLA	B	831	2	69,73,73	1.23	9 (13%)	83,113,113	1.35	5 (6%)
18	CLA	1	614	11	40,45,73	1.67	10 (25%)	50,79,113	1.62	8 (16%)
18	CLA	7	609	16	49,53,73	1.42	8 (16%)	59,89,113	1.66	9 (15%)
21	BCR	B	846	-	41,41,41	0.73	0	56,56,56	2.05	16 (28%)
18	CLA	5	617	14	54,58,73	1.41	8 (14%)	65,95,113	1.53	7 (10%)
18	CLA	7	608	-	54,58,73	1.42	11 (20%)	65,95,113	1.47	9 (13%)
28	NEX	6	624	-	38,46,46	0.93	2 (5%)	50,70,70	2.28	16 (32%)
18	CLA	7	602	16	69,73,73	1.22	10 (14%)	83,113,113	1.32	6 (7%)
27	XAT	8	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.67	19 (35%)
18	CLA	B	822	2	46,50,73	1.52	7 (15%)	55,85,113	1.48	4 (7%)
18	CLA	A	812	1	69,73,73	1.22	8 (11%)	83,113,113	1.37	7 (8%)
18	CLA	K	206	9	49,53,73	1.48	10 (20%)	59,89,113	1.53	5 (8%)
18	CLA	A	820	1	69,73,73	1.27	10 (14%)	83,113,113	1.47	11 (13%)
18	CLA	B	820	2	54,58,73	1.42	7 (12%)	65,95,113	1.49	5 (7%)

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
18	CLA	B	812	2	-	5/13/89/115	-
20	LHG	4	622	18	-	25/53/53/53	-
18	CLA	A	817	-	-	4/15/91/115	-
18	CLA	A	814	1	-	18/39/115/115	-
18	CLA	1	608	-	-	2/13/89/115	-
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
18	CLA	8	608	-	-	11/23/99/115	-
21	BCR	4	621	-	-	4/29/63/63	0/2/2/2
18	CLA	A	837	1	-	10/15/91/115	-
18	CLA	5	603	14	-	7/25/101/115	-
18	CLA	A	832	1	-	6/21/97/115	-
18	CLA	1	606	11	-	3/7/79/115	-
18	CLA	A	805	1	-	3/24/100/115	-
18	CLA	1	616	11	-	4/11/87/115	-
18	CLA	L	304	-	-	9/15/91/115	-
22	SF4	A	853	-	-	-	0/6/5/5
18	CLA	B	832	2	-	8/33/109/115	-
18	CLA	B	827	2	-	17/36/112/115	-
20	LHG	3	624	18	-	27/53/53/53	-
24	LMG	4	623	-	-	12/35/55/70	0/1/1/1
18	CLA	A	824	1	-	4/10/86/115	-
18	CLA	8	609	17	-	6/15/91/115	-
21	BCR	J	102	-	-	7/29/63/63	0/2/2/2
18	CLA	6	613	-	-	16/37/113/115	-
18	CLA	a	601	11	-	8/25/101/115	-
27	XAT	3	619	-	-	2/31/93/93	0/4/4/4
18	CLA	A	845	20	-	13/21/97/115	-
18	CLA	A	806	1	-	15/39/115/115	-
18	CLA	a	610	11	-	6/31/107/115	-
18	CLA	a	602	11	-	8/35/111/115	-
18	CLA	4	604	-	-	10/25/101/115	-
18	CLA	6	609	15	-	6/15/91/115	-
18	CLA	7	613	16	-	14/39/115/115	-
21	BCR	B	845	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMU	8	624	-	-	10/21/61/61	0/2/2/2
18	CLA	a	604	-	-	11/20/96/115	-
18	CLA	3	617	12	-	4/8/84/115	-
18	CLA	4	601	13	-	18/39/115/115	-
18	CLA	8	613	17	-	21/39/115/115	-
20	LHG	7	622	18	-	24/41/41/53	-
23	LMU	A	858	-	-	7/21/57/61	0/2/2/2
18	CLA	5	610	14	-	4/26/102/115	-
18	CLA	B	829	2	-	10/39/115/115	-
18	CLA	B	835	-	-	9/15/91/115	-
18	CLA	3	612	12	-	3/13/89/115	-
18	CLA	a	616	11	-	6/15/91/115	-
18	CLA	7	610	16	-	10/39/115/115	-
20	LHG	8	622	18	-	25/53/53/53	-
21	BCR	a	619	-	-	2/29/63/63	0/2/2/2
18	CLA	6	616	15	-	18/39/115/115	-
21	BCR	B	848	-	-	4/29/63/63	0/2/2/2
18	CLA	4	603	13	-	5/13/89/115	-
18	CLA	6	610	15	-	12/39/115/115	-
18	CLA	3	614	12	-	2/8/84/115	-
18	CLA	3	604	-	-	9/39/115/115	-
18	CLA	7	612	16	-	5/13/89/115	-
18	CLA	5	616	14	-	4/8/84/115	-
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
18	CLA	8	607	-	-	5/10/86/115	-
26	LUT	6	619	-	-	2/29/67/67	0/2/2/2
21	BCR	A	851	-	-	5/29/63/63	0/2/2/2
21	BCR	3	621	-	-	6/29/63/63	0/2/2/2
18	CLA	B	833	2	-	18/39/115/115	-
18	CLA	5	604	-	-	15/35/111/115	-
18	CLA	F	303	-	-	7/12/88/115	-
18	CLA	3	615	-	-	3/8/84/115	-
18	CLA	7	604	-	-	8/25/101/115	-
18	CLA	1	604	-	-	12/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	815	2	-	4/13/89/115	-
24	LMG	A	860	-	-	14/35/55/70	0/1/1/1
21	BCR	6	622	-	-	6/29/63/63	0/2/2/2
18	CLA	1	601	11	-	5/25/101/115	-
18	CLA	A	803	-	-	7/39/115/115	-
21	BCR	7	621	-	-	2/29/63/63	0/2/2/2
25	DGD	J	103	-	-	26/47/87/95	0/2/2/2
27	XAT	6	621	-	-	2/31/93/93	0/4/4/4
18	CLA	5	606	-	-	3/8/84/115	-
18	CLA	7	615	-	-	2/5/81/115	-
18	CLA	5	608	-	-	7/21/97/115	-
18	CLA	A	842	1	-	12/39/115/115	-
18	CLA	4	613	13	-	15/39/115/115	-
18	CLA	7	603	16	-	6/13/89/115	-
18	CLA	5	607	-	-	17/39/115/115	-
18	CLA	1	603	11	-	15/25/101/115	-
23	LMU	K	208	-	-	12/21/61/61	0/2/2/2
18	CLA	A	825	1	-	22/39/115/115	-
18	CLA	5	612	14	-	2/10/86/115	-
18	CLA	6	617	15	-	7/15/91/115	-
18	CLA	8	603	17	-	7/13/89/115	-
18	CLA	A	840	1	-	4/24/100/115	-
18	CLA	A	827	-	-	6/32/108/115	-
18	CLA	6	602	15	-	9/39/115/115	-
18	CLA	L	302	10	-	9/15/91/115	-
18	CLA	B	825	-	-	11/36/112/115	-
18	CLA	4	618	13	-	1/8/84/115	-
18	CLA	5	609	14	-	14/39/115/115	-
18	CLA	5	618	14	-	0/8/84/115	-
18	CLA	8	614	17	-	10/29/105/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
21	BCR	3	622	-	-	8/29/63/63	0/2/2/2
26	LUT	5	620	-	-	2/29/67/67	0/2/2/2
18	CLA	5	602	14	-	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	6	612	15	-	3/10/86/115	-
18	CLA	4	610	13	-	9/35/111/115	-
21	BCR	B	843	-	-	5/29/63/63	0/2/2/2
27	XAT	a	618	-	-	1/31/93/93	0/4/4/4
18	CLA	B	810	2	-	14/39/115/115	-
18	CLA	3	609	12	-	22/33/109/115	-
18	CLA	6	604	-	-	20/39/115/115	-
21	BCR	K	202	-	-	4/29/63/63	0/2/2/2
21	BCR	B	844	-	-	9/29/63/63	0/2/2/2
18	CLA	B	826	2	-	6/27/103/115	-
18	CLA	J	101	8	-	7/12/88/115	-
18	CLA	A	829	1	-	8/39/115/115	-
18	CLA	6	620	-	-	9/15/91/115	-
18	CLA	A	801	1	-	11/39/115/115	-
18	CLA	K	204	9	-	9/17/93/115	-
18	CLA	3	608	-	-	9/27/103/115	-
18	CLA	8	610	17	-	7/33/109/115	-
18	CLA	4	602	13	-	7/33/109/115	-
20	LHG	1	620	18	-	17/53/53/53	-
26	LUT	4	619	-	-	2/29/67/67	0/2/2/2
27	XAT	7	620	-	-	1/31/93/93	0/4/4/4
18	CLA	A	810	1	-	7/21/97/115	-
27	XAT	4	620	-	-	1/31/93/93	0/4/4/4
26	LUT	1	617	-	-	4/29/67/67	0/2/2/2
18	CLA	a	606	11	-	6/12/88/115	-
18	CLA	8	612	17	-	2/10/86/115	-
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
18	CLA	A	822	-	-	13/39/115/115	-
18	CLA	A	808	1	-	6/21/97/115	-
18	CLA	a	607	-	-	7/15/91/115	-
18	CLA	a	614	11	-	9/27/99/115	-
18	CLA	4	606	-	-	4/8/84/115	-
18	CLA	B	808	2	-	16/39/115/115	-
18	CLA	a	609	11	-	22/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	815	1	-	10/21/97/115	-
18	CLA	4	612	13	-	2/10/86/115	-
20	LHG	B	851	18	-	19/39/39/53	-
21	BCR	A	848	-	-	4/29/63/63	0/2/2/2
18	CLA	A	811	1	-	17/39/115/115	-
18	CLA	4	607	-	-	8/15/91/115	-
27	XAT	1	618	-	-	1/31/93/93	0/4/4/4
26	LUT	3	618	-	-	2/29/67/67	0/2/2/2
21	BCR	3	620	-	-	5/29/63/63	0/2/2/2
18	CLA	B	828	2	-	13/39/115/115	-
18	CLA	B	811	2	-	9/25/101/115	-
18	CLA	A	807	1	-	15/39/115/115	-
18	CLA	3	613	12	-	7/23/99/115	-
18	CLA	4	609	13	-	6/35/111/115	-
24	LMG	5	626	-	-	26/35/55/70	0/1/1/1
18	CLA	5	611	20	-	7/12/88/115	-
18	CLA	6	607	-	-	4/10/86/115	-
18	CLA	6	601	15	-	16/39/115/115	-
26	LUT	7	619	-	-	2/29/67/67	0/2/2/2
18	CLA	1	613	-	-	11/39/115/115	-
18	CLA	7	614	16	-	6/12/88/115	-
18	CLA	B	824	-	-	14/39/115/115	-
18	CLA	B	821	2	-	9/16/92/115	-
18	CLA	A	838	1	-	7/21/97/115	-
18	CLA	6	618	15	-	2/8/84/115	-
18	CLA	A	804	1	-	16/39/115/115	-
21	BCR	7	623	-	-	3/29/63/63	0/2/2/2
18	CLA	A	816	1	-	4/15/91/115	-
18	CLA	A	821	1	-	13/25/101/115	-
18	CLA	B	802	2	-	20/39/115/115	-
18	CLA	A	813	1	-	4/26/102/115	-
20	LHG	a	620	18	-	10/53/53/53	-
18	CLA	A	854	-	-	14/39/115/115	-
20	LHG	A	846	-	-	34/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	K	207	-	-	4/29/63/63	0/2/2/2
18	CLA	B	804	2	-	3/10/86/115	-
21	BCR	5	622	-	-	6/29/63/63	0/2/2/2
18	CLA	3	610	12	-	8/39/115/115	-
23	LMU	A	859	-	-	9/21/57/61	0/2/2/2
23	LMU	8	625	-	-	11/21/61/61	0/2/2/2
18	CLA	B	813	2	-	23/39/115/115	-
18	CLA	8	616	17	-	11/11/87/115	-
21	BCR	1	619	-	-	0/29/63/63	0/2/2/2
18	CLA	A	818	1	-	13/33/109/115	-
18	CLA	B	814	2	-	13/38/114/115	-
18	CLA	B	819	-	-	8/27/103/115	-
20	LHG	5	625	-	-	31/53/53/53	-
24	LMG	J	104	-	-	17/35/55/70	0/1/1/1
18	CLA	K	201	9	-	10/15/91/115	-
18	CLA	a	608	-	-	4/13/89/115	-
18	CLA	B	817	2	-	12/32/108/115	-
18	CLA	3	607	12	-	6/28/104/115	-
18	CLA	7	606	-	-	4/10/86/115	-
18	CLA	B	823	2	-	7/15/91/115	-
18	CLA	1	612	11	-	7/15/91/115	-
18	CLA	A	835	1	-	13/35/111/115	-
20	LHG	6	623	18	-	26/52/52/53	-
18	CLA	6	608	-	-	9/23/99/115	-
18	CLA	7	607	-	-	8/12/88/115	-
24	LMG	5	627	-	-	15/35/55/70	0/1/1/1
18	CLA	B	803	-	-	12/39/115/115	-
18	CLA	1	607	-	-	2/8/84/115	-
18	CLA	B	805	2	-	14/39/115/115	-
18	CLA	1	609	11	-	3/8/84/115	-
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
18	CLA	5	614	14	-	9/15/87/115	-
24	LMG	7	624	-	-	15/39/59/70	0/1/1/1
23	LMU	A	857	-	-	9/19/56/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	816	2	-	12/27/103/115	-
18	CLA	K	203	-	-	12/39/115/115	-
18	CLA	A	802	2	-	11/39/115/115	-
18	CLA	L	303	10	-	8/15/91/115	-
18	CLA	1	602	11	-	9/35/111/115	-
18	CLA	8	602	17	-	9/33/109/115	-
23	LMU	5	628	-	-	12/19/59/61	0/2/2/2
28	NEX	5	624	-	-	2/27/83/83	0/3/3/3
18	CLA	A	836	1	-	15/39/115/115	-
20	LHG	3	623	-	-	22/49/49/53	-
18	CLA	B	809	2	-	18/39/115/115	-
18	CLA	A	833	1	-	2/15/91/115	-
18	CLA	B	806	2	-	13/39/115/115	-
18	CLA	6	614	15	-	13/33/109/115	-
18	CLA	a	611	20	-	0/4/80/115	-
18	CLA	B	818	2	-	15/33/109/115	-
18	CLA	B	836	2	-	7/21/97/115	-
18	CLA	3	603	12	-	7/27/103/115	-
18	CLA	F	301	-	-	10/30/106/115	-
22	SF4	C	101	-	-	-	0/6/5/5
18	CLA	A	823	1	-	4/12/88/115	-
18	CLA	4	611	20	-	6/12/88/115	-
18	CLA	8	604	-	-	11/21/97/115	-
18	CLA	B	837	2	-	8/39/115/115	-
18	CLA	5	619	-	-	7/11/87/115	-
20	LHG	A	847	18	-	17/34/34/53	-
18	CLA	B	838	2	-	8/18/94/115	-
21	BCR	A	852	-	-	7/29/63/63	0/2/2/2
18	CLA	B	840	2	-	9/39/115/115	-
18	CLA	7	601	16	-	14/33/109/115	-
21	BCR	8	621	-	-	6/29/63/63	0/2/2/2
18	CLA	3	602	12	-	5/33/109/115	-
18	CLA	a	613	-	-	13/39/115/115	-
18	CLA	6	611	20	-	4/12/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	7	616	16	-	7/11/87/115	-
18	CLA	A	828	1	-	12/37/113/115	-
18	CLA	B	839	-	-	11/39/115/115	-
18	CLA	8	601	17	-	18/39/115/115	-
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
18	CLA	A	834	1	-	14/39/115/115	-
18	CLA	4	614	13	-	14/29/105/115	-
18	CLA	8	606	-	-	9/37/113/115	-
18	CLA	B	807	2	-	7/24/100/115	-
18	CLA	A	831	1	-	9/39/115/115	-
26	LUT	8	619	-	-	2/29/67/67	0/2/2/2
18	CLA	B	834	2	-	13/33/109/115	-
18	CLA	5	613	14	-	22/37/113/115	-
18	CLA	A	841	1	-	20/39/115/115	-
18	CLA	B	841	20	-	7/14/90/115	-
18	CLA	a	603	11	-	8/25/101/115	-
18	CLA	F	304	-	-	6/10/86/115	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
18	CLA	3	606	-	-	10/25/101/115	-
18	CLA	A	830	1	-	20/39/115/115	-
18	CLA	a	612	11	-	5/15/91/115	-
18	CLA	1	610	11	-	2/8/80/115	-
18	CLA	3	611	20	-	0/4/80/115	-
20	LHG	5	623	18	-	24/53/53/53	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	LUT	a	617	-	-	5/29/67/67	0/2/2/2
18	CLA	4	608	-	-	15/39/115/115	-
18	CLA	A	819	1	-	10/32/108/115	-
25	DGD	B	850	-	-	23/51/91/95	0/2/2/2
18	CLA	B	830	2	-	7/13/89/115	-
18	CLA	7	611	20	-	12/31/107/115	-
20	LHG	8	623	-	-	33/53/53/53	-
18	CLA	1	611	20	-	13/39/115/115	-
18	CLA	A	809	1	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	5	601	14	-	8/29/105/115	-
18	CLA	A	826	-	-	13/37/113/115	-
22	SF4	C	102	-	-	-	0/6/5/5
18	CLA	8	611	20	-	6/12/88/115	-
18	CLA	4	616	13	-	7/11/87/115	-
19	PQN	A	844	-	-	7/23/43/43	0/2/2/2
27	XAT	5	621	-	-	2/31/93/93	0/4/4/4
18	CLA	A	843	-	-	18/37/113/115	-
18	CLA	A	839	1	-	6/27/103/115	-
24	LMG	4	624	-	-	13/35/55/70	0/1/1/1
18	CLA	6	606	-	-	4/8/84/115	-
18	CLA	6	603	15	-	7/25/101/115	-
18	CLA	B	831	2	-	10/39/115/115	-
18	CLA	1	614	11	-	0/4/76/115	-
18	CLA	7	609	16	-	6/15/91/115	-
21	BCR	B	846	-	-	2/29/63/63	0/2/2/2
18	CLA	5	617	14	-	10/21/97/115	-
18	CLA	7	608	-	-	5/21/97/115	-
28	NEX	6	624	-	-	4/27/83/83	0/3/3/3
18	CLA	7	602	16	-	15/39/115/115	-
27	XAT	8	620	-	-	2/31/93/93	0/4/4/4
18	CLA	B	822	2	-	4/12/88/115	-
18	CLA	A	812	1	-	15/39/115/115	-
18	CLA	K	206	9	-	9/15/91/115	-
18	CLA	A	820	1	-	16/39/115/115	-
18	CLA	B	820	2	-	10/21/97/115	-

All (2102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	842	PQN	C12-C13	8.68	1.53	1.33
19	A	844	PQN	C12-C13	8.32	1.52	1.33
19	A	844	PQN	O1-C1	8.02	1.40	1.23
19	B	842	PQN	O1-C1	7.81	1.39	1.23
19	B	842	PQN	O4-C4	7.53	1.39	1.23
19	A	844	PQN	O4-C4	7.40	1.38	1.23
19	B	842	PQN	C2-C1	-4.34	1.38	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	609	CLA	C1D-ND	4.30	1.43	1.37
20	8	622	LHG	O8-C23	4.27	1.45	1.33
19	A	844	PQN	C2-C1	-4.25	1.38	1.48
20	8	622	LHG	O7-C7	4.09	1.45	1.34
18	a	609	CLA	C1D-ND	4.05	1.42	1.37
18	B	821	CLA	C1D-ND	4.04	1.42	1.37
18	B	822	CLA	C1D-ND	3.98	1.42	1.37
18	F	303	CLA	C1D-ND	3.98	1.42	1.37
18	3	608	CLA	C4D-ND	-3.97	1.32	1.37
18	B	830	CLA	C1D-ND	3.94	1.42	1.37
18	A	831	CLA	CMB-C2B	-3.93	1.42	1.50
18	J	101	CLA	C1D-ND	3.91	1.42	1.37
18	B	820	CLA	C1D-ND	3.90	1.42	1.37
18	L	302	CLA	C1D-ND	3.90	1.42	1.37
18	B	841	CLA	C1D-ND	3.89	1.42	1.37
23	A	857	LMU	O5'-C1'	3.88	1.50	1.41
23	A	858	LMU	O5B-C1B	3.88	1.51	1.41
18	1	608	CLA	C1D-ND	3.88	1.42	1.37
23	5	628	LMU	O5B-C1B	3.86	1.51	1.41
18	8	616	CLA	C1D-ND	3.84	1.42	1.37
18	a	606	CLA	C1D-ND	3.84	1.42	1.37
18	1	604	CLA	C1D-ND	3.83	1.42	1.37
18	1	603	CLA	C1D-ND	3.82	1.42	1.37
18	5	607	CLA	C1D-ND	3.82	1.42	1.37
18	3	609	CLA	C1D-ND	3.81	1.42	1.37
18	4	609	CLA	C1D-ND	3.81	1.42	1.37
18	1	610	CLA	C1D-ND	3.80	1.42	1.37
18	B	824	CLA	C1D-ND	3.79	1.42	1.37
18	1	607	CLA	C1D-ND	3.79	1.42	1.37
18	B	803	CLA	C4D-ND	-3.78	1.32	1.37
18	K	203	CLA	C1D-ND	3.78	1.42	1.37
18	a	610	CLA	C1D-ND	3.77	1.42	1.37
18	4	610	CLA	C1D-ND	3.77	1.42	1.37
18	K	206	CLA	C1D-ND	3.77	1.42	1.37
18	a	603	CLA	C1D-ND	3.76	1.42	1.37
18	4	616	CLA	C1D-ND	3.76	1.42	1.37
18	a	604	CLA	C1D-ND	3.76	1.42	1.37
18	5	610	CLA	C1D-ND	3.76	1.42	1.37
18	a	611	CLA	C1D-ND	3.75	1.42	1.37
23	K	208	LMU	O5'-C1'	3.75	1.51	1.41
18	L	304	CLA	C1D-ND	3.75	1.42	1.37
18	7	615	CLA	C1D-ND	3.74	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	608	CLA	C1D-ND	3.73	1.42	1.37
23	A	857	LMU	O5B-C1B	3.73	1.51	1.41
18	7	612	CLA	C4B-NB	3.73	1.42	1.37
18	A	817	CLA	C1D-ND	3.72	1.42	1.37
18	1	613	CLA	C1D-ND	3.72	1.42	1.37
18	5	613	CLA	C1D-ND	3.72	1.42	1.37
18	B	810	CLA	C1D-ND	3.71	1.42	1.37
23	8	624	LMU	O5B-C1B	3.71	1.51	1.41
18	4	607	CLA	C1D-ND	3.71	1.42	1.37
18	A	837	CLA	C1D-ND	3.71	1.42	1.37
18	B	812	CLA	C1D-ND	3.71	1.42	1.37
18	1	606	CLA	C1D-ND	3.70	1.42	1.37
23	A	859	LMU	O5'-C1'	3.70	1.51	1.42
18	a	613	CLA	C1D-ND	3.70	1.42	1.37
18	3	615	CLA	C1D-ND	3.69	1.42	1.37
18	B	813	CLA	C1D-ND	3.69	1.42	1.37
18	5	603	CLA	CAB-C3B	-3.69	1.43	1.50
18	7	606	CLA	C1D-ND	3.69	1.42	1.37
18	A	831	CLA	C4D-ND	-3.67	1.32	1.37
18	B	817	CLA	C1D-ND	3.67	1.42	1.37
18	K	204	CLA	C1D-ND	3.67	1.42	1.37
23	K	208	LMU	O5B-C1B	3.66	1.51	1.41
18	B	835	CLA	C1D-ND	3.66	1.42	1.37
18	A	806	CLA	C4D-ND	-3.66	1.32	1.37
18	4	618	CLA	C1D-ND	3.66	1.42	1.37
18	8	609	CLA	C1D-ND	3.66	1.42	1.37
18	4	602	CLA	C1D-ND	3.65	1.42	1.37
23	5	628	LMU	O5'-C1'	3.65	1.51	1.41
18	4	614	CLA	C1D-ND	3.65	1.42	1.37
18	B	829	CLA	CMB-C2B	-3.65	1.43	1.50
18	B	819	CLA	C1D-ND	3.64	1.42	1.37
18	B	825	CLA	C4D-ND	-3.64	1.32	1.37
18	F	304	CLA	C1D-ND	3.64	1.42	1.37
18	A	835	CLA	C1D-ND	3.64	1.42	1.37
18	3	612	CLA	C1D-ND	3.64	1.42	1.37
18	B	823	CLA	C1D-ND	3.64	1.42	1.37
18	A	807	CLA	C4D-ND	-3.63	1.32	1.37
18	3	607	CLA	C1D-ND	3.63	1.42	1.37
18	B	828	CLA	C4D-ND	-3.63	1.32	1.37
18	1	612	CLA	C1D-ND	3.63	1.42	1.37
18	5	616	CLA	C1D-ND	3.63	1.42	1.37
18	8	606	CLA	C1D-ND	3.63	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	611	CLA	C1D-ND	3.63	1.42	1.37
18	B	834	CLA	C1D-ND	3.62	1.42	1.37
18	8	608	CLA	C1D-ND	3.62	1.42	1.37
18	3	603	CLA	C1D-ND	3.62	1.42	1.37
18	A	833	CLA	C1D-ND	3.61	1.42	1.37
18	A	812	CLA	C4D-ND	-3.61	1.32	1.37
18	A	839	CLA	C4D-ND	-3.61	1.32	1.37
18	7	613	CLA	C1D-ND	3.61	1.42	1.37
18	B	815	CLA	C1D-ND	3.61	1.42	1.37
19	B	842	PQN	C3-C2	3.61	1.41	1.35
18	a	607	CLA	C1D-ND	3.60	1.42	1.37
18	5	614	CLA	C1D-ND	3.59	1.42	1.37
18	3	614	CLA	C1D-ND	3.59	1.42	1.37
18	6	614	CLA	C1D-ND	3.58	1.42	1.37
18	5	603	CLA	C4D-ND	-3.57	1.32	1.37
18	7	601	CLA	C4D-ND	-3.57	1.32	1.37
18	A	833	CLA	C4D-ND	-3.56	1.32	1.37
18	3	606	CLA	C1D-ND	3.56	1.42	1.37
18	A	803	CLA	C4D-ND	-3.55	1.32	1.37
18	4	604	CLA	C1D-ND	3.55	1.42	1.37
18	B	824	CLA	C4B-NB	3.55	1.42	1.37
18	1	601	CLA	C1D-ND	3.55	1.42	1.37
18	A	814	CLA	C4D-ND	-3.55	1.32	1.37
18	B	829	CLA	C4D-ND	-3.54	1.32	1.37
18	4	611	CLA	C1D-ND	3.54	1.42	1.37
18	6	601	CLA	C1D-ND	3.54	1.42	1.37
18	7	611	CLA	C1D-ND	3.54	1.42	1.37
18	6	606	CLA	C1D-ND	3.54	1.42	1.37
18	5	611	CLA	C1D-ND	3.54	1.42	1.37
18	4	608	CLA	C1D-ND	3.53	1.42	1.37
18	8	603	CLA	C1D-ND	3.53	1.42	1.37
18	7	612	CLA	C3B-C4B	3.53	1.51	1.42
18	7	608	CLA	C1D-ND	3.53	1.42	1.37
18	6	602	CLA	C1D-ND	3.53	1.42	1.37
18	a	614	CLA	C1D-ND	3.52	1.42	1.37
18	A	845	CLA	C1D-ND	3.52	1.42	1.37
18	6	611	CLA	C1D-ND	3.52	1.42	1.37
18	1	609	CLA	C4B-NB	3.52	1.42	1.37
18	5	612	CLA	C1D-ND	3.52	1.42	1.37
18	A	829	CLA	C1D-ND	3.51	1.42	1.37
18	A	839	CLA	C1D-ND	3.51	1.42	1.37
18	5	619	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)
18	6	604	CLA	C1D-ND	3.51	1.42	1.37
18	A	825	CLA	C4D-ND	-3.51	1.32	1.37
18	A	819	CLA	C4D-ND	-3.51	1.32	1.37
18	4	602	CLA	C4D-ND	-3.50	1.32	1.37
18	B	832	CLA	C4D-ND	-3.50	1.32	1.37
18	A	834	CLA	C1D-ND	3.50	1.42	1.37
18	1	602	CLA	C1D-ND	3.50	1.42	1.37
18	B	805	CLA	C4D-ND	-3.50	1.32	1.37
18	7	603	CLA	C1D-ND	3.50	1.42	1.37
18	7	616	CLA	C1D-ND	3.50	1.42	1.37
18	B	821	CLA	C4B-NB	3.50	1.42	1.37
18	B	831	CLA	C1D-ND	3.50	1.42	1.37
18	A	825	CLA	C1D-ND	3.49	1.42	1.37
18	3	610	CLA	C4D-ND	-3.49	1.32	1.37
18	A	816	CLA	C1D-ND	3.49	1.42	1.37
18	4	603	CLA	C1D-ND	3.49	1.42	1.37
18	5	606	CLA	C3B-C4B	3.49	1.50	1.42
18	5	602	CLA	C4D-ND	-3.48	1.32	1.37
18	3	610	CLA	C1D-ND	3.48	1.42	1.37
18	A	824	CLA	C1D-ND	3.48	1.42	1.37
18	8	608	CLA	C4D-ND	-3.48	1.32	1.37
18	B	826	CLA	C1D-ND	3.48	1.42	1.37
18	5	609	CLA	C1D-ND	3.48	1.42	1.37
18	1	601	CLA	C4D-ND	-3.48	1.32	1.37
18	B	807	CLA	C1D-ND	3.47	1.42	1.37
18	1	614	CLA	C1D-ND	3.47	1.42	1.37
18	B	838	CLA	C4D-ND	-3.47	1.32	1.37
18	5	606	CLA	C4B-NB	3.47	1.42	1.37
23	8	625	LMU	O5'-C1'	3.47	1.50	1.41
18	B	822	CLA	C4B-NB	3.47	1.42	1.37
18	B	833	CLA	C1D-ND	3.47	1.42	1.37
18	1	616	CLA	C4B-NB	3.47	1.42	1.37
18	4	613	CLA	C1D-ND	3.47	1.42	1.37
18	5	601	CLA	C1D-ND	3.47	1.42	1.37
18	6	608	CLA	C1D-ND	3.47	1.42	1.37
18	a	602	CLA	C1D-ND	3.46	1.42	1.37
18	1	608	CLA	C4B-NB	3.46	1.42	1.37
18	8	610	CLA	C1D-ND	3.46	1.42	1.37
18	3	617	CLA	C1D-ND	3.46	1.42	1.37
18	5	617	CLA	C1D-ND	3.46	1.42	1.37
18	A	838	CLA	C4D-ND	-3.46	1.32	1.37
18	3	603	CLA	C4D-ND	-3.46	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	604	CLA	C1D-ND	3.46	1.42	1.37
23	A	858	LMU	O5'-C1'	3.45	1.50	1.41
18	8	604	CLA	C1D-ND	3.45	1.42	1.37
18	7	614	CLA	C1D-ND	3.45	1.42	1.37
18	A	805	CLA	C4D-ND	-3.45	1.33	1.37
18	5	608	CLA	C1D-ND	3.45	1.42	1.37
18	F	303	CLA	C4B-NB	3.45	1.42	1.37
18	6	617	CLA	C1D-ND	3.45	1.42	1.37
18	A	810	CLA	C4D-ND	-3.45	1.33	1.37
18	B	826	CLA	C4D-ND	-3.44	1.33	1.37
18	B	816	CLA	C1D-ND	3.44	1.42	1.37
18	B	806	CLA	C4D-ND	-3.44	1.33	1.37
18	8	614	CLA	C1D-ND	3.44	1.42	1.37
18	4	612	CLA	C1D-ND	3.43	1.42	1.37
18	A	802	CLA	C4D-ND	-3.43	1.33	1.37
18	7	604	CLA	C1D-ND	3.43	1.42	1.37
23	8	625	LMU	O5B-C1B	3.43	1.50	1.41
18	A	854	CLA	C4D-ND	-3.43	1.33	1.37
18	A	807	CLA	C1D-ND	3.43	1.42	1.37
18	5	618	CLA	C1D-ND	3.43	1.42	1.37
18	5	608	CLA	C4D-ND	-3.43	1.33	1.37
18	5	606	CLA	C1D-ND	3.42	1.42	1.37
18	A	836	CLA	C1D-ND	3.42	1.42	1.37
18	7	608	CLA	C4D-ND	-3.42	1.33	1.37
19	A	844	PQN	C3-C2	3.42	1.41	1.35
23	A	859	LMU	O5B-C1B	3.42	1.50	1.41
18	3	611	CLA	C1D-ND	3.42	1.42	1.37
18	B	807	CLA	C4D-ND	-3.41	1.33	1.37
18	A	801	CLA	C1D-ND	3.41	1.42	1.37
18	A	813	CLA	C4D-ND	-3.41	1.33	1.37
18	A	830	CLA	C4D-ND	-3.41	1.33	1.37
18	3	608	CLA	C1D-ND	3.41	1.42	1.37
18	6	616	CLA	C1D-ND	3.41	1.42	1.37
18	7	601	CLA	C1D-ND	3.41	1.42	1.37
18	B	818	CLA	C4D-ND	-3.41	1.33	1.37
18	a	612	CLA	C1D-ND	3.40	1.42	1.37
18	6	612	CLA	C1D-ND	3.40	1.42	1.37
18	B	833	CLA	C4D-ND	-3.40	1.33	1.37
18	B	837	CLA	C1D-ND	3.40	1.42	1.37
18	A	811	CLA	C4D-ND	-3.40	1.33	1.37
18	B	832	CLA	C1D-ND	3.40	1.42	1.37
18	1	603	CLA	C4B-NB	3.40	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	602	CLA	C4D-ND	-3.40	1.33	1.37
18	6	610	CLA	C1D-ND	3.39	1.42	1.37
18	8	613	CLA	C1D-ND	3.39	1.42	1.37
18	B	811	CLA	C1D-ND	3.39	1.41	1.37
18	4	604	CLA	CAB-C3B	-3.39	1.43	1.50
18	7	612	CLA	C4D-ND	-3.39	1.33	1.37
18	B	808	CLA	C1D-ND	3.39	1.41	1.37
18	5	604	CLA	C1D-ND	3.39	1.41	1.37
18	5	607	CLA	C4D-ND	-3.38	1.33	1.37
18	B	836	CLA	C1D-ND	3.38	1.41	1.37
18	8	612	CLA	C1D-ND	3.38	1.41	1.37
18	L	302	CLA	C4B-NB	3.38	1.41	1.37
18	1	616	CLA	C1D-ND	3.38	1.41	1.37
18	K	201	CLA	C4B-NB	3.38	1.41	1.37
18	A	808	CLA	C1D-ND	3.37	1.41	1.37
18	8	602	CLA	C4D-ND	-3.37	1.33	1.37
18	A	828	CLA	C1D-ND	3.37	1.41	1.37
18	B	823	CLA	C4B-NB	3.36	1.41	1.37
18	B	840	CLA	C4D-ND	-3.36	1.33	1.37
18	4	613	CLA	C4D-ND	-3.36	1.33	1.37
18	A	814	CLA	C1D-ND	3.36	1.41	1.37
18	a	616	CLA	C1D-ND	3.36	1.41	1.37
19	B	842	PQN	C3-C4	-3.36	1.38	1.47
18	7	607	CLA	C1D-ND	3.36	1.41	1.37
18	8	614	CLA	C4D-ND	-3.36	1.33	1.37
18	A	842	CLA	C1D-ND	3.36	1.41	1.37
18	A	829	CLA	C4D-ND	-3.35	1.33	1.37
18	B	837	CLA	C4D-ND	-3.35	1.33	1.37
18	B	836	CLA	C4D-ND	-3.35	1.33	1.37
18	8	607	CLA	C1D-ND	3.35	1.41	1.37
18	B	820	CLA	C4B-NB	3.35	1.41	1.37
18	A	820	CLA	C4D-ND	-3.35	1.33	1.37
18	A	840	CLA	C4D-ND	-3.35	1.33	1.37
18	7	602	CLA	C4D-ND	-3.35	1.33	1.37
18	4	606	CLA	C1D-ND	3.35	1.41	1.37
18	B	817	CLA	C4D-ND	-3.35	1.33	1.37
18	4	601	CLA	C4D-ND	-3.35	1.33	1.37
18	B	809	CLA	C4D-ND	-3.35	1.33	1.37
18	L	303	CLA	C1D-ND	3.35	1.41	1.37
18	a	603	CLA	C4B-NB	3.34	1.41	1.37
18	8	606	CLA	C3B-C4B	3.34	1.50	1.42
18	7	602	CLA	C1D-ND	3.34	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	C1D-ND	3.34	1.41	1.37
23	8	624	LMU	O5'-C1'	3.34	1.50	1.41
18	A	823	CLA	C4D-ND	-3.33	1.33	1.37
18	A	827	CLA	C1D-ND	3.33	1.41	1.37
18	1	606	CLA	C4B-NB	3.33	1.41	1.37
18	8	602	CLA	C1D-ND	3.33	1.41	1.37
18	a	612	CLA	C4B-NB	3.32	1.41	1.37
18	a	608	CLA	C4B-NB	3.32	1.41	1.37
18	7	612	CLA	C1D-ND	3.32	1.41	1.37
18	7	614	CLA	C4D-ND	-3.32	1.33	1.37
18	6	607	CLA	C4D-ND	-3.32	1.33	1.37
18	5	602	CLA	C1D-ND	3.32	1.41	1.37
18	6	607	CLA	C1D-ND	3.32	1.41	1.37
18	B	839	CLA	C4D-ND	-3.32	1.33	1.37
18	A	815	CLA	C4D-ND	-3.32	1.33	1.37
18	1	610	CLA	C4B-NB	3.31	1.41	1.37
18	A	822	CLA	C4D-ND	-3.31	1.33	1.37
18	A	826	CLA	C4D-ND	-3.31	1.33	1.37
18	A	820	CLA	C1D-ND	3.31	1.41	1.37
18	B	825	CLA	C1D-ND	3.31	1.41	1.37
18	B	841	CLA	C4B-NB	3.31	1.41	1.37
18	A	843	CLA	C1D-ND	3.31	1.41	1.37
18	8	611	CLA	C4D-ND	-3.31	1.33	1.37
18	1	602	CLA	C4D-ND	-3.30	1.33	1.37
18	a	602	CLA	C4D-ND	-3.30	1.33	1.37
18	A	805	CLA	C1D-ND	3.30	1.41	1.37
18	B	812	CLA	C4B-NB	3.30	1.41	1.37
19	A	844	PQN	C3-C4	-3.30	1.38	1.47
18	6	602	CLA	C4D-ND	-3.30	1.33	1.37
18	3	602	CLA	C1D-ND	3.30	1.41	1.37
18	A	804	CLA	C1D-ND	3.30	1.41	1.37
18	B	818	CLA	C1D-ND	3.30	1.41	1.37
18	1	612	CLA	C4B-NB	3.30	1.41	1.37
18	6	603	CLA	C1D-ND	3.29	1.41	1.37
18	F	301	CLA	C4D-ND	-3.29	1.33	1.37
18	B	827	CLA	C4D-ND	-3.29	1.33	1.37
18	A	818	CLA	C4D-ND	-3.29	1.33	1.37
18	5	613	CLA	C4D-ND	-3.29	1.33	1.37
18	L	304	CLA	C4B-NB	3.29	1.41	1.37
18	4	601	CLA	C1D-ND	3.28	1.41	1.37
18	B	819	CLA	C4B-NB	3.28	1.41	1.37
18	3	604	CLA	C4D-ND	-3.28	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	839	CLA	C1D-ND	3.28	1.41	1.37
18	3	617	CLA	C4D-ND	-3.28	1.33	1.37
18	5	617	CLA	C4D-ND	-3.28	1.33	1.37
18	3	615	CLA	C4B-NB	3.28	1.41	1.37
18	6	608	CLA	C4D-ND	-3.27	1.33	1.37
18	A	809	CLA	C4D-ND	-3.27	1.33	1.37
18	A	827	CLA	C4D-ND	-3.27	1.33	1.37
18	A	841	CLA	C4D-ND	-3.27	1.33	1.37
18	J	101	CLA	C4B-NB	3.27	1.41	1.37
18	A	801	CLA	C4D-ND	-3.27	1.33	1.37
18	8	601	CLA	C1D-ND	3.27	1.41	1.37
18	7	610	CLA	C4D-ND	-3.27	1.33	1.37
18	a	601	CLA	C4B-NB	3.26	1.41	1.37
18	K	206	CLA	C4B-NB	3.26	1.41	1.37
18	B	831	CLA	C4D-ND	-3.26	1.33	1.37
18	A	821	CLA	C4D-ND	-3.26	1.33	1.37
18	A	804	CLA	C4D-ND	-3.26	1.33	1.37
18	4	608	CLA	C4D-ND	-3.26	1.33	1.37
18	8	608	CLA	C4B-NB	3.26	1.41	1.37
18	5	619	CLA	CAB-C3B	-3.26	1.43	1.50
18	B	802	CLA	C4D-ND	-3.26	1.33	1.37
18	8	610	CLA	C4D-ND	-3.26	1.33	1.37
18	8	613	CLA	C4D-ND	-3.25	1.33	1.37
18	B	835	CLA	C4B-NB	3.25	1.41	1.37
18	A	808	CLA	C4D-ND	-3.25	1.33	1.37
18	8	611	CLA	C1D-ND	3.25	1.41	1.37
18	A	828	CLA	C4D-ND	-3.25	1.33	1.37
18	a	601	CLA	C4D-ND	-3.25	1.33	1.37
18	4	612	CLA	C4B-NB	3.24	1.41	1.37
18	A	834	CLA	C4D-ND	-3.24	1.33	1.37
18	3	612	CLA	C4D-ND	-3.24	1.33	1.37
18	4	614	CLA	C4D-ND	-3.24	1.33	1.37
18	B	803	CLA	CMC-C2C	-3.24	1.43	1.50
18	A	837	CLA	C4B-NB	3.24	1.41	1.37
18	6	620	CLA	C4D-ND	-3.24	1.33	1.37
18	a	609	CLA	C4B-NB	3.24	1.41	1.37
18	A	832	CLA	C4D-ND	-3.24	1.33	1.37
18	6	618	CLA	CAB-C3B	-3.24	1.43	1.50
18	8	616	CLA	CAB-C3B	-3.23	1.43	1.50
18	K	201	CLA	C1D-ND	3.23	1.41	1.37
18	A	824	CLA	C4D-ND	-3.23	1.33	1.37
18	7	603	CLA	C4D-ND	-3.23	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	609	CLA	C3B-C4B	3.23	1.50	1.42
18	5	618	CLA	CAB-C3B	-3.23	1.44	1.50
18	B	806	CLA	C1D-ND	3.23	1.41	1.37
18	8	606	CLA	C4B-NB	3.23	1.41	1.37
18	6	603	CLA	CAB-C3B	-3.23	1.44	1.50
18	A	815	CLA	C1D-ND	3.23	1.41	1.37
18	K	203	CLA	C4B-NB	3.23	1.41	1.37
18	8	601	CLA	C4D-ND	-3.22	1.33	1.37
18	a	613	CLA	C4B-NB	3.22	1.41	1.37
18	L	303	CLA	C4B-NB	3.22	1.41	1.37
18	7	616	CLA	C4B-NB	3.22	1.41	1.37
18	1	604	CLA	C4B-NB	3.22	1.41	1.37
18	1	607	CLA	C4B-NB	3.21	1.41	1.37
18	A	813	CLA	C1D-ND	3.21	1.41	1.37
18	A	826	CLA	C1D-ND	3.21	1.41	1.37
18	A	831	CLA	C1B-NB	-3.21	1.33	1.37
18	A	836	CLA	C4D-ND	-3.21	1.33	1.37
18	8	603	CLA	CAB-C3B	-3.20	1.44	1.50
18	3	611	CLA	C4B-NB	3.20	1.41	1.37
18	6	612	CLA	C4B-NB	3.20	1.41	1.37
18	A	842	CLA	C4D-ND	-3.20	1.33	1.37
18	5	616	CLA	CAB-C3B	-3.20	1.44	1.50
18	A	811	CLA	C1D-ND	3.20	1.41	1.37
18	8	604	CLA	C4B-NB	3.20	1.41	1.37
18	4	614	CLA	C4B-NB	3.19	1.41	1.37
18	3	607	CLA	C4D-ND	-3.19	1.33	1.37
18	3	606	CLA	C4B-NB	3.19	1.41	1.37
18	4	604	CLA	C4D-ND	-3.19	1.33	1.37
18	B	840	CLA	C1D-ND	3.19	1.41	1.37
18	B	841	CLA	C4D-ND	-3.19	1.33	1.37
18	3	614	CLA	C4B-NB	3.19	1.41	1.37
18	6	610	CLA	C4D-ND	-3.19	1.33	1.37
18	A	818	CLA	C1D-ND	3.19	1.41	1.37
18	6	603	CLA	C4D-ND	-3.19	1.33	1.37
18	8	607	CLA	CAB-C3B	-3.19	1.44	1.50
18	6	617	CLA	C4D-ND	-3.19	1.33	1.37
18	3	612	CLA	C4B-NB	3.19	1.41	1.37
18	5	601	CLA	C4B-NB	3.19	1.41	1.37
18	5	604	CLA	C4D-ND	-3.18	1.33	1.37
18	A	843	CLA	C4D-ND	-3.18	1.33	1.37
18	6	618	CLA	C4D-ND	-3.18	1.33	1.37
18	A	819	CLA	C1D-ND	3.18	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	614	CLA	CAB-C3B	-3.18	1.44	1.50
18	5	604	CLA	CAB-C3B	-3.18	1.44	1.50
18	4	606	CLA	C4D-ND	-3.18	1.33	1.37
18	A	816	CLA	C4D-ND	-3.18	1.33	1.37
19	B	842	PQN	C11-C12	3.18	1.55	1.50
18	A	845	CLA	C4D-ND	-3.18	1.33	1.37
18	6	609	CLA	C1D-ND	3.17	1.41	1.37
18	3	613	CLA	C4D-ND	-3.17	1.33	1.37
18	1	613	CLA	C4D-ND	-3.17	1.33	1.37
18	A	845	CLA	C4B-NB	3.17	1.41	1.37
18	4	611	CLA	C4D-ND	-3.16	1.33	1.37
18	B	810	CLA	C4D-ND	-3.16	1.33	1.37
18	4	616	CLA	C4B-NB	3.16	1.41	1.37
18	a	607	CLA	C4B-NB	3.16	1.41	1.37
18	a	614	CLA	C4D-ND	-3.15	1.33	1.37
18	3	603	CLA	C4B-NB	3.15	1.41	1.37
18	7	607	CLA	C4B-NB	3.15	1.41	1.37
18	6	613	CLA	C1D-ND	3.15	1.41	1.37
18	A	841	CLA	C1D-ND	3.15	1.41	1.37
18	B	811	CLA	C4D-ND	-3.15	1.33	1.37
18	B	804	CLA	C4D-ND	-3.14	1.33	1.37
18	6	609	CLA	C4B-NB	3.14	1.41	1.37
18	a	611	CLA	CAB-C3B	-3.14	1.44	1.50
18	6	603	CLA	C4B-NB	3.14	1.41	1.37
28	5	624	NEX	C7-C8	-3.14	1.26	1.32
18	a	610	CLA	C4D-ND	-3.14	1.33	1.37
18	3	612	CLA	C3B-C4B	3.14	1.50	1.42
18	3	613	CLA	C4B-NB	3.14	1.41	1.37
18	5	618	CLA	C4B-NB	3.14	1.41	1.37
18	8	609	CLA	C4D-ND	-3.14	1.33	1.37
18	8	616	CLA	C4D-ND	-3.14	1.33	1.37
18	7	611	CLA	C4D-ND	-3.13	1.33	1.37
18	B	813	CLA	C4D-ND	-3.13	1.33	1.37
18	6	607	CLA	CAB-C3B	-3.13	1.44	1.50
19	A	844	PQN	C11-C12	3.13	1.55	1.50
18	B	834	CLA	C4D-ND	-3.13	1.33	1.37
18	A	823	CLA	C1D-ND	3.13	1.41	1.37
18	6	606	CLA	C4D-ND	-3.13	1.33	1.37
18	8	607	CLA	C4D-ND	-3.13	1.33	1.37
18	A	835	CLA	C4D-ND	-3.12	1.33	1.37
18	1	613	CLA	C4B-NB	3.12	1.41	1.37
18	4	603	CLA	C4B-NB	3.12	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	607	CLA	C4D-ND	-3.12	1.33	1.37
18	1	614	CLA	C4B-NB	3.12	1.41	1.37
18	B	808	CLA	C4D-ND	-3.12	1.33	1.37
18	B	828	CLA	C1D-ND	3.12	1.41	1.37
18	B	811	CLA	C4B-NB	3.12	1.41	1.37
18	a	606	CLA	C4B-NB	3.12	1.41	1.37
18	6	604	CLA	C4D-ND	-3.12	1.33	1.37
18	8	606	CLA	C4D-ND	-3.12	1.33	1.37
18	B	814	CLA	C4D-ND	-3.12	1.33	1.37
18	8	612	CLA	C4D-ND	-3.12	1.33	1.37
18	F	304	CLA	C4B-NB	3.11	1.41	1.37
18	a	604	CLA	C4B-NB	3.11	1.41	1.37
18	4	603	CLA	CAB-C3B	-3.11	1.44	1.50
18	6	617	CLA	C4B-NB	3.11	1.41	1.37
18	7	607	CLA	C4D-ND	-3.11	1.33	1.37
18	5	604	CLA	C4B-NB	3.11	1.41	1.37
18	6	613	CLA	C4B-NB	3.11	1.41	1.37
18	4	618	CLA	CAB-C3B	-3.11	1.44	1.50
18	5	610	CLA	C4D-ND	-3.11	1.33	1.37
18	a	611	CLA	C4B-NB	3.11	1.41	1.37
18	5	616	CLA	C4B-NB	3.11	1.41	1.37
18	4	601	CLA	C4B-NB	3.11	1.41	1.37
18	B	823	CLA	C3B-C4B	3.11	1.50	1.42
18	5	611	CLA	C4D-ND	-3.11	1.33	1.37
18	5	614	CLA	C4B-NB	3.11	1.41	1.37
18	a	613	CLA	C4D-ND	-3.10	1.33	1.37
18	7	615	CLA	CAB-C3B	-3.10	1.44	1.50
18	3	607	CLA	C4B-NB	3.10	1.41	1.37
18	3	611	CLA	CAB-C3B	-3.10	1.44	1.50
18	5	611	CLA	C4B-NB	3.10	1.41	1.37
18	A	822	CLA	C1D-ND	3.10	1.41	1.37
18	5	616	CLA	C4D-ND	-3.10	1.33	1.37
18	A	838	CLA	C1D-ND	3.09	1.41	1.37
18	F	301	CLA	C1D-ND	3.09	1.41	1.37
18	8	613	CLA	C4B-NB	3.09	1.41	1.37
18	1	601	CLA	C4B-NB	3.09	1.41	1.37
18	a	614	CLA	C4B-NB	3.09	1.41	1.37
18	7	606	CLA	C4B-NB	3.09	1.41	1.37
18	1	610	CLA	C4D-ND	-3.08	1.33	1.37
18	A	806	CLA	C1D-ND	3.08	1.41	1.37
18	4	616	CLA	CAB-C3B	-3.08	1.44	1.50
18	B	838	CLA	C1D-ND	3.08	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	614	CLA	C4D-ND	-3.08	1.33	1.37
18	B	834	CLA	C4B-NB	3.08	1.41	1.37
18	3	606	CLA	C4D-ND	-3.08	1.33	1.37
18	a	607	CLA	C4D-ND	-3.08	1.33	1.37
18	4	618	CLA	C4B-NB	3.08	1.41	1.37
18	1	616	CLA	CAB-C3B	-3.08	1.44	1.50
18	L	303	CLA	C4D-ND	-3.07	1.33	1.37
18	6	614	CLA	C4D-ND	-3.07	1.33	1.37
18	B	841	CLA	C3B-C4B	3.07	1.49	1.42
18	6	614	CLA	C4B-NB	3.06	1.41	1.37
18	B	811	CLA	CAB-C3B	-3.06	1.44	1.50
18	A	823	CLA	C4B-NB	3.06	1.41	1.37
18	7	615	CLA	C4B-NB	3.06	1.41	1.37
18	8	603	CLA	C4B-NB	3.06	1.41	1.37
18	7	616	CLA	CAB-C3B	-3.06	1.44	1.50
18	3	611	CLA	C4D-ND	-3.06	1.33	1.37
18	4	609	CLA	C4B-NB	3.06	1.41	1.37
18	5	618	CLA	C4D-ND	-3.06	1.33	1.37
18	6	618	CLA	C4B-NB	3.06	1.41	1.37
18	4	604	CLA	C4B-NB	3.05	1.41	1.37
18	7	610	CLA	C1D-ND	3.05	1.41	1.37
18	8	607	CLA	C4B-NB	3.05	1.41	1.37
18	3	604	CLA	C4B-NB	3.05	1.41	1.37
18	A	802	CLA	C3B-C4B	3.05	1.49	1.42
18	B	824	CLA	C3B-C4B	3.05	1.49	1.42
18	K	204	CLA	C4D-ND	-3.05	1.33	1.37
18	A	815	CLA	C4B-NB	3.05	1.41	1.37
18	B	805	CLA	C1D-ND	3.05	1.41	1.37
18	1	608	CLA	C4D-ND	-3.05	1.33	1.37
18	A	810	CLA	C1D-ND	3.05	1.41	1.37
18	a	601	CLA	C1D-ND	3.04	1.41	1.37
18	7	609	CLA	C1D-ND	3.04	1.41	1.37
18	4	613	CLA	C4B-NB	3.04	1.41	1.37
18	B	804	CLA	C1D-ND	3.04	1.41	1.37
18	a	616	CLA	C4B-NB	3.04	1.41	1.37
18	3	607	CLA	CAB-C3B	-3.04	1.44	1.50
18	1	611	CLA	C4B-NB	3.04	1.41	1.37
18	3	615	CLA	C4D-ND	-3.04	1.33	1.37
18	1	604	CLA	C3B-C4B	3.04	1.49	1.42
18	4	603	CLA	C4D-ND	-3.03	1.33	1.37
18	5	603	CLA	C1D-ND	3.03	1.41	1.37
18	F	303	CLA	C4D-ND	-3.03	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	616	CLA	C4D-ND	-3.03	1.33	1.37
18	3	614	CLA	C4D-ND	-3.03	1.33	1.37
18	5	606	CLA	C4D-ND	-3.03	1.33	1.37
18	B	827	CLA	C1D-ND	3.02	1.41	1.37
18	B	833	CLA	C4B-NB	3.02	1.41	1.37
18	B	807	CLA	C4B-NB	3.02	1.41	1.37
18	B	819	CLA	C4D-ND	-3.02	1.33	1.37
18	a	601	CLA	C3B-C4B	3.02	1.49	1.42
18	7	604	CLA	C4B-NB	3.02	1.41	1.37
18	a	608	CLA	C3B-C4B	3.02	1.49	1.42
18	8	609	CLA	C3B-C4B	3.01	1.49	1.42
18	1	609	CLA	CAB-C3B	-3.01	1.44	1.50
18	5	619	CLA	C4D-ND	-3.01	1.33	1.37
18	7	615	CLA	C4D-ND	-3.01	1.33	1.37
18	5	612	CLA	C4B-NB	3.01	1.41	1.37
18	6	616	CLA	C4B-NB	3.01	1.41	1.37
18	a	612	CLA	C3B-C4B	3.01	1.49	1.42
18	3	613	CLA	C1D-ND	3.01	1.41	1.37
18	6	616	CLA	C3B-C4B	3.01	1.49	1.42
18	6	613	CLA	C4D-ND	-3.01	1.33	1.37
18	B	829	CLA	MG-NB	-3.00	1.99	2.05
18	A	822	CLA	C4B-NB	3.00	1.41	1.37
18	1	611	CLA	C3B-C4B	3.00	1.49	1.42
18	4	616	CLA	C4D-ND	-3.00	1.33	1.37
18	B	815	CLA	C4D-ND	-3.00	1.33	1.37
18	7	616	CLA	C4D-ND	-3.00	1.33	1.37
18	A	816	CLA	C4B-NB	3.00	1.41	1.37
18	8	616	CLA	C4B-NB	3.00	1.41	1.37
18	A	837	CLA	C4D-ND	-3.00	1.33	1.37
18	a	612	CLA	C4D-ND	-2.99	1.33	1.37
18	6	608	CLA	C4B-NB	2.99	1.41	1.37
18	4	612	CLA	C4D-ND	-2.99	1.33	1.37
18	1	606	CLA	C4D-ND	-2.99	1.33	1.37
18	6	611	CLA	C4D-ND	-2.99	1.33	1.37
18	A	809	CLA	C1D-ND	2.99	1.41	1.37
18	B	804	CLA	C4B-NB	2.99	1.41	1.37
18	5	609	CLA	C4D-ND	-2.99	1.33	1.37
18	B	810	CLA	C4B-NB	2.98	1.41	1.37
18	5	619	CLA	C4B-NB	2.98	1.41	1.37
18	A	824	CLA	C4B-NB	2.98	1.41	1.37
18	8	611	CLA	C4B-NB	2.98	1.41	1.37
18	5	610	CLA	C4B-NB	2.98	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	C4B-NB	2.98	1.41	1.37
18	A	841	CLA	C4B-NB	2.98	1.41	1.37
18	4	606	CLA	C4B-NB	2.98	1.41	1.37
18	5	609	CLA	C4B-NB	2.98	1.41	1.37
18	B	820	CLA	C4D-ND	-2.98	1.33	1.37
18	B	840	CLA	C4B-NB	2.98	1.41	1.37
18	B	816	CLA	C3B-C4B	2.98	1.49	1.42
18	B	830	CLA	C4B-NB	2.97	1.41	1.37
18	A	818	CLA	C4B-NB	2.97	1.41	1.37
18	4	618	CLA	C4D-ND	-2.97	1.33	1.37
18	7	609	CLA	C4D-ND	-2.97	1.33	1.37
18	7	614	CLA	C4B-NB	2.97	1.41	1.37
18	B	815	CLA	C4B-NB	2.97	1.41	1.37
18	6	601	CLA	C4D-ND	-2.97	1.33	1.37
18	a	602	CLA	C4B-NB	2.97	1.41	1.37
18	4	611	CLA	C4B-NB	2.97	1.41	1.37
18	6	613	CLA	C3B-C4B	2.97	1.49	1.42
18	B	829	CLA	C1B-NB	-2.97	1.34	1.37
18	5	612	CLA	C4D-ND	-2.97	1.33	1.37
18	5	614	CLA	C4D-ND	-2.97	1.33	1.37
18	6	612	CLA	C4D-ND	-2.97	1.33	1.37
18	6	620	CLA	C1D-ND	2.97	1.41	1.37
18	8	612	CLA	C4B-NB	2.96	1.41	1.37
18	A	812	CLA	C1D-ND	2.96	1.41	1.37
18	B	816	CLA	C4B-NB	2.96	1.41	1.37
18	7	604	CLA	C4D-ND	-2.96	1.33	1.37
18	4	608	CLA	C4B-NB	2.96	1.41	1.37
18	A	804	CLA	C4B-NB	2.96	1.41	1.37
18	1	601	CLA	C3B-C4B	2.96	1.49	1.42
18	5	601	CLA	C4D-ND	-2.96	1.33	1.37
18	8	604	CLA	C4D-ND	-2.96	1.33	1.37
18	B	835	CLA	C4D-ND	-2.96	1.33	1.37
18	B	823	CLA	C4D-ND	-2.95	1.33	1.37
18	6	611	CLA	C4B-NB	2.95	1.41	1.37
18	7	603	CLA	C4B-NB	2.95	1.41	1.37
18	A	803	CLA	C1D-ND	2.95	1.41	1.37
18	6	606	CLA	C4B-NB	2.95	1.41	1.37
18	B	821	CLA	C3B-C4B	2.95	1.49	1.42
18	K	203	CLA	C4D-ND	-2.95	1.33	1.37
18	B	837	CLA	C3B-C4B	2.95	1.49	1.42
18	7	613	CLA	C4D-ND	-2.94	1.33	1.37
18	K	206	CLA	C4D-ND	-2.94	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	607	CLA	C4B-NB	2.94	1.41	1.37
18	A	832	CLA	C1D-ND	2.94	1.41	1.37
18	7	608	CLA	C4B-NB	2.94	1.41	1.37
18	F	301	CLA	C4B-NB	2.93	1.41	1.37
18	B	837	CLA	C4B-NB	2.93	1.41	1.37
18	a	610	CLA	C4B-NB	2.93	1.41	1.37
18	1	612	CLA	C4D-ND	-2.93	1.33	1.37
18	B	816	CLA	C4D-ND	-2.93	1.33	1.37
18	A	821	CLA	C1D-ND	2.92	1.41	1.37
18	B	826	CLA	C4B-NB	2.92	1.41	1.37
18	6	608	CLA	C3B-C4B	2.92	1.49	1.42
18	B	812	CLA	C4D-ND	-2.92	1.33	1.37
28	6	624	NEX	C7-C8	-2.92	1.27	1.32
18	1	616	CLA	C4D-ND	-2.92	1.33	1.37
18	B	835	CLA	C3B-C4B	2.92	1.49	1.42
18	a	608	CLA	C4D-ND	-2.92	1.33	1.37
18	A	821	CLA	C4B-NB	2.92	1.41	1.37
18	B	829	CLA	CMD-C2D	-2.91	1.44	1.50
18	7	613	CLA	C4B-NB	2.91	1.41	1.37
18	5	613	CLA	C4B-NB	2.91	1.41	1.37
18	7	606	CLA	C4D-ND	-2.91	1.33	1.37
18	3	617	CLA	C4B-NB	2.91	1.41	1.37
18	a	611	CLA	C4D-ND	-2.91	1.33	1.37
18	A	831	CLA	MG-NB	-2.91	2.00	2.05
18	A	803	CLA	MG-NB	-2.91	2.00	2.05
18	6	618	CLA	C1D-ND	2.90	1.41	1.37
18	4	610	CLA	C4D-ND	-2.90	1.33	1.37
18	1	608	CLA	C3B-C4B	2.90	1.49	1.42
18	L	302	CLA	C3B-C4B	2.90	1.49	1.42
18	B	814	CLA	C4B-NB	2.90	1.41	1.37
18	6	616	CLA	C4D-ND	-2.90	1.33	1.37
18	B	814	CLA	C1D-ND	2.90	1.41	1.37
18	A	842	CLA	C4B-NB	2.90	1.41	1.37
18	A	802	CLA	CMD-C2D	-2.89	1.44	1.50
18	6	604	CLA	C4B-NB	2.89	1.41	1.37
18	A	819	CLA	C4B-NB	2.89	1.41	1.37
18	B	820	CLA	C3B-C4B	2.89	1.49	1.42
18	6	609	CLA	C4D-ND	-2.89	1.33	1.37
18	8	601	CLA	C4B-NB	2.88	1.41	1.37
18	a	606	CLA	C4D-ND	-2.88	1.33	1.37
18	K	204	CLA	C4B-NB	2.88	1.41	1.37
18	B	831	CLA	C4B-NB	2.88	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	812	CLA	C3B-C4B	2.88	1.49	1.42
18	B	829	CLA	C1D-ND	2.88	1.41	1.37
18	6	620	CLA	C4B-NB	2.88	1.41	1.37
18	B	822	CLA	C3B-C4B	2.88	1.49	1.42
18	5	603	CLA	C4B-NB	2.87	1.41	1.37
18	3	610	CLA	C3B-C4B	2.87	1.49	1.42
18	B	836	CLA	C4B-NB	2.87	1.41	1.37
18	8	603	CLA	C4D-ND	-2.87	1.33	1.37
18	B	814	CLA	C3B-C4B	2.87	1.49	1.42
18	B	809	CLA	C1D-ND	2.87	1.41	1.37
18	B	821	CLA	C4D-ND	-2.87	1.33	1.37
18	B	813	CLA	C4B-NB	2.87	1.41	1.37
18	7	604	CLA	C3B-C4B	2.87	1.49	1.42
18	a	604	CLA	C4D-ND	-2.87	1.33	1.37
18	6	610	CLA	C3B-C4B	2.86	1.49	1.42
18	8	609	CLA	C4B-NB	2.86	1.41	1.37
18	6	614	CLA	C3B-C4B	2.86	1.49	1.42
18	B	802	CLA	C1D-ND	2.86	1.41	1.37
18	5	602	CLA	C3B-C4B	2.85	1.49	1.42
18	A	840	CLA	C4B-NB	2.85	1.41	1.37
18	a	606	CLA	C3B-C4B	2.85	1.49	1.42
18	K	203	CLA	C3B-C4B	2.85	1.49	1.42
18	a	604	CLA	C3B-C4B	2.85	1.49	1.42
18	6	612	CLA	C3B-C4B	2.85	1.49	1.42
18	5	610	CLA	C3B-C4B	2.85	1.49	1.42
18	A	817	CLA	C4D-ND	-2.85	1.33	1.37
18	a	603	CLA	C4D-ND	-2.85	1.33	1.37
18	3	614	CLA	C3B-C4B	2.84	1.49	1.42
18	B	804	CLA	C3B-C4B	2.84	1.49	1.42
18	1	607	CLA	C3B-C4B	2.84	1.49	1.42
18	A	854	CLA	C4B-NB	2.84	1.41	1.37
18	7	602	CLA	C4B-NB	2.83	1.41	1.37
18	L	304	CLA	C3B-C4B	2.83	1.49	1.42
18	6	602	CLA	C4B-NB	2.83	1.41	1.37
18	F	301	CLA	CMB-C2B	-2.83	1.44	1.50
18	5	602	CLA	C4B-NB	2.83	1.41	1.37
18	1	610	CLA	C3B-C4B	2.83	1.49	1.42
18	7	609	CLA	C3B-C4B	2.83	1.49	1.42
18	J	101	CLA	C4D-ND	-2.83	1.33	1.37
18	J	101	CLA	C3B-C4B	2.83	1.49	1.42
18	6	611	CLA	C3B-C4B	2.82	1.49	1.42
18	A	833	CLA	C4B-NB	2.82	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	610	CLA	C4B-NB	2.82	1.41	1.37
18	B	822	CLA	C4D-ND	-2.82	1.33	1.37
19	B	842	PQN	C10-C1	-2.82	1.42	1.48
20	A	846	LHG	O7-C5	-2.82	1.39	1.46
18	8	614	CLA	C4B-NB	2.82	1.41	1.37
18	6	620	CLA	C3B-C4B	2.82	1.49	1.42
18	1	607	CLA	C4D-ND	-2.82	1.33	1.37
18	7	611	CLA	C4B-NB	2.82	1.41	1.37
18	A	854	CLA	C1D-ND	2.82	1.41	1.37
18	8	602	CLA	C4B-NB	2.82	1.41	1.37
18	1	606	CLA	C3B-C4B	2.82	1.49	1.42
18	a	603	CLA	C3B-C4B	2.82	1.49	1.42
18	5	612	CLA	C3B-C4B	2.82	1.49	1.42
18	3	609	CLA	C4B-NB	2.82	1.41	1.37
18	7	602	CLA	C3B-C4B	2.82	1.49	1.42
18	B	818	CLA	C4B-NB	2.81	1.41	1.37
18	1	602	CLA	C4B-NB	2.81	1.41	1.37
18	B	836	CLA	C3B-C4B	2.81	1.49	1.42
18	A	820	CLA	CMB-C2B	-2.81	1.44	1.50
18	4	612	CLA	C3B-C4B	2.81	1.49	1.42
18	A	814	CLA	C3B-C4B	2.81	1.49	1.42
18	A	811	CLA	C4B-NB	2.81	1.41	1.37
18	B	808	CLA	C3B-C4B	2.80	1.49	1.42
18	5	613	CLA	C1B-C2B	2.80	1.49	1.43
18	B	827	CLA	C4B-NB	2.80	1.41	1.37
18	K	206	CLA	C3B-C4B	2.80	1.49	1.42
18	F	304	CLA	C4D-ND	-2.80	1.33	1.37
18	4	609	CLA	C4D-ND	-2.80	1.33	1.37
18	A	805	CLA	C3B-C4B	2.80	1.49	1.42
18	A	806	CLA	C4B-NB	2.80	1.41	1.37
18	A	810	CLA	C4B-NB	2.80	1.41	1.37
18	5	617	CLA	C4B-NB	2.80	1.41	1.37
19	A	844	PQN	C11-C3	2.80	1.56	1.51
18	3	608	CLA	MG-NB	-2.79	2.00	2.05
18	B	813	CLA	C3B-C4B	2.79	1.49	1.42
18	A	808	CLA	C4B-NB	2.79	1.41	1.37
18	B	810	CLA	C3B-C4B	2.79	1.49	1.42
18	5	611	CLA	C3B-C4B	2.79	1.49	1.42
18	8	610	CLA	C3B-C4B	2.79	1.49	1.42
18	3	604	CLA	C3B-C4B	2.79	1.49	1.42
18	A	821	CLA	C3B-C4B	2.79	1.49	1.42
18	A	830	CLA	C1D-ND	2.79	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	825	CLA	C3B-C4B	2.78	1.49	1.42
18	A	817	CLA	C4B-NB	2.78	1.41	1.37
18	A	854	CLA	C3B-C4B	2.78	1.49	1.42
18	A	812	CLA	C4B-NB	2.78	1.41	1.37
18	A	818	CLA	C3B-C4B	2.78	1.49	1.42
18	3	606	CLA	C3B-C4B	2.78	1.49	1.42
18	8	604	CLA	C3B-C4B	2.78	1.49	1.42
18	7	614	CLA	C3B-C4B	2.78	1.49	1.42
18	8	608	CLA	C3B-C4B	2.77	1.49	1.42
18	1	604	CLA	C4D-ND	-2.77	1.33	1.37
18	7	601	CLA	C3B-C4B	2.77	1.49	1.42
18	A	801	CLA	C4B-NB	2.77	1.41	1.37
18	B	826	CLA	C3B-C4B	2.77	1.49	1.42
18	B	806	CLA	C4B-NB	2.77	1.41	1.37
18	1	612	CLA	C3B-C4B	2.77	1.49	1.42
18	a	602	CLA	C3B-C4B	2.77	1.49	1.42
18	1	611	CLA	C4D-ND	-2.77	1.33	1.37
18	B	830	CLA	C1B-C2B	2.77	1.49	1.43
18	7	601	CLA	C4B-NB	2.77	1.41	1.37
18	L	303	CLA	C3B-C4B	2.77	1.49	1.42
18	B	826	CLA	CMC-C2C	-2.77	1.44	1.50
18	F	304	CLA	C3B-C4B	2.77	1.49	1.42
18	5	601	CLA	C3B-C4B	2.77	1.49	1.42
18	B	832	CLA	C4B-NB	2.76	1.41	1.37
18	1	603	CLA	C3B-C4B	2.76	1.49	1.42
18	4	611	CLA	C3B-C4B	2.76	1.49	1.42
18	6	617	CLA	C3B-C4B	2.76	1.49	1.42
18	8	611	CLA	C3B-C4B	2.76	1.49	1.42
18	8	613	CLA	C1B-C2B	2.76	1.49	1.43
18	A	803	CLA	CMB-C2B	-2.76	1.44	1.50
18	L	302	CLA	C4D-ND	-2.76	1.33	1.37
18	B	817	CLA	C4B-NB	2.76	1.41	1.37
18	A	841	CLA	C3B-C4B	2.76	1.49	1.42
18	5	607	CLA	C3B-C4B	2.76	1.49	1.42
18	a	607	CLA	C3B-C4B	2.76	1.49	1.42
18	a	614	CLA	C3B-C4B	2.75	1.49	1.42
18	3	615	CLA	C1B-C2B	2.75	1.49	1.43
18	B	833	CLA	C3B-C4B	2.75	1.49	1.42
18	F	303	CLA	C3B-C4B	2.75	1.49	1.42
18	8	612	CLA	C3B-C4B	2.75	1.49	1.42
18	7	610	CLA	C4B-NB	2.75	1.41	1.37
18	6	607	CLA	CMC-C2C	-2.75	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	834	CLA	C3B-C4B	2.75	1.49	1.42
18	A	834	CLA	C4B-NB	2.75	1.41	1.37
18	a	616	CLA	C3B-C4B	2.75	1.49	1.42
18	7	609	CLA	C4B-NB	2.75	1.41	1.37
18	7	613	CLA	C3B-C4B	2.74	1.49	1.42
18	A	810	CLA	C3B-C4B	2.74	1.49	1.42
18	A	805	CLA	C4B-NB	2.74	1.41	1.37
18	A	820	CLA	C4B-NB	2.74	1.41	1.37
18	A	837	CLA	C3B-C4B	2.74	1.49	1.42
18	5	607	CLA	CMC-C2C	-2.74	1.45	1.50
18	6	601	CLA	C4B-NB	2.74	1.41	1.37
18	B	815	CLA	C3B-C4B	2.74	1.49	1.42
18	5	608	CLA	C4B-NB	2.74	1.41	1.37
18	K	204	CLA	C3B-C4B	2.74	1.49	1.42
18	L	304	CLA	C4D-ND	-2.74	1.33	1.37
18	3	609	CLA	C4D-ND	-2.74	1.33	1.37
18	B	838	CLA	C4B-NB	2.74	1.41	1.37
18	B	824	CLA	C4D-ND	-2.74	1.33	1.37
18	B	807	CLA	C3B-C4B	2.73	1.49	1.42
18	A	815	CLA	C3B-C4B	2.73	1.49	1.42
18	8	614	CLA	C3B-C4B	2.73	1.49	1.42
18	F	301	CLA	CMD-C2D	-2.73	1.45	1.50
18	A	831	CLA	C4B-NB	2.73	1.41	1.37
18	6	607	CLA	C4B-NB	2.73	1.41	1.37
23	A	857	LMU	O5'-C5'	2.72	1.48	1.43
18	1	603	CLA	C1B-C2B	2.72	1.49	1.43
18	3	611	CLA	C1B-C2B	2.72	1.49	1.43
18	7	607	CLA	C1B-C2B	2.72	1.49	1.43
18	5	614	CLA	C3B-C4B	2.72	1.49	1.42
18	A	836	CLA	C4B-NB	2.72	1.41	1.37
18	B	809	CLA	CMB-C2B	-2.72	1.45	1.50
18	a	613	CLA	C3B-C4B	2.71	1.49	1.42
18	A	831	CLA	CMD-C2D	-2.71	1.45	1.50
18	L	302	CLA	C1B-C2B	2.71	1.49	1.43
18	B	828	CLA	CMD-C2D	-2.71	1.45	1.50
18	B	831	CLA	C3B-C4B	2.71	1.49	1.42
18	1	613	CLA	C3B-C4B	2.71	1.49	1.42
18	3	610	CLA	C4B-NB	2.71	1.41	1.37
18	B	805	CLA	C4B-NB	2.71	1.41	1.37
18	a	609	CLA	C4D-ND	-2.70	1.34	1.37
18	B	808	CLA	CMC-C2C	-2.70	1.45	1.50
18	7	610	CLA	C3B-C4B	2.70	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	817	CLA	C3B-C4B	2.70	1.49	1.42
18	A	811	CLA	C3B-C4B	2.70	1.49	1.42
18	6	606	CLA	C3B-C4B	2.70	1.49	1.42
18	4	608	CLA	C3B-C4B	2.70	1.49	1.42
18	7	607	CLA	C3B-C4B	2.70	1.49	1.42
18	A	835	CLA	C4B-NB	2.69	1.41	1.37
18	L	304	CLA	C1B-C2B	2.69	1.49	1.43
18	A	830	CLA	CMD-C2D	-2.69	1.45	1.50
18	A	842	CLA	C3B-C4B	2.69	1.49	1.42
18	B	820	CLA	C1B-C2B	2.69	1.49	1.43
18	3	613	CLA	C1B-C2B	2.69	1.49	1.43
18	A	801	CLA	CMD-C2D	-2.69	1.45	1.50
18	1	609	CLA	C4D-ND	-2.69	1.34	1.37
18	A	827	CLA	C3B-C4B	2.68	1.49	1.42
18	B	834	CLA	C3B-C4B	2.68	1.49	1.42
18	A	836	CLA	CMB-C2B	-2.68	1.45	1.50
18	1	603	CLA	C4D-ND	-2.68	1.34	1.37
18	4	607	CLA	C3B-C4B	2.68	1.49	1.42
18	4	603	CLA	C1B-C2B	2.68	1.49	1.43
18	4	610	CLA	C4B-NB	2.68	1.41	1.37
18	A	807	CLA	C4B-NB	2.68	1.41	1.37
18	A	813	CLA	C3B-C4B	2.67	1.49	1.42
18	3	617	CLA	C3B-C4B	2.67	1.49	1.42
18	4	614	CLA	C3B-C4B	2.67	1.49	1.42
18	7	606	CLA	C3B-C4B	2.67	1.49	1.42
18	A	816	CLA	C3B-C4B	2.67	1.49	1.42
18	B	822	CLA	C1B-C2B	2.67	1.49	1.43
18	1	608	CLA	C1B-C2B	2.66	1.49	1.43
18	A	845	CLA	C3B-C4B	2.66	1.49	1.42
18	A	804	CLA	C3B-C4B	2.66	1.49	1.42
18	1	602	CLA	C3B-C4B	2.66	1.49	1.42
18	a	609	CLA	C3B-C4B	2.66	1.49	1.42
18	A	830	CLA	C4B-NB	2.66	1.41	1.37
18	B	819	CLA	C3B-C4B	2.66	1.49	1.42
18	4	601	CLA	C3B-C4B	2.66	1.49	1.42
18	A	822	CLA	C3B-C4B	2.65	1.49	1.42
18	A	809	CLA	C3B-C4B	2.65	1.49	1.42
18	A	826	CLA	C4B-NB	2.65	1.41	1.37
18	K	206	CLA	C1B-C2B	2.65	1.49	1.43
18	B	829	CLA	C4B-NB	2.65	1.41	1.37
18	K	201	CLA	C1B-C2B	2.65	1.49	1.43
18	B	839	CLA	C3B-C4B	2.65	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	8	601	CLA	C3B-C4B	2.65	1.49	1.42
18	A	854	CLA	CHC-C1C	2.65	1.43	1.38
18	K	201	CLA	C3B-C4B	2.65	1.49	1.42
18	A	810	CLA	CMD-C2D	-2.64	1.45	1.50
18	8	602	CLA	C3B-C4B	2.64	1.49	1.42
18	B	821	CLA	C1B-C2B	2.64	1.49	1.43
18	4	618	CLA	C1B-C2B	2.64	1.49	1.43
18	8	607	CLA	C1B-C2B	2.64	1.49	1.43
18	F	301	CLA	MG-NB	-2.64	2.00	2.05
18	1	607	CLA	C1B-C2B	2.64	1.49	1.43
18	A	829	CLA	C4B-NB	2.64	1.41	1.37
18	B	828	CLA	MG-NB	-2.64	2.00	2.05
18	A	805	CLA	MG-NB	-2.63	2.00	2.05
18	3	608	CLA	CMB-C2B	-2.63	1.45	1.50
18	B	802	CLA	C4B-NB	2.63	1.41	1.37
18	B	808	CLA	C4B-NB	2.63	1.41	1.37
18	A	828	CLA	C3B-C4B	2.63	1.48	1.42
18	5	617	CLA	CMB-C2B	-2.63	1.45	1.50
18	A	824	CLA	C1B-C2B	2.63	1.49	1.43
18	A	839	CLA	C4B-NB	2.63	1.41	1.37
18	B	812	CLA	C1B-C2B	2.63	1.49	1.43
18	K	201	CLA	C4D-ND	-2.63	1.34	1.37
18	a	610	CLA	C3B-C4B	2.63	1.48	1.42
18	5	603	CLA	MG-NB	-2.63	2.00	2.05
18	1	602	CLA	C1B-C2B	2.63	1.49	1.43
18	A	833	CLA	C3B-C4B	2.62	1.48	1.42
18	B	805	CLA	C3B-C4B	2.62	1.48	1.42
18	A	823	CLA	C3B-C4B	2.62	1.48	1.42
18	B	809	CLA	C4B-NB	2.62	1.41	1.37
18	A	812	CLA	C3B-C4B	2.62	1.48	1.42
18	A	820	CLA	CMC-C2C	-2.62	1.45	1.50
18	7	616	CLA	C1B-C2B	2.62	1.49	1.43
18	1	609	CLA	C4B-C3B	2.61	1.49	1.43
18	B	825	CLA	C4B-NB	2.61	1.41	1.37
18	1	612	CLA	C1B-C2B	2.61	1.49	1.43
18	6	607	CLA	C1B-C2B	2.61	1.49	1.43
18	A	813	CLA	C4B-NB	2.61	1.41	1.37
18	A	826	CLA	MG-NB	-2.61	2.00	2.05
18	B	824	CLA	CMD-C2D	-2.61	1.45	1.50
18	B	832	CLA	C3B-C4B	2.61	1.48	1.42
18	5	609	CLA	C3B-C4B	2.61	1.48	1.42
18	A	838	CLA	MG-NB	-2.61	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	845	CLA	C1B-C2B	2.61	1.49	1.43
18	A	819	CLA	CMB-C2B	-2.61	1.45	1.50
18	A	832	CLA	CMD-C2D	-2.61	1.45	1.50
18	A	803	CLA	C4B-NB	2.60	1.41	1.37
18	1	609	CLA	C1B-C2B	2.60	1.49	1.43
18	7	608	CLA	C3B-C4B	2.60	1.48	1.42
18	1	606	CLA	C1B-C2B	2.60	1.49	1.43
18	B	825	CLA	CMD-C2D	-2.60	1.45	1.50
18	1	614	CLA	C4B-C3B	2.60	1.49	1.43
18	a	607	CLA	C1B-C2B	2.60	1.49	1.43
18	5	611	CLA	C1B-C2B	2.60	1.49	1.43
18	A	831	CLA	MG-ND	-2.59	2.00	2.05
18	A	822	CLA	CMB-C2B	-2.59	1.45	1.50
18	7	615	CLA	C1B-C2B	2.59	1.49	1.43
18	3	608	CLA	C4B-NB	2.59	1.41	1.37
18	4	613	CLA	C3B-C4B	2.59	1.48	1.42
18	8	613	CLA	C3B-C4B	2.59	1.48	1.42
18	J	101	CLA	C1B-C2B	2.59	1.49	1.43
18	B	819	CLA	C1B-C2B	2.59	1.49	1.43
18	8	616	CLA	C1B-C2B	2.59	1.49	1.43
18	K	204	CLA	C1B-C2B	2.59	1.49	1.43
18	K	203	CLA	C1B-C2B	2.59	1.49	1.43
18	7	616	CLA	C4B-C3B	2.59	1.49	1.43
18	6	604	CLA	C3B-C4B	2.59	1.48	1.42
18	A	843	CLA	C4B-NB	2.59	1.41	1.37
18	3	614	CLA	C1B-C2B	2.58	1.49	1.43
18	5	608	CLA	C3B-C4B	2.58	1.48	1.42
18	B	840	CLA	CMB-C2B	-2.58	1.45	1.50
18	A	806	CLA	CMD-C2D	-2.58	1.45	1.50
18	4	606	CLA	C3B-C4B	2.58	1.48	1.42
18	B	802	CLA	C1B-C2B	2.58	1.49	1.43
18	K	201	CLA	CMD-C2D	-2.58	1.45	1.50
19	A	844	PQN	C10-C5	-2.58	1.36	1.40
18	B	818	CLA	C3B-C4B	2.58	1.48	1.42
18	B	839	CLA	C4B-NB	2.58	1.41	1.37
18	A	839	CLA	C3B-C4B	2.58	1.48	1.42
18	A	835	CLA	C3B-C4B	2.57	1.48	1.42
18	L	303	CLA	C1B-C2B	2.57	1.49	1.43
18	B	802	CLA	CMD-C2D	-2.57	1.45	1.50
18	a	616	CLA	C1B-C2B	2.57	1.49	1.43
18	B	823	CLA	C1B-C2B	2.57	1.49	1.43
18	B	831	CLA	C1B-C2B	2.57	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	609	CLA	C3B-C4B	2.57	1.48	1.42
18	B	811	CLA	C1B-C2B	2.57	1.49	1.43
18	B	815	CLA	C1B-C2B	2.57	1.49	1.43
18	A	824	CLA	C3B-C4B	2.56	1.48	1.42
25	J	103	DGD	C4E-C3E	2.56	1.58	1.52
18	6	602	CLA	C3B-C4B	2.56	1.48	1.42
18	A	809	CLA	C4B-NB	2.56	1.40	1.37
18	F	303	CLA	C1B-C2B	2.56	1.49	1.43
18	B	840	CLA	C3B-C4B	2.56	1.48	1.42
18	A	802	CLA	MG-ND	-2.56	2.00	2.05
18	8	603	CLA	C1B-C2B	2.56	1.49	1.43
18	7	615	CLA	C4B-C3B	2.56	1.49	1.43
18	B	811	CLA	C4B-C3B	2.56	1.49	1.43
18	5	616	CLA	C1B-C2B	2.56	1.49	1.43
18	A	854	CLA	CMC-C2C	-2.55	1.45	1.50
18	a	616	CLA	CMD-C2D	-2.55	1.45	1.50
18	8	610	CLA	C4B-NB	2.55	1.40	1.37
18	8	608	CLA	C1B-C2B	2.55	1.49	1.43
18	B	802	CLA	CMB-C2B	-2.55	1.45	1.50
18	B	803	CLA	C3B-C4B	2.55	1.48	1.42
18	A	808	CLA	C1B-C2B	2.55	1.49	1.43
18	3	611	CLA	C4B-C3B	2.55	1.49	1.43
18	A	803	CLA	MG-ND	-2.55	2.00	2.05
18	A	828	CLA	C4B-NB	2.55	1.40	1.37
18	A	837	CLA	C1B-C2B	2.55	1.49	1.43
18	A	822	CLA	MG-NB	-2.54	2.00	2.05
18	A	832	CLA	MG-NB	-2.54	2.00	2.05
18	5	617	CLA	C1B-C2B	2.54	1.49	1.43
18	B	830	CLA	CMB-C2B	-2.54	1.45	1.50
18	6	609	CLA	C3B-C4B	2.54	1.48	1.42
18	A	817	CLA	C1B-C2B	2.54	1.49	1.43
18	a	611	CLA	C1B-C2B	2.54	1.49	1.43
18	A	825	CLA	C3B-C4B	2.54	1.48	1.42
18	8	602	CLA	C1B-C2B	2.54	1.49	1.43
25	J	103	DGD	C4E-C5E	2.53	1.58	1.53
18	4	607	CLA	C1B-C2B	2.53	1.49	1.43
18	B	830	CLA	C4D-ND	-2.53	1.34	1.37
18	6	618	CLA	C1B-C2B	2.53	1.49	1.43
18	a	613	CLA	C1B-C2B	2.53	1.49	1.43
18	4	604	CLA	C4B-C3B	2.53	1.49	1.43
18	A	806	CLA	CMC-C2C	-2.53	1.45	1.50
18	a	609	CLA	C1B-C2B	2.53	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	613	CLA	C1B-C2B	2.53	1.49	1.43
18	4	616	CLA	C1B-C2B	2.53	1.49	1.43
18	B	829	CLA	MG-ND	-2.52	2.00	2.05
18	4	610	CLA	C3B-C4B	2.52	1.48	1.42
19	A	844	PQN	C5-C4	-2.52	1.43	1.48
18	7	611	CLA	C1B-C2B	2.52	1.49	1.43
18	7	616	CLA	CMD-C2D	-2.52	1.45	1.50
18	a	603	CLA	C1B-C2B	2.52	1.49	1.43
18	5	601	CLA	C1B-C2B	2.52	1.49	1.43
18	B	818	CLA	MG-NB	-2.52	2.00	2.05
18	3	602	CLA	C1B-C2B	2.52	1.49	1.43
18	3	606	CLA	C1B-C2B	2.51	1.49	1.43
18	4	612	CLA	C1B-C2B	2.51	1.49	1.43
20	6	623	LHG	O7-C5	-2.51	1.40	1.46
18	8	616	CLA	C4B-C3B	2.51	1.49	1.43
18	B	841	CLA	CHC-C1C	2.51	1.43	1.38
18	a	611	CLA	C4B-C3B	2.51	1.49	1.43
18	a	614	CLA	C1B-C2B	2.51	1.49	1.43
18	B	809	CLA	MG-NB	-2.51	2.00	2.05
18	7	603	CLA	C3B-C4B	2.51	1.48	1.42
18	3	615	CLA	C3B-C4B	2.51	1.48	1.42
18	B	806	CLA	C3B-C4B	2.51	1.48	1.42
18	5	601	CLA	CMD-C2D	-2.51	1.45	1.50
18	F	304	CLA	C1B-C2B	2.51	1.49	1.43
18	8	604	CLA	C1B-C2B	2.50	1.49	1.43
18	A	827	CLA	C4B-NB	2.50	1.40	1.37
18	7	603	CLA	C1B-C2B	2.50	1.49	1.43
18	a	608	CLA	C1B-C2B	2.50	1.49	1.43
18	4	606	CLA	C1B-C2B	2.50	1.49	1.43
18	B	814	CLA	CMD-C2D	-2.50	1.45	1.50
18	B	830	CLA	C3B-C4B	2.50	1.48	1.42
18	1	614	CLA	C1B-C2B	2.50	1.49	1.43
18	B	808	CLA	CMD-C2D	-2.50	1.45	1.50
18	4	610	CLA	C1B-C2B	2.50	1.49	1.43
18	6	603	CLA	C1B-C2B	2.49	1.49	1.43
18	a	606	CLA	C1B-C2B	2.49	1.49	1.43
18	A	830	CLA	CMC-C2C	-2.49	1.45	1.50
18	B	839	CLA	CMD-C2D	-2.49	1.45	1.50
18	B	823	CLA	CHC-C1C	2.49	1.43	1.38
18	5	614	CLA	C1B-C2B	2.49	1.49	1.43
18	5	604	CLA	C1B-C2B	2.49	1.49	1.43
18	5	607	CLA	C4B-NB	2.49	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	817	CLA	C3B-C4B	2.49	1.48	1.42
18	B	806	CLA	MG-NB	-2.49	2.00	2.05
18	A	808	CLA	C3B-C4B	2.49	1.48	1.42
18	A	819	CLA	MG-NB	-2.48	2.00	2.05
18	4	608	CLA	C1B-C2B	2.48	1.49	1.43
19	A	844	PQN	C10-C1	-2.48	1.43	1.48
18	B	838	CLA	MG-NB	-2.48	2.00	2.05
18	4	602	CLA	C3B-C4B	2.48	1.48	1.42
18	7	606	CLA	CMB-C2B	-2.48	1.45	1.50
18	6	601	CLA	C3B-C4B	2.48	1.48	1.42
18	3	613	CLA	C3B-C4B	2.48	1.48	1.42
18	A	832	CLA	C3B-C4B	2.48	1.48	1.42
18	B	828	CLA	C4B-NB	2.48	1.40	1.37
18	B	803	CLA	MG-NB	-2.48	2.00	2.05
18	B	828	CLA	MG-ND	-2.48	2.00	2.05
18	1	616	CLA	C4B-C3B	2.48	1.49	1.43
18	A	806	CLA	C3B-C4B	2.47	1.48	1.42
18	5	608	CLA	MG-NB	-2.47	2.00	2.05
20	7	622	LHG	O7-C5	-2.47	1.40	1.46
18	A	801	CLA	C1B-C2B	2.47	1.49	1.43
18	A	825	CLA	C4B-NB	2.47	1.40	1.37
23	A	859	LMU	C2'-C3'	-2.47	1.48	1.52
18	B	813	CLA	C1B-C2B	2.47	1.49	1.43
18	A	840	CLA	MG-NB	-2.47	2.00	2.05
18	A	812	CLA	C1B-C2B	2.47	1.49	1.43
20	5	623	LHG	O7-C5	-2.47	1.40	1.46
18	8	614	CLA	C1B-C2B	2.47	1.49	1.43
18	7	611	CLA	CMD-C2D	-2.47	1.45	1.50
18	B	805	CLA	C1B-C2B	2.46	1.49	1.43
18	4	614	CLA	C1B-C2B	2.46	1.49	1.43
18	A	827	CLA	MG-NB	-2.46	2.00	2.05
18	A	802	CLA	C4B-NB	2.46	1.40	1.37
18	F	301	CLA	C3B-C4B	2.46	1.48	1.42
18	5	603	CLA	C4B-C3B	2.46	1.49	1.43
18	1	601	CLA	MG-NB	-2.46	2.00	2.05
18	B	817	CLA	CMC-C2C	-2.45	1.45	1.50
18	1	616	CLA	CMD-C2D	-2.45	1.45	1.50
18	B	833	CLA	C1B-C2B	2.45	1.49	1.43
25	J	103	DGD	O1G-C1G	-2.45	1.39	1.45
18	A	804	CLA	C1B-C2B	2.45	1.49	1.43
18	B	826	CLA	C1B-C2B	2.45	1.49	1.43
18	a	602	CLA	C1B-C2B	2.45	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	821	CLA	CMD-C2D	-2.45	1.45	1.50
18	3	610	CLA	CMC-C2C	-2.45	1.45	1.50
19	B	842	PQN	C5-C4	-2.45	1.43	1.48
18	8	601	CLA	CMD-C2D	-2.45	1.45	1.50
18	A	826	CLA	C1B-C2B	2.45	1.49	1.43
18	4	602	CLA	C1B-C2B	2.45	1.49	1.43
18	5	604	CLA	C4B-C3B	2.45	1.49	1.43
26	7	619	LUT	C22-C21	-2.45	1.51	1.54
18	A	830	CLA	MG-NB	-2.44	2.00	2.05
18	A	829	CLA	MG-NB	-2.44	2.00	2.05
18	A	835	CLA	C1B-C2B	2.44	1.49	1.43
18	3	607	CLA	C4B-C3B	2.44	1.49	1.43
18	A	820	CLA	C3B-C4B	2.44	1.48	1.42
18	B	802	CLA	MG-NB	-2.44	2.01	2.05
18	A	854	CLA	MG-NB	-2.44	2.01	2.05
18	5	618	CLA	C1B-C2B	2.44	1.49	1.43
18	1	616	CLA	C1B-C2B	2.44	1.49	1.43
18	B	839	CLA	MG-NB	-2.44	2.01	2.05
18	A	843	CLA	CMB-C2B	-2.44	1.45	1.50
18	4	618	CLA	C4B-C3B	2.43	1.49	1.43
18	A	834	CLA	MG-NB	-2.43	2.01	2.05
18	6	607	CLA	C4B-C3B	2.43	1.49	1.43
18	6	606	CLA	C1B-C2B	2.43	1.49	1.43
18	A	831	CLA	C1D-ND	2.43	1.40	1.37
18	6	609	CLA	CMB-C2B	-2.43	1.45	1.50
18	B	838	CLA	C3B-C4B	2.43	1.48	1.42
18	B	803	CLA	MG-ND	-2.43	2.01	2.05
18	A	839	CLA	C1B-C2B	2.43	1.49	1.43
18	5	616	CLA	C4B-C3B	2.43	1.49	1.43
18	4	616	CLA	C4B-C3B	2.43	1.49	1.43
18	A	810	CLA	MG-NB	-2.43	2.01	2.05
18	3	603	CLA	MG-NB	-2.43	2.01	2.05
18	6	618	CLA	C4B-C3B	2.43	1.49	1.43
18	A	843	CLA	MG-NB	-2.43	2.01	2.05
18	B	827	CLA	MG-NB	-2.43	2.01	2.05
18	A	826	CLA	CMD-C2D	-2.42	1.45	1.50
18	A	831	CLA	CMC-C2C	-2.42	1.45	1.50
18	a	612	CLA	C1B-C2B	2.42	1.49	1.43
18	3	603	CLA	C1B-C2B	2.42	1.49	1.43
18	3	602	CLA	CMD-C2D	-2.42	1.45	1.50
18	A	820	CLA	MG-NB	-2.42	2.01	2.05
18	4	613	CLA	C1B-C2B	2.42	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	602	CLA	MG-NB	-2.42	2.01	2.05
18	4	601	CLA	C1B-C2B	2.42	1.49	1.43
18	5	617	CLA	CMC-C2C	-2.42	1.45	1.50
18	5	612	CLA	C1B-C2B	2.42	1.49	1.43
18	B	833	CLA	CMC-C2C	-2.42	1.45	1.50
18	3	602	CLA	CMC-C2C	-2.42	1.45	1.50
18	7	613	CLA	C1B-C2B	2.42	1.48	1.43
18	A	840	CLA	C3B-C4B	2.42	1.48	1.42
18	8	610	CLA	C1B-C2B	2.42	1.48	1.43
18	B	834	CLA	C1B-C2B	2.42	1.48	1.43
18	6	604	CLA	C1B-C2B	2.42	1.48	1.43
18	B	825	CLA	MG-NB	-2.42	2.01	2.05
18	5	602	CLA	C1B-C2B	2.42	1.48	1.43
18	7	613	CLA	CMD-C2D	-2.41	1.45	1.50
18	A	807	CLA	C3B-C4B	2.41	1.48	1.42
18	B	810	CLA	C1B-C2B	2.41	1.48	1.43
18	A	813	CLA	C1B-C2B	2.41	1.48	1.43
18	A	836	CLA	C1B-C2B	2.41	1.48	1.43
21	A	852	BCR	C30-C25	-2.41	1.50	1.53
19	B	842	PQN	C10-C5	-2.41	1.36	1.40
18	A	826	CLA	C3B-C4B	2.41	1.48	1.42
18	A	827	CLA	CMD-C2D	-2.41	1.45	1.50
18	A	832	CLA	CMB-C2B	-2.41	1.45	1.50
18	A	824	CLA	CMD-C2D	-2.41	1.45	1.50
18	A	816	CLA	C1B-C2B	2.41	1.48	1.43
18	A	807	CLA	C1B-C2B	2.41	1.48	1.43
19	B	842	PQN	C11-C3	2.40	1.55	1.51
18	A	841	CLA	MG-NB	-2.40	2.01	2.05
18	4	606	CLA	MG-NB	-2.40	2.01	2.05
18	B	804	CLA	MG-NB	-2.40	2.01	2.05
18	7	601	CLA	MG-NB	-2.40	2.01	2.05
18	3	608	CLA	MG-ND	-2.40	2.01	2.05
18	7	611	CLA	C3B-C4B	2.40	1.48	1.42
18	A	842	CLA	C1B-C2B	2.40	1.48	1.43
18	A	838	CLA	CMD-C2D	-2.40	1.45	1.50
18	7	608	CLA	MG-NB	-2.40	2.01	2.05
18	4	602	CLA	C4B-NB	2.39	1.40	1.37
18	A	829	CLA	C3B-C4B	2.39	1.48	1.42
18	3	608	CLA	C3B-C4B	2.39	1.48	1.42
18	B	827	CLA	C3B-C4B	2.39	1.48	1.42
18	A	836	CLA	MG-NB	-2.39	2.01	2.05
18	6	609	CLA	CMD-C2D	-2.39	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	603	CLA	C3B-C4B	2.39	1.48	1.42
18	A	806	CLA	C1B-C2B	2.39	1.48	1.43
18	1	604	CLA	C1B-C2B	2.39	1.48	1.43
18	7	614	CLA	C1B-C2B	2.39	1.48	1.43
18	A	818	CLA	C1B-C2B	2.39	1.48	1.43
18	6	617	CLA	C1B-C2B	2.38	1.48	1.43
18	A	828	CLA	MG-NB	-2.38	2.01	2.05
18	A	843	CLA	C1B-C2B	2.38	1.48	1.43
18	B	835	CLA	C1B-C2B	2.38	1.48	1.43
18	3	613	CLA	CMD-C2D	-2.38	1.45	1.50
18	8	601	CLA	MG-NB	-2.38	2.01	2.05
18	3	602	CLA	C3B-C4B	2.38	1.48	1.42
18	B	836	CLA	MG-NB	-2.38	2.01	2.05
18	A	819	CLA	C3B-C4B	2.38	1.48	1.42
18	8	601	CLA	C1B-C2B	2.38	1.48	1.43
18	B	817	CLA	CMB-C2B	-2.38	1.45	1.50
18	B	832	CLA	MG-NB	-2.37	2.01	2.05
18	4	601	CLA	MG-NB	-2.37	2.01	2.05
20	A	847	LHG	O7-C5	-2.37	1.40	1.46
18	6	614	CLA	C1B-C2B	2.37	1.48	1.43
18	A	833	CLA	MG-NB	-2.37	2.01	2.05
18	1	611	CLA	C1B-C2B	2.37	1.48	1.43
18	A	830	CLA	C3B-C4B	2.37	1.48	1.42
18	A	801	CLA	CMB-C2B	-2.37	1.45	1.50
18	B	840	CLA	MG-NB	-2.37	2.01	2.05
18	7	604	CLA	CMB-C2B	-2.37	1.45	1.50
18	1	616	CLA	CMB-C2B	-2.37	1.45	1.50
18	B	841	CLA	C1B-C2B	2.37	1.48	1.43
18	B	816	CLA	MG-NB	-2.37	2.01	2.05
18	4	604	CLA	C1B-C2B	2.37	1.48	1.43
18	4	608	CLA	MG-NB	-2.37	2.01	2.05
18	6	601	CLA	C1B-C2B	2.37	1.48	1.43
18	5	619	CLA	C4B-C3B	2.36	1.48	1.43
18	8	611	CLA	MG-NB	-2.36	2.01	2.05
18	A	809	CLA	MG-NB	-2.36	2.01	2.05
18	3	603	CLA	CMD-C2D	-2.36	1.45	1.50
18	A	823	CLA	C1B-C2B	2.36	1.48	1.43
18	A	803	CLA	CMD-C2D	-2.36	1.45	1.50
18	6	603	CLA	C4B-C3B	2.36	1.48	1.43
18	5	601	CLA	MG-NB	-2.36	2.01	2.05
18	6	610	CLA	C1B-C2B	2.36	1.48	1.43
18	8	612	CLA	C1B-C2B	2.36	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	617	CLA	C1B-C2B	2.36	1.48	1.43
18	8	611	CLA	C1B-C2B	2.36	1.48	1.43
18	4	607	CLA	CMC-C2C	-2.36	1.45	1.50
18	5	618	CLA	C4B-C3B	2.36	1.48	1.43
18	6	607	CLA	CMD-C2D	-2.35	1.45	1.50
18	7	609	CLA	C1B-C2B	2.35	1.48	1.43
27	3	619	XAT	O4-C5	-2.35	1.42	1.46
18	3	613	CLA	CMB-C2B	-2.35	1.45	1.50
18	A	828	CLA	CMC-C2C	-2.35	1.45	1.50
18	a	608	CLA	CHC-C1C	2.35	1.43	1.38
18	5	603	CLA	CMB-C2B	-2.35	1.45	1.50
18	A	825	CLA	C1B-C2B	2.35	1.48	1.43
18	B	829	CLA	C3B-C4B	2.35	1.48	1.42
18	6	611	CLA	C1B-C2B	2.35	1.48	1.43
18	A	818	CLA	CMC-C2C	-2.35	1.45	1.50
18	B	824	CLA	CHC-C1C	2.35	1.43	1.38
18	4	601	CLA	CMD-C2D	-2.35	1.45	1.50
18	B	837	CLA	MG-NB	-2.34	2.01	2.05
18	6	609	CLA	C1B-C2B	2.34	1.48	1.43
18	6	608	CLA	MG-NB	-2.34	2.01	2.05
18	A	803	CLA	C3B-C4B	2.34	1.48	1.42
18	B	806	CLA	C1B-C2B	2.34	1.48	1.43
18	A	812	CLA	CMD-C2D	-2.34	1.45	1.50
18	5	604	CLA	CMB-C2B	-2.34	1.45	1.50
18	5	610	CLA	CMC-C2C	-2.34	1.45	1.50
18	4	604	CLA	CMB-C2B	-2.34	1.45	1.50
18	3	606	CLA	CMD-C2D	-2.34	1.45	1.50
18	B	828	CLA	CMB-C2B	-2.34	1.45	1.50
18	1	601	CLA	C1B-C2B	2.34	1.48	1.43
18	6	602	CLA	MG-NB	-2.34	2.01	2.05
18	8	607	CLA	CMD-C2D	-2.34	1.45	1.50
18	A	842	CLA	MG-NB	-2.34	2.01	2.05
18	5	604	CLA	MG-NB	-2.34	2.01	2.05
18	7	602	CLA	C1B-C2B	2.33	1.48	1.43
18	A	807	CLA	CMC-C2C	-2.33	1.45	1.50
18	a	601	CLA	C1B-C2B	2.33	1.48	1.43
18	4	611	CLA	C1B-C2B	2.33	1.48	1.43
18	A	839	CLA	CMB-C2B	-2.33	1.45	1.50
18	4	607	CLA	CMD-C2D	-2.33	1.45	1.50
18	a	604	CLA	C1B-C2B	2.33	1.48	1.43
18	B	805	CLA	CMD-C2D	-2.33	1.45	1.50
18	A	809	CLA	CMD-C2D	-2.33	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	838	CLA	C1B-C2B	2.33	1.48	1.43
18	A	836	CLA	CMD-C2D	-2.33	1.45	1.50
18	B	834	CLA	CMD-C2D	-2.33	1.45	1.50
18	a	601	CLA	CMD-C2D	-2.33	1.45	1.50
18	6	601	CLA	MG-NB	-2.33	2.01	2.05
18	B	838	CLA	CMB-C2B	-2.33	1.45	1.50
18	a	610	CLA	MG-NB	-2.33	2.01	2.05
18	5	619	CLA	CMB-C2B	-2.33	1.45	1.50
18	3	609	CLA	CMB-C2B	-2.33	1.45	1.50
18	7	601	CLA	C1B-C2B	2.33	1.48	1.43
18	6	620	CLA	C1B-C2B	2.33	1.48	1.43
18	B	804	CLA	CHC-C1C	2.33	1.43	1.38
18	6	613	CLA	C1B-C2B	2.33	1.48	1.43
18	A	814	CLA	C1B-C2B	2.33	1.48	1.43
18	8	609	CLA	C1B-C2B	2.33	1.48	1.43
18	6	604	CLA	MG-NB	-2.32	2.01	2.05
18	B	819	CLA	CMB-C2B	-2.32	1.45	1.50
18	6	603	CLA	MG-NB	-2.32	2.01	2.05
18	B	809	CLA	C1B-C2B	2.32	1.48	1.43
18	A	815	CLA	CMD-C2D	-2.32	1.45	1.50
18	A	811	CLA	C1B-C2B	2.32	1.48	1.43
18	A	819	CLA	C1B-C2B	2.32	1.48	1.43
18	B	818	CLA	CMB-C2B	-2.32	1.45	1.50
18	B	828	CLA	C3B-C4B	2.32	1.48	1.42
18	A	813	CLA	MG-NB	-2.32	2.01	2.05
18	A	805	CLA	CHC-C1C	2.32	1.43	1.38
18	B	809	CLA	CMD-C2D	-2.32	1.45	1.50
18	A	830	CLA	C1B-C2B	2.32	1.48	1.43
18	B	807	CLA	C1B-C2B	2.32	1.48	1.43
18	5	613	CLA	C3B-C4B	2.32	1.48	1.42
18	3	609	CLA	MG-NB	-2.32	2.01	2.05
18	A	814	CLA	C4B-NB	2.31	1.40	1.37
18	A	814	CLA	MG-NB	-2.31	2.01	2.05
18	A	843	CLA	C3B-C4B	2.31	1.48	1.42
18	A	832	CLA	C1B-C2B	2.31	1.48	1.43
18	3	604	CLA	CMB-C2B	-2.31	1.45	1.50
18	1	616	CLA	MG-NB	-2.31	2.01	2.05
18	F	301	CLA	MG-ND	-2.31	2.01	2.05
18	3	604	CLA	C1B-C2B	2.31	1.48	1.43
18	8	607	CLA	C4B-C3B	2.31	1.48	1.43
18	A	814	CLA	CMC-C2C	-2.31	1.45	1.50
18	3	607	CLA	C1B-C2B	2.31	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	606	CLA	CMC-C2C	-2.31	1.45	1.50
18	A	838	CLA	C3B-C4B	2.31	1.48	1.42
18	A	840	CLA	C1B-C2B	2.31	1.48	1.43
18	4	604	CLA	MG-NB	-2.31	2.01	2.05
18	B	824	CLA	C1B-C2B	2.31	1.48	1.43
18	B	825	CLA	C1B-C2B	2.31	1.48	1.43
18	7	608	CLA	CMB-C2B	-2.31	1.45	1.50
18	A	818	CLA	MG-NB	-2.31	2.01	2.05
18	A	826	CLA	C1B-NB	-2.31	1.34	1.37
18	A	841	CLA	C1B-C2B	2.31	1.48	1.43
18	6	609	CLA	MG-NB	-2.31	2.01	2.05
18	a	601	CLA	MG-NB	-2.31	2.01	2.05
18	A	839	CLA	MG-NB	-2.31	2.01	2.05
18	5	617	CLA	MG-NB	-2.31	2.01	2.05
18	B	809	CLA	C3B-C4B	2.31	1.48	1.42
18	7	608	CLA	C1B-C2B	2.30	1.48	1.43
18	A	801	CLA	MG-NB	-2.30	2.01	2.05
18	7	608	CLA	CMD-C2D	-2.30	1.45	1.50
18	4	613	CLA	MG-NB	-2.30	2.01	2.05
18	A	826	CLA	MG-ND	-2.30	2.01	2.05
18	8	614	CLA	MG-NB	-2.30	2.01	2.05
18	7	604	CLA	MG-NB	-2.30	2.01	2.05
18	A	813	CLA	CMC-C2C	-2.30	1.45	1.50
18	B	814	CLA	C1B-C2B	2.30	1.48	1.43
18	7	610	CLA	MG-NB	-2.30	2.01	2.05
18	B	815	CLA	CMC-C2C	-2.30	1.45	1.50
18	A	825	CLA	MG-NB	-2.30	2.01	2.05
18	7	603	CLA	MG-NB	-2.30	2.01	2.05
18	4	614	CLA	MG-NB	-2.30	2.01	2.05
18	B	828	CLA	C1B-NB	-2.29	1.35	1.37
18	A	820	CLA	C1B-NB	-2.29	1.35	1.37
18	B	803	CLA	CMD-C2D	-2.29	1.45	1.50
18	5	602	CLA	CMB-C2B	-2.29	1.45	1.50
18	5	608	CLA	CMC-C2C	-2.29	1.45	1.50
18	5	617	CLA	C3B-C4B	2.29	1.48	1.42
18	B	840	CLA	CMD-C2D	-2.29	1.45	1.50
18	a	602	CLA	MG-NB	-2.29	2.01	2.05
18	3	615	CLA	CMB-C2B	-2.29	1.45	1.50
18	B	806	CLA	C1B-NB	-2.29	1.35	1.37
18	5	603	CLA	CMD-C2D	-2.29	1.45	1.50
18	3	610	CLA	MG-NB	-2.29	2.01	2.05
18	A	815	CLA	CHC-C1C	2.29	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	603	CLA	C4B-C3B	2.29	1.48	1.43
18	A	825	CLA	MG-ND	-2.29	2.01	2.05
18	A	804	CLA	CMD-C2D	-2.29	1.46	1.50
18	8	601	CLA	CMC-C2C	-2.29	1.46	1.50
18	B	820	CLA	CHC-C1C	2.29	1.43	1.38
18	a	616	CLA	MG-NB	-2.29	2.01	2.05
18	B	817	CLA	MG-NB	-2.29	2.01	2.05
18	B	838	CLA	CMD-C2D	-2.29	1.46	1.50
18	B	807	CLA	MG-NB	-2.29	2.01	2.05
18	8	608	CLA	CMC-C2C	-2.28	1.46	1.50
18	5	618	CLA	CMD-C2D	-2.28	1.46	1.50
18	B	802	CLA	C3B-C4B	2.28	1.48	1.42
18	5	619	CLA	MG-NB	-2.28	2.01	2.05
18	6	604	CLA	CMB-C2B	-2.28	1.46	1.50
18	4	603	CLA	CMD-C2D	-2.28	1.46	1.50
18	6	606	CLA	MG-NB	-2.28	2.01	2.05
18	1	610	CLA	MG-NB	-2.28	2.01	2.05
18	3	604	CLA	MG-NB	-2.28	2.01	2.05
18	6	613	CLA	MG-NB	-2.28	2.01	2.05
18	5	610	CLA	C1B-C2B	2.28	1.48	1.43
18	7	612	CLA	CMC-C2C	-2.28	1.46	1.50
18	A	806	CLA	MG-NB	-2.28	2.01	2.05
18	1	608	CLA	CHC-C1C	2.28	1.43	1.38
18	7	614	CLA	MG-NB	-2.28	2.01	2.05
18	A	810	CLA	MG-ND	-2.28	2.01	2.05
18	6	602	CLA	CMB-C2B	-2.28	1.46	1.50
18	A	840	CLA	CMD-C2D	-2.28	1.46	1.50
18	1	610	CLA	CHC-C1C	2.28	1.43	1.38
18	A	819	CLA	CMC-C2C	-2.28	1.46	1.50
18	B	802	CLA	CMC-C2C	-2.28	1.46	1.50
18	5	602	CLA	MG-NB	-2.28	2.01	2.05
18	6	612	CLA	C1B-C2B	2.27	1.48	1.43
18	A	807	CLA	CMB-C2B	-2.27	1.46	1.50
18	B	834	CLA	CMB-C2B	-2.27	1.46	1.50
18	A	830	CLA	MG-ND	-2.27	2.01	2.05
18	A	812	CLA	CMC-C2C	-2.27	1.46	1.50
18	8	613	CLA	CMB-C2B	-2.27	1.46	1.50
18	6	616	CLA	MG-NB	-2.27	2.01	2.05
18	A	838	CLA	C1B-NB	-2.27	1.35	1.37
18	7	610	CLA	C1B-C2B	2.27	1.48	1.43
18	A	807	CLA	CMD-C2D	-2.27	1.46	1.50
18	4	609	CLA	C1B-C2B	2.27	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	608	CLA	CMC-C2C	-2.27	1.46	1.50
18	A	842	CLA	CMD-C2D	-2.27	1.46	1.50
18	a	604	CLA	MG-NB	-2.27	2.01	2.05
18	A	817	CLA	CMD-C2D	-2.27	1.46	1.50
18	3	608	CLA	CMD-C2D	-2.27	1.46	1.50
18	A	815	CLA	MG-NB	-2.26	2.01	2.05
18	B	837	CLA	CHC-C1C	2.26	1.43	1.38
18	7	606	CLA	C1B-C2B	2.26	1.48	1.43
18	5	618	CLA	MG-NB	-2.26	2.01	2.05
18	7	614	CLA	CMD-C2D	-2.26	1.46	1.50
18	A	821	CLA	C1B-C2B	2.26	1.48	1.43
18	4	601	CLA	CMB-C2B	-2.26	1.46	1.50
18	5	609	CLA	MG-NB	-2.26	2.01	2.05
18	A	814	CLA	CMD-C2D	-2.26	1.46	1.50
18	B	819	CLA	CMD-C2D	-2.26	1.46	1.50
18	8	613	CLA	CMD-C2D	-2.26	1.46	1.50
18	B	831	CLA	MG-NB	-2.26	2.01	2.05
18	A	804	CLA	CMC-C2C	-2.26	1.46	1.50
18	A	831	CLA	CHC-C4B	-2.26	1.34	1.39
18	A	801	CLA	C3B-C4B	2.26	1.48	1.42
18	A	817	CLA	CMB-C2B	-2.26	1.46	1.50
18	A	819	CLA	CMD-C2D	-2.26	1.46	1.50
18	1	602	CLA	MG-NB	-2.26	2.01	2.05
18	4	611	CLA	MG-NB	-2.26	2.01	2.05
18	3	610	CLA	C1B-C2B	2.26	1.48	1.43
26	7	619	LUT	C30-C29	-2.25	1.32	1.35
18	B	827	CLA	CMB-C2B	-2.25	1.46	1.50
18	5	618	CLA	CMC-C2C	-2.25	1.46	1.50
18	B	806	CLA	MG-ND	-2.25	2.01	2.05
18	B	826	CLA	MG-NB	-2.25	2.01	2.05
18	A	811	CLA	CMB-C2B	-2.25	1.46	1.50
20	a	620	LHG	O7-C5	-2.25	1.41	1.46
18	A	825	CLA	CMB-C2B	-2.25	1.46	1.50
18	A	828	CLA	CMB-C2B	-2.25	1.46	1.50
18	7	610	CLA	CMC-C2C	-2.25	1.46	1.50
18	1	613	CLA	CMD-C2D	-2.25	1.46	1.50
18	A	838	CLA	C1B-C2B	2.25	1.48	1.43
18	6	610	CLA	CMD-C2D	-2.25	1.46	1.50
18	7	613	CLA	CMB-C2B	-2.25	1.46	1.50
18	B	819	CLA	MG-NB	-2.25	2.01	2.05
18	A	828	CLA	C1B-C2B	2.25	1.48	1.43
18	8	603	CLA	C4B-C3B	2.24	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	603	CLA	CMB-C2B	-2.24	1.46	1.50
18	A	838	CLA	MG-ND	-2.24	2.01	2.05
18	A	829	CLA	CMD-C2D	-2.24	1.46	1.50
18	a	614	CLA	MG-NB	-2.24	2.01	2.05
18	3	614	CLA	MG-NB	-2.24	2.01	2.05
18	A	808	CLA	MG-NB	-2.24	2.01	2.05
18	B	840	CLA	C1B-C2B	2.24	1.48	1.43
18	6	617	CLA	MG-NB	-2.24	2.01	2.05
18	A	809	CLA	CMB-C2B	-2.24	1.46	1.50
18	8	612	CLA	CMD-C2D	-2.24	1.46	1.50
18	B	814	CLA	MG-NB	-2.24	2.01	2.05
18	3	611	CLA	MG-NB	-2.24	2.01	2.05
27	7	620	XAT	O24-C25	-2.24	1.43	1.46
18	7	601	CLA	CMD-C2D	-2.24	1.46	1.50
18	5	609	CLA	C1B-C2B	2.23	1.48	1.43
18	A	822	CLA	CMD-C2D	-2.23	1.46	1.50
18	B	804	CLA	CMD-C2D	-2.23	1.46	1.50
18	8	611	CLA	CMB-C2B	-2.23	1.46	1.50
18	a	610	CLA	CMB-C2B	-2.23	1.46	1.50
18	6	614	CLA	CMD-C2D	-2.23	1.46	1.50
18	5	604	CLA	CMD-C2D	-2.23	1.46	1.50
18	1	611	CLA	MG-NB	-2.23	2.01	2.05
18	A	810	CLA	CMC-C2C	-2.23	1.46	1.50
18	B	805	CLA	MG-NB	-2.23	2.01	2.05
18	5	607	CLA	MG-NB	-2.23	2.01	2.05
18	B	828	CLA	CMC-C2C	-2.23	1.46	1.50
18	A	834	CLA	CMB-C2B	-2.23	1.46	1.50
18	4	618	CLA	CMC-C2C	-2.23	1.46	1.50
18	5	603	CLA	MG-ND	-2.23	2.01	2.05
18	A	811	CLA	MG-NB	-2.23	2.01	2.05
18	A	841	CLA	CMB-C2B	-2.23	1.46	1.50
18	7	602	CLA	CMC-C2C	-2.23	1.46	1.50
18	7	612	CLA	CHC-C1C	2.23	1.43	1.38
18	B	827	CLA	C1B-C2B	2.23	1.48	1.43
18	3	606	CLA	MG-NB	-2.23	2.01	2.05
18	A	854	CLA	CMD-C2D	-2.23	1.46	1.50
18	5	603	CLA	CMC-C2C	-2.23	1.46	1.50
18	K	204	CLA	MG-NB	-2.23	2.01	2.05
18	3	613	CLA	MG-NB	-2.23	2.01	2.05
18	B	825	CLA	CHC-C1C	2.23	1.43	1.38
18	7	601	CLA	CMC-C2C	-2.22	1.46	1.50
18	7	607	CLA	MG-NB	-2.22	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	803	CLA	C1B-C2B	2.22	1.48	1.43
18	1	610	CLA	C1B-C2B	2.22	1.48	1.43
18	B	827	CLA	CMD-C2D	-2.22	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.22	1.46	1.50
18	5	612	CLA	CMC-C2C	-2.22	1.46	1.50
18	5	606	CLA	CMB-C2B	-2.22	1.46	1.50
18	6	607	CLA	MG-NB	-2.22	2.01	2.05
18	a	604	CLA	CMB-C2B	-2.22	1.46	1.50
18	4	614	CLA	CMD-C2D	-2.22	1.46	1.50
18	A	838	CLA	C4B-NB	2.22	1.40	1.37
18	a	610	CLA	C1B-C2B	2.22	1.48	1.43
18	A	822	CLA	C1B-NB	-2.22	1.35	1.37
18	6	620	CLA	CMC-C2C	-2.22	1.46	1.50
18	A	823	CLA	MG-NB	-2.22	2.01	2.05
18	6	611	CLA	MG-NB	-2.22	2.01	2.05
18	B	813	CLA	CMD-C2D	-2.22	1.46	1.50
18	6	608	CLA	CHC-C1C	2.22	1.43	1.38
18	B	815	CLA	CMD-C2D	-2.22	1.46	1.50
18	3	612	CLA	C1B-C2B	2.22	1.48	1.43
18	6	620	CLA	CHC-C1C	2.22	1.43	1.38
18	6	602	CLA	CMC-C2C	-2.22	1.46	1.50
18	5	603	CLA	C1B-C2B	2.22	1.48	1.43
18	A	805	CLA	CMC-C2C	-2.22	1.46	1.50
18	6	618	CLA	CMC-C2C	-2.22	1.46	1.50
18	A	807	CLA	MG-NB	-2.22	2.01	2.05
18	3	603	CLA	MG-ND	-2.22	2.01	2.05
18	8	610	CLA	MG-NB	-2.22	2.01	2.05
27	6	621	XAT	O24-C25	-2.22	1.43	1.46
18	1	610	CLA	CMB-C2B	-2.21	1.46	1.50
18	5	606	CLA	CMD-C2D	-2.21	1.46	1.50
18	A	821	CLA	CMB-C2B	-2.21	1.46	1.50
18	B	812	CLA	CHC-C1C	2.21	1.43	1.38
18	A	839	CLA	CMC-C2C	-2.21	1.46	1.50
18	6	610	CLA	CMC-C2C	-2.21	1.46	1.50
18	6	616	CLA	CHC-C1C	2.21	1.43	1.38
18	A	816	CLA	CMC-C2C	-2.21	1.46	1.50
18	6	612	CLA	MG-NB	-2.21	2.01	2.05
18	A	832	CLA	MG-ND	-2.21	2.01	2.05
18	B	813	CLA	MG-NB	-2.21	2.01	2.05
18	F	303	CLA	CMB-C2B	-2.21	1.46	1.50
18	7	616	CLA	MG-NB	-2.21	2.01	2.05
18	A	802	CLA	CMC-C2C	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	C1B-C2B	2.21	1.48	1.43
18	4	610	CLA	CMC-C2C	-2.21	1.46	1.50
18	1	614	CLA	MG-NB	-2.21	2.01	2.05
18	B	837	CLA	CMD-C2D	-2.21	1.46	1.50
18	B	841	CLA	MG-NB	-2.21	2.01	2.05
18	A	826	CLA	CMC-C2C	-2.21	1.46	1.50
18	3	602	CLA	C4B-NB	2.21	1.40	1.37
18	5	616	CLA	MG-NB	-2.20	2.01	2.05
18	6	620	CLA	CMD-C2D	-2.20	1.46	1.50
18	5	603	CLA	CHC-C1C	2.20	1.43	1.38
18	8	610	CLA	CMC-C2C	-2.20	1.46	1.50
18	A	804	CLA	MG-NB	-2.20	2.01	2.05
18	4	602	CLA	CMD-C2D	-2.20	1.46	1.50
18	4	611	CLA	CHC-C1C	2.20	1.43	1.38
18	5	612	CLA	CMD-C2D	-2.20	1.46	1.50
18	8	603	CLA	CMC-C2C	-2.20	1.46	1.50
18	1	609	CLA	CHC-C1C	2.20	1.43	1.38
18	B	806	CLA	CMD-C2D	-2.20	1.46	1.50
18	4	608	CLA	CMD-C2D	-2.20	1.46	1.50
18	F	304	CLA	MG-NB	-2.20	2.01	2.05
18	a	612	CLA	MG-NB	-2.20	2.01	2.05
18	B	826	CLA	CMD-C2D	-2.20	1.46	1.50
18	A	824	CLA	MG-NB	-2.20	2.01	2.05
18	A	833	CLA	CMD-C2D	-2.20	1.46	1.50
18	6	616	CLA	CMB-C2B	-2.20	1.46	1.50
18	B	813	CLA	CMC-C2C	-2.20	1.46	1.50
18	3	609	CLA	CMD-C2D	-2.20	1.46	1.50
18	A	810	CLA	CMB-C2B	-2.19	1.46	1.50
18	8	607	CLA	CMB-C2B	-2.19	1.46	1.50
18	6	604	CLA	CMD-C2D	-2.19	1.46	1.50
18	5	608	CLA	C1B-C2B	2.19	1.48	1.43
18	A	816	CLA	CMD-C2D	-2.19	1.46	1.50
18	5	602	CLA	CMC-C2C	-2.19	1.46	1.50
18	6	613	CLA	CMD-C2D	-2.19	1.46	1.50
18	A	842	CLA	CMB-C2B	-2.19	1.46	1.50
18	F	304	CLA	CMD-C2D	-2.19	1.46	1.50
18	A	809	CLA	C1B-C2B	2.19	1.48	1.43
18	1	614	CLA	CHC-C1C	2.19	1.43	1.38
18	A	834	CLA	C1B-C2B	2.19	1.48	1.43
18	A	829	CLA	C1B-C2B	2.19	1.48	1.43
18	B	828	CLA	C1B-C2B	2.19	1.48	1.43
18	B	810	CLA	CMB-C2B	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	837	CLA	CMB-C2B	-2.19	1.46	1.50
18	5	618	CLA	CMB-C2B	-2.19	1.46	1.50
18	A	836	CLA	C3B-C4B	2.19	1.47	1.42
18	B	814	CLA	CHC-C1C	2.19	1.43	1.38
18	3	607	CLA	MG-NB	-2.19	2.01	2.05
18	K	201	CLA	MG-NB	-2.19	2.01	2.05
18	B	807	CLA	CMD-C2D	-2.19	1.46	1.50
18	6	617	CLA	CMD-C2D	-2.19	1.46	1.50
18	6	602	CLA	C1B-C2B	2.19	1.48	1.43
18	6	620	CLA	MG-NB	-2.19	2.01	2.05
18	3	610	CLA	CMD-C2D	-2.19	1.46	1.50
18	6	608	CLA	CMC-C2C	-2.19	1.46	1.50
18	7	610	CLA	CMB-C2B	-2.19	1.46	1.50
18	B	818	CLA	C1B-C2B	2.19	1.48	1.43
18	A	815	CLA	C1B-C2B	2.19	1.48	1.43
18	K	206	CLA	MG-NB	-2.18	2.01	2.05
18	8	606	CLA	CMB-C2B	-2.18	1.46	1.50
18	B	834	CLA	MG-NB	-2.18	2.01	2.05
18	B	806	CLA	CMB-C2B	-2.18	1.46	1.50
18	A	809	CLA	CHC-C1C	2.18	1.43	1.38
27	7	620	XAT	O4-C5	-2.18	1.43	1.46
18	7	614	CLA	CMB-C2B	-2.18	1.46	1.50
18	5	602	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	816	CLA	C1B-C2B	2.18	1.48	1.43
18	B	836	CLA	CMD-C2D	-2.18	1.46	1.50
18	8	601	CLA	CMB-C2B	-2.18	1.46	1.50
18	A	830	CLA	C1B-NB	-2.18	1.35	1.37
18	B	808	CLA	CMB-C2B	-2.18	1.46	1.50
18	4	603	CLA	MG-NB	-2.18	2.01	2.05
18	8	607	CLA	MG-NB	-2.18	2.01	2.05
18	B	836	CLA	CHC-C1C	2.18	1.43	1.38
18	8	601	CLA	MG-ND	-2.18	2.01	2.05
18	8	606	CLA	C1B-C2B	2.18	1.48	1.43
18	3	608	CLA	C1B-C2B	2.18	1.48	1.43
18	A	820	CLA	CMD-C2D	-2.18	1.46	1.50
18	8	603	CLA	MG-NB	-2.18	2.01	2.05
18	B	832	CLA	CMD-C2D	-2.18	1.46	1.50
18	8	609	CLA	CMD-C2D	-2.18	1.46	1.50
18	a	611	CLA	MG-NB	-2.18	2.01	2.05
18	A	840	CLA	CMB-C2B	-2.18	1.46	1.50
18	7	612	CLA	CMD-C2D	-2.18	1.46	1.50
18	5	608	CLA	CMD-C2D	-2.18	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	818	CLA	CMD-C2D	-2.18	1.46	1.50
18	1	607	CLA	CHC-C1C	2.17	1.42	1.38
18	6	617	CLA	CHC-C1C	2.17	1.42	1.38
18	1	604	CLA	MG-NB	-2.17	2.01	2.05
18	8	607	CLA	CMC-C2C	-2.17	1.46	1.50
27	6	621	XAT	O4-C5	-2.17	1.43	1.46
18	A	845	CLA	CMB-C2B	-2.17	1.46	1.50
18	A	828	CLA	CMD-C2D	-2.17	1.46	1.50
18	6	618	CLA	MG-NB	-2.17	2.01	2.05
18	K	204	CLA	CMD-C2D	-2.17	1.46	1.50
18	B	824	CLA	CMB-C2B	-2.17	1.46	1.50
18	B	811	CLA	MG-NB	-2.17	2.01	2.05
18	K	201	CLA	MG-ND	-2.17	2.01	2.05
18	8	608	CLA	CMB-C2B	-2.17	1.46	1.50
18	5	614	CLA	MG-NB	-2.17	2.01	2.05
18	F	304	CLA	CHC-C1C	2.17	1.42	1.38
18	K	203	CLA	CHC-C1C	2.17	1.42	1.38
18	6	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	6	610	CLA	CHC-C1C	2.17	1.42	1.38
18	7	616	CLA	CHC-C1C	2.17	1.42	1.38
18	A	817	CLA	MG-NB	-2.17	2.01	2.05
18	8	602	CLA	CMC-C2C	-2.17	1.46	1.50
18	8	610	CLA	CHC-C1C	2.17	1.42	1.38
18	A	812	CLA	MG-NB	-2.17	2.01	2.05
18	8	604	CLA	MG-NB	-2.17	2.01	2.05
18	a	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	A	829	CLA	CMC-C2C	-2.17	1.46	1.50
18	B	839	CLA	CMB-C2B	-2.17	1.46	1.50
18	1	602	CLA	CMC-C2C	-2.17	1.46	1.50
18	5	611	CLA	CMD-C2D	-2.17	1.46	1.50
18	5	619	CLA	CMD-C2D	-2.17	1.46	1.50
18	7	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	5	611	CLA	MG-NB	-2.17	2.01	2.05
18	A	805	CLA	CMB-C2B	-2.17	1.46	1.50
18	A	845	CLA	CMC-C2C	-2.16	1.46	1.50
18	3	611	CLA	CMD-C2D	-2.16	1.46	1.50
18	8	611	CLA	CMD-C2D	-2.16	1.46	1.50
18	5	606	CLA	C1B-C2B	2.16	1.48	1.43
18	a	607	CLA	CHC-C1C	2.16	1.42	1.38
18	A	826	CLA	CMB-C2B	-2.16	1.46	1.50
18	4	610	CLA	CMD-C2D	-2.16	1.46	1.50
18	3	602	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)
18	6	617	CLA	CMC-C2C	-2.16	1.46	1.50
18	A	831	CLA	C3B-C4B	2.16	1.47	1.42
18	A	813	CLA	CMD-C2D	-2.16	1.46	1.50
18	a	602	CLA	CHC-C1C	2.16	1.42	1.38
18	B	803	CLA	C1D-ND	2.16	1.40	1.37
18	B	812	CLA	CMD-C2D	-2.16	1.46	1.50
18	B	805	CLA	MG-ND	-2.16	2.01	2.05
18	8	603	CLA	CMB-C2B	-2.16	1.46	1.50
24	A	860	LMG	C4-C3	2.16	1.57	1.52
18	a	613	CLA	MG-NB	-2.16	2.01	2.05
18	7	603	CLA	CMB-C2B	-2.16	1.46	1.50
18	B	835	CLA	CHC-C1C	2.16	1.42	1.38
18	4	611	CLA	CMC-C2C	-2.16	1.46	1.50
18	1	606	CLA	MG-NB	-2.16	2.01	2.05
18	a	612	CLA	CHC-C1C	2.16	1.42	1.38
18	a	606	CLA	MG-NB	-2.16	2.01	2.05
18	6	612	CLA	CHC-C1C	2.16	1.42	1.38
18	6	608	CLA	CMB-C2B	-2.16	1.46	1.50
18	B	824	CLA	MG-NB	-2.16	2.01	2.05
18	1	613	CLA	MG-NB	-2.16	2.01	2.05
18	6	610	CLA	MG-NB	-2.16	2.01	2.05
18	B	807	CLA	CMB-C2B	-2.16	1.46	1.50
18	A	803	CLA	CMC-C2C	-2.16	1.46	1.50
18	4	603	CLA	CMB-C2B	-2.16	1.46	1.50
18	A	806	CLA	CMB-C2B	-2.15	1.46	1.50
18	B	809	CLA	MG-ND	-2.15	2.01	2.05
18	7	615	CLA	MG-NB	-2.15	2.01	2.05
18	1	604	CLA	CMB-C2B	-2.15	1.46	1.50
18	6	612	CLA	CMD-C2D	-2.15	1.46	1.50
18	B	836	CLA	C1B-C2B	2.15	1.48	1.43
18	4	613	CLA	CMB-C2B	-2.15	1.46	1.50
18	B	804	CLA	CMC-C2C	-2.15	1.46	1.50
18	5	610	CLA	CMD-C2D	-2.15	1.46	1.50
18	6	606	CLA	CMB-C2B	-2.15	1.46	1.50
18	7	609	CLA	CMD-C2D	-2.15	1.46	1.50
18	5	610	CLA	MG-NB	-2.15	2.01	2.05
18	7	602	CLA	CHC-C1C	2.15	1.42	1.38
18	8	612	CLA	CMC-C2C	-2.15	1.46	1.50
18	A	801	CLA	CMC-C2C	-2.15	1.46	1.50
18	5	616	CLA	CMD-C2D	-2.15	1.46	1.50
18	4	606	CLA	CMB-C2B	-2.15	1.46	1.50
18	4	610	CLA	MG-NB	-2.15	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	CMD-C2D	-2.15	1.46	1.50
18	A	827	CLA	C1B-NB	-2.15	1.35	1.37
18	8	604	CLA	CMD-C2D	-2.15	1.46	1.50
18	5	609	CLA	CMB-C2B	-2.15	1.46	1.50
18	6	613	CLA	CMC-C2C	-2.15	1.46	1.50
18	6	616	CLA	CMD-C2D	-2.15	1.46	1.50
18	4	604	CLA	CHC-C1C	2.15	1.42	1.38
18	A	810	CLA	C1B-C2B	2.15	1.48	1.43
18	a	610	CLA	CHC-C1C	2.15	1.42	1.38
18	A	834	CLA	CMD-C2D	-2.14	1.46	1.50
18	6	614	CLA	CMC-C2C	-2.14	1.46	1.50
18	7	606	CLA	MG-NB	-2.14	2.01	2.05
18	A	841	CLA	CMD-C2D	-2.14	1.46	1.50
18	6	603	CLA	CMB-C2B	-2.14	1.46	1.50
18	A	821	CLA	MG-NB	-2.14	2.01	2.05
18	A	833	CLA	C1B-C2B	2.14	1.48	1.43
18	5	619	CLA	C1B-C2B	2.14	1.48	1.43
18	8	604	CLA	CMB-C2B	-2.14	1.46	1.50
18	a	601	CLA	CHC-C1C	2.14	1.42	1.38
18	7	604	CLA	C1B-C2B	2.14	1.48	1.43
18	7	613	CLA	CMC-C2C	-2.14	1.46	1.50
18	4	610	CLA	CMB-C2B	-2.14	1.46	1.50
18	a	602	CLA	CMC-C2C	-2.14	1.46	1.50
18	8	602	CLA	CMB-C2B	-2.14	1.46	1.50
18	3	604	CLA	CMD-C2D	-2.14	1.46	1.50
18	A	804	CLA	CMB-C2B	-2.14	1.46	1.50
18	A	823	CLA	CMB-C2B	-2.14	1.46	1.50
18	A	845	CLA	MG-NB	-2.14	2.01	2.05
18	1	606	CLA	CHC-C1C	2.14	1.42	1.38
18	A	808	CLA	CMB-C2B	-2.14	1.46	1.50
18	8	612	CLA	MG-NB	-2.14	2.01	2.05
18	A	805	CLA	CMD-C2D	-2.13	1.46	1.50
18	3	617	CLA	CMD-C2D	-2.13	1.46	1.50
18	7	612	CLA	CMB-C2B	-2.13	1.46	1.50
18	B	832	CLA	CMC-C2C	-2.13	1.46	1.50
18	B	833	CLA	CMB-C2B	-2.13	1.46	1.50
18	A	843	CLA	CMD-C2D	-2.13	1.46	1.50
18	5	612	CLA	MG-NB	-2.13	2.01	2.05
18	A	842	CLA	CMC-C2C	-2.13	1.46	1.50
18	a	602	CLA	CMD-C2D	-2.13	1.46	1.50
18	8	603	CLA	CMD-C2D	-2.13	1.46	1.50
18	6	614	CLA	CHC-C1C	2.13	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	603	CLA	CMB-C2B	-2.13	1.46	1.50
18	3	614	CLA	CMC-C2C	-2.13	1.46	1.50
24	A	860	LMG	O7-C8	-2.13	1.41	1.46
18	B	818	CLA	CMD-C2D	-2.13	1.46	1.50
18	6	614	CLA	MG-NB	-2.13	2.01	2.05
18	A	835	CLA	CMB-C2B	-2.13	1.46	1.50
18	4	612	CLA	CMD-C2D	-2.13	1.46	1.50
18	7	604	CLA	CMD-C2D	-2.13	1.46	1.50
18	A	823	CLA	CMD-C2D	-2.13	1.46	1.50
18	A	807	CLA	MG-ND	-2.13	2.01	2.05
18	7	613	CLA	MG-NB	-2.13	2.01	2.05
18	F	301	CLA	C1B-C2B	2.13	1.48	1.43
18	5	607	CLA	CMD-C2D	-2.13	1.46	1.50
18	4	616	CLA	MG-NB	-2.13	2.01	2.05
18	8	611	CLA	CMC-C2C	-2.13	1.46	1.50
18	4	612	CLA	CHC-C1C	2.13	1.42	1.38
18	B	835	CLA	CMD-C2D	-2.13	1.46	1.50
18	4	616	CLA	CHC-C1C	2.13	1.42	1.38
18	7	615	CLA	CHC-C1C	2.13	1.42	1.38
18	B	808	CLA	MG-NB	-2.13	2.01	2.05
18	B	814	CLA	MG-ND	-2.13	2.01	2.05
18	7	603	CLA	CMC-C2C	-2.13	1.46	1.50
18	4	603	CLA	CMC-C2C	-2.12	1.46	1.50
18	6	611	CLA	CHC-C1C	2.12	1.42	1.38
18	B	806	CLA	CMC-C2C	-2.12	1.46	1.50
18	B	816	CLA	CHC-C1C	2.12	1.42	1.38
18	6	613	CLA	CMB-C2B	-2.12	1.46	1.50
18	8	602	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	830	CLA	CMB-C2B	-2.12	1.46	1.50
18	4	612	CLA	MG-NB	-2.12	2.01	2.05
18	3	612	CLA	CMB-C2B	-2.12	1.46	1.50
18	F	303	CLA	MG-NB	-2.12	2.01	2.05
18	A	815	CLA	CMB-C2B	-2.12	1.46	1.50
18	B	827	CLA	CMC-C2C	-2.12	1.46	1.50
18	A	802	CLA	MG-NB	-2.12	2.01	2.05
18	5	606	CLA	MG-NB	-2.12	2.01	2.05
18	7	610	CLA	CHC-C1C	2.12	1.42	1.38
18	3	612	CLA	CMD-C2D	-2.12	1.46	1.50
18	7	601	CLA	CMB-C2B	-2.12	1.46	1.50
18	7	610	CLA	CMD-C2D	-2.12	1.46	1.50
18	1	604	CLA	CHC-C1C	2.12	1.42	1.38
18	A	835	CLA	MG-NB	-2.12	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	612	CLA	MG-NB	-2.12	2.01	2.05
18	4	602	CLA	CMC-C2C	-2.12	1.46	1.50
18	B	825	CLA	CMC-C2C	-2.12	1.46	1.50
18	1	603	CLA	CMD-C2D	-2.12	1.46	1.50
18	7	608	CLA	CAC-C3C	-2.12	1.45	1.51
18	7	602	CLA	MG-NB	-2.12	2.01	2.05
18	6	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	6	612	CLA	CMC-C2C	-2.12	1.46	1.50
18	3	617	CLA	CHC-C1C	2.11	1.42	1.38
18	B	817	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	813	CLA	CHC-C1C	2.11	1.42	1.38
18	a	614	CLA	CMD-C2D	-2.11	1.46	1.50
18	J	101	CLA	CMD-C2D	-2.11	1.46	1.50
18	6	607	CLA	CMB-C2B	-2.11	1.46	1.50
18	B	837	CLA	CMC-C2C	-2.11	1.46	1.50
18	B	836	CLA	C1B-NB	-2.11	1.35	1.37
18	A	854	CLA	MG-ND	-2.11	2.01	2.05
18	5	614	CLA	CHC-C1C	2.11	1.42	1.38
18	B	831	CLA	CMC-C2C	-2.11	1.46	1.50
18	B	832	CLA	C1B-C2B	2.11	1.48	1.43
18	B	817	CLA	CHC-C1C	2.11	1.42	1.38
18	1	604	CLA	CMD-C2D	-2.11	1.46	1.50
18	a	604	CLA	CMD-C2D	-2.11	1.46	1.50
18	7	606	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	815	CLA	MG-NB	-2.11	2.01	2.05
18	a	608	CLA	MG-NB	-2.11	2.01	2.05
18	1	602	CLA	CHC-C1C	2.11	1.42	1.38
18	A	839	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	830	CLA	C3C-C2C	2.11	1.41	1.36
18	A	802	CLA	CHC-C1C	2.11	1.42	1.38
18	B	816	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	803	CLA	C1B-NB	-2.11	1.35	1.37
18	7	607	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	807	CLA	CHC-C1C	2.11	1.42	1.38
18	a	606	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	816	CLA	MG-NB	-2.11	2.01	2.05
18	A	832	CLA	C1B-NB	-2.11	1.35	1.37
24	J	104	LMG	O7-C8	-2.11	1.41	1.46
18	5	616	CLA	CMB-C2B	-2.11	1.46	1.50
18	7	611	CLA	MG-NB	-2.11	2.01	2.05
18	8	608	CLA	CHC-C1C	2.11	1.42	1.38
18	A	843	CLA	MG-ND	-2.11	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	619	XAT	O24-C25	-2.11	1.43	1.46
18	a	612	CLA	CMD-C2D	-2.11	1.46	1.50
18	6	602	CLA	CMD-C2D	-2.11	1.46	1.50
18	6	604	CLA	CMC-C2C	-2.11	1.46	1.50
18	1	612	CLA	MG-NB	-2.11	2.01	2.05
18	8	608	CLA	MG-NB	-2.11	2.01	2.05
18	1	601	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	810	CLA	MG-NB	-2.11	2.01	2.05
18	B	835	CLA	MG-NB	-2.11	2.01	2.05
18	B	833	CLA	MG-NB	-2.10	2.01	2.05
18	4	609	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	613	CLA	CMD-C2D	-2.10	1.46	1.50
18	K	206	CLA	CHC-C1C	2.10	1.42	1.38
18	A	811	CLA	CMD-C2D	-2.10	1.46	1.50
18	6	606	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	804	CLA	CMB-C2B	-2.10	1.46	1.50
18	B	836	CLA	CMC-C2C	-2.10	1.46	1.50
24	4	624	LMG	C4-C5	2.10	1.57	1.53
18	5	608	CLA	MG-ND	-2.10	2.01	2.05
18	6	620	CLA	CMB-C2B	-2.10	1.46	1.50
18	8	606	CLA	CMD-C2D	-2.10	1.46	1.50
18	L	303	CLA	CHC-C1C	2.10	1.42	1.38
18	L	304	CLA	CHC-C1C	2.10	1.42	1.38
18	4	609	CLA	CMB-C2B	-2.10	1.46	1.50
18	A	810	CLA	CHC-C1C	2.10	1.42	1.38
18	B	803	CLA	C4B-NB	2.10	1.40	1.37
18	A	806	CLA	MG-ND	-2.10	2.01	2.05
18	7	614	CLA	CHC-C1C	2.10	1.42	1.38
18	B	826	CLA	CHC-C1C	2.10	1.42	1.38
18	4	618	CLA	CMB-C2B	-2.10	1.46	1.50
18	B	805	CLA	CMC-C2C	-2.09	1.46	1.50
18	6	601	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	808	CLA	CMC-C2C	-2.09	1.46	1.50
18	3	607	CLA	CMB-C2B	-2.09	1.46	1.50
18	L	302	CLA	CHC-C1C	2.09	1.42	1.38
18	A	803	CLA	C1B-NB	-2.09	1.35	1.37
20	4	622	LHG	O7-C5	-2.09	1.41	1.46
18	1	607	CLA	MG-NB	-2.09	2.01	2.05
18	B	831	CLA	CMD-C2D	-2.09	1.46	1.50
18	8	614	CLA	CMD-C2D	-2.09	1.46	1.50
18	1	608	CLA	MG-NB	-2.09	2.01	2.05
18	4	616	CLA	CMB-C2B	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	CMB-C2B	-2.09	1.46	1.50
18	4	616	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	819	CLA	MG-ND	-2.09	2.01	2.05
18	6	620	CLA	O2A-CGA	2.09	1.37	1.30
18	8	614	CLA	CMB-C2B	-2.09	1.46	1.50
18	K	203	CLA	MG-NB	-2.09	2.01	2.05
18	4	618	CLA	MG-NB	-2.09	2.01	2.05
18	4	607	CLA	MG-NB	-2.09	2.01	2.05
18	B	816	CLA	CMB-C2B	-2.09	1.46	1.50
18	4	612	CLA	CMC-C2C	-2.09	1.46	1.50
18	B	818	CLA	CMC-C2C	-2.09	1.46	1.50
18	1	601	CLA	CMB-C2B	-2.09	1.46	1.50
18	a	602	CLA	CMB-C2B	-2.09	1.46	1.50
18	3	612	CLA	CMC-C2C	-2.09	1.46	1.50
18	7	606	CLA	CMC-C2C	-2.09	1.46	1.50
18	A	821	CLA	CMC-C2C	-2.09	1.46	1.50
18	B	837	CLA	C1B-C2B	2.09	1.48	1.43
18	A	813	CLA	CMB-C2B	-2.09	1.46	1.50
18	A	837	CLA	CMD-C2D	-2.09	1.46	1.50
18	7	608	CLA	CMC-C2C	-2.09	1.46	1.50
18	4	606	CLA	CMC-C2C	-2.09	1.46	1.50
18	6	604	CLA	MG-ND	-2.09	2.01	2.05
18	A	827	CLA	CMB-C2B	-2.09	1.46	1.50
18	A	827	CLA	MG-ND	-2.09	2.01	2.05
27	a	618	XAT	O4-C5	-2.09	1.43	1.46
18	3	617	CLA	CMB-C2B	-2.09	1.46	1.50
18	7	602	CLA	CMB-C2B	-2.09	1.46	1.50
18	3	611	CLA	CHC-C1C	2.09	1.42	1.38
18	8	613	CLA	CMC-C2C	-2.09	1.46	1.50
18	K	204	CLA	CMC-C2C	-2.09	1.46	1.50
18	6	611	CLA	CMB-C2B	-2.09	1.46	1.50
18	5	607	CLA	CHC-C1C	2.09	1.42	1.38
18	5	613	CLA	CMB-C2B	-2.08	1.46	1.50
27	8	620	XAT	O4-C5	-2.08	1.43	1.46
18	F	304	CLA	CMB-C2B	-2.08	1.46	1.50
18	1	602	CLA	CMD-C2D	-2.08	1.46	1.50
18	5	601	CLA	CMB-C2B	-2.08	1.46	1.50
18	6	618	CLA	CHC-C1C	2.08	1.42	1.38
18	7	604	CLA	CMC-C2C	-2.08	1.46	1.50
18	B	809	CLA	C1B-NB	-2.08	1.35	1.37
18	3	614	CLA	CMD-C2D	-2.08	1.46	1.50
18	8	606	CLA	CMC-C2C	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	613	CLA	CMC-C2C	-2.08	1.46	1.50
18	5	611	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	816	CLA	CMC-C2C	-2.08	1.46	1.50
18	4	614	CLA	CMB-C2B	-2.08	1.46	1.50
18	8	608	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	820	CLA	MG-ND	-2.08	2.01	2.05
18	6	611	CLA	CMC-C2C	-2.08	1.46	1.50
18	A	845	CLA	CMD-C2D	-2.08	1.46	1.50
18	5	610	CLA	CHC-C1C	2.08	1.42	1.38
18	B	811	CLA	CMB-C2B	-2.08	1.46	1.50
18	K	203	CLA	CMB-C2B	-2.08	1.46	1.50
18	3	610	CLA	CHC-C1C	2.08	1.42	1.38
18	K	206	CLA	CMC-C2C	-2.08	1.46	1.50
18	7	602	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	841	CLA	CMC-C2C	-2.08	1.46	1.50
18	7	612	CLA	C1B-C2B	2.08	1.48	1.43
18	B	833	CLA	CHC-C1C	2.08	1.42	1.38
18	1	614	CLA	CMD-C2D	-2.08	1.46	1.50
18	8	606	CLA	MG-NB	-2.08	2.01	2.05
18	5	608	CLA	CMB-C2B	-2.08	1.46	1.50
18	a	601	CLA	MG-ND	-2.08	2.01	2.05
18	3	617	CLA	CMC-C2C	-2.08	1.46	1.50
18	A	837	CLA	MG-NB	-2.08	2.01	2.05
18	3	615	CLA	MG-NB	-2.07	2.01	2.05
18	K	206	CLA	CMD-C2D	-2.07	1.46	1.50
18	a	608	CLA	CMD-C2D	-2.07	1.46	1.50
18	6	611	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	850	DGD	O2G-C2G	-2.07	1.41	1.46
18	B	831	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	614	CLA	CMB-C2B	-2.07	1.46	1.50
18	1	613	CLA	CHC-C1C	2.07	1.42	1.38
18	A	806	CLA	CAC-C3C	-2.07	1.45	1.51
18	3	610	CLA	CMB-C2B	-2.07	1.46	1.50
18	B	830	CLA	MG-NB	-2.07	2.01	2.05
18	5	618	CLA	CHC-C1C	2.07	1.42	1.38
18	K	203	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	818	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	607	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	811	CLA	CHC-C1C	2.07	1.42	1.38
18	B	839	CLA	C1B-C2B	2.07	1.48	1.43
18	6	612	CLA	CMB-C2B	-2.07	1.46	1.50
18	4	611	CLA	CMD-C2D	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	616	CLA	CMC-C2C	-2.07	1.46	1.50
18	7	604	CLA	CHC-C1C	2.07	1.42	1.38
18	A	843	CLA	CMC-C2C	-2.07	1.46	1.50
18	A	827	CLA	CHC-C1C	2.07	1.42	1.38
18	F	303	CLA	CMC-C2C	-2.07	1.46	1.50
18	5	619	CLA	MG-ND	-2.07	2.01	2.05
18	B	812	CLA	MG-NB	-2.07	2.01	2.05
18	B	809	CLA	CMC-C2C	-2.07	1.46	1.50
18	1	610	CLA	CMD-C2D	-2.07	1.46	1.50
18	1	606	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	606	CLA	CMB-C2B	-2.07	1.46	1.50
18	3	613	CLA	CMC-C2C	-2.07	1.46	1.50
18	6	609	CLA	MG-ND	-2.07	2.01	2.05
18	B	822	CLA	CHC-C1C	2.07	1.42	1.38
18	7	607	CLA	CMC-C2C	-2.07	1.46	1.50
18	7	615	CLA	CMD-C2D	-2.07	1.46	1.50
24	J	104	LMG	O4-C4	-2.07	1.38	1.43
18	a	607	CLA	MG-NB	-2.07	2.01	2.05
18	A	802	CLA	C1B-NB	-2.07	1.35	1.37
18	7	609	CLA	MG-NB	-2.07	2.01	2.05
18	8	616	CLA	CMB-C2B	-2.07	1.46	1.50
18	8	611	CLA	CHC-C1C	2.06	1.42	1.38
18	3	609	CLA	C1B-C2B	2.06	1.48	1.43
18	8	606	CLA	CHC-C1C	2.06	1.42	1.38
18	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	601	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	818	CLA	C1B-NB	-2.06	1.35	1.37
18	a	606	CLA	CMB-C2B	-2.06	1.46	1.50
18	F	301	CLA	C1B-NB	-2.06	1.35	1.37
18	7	609	CLA	CHC-C1C	2.06	1.42	1.38
18	B	824	CLA	CMC-C2C	-2.06	1.46	1.50
18	1	611	CLA	CMB-C2B	-2.06	1.46	1.50
18	7	606	CLA	CAC-C3C	-2.06	1.46	1.50
18	7	607	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	804	CLA	C1B-C2B	2.06	1.48	1.43
18	5	614	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	835	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	813	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	835	CLA	CMC-C2C	-2.06	1.46	1.50
18	1	607	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	610	CLA	CMC-C2C	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	612	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	851	LHG	O7-C5	-2.06	1.41	1.46
18	A	824	CLA	CMB-C2B	-2.06	1.46	1.50
18	5	610	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	817	CLA	C1B-NB	-2.06	1.35	1.37
18	a	613	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	833	CLA	CHC-C1C	2.06	1.42	1.38
18	B	834	CLA	CHC-C1C	2.06	1.42	1.38
18	5	609	CLA	CMD-C2D	-2.06	1.46	1.50
18	1	616	CLA	MG-ND	-2.06	2.01	2.05
18	6	602	CLA	CHC-C1C	2.06	1.42	1.38
18	a	611	CLA	CMD-C2D	-2.06	1.46	1.50
18	7	613	CLA	CHC-C1C	2.05	1.42	1.38
18	B	814	CLA	CMC-C2C	-2.05	1.46	1.50
18	B	835	CLA	CMB-C2B	-2.05	1.46	1.50
18	8	610	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	609	CLA	CMB-C2B	-2.05	1.46	1.50
18	8	614	CLA	CHC-C1C	2.05	1.42	1.38
18	F	303	CLA	CHC-C1C	2.05	1.42	1.38
18	a	611	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	616	CLA	C1B-C2B	2.05	1.48	1.43
18	5	612	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	805	CLA	C1B-NB	-2.05	1.35	1.37
18	B	820	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	610	CLA	CMD-C2D	-2.05	1.46	1.50
18	7	611	CLA	CMC-C2C	-2.05	1.46	1.50
18	K	206	CLA	CMB-C2B	-2.05	1.46	1.50
18	3	603	CLA	CMC-C2C	-2.05	1.46	1.50
18	4	611	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	608	CLA	C1B-C2B	2.05	1.48	1.43
18	1	603	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	610	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
18	4	601	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	827	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	833	CLA	CMB-C2B	-2.05	1.46	1.50
18	L	303	CLA	MG-NB	-2.05	2.01	2.05
18	B	822	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	837	CLA	CMB-C2B	-2.05	1.46	1.50
18	4	607	CLA	CMB-C2B	-2.05	1.46	1.50
18	L	304	CLA	MG-NB	-2.05	2.01	2.05
28	6	624	NEX	O24-C25	-2.05	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	602	CLA	CMB-C2B	-2.05	1.46	1.50
18	6	603	CLA	CMC-C2C	-2.05	1.46	1.50
18	4	613	CLA	CMC-C2C	-2.05	1.46	1.50
18	B	815	CLA	CMB-C2B	-2.05	1.46	1.50
18	4	607	CLA	CHC-C1C	2.04	1.42	1.38
18	B	807	CLA	CMC-C2C	-2.04	1.46	1.50
18	4	618	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	842	CLA	CHC-C1C	2.04	1.42	1.38
18	3	613	CLA	MG-ND	-2.04	2.01	2.05
18	6	601	CLA	CMC-C2C	-2.04	1.46	1.50
18	a	609	CLA	CMD-C2D	-2.04	1.46	1.50
18	8	609	CLA	CMB-C2B	-2.04	1.46	1.50
18	3	608	CLA	CAC-C3C	-2.04	1.45	1.51
18	K	204	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	828	CLA	C1B-NB	-2.04	1.35	1.37
18	4	604	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	854	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	840	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	6	618	CLA	CMB-C2B	-2.04	1.46	1.50
18	5	612	CLA	CHC-C1C	2.04	1.42	1.38
18	a	604	CLA	CMC-C2C	-2.04	1.46	1.50
18	1	611	CLA	CMD-C2D	-2.04	1.46	1.50
18	3	607	CLA	CHC-C1C	2.04	1.42	1.38
18	A	816	CLA	CHC-C1C	2.04	1.42	1.38
18	a	611	CLA	CHC-C1C	2.04	1.42	1.38
18	A	823	CLA	CMC-C2C	-2.04	1.46	1.50
18	6	617	CLA	CMB-C2B	-2.04	1.46	1.50
18	4	601	CLA	CHC-C1C	2.04	1.42	1.38
18	L	304	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	832	CLA	CMB-C2B	-2.04	1.46	1.50
18	a	613	CLA	CMD-C2D	-2.04	1.46	1.50
18	8	602	CLA	MG-NB	-2.04	2.01	2.05
18	A	822	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	814	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	839	CLA	CMC-C2C	-2.03	1.46	1.50
18	a	604	CLA	CHC-C1C	2.03	1.42	1.38
18	1	614	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	823	CLA	CMC-C2C	-2.03	1.46	1.50
18	3	615	CLA	CMC-C2C	-2.03	1.46	1.50
18	4	604	CLA	CMD-C2D	-2.03	1.46	1.50
18	4	613	CLA	CHC-C1C	2.03	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	609	CLA	CHC-C1C	2.03	1.42	1.38
18	3	614	CLA	CHC-C1C	2.03	1.42	1.38
18	8	609	CLA	MG-NB	-2.03	2.01	2.05
18	1	616	CLA	CHC-C1C	2.03	1.42	1.38
18	A	832	CLA	CMC-C2C	-2.03	1.46	1.50
18	8	604	CLA	CHC-C1C	2.03	1.42	1.38
18	A	825	CLA	CMD-C2D	-2.03	1.46	1.50
18	6	614	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	837	CLA	CMC-C2C	-2.03	1.46	1.50
18	J	101	CLA	CMB-C2B	-2.03	1.46	1.50
18	8	609	CLA	CMC-C2C	-2.03	1.46	1.50
18	1	613	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	815	CLA	CMC-C2C	-2.02	1.46	1.50
18	6	601	CLA	CMB-C2B	-2.02	1.46	1.50
18	6	618	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	854	CLA	C1B-C2B	2.02	1.48	1.43
18	F	303	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	606	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	838	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	812	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	825	CLA	MG-ND	-2.02	2.01	2.05
18	5	613	CLA	CMD-C2D	-2.02	1.46	1.50
18	8	612	CLA	CMB-C2B	-2.02	1.46	1.50
18	a	614	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	818	CLA	MG-ND	-2.02	2.01	2.05
18	B	811	CLA	CHC-C1C	2.02	1.42	1.38
18	A	836	CLA	MG-ND	-2.02	2.01	2.05
18	A	829	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	821	CLA	CMB-C2B	-2.02	1.46	1.50
18	3	611	CLA	CMB-C2B	-2.02	1.46	1.50
18	5	616	CLA	MG-ND	-2.02	2.01	2.05
24	4	623	LMG	C4-C5	2.02	1.57	1.53
18	a	614	CLA	CHC-C1C	2.02	1.42	1.38
18	7	604	CLA	C1B-NB	-2.02	1.35	1.37
18	A	817	CLA	CMC-C2C	-2.02	1.46	1.50
18	4	614	CLA	CMC-C2C	-2.02	1.46	1.50
18	B	814	CLA	C1B-NB	-2.02	1.35	1.37
27	4	620	XAT	O24-C25	-2.02	1.43	1.46
18	B	823	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	602	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	607	CLA	CMC-C2C	-2.02	1.46	1.50
18	7	611	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)
18	B	825	CLA	CMB-C2B	-2.01	1.46	1.50
18	4	601	CLA	MG-ND	-2.01	2.01	2.05
18	B	829	CLA	CHC-C4B	-2.01	1.34	1.39
18	a	612	CLA	CMC-C2C	-2.01	1.46	1.50
18	8	614	CLA	CMC-C2C	-2.01	1.46	1.50
18	6	604	CLA	CHC-C1C	2.01	1.42	1.38
18	a	613	CLA	CHC-C1C	2.01	1.42	1.38
27	1	618	XAT	O4-C5	-2.01	1.43	1.46
18	5	604	CLA	CMC-C2C	-2.01	1.46	1.50
18	5	601	CLA	MG-ND	-2.01	2.01	2.05
18	A	837	CLA	CHC-C1C	2.01	1.42	1.38
18	5	616	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	827	CLA	C1B-C2B	2.01	1.48	1.43
18	L	303	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	806	CLA	C1B-NB	-2.01	1.35	1.37
18	a	606	CLA	CHC-C1C	2.01	1.42	1.38
18	5	604	CLA	CHC-C1C	2.01	1.42	1.38
18	1	601	CLA	MG-ND	-2.01	2.01	2.05
18	5	614	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	809	CLA	MG-ND	-2.01	2.01	2.05
18	7	608	CLA	MG-ND	-2.01	2.01	2.05
18	5	607	CLA	C1B-C2B	2.01	1.48	1.43
18	a	601	CLA	CMB-C2B	-2.01	1.46	1.50
18	3	615	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	813	CLA	CHC-C1C	2.01	1.42	1.38
18	4	608	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	803	CLA	CMB-C2B	-2.01	1.46	1.50
18	3	602	CLA	CMA-C3A	-2.01	1.48	1.53
18	a	616	CLA	CMB-C2B	-2.00	1.46	1.50
18	7	616	CLA	CMB-C2B	-2.00	1.46	1.50
18	3	609	CLA	MG-ND	-2.00	2.01	2.05
18	1	601	CLA	CMC-C2C	-2.00	1.46	1.50
18	B	817	CLA	C1B-C2B	2.00	1.48	1.43
18	B	821	CLA	CMD-C2D	-2.00	1.46	1.50
18	1	606	CLA	CMD-C2D	-2.00	1.46	1.50
18	a	607	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	834	CLA	CMC-C2C	-2.00	1.46	1.50

All (2539) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	621	XAT	O24-C25-C24	11.52	122.04	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	803	CLA	C4A-NA-C1A	9.21	110.84	106.71
18	8	613	CLA	C4A-NA-C1A	9.08	110.79	106.71
27	6	621	XAT	O24-C25-C24	8.96	120.11	113.38
27	8	620	XAT	O24-C25-C24	8.87	120.04	113.38
19	A	844	PQN	C11-C12-C13	-8.68	112.35	126.79
18	5	613	CLA	C4A-NA-C1A	8.61	110.58	106.71
18	A	813	CLA	C4A-NA-C1A	8.56	110.55	106.71
27	7	620	XAT	O24-C25-C24	8.55	119.81	113.38
18	3	613	CLA	C4A-NA-C1A	8.55	110.55	106.71
27	1	618	XAT	O4-C5-C4	8.51	119.78	113.38
18	B	840	CLA	C4A-NA-C1A	8.31	110.44	106.71
18	B	808	CLA	C4A-NA-C1A	8.30	110.44	106.71
18	K	201	CLA	C4A-NA-C1A	8.28	110.43	106.71
18	A	817	CLA	C4A-NA-C1A	8.16	110.37	106.71
18	8	608	CLA	C4A-NA-C1A	8.12	110.36	106.71
18	A	808	CLA	C4A-NA-C1A	7.98	110.29	106.71
18	3	615	CLA	C4A-NA-C1A	7.89	110.25	106.71
18	A	837	CLA	C4A-NA-C1A	7.81	110.22	106.71
18	A	842	CLA	C4A-NA-C1A	7.81	110.22	106.71
18	6	607	CLA	C4A-NA-C1A	7.80	110.21	106.71
18	L	302	CLA	C4A-NA-C1A	7.77	110.20	106.71
18	6	618	CLA	C4A-NA-C1A	7.75	110.19	106.71
18	8	607	CLA	C4A-NA-C1A	7.72	110.18	106.71
18	7	611	CLA	C4A-NA-C1A	7.71	110.17	106.71
18	8	609	CLA	C4A-NA-C1A	7.71	110.17	106.71
18	8	616	CLA	C4A-NA-C1A	7.69	110.16	106.71
18	5	607	CLA	C4A-NA-C1A	7.67	110.16	106.71
18	B	826	CLA	C4A-NA-C1A	7.66	110.15	106.71
18	A	818	CLA	C4A-NA-C1A	7.64	110.14	106.71
18	8	603	CLA	C4A-NA-C1A	7.62	110.13	106.71
18	A	845	CLA	C4A-NA-C1A	7.60	110.12	106.71
18	5	617	CLA	C4A-NA-C1A	7.59	110.12	106.71
18	B	805	CLA	C4A-NA-C1A	7.56	110.11	106.71
18	B	815	CLA	C4A-NA-C1A	7.56	110.11	106.71
18	J	101	CLA	C4A-NA-C1A	7.56	110.10	106.71
18	a	613	CLA	C4A-NA-C1A	7.55	110.10	106.71
18	A	821	CLA	C4A-NA-C1A	7.53	110.09	106.71
18	1	603	CLA	C4A-NA-C1A	7.48	110.07	106.71
18	B	818	CLA	C4A-NA-C1A	7.48	110.07	106.71
27	1	618	XAT	O24-C25-C24	7.48	119.00	113.38
18	6	613	CLA	C4A-NA-C1A	7.48	110.07	106.71
18	B	820	CLA	C4A-NA-C1A	7.47	110.06	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	616	CLA	C4A-NA-C1A	7.46	110.06	106.71
18	4	613	CLA	C4A-NA-C1A	7.44	110.05	106.71
18	K	206	CLA	C4A-NA-C1A	7.43	110.05	106.71
18	6	609	CLA	C4A-NA-C1A	7.41	110.04	106.71
18	B	831	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	A	816	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	A	807	CLA	C4A-NA-C1A	7.39	110.03	106.71
21	B	801	BCR	C24-C23-C22	-7.38	115.09	126.23
18	A	835	CLA	C4A-NA-C1A	7.37	110.02	106.71
18	B	838	CLA	C4A-NA-C1A	7.36	110.01	106.71
18	B	809	CLA	C4A-NA-C1A	7.35	110.01	106.71
18	A	806	CLA	C4A-NA-C1A	7.34	110.01	106.71
18	1	613	CLA	C4A-NA-C1A	7.33	110.00	106.71
18	A	826	CLA	C4A-NA-C1A	7.32	110.00	106.71
18	B	819	CLA	C4A-NA-C1A	7.32	110.00	106.71
18	3	611	CLA	C4A-NA-C1A	7.30	109.99	106.71
18	5	602	CLA	C4A-NA-C1A	7.30	109.99	106.71
18	A	804	CLA	C4A-NA-C1A	7.29	109.98	106.71
18	A	823	CLA	C4A-NA-C1A	7.27	109.97	106.71
18	L	304	CLA	C4A-NA-C1A	7.27	109.97	106.71
18	A	839	CLA	C4A-NA-C1A	7.25	109.97	106.71
18	B	827	CLA	C4A-NA-C1A	7.25	109.97	106.71
18	A	836	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	B	835	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	8	614	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	4	609	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	A	814	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	5	619	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	8	601	CLA	C4A-NA-C1A	7.21	109.95	106.71
19	B	842	PQN	C15-C13-C12	-7.21	106.52	121.12
18	A	828	CLA	C4A-NA-C1A	7.21	109.95	106.71
18	A	809	CLA	C4A-NA-C1A	7.21	109.95	106.71
18	3	602	CLA	C4A-NA-C1A	7.20	109.94	106.71
18	8	604	CLA	C4A-NA-C1A	7.20	109.94	106.71
18	A	843	CLA	C4A-NA-C1A	7.18	109.93	106.71
18	B	816	CLA	C4A-NA-C1A	7.17	109.93	106.71
18	4	610	CLA	C4A-NA-C1A	7.17	109.93	106.71
18	B	812	CLA	C4A-NA-C1A	7.16	109.92	106.71
18	a	609	CLA	C4A-NA-C1A	7.15	109.92	106.71
18	A	841	CLA	C4A-NA-C1A	7.15	109.92	106.71
18	4	607	CLA	C4A-NA-C1A	7.15	109.92	106.71
27	7	620	XAT	O4-C5-C4	7.15	118.75	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	829	CLA	C4A-NA-C1A	7.14	109.92	106.71
18	B	807	CLA	C4A-NA-C1A	7.14	109.92	106.71
18	7	613	CLA	C4A-NA-C1A	7.14	109.91	106.71
18	K	204	CLA	C4A-NA-C1A	7.12	109.91	106.71
18	1	611	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	A	844	PQN	C15-C13-C12	-7.11	106.74	121.12
18	3	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
27	a	618	XAT	O4-C5-C4	7.10	118.72	113.38
18	6	601	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	4	602	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	4	608	CLA	C4A-NA-C1A	7.09	109.89	106.71
18	A	811	CLA	C4A-NA-C1A	7.09	109.89	106.71
18	B	832	CLA	C4A-NA-C1A	7.07	109.89	106.71
21	A	851	BCR	C24-C23-C22	-7.05	115.58	126.23
18	6	614	CLA	C4A-NA-C1A	7.04	109.87	106.71
18	a	607	CLA	C4A-NA-C1A	7.04	109.87	106.71
18	A	838	CLA	C4A-NA-C1A	7.03	109.87	106.71
18	A	822	CLA	C4A-NA-C1A	7.01	109.86	106.71
18	5	618	CLA	C4A-NA-C1A	6.99	109.85	106.71
18	8	602	CLA	C4A-NA-C1A	6.99	109.85	106.71
18	A	825	CLA	C4A-NA-C1A	6.98	109.84	106.71
18	A	802	CLA	C4A-NA-C1A	6.96	109.84	106.71
18	5	608	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	7	603	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	B	802	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	6	604	CLA	C4A-NA-C1A	6.95	109.83	106.71
27	4	620	XAT	O4-C5-C4	6.94	118.60	113.38
18	L	303	CLA	C4A-NA-C1A	6.94	109.83	106.71
18	4	603	CLA	C4A-NA-C1A	6.93	109.82	106.71
18	A	801	CLA	C4A-NA-C1A	6.92	109.82	106.71
18	4	614	CLA	C4A-NA-C1A	6.92	109.82	106.71
18	6	620	CLA	C4A-NA-C1A	6.92	109.81	106.71
18	A	812	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	8	610	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	B	821	CLA	C4A-NA-C1A	6.89	109.81	106.71
18	3	606	CLA	C4A-NA-C1A	6.89	109.80	106.71
18	B	814	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	3	604	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	5	604	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	B	822	CLA	C4A-NA-C1A	6.87	109.80	106.71
18	B	830	CLA	C4A-NA-C1A	6.85	109.79	106.71
18	a	603	CLA	C4A-NA-C1A	6.85	109.78	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	602	CLA	C4A-NA-C1A	6.85	109.78	106.71
18	B	811	CLA	C4A-NA-C1A	6.84	109.78	106.71
18	4	606	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	a	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	7	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	7	615	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	A	819	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	5	611	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	A	840	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	3	608	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	7	607	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	a	601	CLA	C4A-NA-C1A	6.77	109.75	106.71
21	3	622	BCR	C11-C10-C9	-6.74	117.69	127.31
27	a	618	XAT	O24-C25-C24	6.74	118.44	113.38
18	7	616	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	820	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	831	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	a	606	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	1	608	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	6	612	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	3	610	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	B	833	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	B	842	PQN	C11-C12-C13	-6.70	115.64	126.79
18	K	203	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	F	303	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	4	618	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	6	602	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	6	606	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	7	614	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	A	834	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	5	610	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	5	601	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	B	834	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	1	612	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	B	806	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	J	102	BCR	C28-C27-C26	-6.58	102.32	114.08
18	5	609	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	1	602	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	813	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	6	610	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	B	810	CLA	C4A-NA-C1A	6.55	109.65	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	619	XAT	O24-C25-C24	6.54	118.30	113.38
18	1	609	CLA	C4A-NA-C1A	6.54	109.65	106.71
27	4	620	XAT	O24-C25-C24	6.53	118.29	113.38
18	7	609	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	3	621	BCR	C11-C10-C9	-6.52	118.00	127.31
27	5	621	XAT	O4-C5-C4	6.49	118.26	113.38
18	A	832	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	a	614	CLA	C4A-NA-C1A	6.47	109.61	106.71
18	B	839	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	1	607	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	6	603	CLA	C4A-NA-C1A	6.43	109.60	106.71
21	A	852	BCR	C20-C21-C22	-6.43	118.14	127.31
18	3	609	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	4	601	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	1	616	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	7	608	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	1	601	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	1	604	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	8	612	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	a	616	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	a	608	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	823	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	5	612	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	F	304	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	a	611	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	6	608	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	A	824	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	5	616	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	7	610	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	a	612	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	4	604	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	A	844	PQN	C14-C13-C12	-6.25	107.65	123.68
18	F	301	CLA	C4A-NA-C1A	6.23	109.51	106.71
21	3	622	BCR	C20-C21-C22	-6.22	118.43	127.31
18	A	833	CLA	C4A-NA-C1A	6.22	109.50	106.71
27	8	620	XAT	O4-C5-C4	6.21	118.05	113.38
18	B	817	CLA	C4A-NA-C1A	6.21	109.50	106.71
18	A	810	CLA	C4A-NA-C1A	6.18	109.48	106.71
21	3	621	BCR	C7-C8-C9	-6.17	116.91	126.23
18	A	854	CLA	C4A-NA-C1A	6.15	109.47	106.71
18	1	606	CLA	C4A-NA-C1A	6.15	109.47	106.71
18	A	827	CLA	C4A-NA-C1A	6.14	109.47	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	621	XAT	O4-C5-C4	6.14	117.99	113.38
18	5	603	CLA	C4A-NA-C1A	6.12	109.46	106.71
18	5	614	CLA	C4A-NA-C1A	6.12	109.46	106.71
18	6	611	CLA	C4A-NA-C1A	6.11	109.45	106.71
21	F	305	BCR	C16-C17-C18	-6.09	118.62	127.31
18	4	612	CLA	C4A-NA-C1A	6.08	109.44	106.71
18	7	606	CLA	C4A-NA-C1A	6.07	109.44	106.71
18	B	837	CLA	C4A-NA-C1A	6.07	109.44	106.71
18	8	611	CLA	C4A-NA-C1A	6.05	109.43	106.71
27	3	619	XAT	O4-C5-C4	6.05	117.93	113.38
18	B	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
18	3	612	CLA	C4A-NA-C1A	5.95	109.38	106.71
18	B	824	CLA	C4A-NA-C1A	5.93	109.37	106.71
18	3	614	CLA	C4A-NA-C1A	5.92	109.37	106.71
18	B	825	CLA	C4A-NA-C1A	5.91	109.36	106.71
18	a	602	CLA	C4A-NA-C1A	5.90	109.36	106.71
18	3	617	CLA	C4A-NA-C1A	5.90	109.36	106.71
18	a	610	CLA	C4A-NA-C1A	5.89	109.35	106.71
18	B	803	CLA	CAC-C3C-C4C	5.86	132.42	124.81
18	3	607	CLA	C4A-NA-C1A	5.82	109.32	106.71
18	4	611	CLA	C4A-NA-C1A	5.80	109.31	106.71
18	5	606	CLA	C4A-NA-C1A	5.80	109.31	106.71
18	B	828	CLA	C4A-NA-C1A	5.76	109.30	106.71
18	1	614	CLA	C4A-NA-C1A	5.74	109.29	106.71
18	6	617	CLA	C4A-NA-C1A	5.73	109.28	106.71
18	B	829	CLA	C4A-NA-C1A	5.72	109.28	106.71
27	3	619	XAT	C38-C25-C26	-5.71	112.69	122.26
27	6	621	XAT	C26-C27-C28	-5.70	113.95	125.99
21	A	852	BCR	C7-C8-C9	-5.68	117.65	126.23
27	4	620	XAT	C38-C25-C26	-5.68	112.74	122.26
21	B	844	BCR	C7-C8-C9	-5.66	117.67	126.23
27	3	619	XAT	C6-C7-C8	-5.65	114.04	125.99
21	B	848	BCR	C24-C23-C22	-5.62	117.75	126.23
21	F	305	BCR	C20-C21-C22	-5.61	119.30	127.31
18	B	841	CLA	C4A-NA-C1A	5.57	109.21	106.71
18	8	606	CLA	C4A-NA-C1A	5.56	109.20	106.71
27	4	620	XAT	C26-C27-C28	-5.54	114.28	125.99
27	8	620	XAT	C6-C7-C8	-5.47	114.42	125.99
18	A	815	CLA	C4A-NA-C1A	5.44	109.15	106.71
18	6	616	CLA	C4A-NA-C1A	5.44	109.15	106.71
28	6	624	NEX	C38-C25-C26	-5.44	113.15	122.26
18	B	836	CLA	C4A-NA-C1A	5.42	109.14	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	851	BCR	C20-C21-C22	-5.41	119.59	127.31
21	3	622	BCR	C7-C8-C9	-5.39	118.09	126.23
27	a	618	XAT	C38-C25-C26	-5.37	113.26	122.26
21	7	621	BCR	C28-C27-C26	-5.37	104.49	114.08
18	A	803	CLA	C4A-NA-C1A	5.37	109.12	106.71
28	5	624	NEX	C38-C25-C26	-5.36	113.28	122.26
21	5	622	BCR	C28-C27-C26	-5.35	104.53	114.08
27	7	620	XAT	C26-C27-C28	-5.34	114.69	125.99
18	7	601	CLA	C4A-NA-C1A	5.33	109.10	106.71
18	A	805	CLA	C4A-NA-C1A	5.33	109.10	106.71
27	5	621	XAT	O4-C5-C18	5.30	121.41	115.06
27	5	621	XAT	C6-C7-C8	-5.30	114.78	125.99
27	8	620	XAT	C38-C25-C26	-5.29	113.40	122.26
27	6	621	XAT	C6-C7-C8	-5.28	114.82	125.99
27	6	621	XAT	C38-C25-C26	-5.28	113.42	122.26
27	a	618	XAT	C6-C7-C8	-5.27	114.85	125.99
27	4	620	XAT	C6-C7-C8	-5.27	114.86	125.99
27	6	621	XAT	C18-C5-C6	-5.25	113.47	122.26
28	5	624	NEX	O24-C25-C38	5.22	121.31	115.06
28	6	624	NEX	O24-C25-C24	5.21	117.30	113.38
21	3	622	BCR	C24-C23-C22	-5.20	118.37	126.23
21	3	621	BCR	C20-C21-C22	-5.19	119.90	127.31
18	1	610	CLA	C4A-NA-C1A	5.18	109.03	106.71
21	5	622	BCR	C15-C14-C13	-5.17	119.93	127.31
27	8	620	XAT	C18-C5-C6	-5.17	113.59	122.26
28	6	624	NEX	O24-C25-C38	5.17	121.25	115.06
19	B	842	PQN	C14-C13-C12	-5.17	110.42	123.68
21	A	852	BCR	C16-C17-C18	-5.14	119.98	127.31
21	B	843	BCR	C28-C27-C26	-5.14	104.91	114.08
18	B	829	CLA	CMB-C2B-C1B	-5.11	117.58	125.37
21	B	845	BCR	C7-C8-C9	-5.11	118.52	126.23
21	3	621	BCR	C35-C13-C14	-5.07	115.81	122.92
21	3	622	BCR	C36-C18-C17	-5.07	115.83	122.92
27	3	619	XAT	C18-C5-C6	-5.06	113.78	122.26
21	K	202	BCR	C28-C27-C26	-5.05	105.06	114.08
21	A	856	BCR	C15-C16-C17	-5.01	113.22	123.47
27	7	620	XAT	C6-C7-C8	-4.99	115.44	125.99
27	a	618	XAT	C18-C5-C6	-4.99	113.90	122.26
28	5	624	NEX	O24-C25-C24	4.98	117.12	113.38
21	B	844	BCR	C30-C25-C26	-4.97	115.61	122.61
18	7	601	CLA	O2D-CGD-O1D	-4.97	114.11	123.84
21	B	843	BCR	C16-C17-C18	-4.97	120.22	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	620	BCR	C3-C4-C5	-4.97	105.21	114.08
21	A	848	BCR	C16-C17-C18	-4.94	120.27	127.31
27	7	620	XAT	C38-C25-C26	-4.93	113.99	122.26
21	B	845	BCR	C24-C23-C22	-4.93	118.79	126.23
27	5	621	XAT	C18-C5-C6	-4.90	114.05	122.26
21	8	621	BCR	C15-C14-C13	-4.90	120.32	127.31
27	a	618	XAT	O24-C25-C38	4.89	120.92	115.06
27	8	620	XAT	C26-C27-C28	-4.89	115.66	125.99
18	5	603	CLA	C3B-C4B-NB	-4.89	106.96	110.23
27	4	620	XAT	C18-C5-C6	-4.88	114.08	122.26
27	5	621	XAT	C26-C27-C28	-4.87	115.70	125.99
18	A	831	CLA	CMB-C2B-C1B	-4.87	117.96	125.37
21	A	852	BCR	C24-C23-C22	-4.83	118.93	126.23
25	J	103	DGD	O3G-C3G-C2G	-4.83	99.26	110.90
27	4	620	XAT	O24-C25-C38	4.82	120.83	115.06
18	A	806	CLA	CAA-C2A-C3A	-4.81	99.62	112.78
21	6	622	BCR	C16-C17-C18	-4.77	120.50	127.31
21	a	619	BCR	C28-C27-C26	-4.77	105.56	114.08
21	A	850	BCR	C28-C27-C26	-4.77	105.56	114.08
21	5	622	BCR	C3-C4-C5	-4.77	105.56	114.08
21	1	619	BCR	C16-C17-C18	-4.76	120.52	127.31
27	7	620	XAT	C18-C5-C6	-4.75	114.30	122.26
27	1	618	XAT	C26-C27-C28	-4.75	115.95	125.99
21	3	620	BCR	C28-C27-C26	-4.75	105.60	114.08
27	1	618	XAT	C18-C5-C6	-4.73	114.33	122.26
18	7	612	CLA	C4A-NA-C1A	4.73	108.83	106.71
27	a	618	XAT	C26-C27-C28	-4.72	116.01	125.99
28	5	624	NEX	C26-C27-C28	-4.70	116.05	125.99
21	4	621	BCR	C28-C27-C26	-4.70	105.69	114.08
21	3	622	BCR	C35-C13-C14	-4.69	116.36	122.92
21	B	848	BCR	C20-C21-C22	-4.67	120.64	127.31
21	6	622	BCR	C3-C4-C5	-4.67	105.74	114.08
21	F	305	BCR	C24-C23-C22	-4.66	119.19	126.23
27	1	618	XAT	C38-C25-C26	-4.66	114.45	122.26
21	B	846	BCR	C11-C10-C9	-4.65	120.67	127.31
21	B	846	BCR	C38-C26-C25	-4.65	119.31	124.53
21	3	621	BCR	C24-C23-C22	-4.64	119.23	126.23
21	A	850	BCR	C7-C8-C9	-4.62	119.25	126.23
21	A	851	BCR	C28-C27-C26	-4.61	105.84	114.08
21	A	849	BCR	C24-C23-C22	-4.59	119.29	126.23
21	A	849	BCR	C20-C21-C22	-4.59	120.76	127.31
21	8	621	BCR	C28-C27-C26	-4.58	105.90	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	620	XAT	C15-C14-C13	-4.57	120.78	127.31
21	J	102	BCR	C3-C4-C5	-4.54	105.96	114.08
21	a	619	BCR	C16-C17-C18	-4.54	120.83	127.31
21	K	202	BCR	C11-C10-C9	-4.50	120.88	127.31
21	K	202	BCR	C16-C17-C18	-4.50	120.89	127.31
27	3	619	XAT	O4-C5-C18	4.49	120.44	115.06
18	A	835	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
21	B	801	BCR	C16-C17-C18	-4.48	120.92	127.31
21	B	844	BCR	C24-C23-C22	-4.47	119.47	126.23
21	L	305	BCR	C7-C8-C9	-4.46	119.50	126.23
27	6	621	XAT	O4-C5-C18	4.45	120.39	115.06
21	A	851	BCR	C16-C17-C18	-4.44	120.97	127.31
21	1	619	BCR	C28-C27-C26	-4.44	106.15	114.08
21	3	622	BCR	C28-C27-C26	-4.42	106.18	114.08
28	6	624	NEX	C26-C27-C28	-4.42	116.64	125.99
21	A	851	BCR	C15-C14-C13	-4.42	121.01	127.31
21	3	621	BCR	C28-C27-C26	-4.40	106.22	114.08
21	B	801	BCR	C20-C21-C22	-4.40	121.03	127.31
21	A	856	BCR	C20-C21-C22	-4.39	121.04	127.31
27	3	619	XAT	C26-C27-C28	-4.39	116.70	125.99
21	K	202	BCR	C24-C23-C22	-4.39	119.60	126.23
18	7	601	CLA	O2D-CGD-CBD	4.39	119.06	111.27
21	A	849	BCR	C11-C10-C9	-4.38	121.05	127.31
28	5	624	NEX	C31-C30-C29	-4.38	121.06	127.31
21	L	305	BCR	C16-C17-C18	-4.38	121.07	127.31
21	B	846	BCR	C7-C8-C9	-4.37	119.64	126.23
18	B	829	CLA	CHB-C1B-NB	4.35	128.86	124.26
19	B	842	PQN	C14-C13-C15	-4.34	107.96	115.27
21	L	301	BCR	C7-C8-C9	-4.34	119.67	126.23
21	4	621	BCR	C15-C14-C13	-4.34	121.11	127.31
21	B	847	BCR	C15-C14-C13	-4.33	121.13	127.31
20	5	623	LHG	O4-P-O5	4.33	133.64	112.24
28	6	624	NEX	C31-C30-C29	-4.33	121.13	127.31
20	A	847	LHG	O4-P-O5	4.33	133.63	112.24
20	4	622	LHG	O4-P-O5	4.32	133.57	112.24
26	5	620	LUT	C35-C34-C33	-4.31	121.16	127.31
21	5	622	BCR	C16-C17-C18	-4.29	121.18	127.31
27	1	618	XAT	C6-C7-C8	-4.29	116.91	125.99
21	A	856	BCR	C3-C4-C5	-4.29	106.41	114.08
20	7	622	LHG	O4-P-O5	4.28	133.38	112.24
18	6	620	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
20	6	623	LHG	O4-P-O5	4.25	133.26	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	843	BCR	C16-C15-C14	-4.24	114.79	123.47
21	K	202	BCR	C15-C14-C13	-4.23	121.27	127.31
21	B	846	BCR	C15-C14-C13	-4.23	121.27	127.31
21	L	301	BCR	C15-C14-C13	-4.23	121.28	127.31
27	3	619	XAT	O24-C25-C38	4.23	120.12	115.06
20	1	620	LHG	O4-P-O5	4.22	133.12	112.24
21	L	301	BCR	C24-C23-C22	-4.22	119.86	126.23
20	a	620	LHG	O4-P-O5	4.21	133.07	112.24
21	7	621	BCR	C16-C17-C18	-4.21	121.30	127.31
20	3	623	LHG	O4-P-O5	4.20	133.00	112.24
21	K	207	BCR	C20-C21-C22	-4.20	121.32	127.31
21	7	623	BCR	C20-C21-C22	-4.18	121.34	127.31
21	K	202	BCR	C3-C4-C5	-4.18	106.61	114.08
20	A	846	LHG	O4-P-O5	4.18	132.90	112.24
21	7	623	BCR	C15-C14-C13	-4.17	121.36	127.31
20	8	623	LHG	O4-P-O5	4.17	132.85	112.24
20	B	851	LHG	O4-P-O5	4.17	132.84	112.24
21	6	622	BCR	C15-C14-C13	-4.16	121.37	127.31
21	3	620	BCR	C20-C21-C22	-4.15	121.39	127.31
21	B	847	BCR	C11-C10-C9	-4.15	121.39	127.31
21	3	620	BCR	C16-C17-C18	-4.14	121.40	127.31
20	3	624	LHG	O4-P-O5	4.14	132.72	112.24
20	5	625	LHG	O4-P-O5	4.14	132.71	112.24
27	a	618	XAT	O4-C5-C18	4.14	120.02	115.06
21	3	622	BCR	C38-C26-C25	-4.11	119.92	124.53
18	1	604	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
21	B	801	BCR	C28-C27-C26	-4.08	106.78	114.08
26	3	618	LUT	C15-C14-C13	-4.08	121.49	127.31
26	4	619	LUT	C35-C34-C33	-4.07	121.50	127.31
21	A	852	BCR	C20-C19-C18	-4.07	114.98	126.42
26	5	620	LUT	C35-C15-C14	-4.07	115.14	123.47
21	K	207	BCR	C16-C17-C18	-4.06	121.51	127.31
28	5	624	NEX	C15-C14-C13	-4.06	121.51	127.31
21	A	849	BCR	C15-C14-C13	-4.06	121.51	127.31
21	K	207	BCR	C15-C14-C13	-4.05	121.53	127.31
21	3	622	BCR	C19-C18-C17	4.04	125.15	118.94
21	4	621	BCR	C16-C17-C18	-4.04	121.54	127.31
21	6	622	BCR	C16-C15-C14	-4.04	115.19	123.47
20	8	622	LHG	O7-C7-C8	4.03	120.19	111.50
27	4	620	XAT	O4-C5-C18	4.03	119.88	115.06
21	B	845	BCR	C33-C5-C6	-4.02	120.02	124.53
21	3	621	BCR	C36-C18-C17	-4.01	117.31	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	856	BCR	C28-C27-C26	-4.00	106.94	114.08
21	A	851	BCR	C7-C8-C9	-4.00	120.20	126.23
21	A	850	BCR	C24-C23-C22	-3.99	120.21	126.23
27	8	620	XAT	O4-C5-C18	3.99	119.83	115.06
21	3	621	BCR	C12-C13-C14	3.97	125.03	118.94
21	A	849	BCR	C7-C8-C9	-3.97	120.24	126.23
26	1	617	LUT	C35-C34-C33	-3.96	121.66	127.31
18	A	802	CLA	CMB-C2B-C1B	-3.92	119.39	125.37
21	8	621	BCR	C3-C4-C5	-3.92	107.08	114.08
28	6	624	NEX	C15-C14-C13	-3.91	121.72	127.31
18	1	611	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
26	7	619	LUT	C35-C34-C33	-3.90	121.75	127.31
21	7	621	BCR	C3-C4-C5	-3.89	107.13	114.08
26	7	619	LUT	C7-C8-C9	-3.89	120.36	126.23
21	7	623	BCR	C24-C23-C22	-3.88	120.36	126.23
21	B	847	BCR	C23-C24-C25	-3.88	116.30	127.20
21	3	620	BCR	C11-C10-C9	-3.88	121.78	127.31
21	B	847	BCR	C7-C8-C9	-3.88	120.38	126.23
26	7	619	LUT	C15-C14-C13	-3.87	121.78	127.31
21	B	845	BCR	C16-C17-C18	-3.87	121.78	127.31
21	7	621	BCR	C15-C14-C13	-3.87	121.79	127.31
21	A	848	BCR	C7-C8-C9	-3.86	120.41	126.23
18	A	831	CLA	CHB-C1B-NB	3.85	128.34	124.26
27	3	619	XAT	C24-C23-C22	-3.85	103.34	110.77
18	5	619	CLA	C2A-C1A-CHA	3.84	130.58	123.86
21	3	622	BCR	C11-C12-C13	-3.84	115.62	126.42
21	3	621	BCR	C33-C5-C6	-3.83	120.22	124.53
28	6	624	NEX	C24-C23-C22	-3.83	103.37	110.77
21	7	623	BCR	C16-C17-C18	-3.83	121.85	127.31
18	B	804	CLA	CAA-C2A-C3A	-3.82	107.19	116.10
21	1	619	BCR	C20-C21-C22	-3.82	121.86	127.31
21	8	621	BCR	C7-C8-C9	-3.81	120.47	126.23
21	B	848	BCR	C16-C17-C18	-3.81	121.87	127.31
21	3	620	BCR	C24-C23-C22	-3.81	120.47	126.23
26	8	619	LUT	C35-C34-C33	-3.81	121.88	127.31
21	J	102	BCR	C16-C17-C18	-3.80	121.89	127.31
21	A	848	BCR	C38-C26-C25	-3.80	120.26	124.53
21	3	622	BCR	C20-C19-C18	-3.79	115.76	126.42
27	3	619	XAT	C15-C14-C13	-3.79	121.90	127.31
21	B	844	BCR	C15-C14-C13	-3.78	121.91	127.31
21	J	102	BCR	C15-C14-C13	-3.78	121.91	127.31
25	B	850	DGD	O3G-C3G-C2G	-3.78	101.77	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	207	BCR	C24-C23-C22	-3.77	120.54	126.23
25	J	103	DGD	O6D-C1D-O3G	-3.77	101.06	109.97
21	B	843	BCR	C11-C10-C9	-3.76	121.94	127.31
18	A	802	CLA	CHB-C4A-NA	3.76	129.71	124.51
27	7	620	XAT	C35-C34-C33	-3.76	121.94	127.31
21	1	619	BCR	C24-C23-C22	-3.73	120.60	126.23
21	3	622	BCR	C38-C26-C27	3.72	120.77	113.62
21	A	848	BCR	C24-C23-C22	-3.72	120.61	126.23
21	a	619	BCR	C33-C5-C6	-3.72	120.35	124.53
21	A	852	BCR	C34-C9-C10	-3.72	117.71	122.92
18	a	604	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
18	1	609	CLA	CAA-C2A-C3A	-3.71	107.43	116.10
21	L	305	BCR	C11-C10-C9	-3.71	122.02	127.31
21	7	623	BCR	C33-C5-C6	-3.71	120.36	124.53
18	1	614	CLA	C2A-C3A-C4A	-3.70	102.19	106.26
27	6	621	XAT	C15-C14-C13	-3.69	122.04	127.31
21	3	621	BCR	C11-C12-C13	-3.69	116.05	126.42
27	8	620	XAT	C10-C11-C12	-3.68	111.72	123.22
23	A	857	LMU	C1B-O1B-C4'	-3.68	109.64	115.33
21	B	844	BCR	C33-C5-C6	-3.68	120.40	124.53
21	A	848	BCR	C20-C21-C22	-3.68	122.06	127.31
27	7	620	XAT	O24-C25-C38	3.68	119.46	115.06
18	A	824	CLA	CMA-C3A-C2A	-3.68	107.52	116.10
18	3	614	CLA	CAA-C2A-C3A	-3.67	107.53	116.10
21	1	619	BCR	C7-C8-C9	-3.67	120.69	126.23
28	6	624	NEX	C17-C1-C6	-3.66	107.19	110.47
18	A	820	CLA	CMB-C2B-C1B	-3.66	119.79	125.37
21	B	845	BCR	C15-C14-C13	-3.66	122.08	127.31
18	A	835	CLA	O2D-CGD-CBD	3.65	117.75	111.27
18	A	854	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
27	7	620	XAT	C15-C14-C13	-3.65	122.10	127.31
18	A	834	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
27	1	618	XAT	C35-C34-C33	-3.64	122.12	127.31
27	5	621	XAT	C15-C14-C13	-3.64	122.12	127.31
27	1	618	XAT	O24-C25-C38	3.62	119.40	115.06
26	6	619	LUT	C35-C34-C33	-3.62	122.14	127.31
18	A	819	CLA	C3B-C4B-NB	-3.62	107.15	110.52
18	4	601	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
18	5	607	CLA	CHB-C4A-NA	3.62	129.52	124.51
18	6	616	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
18	7	602	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
18	6	601	CLA	O2D-CGD-O1D	-3.60	116.80	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	829	CLA	C2D-C1D-ND	-3.60	107.45	110.10
21	8	621	BCR	C16-C17-C18	-3.60	122.18	127.31
21	3	621	BCR	C16-C15-C14	-3.59	116.13	123.47
21	B	846	BCR	C38-C26-C27	3.58	120.50	113.62
18	8	614	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
18	B	836	CLA	CMB-C2B-C1B	-3.58	119.92	125.37
18	A	803	CLA	CMB-C2B-C1B	-3.58	119.92	125.37
18	B	804	CLA	C3B-C4B-NB	-3.57	107.20	110.52
27	6	621	XAT	O24-C25-C38	3.57	119.33	115.06
18	B	802	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
27	7	620	XAT	O4-C5-C18	3.57	119.33	115.06
21	4	621	BCR	C11-C10-C9	-3.56	122.22	127.31
18	4	604	CLA	C3B-C4B-NB	-3.56	107.84	110.23
27	6	621	XAT	C4-C3-C2	-3.56	103.90	110.77
26	a	617	LUT	C35-C34-C33	-3.55	122.25	127.31
27	5	621	XAT	C10-C11-C12	-3.54	112.16	123.22
21	A	848	BCR	C11-C10-C9	-3.54	122.26	127.31
18	B	841	CLA	C3B-C4B-NB	-3.53	107.24	110.52
18	6	620	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
18	K	201	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
21	B	843	BCR	C20-C21-C22	-3.52	122.29	127.31
18	A	833	CLA	CMB-C2B-C1B	-3.51	120.02	125.37
23	5	628	LMU	C2'-C3'-C4'	3.51	117.70	109.68
21	L	301	BCR	C11-C10-C9	-3.51	122.30	127.31
21	1	619	BCR	C33-C5-C6	-3.51	120.59	124.53
27	1	618	XAT	O4-C5-C18	3.50	119.25	115.06
26	1	617	LUT	C35-C15-C14	-3.49	116.32	123.47
21	B	801	BCR	C16-C15-C14	-3.49	116.32	123.47
18	3	611	CLA	C3B-C4B-NB	-3.49	107.89	110.23
21	4	621	BCR	C3-C4-C5	-3.48	107.86	114.08
18	A	837	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
26	a	617	LUT	C35-C15-C14	-3.48	116.34	123.47
21	F	305	BCR	C38-C26-C25	-3.48	120.62	124.53
18	6	618	CLA	C3B-C4B-NB	-3.48	107.90	110.23
18	5	618	CLA	C3B-C4B-NB	-3.48	107.90	110.23
21	A	850	BCR	C33-C5-C6	-3.48	120.62	124.53
21	A	850	BCR	C11-C10-C9	-3.48	122.35	127.31
18	B	824	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
21	A	849	BCR	C16-C17-C18	-3.47	122.36	127.31
21	F	305	BCR	C16-C15-C14	-3.47	116.37	123.47
18	L	302	CLA	CHB-C4A-NA	3.47	129.31	124.51
18	A	831	CLA	O2D-CGD-O1D	-3.47	117.06	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	603	CLA	C3B-C4B-NB	-3.46	107.91	110.23
21	6	622	BCR	C38-C26-C25	-3.46	120.64	124.53
18	4	609	CLA	CHB-C4A-NA	3.45	129.29	124.51
18	7	604	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
21	3	622	BCR	C12-C13-C14	3.45	124.23	118.94
21	4	621	BCR	C33-C5-C6	-3.45	120.66	124.53
21	A	850	BCR	C15-C14-C13	-3.44	122.40	127.31
21	7	623	BCR	C11-C10-C9	-3.44	122.40	127.31
18	6	616	CLA	CMB-C2B-C1B	-3.44	120.14	125.37
18	7	616	CLA	C3B-C4B-NB	-3.44	107.93	110.23
23	K	208	LMU	C1'-C2'-C3'	3.43	117.15	110.00
21	A	850	BCR	C16-C17-C18	-3.43	122.41	127.31
21	a	619	BCR	C11-C10-C9	-3.43	122.41	127.31
27	7	620	XAT	C24-C23-C22	-3.43	104.16	110.77
18	a	611	CLA	CAA-C2A-C3A	-3.42	108.11	116.10
18	A	809	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
21	L	305	BCR	C28-C27-C26	-3.41	107.98	114.08
18	A	805	CLA	C3B-C4B-NB	-3.41	107.36	110.52
21	K	207	BCR	C7-C8-C9	-3.40	121.10	126.23
28	6	624	NEX	C11-C10-C9	-3.40	122.46	127.31
21	B	847	BCR	C20-C21-C22	-3.40	122.46	127.31
27	5	621	XAT	C4-C3-C2	-3.40	104.21	110.77
27	5	621	XAT	C38-C25-C26	-3.39	116.58	122.26
26	4	619	LUT	C35-C15-C14	-3.39	116.54	123.47
18	B	840	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
26	6	619	LUT	C35-C15-C14	-3.38	116.55	123.47
18	3	608	CLA	C3B-C4B-NB	-3.38	107.38	110.52
18	A	817	CLA	CHB-C4A-NA	3.38	129.19	124.51
18	B	810	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
18	4	616	CLA	C3B-C4B-NB	-3.38	107.97	110.23
27	a	618	XAT	C10-C11-C12	-3.37	112.70	123.22
18	a	602	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
27	8	620	XAT	O24-C25-C38	3.37	119.09	115.06
27	3	619	XAT	C4-C3-C2	-3.36	104.28	110.77
18	1	601	CLA	C3B-C4B-NB	-3.35	107.41	110.52
18	A	820	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
21	A	849	BCR	C3-C4-C5	-3.35	108.10	114.08
21	B	847	BCR	C15-C16-C17	-3.34	116.62	123.47
21	8	621	BCR	C21-C20-C19	-3.34	112.78	123.22
18	5	606	CLA	C3B-C4B-NB	-3.34	107.41	110.52
21	A	851	BCR	C11-C10-C9	-3.34	122.54	127.31
18	5	619	CLA	C3B-C4B-NB	-3.34	107.99	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	621	BCR	C20-C19-C18	-3.34	117.05	126.42
18	A	810	CLA	C3B-C4B-NB	-3.33	107.42	110.52
21	B	848	BCR	C15-C14-C13	-3.33	122.56	127.31
18	1	606	CLA	CBD-CHA-C1A	3.32	131.58	128.06
21	7	621	BCR	C21-C20-C19	-3.32	112.84	123.22
18	B	821	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	B	833	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	a	601	CLA	C3B-C4B-NB	-3.32	107.44	110.52
21	1	619	BCR	C11-C10-C9	-3.32	122.58	127.31
26	8	619	LUT	C35-C15-C14	-3.32	116.68	123.47
18	8	616	CLA	CHB-C4A-NA	3.31	129.09	124.51
21	B	847	BCR	C24-C23-C22	-3.31	121.23	126.23
21	a	619	BCR	C20-C21-C22	-3.31	122.58	127.31
18	A	802	CLA	CMB-C2B-C3B	3.31	134.60	126.59
26	4	619	LUT	C10-C11-C12	-3.30	112.91	123.22
18	5	616	CLA	C3B-C4B-NB	-3.30	108.02	110.23
21	B	846	BCR	C3-C4-C5	-3.29	108.19	114.08
18	A	842	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
21	F	305	BCR	C10-C11-C12	-3.29	112.95	123.22
18	5	619	CLA	CHB-C4A-NA	3.29	129.06	124.51
18	3	611	CLA	CAA-C2A-C3A	-3.29	108.42	116.10
18	5	619	CLA	CMB-C2B-C3B	3.29	132.11	123.59
21	B	847	BCR	C3-C4-C5	-3.28	108.22	114.08
27	4	620	XAT	C15-C14-C13	-3.28	122.63	127.31
21	B	847	BCR	C16-C17-C18	-3.28	122.63	127.31
23	A	859	LMU	C1'-O5'-C5'	3.28	118.12	113.03
21	B	801	BCR	C29-C30-C25	3.27	115.52	110.48
18	A	818	CLA	CMB-C2B-C1B	-3.27	120.39	125.37
18	A	826	CLA	C2A-C1A-CHA	3.26	129.57	123.86
18	7	614	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
27	4	620	XAT	C35-C34-C33	-3.26	122.66	127.31
18	7	609	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
21	F	305	BCR	C15-C14-C13	-3.26	122.66	127.31
21	a	619	BCR	C15-C14-C13	-3.25	122.67	127.31
18	1	602	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
18	A	815	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
21	L	305	BCR	C21-C20-C19	-3.25	113.09	123.22
21	B	845	BCR	C11-C10-C9	-3.24	122.69	127.31
18	1	610	CLA	C3B-C4B-NB	-3.24	107.51	110.52
18	8	611	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	A	811	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
21	B	843	BCR	C29-C30-C25	3.23	115.45	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	607	CLA	CAA-C2A-C3A	-3.22	108.58	116.10
27	3	619	XAT	C31-C30-C29	-3.22	122.72	127.31
18	a	610	CLA	C3B-C4B-NB	-3.22	107.53	110.52
23	A	857	LMU	C5'-C4'-C3'	3.22	114.21	109.40
18	B	835	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
18	6	601	CLA	CHB-C4A-NA	3.21	128.96	124.51
21	3	620	BCR	C15-C14-C13	-3.21	122.73	127.31
18	B	808	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	B	817	CLA	CHB-C4A-NA	3.21	128.95	124.51
21	4	621	BCR	C7-C8-C9	-3.21	121.39	126.23
18	A	840	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	3	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
27	a	618	XAT	C35-C34-C33	-3.20	122.74	127.31
18	A	817	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
18	B	814	CLA	CHB-C4A-NA	3.20	128.94	124.51
18	J	101	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
26	1	617	LUT	C10-C11-C12	-3.20	113.24	123.22
18	7	615	CLA	C3B-C4B-NB	-3.20	108.09	110.23
18	A	815	CLA	C3B-C4B-NB	-3.19	107.55	110.52
21	4	621	BCR	C33-C5-C4	3.19	119.75	113.62
18	a	614	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
18	7	602	CLA	C3B-C4B-NB	-3.19	107.55	110.52
28	5	624	NEX	C27-C28-C29	-3.19	120.58	125.53
18	A	813	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
18	B	803	CLA	CBC-CAC-C3C	3.19	121.22	112.43
21	3	621	BCR	C19-C18-C17	3.19	123.83	118.94
18	K	203	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
21	B	844	BCR	C34-C9-C10	-3.19	118.46	122.92
18	F	301	CLA	C3B-C4B-NB	-3.18	107.56	110.52
18	B	811	CLA	C3B-C4B-NB	-3.18	108.10	110.23
21	6	622	BCR	C21-C20-C19	-3.17	113.32	123.22
21	F	305	BCR	C3-C4-C5	-3.17	108.42	114.08
21	L	301	BCR	C38-C26-C25	-3.17	120.97	124.53
18	B	805	CLA	CHB-C4A-NA	3.16	128.89	124.51
21	K	202	BCR	C38-C26-C27	3.16	119.69	113.62
18	7	609	CLA	CHB-C4A-NA	3.16	128.88	124.51
18	B	841	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
21	K	202	BCR	C27-C26-C25	-3.16	118.15	122.73
18	6	617	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
18	7	612	CLA	C3B-C4B-NB	-3.15	107.59	110.52
18	A	828	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
26	7	619	LUT	C35-C15-C14	-3.15	117.02	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	803	CLA	CHB-C4A-NA	3.15	128.87	124.51
21	6	622	BCR	C11-C10-C9	-3.15	122.81	127.31
27	a	618	XAT	C31-C30-C29	-3.15	122.82	127.31
18	a	611	CLA	C3B-C4B-NB	-3.14	108.12	110.23
18	B	818	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
18	A	805	CLA	CMB-C2B-C1B	-3.14	120.58	125.37
21	3	622	BCR	C33-C5-C6	-3.14	121.00	124.53
18	7	601	CLA	C3B-C4B-NB	-3.14	107.60	110.52
28	6	624	NEX	C35-C34-C33	-3.13	122.84	127.31
18	3	609	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
26	7	619	LUT	C30-C31-C32	-3.13	113.45	123.22
25	B	850	DGD	O5D-C6D-C5D	-3.13	103.26	109.05
18	B	839	CLA	C3B-C4B-NB	-3.13	107.61	110.52
18	A	804	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	K	201	CLA	CHB-C4A-NA	3.12	128.83	124.51
18	7	604	CLA	CMB-C2B-C1B	-3.12	120.61	125.37
18	B	816	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
21	B	845	BCR	C20-C21-C22	-3.12	122.85	127.31
18	A	822	CLA	CHB-C1B-NB	3.12	127.56	124.26
28	5	624	NEX	C24-C23-C22	-3.12	104.75	110.77
21	B	848	BCR	C10-C11-C12	-3.12	113.48	123.22
21	1	619	BCR	C16-C15-C14	-3.12	117.09	123.47
18	8	607	CLA	C3B-C4B-NB	-3.11	108.14	110.23
26	4	619	LUT	C30-C31-C32	-3.11	113.50	123.22
18	A	813	CLA	CHB-C4A-NA	3.11	128.82	124.51
18	A	825	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
21	K	207	BCR	C33-C5-C6	-3.11	121.03	124.53
18	B	835	CLA	CHB-C4A-NA	3.11	128.81	124.51
27	4	620	XAT	C24-C23-C22	-3.11	104.77	110.77
18	1	610	CLA	CBD-CHA-C1A	3.11	132.16	128.50
18	A	821	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	A	802	CLA	C3B-C4B-NB	-3.11	107.63	110.52
18	6	604	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
21	A	848	BCR	C33-C5-C6	-3.10	121.04	124.53
18	A	804	CLA	CHB-C4A-NA	3.10	128.80	124.51
18	3	617	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	B	850	DGD	O6D-C1D-O3G	-3.10	102.63	109.97
18	5	611	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
21	5	622	BCR	C4-C5-C6	-3.10	118.23	122.73
18	6	603	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	A	824	CLA	CAA-C2A-C3A	-3.09	108.89	116.10
18	A	805	CLA	O2D-CGD-O1D	-3.09	117.80	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	101	CLA	CHB-C4A-NA	3.09	128.78	124.51
21	8	621	BCR	C4-C5-C6	-3.08	118.25	122.73
27	6	621	XAT	C35-C34-C33	-3.08	122.91	127.31
18	6	608	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	a	611	CLA	O2D-CGD-O1D	-3.08	117.09	124.09
18	A	821	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	8	616	CLA	C2A-C1A-CHA	3.08	129.25	123.86
18	B	826	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
27	6	621	XAT	C24-C23-C22	-3.08	104.82	110.77
27	1	618	XAT	C10-C11-C12	-3.08	113.61	123.22
18	A	801	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	B	830	CLA	CMC-C2C-C1C	-3.08	120.35	125.04
18	B	830	CLA	C2D-C1D-ND	-3.08	107.84	110.10
26	8	619	LUT	C15-C14-C13	-3.07	122.93	127.31
18	A	841	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	8	606	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	5	608	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	5	613	CLA	CHB-C4A-NA	3.06	128.75	124.51
21	4	621	BCR	C21-C20-C19	-3.06	113.66	123.22
18	4	609	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	7	616	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	6	620	CLA	CHB-C4A-NA	3.06	128.74	124.51
18	3	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
18	B	832	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
27	4	620	XAT	C10-C11-C12	-3.05	113.68	123.22
18	A	831	CLA	C2B-C1B-NB	-3.05	108.19	110.23
18	4	604	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
18	3	617	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
18	F	304	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
18	B	820	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
26	3	618	LUT	C10-C11-C12	-3.05	113.71	123.22
18	B	825	CLA	C3B-C4B-NB	-3.05	107.69	110.52
21	5	622	BCR	C8-C7-C6	-3.04	118.66	127.20
18	a	613	CLA	CHB-C4A-NA	3.04	128.72	124.51
18	B	808	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
18	A	808	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	B	826	CLA	CMB-C2B-C1B	-3.04	120.74	125.37
21	A	856	BCR	C10-C11-C12	-3.04	113.73	123.22
18	5	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	a	618	XAT	C15-C14-C13	-3.04	122.98	127.31
27	7	620	XAT	C4-C3-C2	-3.03	104.91	110.77
18	3	612	CLA	C3B-C4B-NB	-3.03	107.70	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	603	CLA	CHB-C4A-NA	3.03	128.71	124.51
18	B	837	CLA	C3B-C4B-NB	-3.03	107.70	110.52
18	4	602	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	B	846	BCR	C16-C17-C18	-3.03	122.98	127.31
21	B	846	BCR	C33-C5-C6	-3.03	121.12	124.53
18	4	602	CLA	CMB-C2B-C1B	-3.03	120.76	125.37
18	3	610	CLA	CHB-C4A-NA	3.03	128.70	124.51
18	A	829	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
21	A	850	BCR	C1-C6-C5	-3.02	118.36	122.61
18	A	826	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
18	5	604	CLA	C3B-C4B-NB	-3.02	108.21	110.23
23	A	857	LMU	C2'-C3'-C4'	3.02	115.63	110.24
21	a	619	BCR	C7-C8-C9	-3.02	121.68	126.23
18	3	607	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	8	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	6	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	A	825	CLA	CHB-C4A-NA	3.01	128.67	124.51
18	7	607	CLA	CAA-C2A-C3A	-3.01	106.74	114.26
18	A	838	CLA	CHB-C4A-NA	3.01	128.67	124.51
18	5	613	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	B	829	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
18	K	206	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	B	808	CLA	CBA-CAA-C2A	3.00	122.73	113.86
18	B	808	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	5	619	CLA	CAB-C3B-C2B	3.00	131.37	123.59
21	A	848	BCR	C15-C14-C13	-3.00	123.03	127.31
18	L	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	5	614	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	4	603	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	8	613	CLA	CHB-C4A-NA	2.99	128.65	124.51
18	6	608	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
18	B	833	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
21	5	622	BCR	C33-C5-C4	2.99	119.36	113.62
18	B	836	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	6	620	CLA	C3B-C4B-NB	-2.99	107.75	110.52
21	5	622	BCR	C20-C21-C22	-2.98	123.05	127.31
18	A	822	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
21	a	619	BCR	C24-C23-C22	-2.98	121.73	126.23
27	5	621	XAT	C24-C23-C22	-2.98	105.01	110.77
18	B	803	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	7	619	LUT	C20-C13-C12	2.98	122.78	118.08
21	B	843	BCR	C7-C8-C9	-2.98	121.73	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	204	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	B	832	CLA	CMB-C2B-C1B	-2.98	120.83	125.37
18	3	609	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	A	806	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	8	608	CLA	CHB-C4A-NA	2.98	128.63	124.51
27	8	620	XAT	C4-C3-C2	-2.97	105.03	110.77
18	A	814	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	8	625	LMU	C3B-C4B-C5B	2.97	115.54	110.24
21	L	305	BCR	C16-C15-C14	-2.97	117.39	123.47
18	a	603	CLA	CHB-C4A-NA	2.97	128.62	124.51
18	4	608	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	7	609	CLA	O2D-CGD-CBD	2.96	116.54	111.27
18	8	607	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	A	806	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	7	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	B	816	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	5	603	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	6	604	CLA	C3B-C4B-NB	-2.96	107.77	110.52
18	A	840	CLA	CHB-C4A-NA	2.96	128.60	124.51
18	8	609	CLA	CHB-C4A-NA	2.96	128.60	124.51
21	L	301	BCR	C33-C5-C6	-2.96	121.21	124.53
21	B	843	BCR	C27-C26-C25	-2.96	118.44	122.73
23	K	208	LMU	C2'-C3'-C4'	2.95	116.42	109.68
18	A	839	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	806	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	B	845	BCR	C33-C5-C4	2.95	119.29	113.62
18	B	816	CLA	C3B-C4B-NB	-2.95	107.78	110.52
21	A	856	BCR	C15-C14-C13	-2.95	123.10	127.31
18	4	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	B	846	BCR	C24-C23-C22	-2.95	121.78	126.23
18	B	815	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	6	622	BCR	C7-C8-C9	-2.95	121.78	126.23
18	4	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	A	816	CLA	CHB-C4A-NA	2.95	128.59	124.51
18	A	835	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	3	622	BCR	C16-C15-C14	-2.95	117.44	123.47
18	A	828	CLA	CHB-C4A-NA	2.94	128.58	124.51
18	7	608	CLA	C3B-C4B-NB	-2.94	107.78	110.52
18	7	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	8	625	LMU	O5'-C1'-C2'	2.94	116.58	110.35
27	4	620	XAT	C19-C9-C8	2.94	122.71	118.08
18	B	817	CLA	C3B-C4B-NB	-2.94	107.79	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	604	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
21	L	305	BCR	C29-C30-C25	2.94	115.00	110.48
21	A	849	BCR	C38-C26-C27	2.93	119.25	113.62
18	a	602	CLA	C3B-C4B-NB	-2.93	107.79	110.52
18	A	818	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
21	A	851	BCR	C10-C11-C12	-2.93	114.06	123.22
18	K	204	CLA	CHB-C4A-NA	2.93	128.57	124.51
18	8	603	CLA	CHB-C4A-NA	2.93	128.57	124.51
23	A	858	LMU	C6B-C5B-C4B	-2.93	109.45	113.54
18	B	832	CLA	CHB-C4A-NA	2.93	128.56	124.51
23	8	625	LMU	C1'-C2'-C3'	2.93	116.10	110.00
18	B	824	CLA	O2D-CGD-CBD	2.93	116.47	111.27
18	6	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	1	614	CLA	C3B-C4B-NB	-2.93	108.27	110.23
18	B	840	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	A	850	BCR	C33-C5-C4	2.93	119.24	113.62
18	A	809	CLA	CHB-C4A-NA	2.93	128.56	124.51
18	A	829	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
27	1	618	XAT	C24-C23-C22	-2.92	105.13	110.77
18	8	611	CLA	C3B-C4B-NB	-2.92	107.81	110.52
18	B	830	CLA	CHB-C4A-NA	2.92	128.55	124.51
18	B	827	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
21	B	801	BCR	C3-C4-C5	-2.92	108.87	114.08
18	a	609	CLA	CHB-C4A-NA	2.92	128.55	124.51
21	L	301	BCR	C28-C27-C26	-2.92	108.87	114.08
18	6	611	CLA	C3B-C4B-NB	-2.92	107.81	110.52
21	a	619	BCR	C33-C5-C4	2.92	119.22	113.62
18	6	607	CLA	CHB-C4A-NA	2.92	128.54	124.51
18	A	824	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	B	819	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	7	611	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
18	3	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	4	601	CLA	C3B-C4B-NB	-2.91	107.81	110.52
18	A	838	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	B	839	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	A	808	CLA	CHB-C4A-NA	2.91	128.54	124.51
18	A	838	CLA	CMB-C2B-C1B	-2.91	120.94	125.37
24	A	860	LMG	O1-C7-C8	-2.91	103.88	110.90
18	A	836	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	6	602	CLA	C3B-C4B-NB	-2.91	107.82	110.52
18	3	604	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	4	610	CLA	CHB-C4A-NA	2.91	128.53	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	603	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
21	3	620	BCR	C33-C5-C4	2.90	119.19	113.62
21	B	844	BCR	C3-C4-C5	-2.90	108.90	114.08
21	A	850	BCR	C20-C21-C22	-2.90	123.17	127.31
18	5	602	CLA	CMB-C2B-C1B	-2.90	120.96	125.37
28	5	624	NEX	C15-C35-C34	-2.90	117.54	123.47
18	7	612	CLA	CHB-C1B-NB	2.90	127.32	124.26
21	5	622	BCR	C16-C15-C14	-2.90	117.54	123.47
18	A	822	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	A	807	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	7	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
18	A	805	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	B	838	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	3	615	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	A	837	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	L	304	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	B	812	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
21	K	202	BCR	C20-C21-C22	-2.88	123.20	127.31
21	B	846	BCR	C21-C20-C19	-2.88	114.24	123.22
18	8	601	CLA	CHB-C4A-NA	2.88	128.49	124.51
18	6	618	CLA	CHB-C4A-NA	2.88	128.49	124.51
20	A	847	LHG	O8-C23-C24	2.88	120.93	111.91
18	3	608	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
18	A	809	CLA	C3B-C4B-NB	-2.87	107.85	110.52
18	5	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	A	849	BCR	C15-C16-C17	-2.87	117.59	123.47
18	B	805	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	1	610	CLA	CHB-C1B-NB	2.87	127.30	124.26
18	F	303	CLA	CAA-C2A-C3A	-2.87	107.09	114.26
21	B	845	BCR	C34-C9-C10	-2.87	118.90	122.92
21	K	202	BCR	C30-C25-C26	-2.87	118.57	122.61
21	A	851	BCR	C33-C5-C6	-2.87	121.31	124.53
27	4	620	XAT	C35-C15-C14	-2.87	117.60	123.47
21	L	305	BCR	C15-C14-C13	-2.87	123.22	127.31
18	4	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	B	826	CLA	CHB-C4A-NA	2.87	128.47	124.51
18	A	821	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	B	809	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	5	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	6	608	CLA	CMB-C2B-C1B	-2.86	121.01	125.37
18	A	805	CLA	CHB-C1B-NB	2.86	127.29	124.26
18	A	854	CLA	CMB-C2B-C1B	-2.86	121.01	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	619	LUT	C10-C11-C12	-2.86	114.28	123.22
18	A	819	CLA	CHB-C4A-NA	2.86	128.47	124.51
27	8	620	XAT	C19-C9-C8	2.86	122.58	118.08
18	A	823	CLA	CAA-C2A-C3A	-2.86	107.11	114.26
18	6	610	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	B	837	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	B	834	CLA	CHB-C4A-NA	2.86	128.46	124.51
18	A	816	CLA	CMB-C2B-C1B	-2.86	121.02	125.37
18	8	601	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	J	103	DGD	O6E-C5E-C4E	2.85	114.88	109.69
18	4	616	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
20	A	846	LHG	O8-C23-C24	2.85	120.86	111.91
18	A	826	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	a	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
27	8	620	XAT	C35-C34-C33	-2.85	123.24	127.31
21	7	621	BCR	C24-C23-C22	-2.85	121.93	126.23
27	1	618	XAT	C35-C15-C14	-2.85	117.64	123.47
21	B	847	BCR	C33-C5-C4	2.85	119.09	113.62
18	6	620	CLA	CAA-CBA-CGA	-2.85	104.95	112.51
18	7	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	1	611	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	7	613	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	1	604	CLA	O2D-CGD-CBD	2.85	116.33	111.27
18	6	609	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	a	613	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	6	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	7	620	XAT	C31-C30-C29	-2.84	123.25	127.31
27	4	620	XAT	C8-C9-C10	-2.84	114.58	118.94
18	A	804	CLA	C3B-C4B-NB	-2.84	107.88	110.52
18	6	614	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	B	813	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	8	616	CLA	C3B-C4B-NB	-2.84	108.33	110.23
18	1	608	CLA	C3B-C4B-NB	-2.84	107.88	110.52
18	B	827	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	A	856	BCR	C11-C10-C9	-2.84	123.26	127.31
18	8	602	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	3	609	CLA	CHB-C1B-NB	2.84	127.26	124.26
26	5	620	LUT	C30-C31-C32	-2.84	114.36	123.22
18	5	608	CLA	C3B-C4B-NB	-2.84	107.88	110.52
18	6	612	CLA	CHB-C4A-NA	2.84	128.43	124.51
18	A	801	CLA	C1D-ND-C4D	-2.84	104.32	106.33
18	7	602	CLA	CHB-C4A-NA	2.83	128.43	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	301	BCR	C15-C16-C17	-2.83	117.67	123.47
21	8	621	BCR	C29-C30-C25	2.83	114.84	110.48
21	1	619	BCR	C15-C14-C13	-2.83	123.27	127.31
21	3	622	BCR	C30-C25-C26	-2.83	118.63	122.61
26	8	619	LUT	C10-C11-C12	-2.83	114.39	123.22
26	3	618	LUT	C35-C34-C33	-2.83	123.28	127.31
18	8	616	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
18	K	206	CLA	CHB-C4A-NA	2.83	128.42	124.51
18	8	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	1	606	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	A	819	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	L	302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	6	613	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	A	833	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	6	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	F	303	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	1	604	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	3	606	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	B	836	CLA	CMB-C2B-C3B	2.82	133.42	126.59
18	5	608	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
21	F	305	BCR	C36-C18-C17	-2.82	118.97	122.92
18	1	602	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	5	609	CLA	C3B-C4B-NB	-2.82	107.90	110.52
26	6	619	LUT	C10-C11-C12	-2.82	114.42	123.22
18	6	613	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	3	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	8	609	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	A	827	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	4	618	CLA	CAA-C2A-C3A	-2.81	107.23	114.26
18	3	613	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	5	618	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	7	603	CLA	O2D-CGD-O1D	-2.81	117.70	124.09
18	7	610	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	4	602	CLA	CHB-C4A-NA	2.81	128.40	124.51
21	K	202	BCR	C2-C1-C6	2.81	114.80	110.48
18	8	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	B	823	CLA	C3B-C4B-NB	-2.81	107.91	110.52
21	L	305	BCR	C3-C4-C5	-2.81	109.06	114.08
18	A	841	CLA	CHB-C4A-NA	2.81	128.39	124.51
18	A	837	CLA	O2D-CGD-CBD	2.80	116.25	111.27
20	3	623	LHG	O8-C23-C24	2.80	120.71	111.91
18	B	807	CLA	C3B-C4B-NB	-2.80	107.92	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	842	CLA	CHB-C4A-NA	2.80	128.39	124.51
27	4	620	XAT	C4-C3-C2	-2.80	105.36	110.77
18	4	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	F	305	BCR	C38-C26-C27	2.80	118.99	113.62
18	B	839	CLA	CHB-C1B-NB	2.80	127.22	124.26
18	A	803	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	B	802	CLA	C3B-C4B-NB	-2.80	107.92	110.52
18	6	602	CLA	CHB-C4A-NA	2.79	128.38	124.51
18	A	833	CLA	CMB-C2B-C3B	2.79	133.35	126.59
21	3	620	BCR	C7-C8-C9	-2.79	122.02	126.23
18	B	806	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	8	614	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	B	807	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	8	613	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	B	824	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	B	803	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
18	K	203	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	3	617	CLA	CMA-C3A-C2A	-2.79	109.60	116.10
18	3	602	CLA	CHB-C4A-NA	2.78	128.36	124.51
21	K	207	BCR	C38-C26-C25	-2.78	121.40	124.53
21	J	102	BCR	C20-C21-C22	-2.78	123.34	127.31
18	B	829	CLA	CMB-C2B-C3B	2.78	133.33	126.59
18	7	611	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	B	818	CLA	C4-C3-C5	2.78	119.95	115.27
21	6	622	BCR	C20-C21-C22	-2.78	123.34	127.31
18	A	836	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	1	613	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	B	850	DGD	CDB-CCB-CBB	-2.78	100.32	114.42
18	B	811	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	B	812	CLA	CHB-C4A-NA	2.78	128.35	124.51
18	B	825	CLA	CAA-C2A-C1A	-2.78	102.88	111.97
18	4	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	8	610	CLA	CMB-C2B-C1B	-2.77	121.14	125.37
26	7	619	LUT	C22-C23-C24	-2.77	108.58	111.74
27	7	620	XAT	C10-C11-C12	-2.77	114.56	123.22
18	6	604	CLA	CHB-C4A-NA	2.77	128.35	124.51
18	3	610	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	4	602	CLA	CMB-C2B-C3B	2.77	133.30	126.59
21	3	621	BCR	C29-C30-C25	2.77	114.75	110.48
18	B	834	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	8	603	CLA	CAB-C3B-C2B	2.77	130.77	123.59
18	A	845	CLA	CHB-C4A-NA	2.77	128.34	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	612	CLA	CHB-C4A-NA	2.77	128.34	124.51
27	a	618	XAT	C4-C3-C2	-2.77	105.43	110.77
18	5	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	3	620	BCR	C4-C5-C6	-2.77	118.71	122.73
28	5	624	NEX	C11-C10-C9	-2.77	123.36	127.31
18	B	814	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
18	B	830	CLA	CMC-C2C-C3C	2.76	133.62	126.12
18	3	611	CLA	O2D-CGD-O1D	-2.76	117.82	124.09
18	6	607	CLA	CAB-C3B-C2B	2.76	130.75	123.59
18	3	602	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	1	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	B	814	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	8	601	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	6	601	CLA	O2D-CGD-CBD	2.76	116.17	111.27
18	a	606	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	5	617	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	A	858	LMU	O5B-C1B-C2B	2.76	116.24	111.31
18	A	802	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
28	6	624	NEX	C27-C28-C29	-2.75	121.26	125.53
18	A	834	CLA	CHB-C4A-NA	2.75	128.32	124.51
21	J	102	BCR	C20-C19-C18	-2.75	118.68	126.42
18	B	839	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	A	805	CLA	CMB-C2B-C3B	2.75	133.26	126.59
18	B	823	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
18	K	203	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	B	836	CLA	C3B-C4B-NB	-2.75	107.96	110.52
18	B	804	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
18	7	609	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
27	5	621	XAT	C35-C34-C33	-2.75	123.38	127.31
18	A	822	CLA	C3B-C4B-NB	-2.75	107.96	110.52
18	7	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	8	620	XAT	C31-C30-C29	-2.75	123.39	127.31
27	3	619	XAT	C10-C11-C12	-2.75	114.64	123.22
18	B	820	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	K	201	CLA	C2A-C1A-CHA	2.75	128.66	123.86
27	8	620	XAT	C24-C23-C22	-2.75	105.47	110.77
24	5	627	LMG	O6-C1-O1	-2.74	103.47	109.97
18	5	609	CLA	CHB-C4A-NA	2.74	128.31	124.51
18	A	811	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	J	102	BCR	C27-C26-C25	-2.74	118.75	122.73
18	6	618	CLA	O2D-CGD-O1D	-2.74	117.86	124.09
18	B	830	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	5	606	CLA	CHB-C1B-NB	2.74	127.16	124.26
18	6	609	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	1	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	5	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	A	852	BCR	C8-C9-C10	2.74	123.15	118.94
21	B	844	BCR	C28-C27-C26	-2.74	109.18	114.08
18	4	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	7	619	LUT	C38-C25-C24	-2.74	117.70	123.56
18	B	817	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	B	847	BCR	C33-C5-C6	-2.74	121.45	124.53
21	A	852	BCR	C27-C26-C25	-2.74	118.76	122.73
18	A	832	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	6	622	BCR	C33-C5-C4	2.74	118.87	113.62
26	1	617	LUT	C30-C31-C32	-2.73	114.68	123.22
21	7	621	BCR	C11-C10-C9	-2.73	123.41	127.31
21	L	301	BCR	C16-C17-C18	-2.73	123.41	127.31
18	a	613	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	a	601	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	a	608	CLA	C3B-C4B-NB	-2.73	107.98	110.52
21	B	846	BCR	C28-C27-C26	-2.73	109.20	114.08
18	8	612	CLA	O2D-CGD-O1D	-2.73	117.89	124.09
27	a	618	XAT	C24-C23-C22	-2.73	105.50	110.77
18	3	607	CLA	CMB-C2B-C3B	2.73	130.66	123.59
18	A	817	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
18	B	803	CLA	CAC-C3C-C2C	-2.73	122.86	127.53
18	6	609	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	B	828	CLA	CMB-C2B-C1B	-2.73	121.22	125.37
18	1	609	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
18	5	601	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	4	608	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	3	614	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	A	843	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	a	610	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
21	B	844	BCR	C8-C9-C10	2.72	123.11	118.94
21	a	619	BCR	C16-C15-C14	-2.72	117.91	123.47
18	B	828	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	A	830	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	4	613	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
18	B	824	CLA	C3B-C4B-NB	-2.72	108.00	110.52
18	a	601	CLA	O2D-CGD-O1D	-2.72	117.92	124.09
18	A	820	CLA	CHB-C4A-NA	2.72	128.27	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	613	CLA	C3B-C4B-NB	-2.72	108.00	110.52
18	8	612	CLA	CAA-C2A-C3A	-2.72	107.47	114.26
26	3	618	LUT	C38-C25-C24	-2.71	117.75	123.56
18	B	818	CLA	CHB-C4A-NA	2.71	128.27	124.51
21	J	102	BCR	C24-C23-C22	-2.71	122.14	126.23
27	7	620	XAT	C35-C15-C14	-2.71	117.92	123.47
18	5	612	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	5	606	CLA	O2D-CGD-O1D	-2.71	117.93	124.09
21	F	305	BCR	C20-C19-C18	-2.71	118.80	126.42
18	8	608	CLA	C3B-C4B-NB	-2.71	108.00	110.52
18	1	612	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
18	B	811	CLA	CHB-C4A-NA	2.71	128.26	124.51
21	L	301	BCR	C39-C30-C25	-2.71	105.90	110.30
18	B	822	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
18	B	812	CLA	C3B-C4B-NB	-2.71	108.00	110.52
21	7	621	BCR	C15-C16-C17	-2.71	117.92	123.47
18	8	604	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	B	818	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
21	B	845	BCR	C37-C22-C21	-2.70	119.13	122.92
18	A	845	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
18	6	616	CLA	CMB-C2B-C3B	2.70	133.13	126.59
20	a	620	LHG	O8-C23-C24	2.70	120.39	111.91
18	6	611	CLA	CAA-C2A-C3A	-2.70	107.51	114.26
21	A	848	BCR	C16-C15-C14	-2.70	117.94	123.47
18	4	618	CLA	CAB-C3B-C2B	2.70	130.59	123.59
18	F	304	CLA	CAA-C2A-C3A	-2.70	109.80	116.10
21	L	301	BCR	C20-C21-C22	-2.70	123.46	127.31
18	5	601	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	4	616	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	4	613	CLA	C3B-C4B-NB	-2.69	108.02	110.52
18	A	822	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
18	1	614	CLA	CMB-C2B-C3B	2.69	130.56	123.59
18	A	823	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	B	837	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	B	820	CLA	C3B-C4B-NB	-2.69	108.02	110.52
18	4	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	a	610	CLA	CHB-C1B-NB	2.69	127.10	124.26
26	5	620	LUT	C10-C11-C12	-2.69	114.83	123.22
26	4	619	LUT	C15-C14-C13	-2.69	123.47	127.31
18	6	606	CLA	CAA-C2A-C3A	-2.69	107.54	114.26
18	a	610	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	7	604	CLA	CHB-C4A-NA	2.69	128.23	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	A	848	BCR	C38-C26-C27	2.69	118.78	113.62
21	7	623	BCR	C28-C27-C26	-2.69	109.28	114.08
18	7	601	CLA	CHD-C1D-ND	-2.69	121.99	124.45
18	4	603	CLA	CAB-C3B-C2B	2.68	130.54	123.59
18	8	613	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
18	8	616	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
18	6	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	805	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
21	B	847	BCR	C21-C20-C19	-2.68	114.85	123.22
18	A	838	CLA	CMB-C2B-C3B	2.68	133.08	126.59
18	7	615	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	8	610	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	6	620	CLA	O2D-CGD-CBD	2.68	116.03	111.27
18	8	603	CLA	C3B-C4B-NB	-2.68	108.44	110.23
18	4	609	CLA	C3B-C4B-NB	-2.68	108.03	110.52
18	A	812	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
18	1	609	CLA	C3B-C4B-NB	-2.68	108.44	110.23
20	8	623	LHG	O8-C23-C24	2.68	120.31	111.91
18	1	612	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	8	611	CLA	O2D-CGD-CBD	2.67	116.02	111.27
18	A	807	CLA	C3B-C4B-NB	-2.67	108.03	110.52
18	B	804	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
18	A	823	CLA	C3B-C4B-NB	-2.67	108.04	110.52
21	A	849	BCR	C10-C11-C12	-2.67	114.88	123.22
18	A	843	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	A	860	LMG	O6-C1-O1	-2.67	103.65	109.97
27	6	621	XAT	C19-C9-C8	2.67	122.28	118.08
18	4	611	CLA	C3B-C4B-NB	-2.67	108.04	110.52
18	A	802	CLA	CMD-C2D-C1D	-2.67	120.01	124.71
18	7	609	CLA	C3B-C4B-NB	-2.67	108.04	110.52
27	5	621	XAT	O24-C25-C38	2.67	118.25	115.06
20	a	620	LHG	C11-C10-C9	-2.67	100.89	114.42
18	3	613	CLA	O2D-CGD-O1D	-2.67	118.04	124.09
18	A	828	CLA	C3B-C4B-NB	-2.67	108.04	110.52
20	B	851	LHG	O8-C23-C24	2.66	120.27	111.91
18	6	618	CLA	CAB-C3B-C2B	2.66	130.49	123.59
18	3	612	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	L	304	CLA	C3B-C4B-NB	-2.66	108.05	110.52
18	A	803	CLA	CMB-C2B-C3B	2.66	133.03	126.59
18	B	819	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	A	827	CLA	CMB-C2B-C1B	-2.66	121.33	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	607	CLA	C3B-C4B-NB	-2.66	108.45	110.23
18	A	839	CLA	C3B-C4B-NB	-2.65	108.05	110.52
18	5	619	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
18	A	816	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
18	B	841	CLA	CHB-C1B-NB	2.65	127.06	124.26
18	a	608	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
21	J	102	BCR	C38-C26-C27	2.65	118.71	113.62
18	3	615	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
18	5	618	CLA	CAB-C3B-C2B	2.65	130.46	123.59
18	5	609	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
18	A	818	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	A	813	CLA	CMB-C2B-C1B	-2.65	121.34	125.37
18	A	830	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
18	7	603	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	B	832	CLA	O2D-CGD-CBD	2.65	115.97	111.27
18	1	602	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	6	613	CLA	O2D-CGD-O1D	-2.65	118.08	124.09
21	4	621	BCR	C8-C7-C6	-2.64	119.77	127.20
18	7	615	CLA	CAB-C3B-C2B	2.64	130.44	123.59
18	3	603	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	8	614	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	A	841	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
20	8	622	LHG	O8-C23-C24	2.64	120.20	111.91
21	K	207	BCR	C10-C11-C12	-2.64	114.98	123.22
18	7	609	CLA	CAC-C3C-C4C	2.64	128.24	124.81
21	A	856	BCR	C33-C5-C6	-2.64	121.56	124.53
21	L	305	BCR	C38-C26-C25	-2.64	121.56	124.53
20	5	623	LHG	O8-C23-C24	2.64	120.19	111.91
18	a	607	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	813	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	5	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	7	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	4	618	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	5	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	836	CLA	CHB-C1B-NB	2.63	127.05	124.26
18	a	616	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	8	619	LUT	C30-C31-C32	-2.63	115.00	123.22
18	4	616	CLA	CAB-C3B-C2B	2.63	130.41	123.59
18	5	619	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
18	A	807	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	5	623	LHG	C11-C10-C9	-2.63	101.07	114.42
21	K	207	BCR	C30-C25-C26	-2.63	118.91	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	842	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	A	827	CLA	CAA-C2A-C1A	-2.63	103.36	111.97
18	B	804	CLA	CHB-C1B-NB	2.63	127.04	124.26
23	8	625	LMU	O5B-C5B-C4B	2.63	114.47	109.69
18	A	839	CLA	CHB-C4A-NA	2.63	128.14	124.51
27	1	618	XAT	C4-C3-C2	-2.63	105.70	110.77
18	3	604	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	7	608	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
18	1	611	CLA	O2D-CGD-CBD	2.62	115.93	111.27
18	B	815	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	A	854	CLA	CMB-C2B-C3B	2.62	132.94	126.59
18	1	601	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	829	CLA	CMB-C2B-C3B	2.62	132.94	126.59
18	B	814	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	1	607	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	a	607	CLA	C3B-C4B-NB	-2.62	108.08	110.52
28	6	624	NEX	C15-C35-C34	-2.62	118.11	123.47
18	3	607	CLA	CAB-C3B-C2B	2.62	130.38	123.59
18	6	616	CLA	C3B-C4B-NB	-2.62	108.09	110.52
18	B	827	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	3	624	LHG	O8-C23-C24	2.62	120.12	111.91
26	3	618	LUT	C35-C15-C14	-2.62	118.11	123.47
18	3	610	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	B	819	CLA	C3B-C4B-NB	-2.62	108.09	110.52
18	A	802	CLA	C1-C2-C3	-2.61	121.52	126.04
18	L	303	CLA	CHB-C4A-NA	2.61	128.13	124.51
21	7	623	BCR	C15-C16-C17	-2.61	118.12	123.47
27	6	621	XAT	C31-C30-C29	-2.61	123.58	127.31
18	A	832	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
18	B	831	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
21	L	305	BCR	C20-C21-C22	-2.61	123.58	127.31
18	5	617	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	5	618	CLA	O2D-CGD-O1D	-2.61	118.16	124.09
21	1	619	BCR	C33-C5-C4	2.61	118.63	113.62
18	5	606	CLA	CAA-C2A-C3A	-2.61	107.74	114.26
18	5	612	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
18	F	303	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	1	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	7	614	CLA	O2D-CGD-CBD	2.61	115.90	111.27
21	a	619	BCR	C29-C30-C25	2.61	114.49	110.48
18	A	811	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	7	607	CLA	C3B-C4B-NB	-2.60	108.10	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	618	XAT	C19-C9-C8	2.60	122.18	118.08
18	B	805	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
21	J	102	BCR	C2-C1-C6	2.60	114.48	110.48
18	F	301	CLA	CHC-C4B-NB	2.60	127.01	124.26
18	K	201	CLA	CMD-C2D-C1D	-2.60	120.13	124.71
24	7	624	LMG	O1-C7-C8	-2.60	104.63	110.90
18	A	827	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	4	614	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	5	610	CLA	CHB-C1B-NB	2.60	127.01	124.26
21	A	849	BCR	C27-C26-C25	-2.60	118.96	122.73
18	6	616	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	B	846	BCR	C23-C24-C25	-2.60	119.91	127.20
20	6	623	LHG	C11-C10-C9	-2.59	101.26	114.42
26	8	619	LUT	C31-C30-C29	-2.59	123.61	127.31
18	3	606	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
18	B	834	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	A	818	CLA	CMB-C2B-C3B	2.59	132.87	126.59
21	F	305	BCR	C7-C8-C9	-2.59	122.32	126.23
18	6	612	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
18	a	611	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	A	827	CLA	CHB-C1B-NB	2.59	127.00	124.26
18	7	606	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	7	615	CLA	CMB-C2B-C3B	2.59	130.30	123.59
18	B	817	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
18	7	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	1	613	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
18	B	822	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	1	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	A	803	CLA	C4D-C3D-CAD	-2.59	105.05	108.10
18	A	810	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	6	617	CLA	C3B-C4B-NB	-2.59	108.12	110.52
18	5	607	CLA	CMB-C2B-C3B	2.59	132.85	126.59
21	3	620	BCR	C1-C6-C5	-2.59	118.97	122.61
18	A	836	CLA	C3B-C4B-NB	-2.58	108.12	110.52
27	6	621	XAT	C35-C15-C14	-2.58	118.18	123.47
27	5	621	XAT	C19-C9-C8	2.58	122.15	118.08
21	B	846	BCR	C30-C25-C24	2.58	123.08	115.78
26	4	619	LUT	C39-C29-C28	2.58	122.15	118.08
18	a	604	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
18	B	833	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	4	619	LUT	C7-C8-C9	-2.58	122.33	126.23
18	7	613	CLA	C3B-C4B-NB	-2.58	108.12	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	609	CLA	CHD-C1D-ND	-2.58	122.08	124.45
18	B	832	CLA	CMB-C2B-C3B	2.58	132.84	126.59
18	J	101	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	1	604	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	7	603	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	7	616	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	B	846	BCR	C30-C25-C26	-2.58	118.98	122.61
18	3	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	5	618	CLA	CMB-C2B-C3B	2.58	130.27	123.59
18	1	609	CLA	CAB-C3B-C2B	2.58	130.26	123.59
18	A	812	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	4	612	CLA	CAA-C2A-C3A	-2.57	107.83	114.26
18	8	607	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	a	609	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	4	608	CLA	C3B-C4B-NB	-2.57	108.13	110.52
18	B	831	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	4	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	A	852	BCR	C10-C11-C12	-2.57	115.19	123.22
18	B	838	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	6	619	LUT	C30-C31-C32	-2.57	115.20	123.22
18	8	614	CLA	O2D-CGD-CBD	2.57	115.83	111.27
18	6	611	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	A	814	CLA	C3B-C4B-NB	-2.57	108.13	110.52
18	A	854	CLA	C3B-C4B-NB	-2.57	108.13	110.52
18	B	802	CLA	CHC-C4B-NB	2.57	126.97	124.26
21	5	622	BCR	C23-C24-C25	-2.57	119.99	127.20
18	A	854	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	3	619	XAT	C38-C25-C24	2.57	117.17	114.28
27	3	619	XAT	C35-C34-C33	-2.57	123.65	127.31
18	1	616	CLA	C3B-C4B-NB	-2.57	108.51	110.23
18	A	833	CLA	C3B-C4B-NB	-2.57	108.14	110.52
18	B	835	CLA	CMB-C2B-C1B	-2.57	121.46	125.37
23	A	858	LMU	O5'-C5'-C4'	2.56	115.16	109.75
26	7	619	LUT	C39-C29-C28	2.56	122.12	118.08
21	3	622	BCR	C1-C6-C7	2.56	123.03	115.78
24	4	623	LMG	O6-C1-O1	-2.56	103.91	109.97
18	B	816	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
18	A	823	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
18	A	801	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
18	1	601	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
26	a	617	LUT	C10-C11-C12	-2.56	115.23	123.22
18	A	820	CLA	CMB-C2B-C3B	2.56	132.78	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	808	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
18	7	612	CLA	O2A-CGA-O1A	-2.56	116.92	123.30
18	F	304	CLA	C3B-C4B-NB	-2.56	108.14	110.52
18	B	836	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	B	851	LHG	C11-C10-C9	-2.55	101.45	114.42
27	3	619	XAT	C19-C9-C8	2.55	122.10	118.08
20	5	625	LHG	O8-C23-C24	2.55	119.92	111.91
21	K	207	BCR	C11-C10-C9	-2.55	123.67	127.31
18	3	615	CLA	CAA-C2A-C3A	-2.55	107.88	114.26
18	5	612	CLA	O2D-CGD-O1D	-2.55	118.29	124.09
18	B	831	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
18	7	606	CLA	CMB-C2B-C1B	-2.55	121.48	125.37
21	B	848	BCR	C39-C30-C25	-2.55	106.16	110.30
18	3	617	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
18	A	836	CLA	CHC-C4B-NB	2.55	126.95	124.26
18	6	606	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	7	614	CLA	C3B-C4B-NB	-2.55	108.15	110.52
18	8	606	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	7	609	CLA	CMB-C2B-C3B	2.55	132.76	126.59
18	F	304	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	B	813	CLA	C3B-C4B-NB	-2.55	108.15	110.52
18	B	816	CLA	CHB-C1B-NB	2.55	126.95	124.26
26	a	617	LUT	C19-C9-C8	2.55	122.09	118.08
21	7	621	BCR	C38-C26-C27	2.54	118.50	113.62
21	6	622	BCR	C8-C7-C6	-2.54	120.06	127.20
18	3	609	CLA	C2A-C1A-CHA	2.54	128.31	123.86
21	8	621	BCR	C33-C5-C4	2.54	118.50	113.62
18	1	604	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
21	B	843	BCR	C38-C26-C27	2.54	118.50	113.62
18	6	612	CLA	O2D-CGD-O1D	-2.54	118.31	124.09
18	B	824	CLA	CHB-C1B-NB	2.54	126.95	124.26
18	5	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	4	606	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
18	A	826	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	B	844	BCR	C38-C26-C27	2.54	118.50	113.62
18	7	616	CLA	CAB-C3B-C2B	2.54	130.17	123.59
18	A	829	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	835	CLA	C3B-C4B-NB	-2.54	108.16	110.52
21	7	621	BCR	C33-C5-C4	2.54	118.49	113.62
21	A	856	BCR	C29-C30-C25	2.54	114.39	110.48
18	B	823	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	5	611	CLA	C3B-C4B-NB	-2.54	108.16	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	619	CLA	CAA-C2A-C1A	2.54	120.29	111.97
18	K	204	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	a	608	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	6	612	CLA	CAA-C2A-C3A	-2.54	107.92	114.26
18	7	607	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	B	801	BCR	C7-C8-C9	-2.54	122.40	126.23
18	5	616	CLA	CHB-C4A-NA	2.53	128.02	124.51
18	1	616	CLA	CMB-C2B-C3B	2.53	130.15	123.59
18	L	303	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	6	607	CLA	CMB-C2B-C3B	2.53	130.15	123.59
23	5	628	LMU	C1B-O1B-C4'	-2.53	111.70	117.96
18	6	607	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
18	8	606	CLA	CHB-C1B-NB	2.53	126.93	124.26
18	5	619	CLA	CAB-C3B-C4B	-2.53	121.52	125.37
18	5	607	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
21	7	621	BCR	C7-C8-C9	-2.53	122.42	126.23
20	A	847	LHG	C11-C10-C9	-2.53	101.61	114.42
18	1	608	CLA	O2D-CGD-O1D	-2.53	118.36	124.09
18	1	609	CLA	CMB-C2B-C3B	2.52	130.13	123.59
18	6	606	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
18	a	607	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
18	B	837	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
18	B	839	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
18	1	614	CLA	O2D-CGD-O1D	-2.52	118.36	124.09
18	A	802	CLA	CHB-C1B-NB	2.52	126.93	124.26
28	5	624	NEX	C38-C25-C24	2.52	117.12	114.28
18	3	608	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	7	614	CLA	CAA-C2A-C3A	-2.52	107.96	114.26
20	8	623	LHG	C20-C19-C18	-2.52	101.63	114.42
21	a	619	BCR	C1-C6-C5	-2.52	119.07	122.61
18	5	618	CLA	CAA-C2A-C3A	-2.52	107.97	114.26
18	A	838	CLA	C1-C2-C3	-2.52	122.68	126.75
21	7	623	BCR	C38-C26-C25	-2.52	121.70	124.53
18	1	616	CLA	CAB-C3B-C2B	2.52	130.11	123.59
20	1	620	LHG	C11-C10-C9	-2.52	101.65	114.42
18	B	806	CLA	C3B-C4B-NB	-2.51	108.18	110.52
18	B	821	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	4	601	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	B	826	CLA	C3B-C4B-NB	-2.51	108.18	110.52
18	B	804	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	B	817	CLA	CHB-C1B-NB	2.51	126.92	124.26
18	B	828	CLA	C2D-C1D-ND	-2.51	108.25	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	602	CLA	C3B-C4B-NB	-2.51	108.19	110.52
23	A	858	LMU	C6'-C5'-C4'	-2.51	106.02	113.33
18	3	614	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
27	5	621	XAT	C15-C35-C34	-2.51	118.33	123.47
18	5	614	CLA	C3B-C4B-NB	-2.51	108.19	110.52
18	F	301	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
21	4	621	BCR	C29-C30-C25	2.51	114.34	110.48
18	4	604	CLA	CHB-C1B-NB	2.51	126.91	124.26
18	A	840	CLA	CHC-C4B-NB	2.51	126.91	124.26
18	B	834	CLA	CHD-C1D-ND	-2.51	122.15	124.45
18	7	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	814	CLA	CAC-C3C-C4C	2.51	128.06	124.81
21	A	852	BCR	C38-C26-C27	2.51	118.43	113.62
21	3	621	BCR	C33-C5-C4	2.51	118.43	113.62
18	7	616	CLA	CMB-C2B-C3B	2.50	130.08	123.59
18	3	606	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
18	A	806	CLA	CAC-C3C-C4C	2.50	128.06	124.81
18	8	607	CLA	CAB-C3B-C2B	2.50	130.07	123.59
26	8	619	LUT	C38-C25-C24	-2.50	118.21	123.56
18	3	606	CLA	C3B-C4B-NB	-2.50	108.19	110.52
20	5	625	LHG	C20-C19-C18	-2.50	101.73	114.42
18	A	833	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	a	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	3	617	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	5	607	CLA	C3B-C4B-NB	-2.50	108.20	110.52
18	7	611	CLA	CMB-C2B-C3B	2.50	132.63	126.59
18	6	601	CLA	C3B-C4B-NB	-2.50	108.20	110.52
21	A	852	BCR	C33-C5-C6	-2.50	121.73	124.53
18	4	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	6	606	CLA	O2D-CGD-O1D	-2.49	118.42	124.09
21	7	623	BCR	C7-C8-C9	-2.49	122.47	126.23
18	A	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	A	815	CLA	CHB-C1B-NB	2.49	126.90	124.26
18	B	832	CLA	CHB-C1B-NB	2.49	126.90	124.26
18	3	611	CLA	CAB-C3B-C2B	2.49	130.05	123.59
18	6	608	CLA	CHB-C1B-NB	2.49	126.90	124.26
18	3	609	CLA	CMB-C2B-C3B	2.49	132.62	126.59
18	a	612	CLA	CMB-C2B-C1B	-2.49	121.57	125.37
18	1	614	CLA	CAB-C3B-C2B	2.49	130.05	123.59
21	A	849	BCR	C38-C26-C25	-2.49	121.73	124.53
21	A	852	BCR	C16-C15-C14	-2.49	118.37	123.47
21	B	844	BCR	C20-C21-C22	-2.49	123.76	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	832	CLA	C3B-C4B-NB	-2.49	108.20	110.52
18	1	608	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	B	848	BCR	C15-C16-C17	-2.49	118.38	123.47
18	1	607	CLA	O2D-CGD-O1D	-2.49	118.44	124.09
18	3	608	CLA	CHB-C1B-NB	2.49	126.89	124.26
18	4	603	CLA	CHC-C4B-NB	2.49	126.89	124.26
18	L	303	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
18	7	604	CLA	CHB-C1B-NB	2.49	126.89	124.26
21	A	856	BCR	C16-C17-C18	-2.48	123.77	127.31
18	K	201	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
21	7	621	BCR	C33-C5-C6	-2.48	121.74	124.53
18	B	826	CLA	CMB-C2B-C3B	2.48	132.60	126.59
18	1	610	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
18	B	808	CLA	C1-C2-C3	-2.48	121.75	126.04
21	K	207	BCR	C38-C26-C27	2.48	118.38	113.62
18	8	604	CLA	C3B-C4B-NB	-2.48	108.21	110.52
18	4	612	CLA	O2D-CGD-O1D	-2.48	118.46	124.09
18	4	602	CLA	C3B-C4B-NB	-2.48	108.22	110.52
18	4	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	A	828	CLA	CBA-CAA-C2A	-2.48	109.83	114.28
18	B	809	CLA	CHC-C4B-NB	2.48	126.88	124.26
21	5	622	BCR	C21-C20-C19	-2.48	115.48	123.22
18	5	609	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
18	A	804	CLA	O2D-CGD-CBD	2.48	115.67	111.27
18	6	618	CLA	CMB-C2B-C3B	2.48	130.01	123.59
25	B	850	DGD	C3G-C2G-C1G	-2.48	105.93	111.79
18	a	612	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
18	5	610	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
26	1	617	LUT	C39-C29-C28	2.48	121.98	118.08
18	5	604	CLA	CAB-C3B-C2B	2.48	130.00	123.59
18	B	827	CLA	CMB-C2B-C3B	2.47	132.58	126.59
23	K	208	LMU	C4B-C3B-C2B	2.47	115.14	110.82
26	5	620	LUT	C21-C26-C27	-2.47	109.58	112.70
27	6	621	XAT	C39-C29-C28	2.47	121.97	118.08
18	3	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	B	808	CLA	O2D-CGD-CBD	2.47	115.65	111.27
21	J	102	BCR	C10-C11-C12	-2.47	115.52	123.22
21	7	621	BCR	C23-C24-C25	-2.47	120.27	127.20
18	1	603	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
18	5	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	7	608	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	B	825	CLA	CHB-C4A-NA	2.47	127.92	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	606	CLA	C3B-C4B-NB	-2.47	108.23	110.52
18	6	606	CLA	C3B-C4B-NB	-2.47	108.23	110.52
18	A	826	CLA	CMB-C2B-C3B	2.46	132.56	126.59
25	B	850	DGD	CFB-CEB-CDB	-2.46	101.91	114.42
21	3	620	BCR	C38-C26-C25	-2.46	121.76	124.53
18	a	606	CLA	C3B-C4B-NB	-2.46	108.23	110.52
27	1	618	XAT	C31-C30-C29	-2.46	123.80	127.31
18	1	616	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
18	B	811	CLA	CAB-C3B-C2B	2.46	129.97	123.59
18	5	606	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	a	616	CLA	C3B-C4B-NB	-2.46	108.23	110.52
18	3	607	CLA	O2D-CGD-CBD	2.46	115.64	111.27
18	A	818	CLA	CHB-C1B-NB	2.46	126.86	124.26
18	5	609	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
18	A	808	CLA	CHD-C1D-ND	-2.46	122.19	124.45
18	1	603	CLA	O2D-CGD-O1D	-2.46	118.50	124.09
18	B	807	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	3	619	XAT	C30-C31-C32	-2.46	115.55	123.22
21	B	846	BCR	C15-C16-C17	-2.46	118.44	123.47
18	8	610	CLA	CMB-C2B-C3B	2.46	132.54	126.59
21	8	621	BCR	C27-C26-C25	-2.46	119.17	122.73
18	8	616	CLA	CAB-C3B-C2B	2.45	129.95	123.59
21	B	844	BCR	C33-C5-C4	2.45	118.33	113.62
18	B	832	CLA	CHD-C1D-ND	-2.45	122.20	124.45
18	5	616	CLA	CAB-C3B-C2B	2.45	129.95	123.59
21	7	621	BCR	C8-C7-C6	-2.45	120.31	127.20
19	A	844	PQN	C2M-C2-C3	-2.45	120.40	124.40
21	B	847	BCR	C8-C7-C6	-2.45	120.32	127.20
21	K	202	BCR	C15-C16-C17	-2.45	118.45	123.47
21	3	620	BCR	C1-C6-C7	2.45	122.71	115.78
18	5	603	CLA	CHB-C1B-NB	2.45	126.85	124.26
18	7	610	CLA	CHB-C1B-NB	2.45	126.85	124.26
27	7	620	XAT	C11-C10-C9	-2.45	123.81	127.31
18	4	618	CLA	C3B-C4B-NB	-2.45	108.59	110.23
21	F	305	BCR	C35-C13-C12	2.45	121.94	118.08
18	5	613	CLA	CHC-C4B-NB	2.45	126.85	124.26
21	B	844	BCR	C16-C17-C18	-2.45	123.81	127.31
21	B	843	BCR	C30-C25-C26	-2.45	119.16	122.61
18	B	803	CLA	CHC-C1C-NC	2.45	127.92	124.20
18	6	616	CLA	O2D-CGD-CBD	2.45	115.62	111.27
18	a	611	CLA	CMB-C2B-C3B	2.45	129.93	123.59
18	L	303	CLA	CHD-C1D-ND	-2.45	122.21	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	826	CLA	CHA-C1A-NA	-2.45	120.80	126.40
18	B	835	CLA	C2A-C1A-CHA	2.45	128.14	123.86
18	A	843	CLA	C3B-C4B-NB	-2.45	108.25	110.52
21	A	849	BCR	C30-C25-C26	-2.45	119.17	122.61
18	A	831	CLA	CHC-C1C-NC	2.45	127.91	124.20
27	6	621	XAT	C10-C11-C12	-2.45	115.59	123.22
18	B	841	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	a	612	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	3	612	CLA	CHB-C1B-NB	2.44	126.84	124.26
21	A	851	BCR	C38-C26-C25	-2.44	121.78	124.53
18	B	810	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	A	815	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
18	B	803	CLA	CMB-C2B-C3B	2.44	132.50	126.59
18	a	616	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	5	622	BCR	C2-C1-C6	2.44	114.24	110.48
21	A	848	BCR	C30-C25-C26	-2.44	119.18	122.61
23	K	208	LMU	O5'-C1'-C2'	2.44	115.51	110.35
18	4	616	CLA	CMB-C2B-C3B	2.44	129.91	123.59
21	5	622	BCR	C11-C10-C9	-2.44	123.83	127.31
28	5	624	NEX	C4-C3-C2	-2.44	106.07	110.77
18	4	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	B	805	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	1	617	LUT	C7-C8-C9	-2.44	122.55	126.23
26	a	617	LUT	C39-C29-C28	2.44	121.92	118.08
21	B	844	BCR	C30-C25-C24	2.44	122.67	115.78
18	6	616	CLA	CHB-C1B-NB	2.43	126.83	124.26
18	A	809	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	A	854	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	A	817	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	A	814	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	3	603	CLA	CHC-C4B-NB	2.43	126.83	124.26
18	A	805	CLA	O2D-CGD-CBD	2.43	115.59	111.27
21	A	848	BCR	C23-C24-C25	-2.43	120.38	127.20
27	3	619	XAT	C15-C35-C34	-2.43	118.50	123.47
18	7	609	CLA	CHD-C1D-ND	-2.43	122.22	124.45
18	3	607	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	B	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	A	810	CLA	CHB-C1B-NB	2.43	126.83	124.26
18	A	810	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
25	B	850	DGD	CBB-CAB-C9B	-2.43	102.11	114.42
18	B	833	CLA	C3B-C4B-NB	-2.43	108.27	110.52
18	8	610	CLA	C3B-C4B-NB	-2.43	108.27	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	830	CLA	CMC-C2C-C1C	-2.42	121.35	125.04
21	B	845	BCR	C1-C6-C5	-2.42	119.20	122.61
18	6	610	CLA	CHB-C1B-NB	2.42	126.82	124.26
21	J	102	BCR	C29-C30-C25	2.42	114.21	110.48
18	1	611	CLA	C3B-C4B-NB	-2.42	108.27	110.52
18	a	604	CLA	CHB-C1B-NB	2.42	126.82	124.26
26	3	618	LUT	C19-C9-C8	2.42	121.90	118.08
27	1	618	XAT	C19-C9-C8	2.42	121.90	118.08
21	A	849	BCR	C8-C7-C6	-2.42	120.40	127.20
27	5	621	XAT	C31-C32-C33	-2.42	119.61	126.42
18	7	607	CLA	CAC-C3C-C4C	2.42	127.95	124.81
18	5	607	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
18	B	838	CLA	CHC-C4B-NB	2.42	126.82	124.26
21	A	856	BCR	C23-C24-C25	-2.42	120.41	127.20
20	5	625	LHG	C11-C10-C9	-2.42	102.15	114.42
18	A	826	CLA	CBA-CAA-C2A	2.42	118.63	114.28
27	3	619	XAT	C27-C28-C29	-2.42	121.78	125.53
18	B	814	CLA	CMB-C2B-C3B	2.42	132.44	126.59
26	5	620	LUT	C18-C5-C6	-2.42	121.81	124.53
18	7	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
18	5	611	CLA	CAA-C2A-C3A	-2.42	108.22	114.26
18	a	611	CLA	CAB-C3B-C2B	2.42	129.85	123.59
18	A	845	CLA	C3B-C4B-NB	-2.42	108.27	110.52
18	8	604	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
20	A	846	LHG	C20-C19-C18	-2.41	102.17	114.42
26	a	617	LUT	C30-C31-C32	-2.41	115.69	123.22
18	B	833	CLA	CAA-C2A-C1A	-2.41	104.07	111.97
21	6	622	BCR	C4-C5-C6	-2.41	119.23	122.73
21	8	621	BCR	C38-C26-C27	2.41	118.24	113.62
18	A	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	A	816	CLA	CMB-C2B-C3B	2.41	132.42	126.59
18	B	835	CLA	O2D-CGD-CBD	2.41	115.54	111.27
18	3	608	CLA	CHC-C4B-NB	2.40	126.80	124.26
18	6	603	CLA	CAB-C3B-C2B	2.40	129.82	123.59
18	B	809	CLA	CHB-C4A-NA	2.40	127.84	124.51
21	8	621	BCR	C1-C6-C5	-2.40	119.23	122.61
18	7	601	CLA	CHB-C1B-NB	2.40	126.80	124.26
18	B	828	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	5	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	B	803	CLA	C3B-C4B-NB	-2.40	108.29	110.52
20	3	623	LHG	C11-C10-C9	-2.40	102.24	114.42
18	6	608	CLA	CHB-C4A-NA	2.40	127.83	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	831	CLA	CMC-C2C-C1C	-2.40	121.39	125.04
18	B	825	CLA	O1D-CGD-CBD	2.40	129.39	124.48
23	5	628	LMU	O5'-C1'-C2'	2.40	115.42	110.35
18	3	610	CLA	CHB-C1B-NB	2.40	126.80	124.26
21	8	621	BCR	C11-C10-C9	-2.40	123.89	127.31
21	A	848	BCR	C28-C27-C26	-2.40	109.80	114.08
18	B	808	CLA	C3B-C4B-NB	-2.39	108.29	110.52
18	K	206	CLA	C3B-C4B-NB	-2.39	108.29	110.52
18	A	819	CLA	CHC-C4B-NB	2.39	126.79	124.26
23	5	628	LMU	C1'-O5'-C5'	2.39	118.39	113.69
26	5	620	LUT	C28-C29-C30	-2.39	115.27	118.94
21	3	622	BCR	C27-C26-C25	-2.39	119.26	122.73
18	A	831	CLA	CMD-C2D-C1D	-2.39	120.50	124.71
18	A	816	CLA	CHD-C1D-ND	-2.39	122.26	124.45
27	6	621	XAT	C8-C9-C10	-2.39	115.27	118.94
18	B	804	CLA	CMB-C2B-C3B	2.39	132.38	126.59
18	4	618	CLA	CMB-C2B-C3B	2.39	129.78	123.59
20	3	623	LHG	C20-C19-C18	-2.39	102.31	114.42
18	8	610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
18	4	602	CLA	O2D-CGD-CBD	2.39	115.51	111.27
18	B	810	CLA	C3B-C4B-NB	-2.39	108.30	110.52
18	4	606	CLA	CAA-C2A-C3A	-2.39	108.30	114.26
18	A	811	CLA	CHB-C1B-NB	2.38	126.78	124.26
18	8	611	CLA	CAA-C2A-C3A	-2.38	108.30	114.26
18	7	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	8	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	A	859	LMU	C4B-C3B-C2B	2.38	114.98	110.82
18	3	603	CLA	CHB-C1B-NB	2.38	126.78	124.26
18	6	614	CLA	C3B-C4B-NB	-2.38	108.31	110.52
28	6	624	NEX	C2-C1-C6	2.38	111.53	109.21
21	B	848	BCR	C35-C13-C12	2.38	121.83	118.08
18	A	840	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	B	811	CLA	CMB-C2B-C3B	2.38	129.76	123.59
18	B	821	CLA	O2D-CGD-CBD	2.38	115.50	111.27
21	6	622	BCR	C33-C5-C6	-2.38	121.86	124.53
18	A	801	CLA	CHC-C4B-NB	2.38	126.78	124.26
26	1	617	LUT	C38-C25-C24	-2.38	118.47	123.56
21	3	620	BCR	C34-C9-C10	-2.38	119.59	122.92
18	A	841	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
18	7	604	CLA	C3B-C4B-NB	-2.38	108.31	110.52
21	a	619	BCR	C8-C7-C6	-2.38	120.53	127.20
24	J	104	LMG	O2-C2-C1	-2.37	104.28	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	604	CLA	CHB-C1B-NB	2.37	126.77	124.26
21	A	856	BCR	C21-C20-C19	-2.37	115.81	123.22
21	F	305	BCR	C30-C25-C26	-2.37	119.27	122.61
18	5	604	CLA	CMB-C2B-C3B	2.37	129.74	123.59
18	K	201	CLA	C3B-C4B-NB	-2.37	108.31	110.52
24	4	624	LMG	O6-C1-O1	-2.37	104.35	109.97
18	A	814	CLA	C16-C15-C13	-2.37	108.25	115.92
18	5	608	CLA	CMB-C2B-C3B	2.37	132.34	126.59
21	B	847	BCR	C38-C26-C27	2.37	118.17	113.62
18	A	840	CLA	O2D-CGD-CBD	2.37	115.48	111.27
23	5	628	LMU	O5B-C1B-C2B	2.37	115.37	110.35
20	8	622	LHG	C5-O7-C7	-2.37	111.95	117.79
26	5	620	LUT	C39-C29-C28	2.37	121.81	118.08
18	5	617	CLA	CHC-C4B-NB	2.37	126.76	124.26
21	3	620	BCR	C38-C26-C27	2.37	118.17	113.62
21	B	844	BCR	C38-C26-C25	-2.37	121.87	124.53
18	A	827	CLA	C2D-C1D-ND	-2.37	108.36	110.10
18	6	604	CLA	O2D-CGD-CBD	2.37	115.47	111.27
18	a	601	CLA	CHB-C1B-NB	2.37	126.76	124.26
18	6	608	CLA	CMB-C2B-C3B	2.37	132.32	126.59
26	7	619	LUT	C3-C4-C5	-2.36	107.14	111.85
18	5	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
18	3	613	CLA	C1-C2-C3	-2.36	121.96	126.04
18	7	604	CLA	O2D-CGD-CBD	2.36	115.47	111.27
25	J	103	DGD	O5D-C6D-C5D	-2.36	104.67	109.05
18	K	201	CLA	CMD-C2D-C3D	2.36	133.05	127.61
18	B	809	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
18	4	604	CLA	CMB-C2B-C3B	2.36	129.71	123.59
21	A	851	BCR	C16-C15-C14	-2.36	118.64	123.47
27	3	619	XAT	O4-C5-C6	-2.36	57.00	58.96
18	1	602	CLA	O1D-CGD-CBD	2.36	129.31	124.48
26	3	618	LUT	C30-C31-C32	-2.36	115.85	123.22
18	5	607	CLA	C2D-C1D-ND	-2.36	108.37	110.10
20	4	622	LHG	C11-C10-C9	-2.36	102.45	114.42
26	1	617	LUT	C19-C9-C8	2.36	121.79	118.08
20	8	623	LHG	C11-C10-C9	-2.36	102.46	114.42
18	A	827	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	6	619	LUT	C38-C25-C24	-2.36	118.52	123.56
18	4	618	CLA	O2D-CGD-O1D	-2.36	118.74	124.09
18	5	619	CLA	CHA-C1A-NA	-2.36	121.00	126.40
20	7	622	LHG	C11-C10-C9	-2.36	102.47	114.42
18	A	839	CLA	O2A-CGA-O1A	-2.35	117.65	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	301	CLA	C2D-C1D-ND	-2.35	108.37	110.10
18	a	608	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
18	A	802	CLA	CMD-C2D-C3D	2.35	133.02	127.61
20	3	624	LHG	C20-C19-C18	-2.35	102.49	114.42
23	A	857	LMU	O5B-C5B-C4B	2.35	113.96	109.69
18	B	803	CLA	C1C-C2C-C3C	2.35	109.42	106.96
18	B	824	CLA	C2D-C1D-ND	-2.35	108.37	110.10
18	F	301	CLA	CHB-C1B-NB	2.35	126.74	124.26
21	B	843	BCR	C15-C14-C13	-2.35	123.96	127.31
18	B	833	CLA	CHD-C1D-ND	-2.35	122.30	124.45
18	8	606	CLA	CHB-C4A-NA	2.35	127.76	124.51
21	B	845	BCR	C28-C27-C26	-2.35	109.89	114.08
21	J	102	BCR	C11-C10-C9	-2.35	123.96	127.31
21	A	856	BCR	C35-C13-C12	2.35	121.77	118.08
21	A	850	BCR	C38-C26-C27	2.35	118.12	113.62
18	B	834	CLA	C2D-C1D-ND	-2.34	108.38	110.10
21	A	851	BCR	C20-C19-C18	-2.34	119.83	126.42
27	6	621	XAT	C31-C32-C33	-2.34	119.83	126.42
18	a	604	CLA	C3B-C4B-NB	-2.34	108.34	110.52
27	5	621	XAT	C8-C9-C10	-2.34	115.34	118.94
24	A	860	LMG	O3-C3-C2	-2.34	104.93	110.35
18	7	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	5	622	BCR	C34-C9-C8	2.34	121.77	118.08
21	B	801	BCR	C10-C11-C12	-2.34	115.92	123.22
18	1	606	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	a	613	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
20	A	846	LHG	C18-C17-C16	-2.34	102.56	114.42
21	F	305	BCR	C33-C5-C6	-2.34	121.90	124.53
18	5	601	CLA	C2D-C1D-ND	-2.34	108.38	110.10
18	3	613	CLA	CHC-C4B-NB	2.33	126.73	124.26
21	K	207	BCR	C15-C16-C17	-2.33	118.69	123.47
21	8	621	BCR	C24-C23-C22	-2.33	122.71	126.23
18	5	613	CLA	O2D-CGD-CBD	2.33	115.41	111.27
21	F	305	BCR	C34-C9-C8	2.33	121.75	118.08
25	J	103	DGD	C2G-O2G-C1B	2.33	123.53	117.79
18	a	601	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
18	7	604	CLA	CMB-C2B-C3B	2.33	132.23	126.59
18	A	806	CLA	CHD-C1D-ND	-2.33	122.31	124.45
18	a	609	CLA	C2A-C1A-CHA	2.33	127.93	123.86
21	3	620	BCR	C16-C15-C14	-2.33	118.70	123.47
18	8	610	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
18	6	617	CLA	CHB-C4A-NA	2.33	127.73	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	611	CLA	CMA-C3A-C2A	-2.33	110.67	116.10
21	3	622	BCR	C7-C6-C5	-2.32	115.83	121.46
18	B	805	CLA	CMB-C2B-C3B	2.32	132.22	126.59
26	a	617	LUT	C8-C7-C6	-2.32	120.68	127.20
18	K	203	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	6	610	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	A	827	CLA	CMB-C2B-C3B	2.32	132.21	126.59
18	B	822	CLA	CAA-C2A-C3A	-2.32	108.46	114.26
21	5	622	BCR	C29-C30-C25	2.32	114.05	110.48
26	5	620	LUT	C16-C1-C6	-2.32	106.54	110.30
18	8	603	CLA	CHC-C4B-NB	2.32	126.71	124.26
27	7	620	XAT	C19-C9-C8	2.32	121.73	118.08
18	4	607	CLA	C3B-C4B-NB	-2.32	108.36	110.52
18	B	807	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
18	A	835	CLA	CHD-C1D-ND	-2.32	122.32	124.45
21	4	621	BCR	C1-C6-C5	-2.32	119.35	122.61
21	A	850	BCR	C27-C26-C25	-2.32	119.37	122.73
25	J	103	DGD	C5B-C4B-C3B	-2.32	102.67	114.42
18	F	301	CLA	CHB-C4A-NA	2.32	127.71	124.51
21	K	207	BCR	C23-C24-C25	-2.32	120.70	127.20
21	B	843	BCR	C1-C6-C5	-2.31	119.35	122.61
21	7	621	BCR	C34-C9-C8	2.31	121.72	118.08
21	K	202	BCR	C10-C11-C12	-2.31	116.00	123.22
18	A	801	CLA	C2B-C1B-NB	-2.31	108.68	110.23
18	6	607	CLA	C3B-C4B-NB	-2.31	108.68	110.23
20	6	623	LHG	C18-C17-C16	-2.31	102.70	114.42
18	4	611	CLA	O2D-CGD-CBD	2.31	115.37	111.27
20	6	623	LHG	O8-C23-C24	2.31	119.15	111.91
18	B	837	CLA	CHB-C1B-NB	2.31	126.70	124.26
21	L	305	BCR	C23-C24-C25	-2.31	120.72	127.20
18	6	601	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
18	A	820	CLA	CMC-C2C-C1C	-2.31	121.53	125.04
18	3	611	CLA	CMB-C2B-C3B	2.31	129.57	123.59
18	5	604	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	A	856	BCR	C2-C1-C6	2.31	114.03	110.48
27	5	621	XAT	C28-C29-C30	-2.30	115.40	118.94
18	A	824	CLA	O2D-CGD-CBD	2.30	115.36	111.27
18	B	835	CLA	CHB-C1B-NB	2.30	126.70	124.26
24	4	624	LMG	O3-C3-C2	-2.30	105.02	110.35
18	5	607	CLA	CMC-C2C-C1C	-2.30	121.53	125.04
18	4	612	CLA	CHB-C1B-NB	2.30	126.69	124.26
21	B	843	BCR	C24-C23-C22	-2.30	122.76	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	624	NEX	C16-C1-C6	2.30	112.53	110.47
18	B	821	CLA	C3B-C4B-NB	-2.30	108.38	110.52
18	1	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
18	A	831	CLA	CMB-C2B-C3B	2.30	132.15	126.59
20	3	624	LHG	C11-C10-C9	-2.30	102.77	114.42
18	8	612	CLA	C3B-C4B-NB	-2.30	108.39	110.52
18	6	603	CLA	CMB-C2B-C3B	2.30	129.54	123.59
18	A	832	CLA	C1-C2-C3	-2.29	123.04	126.75
18	A	834	CLA	C3B-C4B-NB	-2.29	108.39	110.52
18	4	612	CLA	C3B-C4B-NB	-2.29	108.39	110.52
26	5	620	LUT	C38-C25-C24	-2.29	118.65	123.56
18	1	601	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	3	602	CLA	C3B-C4B-NB	-2.29	108.39	110.52
20	a	620	LHG	C20-C19-C18	-2.29	102.80	114.42
21	L	301	BCR	C34-C9-C10	-2.29	119.72	122.92
25	J	103	DGD	C3G-C2G-C1G	-2.29	106.37	111.79
18	1	609	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	7	608	CLA	CHB-C1B-NB	2.29	126.68	124.26
20	7	622	LHG	O8-C23-O10	-2.29	117.82	123.59
18	A	808	CLA	O2D-CGD-CBD	2.29	115.33	111.27
18	3	615	CLA	C3B-C4B-NB	-2.29	108.39	110.52
18	A	813	CLA	CMB-C2B-C3B	2.29	132.12	126.59
20	5	623	LHG	C20-C19-C18	-2.29	102.82	114.42
18	6	616	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
18	A	833	CLA	CHB-C1B-NB	2.28	126.67	124.26
21	7	621	BCR	C27-C26-C25	-2.28	119.42	122.73
18	A	817	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
18	J	101	CLA	O2D-CGD-CBD	2.28	115.32	111.27
18	B	839	CLA	C2D-C1D-ND	-2.28	108.42	110.10
18	A	825	CLA	C3B-C4B-NB	-2.28	108.40	110.52
28	5	624	NEX	C35-C34-C33	-2.28	124.06	127.31
18	B	807	CLA	CHB-C1B-NB	2.28	126.67	124.26
18	A	827	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
18	3	603	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
23	A	858	LMU	C1B-O5B-C5B	2.28	118.16	113.69
18	7	607	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	A	838	CLA	C2A-C1A-CHA	2.28	127.84	123.86
18	8	604	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	F	305	BCR	C8-C7-C6	-2.28	120.81	127.20
26	a	617	LUT	C16-C1-C6	-2.28	106.61	110.30
20	A	846	LHG	C11-C10-C9	-2.28	102.87	114.42
24	J	104	LMG	O1-C7-C8	-2.28	105.41	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	839	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	6	619	LUT	C39-C29-C28	2.28	121.66	118.08
18	1	614	CLA	CAA-C2A-C3A	-2.27	107.85	114.44
18	6	609	CLA	O2D-CGD-CBD	2.27	115.31	111.27
20	4	622	LHG	C20-C19-C18	-2.27	102.89	114.42
25	B	850	DGD	O3D-C3D-C4D	-2.27	105.10	110.35
18	B	829	CLA	C3C-C4C-NC	-2.27	108.02	110.57
21	B	847	BCR	C4-C5-C6	-2.27	119.43	122.73
18	A	815	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	1	616	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	B	815	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
18	1	603	CLA	C2A-C1A-CHA	2.27	127.83	123.86
18	B	828	CLA	CHC-C4B-NB	2.27	126.66	124.26
18	3	604	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	7	610	CLA	C1-C2-C3	-2.27	122.12	126.04
18	A	820	CLA	CHB-C1B-NB	2.27	126.66	124.26
23	8	625	LMU	C2'-C3'-C4'	2.26	114.85	109.68
26	4	619	LUT	C28-C29-C30	-2.26	115.47	118.94
18	A	835	CLA	C2D-C1D-ND	-2.26	108.44	110.10
18	4	601	CLA	O2D-CGD-CBD	2.26	115.29	111.27
27	1	618	XAT	C38-C25-C24	2.26	116.82	114.28
18	8	616	CLA	CMB-C2B-C3B	2.26	129.45	123.59
18	8	603	CLA	CMB-C2B-C3B	2.26	129.44	123.59
18	A	824	CLA	C3B-C4B-NB	-2.26	108.42	110.52
18	B	840	CLA	C3B-C4B-NB	-2.26	108.42	110.52
18	3	603	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
26	1	617	LUT	C11-C10-C9	-2.26	124.09	127.31
21	B	845	BCR	C15-C16-C17	-2.25	118.86	123.47
18	A	818	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
18	a	603	CLA	C3B-C4B-NB	-2.25	108.42	110.52
18	A	806	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
24	J	104	LMG	O6-C1-O1	-2.25	104.64	109.97
20	4	622	LHG	O8-C23-C24	2.25	118.97	111.91
18	7	611	CLA	CHC-C4B-NB	2.25	126.64	124.26
21	B	848	BCR	C20-C19-C18	-2.25	120.09	126.42
18	7	610	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
18	A	837	CLA	C2A-C1A-CHA	2.25	127.80	123.86
18	6	612	CLA	C3B-C4B-NB	-2.25	108.43	110.52
20	1	620	LHG	C20-C19-C18	-2.25	103.00	114.42
18	3	609	CLA	CMC-C2C-C1C	-2.25	121.61	125.04
20	5	625	LHG	C18-C17-C16	-2.25	103.01	114.42
18	8	612	CLA	CMB-C2B-C1B	-2.25	121.94	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	805	CLA	CHD-C1D-ND	-2.25	122.39	124.45
18	B	828	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
18	B	804	CLA	CMA-C3A-C2A	-2.25	110.86	116.10
18	A	814	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
21	B	847	BCR	C38-C26-C25	-2.25	122.01	124.53
27	1	618	XAT	C20-C13-C12	2.24	121.61	118.08
26	6	619	LUT	C16-C1-C6	-2.24	106.66	110.30
20	3	624	LHG	C18-C17-C16	-2.24	103.03	114.42
18	B	805	CLA	CHC-C4B-NB	2.24	126.63	124.26
26	1	617	LUT	C31-C30-C29	-2.24	124.11	127.31
18	5	614	CLA	C3A-C4A-CHB	-2.24	120.20	124.24
18	A	828	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
18	4	612	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
18	B	831	CLA	CMB-C2B-C3B	2.24	132.01	126.59
20	B	851	LHG	O3-C3-C2	-2.24	100.11	109.69
20	1	620	LHG	O8-C23-C24	2.24	118.94	111.91
18	A	834	CLA	O2D-CGD-CBD	2.24	115.25	111.27
26	7	619	LUT	C28-C29-C30	-2.24	115.51	118.94
18	A	815	CLA	CHD-C1D-ND	-2.24	122.40	124.45
18	A	816	CLA	C3B-C4B-NB	-2.24	108.44	110.52
18	4	607	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
26	7	619	LUT	C36-C21-C26	2.24	112.93	109.55
18	A	806	CLA	C3C-C4C-NC	-2.24	108.06	110.57
23	K	208	LMU	O5'-C5'-C4'	2.23	114.46	109.75
21	1	619	BCR	C1-C6-C5	-2.23	119.47	122.61
18	3	610	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
18	5	607	CLA	C2A-C1A-CHA	2.23	127.77	123.86
18	A	820	CLA	CHC-C1C-NC	2.23	127.59	124.20
18	A	843	CLA	CHC-C4B-NB	2.23	126.62	124.26
18	8	608	CLA	C4-C3-C5	2.23	118.53	115.98
18	B	839	CLA	CMB-C2B-C3B	2.23	131.99	126.59
26	8	619	LUT	C39-C29-C28	2.23	121.59	118.08
18	A	812	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
18	A	825	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	A	809	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
18	A	817	CLA	C3C-C4C-NC	-2.23	108.07	110.57
18	6	613	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
18	3	613	CLA	C3B-C4B-NB	-2.23	108.45	110.52
18	3	603	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	A	831	CLA	C3B-C2B-C1B	2.23	109.85	107.16
18	A	808	CLA	C3B-C4B-NB	-2.23	108.45	110.52
18	B	813	CLA	O2A-CGA-O1A	-2.23	117.97	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	816	CLA	CMB-C2B-C3B	2.23	131.98	126.59
18	B	817	CLA	CHD-C1D-ND	-2.23	122.41	124.45
27	8	620	XAT	O4-C5-C6	-2.23	57.12	58.96
18	6	616	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
18	5	612	CLA	C3B-C4B-NB	-2.22	108.45	110.52
18	A	840	CLA	CAA-CBA-CGA	-2.22	106.75	113.25
18	5	609	CLA	CHB-C1B-NB	2.22	126.61	124.26
18	4	602	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	7	621	BCR	C10-C11-C12	-2.22	116.28	123.22
18	A	820	CLA	C2D-C1D-ND	-2.22	108.47	110.10
18	5	603	CLA	CHC-C4B-NB	2.22	126.61	124.26
18	A	835	CLA	CMC-C2C-C1C	-2.22	121.66	125.04
18	A	801	CLA	C2A-C1A-CHA	2.22	127.74	123.86
21	A	851	BCR	C15-C16-C17	-2.22	118.93	123.47
27	7	620	XAT	C39-C29-C28	2.22	121.58	118.08
18	8	601	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
24	A	860	LMG	O2-C2-C1	-2.22	104.66	110.05
18	3	612	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
18	A	817	CLA	CMB-C2B-C3B	2.22	131.96	126.59
24	J	104	LMG	O3-C3-C2	-2.22	105.22	110.35
18	A	819	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
21	6	622	BCR	C24-C23-C22	-2.22	122.89	126.23
18	3	603	CLA	CMB-C2B-C3B	2.22	131.96	126.59
18	A	810	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
23	A	859	LMU	O5B-C5B-C4B	2.22	113.72	109.69
18	5	603	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
18	8	602	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	B	827	CLA	C3B-C4B-NB	-2.21	108.46	110.52
27	1	618	XAT	O24-C25-C26	-2.21	57.13	58.96
18	3	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	1	612	CLA	C2A-C1A-CHA	2.21	127.73	123.86
18	B	819	CLA	CHC-C4B-NB	2.21	126.60	124.26
18	3	609	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	B	841	CLA	C2A-C1A-CHA	2.21	127.73	123.86
18	5	603	CLA	CMB-C2B-C3B	2.21	129.32	123.59
18	6	609	CLA	CHB-C1B-NB	2.21	126.60	124.26
20	7	622	LHG	C27-C26-C25	-2.21	103.20	114.42
18	B	806	CLA	C2D-C1D-ND	-2.21	108.47	110.10
18	a	610	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	4	624	LMG	O2-C2-C1	-2.21	104.68	110.05
18	a	602	CLA	O1D-CGD-CBD	2.21	129.00	124.48
21	3	620	BCR	C33-C5-C6	-2.21	122.05	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	612	CLA	C2A-C1A-CHA	2.21	127.72	123.86
18	5	616	CLA	CMB-C2B-C3B	2.21	129.31	123.59
18	5	609	CLA	CMB-C2B-C3B	2.21	131.94	126.59
24	5	626	LMG	O6-C1-O1	-2.21	104.75	109.97
18	7	612	CLA	CHA-C1A-NA	-2.21	121.35	126.40
18	6	602	CLA	O2D-CGD-CBD	2.20	115.19	111.27
18	A	843	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
21	7	621	BCR	C38-C26-C25	-2.20	122.05	124.53
18	4	603	CLA	C2D-C1D-ND	-2.20	108.48	110.10
18	6	601	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
21	B	844	BCR	C15-C16-C17	-2.20	118.96	123.47
21	5	622	BCR	C38-C26-C27	2.20	117.85	113.62
21	J	102	BCR	C15-C16-C17	-2.20	118.97	123.47
27	5	621	XAT	C39-C29-C28	2.20	121.55	118.08
18	7	613	CLA	C2D-C1D-ND	-2.20	108.48	110.10
18	B	837	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
18	A	803	CLA	CHB-C1B-NB	2.20	126.59	124.26
18	a	604	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
18	a	604	CLA	O2D-CGD-CBD	2.20	115.18	111.27
21	K	202	BCR	C38-C26-C25	-2.20	122.06	124.53
27	7	620	XAT	O4-C5-C6	-2.20	57.14	58.96
21	A	848	BCR	C20-C19-C18	-2.20	120.24	126.42
18	B	834	CLA	C3C-C4C-NC	-2.20	108.11	110.57
18	L	302	CLA	C3B-C4B-NB	-2.20	108.48	110.52
18	A	826	CLA	CHC-C4B-NB	2.20	126.58	124.26
18	1	616	CLA	CHB-C1B-NB	2.20	126.58	124.26
18	3	604	CLA	CMB-C2B-C1B	-2.20	122.03	125.37
18	A	831	CLA	C2D-C1D-ND	-2.20	108.49	110.10
21	B	845	BCR	C3-C4-C5	-2.20	110.16	114.08
18	4	613	CLA	CHB-C1B-NB	2.20	126.58	124.26
26	6	619	LUT	C19-C9-C8	2.19	121.53	118.08
18	6	620	CLA	CAC-C3C-C4C	2.19	127.66	124.81
18	5	614	CLA	CHB-C4A-NA	2.19	127.70	124.34
18	a	614	CLA	C3B-C4B-NB	-2.19	108.48	110.52
21	L	301	BCR	C30-C25-C26	-2.19	119.53	122.61
18	A	814	CLA	C11-C10-C8	-2.19	108.83	115.92
18	6	613	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	F	303	CLA	C3B-C4B-NB	-2.19	108.48	110.52
21	5	622	BCR	C11-C12-C13	-2.19	120.26	126.42
18	8	616	CLA	CHA-C1A-NA	-2.19	121.38	126.40
18	A	822	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	1	610	CLA	CMA-C3A-C2A	-2.19	108.09	114.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	602	CLA	CHC-C4B-NB	2.19	126.58	124.26
18	B	824	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
18	A	811	CLA	O1D-CGD-CBD	2.19	128.96	124.48
26	4	619	LUT	C3-C4-C5	-2.19	107.50	111.85
21	4	621	BCR	C1-C6-C7	2.19	121.96	115.78
18	7	603	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
18	5	608	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	6	618	CLA	CAA-C2A-C3A	-2.18	108.80	114.26
18	5	609	CLA	C2A-C1A-CHA	2.18	127.68	123.86
21	4	621	BCR	C16-C15-C14	-2.18	119.00	123.47
21	8	621	BCR	C37-C22-C23	2.18	121.52	118.08
24	4	623	LMG	O1-C7-C8	-2.18	105.63	110.90
18	A	812	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	A	830	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
18	A	831	CLA	CMD-C2D-C3D	2.18	132.63	127.61
21	7	621	BCR	C16-C15-C14	-2.18	119.01	123.47
18	4	609	CLA	CMC-C2C-C3C	2.18	132.04	126.12
18	A	840	CLA	C3B-C4B-NB	-2.18	108.49	110.52
18	a	614	CLA	CHB-C4A-NA	2.18	127.68	124.34
18	A	817	CLA	C2D-C1D-ND	-2.18	108.50	110.10
21	3	621	BCR	C16-C17-C18	-2.18	124.20	127.31
26	5	620	LUT	C1-C2-C3	2.18	118.56	113.64
20	6	623	LHG	C5-O7-C7	-2.18	112.43	117.79
27	8	620	XAT	C18-C5-C4	2.18	116.73	114.28
27	1	618	XAT	C11-C10-C9	-2.18	124.20	127.31
18	3	609	CLA	CMC-C2C-C3C	2.18	132.03	126.12
21	6	622	BCR	C37-C22-C23	2.18	121.51	118.08
20	3	623	LHG	C27-C26-C25	-2.18	103.38	114.42
21	4	621	BCR	C4-C5-C6	-2.17	119.57	122.73
18	A	813	CLA	C3B-C4B-NB	-2.17	108.50	110.52
24	5	626	LMG	O3-C3-C2	-2.17	105.32	110.35
18	a	612	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	4	616	CLA	CHC-C4B-NB	2.17	126.56	124.26
18	B	828	CLA	CMB-C2B-C3B	2.17	131.85	126.59
27	a	618	XAT	O24-C25-C26	-2.17	57.16	58.96
18	5	607	CLA	CHC-C1C-NC	2.17	127.50	124.20
18	3	609	CLA	C3B-C4B-NB	-2.17	108.50	110.52
18	3	607	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	A	802	CLA	C3C-C4C-NC	-2.17	108.14	110.57
20	1	620	LHG	C27-C26-C25	-2.17	103.40	114.42
21	B	845	BCR	C29-C30-C25	2.17	113.82	110.48
21	3	622	BCR	C15-C16-C17	-2.17	119.03	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	806	CLA	C2A-C1A-CHA	2.17	127.65	123.86
18	B	841	CLA	CHA-C1A-NA	-2.17	121.43	126.40
28	6	624	NEX	C38-C25-C24	2.17	116.72	114.28
18	5	604	CLA	CHB-C1B-NB	2.17	126.55	124.26
20	3	623	LHG	C18-C17-C16	-2.17	103.41	114.42
18	B	813	CLA	C16-C15-C13	-2.17	108.91	115.92
20	5	625	LHG	C27-C26-C25	-2.17	103.42	114.42
18	B	823	CLA	CHB-C1B-NB	2.17	126.55	124.26
27	7	620	XAT	O24-C25-C26	-2.17	57.16	58.96
21	3	620	BCR	C29-C30-C25	2.17	113.82	110.48
20	B	851	LHG	C27-C26-C25	-2.17	103.43	114.42
18	B	841	CLA	O2D-CGD-CBD	2.16	115.11	111.27
18	4	612	CLA	C2A-C1A-CHA	2.16	127.64	123.86
21	B	847	BCR	C11-C12-C13	-2.16	120.34	126.42
18	4	613	CLA	CHC-C4B-NB	2.16	126.55	124.26
18	7	613	CLA	CHB-C1B-NB	2.16	126.55	124.26
18	B	817	CLA	CMB-C2B-C3B	2.16	131.83	126.59
18	A	804	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
21	B	801	BCR	C20-C19-C18	-2.16	120.34	126.42
24	5	626	LMG	O7-C10-O9	-2.16	118.47	123.70
18	5	602	CLA	C16-C15-C13	-2.16	108.93	115.92
21	A	850	BCR	C3-C4-C5	-2.16	110.22	114.08
18	5	612	CLA	CMB-C2B-C3B	2.16	131.82	126.59
18	7	613	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
20	8	623	LHG	C27-C26-C25	-2.16	103.46	114.42
18	B	806	CLA	CHA-C1A-NA	-2.16	121.45	126.40
18	A	817	CLA	CHD-C1D-ND	-2.16	122.47	124.45
18	5	608	CLA	C2A-C1A-CHA	2.16	127.64	123.86
27	a	618	XAT	C20-C13-C12	2.16	121.48	118.08
18	6	612	CLA	CHB-C1B-NB	2.16	126.54	124.26
21	A	852	BCR	C33-C5-C4	2.16	117.76	113.62
18	A	837	CLA	C3B-C4B-NB	-2.16	108.51	110.52
18	A	832	CLA	C2D-C1D-ND	-2.16	108.51	110.10
18	a	608	CLA	CHB-C1B-NB	2.16	126.54	124.26
21	6	622	BCR	C11-C12-C13	-2.16	120.36	126.42
21	1	619	BCR	C38-C26-C25	-2.16	122.11	124.53
18	8	603	CLA	O2A-CGA-O1A	-2.16	117.93	123.30
18	6	613	CLA	CHB-C1B-NB	2.16	126.54	124.26
20	1	620	LHG	C18-C17-C16	-2.15	103.48	114.42
18	A	824	CLA	C2D-C1D-ND	-2.15	108.52	110.10
18	B	825	CLA	CHB-C1B-NB	2.15	126.54	124.26
18	6	614	CLA	CHD-C1D-ND	-2.15	122.47	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	619	LUT	C15-C35-C34	-2.15	119.06	123.47
18	8	616	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
18	5	610	CLA	CMB-C2B-C3B	2.15	131.80	126.59
20	a	620	LHG	C18-C17-C16	-2.15	103.50	114.42
18	4	609	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	4	614	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	4	604	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	a	612	CLA	CMB-C2B-C3B	2.15	131.80	126.59
18	K	201	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
18	A	810	CLA	C2D-C1D-ND	-2.15	108.52	110.10
19	A	844	PQN	C14-C13-C15	-2.15	111.65	115.27
18	B	807	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	5	626	LMG	O2-C2-C1	-2.15	104.82	110.05
20	4	622	LHG	C18-C17-C16	-2.15	103.51	114.42
18	5	602	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	4	603	CLA	CMB-C2B-C3B	2.15	129.16	123.59
21	J	102	BCR	C23-C24-C25	-2.15	121.17	127.20
18	5	602	CLA	C3B-C4B-NB	-2.15	108.52	110.52
18	6	607	CLA	CHC-C1C-NC	2.15	127.46	124.20
21	A	852	BCR	C1-C6-C5	-2.15	119.59	122.61
18	A	820	CLA	O2D-CGD-CBD	2.15	115.08	111.27
20	8	623	LHG	C18-C17-C16	-2.15	103.52	114.42
18	5	616	CLA	O2A-CGA-O1A	-2.15	117.95	123.30
21	A	852	BCR	C23-C24-C25	-2.15	121.17	127.20
21	A	848	BCR	C10-C11-C12	-2.15	116.52	123.22
23	8	624	LMU	O5B-C5B-C4B	2.15	113.59	109.69
21	B	848	BCR	C34-C9-C8	2.15	121.46	118.08
21	1	619	BCR	C29-C30-C25	2.14	113.78	110.48
18	A	831	CLA	CMC-C2C-C3C	2.14	131.94	126.12
18	3	608	CLA	CHA-C4D-ND	2.14	136.98	132.50
18	7	602	CLA	CHD-C1D-ND	-2.14	122.48	124.45
18	6	604	CLA	CHC-C4B-NB	2.14	126.53	124.26
18	A	854	CLA	C6-C7-C8	-2.14	109.00	115.92
20	6	623	LHG	C27-C26-C25	-2.14	103.55	114.42
21	A	856	BCR	C7-C8-C9	-2.14	123.00	126.23
18	B	830	CLA	CBC-CAC-C3C	2.14	118.33	112.43
20	a	620	LHG	C27-C26-C25	-2.14	103.56	114.42
21	B	844	BCR	C27-C26-C25	-2.14	119.62	122.73
18	6	616	CLA	CAC-C3C-C4C	2.14	127.59	124.81
18	B	818	CLA	CMB-C2B-C3B	2.14	131.77	126.59
18	4	610	CLA	C3B-C4B-NB	-2.14	108.53	110.52
18	A	814	CLA	CMB-C2B-C3B	2.14	131.77	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	618	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	4	620	XAT	C39-C29-C28	2.14	121.44	118.08
18	B	835	CLA	CMB-C2B-C3B	2.14	131.76	126.59
18	8	601	CLA	CHC-C4B-NB	2.14	126.52	124.26
21	J	102	BCR	C34-C9-C8	2.14	121.44	118.08
18	A	814	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	A	821	CLA	CAC-C3C-C4C	2.14	127.58	124.81
21	B	844	BCR	C21-C20-C19	-2.14	116.55	123.22
18	A	814	CLA	C11-C12-C13	-2.14	109.02	115.92
18	7	610	CLA	O2D-CGD-CBD	2.14	115.06	111.27
18	3	602	CLA	CMB-C2B-C3B	2.14	131.76	126.59
18	A	830	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	5	607	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	A	810	CLA	C2A-C1A-CHA	2.13	127.59	123.86
18	7	612	CLA	O1D-CGD-CBD	2.13	128.85	124.48
18	1	606	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	4	619	LUT	C38-C25-C24	-2.13	119.00	123.56
18	A	838	CLA	C3B-C4B-NB	-2.13	108.54	110.52
18	7	608	CLA	CHC-C4B-NB	2.13	126.51	124.26
25	B	850	DGD	C5B-C4B-C3B	-2.13	103.61	114.42
28	5	624	NEX	C25-C24-C23	-2.13	108.53	112.75
18	K	203	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	F	301	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	A	840	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	4	610	CLA	C1-C2-C3	-2.13	122.36	126.04
21	7	621	BCR	C29-C30-C25	2.13	113.76	110.48
23	8	625	LMU	O1B-C4'-C3'	2.13	112.94	107.28
24	4	624	LMG	O1-C7-C8	-2.13	105.77	110.90
18	B	832	CLA	C1-C2-C3	-2.13	122.37	126.04
18	a	603	CLA	C2D-C1D-ND	-2.13	108.54	110.10
18	8	601	CLA	O2D-CGD-CBD	2.12	115.04	111.27
21	A	851	BCR	C38-C26-C27	2.12	117.70	113.62
18	5	604	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	3	618	LUT	C16-C1-C6	-2.12	106.85	110.30
26	1	617	LUT	C8-C7-C6	-2.12	121.24	127.20
24	7	624	LMG	O2-C2-C1	-2.12	104.89	110.05
18	5	612	CLA	CAA-C2A-C3A	-2.12	108.95	114.26
18	6	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
18	8	614	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
27	5	621	XAT	O4-C5-C6	-2.12	57.20	58.96
18	4	610	CLA	CMC-C2C-C1C	-2.12	121.81	125.04
18	B	802	CLA	CHB-C4A-NA	2.12	127.45	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	833	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	J	103	DGD	O2D-C2D-C1D	-2.12	104.89	110.05
21	3	622	BCR	C3-C4-C5	-2.12	110.29	114.08
18	7	606	CLA	C3B-C4B-NB	-2.12	108.55	110.52
18	A	835	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	B	833	CLA	O2D-CGD-CBD	2.12	115.03	111.27
21	8	621	BCR	C23-C24-C25	-2.12	121.25	127.20
21	A	850	BCR	C21-C20-C19	-2.12	116.61	123.22
18	6	616	CLA	C2D-C1D-ND	-2.12	108.54	110.10
21	3	621	BCR	C34-C9-C10	-2.12	119.96	122.92
18	6	602	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	6	609	CLA	CHC-C4B-NB	2.12	126.50	124.26
18	A	829	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	3	621	BCR	C31-C1-C6	-2.12	106.86	110.30
18	1	601	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	L	304	CLA	CHC-C4B-NB	2.12	126.50	124.26
21	B	801	BCR	C1-C6-C5	-2.12	119.63	122.61
20	4	622	LHG	O8-C23-O10	-2.12	118.25	123.59
21	1	619	BCR	C8-C7-C6	-2.11	121.26	127.20
18	1	614	CLA	CHB-C4A-NA	2.11	127.58	124.34
18	7	611	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	7	602	CLA	O2D-CGD-CBD	2.11	115.02	111.27
26	1	617	LUT	C12-C13-C14	-2.11	115.70	118.94
18	a	603	CLA	CBA-CAA-C2A	-2.11	110.49	114.28
27	8	620	XAT	O24-C25-C26	-2.11	57.21	58.96
18	5	617	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	4	614	CLA	C3B-C4B-NB	-2.11	108.56	110.52
18	5	607	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	3	615	CLA	CHC-C4B-NB	2.11	126.49	124.26
18	5	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	3	603	CLA	C1-C2-C3	-2.11	122.39	126.04
24	5	627	LMG	O2-C2-C1	-2.11	104.92	110.05
18	a	614	CLA	O2D-CGD-CBD	2.11	115.02	111.27
26	1	617	LUT	C21-C26-C27	-2.11	110.04	112.70
18	B	810	CLA	O1D-CGD-CBD	2.11	128.80	124.48
18	6	607	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
23	8	624	LMU	C1B-O5B-C5B	2.11	117.82	113.69
18	1	604	CLA	CMB-C2B-C3B	2.11	131.69	126.59
18	1	606	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	830	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
18	B	802	CLA	C1-C2-C3	-2.10	122.41	126.04
24	A	860	LMG	O7-C10-O9	-2.10	118.62	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	832	CLA	CHC-C4B-NB	2.10	126.48	124.26
18	8	613	CLA	C3A-C2A-C1A	2.10	104.49	101.34
18	A	807	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	a	613	CLA	C1-C2-C3	-2.10	122.41	126.04
18	6	613	CLA	C16-C15-C13	-2.10	109.12	115.92
18	a	609	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	L	302	CLA	C2A-C1A-CHA	2.10	127.53	123.86
18	4	611	CLA	CAA-C2A-C3A	-2.10	109.01	114.26
18	B	818	CLA	O2D-CGD-CBD	2.10	115.00	111.27
18	B	805	CLA	O2A-C1-C2	-2.10	103.11	108.64
27	a	618	XAT	C35-C15-C14	-2.10	119.17	123.47
18	B	811	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	8	610	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	B	824	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	8	621	BCR	C15-C16-C17	-2.10	119.17	123.47
18	8	603	CLA	CAB-C3B-C4B	-2.10	122.17	125.37
27	1	618	XAT	C12-C13-C14	-2.10	115.72	118.94
18	6	609	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
18	5	602	CLA	CMB-C2B-C3B	2.10	131.67	126.59
18	3	613	CLA	CMD-C2D-C3D	2.10	132.44	127.61
18	1	609	CLA	C2A-C1A-CHA	2.10	127.51	123.85
21	a	619	BCR	C38-C26-C27	2.10	117.64	113.62
18	A	825	CLA	O1D-CGD-CBD	2.10	128.77	124.48
18	8	611	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	B	845	BCR	C10-C11-C12	-2.10	116.68	123.22
21	6	622	BCR	C23-C24-C25	-2.10	121.32	127.20
18	B	807	CLA	O2D-CGD-CBD	2.10	114.99	111.27
21	5	622	BCR	C37-C22-C23	2.10	121.38	118.08
18	B	825	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	A	852	BCR	C15-C14-C13	-2.09	124.32	127.31
21	L	301	BCR	C21-C20-C19	-2.09	116.68	123.22
21	J	102	BCR	C36-C18-C19	2.09	121.38	118.08
18	B	832	CLA	C3B-C4B-NB	-2.09	108.57	110.52
18	6	603	CLA	CHC-C4B-NB	2.09	126.47	124.26
18	5	612	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	A	806	CLA	CHC-C1C-NC	2.09	127.37	124.20
18	a	616	CLA	C2D-C1D-ND	-2.09	108.56	110.10
18	4	606	CLA	CHC-C4B-NB	2.09	126.47	124.26
18	6	610	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
18	A	841	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	B	835	CLA	C3A-C2A-C1A	2.09	104.47	101.34
28	5	624	NEX	C30-C31-C32	-2.09	116.70	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	624	LHG	C27-C26-C25	-2.09	103.83	114.42
18	4	609	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	B	802	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	1	613	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	A	812	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
21	7	621	BCR	C1-C6-C5	-2.09	119.68	122.61
18	B	827	CLA	CHD-C1D-ND	-2.08	122.54	124.45
26	5	620	LUT	C7-C8-C9	-2.08	123.08	126.23
18	7	601	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	B	838	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	3	607	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	A	818	CLA	C3B-C4B-NB	-2.08	108.58	110.52
26	6	619	LUT	C20-C13-C12	2.08	121.36	118.08
21	A	849	BCR	C33-C5-C4	2.08	117.61	113.62
21	1	619	BCR	C38-C26-C27	2.08	117.61	113.62
18	6	612	CLA	CMB-C2B-C3B	2.08	131.63	126.59
18	B	809	CLA	C3B-C4B-NB	-2.08	108.58	110.52
18	A	854	CLA	C1-C2-C3	-2.08	122.44	126.04
18	A	840	CLA	C2A-C1A-CHA	2.08	127.50	123.86
27	8	620	XAT	C15-C35-C34	-2.08	119.22	123.47
18	5	617	CLA	C1-C2-C3	-2.08	123.39	126.75
26	5	620	LUT	C8-C7-C6	-2.08	121.36	127.20
18	B	839	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	6	601	CLA	CMB-C2B-C3B	2.08	131.62	126.59
27	5	621	XAT	O24-C25-C26	-2.08	57.24	58.96
21	K	202	BCR	C8-C7-C6	-2.08	121.37	127.20
18	B	837	CLA	CHD-C1D-ND	-2.08	122.55	124.45
23	5	628	LMU	C1B-C2B-C3B	2.08	114.32	110.00
18	A	812	CLA	C3B-C4B-NB	-2.08	108.59	110.52
21	K	207	BCR	C20-C19-C18	-2.08	120.58	126.42
28	6	624	NEX	O24-C25-C26	-2.08	57.24	58.96
18	6	606	CLA	CMB-C2B-C3B	2.07	131.61	126.59
18	A	801	CLA	CBA-CAA-C2A	-2.07	107.74	113.86
26	6	619	LUT	C31-C30-C29	-2.07	124.35	127.31
18	K	206	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
18	a	607	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
18	7	608	CLA	O2D-CGD-CBD	2.07	114.95	111.27
26	a	617	LUT	C28-C29-C30	-2.07	115.76	118.94
18	5	612	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	5	617	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	A	822	CLA	CMB-C2B-C3B	2.07	131.61	126.59
18	8	612	CLA	C2A-C1A-CHA	2.07	127.48	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	612	CLA	CBA-CAA-C2A	-2.07	108.85	113.47
26	6	619	LUT	C1-C2-C3	2.07	118.32	113.64
18	A	827	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
21	B	846	BCR	C33-C5-C4	2.07	117.59	113.62
18	A	835	CLA	CMC-C2C-C3C	2.07	131.74	126.12
18	8	607	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	7	608	CLA	C1-C2-C3	-2.07	123.40	126.75
21	5	622	BCR	C39-C30-C25	-2.07	106.94	110.30
24	4	623	LMG	O3-C3-C2	-2.07	105.57	110.35
20	A	846	LHG	C27-C26-C25	-2.07	103.93	114.42
18	A	803	CLA	C3B-C4B-NB	-2.07	108.60	110.52
18	8	602	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	3	621	BCR	C1-C6-C5	-2.07	119.70	122.61
26	8	619	LUT	C7-C8-C9	-2.06	123.11	126.23
21	7	623	BCR	C8-C7-C6	-2.06	121.40	127.20
18	B	838	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	8	616	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	5	614	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
18	4	609	CLA	CMC-C2C-C1C	-2.06	121.90	125.04
21	7	621	BCR	C4-C5-C6	-2.06	119.74	122.73
21	A	856	BCR	C36-C18-C19	2.06	121.33	118.08
18	3	603	CLA	C2D-C1D-ND	-2.06	108.58	110.10
18	1	613	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
18	1	611	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	K	203	CLA	O2D-CGD-CBD	2.06	114.93	111.27
18	5	618	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	3	612	CLA	O1D-CGD-CBD	2.06	128.70	124.48
18	8	601	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
18	6	618	CLA	CAB-C3B-C4B	-2.06	122.23	125.37
18	7	606	CLA	CAA-C2A-C3A	-2.06	109.11	114.26
18	B	806	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	6	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	A	823	CLA	CHB-C1B-NB	2.06	126.44	124.26
21	B	801	BCR	C15-C14-C13	-2.06	124.37	127.31
18	4	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	a	603	CLA	CHB-C1B-NB	2.06	126.43	124.26
21	A	849	BCR	C28-C27-C26	-2.06	110.41	114.08
18	A	825	CLA	C2D-C1D-ND	-2.06	108.59	110.10
18	6	603	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	1	617	LUT	C20-C13-C12	2.06	121.31	118.08
26	a	617	LUT	C38-C25-C24	-2.05	119.16	123.56
18	1	610	CLA	CMB-C2B-C3B	2.05	131.56	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	607	CLA	O2D-CGD-CBD	2.05	114.92	111.27
18	a	607	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	809	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	8	608	CLA	C2A-C1A-CHA	2.05	127.45	123.86
21	L	301	BCR	C10-C11-C12	-2.05	116.81	123.22
18	A	836	CLA	C2D-C1D-ND	-2.05	108.59	110.10
18	6	620	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
21	1	619	BCR	C10-C11-C12	-2.05	116.82	123.22
18	K	201	CLA	O2D-CGD-CBD	2.05	114.91	111.27
18	a	604	CLA	C2D-C1D-ND	-2.05	108.59	110.10
18	5	608	CLA	CHC-C4B-NB	2.05	126.43	124.26
18	1	611	CLA	C2A-C1A-CHA	2.05	127.44	123.86
18	4	604	CLA	CAB-C3B-C2B	2.05	128.90	123.59
19	A	844	PQN	C16-C17-C18	-2.05	109.30	115.92
20	5	623	LHG	C18-C17-C16	-2.05	104.03	114.42
18	3	603	CLA	CHA-C4D-ND	2.05	136.78	132.50
18	6	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	816	CLA	CHB-C1B-NB	2.05	126.42	124.26
27	a	618	XAT	C15-C35-C34	-2.05	119.28	123.47
18	A	837	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
18	a	608	CLA	CMB-C2B-C3B	2.05	131.55	126.59
26	6	619	LUT	C15-C14-C13	-2.05	124.39	127.31
18	3	602	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
21	B	843	BCR	C35-C13-C12	2.05	121.30	118.08
18	A	831	CLA	CHB-C4A-NA	2.05	127.34	124.51
26	8	619	LUT	C21-C26-C27	-2.05	110.11	112.70
18	a	610	CLA	CHC-C4B-NB	2.04	126.42	124.26
18	3	609	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	5	622	BCR	C24-C23-C22	-2.04	123.15	126.23
18	B	817	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	5	623	LHG	C27-C26-C25	-2.04	104.06	114.42
18	8	607	CLA	CMB-C2B-C3B	2.04	128.88	123.59
18	B	841	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
21	a	619	BCR	C38-C26-C25	-2.04	122.24	124.53
18	A	803	CLA	C2A-C1A-CHA	2.04	127.43	123.86
18	A	830	CLA	C3B-C4B-NB	-2.04	108.62	110.52
18	B	802	CLA	O1D-CGD-CBD	2.04	128.66	124.48
18	A	807	CLA	CHC-C4B-NB	2.04	126.42	124.26
18	B	803	CLA	CMC-C2C-C1C	-2.04	121.93	125.04
18	7	615	CLA	CAA-C2A-C3A	-2.04	109.17	114.26
18	A	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	A	850	BCR	C39-C30-C25	-2.04	107.00	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	619	LUT	C21-C26-C27	-2.03	110.13	112.70
21	3	620	BCR	C37-C22-C21	-2.03	120.07	122.92
21	A	849	BCR	C21-C20-C19	-2.03	116.87	123.22
18	a	604	CLA	CMB-C2B-C3B	2.03	131.51	126.59
21	A	849	BCR	C36-C18-C19	2.03	121.28	118.08
18	B	818	CLA	CHB-C1B-NB	2.03	126.41	124.26
27	6	621	XAT	C28-C29-C30	-2.03	115.82	118.94
18	A	818	CLA	CHC-C4B-NB	2.03	126.41	124.26
21	F	305	BCR	C37-C22-C21	-2.03	120.08	122.92
18	A	815	CLA	O2D-CGD-CBD	2.03	114.88	111.27
27	3	619	XAT	O24-C25-C26	-2.03	57.28	58.96
26	3	618	LUT	C15-C35-C34	-2.03	119.32	123.47
24	5	627	LMG	O3-C3-C2	-2.03	105.66	110.35
18	K	203	CLA	CHA-C1A-NA	-2.03	121.75	126.40
18	F	304	CLA	C2D-C1D-ND	-2.03	108.61	110.10
18	A	831	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	3	621	BCR	C38-C26-C25	-2.03	122.25	124.53
18	A	837	CLA	C3A-C2A-C1A	2.03	104.37	101.34
18	B	827	CLA	CHC-C4B-NB	2.03	126.40	124.26
28	5	624	NEX	C10-C11-C12	-2.03	116.89	123.22
21	A	856	BCR	C33-C5-C4	2.03	117.51	113.62
21	B	848	BCR	C33-C5-C6	-2.03	122.25	124.53
18	4	608	CLA	O2D-CGD-CBD	2.03	114.87	111.27
18	5	607	CLA	C2B-C1B-NB	2.03	111.59	110.23
18	7	604	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
18	A	826	CLA	C3B-C4B-NB	-2.03	108.64	110.52
18	4	601	CLA	CHB-C1B-NB	2.03	126.40	124.26
18	4	614	CLA	CHC-C4B-NB	2.03	126.40	124.26
19	B	842	PQN	C9-C10-C5	2.02	121.51	119.26
18	7	606	CLA	CHB-C1B-NB	2.02	126.40	124.26
18	6	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	B	850	DGD	C7B-C6B-C5B	-2.02	104.15	114.42
27	4	620	XAT	O24-C25-C26	-2.02	57.28	58.96
21	4	621	BCR	C24-C23-C22	-2.02	123.18	126.23
18	5	618	CLA	CHB-C1B-NB	2.02	126.40	124.26
19	A	844	PQN	C2M-C2-C1	2.02	119.62	116.27
18	1	612	CLA	CHC-C4B-NB	2.02	126.40	124.26
18	8	601	CLA	CHB-C1B-NB	2.02	126.40	124.26
18	1	601	CLA	CHA-C1A-NA	-2.02	121.77	126.40
18	1	604	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	4	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	B	829	CLA	O1D-CGD-CBD	2.02	128.62	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	622	LHG	C27-C26-C25	-2.02	104.17	114.42
18	1	602	CLA	CHC-C4B-NB	2.02	126.39	124.26
18	a	602	CLA	CHB-C1B-NB	2.02	126.39	124.26
18	B	815	CLA	C2A-C1A-CHA	2.02	127.39	123.86
18	A	817	CLA	CHC-C4B-NB	2.02	126.39	124.26
18	A	829	CLA	C3B-C4B-NB	-2.02	108.64	110.52
18	7	603	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	7	624	LMG	O3-C3-C2	-2.02	105.69	110.35
18	1	613	CLA	CHC-C4B-NB	2.02	126.39	124.26
18	8	601	CLA	C2D-C1D-ND	-2.02	108.62	110.10
18	8	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	A	859	LMU	O5'-C1'-C2'	2.02	113.91	110.87
18	B	813	CLA	C1-C2-C3	-2.02	122.56	126.04
18	F	301	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
18	3	607	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	4	613	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	7	610	CLA	CHD-C1D-ND	-2.01	122.60	124.45
21	8	621	BCR	C34-C9-C8	2.01	121.25	118.08
18	8	612	CLA	CHB-C1B-NB	2.01	126.39	124.26
21	7	623	BCR	C34-C9-C8	2.01	121.25	118.08
18	A	854	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	B	801	BCR	C4-C5-C6	-2.01	119.81	122.73
21	B	843	BCR	C3-C4-C5	-2.01	110.49	114.08
18	A	810	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	a	619	BCR	C3-C4-C5	-2.01	110.49	114.08
21	B	847	BCR	C27-C26-C25	-2.01	119.81	122.73
18	A	854	CLA	C2A-C1A-CHA	2.01	127.37	123.86
26	a	617	LUT	C1-C2-C3	2.01	118.18	113.64
26	a	617	LUT	C11-C10-C9	-2.01	124.44	127.31
27	a	618	XAT	C11-C10-C9	-2.01	124.44	127.31
21	7	623	BCR	C38-C26-C27	2.01	117.47	113.62
21	B	845	BCR	C1-C6-C7	2.01	121.46	115.78
18	A	820	CLA	C2A-C1A-CHA	2.01	127.37	123.86
18	5	616	CLA	CHC-C4B-NB	2.01	126.38	124.26
18	A	832	CLA	CMB-C2B-C3B	2.01	131.45	126.59
18	B	803	CLA	CMD-C2D-C3D	2.01	132.23	127.61
18	B	821	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	A	830	CLA	CMD-C2D-C1D	-2.01	121.18	124.71
24	7	624	LMG	C1-C2-C3	-2.01	105.82	110.00
18	L	302	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
18	7	613	CLA	O2A-C1-C2	-2.01	103.36	108.64
18	4	603	CLA	CAA-C2A-C3A	-2.01	107.29	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	834	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	4	623	LMG	C1-C2-C3	-2.00	105.82	110.00
18	F	304	CLA	O2D-CGD-CBD	2.00	114.83	111.27
21	J	102	BCR	C7-C8-C9	-2.00	123.21	126.23
18	B	838	CLA	C3B-C4B-NB	-2.00	108.66	110.52
18	a	608	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
24	7	624	LMG	O6-C1-O1	-2.00	105.23	109.97
25	B	850	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
18	a	609	CLA	C3B-C4B-NB	-2.00	108.66	110.52
23	5	628	LMU	C3'-C4'-C5'	2.00	115.52	110.93
25	J	103	DGD	O6D-C5D-C6D	-2.00	102.62	106.67
25	J	103	DGD	O3G-C1D-C2D	-2.00	105.18	108.30
18	A	831	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
18	B	820	CLA	O2D-CGD-CBD	2.00	114.83	111.27
18	a	613	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	J	101	CLA	C2A-C1A-CHA	2.00	127.36	123.86
24	5	626	LMG	O8-C28-O10	-2.00	118.54	123.59
18	1	601	CLA	CAA-C2A-C3A	-2.00	107.30	112.78

There are no chirality outliers.

All (2755) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	C2B-C3B-CAB-CBB
18	A	801	CLA	C4B-C3B-CAB-CBB
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C4B-C3B-CAB-CBB
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3-C5-C6-C7
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	807	CLA	C4B-C3B-CAB-CBB
18	A	812	CLA	C2-C3-C5-C6
18	A	812	CLA	C4-C3-C5-C6
18	A	814	CLA	C2-C3-C5-C6
18	A	814	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	815	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	CHA-CBD-CGD-O1D
18	A	817	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	CHA-CBD-CGD-O1D
18	A	820	CLA	CHA-CBD-CGD-O2D
18	A	821	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	C4B-C3B-CAB-CBB
18	A	823	CLA	C2B-C3B-CAB-CBB
18	A	823	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C3A-C2A-CAA-CBA
18	A	828	CLA	CHA-CBD-CGD-O1D
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	C1A-C2A-CAA-CBA
18	A	837	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	CBD-CGD-O2D-CED
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	C4B-C3B-CAB-CBB
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	842	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	CHA-CBD-CGD-O1D
18	A	845	CLA	CHA-CBD-CGD-O2D
18	A	854	CLA	C4-C3-C5-C6
18	B	802	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	CHA-CBD-CGD-O2D
18	B	802	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	802	CLA	C12-C13-C15-C16
18	B	803	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	804	CLA	CBD-CGD-O2D-CED
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C14-C13-C15-C16
18	B	807	CLA	C2B-C3B-CAB-CBB
18	B	807	CLA	C4B-C3B-CAB-CBB
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CHA-CBD-CGD-O1D
18	B	808	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	C2B-C3B-CAB-CBB
18	B	812	CLA	C4B-C3B-CAB-CBB
18	B	812	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	813	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	CBD-CGD-O2D-CED
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C2-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6
18	B	834	CLA	C2B-C3B-CAB-CBB
18	B	834	CLA	C4B-C3B-CAB-CBB
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	303	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	F	303	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	CBD-CGD-O2D-CED
18	F	304	CLA	CBD-CGD-O2D-CED
18	J	101	CLA	C1A-C2A-CAA-CBA
18	J	101	CLA	CBD-CGD-O2D-CED
18	K	201	CLA	C1A-C2A-CAA-CBA
18	K	201	CLA	C3A-C2A-CAA-CBA
18	K	201	CLA	C4B-C3B-CAB-CBB
18	K	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	CBA-CGA-O2A-C1
18	L	302	CLA	C3A-C2A-CAA-CBA
18	L	303	CLA	C2B-C3B-CAB-CBB
18	L	303	CLA	C4B-C3B-CAB-CBB
18	L	303	CLA	CHA-CBD-CGD-O1D
18	L	304	CLA	C2B-C3B-CAB-CBB
18	L	304	CLA	C4B-C3B-CAB-CBB
18	1	602	CLA	C2B-C3B-CAB-CBB
18	1	602	CLA	C4B-C3B-CAB-CBB
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	C4B-C3B-CAB-CBB
18	1	604	CLA	CAD-CBD-CGD-O1D
18	1	604	CLA	CAD-CBD-CGD-O2D
18	1	609	CLA	CBD-CGD-O2D-CED
18	1	610	CLA	C2B-C3B-CAB-CBB
18	1	612	CLA	CBD-CGD-O2D-CED
18	a	602	CLA	CBD-CGD-O2D-CED
18	a	604	CLA	CHA-CBD-CGD-O1D
18	a	604	CLA	CHA-CBD-CGD-O2D
18	a	604	CLA	CAD-CBD-CGD-O1D
18	a	604	CLA	CBD-CGD-O2D-CED
18	a	609	CLA	C1A-C2A-CAA-CBA
18	a	609	CLA	C3A-C2A-CAA-CBA
18	a	612	CLA	CBD-CGD-O2D-CED
18	a	614	CLA	C1A-C2A-CAA-CBA
18	a	614	CLA	C2B-C3B-CAB-CBB
18	a	614	CLA	C4B-C3B-CAB-CBB
18	a	614	CLA	CBD-CGD-O2D-CED
18	a	616	CLA	C4B-C3B-CAB-CBB
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	606	CLA	CHA-CBD-CGD-O2D
18	3	608	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	3	608	CLA	C4B-C3B-CAB-CBB
18	3	609	CLA	C1A-C2A-CAA-CBA
18	3	609	CLA	C3A-C2A-CAA-CBA
18	3	609	CLA	C4B-C3B-CAB-CBB
18	3	610	CLA	C1A-C2A-CAA-CBA
18	3	610	CLA	C3A-C2A-CAA-CBA
18	3	612	CLA	CBD-CGD-O2D-CED
18	3	613	CLA	C4B-C3B-CAB-CBB
18	3	614	CLA	C4B-C3B-CAB-CBB
18	3	615	CLA	C2B-C3B-CAB-CBB
18	3	615	CLA	C4B-C3B-CAB-CBB
18	3	617	CLA	C2B-C3B-CAB-CBB
18	3	617	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C1A-C2A-CAA-CBA
18	4	601	CLA	C3A-C2A-CAA-CBA
18	4	601	CLA	C4B-C3B-CAB-CBB
18	4	606	CLA	C1A-C2A-CAA-CBA
18	4	606	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C12-C13-C15-C16
18	4	611	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C3A-C2A-CAA-CBA
18	4	611	CLA	C2B-C3B-CAB-CBB
18	4	611	CLA	C4B-C3B-CAB-CBB
18	4	612	CLA	C1A-C2A-CAA-CBA
18	4	613	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	C2B-C3B-CAB-CBB
18	4	614	CLA	C4B-C3B-CAB-CBB
18	4	614	CLA	C2-C3-C5-C6
18	4	614	CLA	C4-C3-C5-C6
18	5	601	CLA	C1A-C2A-CAA-CBA
18	5	601	CLA	C4B-C3B-CAB-CBB
18	5	606	CLA	C1A-C2A-CAA-CBA
18	5	606	CLA	C3A-C2A-CAA-CBA
18	5	607	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	C1A-C2A-CAA-CBA
18	5	609	CLA	C1A-C2A-CAA-CBA
18	5	609	CLA	C3A-C2A-CAA-CBA
18	5	611	CLA	C1A-C2A-CAA-CBA
18	5	611	CLA	C3A-C2A-CAA-CBA
18	5	611	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	5	612	CLA	C1A-C2A-CAA-CBA
18	5	612	CLA	C3A-C2A-CAA-CBA
18	5	613	CLA	CHA-CBD-CGD-O1D
18	5	613	CLA	CHA-CBD-CGD-O2D
18	5	614	CLA	C1A-C2A-CAA-CBA
18	5	614	CLA	C3A-C2A-CAA-CBA
18	5	614	CLA	CBD-CGD-O2D-CED
18	5	619	CLA	C1A-C2A-CAA-CBA
18	6	601	CLA	CHA-CBD-CGD-O1D
18	6	601	CLA	CHA-CBD-CGD-O2D
18	6	604	CLA	C2B-C3B-CAB-CBB
18	6	604	CLA	C4B-C3B-CAB-CBB
18	6	606	CLA	C1A-C2A-CAA-CBA
18	6	606	CLA	C3A-C2A-CAA-CBA
18	6	607	CLA	C1A-C2A-CAA-CBA
18	6	607	CLA	C3A-C2A-CAA-CBA
18	6	607	CLA	CHA-CBD-CGD-O1D
18	6	607	CLA	CHA-CBD-CGD-O2D
18	6	608	CLA	C2-C3-C5-C6
18	6	609	CLA	C1A-C2A-CAA-CBA
18	6	609	CLA	C3A-C2A-CAA-CBA
18	6	609	CLA	C2B-C3B-CAB-CBB
18	6	609	CLA	C4B-C3B-CAB-CBB
18	6	611	CLA	C1A-C2A-CAA-CBA
18	6	611	CLA	C3A-C2A-CAA-CBA
18	6	611	CLA	C2B-C3B-CAB-CBB
18	6	611	CLA	C4B-C3B-CAB-CBB
18	6	612	CLA	C1A-C2A-CAA-CBA
18	6	612	CLA	C3A-C2A-CAA-CBA
18	6	617	CLA	CBD-CGD-O2D-CED
18	6	618	CLA	C1A-C2A-CAA-CBA
18	6	618	CLA	C3A-C2A-CAA-CBA
18	6	620	CLA	C1A-C2A-CAA-CBA
18	6	620	CLA	C2B-C3B-CAB-CBB
18	6	620	CLA	C4B-C3B-CAB-CBB
18	7	603	CLA	C2B-C3B-CAB-CBB
18	7	603	CLA	C4B-C3B-CAB-CBB
18	7	606	CLA	C1A-C2A-CAA-CBA
18	7	606	CLA	C3A-C2A-CAA-CBA
18	7	607	CLA	C1A-C2A-CAA-CBA
18	7	607	CLA	C4B-C3B-CAB-CBB
18	7	607	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	7	607	CLA	CBD-CGD-O2D-CED
18	7	608	CLA	C4B-C3B-CAB-CBB
18	7	609	CLA	C3A-C2A-CAA-CBA
18	7	610	CLA	C6-C7-C8-C10
18	7	613	CLA	C2B-C3B-CAB-CBB
18	7	613	CLA	C4B-C3B-CAB-CBB
18	7	613	CLA	CHA-CBD-CGD-O1D
18	7	613	CLA	CHA-CBD-CGD-O2D
18	7	614	CLA	C1A-C2A-CAA-CBA
18	7	614	CLA	C2B-C3B-CAB-CBB
18	7	614	CLA	C4B-C3B-CAB-CBB
18	7	615	CLA	C1A-C2A-CAA-CBA
18	7	616	CLA	CHA-CBD-CGD-O1D
18	7	616	CLA	CHA-CBD-CGD-O2D
18	7	616	CLA	CAD-CBD-CGD-O1D
18	8	601	CLA	CHA-CBD-CGD-O1D
18	8	601	CLA	CHA-CBD-CGD-O2D
18	8	602	CLA	CBD-CGD-O2D-CED
18	8	603	CLA	C2A-CAA-CBA-CGA
18	8	604	CLA	C1A-C2A-CAA-CBA
18	8	604	CLA	CBD-CGD-O2D-CED
18	8	607	CLA	C1A-C2A-CAA-CBA
18	8	607	CLA	C3A-C2A-CAA-CBA
18	8	607	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	C2B-C3B-CAB-CBB
18	8	608	CLA	C4B-C3B-CAB-CBB
18	8	608	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	C2-C3-C5-C6
18	8	608	CLA	C4-C3-C5-C6
18	8	609	CLA	C1A-C2A-CAA-CBA
18	8	609	CLA	C3A-C2A-CAA-CBA
18	8	611	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C3A-C2A-CAA-CBA
18	8	611	CLA	C2B-C3B-CAB-CBB
18	8	611	CLA	C4B-C3B-CAB-CBB
18	8	613	CLA	CHA-CBD-CGD-O1D
18	8	613	CLA	CHA-CBD-CGD-O2D
18	8	616	CLA	C1A-C2A-CAA-CBA
18	8	616	CLA	CAD-CBD-CGD-O1D
18	8	616	CLA	CAD-CBD-CGD-O2D
19	B	842	PQN	C11-C12-C13-C14
19	B	842	PQN	C19-C18-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	846	LHG	O1-C1-C2-C3
20	A	846	LHG	C3-O3-P-O4
20	A	847	LHG	C3-O3-P-O4
20	A	847	LHG	C3-O3-P-O5
20	A	847	LHG	C3-O3-P-O6
20	B	851	LHG	C4-O6-P-O5
20	1	620	LHG	C1-C2-C3-O3
20	3	623	LHG	O1-C1-C2-C3
20	3	623	LHG	C3-O3-P-O4
20	3	623	LHG	C3-O3-P-O5
20	3	623	LHG	C3-O3-P-O6
20	3	624	LHG	C3-O3-P-O5
20	3	624	LHG	C4-O6-P-O5
20	3	624	LHG	C24-C23-O8-C6
20	5	623	LHG	O1-C1-C2-C3
20	5	623	LHG	C4-O6-P-O5
20	5	625	LHG	C3-O3-P-O4
20	6	623	LHG	C3-O3-P-O4
20	7	622	LHG	C3-O3-P-O4
20	7	622	LHG	C3-O3-P-O6
20	7	622	LHG	C4-O6-P-O3
20	7	622	LHG	C4-O6-P-O4
20	7	622	LHG	C4-O6-P-O5
20	8	623	LHG	C1-C2-C3-O3
20	8	623	LHG	C2-C3-O3-P
20	8	623	LHG	C3-O3-P-O4
20	8	623	LHG	C4-O6-P-O3
20	8	623	LHG	C4-O6-P-O4
20	8	623	LHG	C4-O6-P-O5
20	8	623	LHG	O7-C5-C6-O8
21	A	848	BCR	C21-C22-C23-C24
21	A	848	BCR	C37-C22-C23-C24
21	A	851	BCR	C21-C22-C23-C24
21	A	851	BCR	C37-C22-C23-C24
21	A	852	BCR	C17-C18-C19-C20
21	A	852	BCR	C36-C18-C19-C20
21	A	856	BCR	C21-C22-C23-C24
21	A	856	BCR	C37-C22-C23-C24
21	B	843	BCR	C7-C8-C9-C10
21	B	843	BCR	C7-C8-C9-C34
21	B	844	BCR	C7-C8-C9-C34
21	B	844	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	844	BCR	C37-C22-C23-C24
21	B	844	BCR	C23-C24-C25-C30
21	B	848	BCR	C21-C22-C23-C24
21	B	848	BCR	C37-C22-C23-C24
21	J	102	BCR	C21-C22-C23-C24
21	J	102	BCR	C37-C22-C23-C24
21	K	202	BCR	C7-C8-C9-C10
21	K	202	BCR	C7-C8-C9-C34
21	K	207	BCR	C21-C22-C23-C24
21	K	207	BCR	C37-C22-C23-C24
21	L	305	BCR	C7-C8-C9-C10
21	L	305	BCR	C7-C8-C9-C34
21	3	620	BCR	C21-C22-C23-C24
21	3	620	BCR	C37-C22-C23-C24
21	3	620	BCR	C23-C24-C25-C30
21	3	622	BCR	C1-C6-C7-C8
21	3	622	BCR	C5-C6-C7-C8
21	3	622	BCR	C21-C22-C23-C24
21	3	622	BCR	C37-C22-C23-C24
21	5	622	BCR	C23-C24-C25-C30
21	8	621	BCR	C7-C8-C9-C10
21	8	621	BCR	C7-C8-C9-C34
23	K	208	LMU	O5'-C1'-O1'-C1
23	5	628	LMU	O5'-C1'-O1'-C1
23	5	628	LMU	C2-C1-O1'-C1'
24	A	860	LMG	C11-C10-O7-C8
24	J	104	LMG	C11-C10-O7-C8
25	B	850	DGD	O1B-C1B-O2G-C2G
25	B	850	DGD	O2G-C2G-C3G-O3G
25	J	103	DGD	C2B-C1B-O2G-C2G
25	J	103	DGD	O6E-C1E-O5D-C6D
26	1	617	LUT	C27-C28-C29-C39
26	a	617	LUT	C1-C6-C7-C8
26	4	619	LUT	C1-C6-C7-C8
26	5	620	LUT	C1-C6-C7-C8
26	6	619	LUT	C1-C6-C7-C8
27	5	621	XAT	C27-C28-C29-C30
27	5	621	XAT	C27-C28-C29-C39
27	6	621	XAT	O4-C6-C7-C8
18	B	822	CLA	O1D-CGD-O2D-CED
18	F	303	CLA	O1D-CGD-O2D-CED
18	7	608	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	7	616	CLA	O1D-CGD-O2D-CED
18	A	801	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	A	817	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	O1D-CGD-O2D-CED
18	J	101	CLA	O1D-CGD-O2D-CED
18	1	609	CLA	O1D-CGD-O2D-CED
18	5	607	CLA	O1D-CGD-O2D-CED
18	7	607	CLA	O1D-CGD-O2D-CED
18	8	604	CLA	O1D-CGD-O2D-CED
18	8	608	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	A	835	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
18	B	815	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED
18	B	829	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	CBD-CGD-O2D-CED
18	L	302	CLA	CBD-CGD-O2D-CED
18	1	604	CLA	CBD-CGD-O2D-CED
18	a	607	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	4	601	CLA	CBD-CGD-O2D-CED
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	607	CLA	CBD-CGD-O2D-CED
18	4	608	CLA	CBD-CGD-O2D-CED
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	611	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	614	CLA	CBD-CGD-O2D-CED
18	4	616	CLA	CBD-CGD-O2D-CED
18	5	604	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	CBD-CGD-O2D-CED
18	5	617	CLA	CBD-CGD-O2D-CED
18	6	603	CLA	CBD-CGD-O2D-CED
18	6	620	CLA	CBD-CGD-O2D-CED
18	7	602	CLA	CBD-CGD-O2D-CED
18	7	604	CLA	CBD-CGD-O2D-CED
18	7	608	CLA	CBD-CGD-O2D-CED
18	7	614	CLA	CBD-CGD-O2D-CED
18	7	616	CLA	CBD-CGD-O2D-CED
18	8	611	CLA	CBD-CGD-O2D-CED
18	8	614	CLA	CBD-CGD-O2D-CED
18	8	616	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	O1A-CGA-O2A-C1
18	8	613	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	O10-C23-O8-C6
24	J	104	LMG	O10-C28-O8-C9
23	K	208	LMU	O5B-C1B-O1B-C4'
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	B	823	CLA	O1D-CGD-O2D-CED
18	L	302	CLA	O1D-CGD-O2D-CED
18	a	607	CLA	O1D-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	4	607	CLA	O1D-CGD-O2D-CED
18	4	611	CLA	O1D-CGD-O2D-CED
18	5	608	CLA	O1D-CGD-O2D-CED
18	7	604	CLA	O1D-CGD-O2D-CED
18	B	802	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	K	201	CLA	O1D-CGD-O2D-CED
18	1	612	CLA	O1D-CGD-O2D-CED
18	a	604	CLA	O1D-CGD-O2D-CED
18	8	602	CLA	O1D-CGD-O2D-CED
18	8	611	CLA	O1D-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	838	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	K	206	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	CBD-CGD-O2D-CED
18	3	609	CLA	CBD-CGD-O2D-CED
18	4	602	CLA	CBD-CGD-O2D-CED
18	5	611	CLA	CBD-CGD-O2D-CED
18	6	602	CLA	CBD-CGD-O2D-CED
18	6	608	CLA	CBD-CGD-O2D-CED
18	6	614	CLA	CBD-CGD-O2D-CED
18	7	612	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	821	CLA	O1A-CGA-O2A-C1
18	4	609	CLA	O1A-CGA-O2A-C1
18	5	603	CLA	O1A-CGA-O2A-C1
18	7	604	CLA	O1A-CGA-O2A-C1
18	8	604	CLA	O1A-CGA-O2A-C1
20	A	847	LHG	O10-C23-O8-C6
20	B	851	LHG	O10-C23-O8-C6
18	K	204	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	O1D-CGD-O2D-CED
18	a	612	CLA	O1D-CGD-O2D-CED
18	a	614	CLA	O1D-CGD-O2D-CED
18	4	613	CLA	O1D-CGD-O2D-CED
18	5	614	CLA	O1D-CGD-O2D-CED
18	B	804	CLA	O1D-CGD-O2D-CED
18	B	812	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	a	602	CLA	O1D-CGD-O2D-CED
18	3	612	CLA	O1D-CGD-O2D-CED
18	8	607	CLA	O1D-CGD-O2D-CED
18	A	854	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	839	CLA	CBD-CGD-O2D-CED
18	1	613	CLA	CBD-CGD-O2D-CED
18	a	613	CLA	CBD-CGD-O2D-CED
18	3	604	CLA	CBD-CGD-O2D-CED
18	8	613	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	O1D-CGD-O2D-CED
20	5	625	LHG	O9-C7-O7-C5
24	J	104	LMG	O9-C10-O7-C8
25	J	103	DGD	O1B-C1B-O2G-C2G
18	3	610	CLA	O1A-CGA-O2A-C1
18	5	607	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C3-C5-C6-C7
18	A	854	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	809	CLA	C3-C5-C6-C7
18	1	611	CLA	C3-C5-C6-C7
18	3	607	CLA	C3-C5-C6-C7
18	4	604	CLA	C3-C5-C6-C7
18	5	607	CLA	C3-C5-C6-C7
18	6	603	CLA	C3-C5-C6-C7
18	6	616	CLA	C3-C5-C6-C7
18	7	613	CLA	C3-C5-C6-C7
19	A	844	PQN	C13-C15-C16-C17
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	834	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	CBA-CGA-O2A-C1
18	1	603	CLA	CBA-CGA-O2A-C1
18	a	604	CLA	CBA-CGA-O2A-C1
18	4	604	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	CBA-CGA-O2A-C1
18	5	603	CLA	CBA-CGA-O2A-C1
18	8	613	CLA	CBA-CGA-O2A-C1
20	A	847	LHG	C24-C23-O8-C6
20	B	851	LHG	C24-C23-O8-C6
18	B	803	CLA	C2C-C3C-CAC-CBC
23	A	858	LMU	O5B-C5B-C6B-O6B
25	B	850	DGD	C2B-C1B-O2G-C2G
18	4	604	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	6	617	CLA	O1D-CGD-O2D-CED
18	A	840	CLA	CBD-CGD-O2D-CED
25	J	103	DGD	C4D-C5D-C6D-O5D
23	8	624	LMU	O5B-C1B-O1B-C4'
18	5	613	CLA	C4-C3-C5-C6
18	7	601	CLA	C4-C3-C5-C6
18	8	606	CLA	C4-C3-C5-C6
18	A	854	CLA	C2-C3-C5-C6
18	7	601	CLA	C2-C3-C5-C6
18	8	606	CLA	C2-C3-C5-C6
18	A	820	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	6	604	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	K	206	CLA	C2A-CAA-CBA-CGA
18	a	616	CLA	C2A-CAA-CBA-CGA
18	4	601	CLA	C2A-CAA-CBA-CGA
18	4	607	CLA	C2A-CAA-CBA-CGA
24	4	624	LMG	O10-C28-O8-C9
18	A	835	CLA	O1D-CGD-O2D-CED
18	4	608	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	821	CLA	C3-C5-C6-C7
18	B	829	CLA	C3-C5-C6-C7
18	4	601	CLA	C3-C5-C6-C7
18	7	601	CLA	C3-C5-C6-C7
18	8	601	CLA	C3-C5-C6-C7
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBA-CGA-O2A-C1
18	B	810	CLA	CBA-CGA-O2A-C1
18	B	818	CLA	CBA-CGA-O2A-C1
18	B	831	CLA	CBA-CGA-O2A-C1
18	1	611	CLA	CBA-CGA-O2A-C1
18	3	603	CLA	CBA-CGA-O2A-C1
18	3	610	CLA	CBA-CGA-O2A-C1
18	4	613	CLA	CBA-CGA-O2A-C1
18	5	607	CLA	CBA-CGA-O2A-C1
18	6	608	CLA	CBA-CGA-O2A-C1
18	7	604	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	8	604	CLA	CBA-CGA-O2A-C1
23	A	859	LMU	C3'-C4'-O1B-C1B
25	J	103	DGD	O6D-C5D-C6D-O5D
18	A	815	CLA	O1D-CGD-O2D-CED
18	B	831	CLA	O1D-CGD-O2D-CED
18	4	614	CLA	O1D-CGD-O2D-CED
18	5	604	CLA	O1D-CGD-O2D-CED
18	7	614	CLA	O1D-CGD-O2D-CED
19	A	844	PQN	C11-C12-C13-C14
18	B	824	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	O1A-CGA-O2A-C1
18	B	818	CLA	O1A-CGA-O2A-C1
18	B	831	CLA	O1A-CGA-O2A-C1
18	4	604	CLA	O1A-CGA-O2A-C1
18	4	613	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1D-CGD-O2D-CED
18	8	616	CLA	O1D-CGD-O2D-CED
23	8	624	LMU	O5'-C5'-C6'-O6'
24	A	860	LMG	O6-C5-C6-O5
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	821	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	CBD-CGD-O2D-CED
18	A	831	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	5	613	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	O1D-CGD-O2D-CED
20	1	620	LHG	O2-C2-C3-O3
18	A	807	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	B	832	CLA	C3-C5-C6-C7
18	F	301	CLA	C3-C5-C6-C7
18	7	602	CLA	C3-C5-C6-C7
18	B	819	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	CBA-CGA-O2A-C1
18	a	614	CLA	CBA-CGA-O2A-C1
18	6	614	CLA	CBA-CGA-O2A-C1
24	J	104	LMG	C29-C28-O8-C9
24	4	623	LMG	C29-C28-O8-C9
18	A	839	CLA	O1A-CGA-O2A-C1
18	1	604	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	604	CLA	O1A-CGA-O2A-C1
18	6	608	CLA	O1A-CGA-O2A-C1
23	A	857	LMU	O5B-C5B-C6B-O6B
24	4	623	LMG	O6-C5-C6-O5
24	A	860	LMG	C4-C5-C6-O5
18	4	609	CLA	O1D-CGD-O2D-CED
18	5	617	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	C11-C10-O7-C8
18	B	829	CLA	O1D-CGD-O2D-CED
18	A	845	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	828	CLA	CBD-CGD-O2D-CED
18	6	601	CLA	CBD-CGD-O2D-CED
23	K	208	LMU	O5'-C5'-C6'-O6'
23	K	208	LMU	C4'-C5'-C6'-O6'
23	8	625	LMU	C3'-C4'-O1B-C1B
18	1	611	CLA	O1A-CGA-O2A-C1
18	B	815	CLA	O1D-CGD-O2D-CED
18	4	601	CLA	O1D-CGD-O2D-CED
18	8	603	CLA	CBD-CGD-O2D-CED
18	6	613	CLA	C3-C5-C6-C7
18	A	839	CLA	CBA-CGA-O2A-C1
18	a	614	CLA	O1A-CGA-O2A-C1
18	3	603	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C4-C3-C5-C6
18	B	818	CLA	C4-C3-C5-C6
18	8	610	CLA	C4-C3-C5-C6
24	4	623	LMG	C4-C5-C6-O5
18	A	836	CLA	C2-C3-C5-C6
18	B	818	CLA	C2-C3-C5-C6
18	8	610	CLA	C2-C3-C5-C6
18	A	843	CLA	C2A-CAA-CBA-CGA
18	K	201	CLA	C2A-CAA-CBA-CGA
18	5	616	CLA	C2A-CAA-CBA-CGA
18	8	616	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	O1D-CGD-O2D-CED
18	6	620	CLA	O1D-CGD-O2D-CED
18	8	614	CLA	O1D-CGD-O2D-CED
23	8	625	LMU	O5B-C5B-C6B-O6B
18	B	819	CLA	O1A-CGA-O2A-C1
24	4	623	LMG	O10-C28-O8-C9
24	7	624	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	C24-C23-O8-C6
20	8	622	LHG	C24-C23-O8-C6
18	B	821	CLA	O1D-CGD-O2D-CED
23	A	858	LMU	C4B-C5B-C6B-O6B
18	4	616	CLA	O1D-CGD-O2D-CED
18	6	603	CLA	O1D-CGD-O2D-CED
18	6	614	CLA	O1A-CGA-O2A-C1
23	A	857	LMU	C4B-C5B-C6B-O6B
18	A	818	CLA	O1D-CGD-O2D-CED
18	B	819	CLA	O1D-CGD-O2D-CED
18	B	833	CLA	O1D-CGD-O2D-CED
18	K	206	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	3	609	CLA	O1D-CGD-O2D-CED
18	7	602	CLA	O1D-CGD-O2D-CED
18	7	612	CLA	O1D-CGD-O2D-CED
18	6	608	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C1-C2-C3-O3
20	A	847	LHG	C1-C2-C3-O3
23	8	625	LMU	C4B-C5B-C6B-O6B
18	A	801	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	811	CLA	O1A-CGA-O2A-C1
18	B	833	CLA	C3-C5-C6-C7
18	A	835	CLA	CBA-CGA-O2A-C1
18	A	843	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	CBA-CGA-O2A-C1
18	a	613	CLA	CBA-CGA-O2A-C1
18	4	614	CLA	CBA-CGA-O2A-C1
18	6	604	CLA	CBA-CGA-O2A-C1
18	6	616	CLA	CBA-CGA-O2A-C1
18	7	613	CLA	CBA-CGA-O2A-C1
20	7	622	LHG	C24-C23-O8-C6
24	4	624	LMG	C29-C28-O8-C9
24	7	624	LMG	C29-C28-O8-C9
18	4	603	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	803	CLA	C4C-C3C-CAC-CBC
23	5	628	LMU	O5B-C1B-O1B-C4'
18	A	814	CLA	C13-C15-C16-C17
18	4	601	CLA	C15-C16-C17-C18
23	K	208	LMU	O1'-C1-C2-C3
18	6	614	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	C15-C16-C17-C18
18	B	828	CLA	C13-C15-C16-C17
19	B	842	PQN	C25-C26-C27-C28
20	A	846	LHG	O2-C2-C3-O3
20	8	623	LHG	O2-C2-C3-O3
18	A	841	CLA	C3-C5-C6-C7
20	6	623	LHG	C23-C24-C25-C26
23	5	628	LMU	C2'-C1'-O1'-C1
24	J	104	LMG	C2-C1-O1-C7
24	7	624	LMG	C2-C1-O1-C7
24	4	624	LMG	O7-C8-C9-O8
20	B	851	LHG	C29-C30-C31-C32
18	A	835	CLA	O1A-CGA-O2A-C1
18	4	614	CLA	O1A-CGA-O2A-C1
24	5	626	LMG	O10-C28-O8-C9
18	5	613	CLA	C2-C3-C5-C6
18	A	829	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C12-C13-C14
18	B	818	CLA	C6-C7-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	6	604	CLA	C6-C7-C8-C9
18	B	818	CLA	O1D-CGD-O2D-CED
18	6	602	CLA	O1D-CGD-O2D-CED
18	7	611	CLA	C10-C11-C12-C13
18	A	821	CLA	C2A-CAA-CBA-CGA
18	A	854	CLA	C2A-CAA-CBA-CGA
18	3	609	CLA	C2A-CAA-CBA-CGA
18	5	609	CLA	C2A-CAA-CBA-CGA
21	B	801	BCR	C37-C22-C23-C24
21	B	847	BCR	C37-C22-C23-C24
21	J	102	BCR	C11-C12-C13-C35
21	J	102	BCR	C36-C18-C19-C20
21	K	202	BCR	C37-C22-C23-C24
21	L	305	BCR	C36-C18-C19-C20
21	6	622	BCR	C11-C12-C13-C35
27	8	620	XAT	C27-C28-C29-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	6	624	NEX	C11-C12-C13-C20
21	J	102	BCR	C17-C18-C19-C20
21	K	202	BCR	C21-C22-C23-C24
23	8	624	LMU	O5B-C5B-C6B-O6B
20	5	625	LHG	C8-C7-O7-C5
20	B	851	LHG	C23-C24-C25-C26
20	7	622	LHG	C23-C24-C25-C26
18	A	843	CLA	O1A-CGA-O2A-C1
18	a	613	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	C15-C16-C17-C18
18	A	811	CLA	C5-C6-C7-C8
18	B	825	CLA	C10-C11-C12-C13
18	B	837	CLA	C15-C16-C17-C18
18	a	613	CLA	C10-C11-C12-C13
18	3	607	CLA	C5-C6-C7-C8
18	5	602	CLA	C10-C11-C12-C13
18	A	824	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	O6-C5-C6-O5
23	8	624	LMU	C4'-C5'-C6'-O6'
18	1	601	CLA	CBA-CGA-O2A-C1
18	5	604	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	C13-C15-C16-C17
18	a	601	CLA	C5-C6-C7-C8
18	a	603	CLA	C5-C6-C7-C8
18	3	604	CLA	C5-C6-C7-C8
18	5	607	CLA	C8-C10-C11-C12
18	6	601	CLA	C15-C16-C17-C18
18	7	601	CLA	C5-C6-C7-C8
19	A	844	PQN	C18-C20-C21-C22
20	4	622	LHG	C23-C24-C25-C26
20	5	623	LHG	C23-C24-C25-C26
18	A	813	CLA	O1D-CGD-O2D-CED
18	6	616	CLA	O1A-CGA-O2A-C1
24	J	104	LMG	O6-C5-C6-O5
18	A	804	CLA	C13-C15-C16-C17
18	A	806	CLA	C5-C6-C7-C8
18	A	812	CLA	C8-C10-C11-C12
18	A	834	CLA	C10-C11-C12-C13
18	B	833	CLA	C5-C6-C7-C8
18	B	833	CLA	C13-C15-C16-C17
18	1	603	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	1	613	CLA	C10-C11-C12-C13
18	3	609	CLA	C5-C6-C7-C8
18	3	609	CLA	C10-C11-C12-C13
18	4	601	CLA	C13-C15-C16-C17
18	5	602	CLA	C8-C10-C11-C12
18	5	603	CLA	C5-C6-C7-C8
18	5	604	CLA	C5-C6-C7-C8
18	5	609	CLA	C15-C16-C17-C18
18	6	601	CLA	C5-C6-C7-C8
18	6	613	CLA	C5-C6-C7-C8
18	L	304	CLA	O1D-CGD-O2D-CED
20	3	623	LHG	O1-C1-C2-O2
20	5	623	LHG	O1-C1-C2-O2
20	7	622	LHG	O1-C1-C2-O2
18	6	604	CLA	O1A-CGA-O2A-C1
20	3	623	LHG	C7-C8-C9-C10
20	5	625	LHG	C23-C24-C25-C26
24	7	624	LMG	C10-C11-C12-C13
25	B	850	DGD	C1B-C2B-C3B-C4B
18	K	204	CLA	CBD-CGD-O2D-CED
18	L	303	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	C15-C16-C17-C18
18	B	806	CLA	C5-C6-C7-C8
18	1	601	CLA	C5-C6-C7-C8
18	3	610	CLA	C13-C15-C16-C17
18	5	604	CLA	C13-C15-C16-C17
18	6	616	CLA	C10-C11-C12-C13
18	7	610	CLA	C5-C6-C7-C8
18	B	803	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	838	CLA	O1D-CGD-O2D-CED
23	8	625	LMU	O5'-C5'-C6'-O6'
18	A	843	CLA	C2-C1-O2A-CGA
18	A	812	CLA	C15-C16-C17-C18
18	A	836	CLA	C13-C15-C16-C17
18	B	824	CLA	C10-C11-C12-C13
18	B	831	CLA	C15-C16-C17-C18
18	1	611	CLA	C8-C10-C11-C12
18	A	833	CLA	CBD-CGD-O2D-CED
18	A	841	CLA	CBD-CGD-O2D-CED
18	a	609	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C13-C15-C16-C17
18	B	827	CLA	C13-C15-C16-C17
18	B	824	CLA	C13-C15-C16-C17
18	6	610	CLA	C15-C16-C17-C18
18	8	601	CLA	C8-C10-C11-C12
18	B	806	CLA	O1D-CGD-O2D-CED
18	8	613	CLA	O1D-CGD-O2D-CED
18	a	609	CLA	C11-C12-C13-C15
18	8	613	CLA	C11-C10-C8-C7
18	8	610	CLA	C3-C5-C6-C7
18	7	613	CLA	O1A-CGA-O2A-C1
18	3	613	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	4	613	CLA	C2A-CAA-CBA-CGA
18	1	613	CLA	O1D-CGD-O2D-CED
18	4	602	CLA	O1D-CGD-O2D-CED
18	5	611	CLA	O1D-CGD-O2D-CED
18	B	808	CLA	C5-C6-C7-C8
18	B	814	CLA	C8-C10-C11-C12
18	6	613	CLA	C10-C11-C12-C13
18	6	614	CLA	C5-C6-C7-C8
18	8	601	CLA	C13-C15-C16-C17
18	8	606	CLA	C8-C10-C11-C12
18	B	824	CLA	O1A-CGA-O2A-C1
18	6	604	CLA	C5-C6-C7-C8
18	7	613	CLA	C15-C16-C17-C18
18	a	613	CLA	O1D-CGD-O2D-CED
20	A	847	LHG	O2-C2-C3-O3
20	6	623	LHG	O2-C2-C3-O3
24	A	860	LMG	O9-C10-O7-C8
18	A	806	CLA	C13-C15-C16-C17
18	A	812	CLA	C13-C15-C16-C17
18	B	834	CLA	C8-C10-C11-C12
18	B	837	CLA	C5-C6-C7-C8
18	A	808	CLA	CBA-CGA-O2A-C1
20	4	622	LHG	C24-C23-O8-C6
18	A	854	CLA	O1D-CGD-O2D-CED
18	B	839	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	1	601	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	5	604	CLA	O1A-CGA-O2A-C1
20	8	622	LHG	O10-C23-O8-C6
18	A	807	CLA	C15-C16-C17-C18
18	A	812	CLA	C5-C6-C7-C8
18	A	830	CLA	C8-C10-C11-C12
18	B	814	CLA	C13-C15-C16-C17
18	K	203	CLA	C5-C6-C7-C8
18	3	609	CLA	C8-C10-C11-C12
18	6	601	CLA	C13-C15-C16-C17
18	7	611	CLA	C5-C6-C7-C8
18	7	613	CLA	C13-C15-C16-C17
18	8	613	CLA	C15-C16-C17-C18
18	A	842	CLA	C10-C11-C12-C13
18	B	805	CLA	C13-C15-C16-C17
18	B	813	CLA	C5-C6-C7-C8
18	5	601	CLA	C5-C6-C7-C8
18	5	609	CLA	C13-C15-C16-C17
18	6	613	CLA	C15-C16-C17-C18
18	6	616	CLA	C13-C15-C16-C17
20	a	620	LHG	C3-O3-P-O6
20	5	625	LHG	C3-O3-P-O6
20	6	623	LHG	C3-O3-P-O6
20	8	622	LHG	C4-O6-P-O3
20	8	623	LHG	C3-O3-P-O6
24	5	627	LMG	C10-C11-C12-C13
18	A	825	CLA	C3-C5-C6-C7
18	5	603	CLA	C3-C5-C6-C7
18	A	838	CLA	CBA-CGA-O2A-C1
18	1	613	CLA	CBA-CGA-O2A-C1
18	A	840	CLA	O1D-CGD-O2D-CED
24	5	627	LMG	C28-C29-C30-C31
18	B	817	CLA	O1D-CGD-O2D-CED
18	3	604	CLA	O1D-CGD-O2D-CED
18	B	829	CLA	C4-C3-C5-C6
18	A	828	CLA	CAA-CBA-CGA-O2A
18	a	609	CLA	C8-C10-C11-C12
18	3	602	CLA	C8-C10-C11-C12
18	B	830	CLA	C2C-C3C-CAC-CBC
18	A	818	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C2A-CAA-CBA-CGA
18	A	801	CLA	C3-C5-C6-C7
18	1	603	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	841	CLA	C5-C6-C7-C8
18	B	802	CLA	C10-C11-C12-C13
20	3	624	LHG	C26-C27-C28-C29
20	3	624	LHG	C33-C34-C35-C36
20	8	623	LHG	C32-C33-C34-C35
20	6	623	LHG	C8-C7-O7-C5
24	4	623	LMG	C11-C10-O7-C8
18	5	613	CLA	C2A-CAA-CBA-CGA
20	A	846	LHG	C32-C33-C34-C35
20	5	625	LHG	C15-C16-C17-C18
20	8	622	LHG	C11-C10-C9-C8
20	8	622	LHG	C31-C32-C33-C34
25	J	103	DGD	C3A-C4A-C5A-C6A
18	A	822	CLA	C16-C17-C18-C20
18	B	809	CLA	C16-C17-C18-C19
18	B	826	CLA	C6-C7-C8-C10
18	1	603	CLA	C6-C7-C8-C9
18	5	613	CLA	C16-C17-C18-C20
18	7	601	CLA	C11-C12-C13-C15
18	7	602	CLA	C16-C17-C18-C20
18	B	809	CLA	CBA-CGA-O2A-C1
20	1	620	LHG	C25-C26-C27-C28
20	5	625	LHG	C13-C14-C15-C16
20	8	623	LHG	C15-C16-C17-C18
23	8	625	LMU	C2-C3-C4-C5
25	J	103	DGD	C6A-C7A-C8A-C9A
25	J	103	DGD	C4B-C5B-C6B-C7B
18	A	827	CLA	CBD-CGD-O2D-CED
20	A	846	LHG	C31-C32-C33-C34
20	3	623	LHG	C11-C10-C9-C8
20	5	623	LHG	C16-C17-C18-C19
20	6	623	LHG	C27-C28-C29-C30
24	J	104	LMG	C31-C32-C33-C34
24	5	626	LMG	C30-C31-C32-C33
18	A	820	CLA	O1D-CGD-O2D-CED
18	6	604	CLA	O1D-CGD-O2D-CED
20	8	622	LHG	C2-C3-O3-P
20	5	623	LHG	C12-C13-C14-C15
20	5	625	LHG	C30-C31-C32-C33
24	A	860	LMG	C17-C18-C19-C20
24	J	104	LMG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	809	CLA	O1D-CGD-O2D-CED
20	3	623	LHG	O2-C2-C3-O3
20	1	620	LHG	C23-C24-C25-C26
18	A	830	CLA	O1D-CGD-O2D-CED
23	A	859	LMU	O5'-C1'-O1'-C1
23	8	624	LMU	C2'-C1'-O1'-C1
25	J	103	DGD	C2D-C1D-O3G-C3G
18	a	609	CLA	CBA-CGA-O2A-C1
24	5	626	LMG	C29-C28-O8-C9
20	3	624	LHG	C12-C13-C14-C15
18	5	613	CLA	C10-C11-C12-C13
18	B	805	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C20
18	a	609	CLA	C16-C17-C18-C20
18	4	602	CLA	C11-C12-C13-C14
18	5	603	CLA	C6-C7-C8-C10
18	A	809	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	C4-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
20	3	624	LHG	C28-C29-C30-C31
20	8	623	LHG	C10-C11-C12-C13
20	8	623	LHG	C27-C28-C29-C30
23	8	625	LMU	C7-C8-C9-C10
25	J	103	DGD	C5B-C6B-C7B-C8B
18	A	807	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C10-C8-C9
18	K	203	CLA	C11-C10-C8-C9
18	4	608	CLA	C11-C12-C13-C14
18	A	843	CLA	C8-C10-C11-C12
20	1	620	LHG	C27-C28-C29-C30
20	3	624	LHG	C24-C25-C26-C27
20	5	623	LHG	C15-C16-C17-C18
20	8	622	LHG	C32-C33-C34-C35
23	A	858	LMU	C6-C7-C8-C9
24	5	627	LMG	C32-C33-C34-C35
25	B	850	DGD	C6A-C7A-C8A-C9A
25	J	103	DGD	C7A-C8A-C9A-CAA
25	J	103	DGD	C3B-C4B-C5B-C6B
18	A	820	CLA	C15-C16-C17-C18
18	A	854	CLA	C8-C10-C11-C12
18	A	822	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	820	CLA	C2A-CAA-CBA-CGA
18	1	604	CLA	C2A-CAA-CBA-CGA
18	a	609	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	C2A-CAA-CBA-CGA
18	4	608	CLA	C2A-CAA-CBA-CGA
18	5	608	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O1A-CGA-O2A-C1
21	L	305	BCR	C37-C22-C23-C24
20	A	847	LHG	C11-C10-C9-C8
20	3	624	LHG	C9-C10-C11-C12
20	6	623	LHG	C31-C32-C33-C34
25	J	103	DGD	C4A-C5A-C6A-C7A
25	J	103	DGD	C9A-CAA-CBA-CCA
20	4	622	LHG	O1-C1-C2-C3
20	5	625	LHG	O1-C1-C2-C3
20	7	622	LHG	O1-C1-C2-C3
21	B	801	BCR	C21-C22-C23-C24
21	B	844	BCR	C7-C8-C9-C10
21	L	305	BCR	C21-C22-C23-C24
18	A	814	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	827	CLA	C3-C5-C6-C7
20	A	846	LHG	O9-C7-O7-C5
18	B	818	CLA	C5-C6-C7-C8
24	A	860	LMG	C11-C12-C13-C14
24	4	623	LMG	C17-C18-C19-C20
24	5	626	LMG	C16-C17-C18-C19
24	5	626	LMG	C28-C29-C30-C31
20	3	623	LHG	C29-C30-C31-C32
20	5	625	LHG	C34-C35-C36-C37
20	8	622	LHG	C28-C29-C30-C31
20	8	623	LHG	C14-C15-C16-C17
24	A	860	LMG	C32-C33-C34-C35
24	5	626	LMG	C32-C33-C34-C35
24	5	627	LMG	C17-C18-C19-C20
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	836	CLA	C4B-C3B-CAB-CBB
18	A	839	CLA	C4B-C3B-CAB-CBB
18	B	802	CLA	C4B-C3B-CAB-CBB
18	B	819	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	821	CLA	C4B-C3B-CAB-CBB
18	B	830	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C4B-C3B-CAB-CBB
18	F	301	CLA	C4B-C3B-CAB-CBB
18	J	101	CLA	C4B-C3B-CAB-CBB
18	K	203	CLA	C4B-C3B-CAB-CBB
18	K	204	CLA	C4B-C3B-CAB-CBB
18	K	206	CLA	C4B-C3B-CAB-CBB
18	L	302	CLA	C4B-C3B-CAB-CBB
18	1	606	CLA	C4B-C3B-CAB-CBB
18	1	608	CLA	C4B-C3B-CAB-CBB
18	1	610	CLA	C4B-C3B-CAB-CBB
18	a	610	CLA	C4B-C3B-CAB-CBB
18	a	613	CLA	C4B-C3B-CAB-CBB
18	5	613	CLA	C4B-C3B-CAB-CBB
18	5	614	CLA	C4B-C3B-CAB-CBB
18	5	617	CLA	C4B-C3B-CAB-CBB
18	6	613	CLA	C4B-C3B-CAB-CBB
18	7	602	CLA	C4B-C3B-CAB-CBB
18	8	601	CLA	C4B-C3B-CAB-CBB
18	8	602	CLA	C4B-C3B-CAB-CBB
18	8	613	CLA	C4B-C3B-CAB-CBB
18	B	809	CLA	C16-C17-C18-C20
18	B	816	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C10
18	B	832	CLA	C11-C12-C13-C14
18	B	832	CLA	C11-C12-C13-C15
18	1	603	CLA	C6-C7-C8-C10
18	1	611	CLA	C16-C17-C18-C19
23	8	624	LMU	O5'-C1'-O1'-C1
25	J	103	DGD	O6D-C1D-O3G-C3G
18	A	836	CLA	C8-C10-C11-C12
20	3	623	LHG	C28-C29-C30-C31
20	5	623	LHG	C11-C12-C13-C14
20	5	625	LHG	C27-C28-C29-C30
20	8	623	LHG	C17-C18-C19-C20
24	7	624	LMG	C30-C31-C32-C33
18	A	831	CLA	O1D-CGD-O2D-CED
18	B	828	CLA	O1D-CGD-O2D-CED
20	a	620	LHG	C27-C28-C29-C30
20	8	622	LHG	C18-C19-C20-C21
20	8	622	LHG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	8	623	LHG	C33-C34-C35-C36
23	8	624	LMU	C4-C5-C6-C7
24	7	624	LMG	C17-C18-C19-C20
20	A	847	LHG	C23-C24-C25-C26
20	3	623	LHG	C17-C18-C19-C20
20	4	622	LHG	C29-C30-C31-C32
20	8	622	LHG	C33-C34-C35-C36
24	4	624	LMG	C32-C33-C34-C35
18	B	824	CLA	O1D-CGD-O2D-CED
25	B	850	DGD	O6E-C5E-C6E-O5E
20	7	622	LHG	C29-C30-C31-C32
18	A	828	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	F	301	CLA	C3A-C2A-CAA-CBA
18	a	606	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	5	601	CLA	C3A-C2A-CAA-CBA
18	5	619	CLA	C3A-C2A-CAA-CBA
18	6	616	CLA	C3A-C2A-CAA-CBA
18	7	615	CLA	CBD-CGD-O2D-CED
18	8	616	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	C13-C15-C16-C17
18	B	828	CLA	C8-C10-C11-C12
18	3	602	CLA	C10-C11-C12-C13
23	A	857	LMU	C2-C1-O1'-C1'
23	8	625	LMU	C2-C1-O1'-C1'
20	A	846	LHG	C25-C26-C27-C28
24	7	624	LMG	C20-C21-C22-C23
25	B	850	DGD	CEB-CFB-CGB-CHB
18	1	613	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	1	611	CLA	C16-C17-C18-C20
18	a	609	CLA	C16-C17-C18-C19
18	5	613	CLA	C16-C17-C18-C19
18	7	601	CLA	C11-C12-C13-C14
20	B	851	LHG	C24-C25-C26-C27
18	5	613	CLA	O1D-CGD-O2D-CED
20	5	623	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	610	CLA	C5-C6-C7-C8
18	4	610	CLA	C10-C11-C12-C13
18	4	613	CLA	C13-C15-C16-C17
18	3	608	CLA	C4-C3-C5-C6
19	B	842	PQN	C14-C13-C15-C16
18	4	601	CLA	CBA-CGA-O2A-C1
18	3	608	CLA	C2-C3-C5-C6
20	A	846	LHG	O1-C1-C2-O2
20	4	622	LHG	O1-C1-C2-O2
20	5	625	LHG	O1-C1-C2-O2
23	A	858	LMU	C3'-C4'-O1B-C1B
23	A	858	LMU	C5'-C4'-O1B-C1B
24	4	623	LMG	C16-C17-C18-C19
24	5	626	LMG	C15-C16-C17-C18
18	7	611	CLA	C3-C5-C6-C7
18	A	838	CLA	O1A-CGA-O2A-C1
24	A	860	LMG	C10-C11-C12-C13
18	A	822	CLA	C16-C17-C18-C19
18	B	826	CLA	C6-C7-C8-C9
23	8	625	LMU	C11-C10-C9-C8
18	A	804	CLA	C2B-C3B-CAB-CBB
18	A	807	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	815	CLA	C2B-C3B-CAB-CBB
18	A	821	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	836	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	A	839	CLA	C2B-C3B-CAB-CBB
18	A	841	CLA	C2B-C3B-CAB-CBB
18	A	842	CLA	C2B-C3B-CAB-CBB
18	B	802	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	821	CLA	C2B-C3B-CAB-CBB
18	B	830	CLA	C2B-C3B-CAB-CBB
18	B	840	CLA	C2B-C3B-CAB-CBB
18	F	301	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	J	101	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	K	203	CLA	C2B-C3B-CAB-CBB
18	K	204	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	K	206	CLA	C2B-C3B-CAB-CBB
18	L	302	CLA	C2B-C3B-CAB-CBB
18	1	603	CLA	C2B-C3B-CAB-CBB
18	1	608	CLA	C2B-C3B-CAB-CBB
18	1	613	CLA	C2B-C3B-CAB-CBB
18	a	610	CLA	C2B-C3B-CAB-CBB
18	a	613	CLA	C2B-C3B-CAB-CBB
18	a	616	CLA	C2B-C3B-CAB-CBB
18	3	609	CLA	C2B-C3B-CAB-CBB
18	3	610	CLA	C2B-C3B-CAB-CBB
18	3	613	CLA	C2B-C3B-CAB-CBB
18	3	614	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	5	601	CLA	C2B-C3B-CAB-CBB
18	5	611	CLA	C2B-C3B-CAB-CBB
18	5	613	CLA	C2B-C3B-CAB-CBB
18	5	614	CLA	C2B-C3B-CAB-CBB
18	5	617	CLA	C2B-C3B-CAB-CBB
18	7	601	CLA	C2B-C3B-CAB-CBB
18	7	602	CLA	C2B-C3B-CAB-CBB
18	7	607	CLA	C2B-C3B-CAB-CBB
18	7	608	CLA	C2B-C3B-CAB-CBB
18	8	601	CLA	C2B-C3B-CAB-CBB
18	8	602	CLA	C2B-C3B-CAB-CBB
18	8	613	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C3-C5-C6-C7
20	A	846	LHG	C17-C18-C19-C20
20	8	623	LHG	C29-C30-C31-C32
18	B	813	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	C13-C15-C16-C17
18	6	613	CLA	C8-C10-C11-C12
18	6	601	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	C14-C15-C16-C17
20	3	623	LHG	C30-C31-C32-C33
23	K	208	LMU	C5-C6-C7-C8
18	B	810	CLA	C10-C11-C12-C13
18	B	809	CLA	O1A-CGA-O2A-C1
24	7	624	LMG	O10-C28-O8-C9
20	4	622	LHG	C12-C13-C14-C15
18	5	603	CLA	C6-C7-C8-C9
18	A	806	CLA	C3-C5-C6-C7
18	4	614	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	848	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	851	BCR	C23-C24-C25-C26
21	A	851	BCR	C23-C24-C25-C30
21	A	856	BCR	C1-C6-C7-C8
21	A	856	BCR	C5-C6-C7-C8
21	A	856	BCR	C23-C24-C25-C26
21	A	856	BCR	C23-C24-C25-C30
21	B	843	BCR	C1-C6-C7-C8
21	B	843	BCR	C5-C6-C7-C8
21	B	844	BCR	C23-C24-C25-C26
21	B	848	BCR	C5-C6-C7-C8
21	L	301	BCR	C1-C6-C7-C8
21	L	301	BCR	C5-C6-C7-C8
21	L	305	BCR	C5-C6-C7-C8
21	L	305	BCR	C23-C24-C25-C26
21	L	305	BCR	C23-C24-C25-C30
21	3	620	BCR	C23-C24-C25-C26
21	5	622	BCR	C23-C24-C25-C26
21	6	622	BCR	C23-C24-C25-C26
21	6	622	BCR	C23-C24-C25-C30
21	8	621	BCR	C1-C6-C7-C8
21	8	621	BCR	C5-C6-C7-C8
26	1	617	LUT	C1-C6-C7-C8
26	1	617	LUT	C5-C6-C7-C8
26	a	617	LUT	C5-C6-C7-C8
26	4	619	LUT	C5-C6-C7-C8
26	5	620	LUT	C5-C6-C7-C8
26	6	619	LUT	C5-C6-C7-C8
26	8	619	LUT	C1-C6-C7-C8
26	8	619	LUT	C5-C6-C7-C8
24	4	624	LMG	O6-C5-C6-O5
20	3	623	LHG	C9-C10-C11-C12
20	5	625	LHG	C14-C15-C16-C17
20	5	625	LHG	C32-C33-C34-C35
23	8	624	LMU	O1'-C1-C2-C3
20	6	623	LHG	C24-C23-O8-C6
24	5	627	LMG	C29-C28-O8-C9
18	B	809	CLA	C10-C11-C12-C13
18	B	827	CLA	C5-C6-C7-C8
18	4	608	CLA	C5-C6-C7-C8
18	8	613	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	8	623	LHG	C8-C7-O7-C5
18	a	609	CLA	O1A-CGA-O2A-C1
24	5	626	LMG	C17-C18-C19-C20
23	A	858	LMU	C1-C2-C3-C4
18	A	825	CLA	C13-C15-C16-C17
18	5	613	CLA	C13-C15-C16-C17
20	A	846	LHG	C13-C14-C15-C16
20	4	622	LHG	C31-C32-C33-C34
18	B	808	CLA	C4-C3-C5-C6
18	A	826	CLA	C11-C10-C8-C7
18	A	828	CLA	C11-C10-C8-C7
18	A	836	CLA	C11-C12-C13-C15
18	B	803	CLA	C11-C10-C8-C7
18	B	808	CLA	C2-C3-C5-C6
18	B	809	CLA	C12-C13-C15-C16
18	B	814	CLA	C2-C3-C5-C6
18	B	818	CLA	C6-C7-C8-C10
18	B	832	CLA	C2-C3-C5-C6
18	K	203	CLA	C11-C10-C8-C7
18	4	608	CLA	C11-C12-C13-C15
18	4	608	CLA	C12-C13-C15-C16
18	6	614	CLA	C11-C10-C8-C7
18	8	613	CLA	C12-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C25
18	4	601	CLA	O1A-CGA-O2A-C1
18	B	830	CLA	C4C-C3C-CAC-CBC
20	A	846	LHG	C27-C28-C29-C30
18	8	606	CLA	C13-C15-C16-C17
24	5	626	LMG	O9-C10-O7-C8
18	A	804	CLA	CBA-CGA-O2A-C1
18	A	807	CLA	CBA-CGA-O2A-C1
18	8	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
18	6	610	CLA	C2A-CAA-CBA-CGA
18	A	825	CLA	C8-C10-C11-C12
18	B	829	CLA	C10-C11-C12-C13
18	5	607	CLA	C5-C6-C7-C8
18	6	616	CLA	C15-C16-C17-C18
18	A	826	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	8	623	LHG	C25-C26-C27-C28
23	A	857	LMU	O5B-C1B-O1B-C4'
18	A	845	CLA	O1D-CGD-O2D-CED
20	3	624	LHG	C31-C32-C33-C34
23	K	208	LMU	C4-C5-C6-C7
18	B	816	CLA	O1D-CGD-O2D-CED
18	B	838	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	C8-C10-C11-C12
18	A	806	CLA	C15-C16-C17-C18
20	4	622	LHG	C32-C33-C34-C35
20	B	851	LHG	C8-C7-O7-C5
20	8	622	LHG	C8-C7-O7-C5
24	7	624	LMG	C11-C10-O7-C8
20	8	622	LHG	C25-C26-C27-C28
18	4	601	CLA	C5-C6-C7-C8
18	B	841	CLA	CBD-CGD-O2D-CED
20	6	623	LHG	O9-C7-O7-C5
20	8	622	LHG	O9-C7-O7-C5
20	8	623	LHG	O9-C7-O7-C5
24	4	623	LMG	O9-C10-O7-C8
18	B	818	CLA	C3-C5-C6-C7
20	5	623	LHG	C13-C14-C15-C16
23	A	859	LMU	C3-C4-C5-C6
24	5	627	LMG	C30-C31-C32-C33
25	J	103	DGD	C2E-C1E-O5D-C6D
20	A	846	LHG	O7-C5-C6-O8
24	5	626	LMG	O1-C7-C8-O7
23	5	628	LMU	O5'-C5'-C6'-O6'
18	A	843	CLA	C5-C6-C7-C8
20	5	623	LHG	C30-C31-C32-C33
25	B	850	DGD	C4A-C5A-C6A-C7A
18	B	814	CLA	C15-C16-C17-C18
24	7	624	LMG	C18-C19-C20-C21
18	8	603	CLA	O1D-CGD-O2D-CED
18	B	832	CLA	C4-C3-C5-C6
18	B	807	CLA	C2-C3-C5-C6
18	B	829	CLA	C2-C3-C5-C6
20	A	846	LHG	C30-C31-C32-C33
18	A	809	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	836	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	802	CLA	C11-C10-C8-C9
18	B	805	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	a	609	CLA	C11-C12-C13-C14
18	4	608	CLA	C14-C13-C15-C16
18	5	604	CLA	C6-C7-C8-C9
18	5	604	CLA	C11-C10-C8-C9
18	6	614	CLA	C11-C10-C8-C9
18	8	602	CLA	C11-C10-C8-C9
19	A	844	PQN	C21-C22-C23-C24
18	B	811	CLA	C3-C5-C6-C7
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	1	616	CLA	C2A-CAA-CBA-CGA
18	5	602	CLA	C2A-CAA-CBA-CGA
18	8	602	CLA	C2A-CAA-CBA-CGA
20	4	622	LHG	C13-C14-C15-C16
20	5	625	LHG	C29-C30-C31-C32
24	A	860	LMG	C16-C17-C18-C19
25	J	103	DGD	CEA-CFA-CGA-CHA
26	a	617	LUT	C27-C28-C29-C39
18	A	804	CLA	O1A-CGA-O2A-C1
20	A	846	LHG	O10-C23-O8-C6
18	A	809	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	811	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	828	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
18	L	302	CLA	C1A-C2A-CAA-CBA
18	L	303	CLA	C1A-C2A-CAA-CBA
18	1	602	CLA	C1A-C2A-CAA-CBA
18	1	616	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	606	CLA	C1A-C2A-CAA-CBA
18	a	610	CLA	C1A-C2A-CAA-CBA
18	3	607	CLA	C1A-C2A-CAA-CBA
18	4	610	CLA	C1A-C2A-CAA-CBA
18	4	616	CLA	C1A-C2A-CAA-CBA
18	5	610	CLA	C1A-C2A-CAA-CBA
18	5	617	CLA	C1A-C2A-CAA-CBA
18	6	610	CLA	C1A-C2A-CAA-CBA
18	6	616	CLA	C1A-C2A-CAA-CBA
18	7	609	CLA	C1A-C2A-CAA-CBA
18	8	614	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	C11-C12-C13-C15
20	A	846	LHG	C8-C7-O7-C5
18	7	611	CLA	C2-C3-C5-C6
21	A	849	BCR	C9-C10-C11-C12
18	B	803	CLA	C8-C10-C11-C12
18	B	803	CLA	C10-C11-C12-C13
20	B	851	LHG	C4-O6-P-O3
20	3	623	LHG	C24-C25-C26-C27
18	A	834	CLA	C3-C5-C6-C7
23	5	628	LMU	C4B-C5B-C6B-O6B
24	4	624	LMG	C17-C18-C19-C20
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	C5-C6-C7-C8
20	7	622	LHG	O6-C4-C5-C6
23	8	625	LMU	C1-C2-C3-C4
18	7	602	CLA	C16-C17-C18-C19
18	A	836	CLA	C15-C16-C17-C18
20	6	623	LHG	C7-C8-C9-C10
24	J	104	LMG	C28-C29-C30-C31
18	F	303	CLA	C3A-C2A-CAA-CBA
18	4	612	CLA	C3A-C2A-CAA-CBA
18	7	607	CLA	C3A-C2A-CAA-CBA
20	3	624	LHG	C11-C10-C9-C8
18	B	829	CLA	C13-C15-C16-C17
18	3	607	CLA	O1A-CGA-O2A-C1
24	J	104	LMG	C30-C31-C32-C33
18	a	608	CLA	C2A-CAA-CBA-CGA
18	6	616	CLA	C2A-CAA-CBA-CGA
18	7	610	CLA	C3-C5-C6-C7
20	A	846	LHG	C4-C5-C6-O8
20	A	846	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	5	623	LHG	C29-C30-C31-C32
20	6	623	LHG	C4-C5-C6-O8
20	8	623	LHG	C4-C5-C6-O8
24	J	104	LMG	O1-C7-C8-C9
24	5	626	LMG	O1-C7-C8-C9
24	5	626	LMG	C31-C32-C33-C34
24	7	624	LMG	C7-C8-C9-O8
25	J	103	DGD	O1G-C1G-C2G-C3G
24	4	623	LMG	C8-C7-O1-C1
20	1	620	LHG	C31-C32-C33-C34
20	a	620	LHG	C25-C26-C27-C28
18	a	609	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	C13-C15-C16-C17
18	5	604	CLA	C15-C16-C17-C18
20	5	623	LHG	C35-C36-C37-C38
20	8	622	LHG	C17-C18-C19-C20
24	4	623	LMG	C33-C34-C35-C36
18	A	819	CLA	C10-C11-C12-C13
20	3	623	LHG	C15-C16-C17-C18
24	4	624	LMG	C15-C16-C17-C18
24	J	104	LMG	O6-C1-O1-C7
18	A	822	CLA	C15-C16-C17-C18
20	7	622	LHG	C25-C26-C27-C28
23	5	628	LMU	C4-C5-C6-C7
18	A	843	CLA	C15-C16-C17-C18
23	A	859	LMU	C2'-C1'-O1'-C1
20	B	851	LHG	C11-C10-C9-C8
20	6	623	LHG	C32-C33-C34-C35
20	B	851	LHG	C27-C28-C29-C30
18	4	603	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	C10-C11-C12-C13
18	3	613	CLA	C2A-CAA-CBA-CGA
18	A	807	CLA	C4-C3-C5-C6
18	A	820	CLA	C4-C3-C5-C6
18	8	613	CLA	C16-C17-C18-C20
18	B	802	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	3	604	CLA	CBA-CGA-O2A-C1
18	7	601	CLA	CBA-CGA-O2A-C1
20	5	625	LHG	C24-C23-O8-C6
18	A	843	CLA	C13-C15-C16-C17
18	8	613	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	8	614	CLA	C5-C6-C7-C8
18	B	817	CLA	C11-C12-C13-C14
25	J	103	DGD	C3G-C2G-O2G-C1B
18	B	816	CLA	C2A-CAA-CBA-CGA
18	B	829	CLA	C2A-CAA-CBA-CGA
18	4	604	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	CAA-CBA-CGA-O2A
23	5	628	LMU	C3'-C4'-O1B-C1B
25	B	850	DGD	C8A-C9A-CAA-CBA
18	L	303	CLA	O1D-CGD-O2D-CED
20	4	622	LHG	C27-C28-C29-C30
20	8	623	LHG	C9-C10-C11-C12
24	5	627	LMG	C13-C14-C15-C16
18	A	815	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	O6-C4-C5-O7
18	K	204	CLA	O1D-CGD-O2D-CED
18	5	607	CLA	C16-C17-C18-C19
18	5	607	CLA	C16-C17-C18-C20
20	B	851	LHG	C10-C11-C12-C13
18	8	602	CLA	O1A-CGA-O2A-C1
18	a	609	CLA	C3-C5-C6-C7
20	A	846	LHG	C23-C24-C25-C26
18	A	804	CLA	C15-C16-C17-C18
18	A	818	CLA	C10-C11-C12-C13
18	B	806	CLA	C13-C15-C16-C17
20	6	623	LHG	O7-C5-C6-O8
20	3	624	LHG	C16-C17-C18-C19
20	4	622	LHG	C30-C31-C32-C33
23	K	208	LMU	C3-C4-C5-C6
24	5	626	LMG	C11-C12-C13-C14
24	J	104	LMG	C18-C19-C20-C21
24	5	626	LMG	C12-C13-C14-C15
18	A	826	CLA	C2-C1-O2A-CGA
18	5	613	CLA	C2-C1-O2A-CGA
25	B	850	DGD	C7B-C8B-C9B-CAB
18	A	804	CLA	C12-C13-C15-C16
18	A	809	CLA	C11-C12-C13-C15
18	A	809	CLA	C12-C13-C15-C16
18	A	814	CLA	C11-C10-C8-C7
18	A	825	CLA	C6-C7-C8-C10
18	A	825	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	830	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	805	CLA	C11-C12-C13-C15
18	B	806	CLA	C11-C12-C13-C15
18	B	806	CLA	C12-C13-C15-C16
18	B	828	CLA	C12-C13-C15-C16
18	B	834	CLA	C6-C7-C8-C10
18	B	834	CLA	C11-C10-C8-C7
18	B	840	CLA	C6-C7-C8-C10
18	1	613	CLA	C6-C7-C8-C10
18	a	609	CLA	C12-C13-C15-C16
18	a	613	CLA	C6-C7-C8-C10
18	5	604	CLA	C11-C10-C8-C7
18	6	604	CLA	C6-C7-C8-C10
18	6	613	CLA	C11-C10-C8-C7
18	6	616	CLA	C6-C7-C8-C10
18	7	602	CLA	C11-C10-C8-C7
18	8	602	CLA	C11-C10-C8-C7
19	A	844	PQN	C21-C22-C23-C25
19	B	842	PQN	C17-C18-C20-C21
18	3	609	CLA	C3-C5-C6-C7
24	A	860	LMG	O10-C28-O8-C9
18	A	803	CLA	C14-C13-C15-C16
18	A	809	CLA	C11-C12-C13-C14
18	A	811	CLA	C11-C10-C8-C9
18	A	814	CLA	C11-C10-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	825	CLA	C6-C7-C8-C9
18	A	825	CLA	C11-C12-C13-C14
18	A	826	CLA	C14-C13-C15-C16
18	A	830	CLA	C6-C7-C8-C9
18	A	831	CLA	C14-C13-C15-C16
18	A	836	CLA	C11-C10-C8-C9
18	A	841	CLA	C11-C10-C8-C9
18	A	854	CLA	C14-C13-C15-C16
18	B	802	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	806	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C14
18	B	817	CLA	C6-C7-C8-C9
18	B	828	CLA	C11-C10-C8-C9
18	B	834	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	837	CLA	C14-C13-C15-C16
18	1	613	CLA	C6-C7-C8-C9
18	a	609	CLA	C14-C13-C15-C16
18	a	610	CLA	C11-C10-C8-C9
18	a	613	CLA	C6-C7-C8-C9
18	4	608	CLA	C11-C10-C8-C9
18	4	613	CLA	C11-C10-C8-C9
18	4	614	CLA	C6-C7-C8-C9
18	5	607	CLA	C14-C13-C15-C16
18	5	609	CLA	C11-C10-C8-C9
18	6	604	CLA	C11-C12-C13-C14
18	6	613	CLA	C6-C7-C8-C9
18	7	602	CLA	C6-C7-C8-C9
18	8	601	CLA	C11-C12-C13-C14
18	8	613	CLA	C14-C13-C15-C16
27	1	618	XAT	C29-C30-C31-C32
18	K	203	CLA	CBA-CGA-O2A-C1
18	a	601	CLA	CBA-CGA-O2A-C1
18	8	601	CLA	CBA-CGA-O2A-C1
18	8	614	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C2A-CAA-CBA-CGA
18	6	602	CLA	C2A-CAA-CBA-CGA
18	7	601	CLA	O1A-CGA-O2A-C1
21	4	621	BCR	C36-C18-C19-C20
18	A	842	CLA	C16-C17-C18-C20
18	a	603	CLA	C6-C7-C8-C9
20	A	847	LHG	O1-C1-C2-C3
18	A	841	CLA	O1D-CGD-O2D-CED
20	6	623	LHG	C12-C13-C14-C15
24	A	860	LMG	C33-C34-C35-C36
18	B	825	CLA	C3-C5-C6-C7
18	A	833	CLA	O1D-CGD-O2D-CED
18	B	817	CLA	C8-C10-C11-C12
20	A	846	LHG	C14-C15-C16-C17
18	B	825	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
23	8	624	LMU	C1-C2-C3-C4
20	1	620	LHG	C28-C29-C30-C31
20	5	625	LHG	C9-C10-C11-C12
18	B	836	CLA	CBD-CGD-O2D-CED
20	5	623	LHG	C11-C10-C9-C8
18	A	811	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	815	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	843	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	B	806	CLA	C4B-C3B-CAB-CBB
18	B	808	CLA	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	820	CLA	C4B-C3B-CAB-CBB
18	B	824	CLA	C4B-C3B-CAB-CBB
18	B	825	CLA	C4B-C3B-CAB-CBB
18	B	833	CLA	C4B-C3B-CAB-CBB
18	B	839	CLA	C4B-C3B-CAB-CBB
18	B	841	CLA	C4B-C3B-CAB-CBB
18	F	304	CLA	C4B-C3B-CAB-CBB
18	1	601	CLA	C4B-C3B-CAB-CBB
18	1	607	CLA	C4B-C3B-CAB-CBB
18	1	613	CLA	C4B-C3B-CAB-CBB
18	a	602	CLA	C4B-C3B-CAB-CBB
18	a	603	CLA	C4B-C3B-CAB-CBB
18	a	606	CLA	C4B-C3B-CAB-CBB
18	3	604	CLA	C4B-C3B-CAB-CBB
18	3	606	CLA	C4B-C3B-CAB-CBB
18	3	610	CLA	C4B-C3B-CAB-CBB
18	4	607	CLA	C4B-C3B-CAB-CBB
18	4	613	CLA	C4B-C3B-CAB-CBB
18	5	607	CLA	C4B-C3B-CAB-CBB
18	6	602	CLA	C4B-C3B-CAB-CBB
18	6	614	CLA	C4B-C3B-CAB-CBB
18	6	617	CLA	C4B-C3B-CAB-CBB
18	7	601	CLA	C4B-C3B-CAB-CBB
18	8	609	CLA	C4B-C3B-CAB-CBB
18	8	614	CLA	C4B-C3B-CAB-CBB
18	8	613	CLA	C16-C17-C18-C19
20	A	847	LHG	O6-C4-C5-C6
20	5	625	LHG	O6-C4-C5-C6
20	8	623	LHG	O6-C4-C5-C6
18	A	828	CLA	C15-C16-C17-C18
18	A	839	CLA	C5-C6-C7-C8
18	6	604	CLA	C10-C11-C12-C13
18	A	820	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	609	CLA	C14-C13-C15-C16
20	A	846	LHG	C34-C35-C36-C37
18	B	824	CLA	C16-C17-C18-C19
20	A	847	LHG	C10-C11-C12-C13
25	J	103	DGD	C2B-C3B-C4B-C5B
18	8	606	CLA	C15-C16-C17-C18
18	A	827	CLA	O1D-CGD-O2D-CED
18	5	604	CLA	C2A-CAA-CBA-CGA
18	7	611	CLA	C2A-CAA-CBA-CGA
18	A	810	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	837	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	1	606	CLA	CBD-CGD-O2D-CED
18	a	606	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	C3A-C2A-CAA-CBA
18	5	616	CLA	CBD-CGD-O2D-CED
18	8	604	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C8-C10-C11-C12
18	K	203	CLA	C15-C16-C17-C18
20	a	620	LHG	C31-C32-C33-C34
27	a	618	XAT	C29-C30-C31-C32
23	A	858	LMU	C2-C1-O1'-C1'
20	1	620	LHG	C35-C36-C37-C38
20	8	622	LHG	C9-C10-C11-C12
25	B	850	DGD	C4B-C5B-C6B-C7B
18	B	808	CLA	C15-C16-C17-C18
20	3	623	LHG	C16-C17-C18-C19
25	J	103	DGD	CFA-CGA-CHA-CIA
18	B	818	CLA	C8-C10-C11-C12
24	4	624	LMG	C7-C8-C9-O8
24	5	626	LMG	C7-C8-C9-O8
24	5	627	LMG	C7-C8-C9-O8
25	B	850	DGD	O1G-C1G-C2G-C3G
25	B	850	DGD	C1G-C2G-C3G-O3G
23	8	625	LMU	C4'-C5'-C6'-O6'
24	A	860	LMG	C18-C19-C20-C21
24	4	624	LMG	C33-C34-C35-C36
24	5	626	LMG	C18-C19-C20-C21
18	4	613	CLA	C15-C16-C17-C18
20	a	620	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C3-C5-C6-C7
18	A	822	CLA	C4-C3-C5-C6
24	7	624	LMG	C29-C30-C31-C32
20	6	623	LHG	C11-C10-C9-C8
20	6	623	LHG	C30-C31-C32-C33
18	A	806	CLA	C10-C11-C12-C13
20	A	846	LHG	C4-O6-P-O3
18	A	815	CLA	O1A-CGA-O2A-C1
18	a	601	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	C2A-CAA-CBA-CGA
18	a	614	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C13-C15-C16-C17
18	B	808	CLA	C8-C10-C11-C12
18	4	613	CLA	C10-C11-C12-C13
20	5	625	LHG	O6-C4-C5-O7
23	A	857	LMU	C1-C2-C3-C4
18	A	832	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	CBA-CGA-O2A-C1
20	4	622	LHG	C35-C36-C37-C38
18	B	817	CLA	O1A-CGA-O2A-C1
18	3	604	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	C16-C17-C18-C20
18	A	807	CLA	C10-C11-C12-C13
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	811	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C2B-C3B-CAB-CBB
18	B	806	CLA	C2B-C3B-CAB-CBB
18	B	808	CLA	C2B-C3B-CAB-CBB
18	B	820	CLA	C2B-C3B-CAB-CBB
18	B	825	CLA	C2B-C3B-CAB-CBB
18	B	833	CLA	C2B-C3B-CAB-CBB
18	B	841	CLA	C2B-C3B-CAB-CBB
18	F	304	CLA	C2B-C3B-CAB-CBB
18	1	601	CLA	C2B-C3B-CAB-CBB
18	1	606	CLA	C2B-C3B-CAB-CBB
18	1	607	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
18	4	613	CLA	C2B-C3B-CAB-CBB
18	6	602	CLA	C2B-C3B-CAB-CBB
18	6	613	CLA	C2B-C3B-CAB-CBB
18	6	614	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	8	609	CLA	C2B-C3B-CAB-CBB
18	8	614	CLA	C2B-C3B-CAB-CBB
20	A	847	LHG	C24-C25-C26-C27
23	A	859	LMU	C4-C5-C6-C7
18	6	604	CLA	C13-C15-C16-C17
18	B	802	CLA	O1A-CGA-O2A-C1
18	K	203	CLA	O1A-CGA-O2A-C1
20	A	847	LHG	C11-C12-C13-C14
18	a	603	CLA	C6-C7-C8-C10
18	A	819	CLA	C11-C12-C13-C14
20	6	623	LHG	C10-C11-C12-C13
24	4	624	LMG	O6-C1-O1-C7
18	7	613	CLA	CBD-CGD-O2D-CED
20	8	622	LHG	C11-C12-C13-C14
18	A	826	CLA	C4-C3-C5-C6
18	A	827	CLA	C2-C1-O2A-CGA
18	A	835	CLA	C2-C1-O2A-CGA
18	B	839	CLA	C2-C1-O2A-CGA
18	5	609	CLA	C2-C1-O2A-CGA
18	B	824	CLA	C15-C16-C17-C18
18	A	804	CLA	C11-C12-C13-C14
18	A	811	CLA	C6-C7-C8-C9
18	A	820	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C10-C8-C9
18	A	843	CLA	C14-C13-C15-C16
18	B	802	CLA	C14-C13-C15-C16
18	B	814	CLA	C14-C13-C15-C16
18	B	833	CLA	C11-C10-C8-C9
18	4	601	CLA	C11-C12-C13-C14
18	4	604	CLA	C6-C7-C8-C9
18	7	601	CLA	C6-C7-C8-C9
18	7	602	CLA	C11-C10-C8-C9
18	7	610	CLA	C6-C7-C8-C9
18	8	601	CLA	C14-C13-C15-C16
24	4	623	LMG	C18-C19-C20-C21
18	A	854	CLA	C5-C6-C7-C8
18	1	611	CLA	C5-C6-C7-C8
18	a	613	CLA	C5-C6-C7-C8
23	A	857	LMU	C7-C8-C9-C10
18	8	613	CLA	C2A-CAA-CBA-CGA
18	A	842	CLA	C16-C17-C18-C19
21	B	848	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	K	207	BCR	C5-C6-C7-C8
21	L	305	BCR	C1-C6-C7-C8
21	3	621	BCR	C23-C24-C25-C26
21	7	621	BCR	C23-C24-C25-C26
21	7	621	BCR	C23-C24-C25-C30
21	7	623	BCR	C1-C6-C7-C8
21	7	623	BCR	C5-C6-C7-C8
21	8	621	BCR	C23-C24-C25-C26
21	8	621	BCR	C23-C24-C25-C30
26	3	618	LUT	C1-C6-C7-C8
26	3	618	LUT	C5-C6-C7-C8
26	7	619	LUT	C1-C6-C7-C8
18	5	607	CLA	C15-C16-C17-C18
20	5	623	LHG	C27-C28-C29-C30
18	3	612	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	C1A-C2A-CAA-CBA
18	3	615	CLA	C1A-C2A-CAA-CBA
18	8	612	CLA	C1A-C2A-CAA-CBA
21	L	305	BCR	C17-C18-C19-C20
21	6	622	BCR	C11-C12-C13-C14
26	1	617	LUT	C27-C28-C29-C30
18	6	610	CLA	C8-C10-C11-C12
18	B	838	CLA	O1D-CGD-O2D-CED
18	A	831	CLA	C8-C10-C11-C12
18	B	814	CLA	C5-C6-C7-C8
18	6	604	CLA	C8-C10-C11-C12
18	8	601	CLA	O1A-CGA-O2A-C1
18	8	614	CLA	O1A-CGA-O2A-C1
20	A	846	LHG	O6-C4-C5-C6
18	A	804	CLA	C11-C12-C13-C15
18	A	811	CLA	C6-C7-C8-C10
18	A	811	CLA	C11-C10-C8-C7
18	A	811	CLA	C11-C12-C13-C15
18	A	820	CLA	C6-C7-C8-C10
18	A	820	CLA	C11-C10-C8-C7
18	A	825	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	A	836	CLA	C11-C10-C8-C7
18	A	841	CLA	C11-C10-C8-C7
18	A	843	CLA	C12-C13-C15-C16
18	A	854	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	802	CLA	C6-C7-C8-C10
18	B	805	CLA	C12-C13-C15-C16
18	B	808	CLA	C11-C12-C13-C15
18	B	808	CLA	C12-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C10-C8-C7
18	B	813	CLA	C11-C12-C13-C15
18	B	814	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	827	CLA	C12-C13-C15-C16
18	B	828	CLA	C11-C10-C8-C7
18	B	831	CLA	C12-C13-C15-C16
18	B	833	CLA	C11-C10-C8-C7
18	B	837	CLA	C12-C13-C15-C16
18	a	610	CLA	C11-C10-C8-C7
18	4	601	CLA	C11-C12-C13-C15
18	4	604	CLA	C6-C7-C8-C10
18	4	608	CLA	C11-C10-C8-C7
18	4	610	CLA	C6-C7-C8-C10
18	4	613	CLA	C6-C7-C8-C10
18	4	613	CLA	C11-C10-C8-C7
18	4	614	CLA	C6-C7-C8-C10
18	5	604	CLA	C12-C13-C15-C16
18	5	607	CLA	C12-C13-C15-C16
18	5	609	CLA	C11-C10-C8-C7
18	6	601	CLA	C12-C13-C15-C16
18	6	604	CLA	C11-C12-C13-C15
18	7	602	CLA	C6-C7-C8-C10
18	8	601	CLA	C11-C12-C13-C15
18	8	614	CLA	C6-C7-C8-C10
20	1	620	LHG	C16-C17-C18-C19
20	3	624	LHG	C30-C31-C32-C33
27	4	620	XAT	C29-C30-C31-C32
20	6	623	LHG	C15-C16-C17-C18
18	B	825	CLA	O1A-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
18	a	604	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C5-C6-C7-C8
23	8	625	LMU	C5'-C4'-O1B-C1B
18	A	825	CLA	C5-C6-C7-C8
18	A	818	CLA	CAD-CBD-CGD-O2D
18	A	837	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	804	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	830	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	1	612	CLA	CAD-CBD-CGD-O2D
18	a	604	CLA	CAD-CBD-CGD-O2D
18	a	612	CLA	CAD-CBD-CGD-O2D
18	3	610	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	610	CLA	CAD-CBD-CGD-O2D
18	5	610	CLA	CAD-CBD-CGD-O2D
18	5	611	CLA	CAD-CBD-CGD-O2D
18	5	614	CLA	CAD-CBD-CGD-O2D
18	6	614	CLA	CAD-CBD-CGD-O2D
18	6	617	CLA	CAD-CBD-CGD-O2D
18	7	601	CLA	CAD-CBD-CGD-O2D
18	7	612	CLA	CAD-CBD-CGD-O2D
18	7	614	CLA	CAD-CBD-CGD-O2D
18	8	607	CLA	CAD-CBD-CGD-O2D
23	5	628	LMU	C5'-C4'-O1B-C1B
18	B	828	CLA	O1A-CGA-O2A-C1
18	7	611	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	C2-C3-C5-C6
20	8	622	LHG	C24-C25-C26-C27
20	4	622	LHG	C4-C5-C6-O8
20	5	625	LHG	C2-C3-O3-P
20	A	847	LHG	O6-C4-C5-O7
20	3	624	LHG	O6-C4-C5-O7
20	7	622	LHG	O6-C4-C5-O7
18	B	825	CLA	C8-C10-C11-C12
18	B	827	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	C2A-CAA-CBA-CGA
18	L	302	CLA	C2A-CAA-CBA-CGA
18	3	607	CLA	C2A-CAA-CBA-CGA
20	3	624	LHG	C34-C35-C36-C37
20	8	622	LHG	C12-C13-C14-C15
24	5	626	LMG	C13-C14-C15-C16
20	3	624	LHG	C11-C12-C13-C14
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O1D
18	B	805	CLA	CHA-CBD-CGD-O1D
18	B	813	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	827	CLA	CHA-CBD-CGD-O1D
18	F	304	CLA	CHA-CBD-CGD-O1D
18	F	304	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CHA-CBD-CGD-O1D
18	J	101	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	206	CLA	CHA-CBD-CGD-O1D
18	K	206	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	CHA-CBD-CGD-O2D
18	1	604	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CHA-CBD-CGD-O2D
18	5	601	CLA	CHA-CBD-CGD-O1D
18	5	617	CLA	CHA-CBD-CGD-O1D
18	5	617	CLA	CHA-CBD-CGD-O2D
18	6	604	CLA	CHA-CBD-CGD-O1D
18	6	604	CLA	CHA-CBD-CGD-O2D
18	6	616	CLA	CHA-CBD-CGD-O1D
18	6	616	CLA	CHA-CBD-CGD-O2D
18	7	602	CLA	CHA-CBD-CGD-O1D
18	7	602	CLA	CHA-CBD-CGD-O2D
18	7	604	CLA	CHA-CBD-CGD-O1D
18	7	604	CLA	CHA-CBD-CGD-O2D
18	7	607	CLA	CHA-CBD-CGD-O2D
18	A	828	CLA	C3-C5-C6-C7
18	6	604	CLA	C3-C5-C6-C7
18	6	614	CLA	C3-C5-C6-C7
18	A	810	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C35-C36-C37-C38
20	1	620	LHG	C11-C10-C9-C8
20	1	620	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4	622	LHG	C34-C35-C36-C37
20	A	847	LHG	O7-C5-C6-O8
20	4	622	LHG	O7-C5-C6-O8
24	J	104	LMG	O1-C7-C8-O7
24	5	626	LMG	O7-C8-C9-O8
25	B	850	DGD	O1G-C1G-C2G-O2G
25	J	103	DGD	O1G-C1G-C2G-O2G
20	5	623	LHG	C28-C29-C30-C31
18	A	819	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C29-C30-C31-C32
18	A	807	CLA	C16-C17-C18-C20
20	8	623	LHG	O1-C1-C2-O2
24	4	624	LMG	C16-C17-C18-C19
18	B	827	CLA	C4-C3-C5-C6
20	8	623	LHG	C11-C12-C13-C14
18	A	832	CLA	O1A-CGA-O2A-C1
24	5	627	LMG	O10-C28-O8-C9
18	A	807	CLA	C2-C3-C5-C6
18	A	822	CLA	C2-C3-C5-C6
25	B	850	DGD	CFB-CGB-CHB-CIB
18	A	811	CLA	C11-C12-C13-C14
18	A	825	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	4	613	CLA	C6-C7-C8-C9
18	6	614	CLA	C6-C7-C8-C9
18	3	606	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C23-C24-C25-C26
18	6	610	CLA	C13-C15-C16-C17
18	L	304	CLA	C2A-CAA-CBA-CGA
18	7	610	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	CBA-CGA-O2A-C1
21	5	622	BCR	C11-C12-C13-C35
21	B	847	BCR	C21-C22-C23-C24
26	a	617	LUT	C27-C28-C29-C30
20	a	620	LHG	C24-C25-C26-C27
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	832	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	616	CLA	C1A-C2A-CAA-CBA
18	3	617	CLA	CHA-CBD-CGD-O2D
18	4	607	CLA	C1A-C2A-CAA-CBA
18	7	601	CLA	C1A-C2A-CAA-CBA
18	7	603	CLA	CHA-CBD-CGD-O2D
18	7	610	CLA	C1A-C2A-CAA-CBA
18	8	610	CLA	C1A-C2A-CAA-CBA
18	A	811	CLA	C10-C11-C12-C13
18	B	809	CLA	C2-C1-O2A-CGA
18	3	606	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	C3-O3-P-O6
20	8	623	LHG	C16-C17-C18-C19
20	7	622	LHG	O2-C2-C3-O3
20	1	620	LHG	C30-C31-C32-C33
18	A	802	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
20	3	624	LHG	C2-C3-O3-P
24	5	627	LMG	C15-C16-C17-C18
18	7	611	CLA	O1A-CGA-O2A-C1
18	1	611	CLA	C4B-C3B-CAB-CBB
18	a	601	CLA	C4B-C3B-CAB-CBB
20	A	846	LHG	C4-O6-P-O4
20	a	620	LHG	C3-O3-P-O5
20	5	625	LHG	C3-O3-P-O5
20	8	622	LHG	C4-O6-P-O4
20	8	622	LHG	C4-O6-P-O5
20	8	623	LHG	C19-C20-C21-C22
24	A	860	LMG	O6-C1-O1-C7
18	A	818	CLA	C8-C10-C11-C12
18	A	812	CLA	CBA-CGA-O2A-C1
20	3	624	LHG	O6-C4-C5-C6
18	5	610	CLA	C6-C7-C8-C9
24	5	627	LMG	C33-C34-C35-C36
20	5	623	LHG	C24-C25-C26-C27
18	1	602	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	C3-C5-C6-C7
25	J	103	DGD	CCA-CDA-CEA-CFA
24	5	627	LMG	C11-C10-O7-C8
18	A	807	CLA	C16-C17-C18-C19
18	5	604	CLA	C16-C17-C18-C20
18	A	815	CLA	CAD-CBD-CGD-O1D
18	A	825	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	828	CLA	CAD-CBD-CGD-O1D
18	A	845	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CAD-CBD-CGD-O1D
18	B	805	CLA	CAD-CBD-CGD-O1D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	K	204	CLA	CAD-CBD-CGD-O1D
18	5	617	CLA	CAD-CBD-CGD-O1D
18	6	601	CLA	CAD-CBD-CGD-O1D
18	6	620	CLA	CAD-CBD-CGD-O1D
18	7	602	CLA	CAD-CBD-CGD-O1D
18	8	601	CLA	CAD-CBD-CGD-O1D
18	5	617	CLA	CAA-CBA-CGA-O2A
18	8	608	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	C3-C5-C6-C7
18	6	616	CLA	C5-C6-C7-C8
20	A	847	LHG	C7-C8-C9-C10
20	5	625	LHG	C7-C8-C9-C10
18	8	613	CLA	C13-C15-C16-C17
18	7	609	CLA	C2C-C3C-CAC-CBC
18	A	812	CLA	C12-C13-C15-C16
18	A	818	CLA	C6-C7-C8-C10
18	A	829	CLA	C12-C13-C15-C16
18	A	830	CLA	C12-C13-C15-C16
18	A	841	CLA	C12-C13-C15-C16
18	a	606	CLA	CHA-CBD-CGD-O2D
18	3	604	CLA	C6-C7-C8-C10
18	4	618	CLA	C3A-C2A-CAA-CBA
18	5	613	CLA	C11-C12-C13-C15
18	6	602	CLA	C11-C12-C13-C15
18	6	610	CLA	C6-C7-C8-C10
18	6	614	CLA	C6-C7-C8-C10
18	7	611	CLA	C6-C7-C8-C10
18	8	612	CLA	C3A-C2A-CAA-CBA
20	B	851	LHG	C7-C8-C9-C10
20	8	623	LHG	O6-C4-C5-O7
18	4	608	CLA	C3-C5-C6-C7
21	6	622	BCR	C9-C10-C11-C12
20	4	622	LHG	C9-C10-C11-C12
18	7	613	CLA	O1D-CGD-O2D-CED
20	7	622	LHG	C26-C27-C28-C29
23	8	624	LMU	C4B-C5B-C6B-O6B
24	5	627	LMG	O7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	8	622	LHG	C13-C14-C15-C16
23	A	859	LMU	C5'-C4'-O1B-C1B
18	A	814	CLA	C8-C10-C11-C12
18	A	826	CLA	C10-C11-C12-C13
20	1	620	LHG	C29-C30-C31-C32
20	5	623	LHG	C9-C10-C11-C12
24	4	624	LMG	C8-C7-O1-C1
18	3	608	CLA	C5-C6-C7-C8
18	7	610	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C2-C3-O3-P
18	3	613	CLA	C4-C3-C5-C6
18	A	827	CLA	CBA-CGA-O2A-C1
24	A	860	LMG	C29-C28-O8-C9
18	A	826	CLA	C2-C3-C5-C6
18	B	808	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C10-C8-C9
18	B	818	CLA	C11-C10-C8-C9
18	5	604	CLA	C14-C13-C15-C16
18	5	613	CLA	C11-C12-C13-C14
18	6	601	CLA	C14-C13-C15-C16
18	8	613	CLA	C11-C10-C8-C9
18	8	614	CLA	C6-C7-C8-C9
18	A	812	CLA	O1A-CGA-O2A-C1
18	6	603	CLA	O1A-CGA-O2A-C1
18	7	602	CLA	C2A-CAA-CBA-CGA
20	5	623	LHG	C33-C34-C35-C36
27	7	620	XAT	C29-C30-C31-C32
20	8	623	LHG	C30-C31-C32-C33
20	B	851	LHG	C11-C12-C13-C14
25	B	850	DGD	C8B-C9B-CAB-CBB
20	3	623	LHG	C23-C24-C25-C26
23	K	208	LMU	O5B-C5B-C6B-O6B
18	A	809	CLA	C2B-C3B-CAB-CBB
18	A	822	CLA	C2B-C3B-CAB-CBB
18	A	828	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C2B-C3B-CAB-CBB
18	B	810	CLA	C2B-C3B-CAB-CBB
18	B	813	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	823	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	837	CLA	C2B-C3B-CAB-CBB
18	B	838	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C2B-C3B-CAB-CBB
18	1	611	CLA	C2B-C3B-CAB-CBB
18	a	601	CLA	C2B-C3B-CAB-CBB
18	a	602	CLA	C2B-C3B-CAB-CBB
18	a	603	CLA	C2B-C3B-CAB-CBB
18	a	606	CLA	C2B-C3B-CAB-CBB
18	a	609	CLA	C2B-C3B-CAB-CBB
18	3	604	CLA	C2B-C3B-CAB-CBB
18	3	606	CLA	C2B-C3B-CAB-CBB
18	4	607	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
18	5	607	CLA	C2B-C3B-CAB-CBB
18	5	609	CLA	C2B-C3B-CAB-CBB
18	6	608	CLA	C2B-C3B-CAB-CBB
18	6	610	CLA	C2B-C3B-CAB-CBB
18	6	617	CLA	C2B-C3B-CAB-CBB
18	7	606	CLA	C2B-C3B-CAB-CBB
18	7	610	CLA	C2B-C3B-CAB-CBB
18	A	827	CLA	O1A-CGA-O2A-C1
18	A	814	CLA	C10-C11-C12-C13
18	A	830	CLA	C5-C6-C7-C8
19	B	842	PQN	C23-C25-C26-C27
18	5	609	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	C15-C16-C17-C18
18	a	609	CLA	C13-C15-C16-C17
24	7	624	LMG	C13-C14-C15-C16
18	6	616	CLA	C8-C10-C11-C12
18	1	604	CLA	C1-C2-C3-C4
18	a	604	CLA	C1-C2-C3-C4
18	B	841	CLA	O1D-CGD-O2D-CED
23	K	208	LMU	C1-C2-C3-C4
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	6	613	CLA	C2A-CAA-CBA-CGA
18	7	613	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	C5-C6-C7-C8
18	A	841	CLA	C2-C1-O2A-CGA
18	3	606	CLA	C2-C1-O2A-CGA
18	6	616	CLA	C2-C1-O2A-CGA
18	8	610	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	3	623	LHG	C11-C12-C13-C14
20	7	622	LHG	C12-C13-C14-C15
18	B	836	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	C3-C5-C6-C7
23	A	857	LMU	C2B-C1B-O1B-C4'
18	6	603	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C5-C6-C7-C8
18	1	603	CLA	C4-C3-C5-C6
21	K	207	BCR	C1-C6-C7-C8
26	7	619	LUT	C5-C6-C7-C8
20	7	622	LHG	O10-C23-O8-C6
18	B	832	CLA	CAA-CBA-CGA-O2A
20	B	851	LHG	C12-C13-C14-C15
20	8	623	LHG	C28-C29-C30-C31
20	6	623	LHG	C17-C18-C19-C20
20	7	622	LHG	C8-C7-O7-C5
18	B	821	CLA	C2A-CAA-CBA-CGA
18	8	608	CLA	C2A-CAA-CBA-CGA
24	7	624	LMG	O7-C8-C9-O8
20	1	620	LHG	C3-O3-P-O6
20	3	624	LHG	C4-O6-P-O3
20	4	622	LHG	C3-O3-P-O6
20	5	623	LHG	C3-O3-P-O6
20	5	625	LHG	C4-O6-P-O3
20	8	622	LHG	C3-O3-P-O6
18	5	613	CLA	C15-C16-C17-C18
23	A	859	LMU	C11-C10-C9-C8
18	B	813	CLA	C6-C7-C8-C10
18	3	613	CLA	C2-C3-C5-C6
18	6	613	CLA	C6-C7-C8-C10
18	8	601	CLA	C12-C13-C15-C16
18	A	804	CLA	C14-C13-C15-C16
18	B	831	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	4	610	CLA	C6-C7-C8-C9
18	6	613	CLA	C11-C10-C8-C9
18	A	842	CLA	C13-C15-C16-C17
18	B	829	CLA	C5-C6-C7-C8
21	L	301	BCR	C13-C14-C15-C16
21	5	622	BCR	C13-C14-C15-C16
18	5	604	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	a	620	LHG	C11-C10-C9-C8
24	5	626	LMG	C10-C11-C12-C13
25	B	850	DGD	C3B-C4B-C5B-C6B
18	5	619	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	CBA-CGA-O2A-C1
18	6	601	CLA	O1A-CGA-O2A-C1
21	B	801	BCR	C7-C8-C9-C34
18	6	601	CLA	CBA-CGA-O2A-C1
20	a	620	LHG	C2-C3-O3-P
20	3	623	LHG	C2-C3-O3-P
20	4	622	LHG	C2-C3-O3-P
20	5	625	LHG	C5-C4-O6-P
20	7	622	LHG	C2-C3-O3-P
28	6	624	NEX	C11-C12-C13-C14
20	5	625	LHG	C18-C19-C20-C21
18	3	602	CLA	C3-C5-C6-C7
18	A	819	CLA	CAA-CBA-CGA-O2A
20	5	625	LHG	C17-C18-C19-C20
18	A	814	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	5	609	CLA	CBA-CGA-O2A-C1
20	5	625	LHG	C24-C25-C26-C27
18	B	802	CLA	CAA-CBA-CGA-O2A
18	1	613	CLA	C5-C6-C7-C8
18	8	606	CLA	CBD-CGD-O2D-CED
18	5	602	CLA	CBA-CGA-O2A-C1
18	6	613	CLA	CBA-CGA-O2A-C1
18	A	809	CLA	C4B-C3B-CAB-CBB
18	A	822	CLA	C4B-C3B-CAB-CBB
18	A	832	CLA	C4B-C3B-CAB-CBB
18	B	813	CLA	C4B-C3B-CAB-CBB
18	B	816	CLA	C4B-C3B-CAB-CBB
18	B	823	CLA	C4B-C3B-CAB-CBB
18	B	835	CLA	C4B-C3B-CAB-CBB
18	B	837	CLA	C4B-C3B-CAB-CBB
18	1	604	CLA	C4B-C3B-CAB-CBB
18	a	604	CLA	C4B-C3B-CAB-CBB
18	a	607	CLA	C4B-C3B-CAB-CBB
18	a	609	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C4B-C3B-CAB-CBB
18	4	610	CLA	C4B-C3B-CAB-CBB
18	6	608	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	6	610	CLA	C4B-C3B-CAB-CBB
18	7	606	CLA	C4B-C3B-CAB-CBB
18	7	610	CLA	C4B-C3B-CAB-CBB
21	A	856	BCR	C13-C14-C15-C16
21	6	622	BCR	C13-C14-C15-C16
27	3	619	XAT	C29-C30-C31-C32
20	3	624	LHG	C27-C28-C29-C30
18	6	601	CLA	C8-C10-C11-C12
20	8	623	LHG	C31-C32-C33-C34
18	B	816	CLA	C3-C5-C6-C7
18	8	613	CLA	C4-C3-C5-C6
20	7	622	LHG	C10-C11-C12-C13
18	A	826	CLA	C8-C10-C11-C12
20	6	623	LHG	C9-C10-C11-C12
18	A	808	CLA	C2-C1-O2A-CGA
18	B	831	CLA	C2-C1-O2A-CGA
18	B	836	CLA	C2-C1-O2A-CGA
18	a	609	CLA	C2-C1-O2A-CGA
18	5	617	CLA	C2-C1-O2A-CGA
18	A	826	CLA	C13-C15-C16-C17
18	7	603	CLA	CAA-CBA-CGA-O1A
18	B	835	CLA	C2A-CAA-CBA-CGA
18	a	601	CLA	C2A-CAA-CBA-CGA
18	a	602	CLA	C2A-CAA-CBA-CGA
18	6	620	CLA	C2A-CAA-CBA-CGA
20	3	623	LHG	C27-C28-C29-C30
25	J	103	DGD	C8A-C9A-CAA-CBA
18	B	839	CLA	CBA-CGA-O2A-C1
20	6	623	LHG	C14-C15-C16-C17
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
23	A	859	LMU	C5-C6-C7-C8
26	a	617	LUT	C29-C30-C31-C32
18	5	613	CLA	CBA-CGA-O2A-C1
20	6	623	LHG	C28-C29-C30-C31
18	B	835	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CAA-CBA-CGA-O1A
23	A	857	LMU	C3-C4-C5-C6
18	A	802	CLA	C2-C3-C5-C6
18	F	301	CLA	C2-C3-C5-C6
25	B	850	DGD	C9A-CAA-CBA-CCA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	818	CLA	C6-C7-C8-C9
18	1	611	CLA	C6-C7-C8-C9
18	3	604	CLA	C6-C7-C8-C9
18	8	601	CLA	C6-C7-C8-C9
25	J	103	DGD	C5A-C6A-C7A-C8A
18	7	611	CLA	C8-C10-C11-C12
18	8	601	CLA	C10-C11-C12-C13
20	5	625	LHG	C4-C5-C6-O8
21	A	852	BCR	C11-C10-C9-C34
21	A	852	BCR	C16-C17-C18-C36
21	B	844	BCR	C11-C10-C9-C34
21	B	845	BCR	C11-C10-C9-C34
21	B	845	BCR	C20-C21-C22-C37
21	F	305	BCR	C16-C17-C18-C36
21	L	301	BCR	C11-C10-C9-C34
21	3	621	BCR	C35-C13-C14-C15
21	3	621	BCR	C16-C17-C18-C36
21	3	622	BCR	C35-C13-C14-C15
21	3	622	BCR	C16-C17-C18-C36
28	5	624	NEX	C39-C29-C30-C31
28	6	624	NEX	C39-C29-C30-C31
18	5	614	CLA	CAA-CBA-CGA-O1A
18	A	825	CLA	C2A-CAA-CBA-CGA
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O2A-C1-C2-C3
18	6	617	CLA	CAA-CBA-CGA-O2A
21	A	849	BCR	C7-C8-C9-C34
18	L	302	CLA	CAA-CBA-CGA-O1A
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C1A-C2A-CAA-CBA
18	B	839	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C1A-C2A-CAA-CBA
18	1	603	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	C1A-C2A-CAA-CBA
18	a	607	CLA	C1A-C2A-CAA-CBA
18	4	614	CLA	C1A-C2A-CAA-CBA
18	6	608	CLA	C1A-C2A-CAA-CBA
18	7	608	CLA	C1A-C2A-CAA-CBA
18	8	603	CLA	C1A-C2A-CAA-CBA
18	8	606	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C6-C7-C8-C10
18	A	814	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C6-C7-C8-C10
18	4	601	CLA	C6-C7-C8-C10
18	7	601	CLA	C6-C7-C8-C10
18	A	811	CLA	C15-C16-C17-C18
18	A	841	CLA	O1A-CGA-O2A-C1
18	6	617	CLA	CAA-CBA-CGA-O1A
20	8	622	LHG	C35-C36-C37-C38
20	1	620	LHG	C24-C23-O8-C6
18	B	835	CLA	CAA-CBA-CGA-O1A
18	a	612	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C5-C6-C7-C8
18	3	609	CLA	C11-C12-C13-C14
18	A	802	CLA	C2A-CAA-CBA-CGA
18	L	303	CLA	C2A-CAA-CBA-CGA
18	3	606	CLA	C5-C6-C7-C8
18	4	613	CLA	C8-C10-C11-C12
18	6	603	CLA	C5-C6-C7-C8
18	4	603	CLA	CAA-CBA-CGA-O2A
18	5	614	CLA	CAA-CBA-CGA-O2A
18	7	603	CLA	CAA-CBA-CGA-O2A
24	7	624	LMG	C11-C12-C13-C14
18	5	613	CLA	C5-C6-C7-C8
18	a	609	CLA	C4-C3-C5-C6
18	A	835	CLA	C8-C10-C11-C12
18	A	808	CLA	C2B-C3B-CAB-CBB
18	A	832	CLA	C2B-C3B-CAB-CBB
18	B	816	CLA	C2B-C3B-CAB-CBB
18	B	822	CLA	C2B-C3B-CAB-CBB
18	B	835	CLA	C2B-C3B-CAB-CBB
18	1	604	CLA	C2B-C3B-CAB-CBB
18	a	607	CLA	C2B-C3B-CAB-CBB
18	a	608	CLA	C2B-C3B-CAB-CBB
18	4	606	CLA	C2B-C3B-CAB-CBB
18	a	612	CLA	CAA-CBA-CGA-O1A
18	B	802	CLA	C13-C15-C16-C17
21	A	852	BCR	C11-C10-C9-C8
21	A	852	BCR	C16-C17-C18-C19
21	B	844	BCR	C11-C10-C9-C8
21	B	845	BCR	C11-C10-C9-C8
21	B	845	BCR	C20-C21-C22-C23
21	F	305	BCR	C16-C17-C18-C19
21	L	301	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3	621	BCR	C12-C13-C14-C15
21	3	621	BCR	C16-C17-C18-C19
21	3	622	BCR	C12-C13-C14-C15
21	3	622	BCR	C16-C17-C18-C19
23	K	208	LMU	C2'-C1'-O1'-C1
28	5	624	NEX	C28-C29-C30-C31
28	6	624	NEX	C28-C29-C30-C31
18	5	609	CLA	C8-C10-C11-C12
19	B	842	PQN	C15-C16-C17-C18
18	4	603	CLA	CAA-CBA-CGA-O1A
18	5	619	CLA	CAA-CBA-CGA-O1A
18	6	613	CLA	O1A-CGA-O2A-C1
20	5	625	LHG	O7-C5-C6-O8
20	7	622	LHG	O7-C5-C6-O8
27	6	621	XAT	C29-C30-C31-C32
18	5	619	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CAA-CBA-CGA-O2A
18	B	802	CLA	C4-C3-C5-C6
19	A	844	PQN	C14-C13-C15-C16
18	A	802	CLA	C2-C1-O2A-CGA
18	B	816	CLA	C2-C1-O2A-CGA
18	3	603	CLA	C2-C1-O2A-CGA
18	6	608	CLA	C2-C1-O2A-CGA
18	7	604	CLA	C2-C1-O2A-CGA
18	B	833	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	O1A-CGA-O2A-C1
18	L	302	CLA	CAA-CBA-CGA-O2A
18	a	603	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C11-C12-C13-C14
18	6	601	CLA	C11-C10-C8-C9
18	A	814	CLA	O1A-CGA-O2A-C1
18	8	601	CLA	CAA-CBA-CGA-O2A
18	5	602	CLA	O1A-CGA-O2A-C1
18	7	604	CLA	C5-C6-C7-C8
18	8	604	CLA	C2A-CAA-CBA-CGA
21	B	846	BCR	C1-C6-C7-C8
21	B	846	BCR	C5-C6-C7-C8
21	J	102	BCR	C1-C6-C7-C8
21	a	619	BCR	C23-C24-C25-C30
21	3	621	BCR	C23-C24-C25-C30
21	4	621	BCR	C23-C24-C25-C26
21	4	621	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	852	BCR	C19-C20-C21-C22
18	B	813	CLA	C4-C3-C5-C6
18	6	613	CLA	C4-C3-C5-C6
21	J	102	BCR	C11-C12-C13-C14
21	5	622	BCR	C11-C12-C13-C14
18	A	835	CLA	C5-C6-C7-C8
18	6	620	CLA	CAA-CBA-CGA-O2A
18	7	612	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	CAA-CBA-CGA-O2A
23	A	859	LMU	C6-C7-C8-C9
18	A	842	CLA	C15-C16-C17-C18
23	5	628	LMU	O5B-C5B-C6B-O6B
18	B	819	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C30-C31-C32-C33
18	B	802	CLA	C3-C5-C6-C7
18	5	616	CLA	CAA-CBA-CGA-O2A
18	A	808	CLA	C4B-C3B-CAB-CBB
18	A	828	CLA	C4B-C3B-CAB-CBB
18	A	830	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C4B-C3B-CAB-CBB
18	B	838	CLA	C4B-C3B-CAB-CBB
18	a	608	CLA	C4B-C3B-CAB-CBB
18	4	606	CLA	C4B-C3B-CAB-CBB
18	5	609	CLA	C4B-C3B-CAB-CBB
18	B	831	CLA	C4-C3-C5-C6
18	6	604	CLA	C4-C3-C5-C6
18	6	601	CLA	C11-C10-C8-C7
18	6	616	CLA	C12-C13-C15-C16
18	B	833	CLA	CBA-CGA-O2A-C1
20	3	623	LHG	C10-C11-C12-C13
20	a	620	LHG	C10-C11-C12-C13
24	5	626	LMG	C29-C30-C31-C32
18	6	620	CLA	CAA-CBA-CGA-O1A
20	4	622	LHG	C1-C2-C3-O3
20	6	623	LHG	C1-C2-C3-O3
18	4	602	CLA	C5-C6-C7-C8
18	B	823	CLA	CAA-CBA-CGA-O2A
18	7	612	CLA	CAA-CBA-CGA-O1A
18	7	611	CLA	O2A-C1-C2-C3
25	B	850	DGD	CBB-CCB-CDB-CEB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	1	612	CLA	CAA-CBA-CGA-O2A
18	1	616	CLA	CAA-CBA-CGA-O2A
18	8	609	CLA	CAA-CBA-CGA-O2A
18	A	854	CLA	CBA-CGA-O2A-C1
18	5	608	CLA	CBA-CGA-O2A-C1
18	1	603	CLA	CAA-CBA-CGA-O2A
18	6	616	CLA	CAA-CBA-CGA-O2A
20	4	622	LHG	O8-C23-C24-C25
18	A	803	CLA	C4-C3-C5-C6
18	B	834	CLA	C4-C3-C5-C6
18	A	811	CLA	C13-C15-C16-C17
20	4	622	LHG	C11-C12-C13-C14
20	B	851	LHG	C3-O3-P-O6
18	A	841	CLA	CAA-CBA-CGA-O2A
20	7	622	LHG	C9-C10-C11-C12
18	A	806	CLA	C6-C7-C8-C9
18	A	812	CLA	C14-C13-C15-C16
18	A	814	CLA	C11-C12-C13-C14
18	A	830	CLA	C14-C13-C15-C16
18	A	841	CLA	C11-C12-C13-C14
18	A	841	CLA	C14-C13-C15-C16
18	6	602	CLA	C11-C12-C13-C14
18	6	610	CLA	C6-C7-C8-C9
18	7	611	CLA	C6-C7-C8-C9
18	7	611	CLA	C11-C10-C8-C9
18	7	613	CLA	C11-C10-C8-C9
20	1	620	LHG	C34-C35-C36-C37
18	8	606	CLA	C3A-C2A-CAA-CBA
18	A	854	CLA	O1A-CGA-O2A-C1
18	3	609	CLA	O1A-CGA-O2A-C1
18	5	608	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	CAA-CBA-CGA-O2A
20	6	623	LHG	O8-C23-C24-C25
25	J	103	DGD	CBA-CCA-CDA-CEA
18	1	612	CLA	CAA-CBA-CGA-O1A
18	7	616	CLA	CAA-CBA-CGA-O2A
18	8	603	CLA	CAA-CBA-CGA-O2A
18	A	808	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	831	CLA	CAD-CBD-CGD-O2D
18	A	834	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	838	CLA	CAD-CBD-CGD-O2D
18	B	825	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	833	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	B	836	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	F	303	CLA	CAD-CBD-CGD-O2D
18	K	201	CLA	CAD-CBD-CGD-O2D
18	1	609	CLA	CAD-CBD-CGD-O2D
18	1	613	CLA	CAD-CBD-CGD-O2D
18	a	614	CLA	CAD-CBD-CGD-O2D
18	4	604	CLA	CAD-CBD-CGD-O2D
18	4	614	CLA	CAD-CBD-CGD-O2D
18	A	801	CLA	C16-C17-C18-C19
20	B	851	LHG	O9-C7-O7-C5
18	6	604	CLA	C15-C16-C17-C18
18	A	816	CLA	CAA-CBA-CGA-O2A
18	a	607	CLA	CAA-CBA-CGA-O2A
18	3	609	CLA	C4-C3-C5-C6
18	a	616	CLA	CAA-CBA-CGA-O2A
18	B	802	CLA	C2-C3-C5-C6
18	6	613	CLA	C2-C3-C5-C6
18	B	813	CLA	CAA-CBA-CGA-O2A
18	B	838	CLA	CAA-CBA-CGA-O2A
24	4	623	LMG	O8-C28-C29-C30
24	5	626	LMG	O8-C28-C29-C30
21	B	801	BCR	C7-C8-C9-C10
21	4	621	BCR	C17-C18-C19-C20
27	8	620	XAT	C27-C28-C29-C30
24	J	104	LMG	C7-C8-C9-O8
27	3	619	XAT	O24-C26-C27-C28
18	B	823	CLA	CAA-CBA-CGA-O1A
18	5	616	CLA	CAA-CBA-CGA-O1A
18	A	843	CLA	C6-C7-C8-C10
18	A	821	CLA	CAA-CBA-CGA-O2A
18	3	609	CLA	CAA-CBA-CGA-O2A
24	5	627	LMG	O7-C10-C11-C12
20	3	623	LHG	C31-C32-C33-C34
20	4	622	LHG	C17-C18-C19-C20
18	a	616	CLA	CAA-CBA-CGA-O1A
18	4	607	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	607	CLA	CAA-CBA-CGA-O2A
18	4	616	CLA	CAA-CBA-CGA-O2A
18	A	804	CLA	O2A-C1-C2-C3
18	A	811	CLA	O2A-C1-C2-C3
18	B	807	CLA	C2A-CAA-CBA-CGA
18	a	613	CLA	C2A-CAA-CBA-CGA
18	4	610	CLA	C2A-CAA-CBA-CGA
18	A	854	CLA	C13-C15-C16-C17
18	4	604	CLA	C5-C6-C7-C8
25	B	850	DGD	C4E-C5E-C6E-O5E
18	A	842	CLA	CAA-CBA-CGA-O1A
18	1	616	CLA	CAA-CBA-CGA-O1A
18	8	603	CLA	CAA-CBA-CGA-O1A
20	8	623	LHG	C18-C19-C20-C21
18	4	601	CLA	C16-C17-C18-C19
18	8	606	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	815	CLA	CHA-CBD-CGD-O2D
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	830	CLA	CHA-CBD-CGD-O1D
18	A	830	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	CHA-CBD-CGD-O2D
18	B	805	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	815	CLA	CHA-CBD-CGD-O1D
18	B	827	CLA	CHA-CBD-CGD-O2D
18	B	841	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	L	304	CLA	CHA-CBD-CGD-O1D
18	L	304	CLA	CHA-CBD-CGD-O2D
18	1	602	CLA	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	602	CLA	CHA-CBD-CGD-O2D
18	a	603	CLA	CHA-CBD-CGD-O1D
18	a	603	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	4	616	CLA	CHA-CBD-CGD-O1D
18	5	601	CLA	CHA-CBD-CGD-O2D
18	5	603	CLA	CHA-CBD-CGD-O1D
18	5	607	CLA	CHA-CBD-CGD-O1D
18	5	607	CLA	CHA-CBD-CGD-O2D
18	5	619	CLA	CHA-CBD-CGD-O1D
18	5	619	CLA	CHA-CBD-CGD-O2D
18	6	603	CLA	CHA-CBD-CGD-O1D
18	8	604	CLA	CHA-CBD-CGD-O1D
18	8	604	CLA	CHA-CBD-CGD-O2D
18	8	616	CLA	CHA-CBD-CGD-O1D
18	8	616	CLA	CHA-CBD-CGD-O2D
21	A	851	BCR	C19-C20-C21-C22
18	7	616	CLA	CAA-CBA-CGA-O1A
18	8	609	CLA	CAA-CBA-CGA-O1A
18	B	813	CLA	C2-C3-C5-C6
20	4	622	LHG	C18-C19-C20-C21
23	5	628	LMU	C2B-C1B-O1B-C4'
20	5	625	LHG	C35-C36-C37-C38
18	A	816	CLA	CAA-CBA-CGA-O1A
18	4	616	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	C11-C12-C13-C15
18	A	807	CLA	CAA-CBA-CGA-O2A
18	A	818	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	CAA-CBA-CGA-O2A
18	B	810	CLA	CAA-CBA-CGA-O2A
18	8	608	CLA	CAA-CBA-CGA-O2A
20	3	624	LHG	O7-C5-C6-O8
18	4	610	CLA	C8-C10-C11-C12
18	A	813	CLA	C6-C7-C8-C9
18	A	835	CLA	CAA-CBA-CGA-O2A
18	B	834	CLA	CAA-CBA-CGA-O2A
18	8	604	CLA	CAA-CBA-CGA-O2A
18	6	609	CLA	CAA-CBA-CGA-O2A
20	B	851	LHG	O2-C2-C3-O3
18	B	819	CLA	C3-C5-C6-C7
18	A	845	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4	622	LHG	O10-C23-O8-C6
18	a	609	CLA	C5-C6-C7-C8
18	A	802	CLA	C12-C13-C15-C16
18	A	830	CLA	C11-C12-C13-C15
18	K	203	CLA	C6-C7-C8-C10
18	1	603	CLA	C2-C3-C5-C6
18	3	609	CLA	C2-C3-C5-C6
20	7	622	LHG	C5-C4-O6-P
24	5	626	LMG	C4-C5-C6-O5
24	5	626	LMG	O6-C1-O1-C7
18	B	833	CLA	CAA-CBA-CGA-O2A
18	a	607	CLA	CAA-CBA-CGA-O1A
18	A	802	CLA	C11-C10-C8-C9
18	A	812	CLA	C6-C7-C8-C9
18	B	825	CLA	C6-C7-C8-C9
18	K	203	CLA	C6-C7-C8-C9
18	5	613	CLA	C14-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C24
21	3	620	BCR	C13-C14-C15-C16
18	A	830	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	5	610	CLA	C2B-C3B-CAB-CBB
18	B	826	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C16-C17-C18-C19
18	3	609	CLA	CBA-CGA-O2A-C1
18	3	606	CLA	CAA-CBA-CGA-O2A
18	A	802	CLA	C10-C11-C12-C13
18	3	609	CLA	C4C-C3C-CAC-CBC
20	A	846	LHG	C29-C30-C31-C32
18	B	838	CLA	CAA-CBA-CGA-O1A
18	1	603	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C4-C3-C5-C6
20	8	623	LHG	O1-C1-C2-C3
18	8	613	CLA	C2-C3-C5-C6
20	A	846	LHG	O10-C23-C24-C25
18	B	826	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	835	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C1A-C2A-CAA-CBA
18	1	603	CLA	CHA-CBD-CGD-O2D
18	a	608	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	613	CLA	C1A-C2A-CAA-CBA
18	5	606	CLA	CHA-CBD-CGD-O2D
18	6	612	CLA	CHA-CBD-CGD-O2D
20	A	846	LHG	C11-C10-C9-C8
18	A	843	CLA	C16-C17-C18-C20
18	4	601	CLA	C16-C17-C18-C20
24	J	104	LMG	O10-C28-C29-C30
18	8	610	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	CAA-CBA-CGA-O1A
18	A	845	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O1A
18	A	839	CLA	C2A-CAA-CBA-CGA
18	a	601	CLA	C6-C7-C8-C10
18	6	616	CLA	CAA-CBA-CGA-O1A
18	8	601	CLA	C5-C6-C7-C8
23	5	628	LMU	C2-C3-C4-C5
20	6	623	LHG	C33-C34-C35-C36
18	A	841	CLA	CAA-CBA-CGA-O1A
24	5	627	LMG	O9-C10-C11-C12
18	A	837	CLA	CAA-CBA-CGA-O2A
24	4	624	LMG	C2-C1-O1-C7
20	A	846	LHG	C3-O3-P-O5
20	A	846	LHG	C4-O6-P-O5
20	B	851	LHG	C3-O3-P-O5
20	1	620	LHG	C3-O3-P-O5
20	4	622	LHG	C3-O3-P-O5
20	5	623	LHG	C3-O3-P-O5
20	5	625	LHG	C4-O6-P-O5
18	A	830	CLA	CAA-CBA-CGA-O1A
25	B	850	DGD	O1B-C1B-C2B-C3B
18	a	613	CLA	C15-C16-C17-C18
21	B	844	BCR	C5-C6-C7-C8
21	a	619	BCR	C23-C24-C25-C26
18	A	829	CLA	C15-C16-C17-C18
18	A	818	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	CAA-CBA-CGA-O1A
24	J	104	LMG	O8-C28-C29-C30
18	6	609	CLA	CAA-CBA-CGA-O1A
18	8	616	CLA	CAA-CBA-CGA-O2A
18	A	835	CLA	CAA-CBA-CGA-O1A
18	3	606	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	811	CLA	CAD-CBD-CGD-O1D
18	A	814	CLA	CAD-CBD-CGD-O1D
18	A	830	CLA	CAD-CBD-CGD-O1D
18	A	832	CLA	CAD-CBD-CGD-O1D
18	B	815	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
18	B	841	CLA	CAD-CBD-CGD-O1D
18	K	201	CLA	CAD-CBD-CGD-O1D
18	4	616	CLA	CAD-CBD-CGD-O1D
18	5	601	CLA	CAD-CBD-CGD-O1D
18	5	607	CLA	CAD-CBD-CGD-O1D
18	B	833	CLA	CAA-CBA-CGA-O1A
18	8	608	CLA	CAA-CBA-CGA-O1A
23	A	857	LMU	C6-C7-C8-C9
18	A	804	CLA	C10-C11-C12-C13
18	A	814	CLA	C6-C7-C8-C9
18	A	822	CLA	C6-C7-C8-C9
18	A	834	CLA	C11-C12-C13-C14
18	B	813	CLA	C6-C7-C8-C9
18	6	610	CLA	C11-C12-C13-C14
19	A	844	PQN	C16-C17-C18-C19
20	7	622	LHG	C30-C31-C32-C33
18	B	827	CLA	CAA-CBA-CGA-O1A
18	8	604	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	O10-C23-C24-C25
18	5	613	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	C16-C17-C18-C20
18	1	602	CLA	CAA-CBA-CGA-O2A
18	a	602	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	C15-C16-C17-C18
18	A	837	CLA	CAA-CBA-CGA-O1A
18	K	206	CLA	CAA-CBA-CGA-O1A
18	3	613	CLA	CBA-CGA-O2A-C1
18	5	609	CLA	CAA-CBA-CGA-O2A
18	6	602	CLA	CAA-CBA-CGA-O2A
18	6	610	CLA	CAA-CBA-CGA-O2A
20	A	846	LHG	O8-C23-C24-C25
20	3	624	LHG	C1-C2-C3-O3
18	A	801	CLA	C5-C6-C7-C8
18	7	613	CLA	C10-C11-C12-C13
18	B	810	CLA	CAA-CBA-CGA-O1A
18	7	610	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	614	CLA	C5-C6-C7-C8
18	A	802	CLA	C11-C10-C8-C7
18	A	807	CLA	C12-C13-C15-C16
18	A	812	CLA	C6-C7-C8-C10
18	A	814	CLA	C6-C7-C8-C10
18	A	822	CLA	C6-C7-C8-C10
18	A	834	CLA	C11-C12-C13-C15
18	A	838	CLA	C3A-C2A-CAA-CBA
18	B	818	CLA	C11-C10-C8-C7
18	1	603	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	a	601	CLA	CAD-CBD-CGD-O2D
18	a	602	CLA	C11-C12-C13-C15
18	a	609	CLA	C2-C3-C5-C6
18	3	606	CLA	CHA-CBD-CGD-O1D
18	3	617	CLA	CAD-CBD-CGD-O2D
18	5	613	CLA	C12-C13-C15-C16
18	6	604	CLA	C11-C10-C8-C7
18	6	606	CLA	CHA-CBD-CGD-O1D
18	6	606	CLA	CAD-CBD-CGD-O2D
18	7	603	CLA	CHA-CBD-CGD-O1D
18	8	603	CLA	C3A-C2A-CAA-CBA
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	836	CLA	CAA-CBA-CGA-O2A
18	B	806	CLA	CAA-CBA-CGA-O2A
20	8	622	LHG	O7-C7-C8-C9
21	B	843	BCR	C11-C12-C13-C14
21	7	623	BCR	C17-C18-C19-C20
18	6	610	CLA	CAA-CBA-CGA-O1A
20	6	623	LHG	O10-C23-C24-C25
21	5	622	BCR	C9-C10-C11-C12
23	K	208	LMU	C2-C1-O1'-C1'
18	K	203	CLA	CAA-CBA-CGA-O2A
25	B	850	DGD	O2G-C1B-C2B-C3B
25	B	850	DGD	C5B-C6B-C7B-C8B
18	B	806	CLA	CAA-CBA-CGA-O1A
18	B	834	CLA	CAA-CBA-CGA-O1A
18	6	602	CLA	CAA-CBA-CGA-O1A
18	8	610	CLA	CBA-CGA-O2A-C1
18	1	611	CLA	C15-C16-C17-C18
18	6	601	CLA	CAA-CBA-CGA-O2A
20	3	624	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	836	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	C2A-CAA-CBA-CGA
18	8	616	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	O9-C7-C8-C9
18	K	201	CLA	CAA-CBA-CGA-O2A
18	K	206	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

231 monomers are involved in 500 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	812	CLA	2	0
20	4	622	LHG	4	0
18	A	817	CLA	2	0
18	A	814	CLA	6	0
18	1	608	CLA	1	0
21	A	850	BCR	4	0
18	8	608	CLA	2	0
21	4	621	BCR	3	0
18	A	837	CLA	1	0
18	1	616	CLA	1	0
18	L	304	CLA	1	0
18	B	832	CLA	2	0
18	B	827	CLA	4	0
20	3	624	LHG	5	0
18	A	824	CLA	1	0
21	J	102	BCR	2	0
18	6	613	CLA	2	0
27	3	619	XAT	3	0
18	A	845	CLA	1	0
18	A	806	CLA	6	0
18	a	610	CLA	3	0
18	6	609	CLA	1	0
21	B	845	BCR	2	0
23	8	624	LMU	1	0
18	a	604	CLA	1	0
18	3	617	CLA	4	0
18	4	601	CLA	4	0
18	8	613	CLA	4	0
20	7	622	LHG	5	0
23	A	858	LMU	2	0
18	5	610	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	829	CLA	6	0
18	B	835	CLA	1	0
18	3	612	CLA	2	0
18	a	616	CLA	1	0
18	7	610	CLA	3	0
20	8	622	LHG	7	0
21	a	619	BCR	1	0
18	6	616	CLA	5	0
21	B	848	BCR	2	0
18	4	603	CLA	1	0
18	6	610	CLA	2	0
18	7	612	CLA	3	0
21	L	301	BCR	4	0
18	8	607	CLA	1	0
26	6	619	LUT	2	0
21	A	851	BCR	4	0
21	3	621	BCR	4	0
18	B	833	CLA	3	0
18	5	604	CLA	2	0
18	7	604	CLA	2	0
21	6	622	BCR	4	0
18	1	601	CLA	1	0
18	A	803	CLA	1	0
21	7	621	BCR	4	0
25	J	103	DGD	3	0
27	6	621	XAT	2	0
18	5	606	CLA	2	0
18	5	608	CLA	1	0
18	A	842	CLA	5	0
18	4	613	CLA	3	0
18	5	607	CLA	5	0
18	1	603	CLA	5	0
18	A	825	CLA	3	0
18	5	612	CLA	3	0
18	6	617	CLA	2	0
18	A	840	CLA	2	0
18	A	827	CLA	2	0
18	6	602	CLA	1	0
18	L	302	CLA	4	0
18	B	825	CLA	3	0
18	5	609	CLA	3	0
18	5	618	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	849	BCR	5	0
21	3	622	BCR	3	0
26	5	620	LUT	3	0
18	5	602	CLA	5	0
18	6	612	CLA	2	0
18	4	610	CLA	3	0
21	B	843	BCR	3	0
27	a	618	XAT	3	0
18	B	810	CLA	3	0
18	3	609	CLA	3	0
18	6	604	CLA	4	0
21	K	202	BCR	2	0
21	B	844	BCR	3	0
18	B	826	CLA	1	0
18	A	829	CLA	7	0
18	6	620	CLA	3	0
18	A	801	CLA	4	0
18	K	204	CLA	2	0
18	3	608	CLA	3	0
18	8	610	CLA	3	0
18	4	602	CLA	3	0
20	1	620	LHG	2	0
26	4	619	LUT	6	0
27	7	620	XAT	4	0
18	A	810	CLA	1	0
27	4	620	XAT	2	0
26	1	617	LUT	3	0
18	a	606	CLA	2	0
21	B	801	BCR	2	0
21	L	305	BCR	4	0
18	A	822	CLA	2	0
18	A	808	CLA	1	0
18	a	607	CLA	1	0
18	B	808	CLA	4	0
18	a	609	CLA	3	0
18	A	815	CLA	2	0
18	4	612	CLA	1	0
20	B	851	LHG	1	0
21	A	848	BCR	3	0
18	A	811	CLA	5	0
27	1	618	XAT	3	0
26	3	618	LUT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	620	BCR	5	0
18	B	828	CLA	3	0
18	B	811	CLA	4	0
18	A	807	CLA	2	0
18	4	609	CLA	1	0
18	6	607	CLA	1	0
18	6	601	CLA	3	0
26	7	619	LUT	3	0
18	1	613	CLA	2	0
18	B	824	CLA	3	0
18	B	821	CLA	1	0
18	A	838	CLA	2	0
18	A	804	CLA	3	0
21	7	623	BCR	1	0
18	A	821	CLA	1	0
18	B	802	CLA	1	0
18	A	813	CLA	2	0
20	a	620	LHG	7	0
18	A	854	CLA	5	0
20	A	846	LHG	3	0
21	K	207	BCR	4	0
21	5	622	BCR	3	0
18	3	610	CLA	5	0
23	A	859	LMU	3	0
18	B	813	CLA	6	0
18	8	616	CLA	1	0
21	1	619	BCR	1	0
18	A	818	CLA	5	0
18	B	814	CLA	1	0
18	B	819	CLA	1	0
20	5	625	LHG	3	0
24	J	104	LMG	4	0
18	K	201	CLA	2	0
18	a	608	CLA	1	0
18	B	817	CLA	5	0
18	3	607	CLA	1	0
18	1	612	CLA	1	0
18	A	835	CLA	4	0
20	6	623	LHG	1	0
24	5	627	LMG	3	0
18	B	803	CLA	3	0
18	B	805	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	609	CLA	3	0
21	F	305	BCR	6	0
23	A	857	LMU	1	0
18	K	203	CLA	1	0
18	A	802	CLA	5	0
18	L	303	CLA	1	0
18	1	602	CLA	2	0
28	5	624	NEX	4	0
18	A	836	CLA	5	0
20	3	623	LHG	1	0
18	B	809	CLA	2	0
18	B	806	CLA	3	0
18	a	611	CLA	1	0
18	B	818	CLA	4	0
18	3	603	CLA	1	0
18	F	301	CLA	2	0
18	A	823	CLA	1	0
18	8	604	CLA	1	0
18	B	837	CLA	5	0
18	5	619	CLA	1	0
18	B	838	CLA	3	0
21	A	852	BCR	2	0
18	B	840	CLA	2	0
18	7	601	CLA	2	0
21	8	621	BCR	2	0
18	a	613	CLA	4	0
18	6	611	CLA	1	0
18	A	828	CLA	8	0
18	B	839	CLA	1	0
18	8	601	CLA	1	0
21	A	856	BCR	6	0
18	A	834	CLA	3	0
18	4	614	CLA	1	0
18	8	606	CLA	1	0
18	B	807	CLA	3	0
18	A	831	CLA	2	0
26	8	619	LUT	5	0
18	B	834	CLA	3	0
18	5	613	CLA	4	0
18	A	841	CLA	3	0
18	B	841	CLA	3	0
18	a	603	CLA	2	0

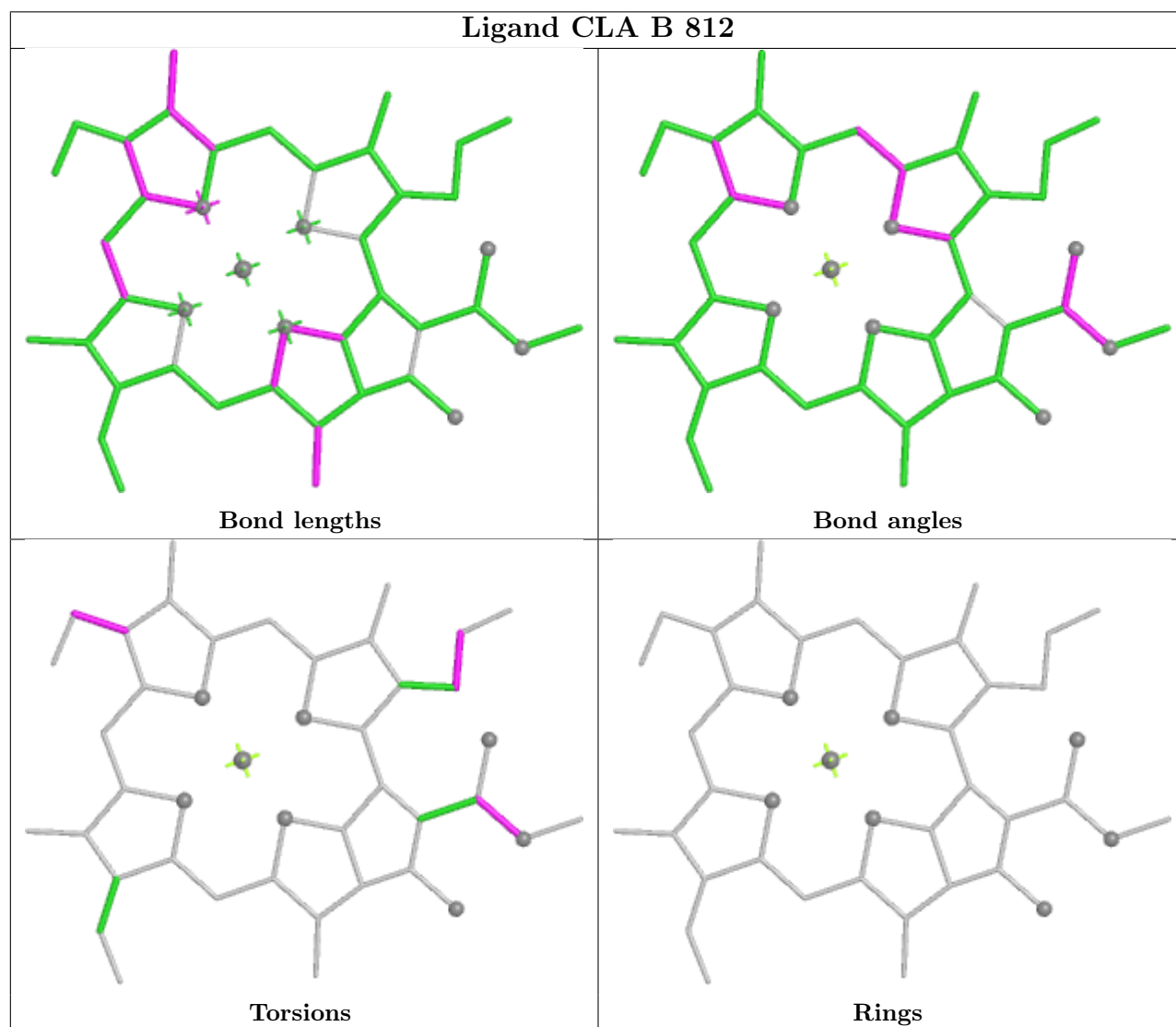
Continued on next page...

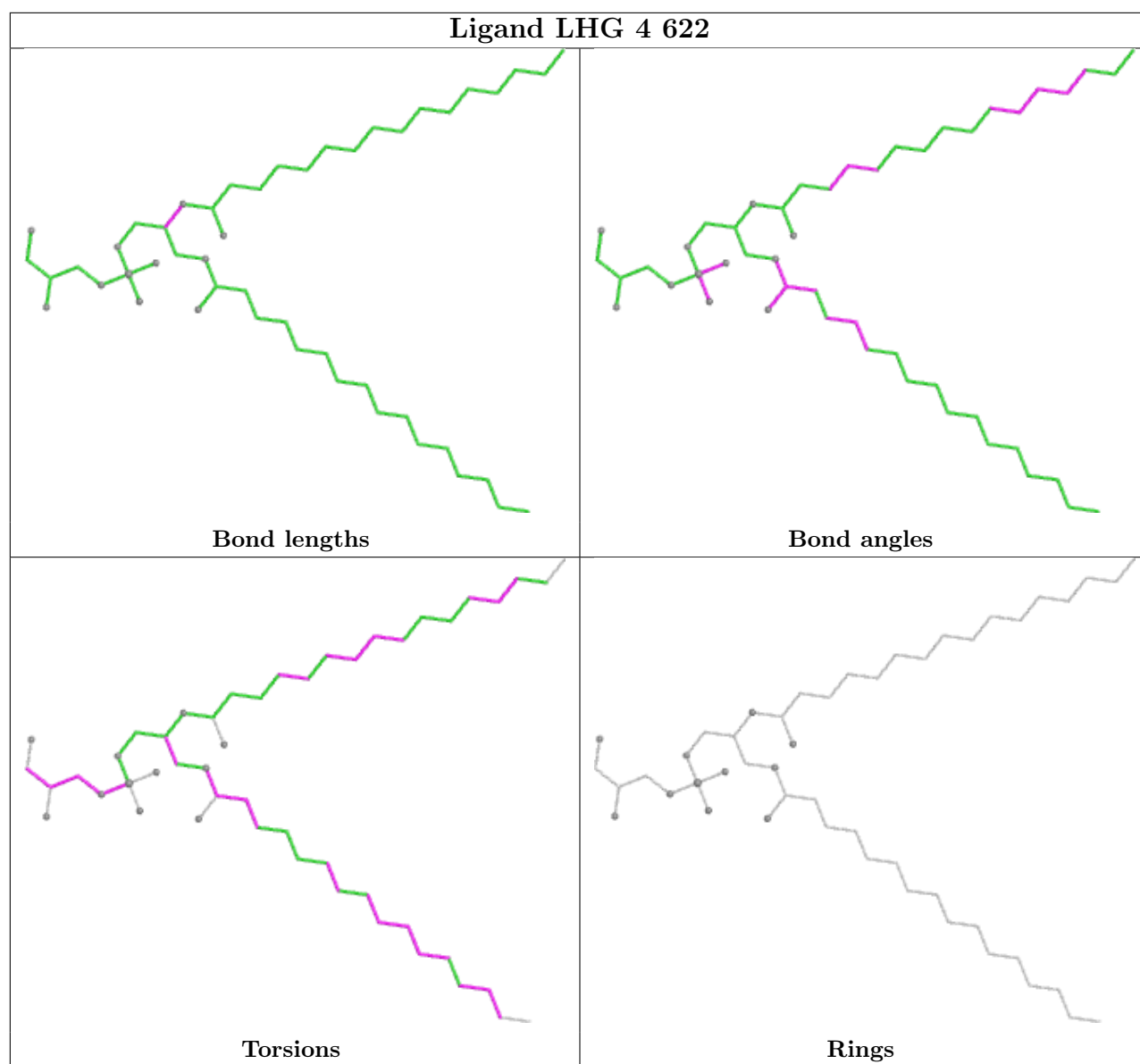
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	304	CLA	1	0
19	B	842	PQN	2	0
18	3	606	CLA	1	0
18	A	830	CLA	5	0
18	1	610	CLA	1	0
20	5	623	LHG	2	0
21	B	847	BCR	4	0
26	a	617	LUT	4	0
18	4	608	CLA	1	0
18	A	819	CLA	3	0
25	B	850	DGD	3	0
18	7	611	CLA	3	0
20	8	623	LHG	2	0
18	1	611	CLA	1	0
18	A	809	CLA	1	0
18	8	611	CLA	2	0
18	4	616	CLA	1	0
19	A	844	PQN	3	0
27	5	621	XAT	5	0
18	A	843	CLA	1	0
18	A	839	CLA	2	0
18	6	603	CLA	1	0
18	B	831	CLA	4	0
21	B	846	BCR	3	0
18	5	617	CLA	1	0
18	7	608	CLA	4	0
28	6	624	NEX	4	0
18	7	602	CLA	2	0
27	8	620	XAT	2	0
18	A	812	CLA	4	0
18	K	206	CLA	1	0
18	A	820	CLA	5	0

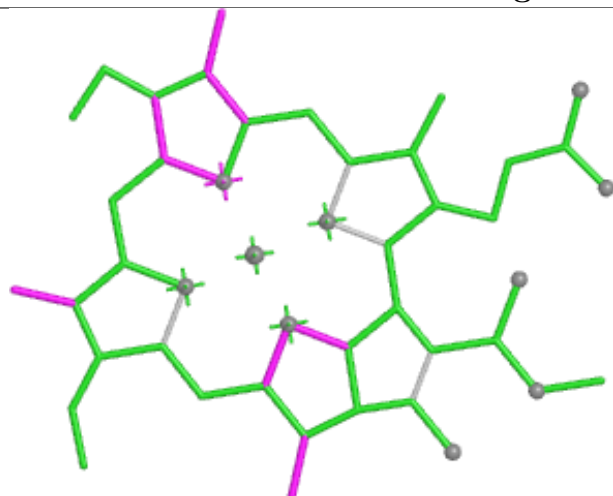
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

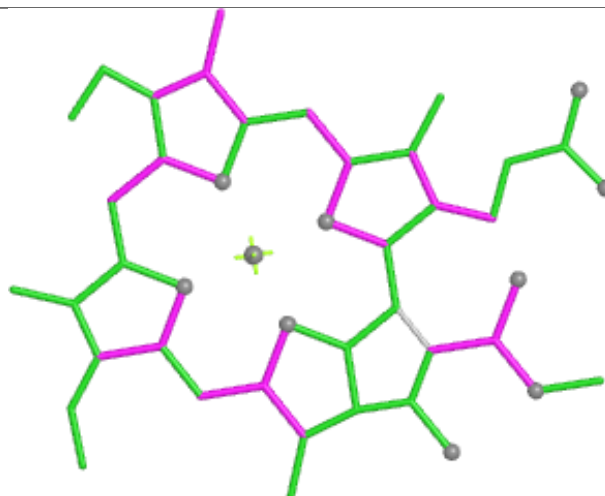




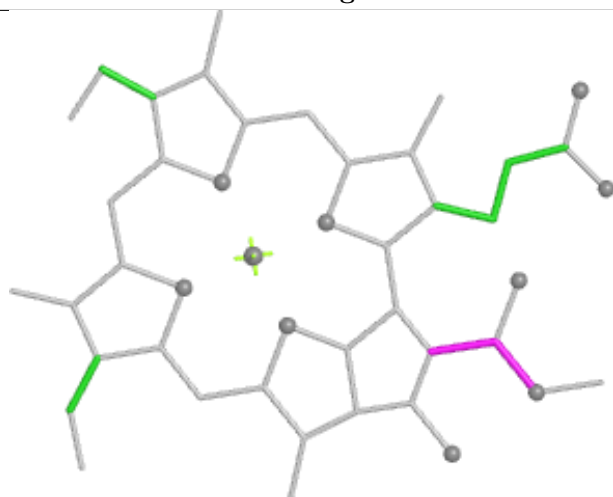
Ligand CLA A 817



Bond lengths



Bond angles

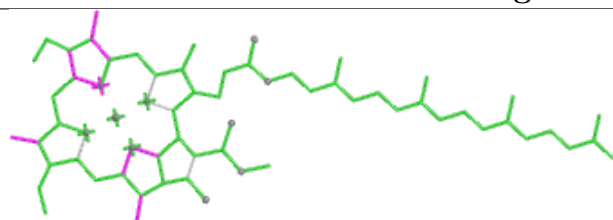


Torsions

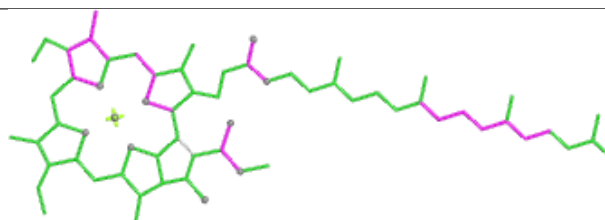


Rings

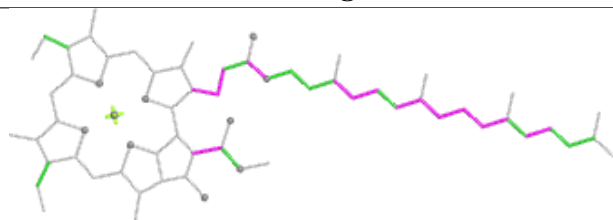
Ligand CLA A 814



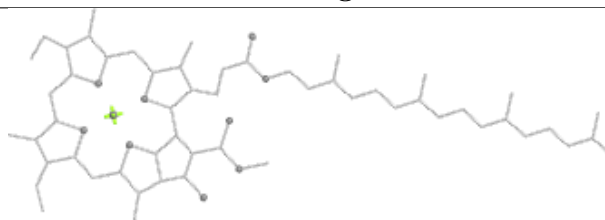
Bond lengths



Bond angles

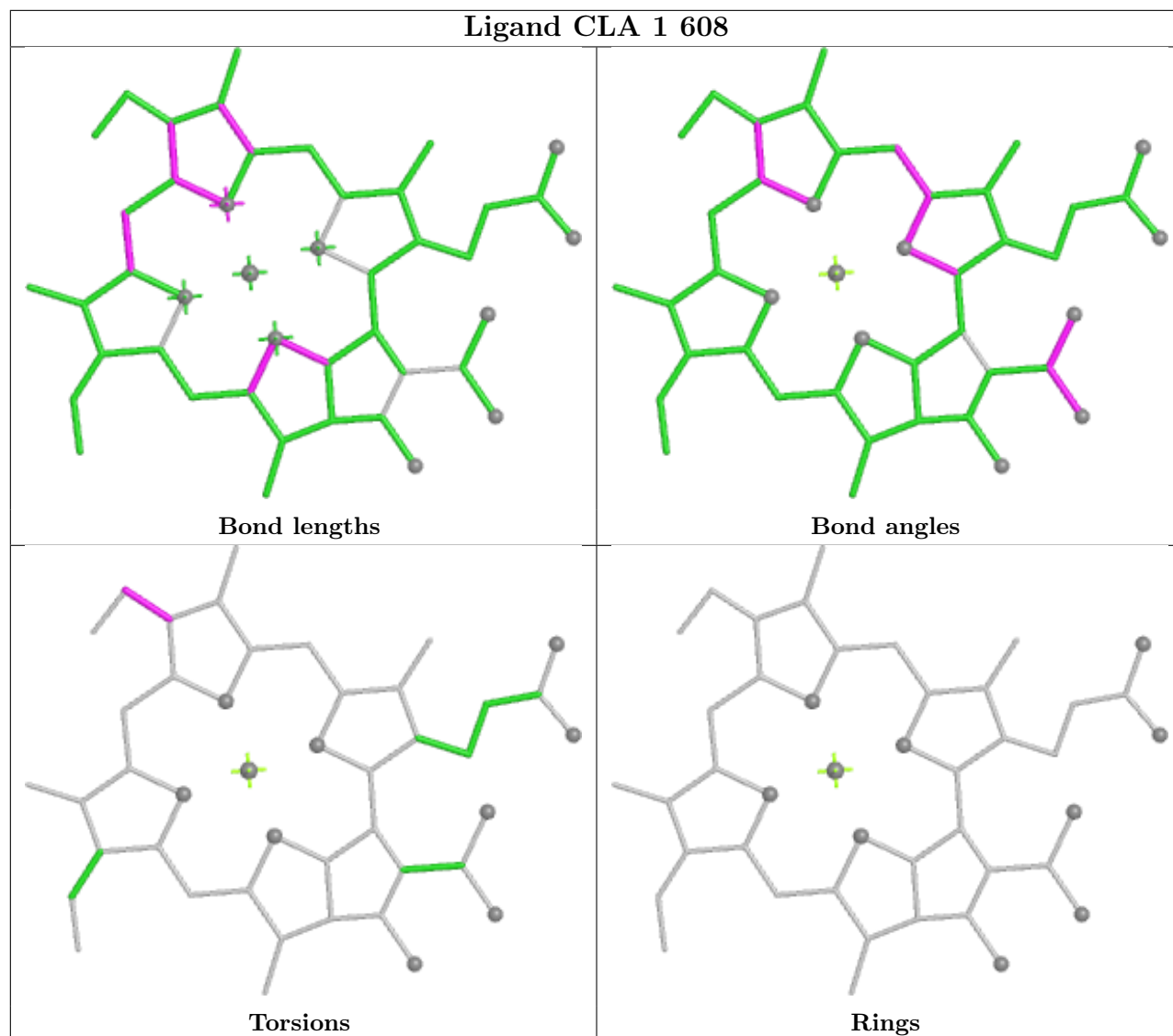


Torsions

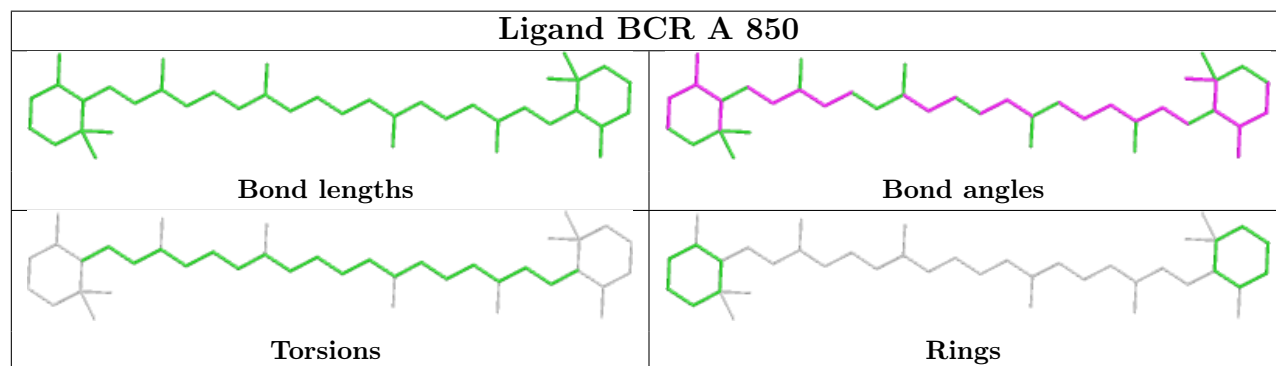


Rings

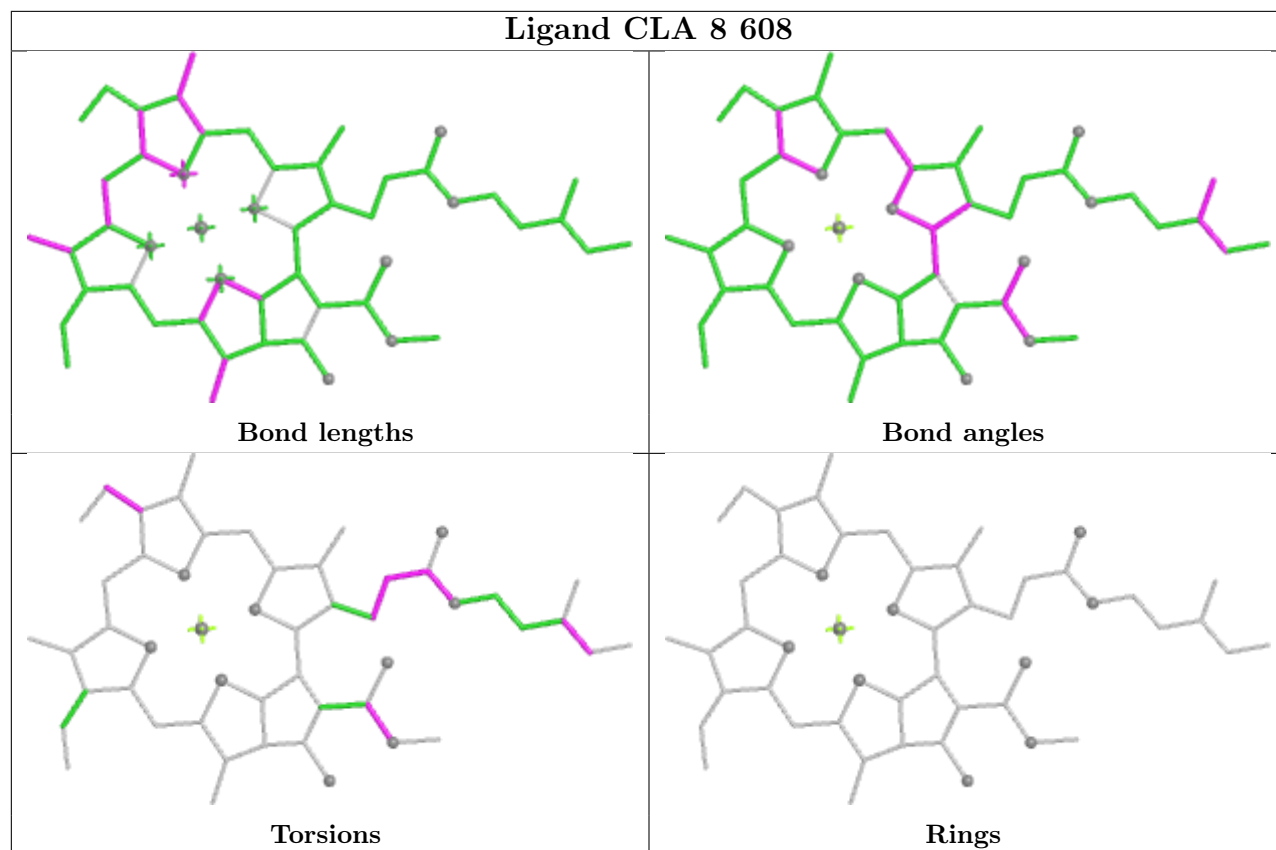
Ligand CLA 1 608



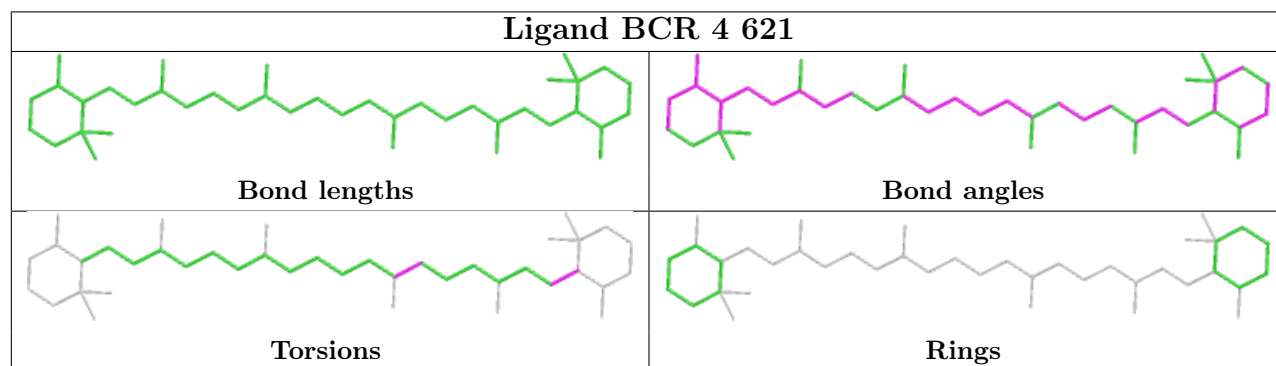
Ligand BCR A 850



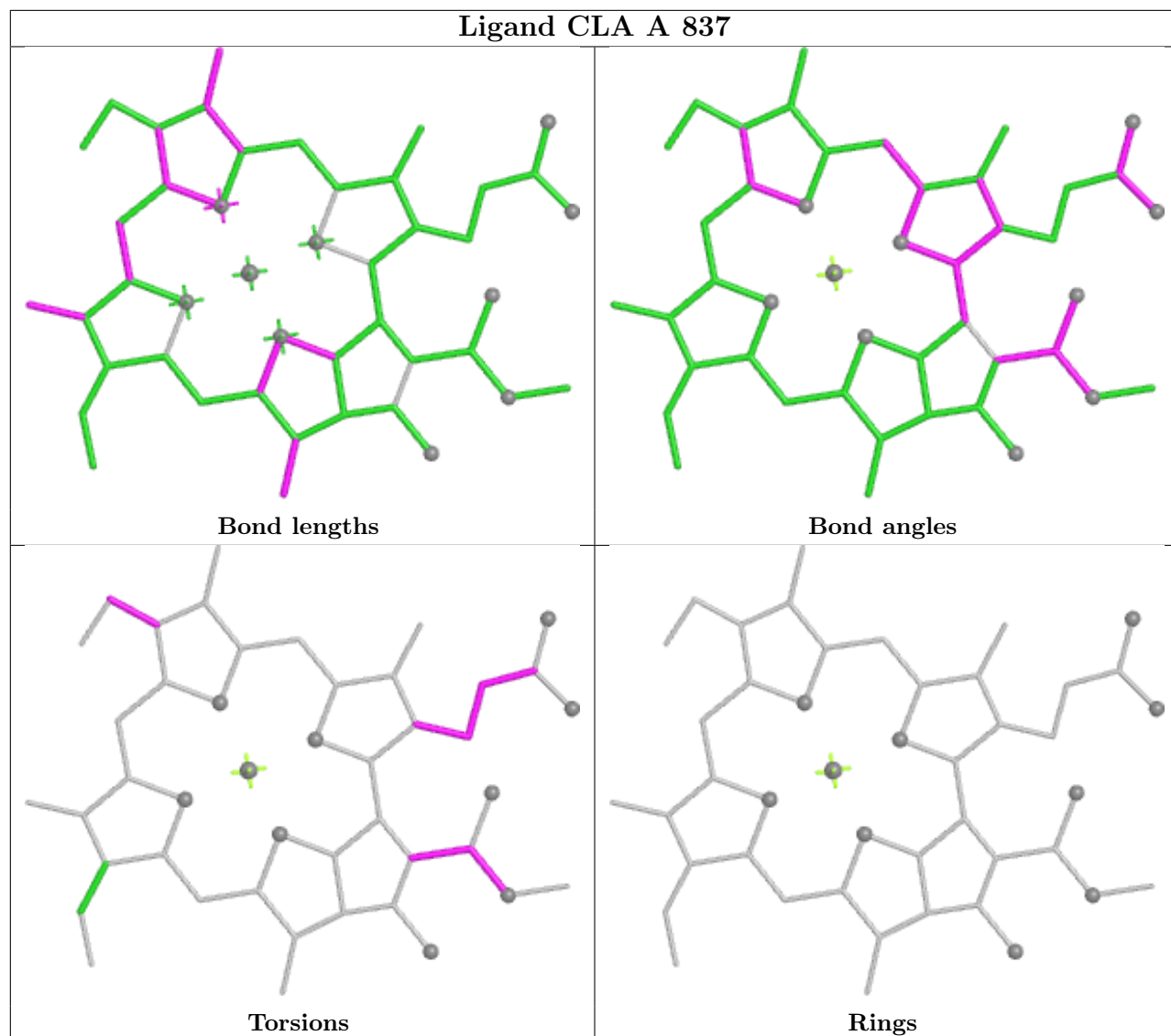
Ligand CLA 8 608



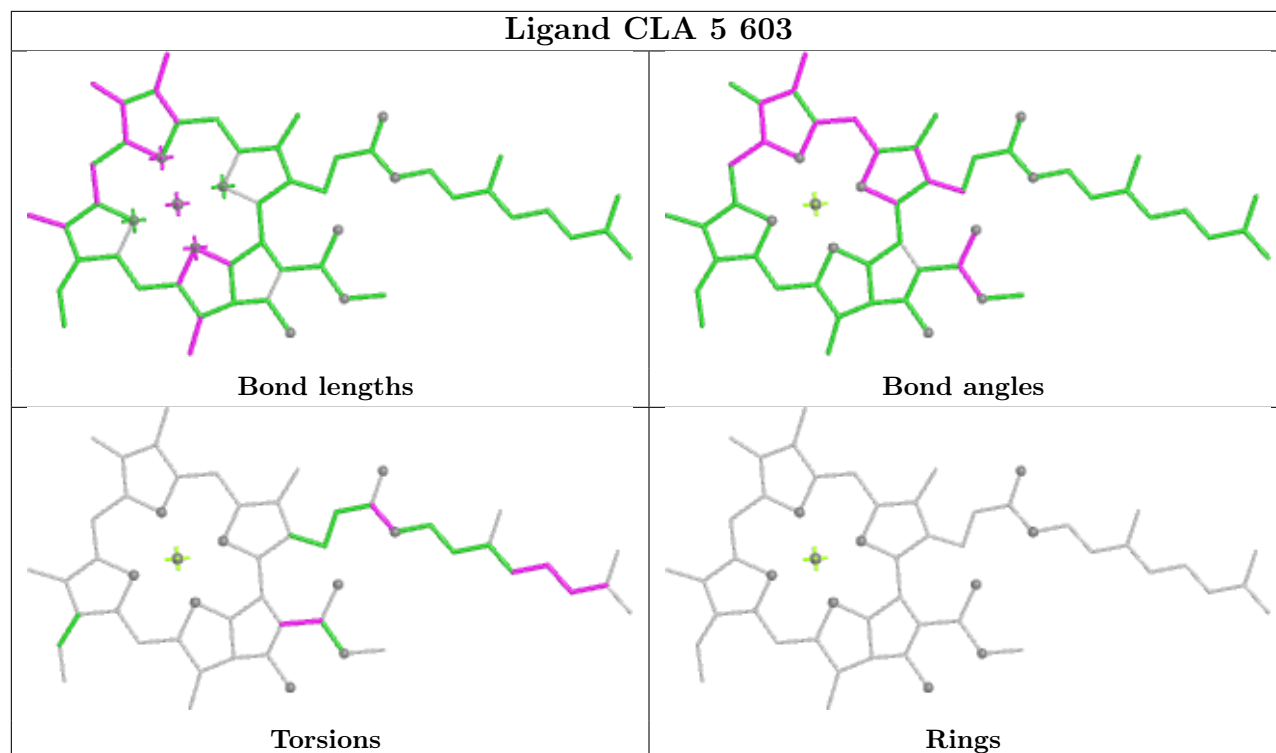
Ligand BCR 4 621



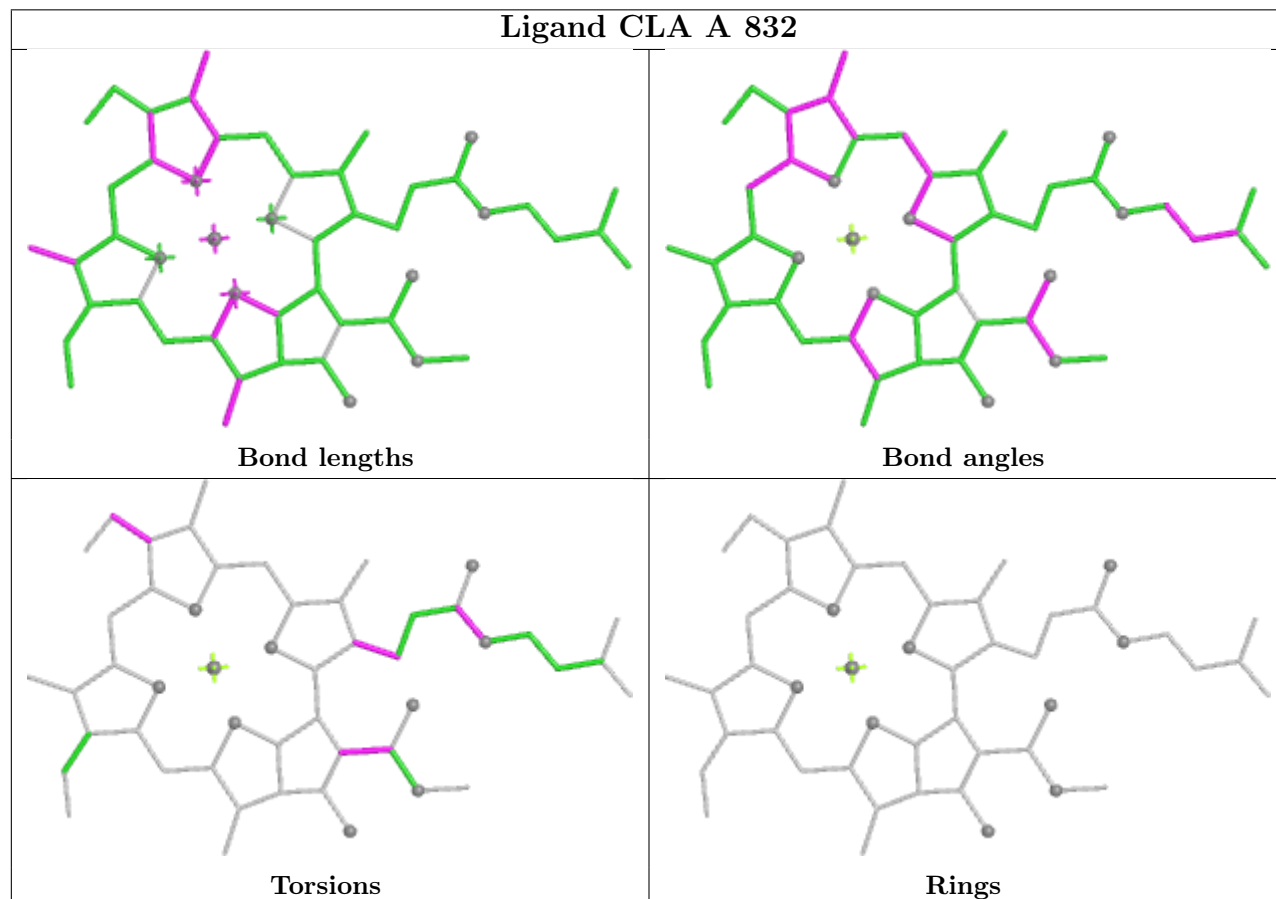
Ligand CLA A 837



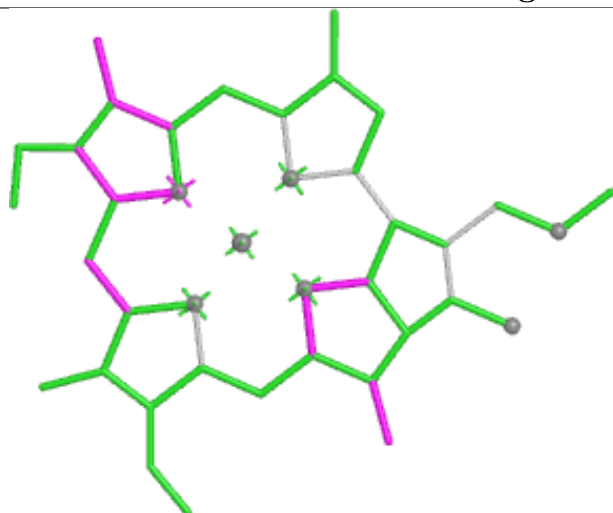
Ligand CLA 5 603



Ligand CLA A 832



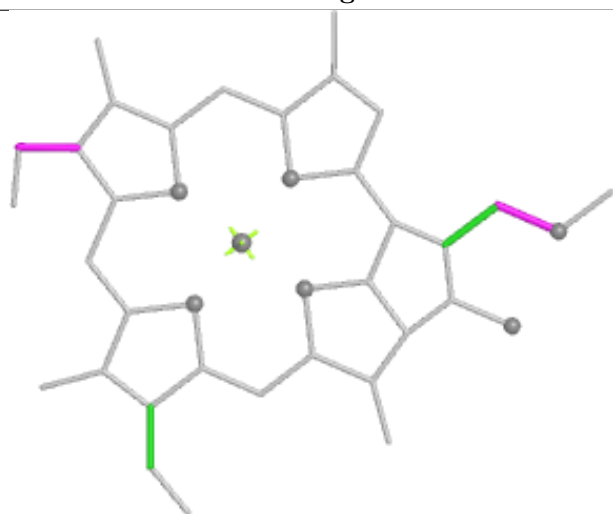
Ligand CLA 1 606



Bond lengths



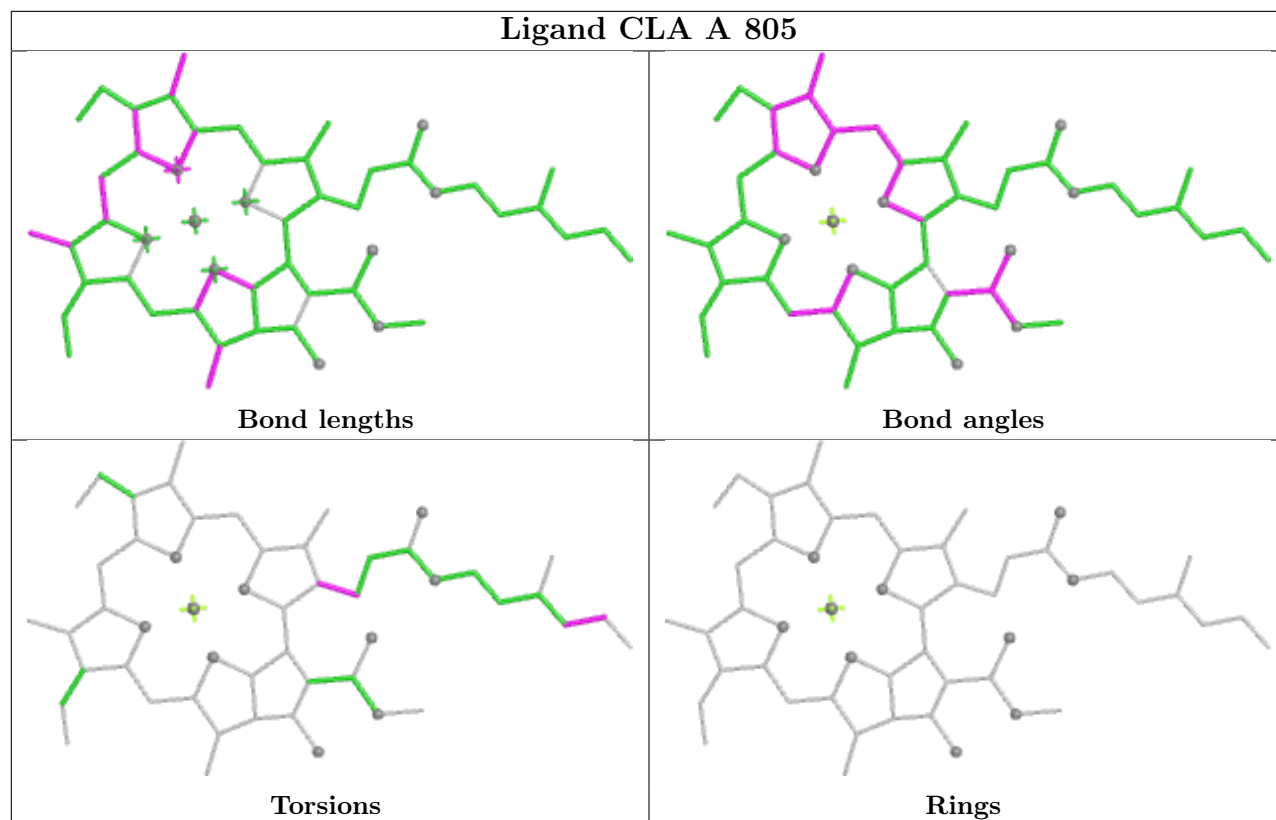
Bond angles



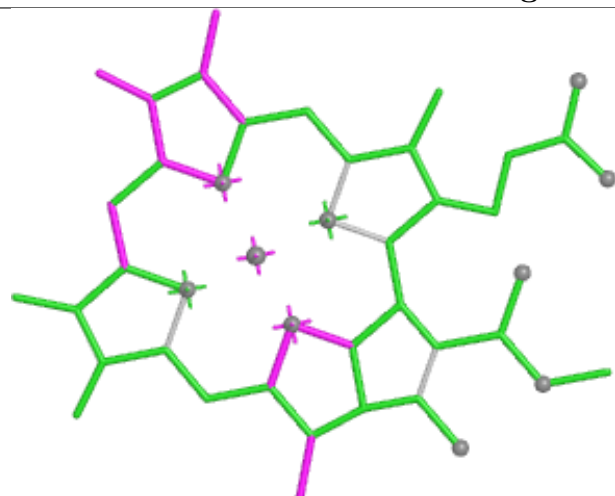
Torsions



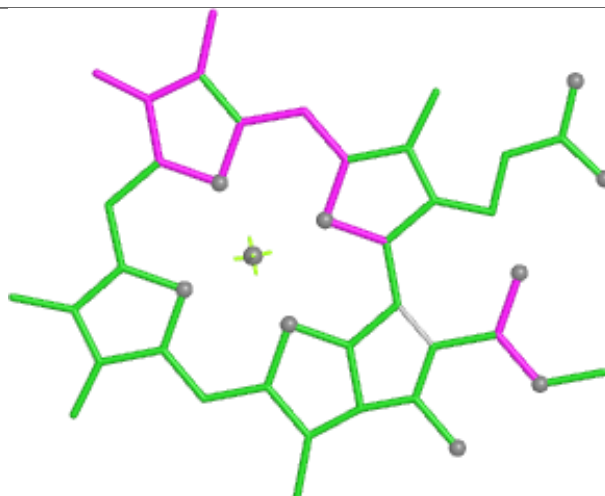
Rings



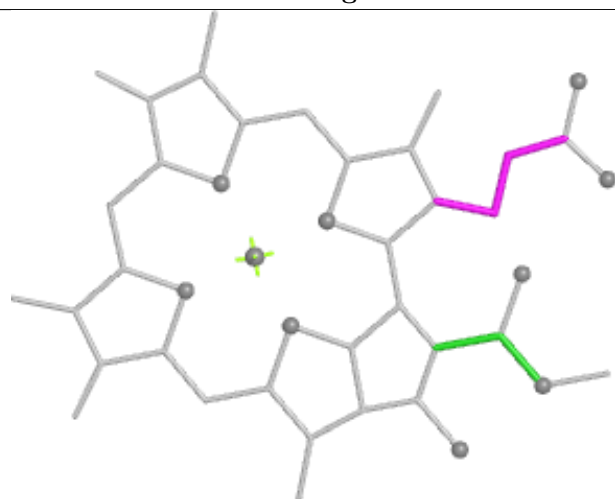
Ligand CLA 1 616



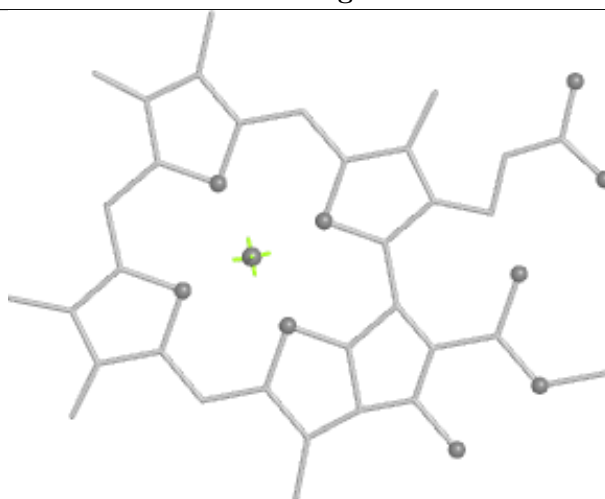
Bond lengths



Bond angles

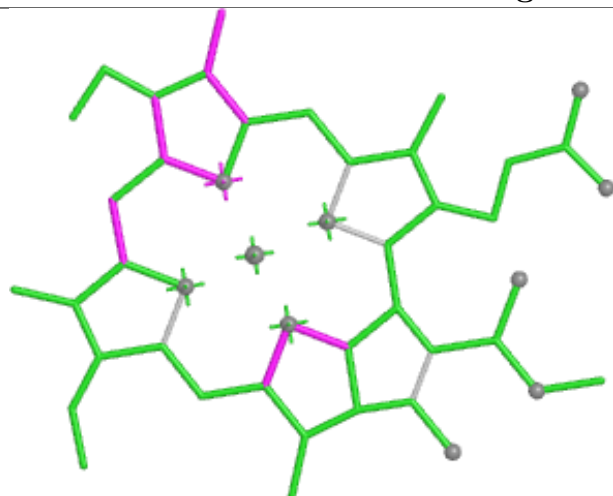


Torsions

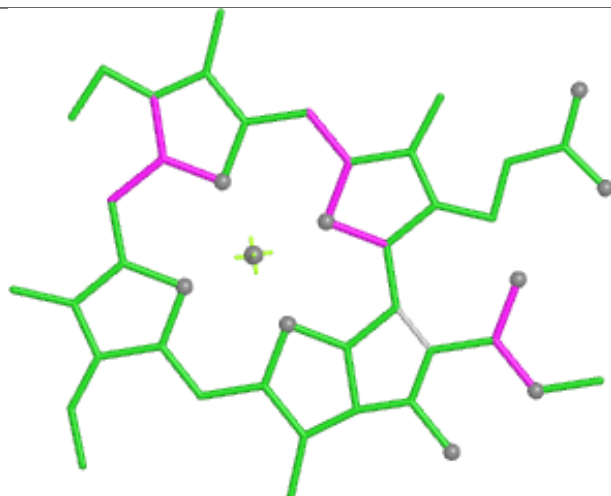


Rings

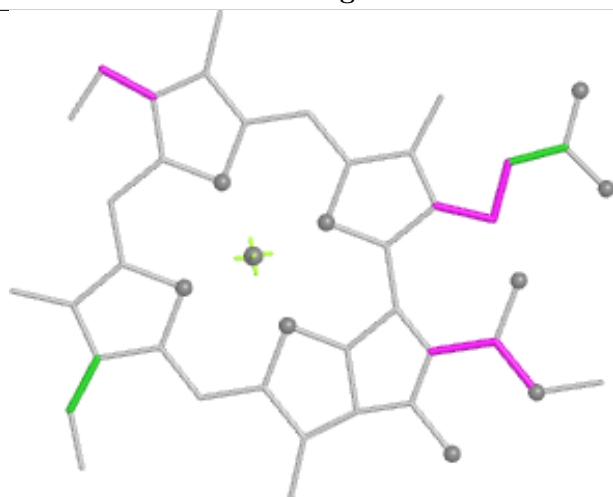
Ligand CLA L 304



Bond lengths



Bond angles

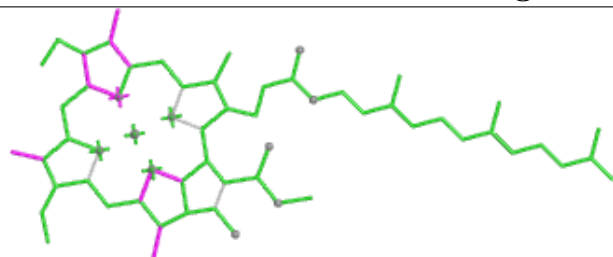


Torsions

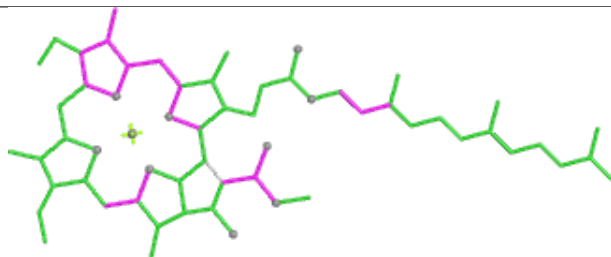


Rings

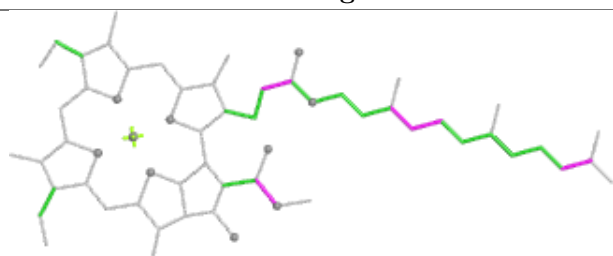
Ligand CLA B 832



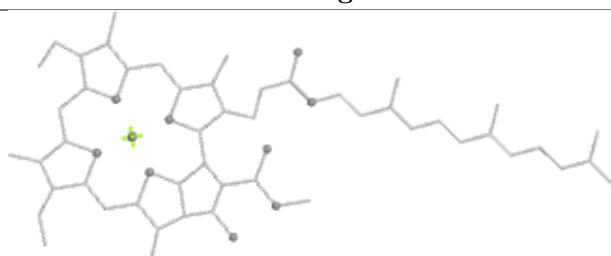
Bond lengths



Bond angles

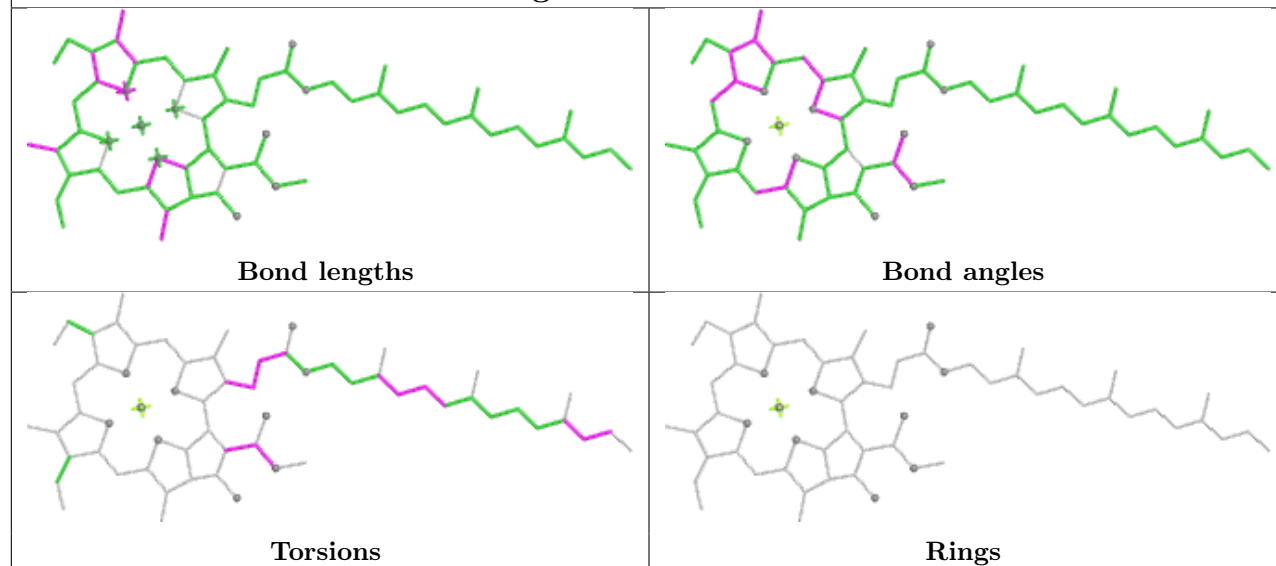


Torsions

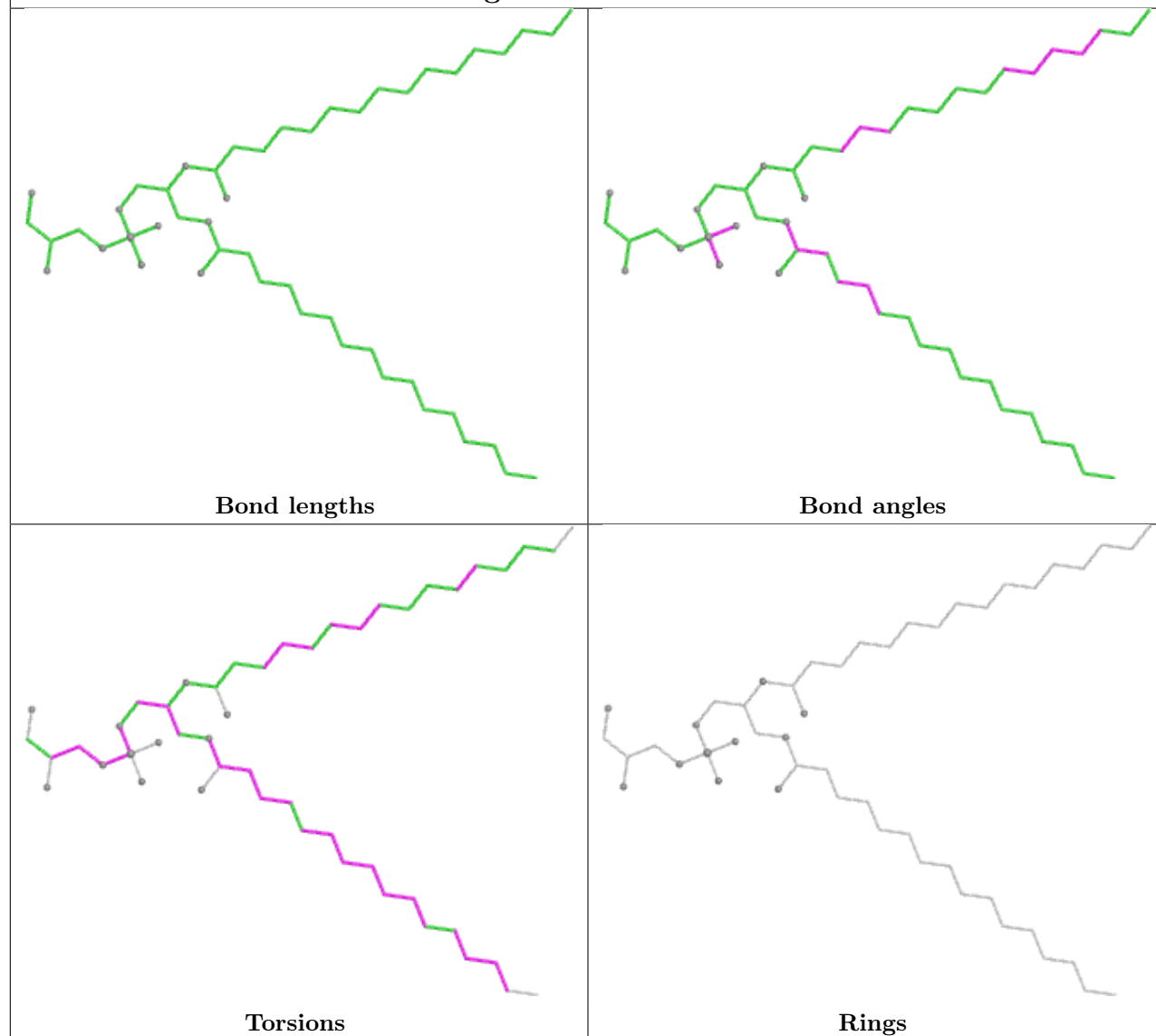


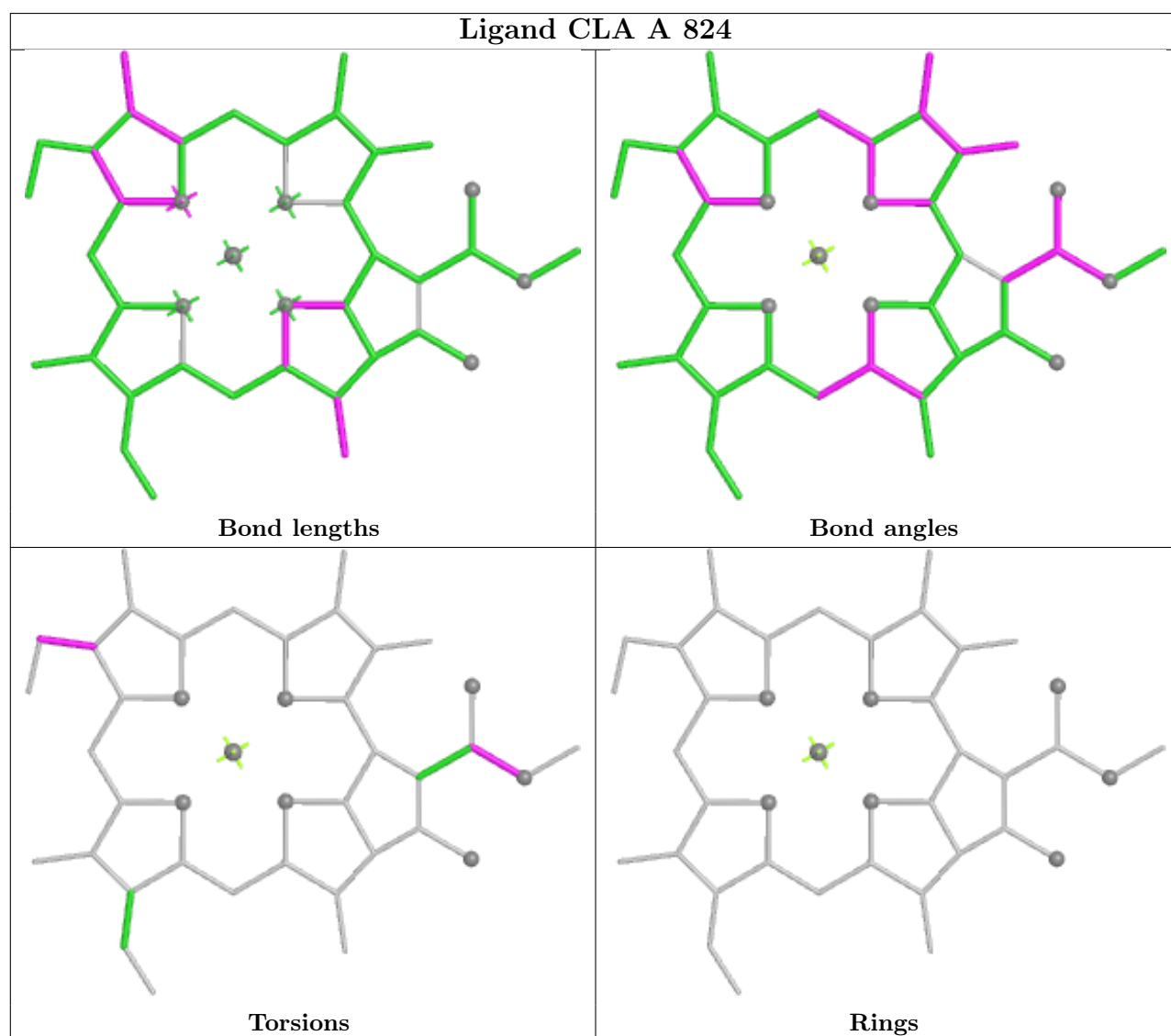
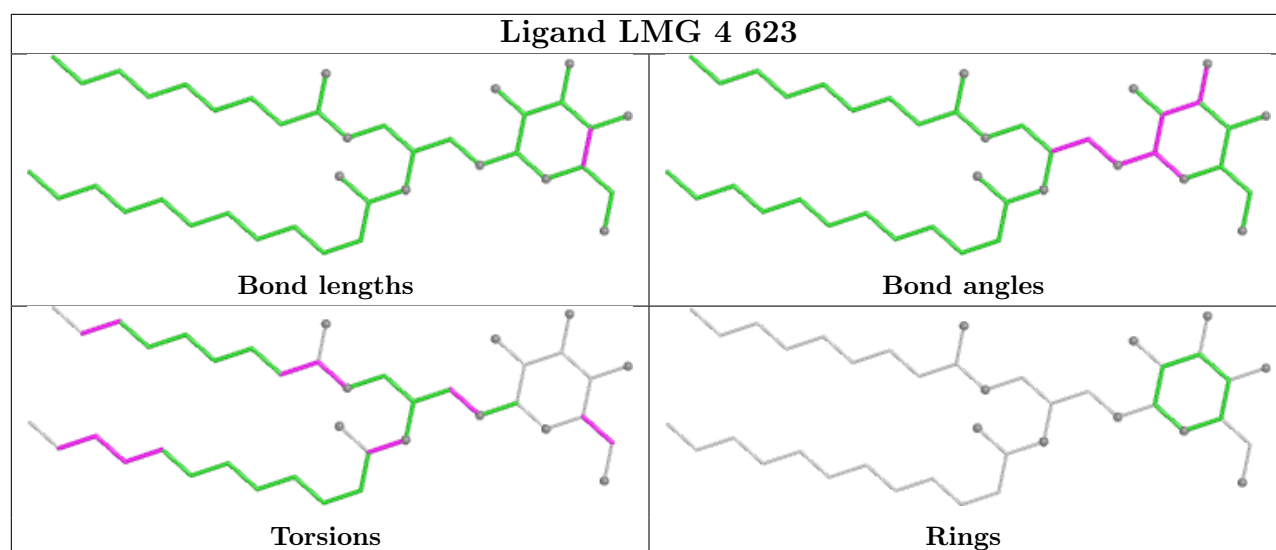
Rings

Ligand CLA B 827

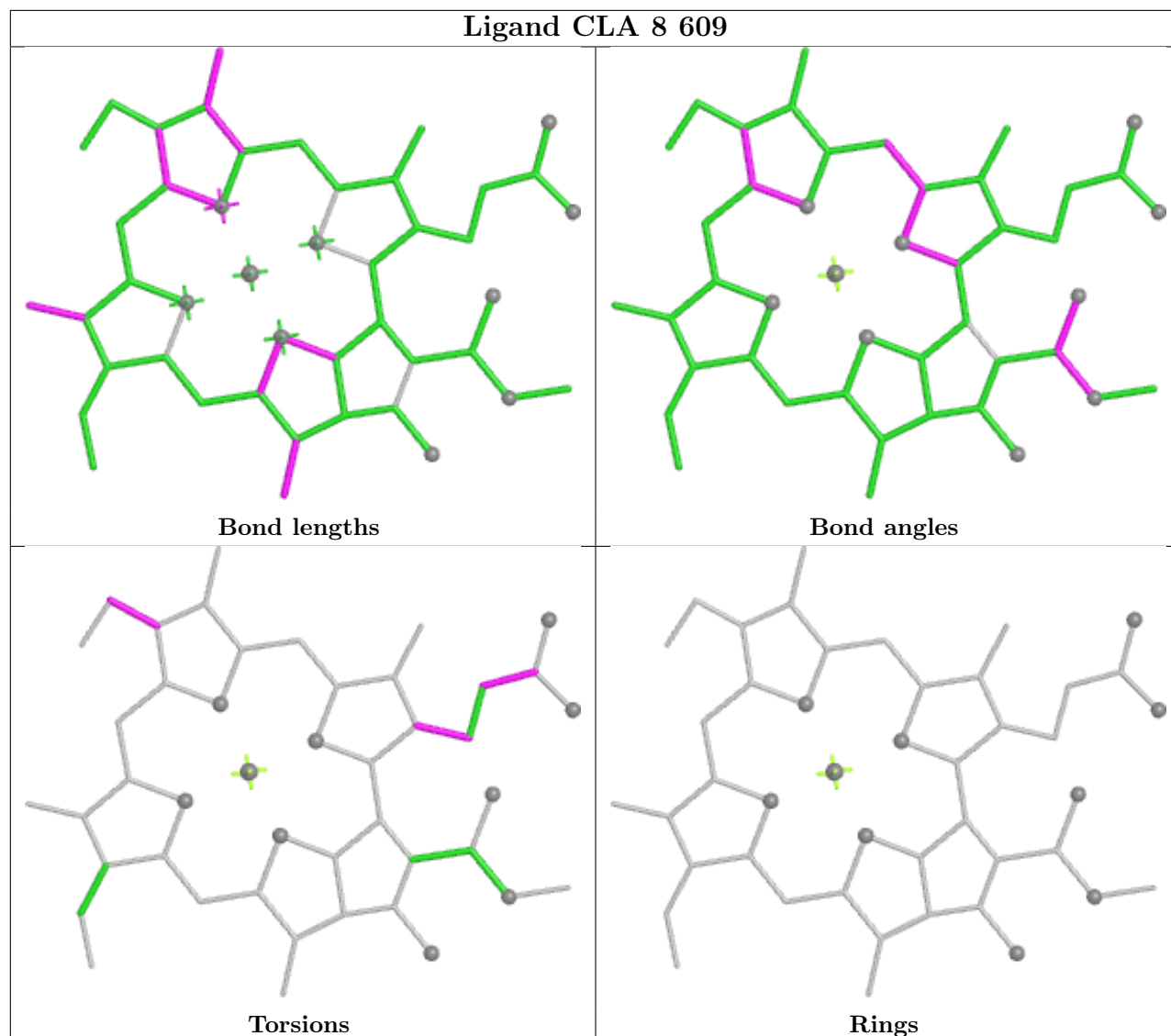


Ligand LHG 3 624

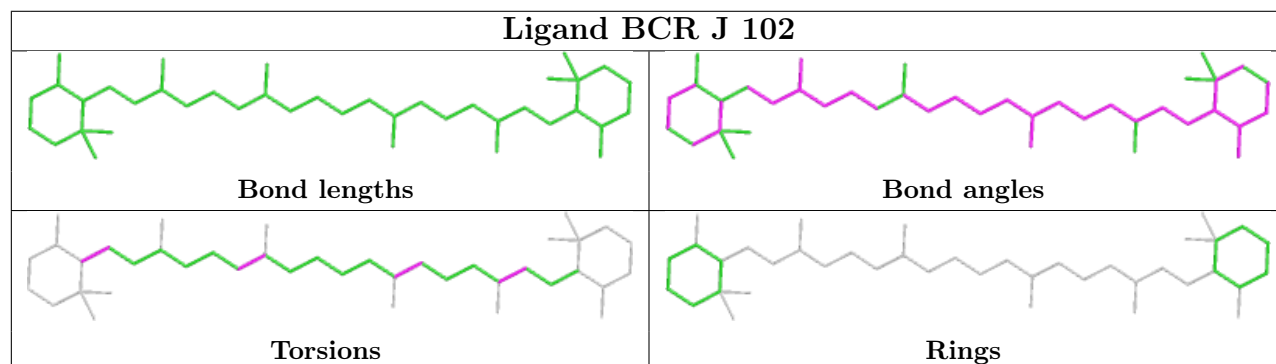




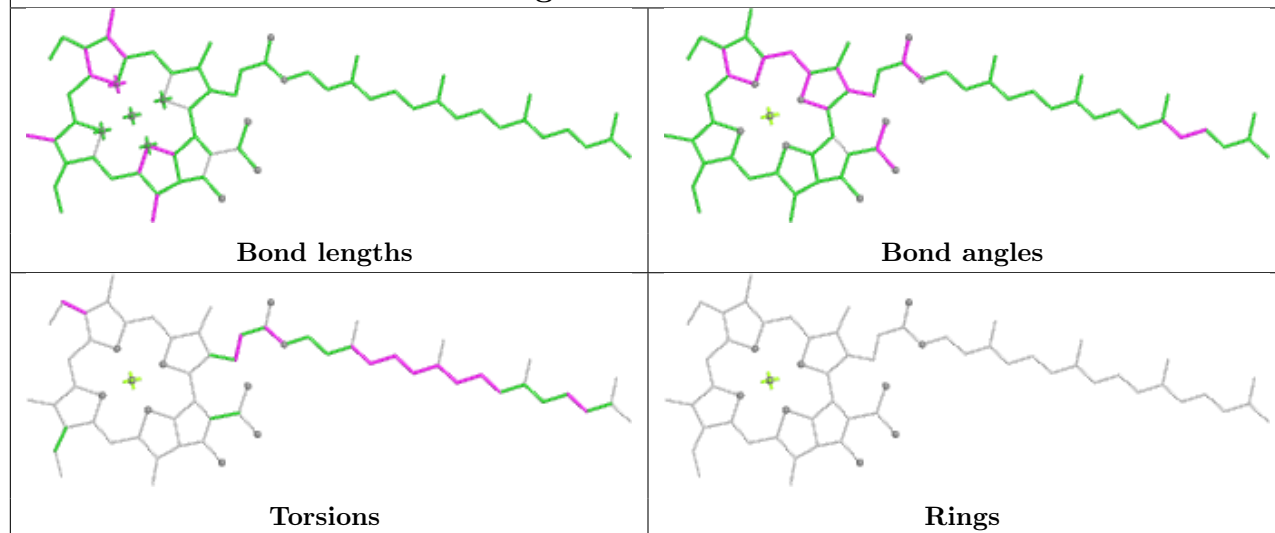
Ligand CLA 8 609



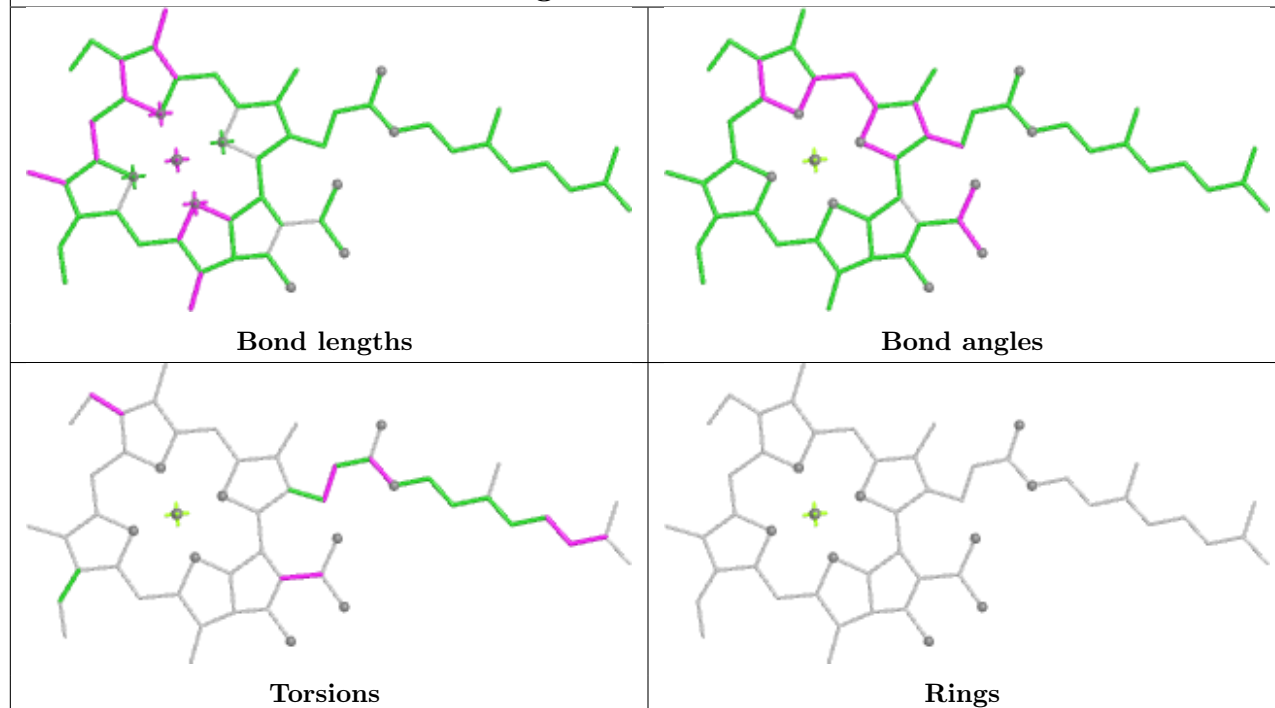
Ligand BCR J 102



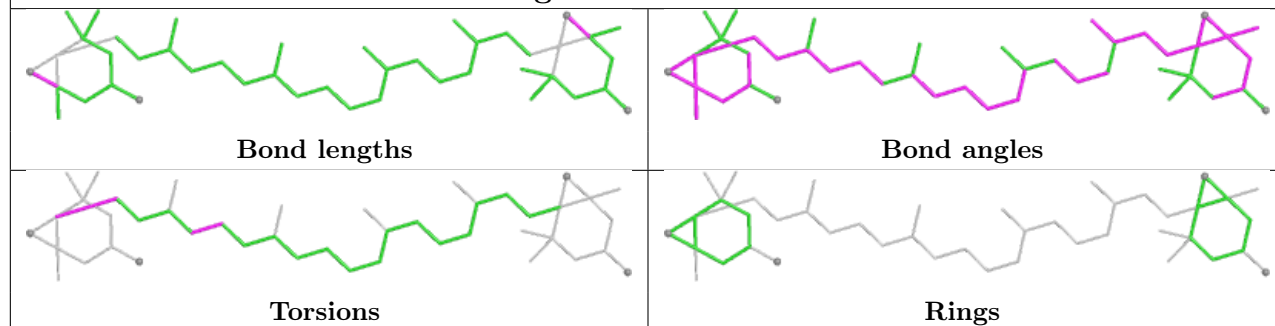
Ligand CLA 6 613



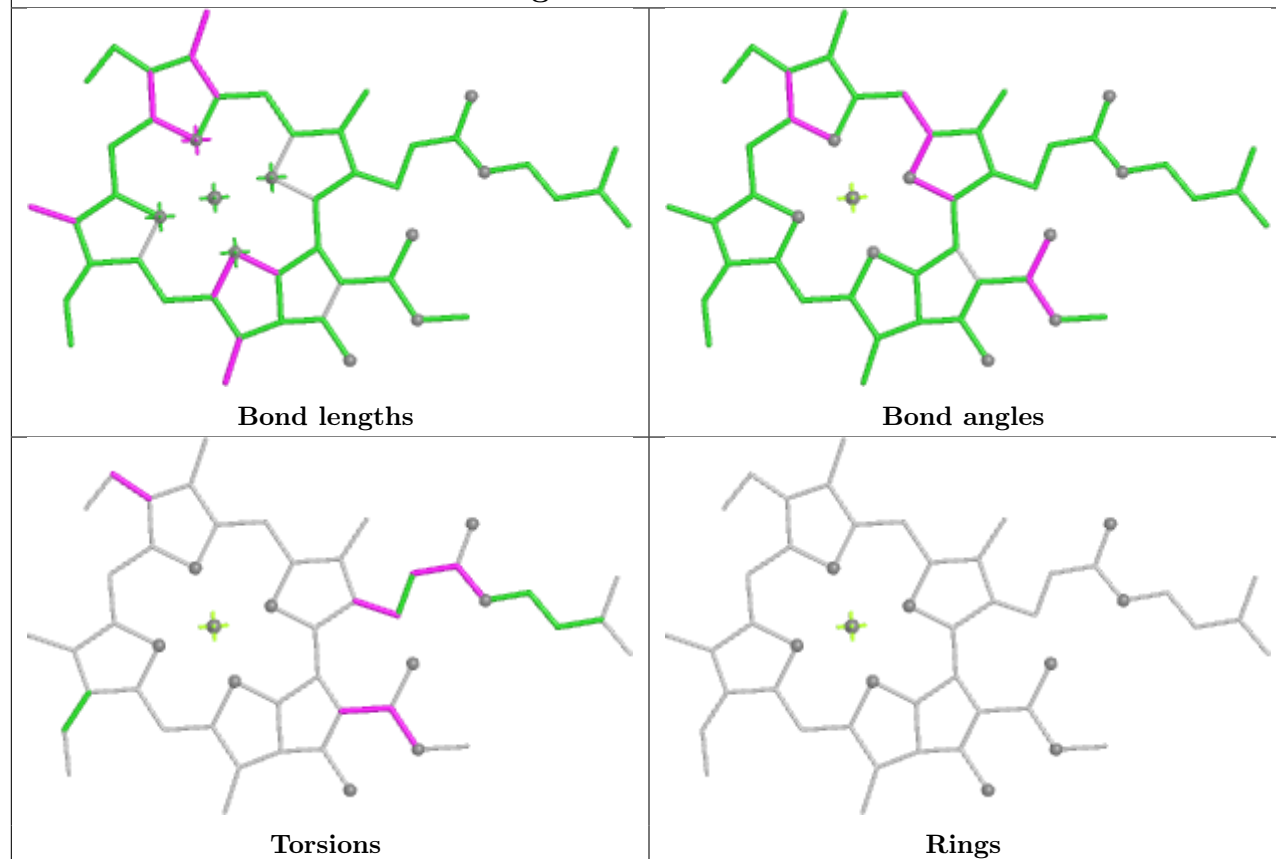
Ligand CLA a 601



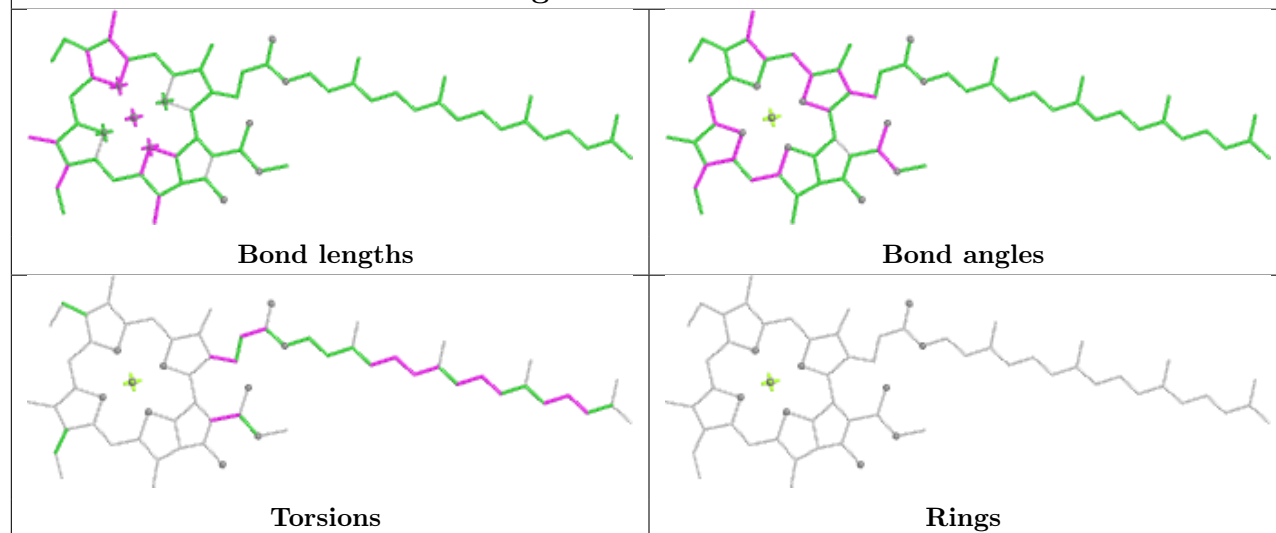
Ligand XAT 3 619

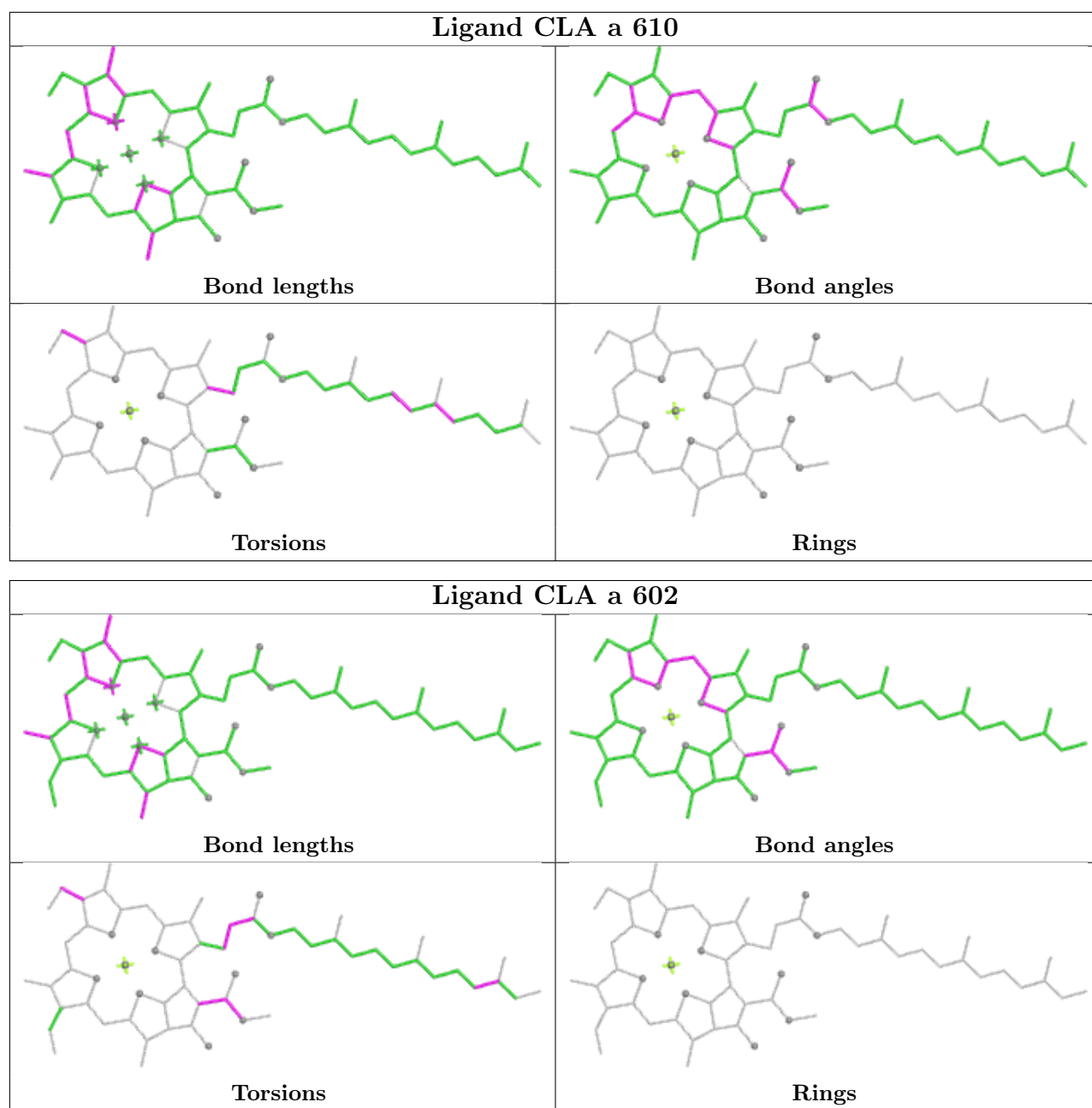


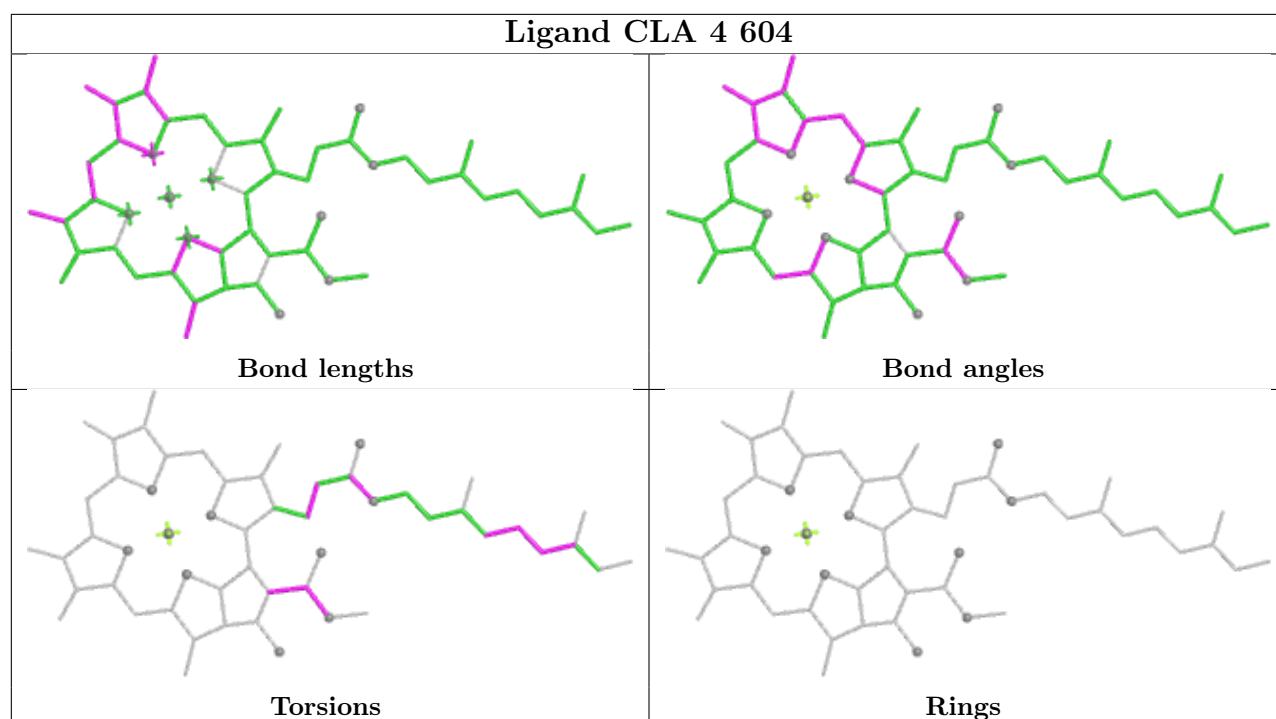
Ligand CLA A 845



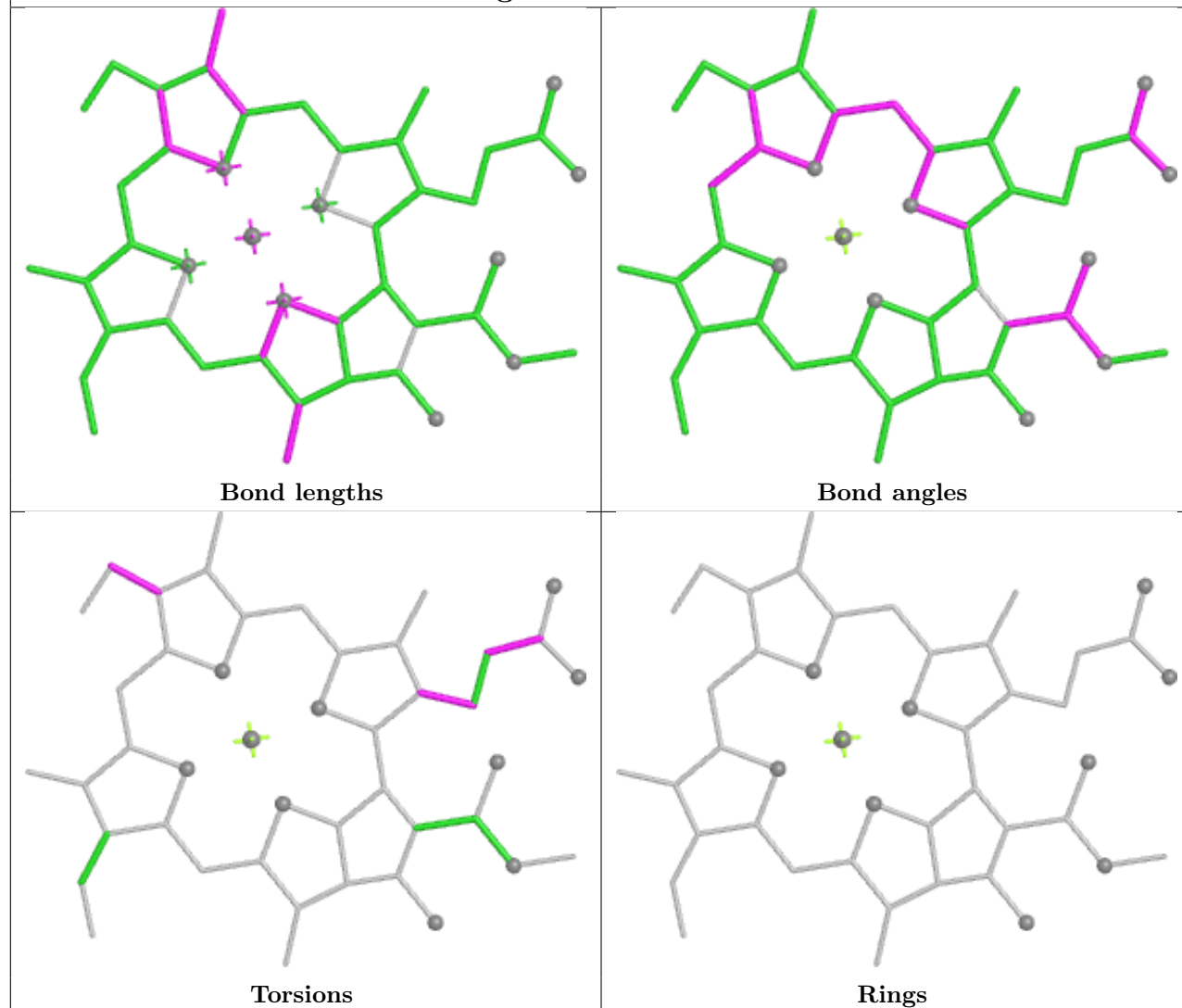
Ligand CLA A 806



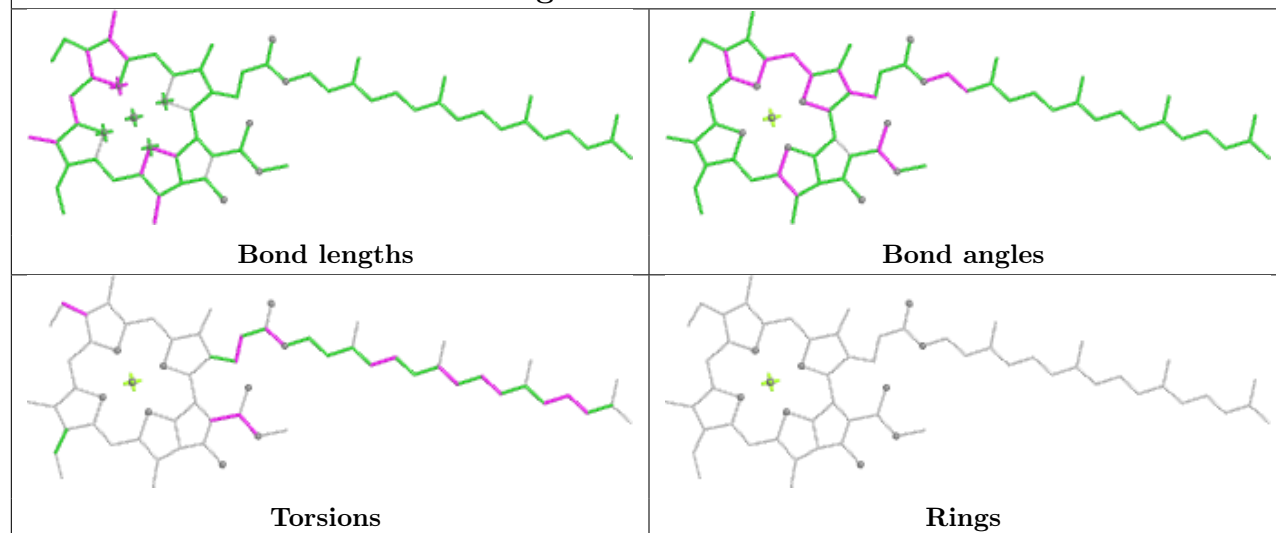


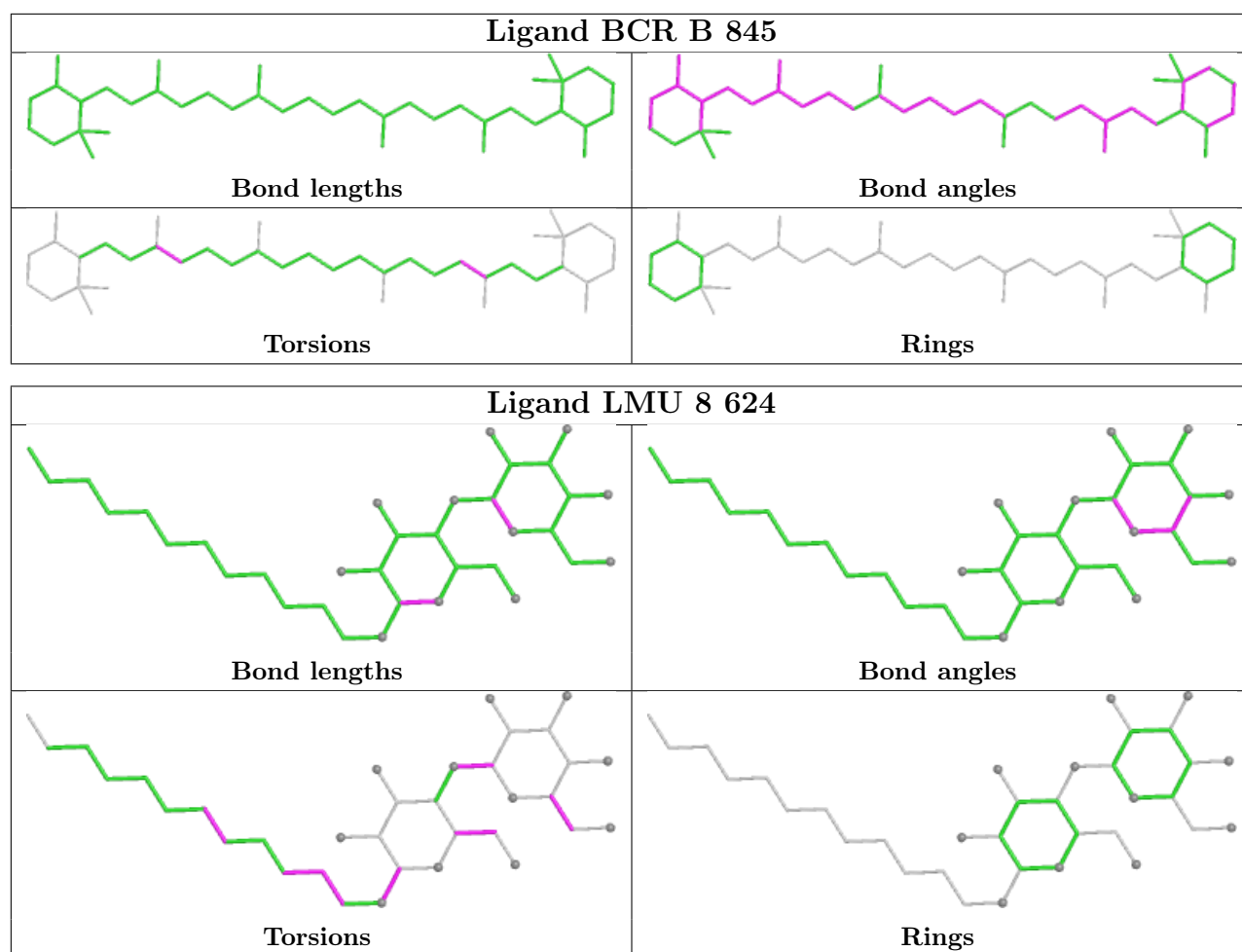


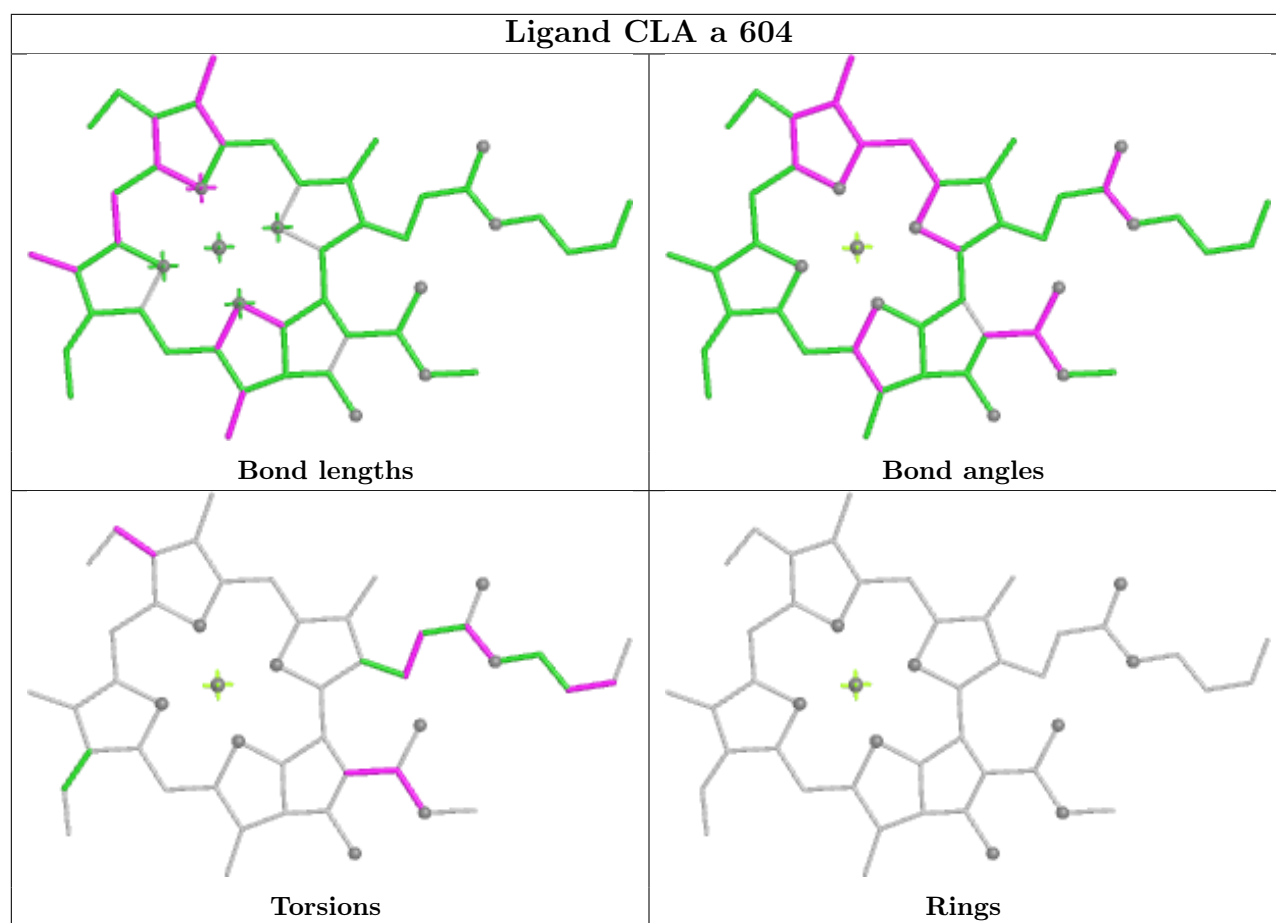
Ligand CLA 6 609



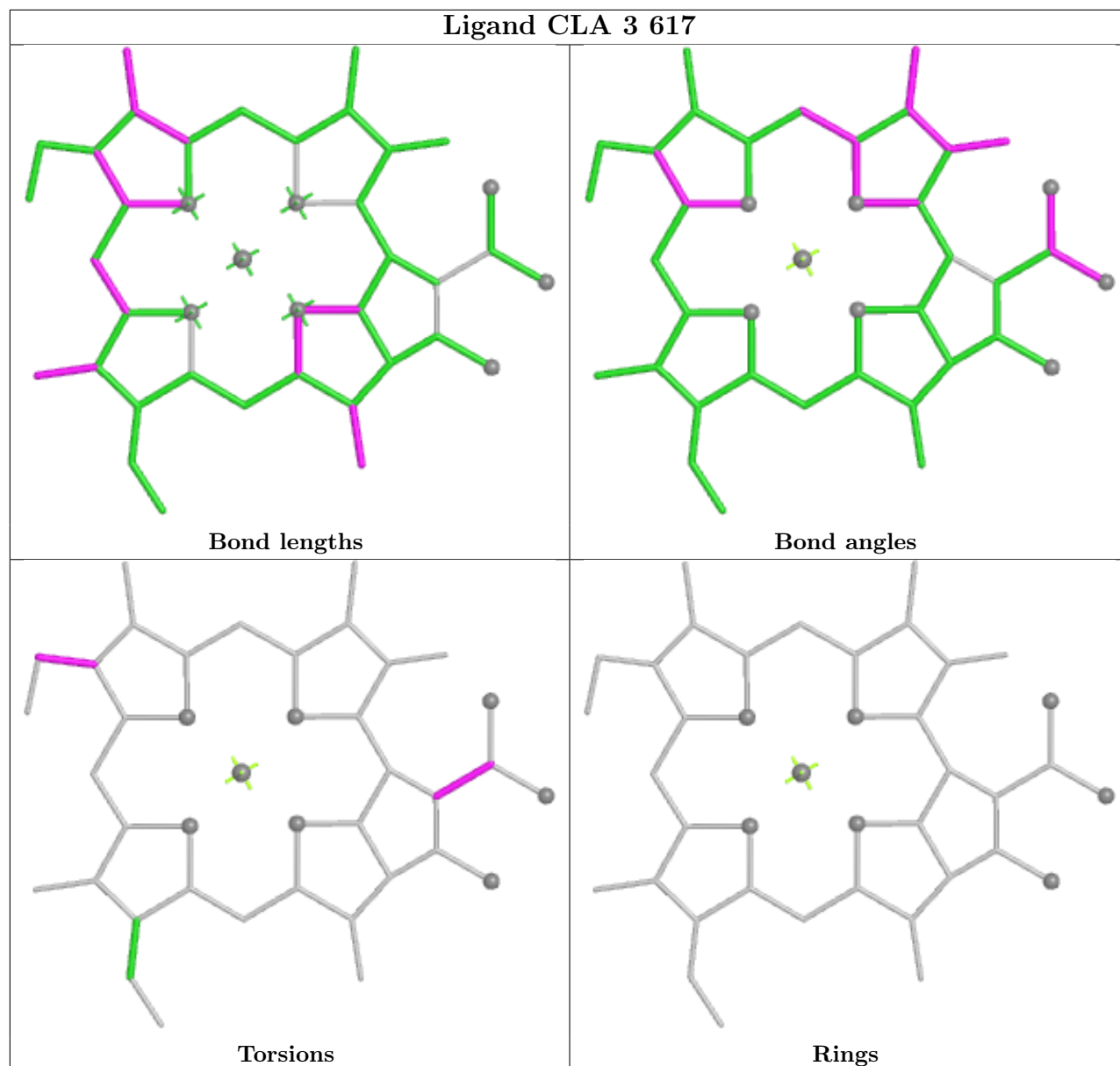
Ligand CLA 7 613



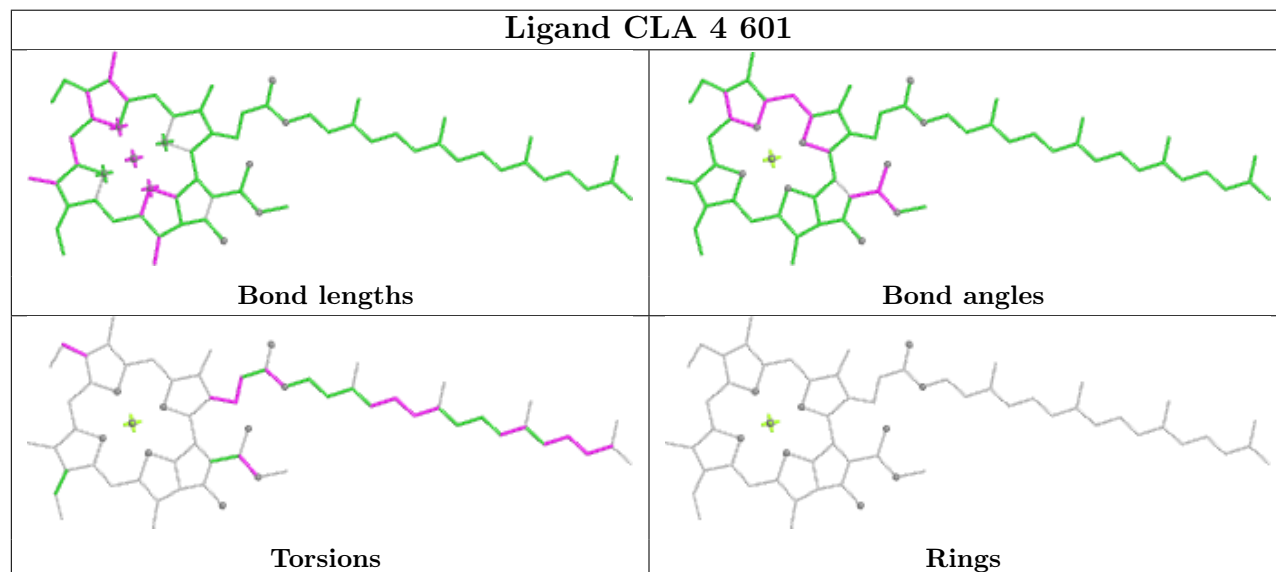




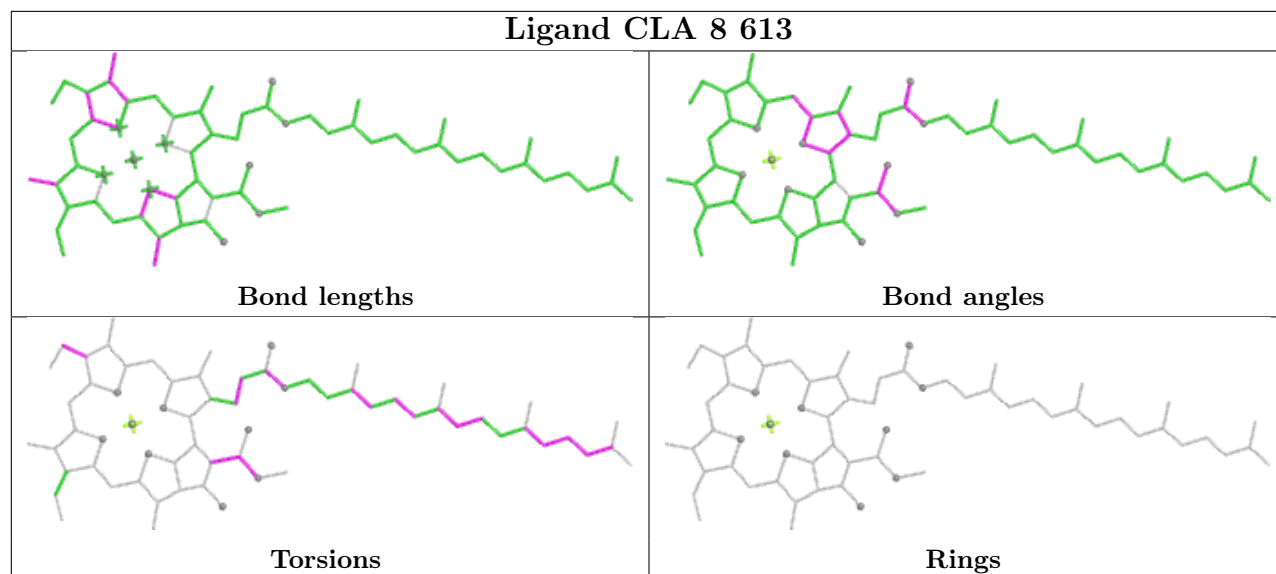
Ligand CLA 3 617



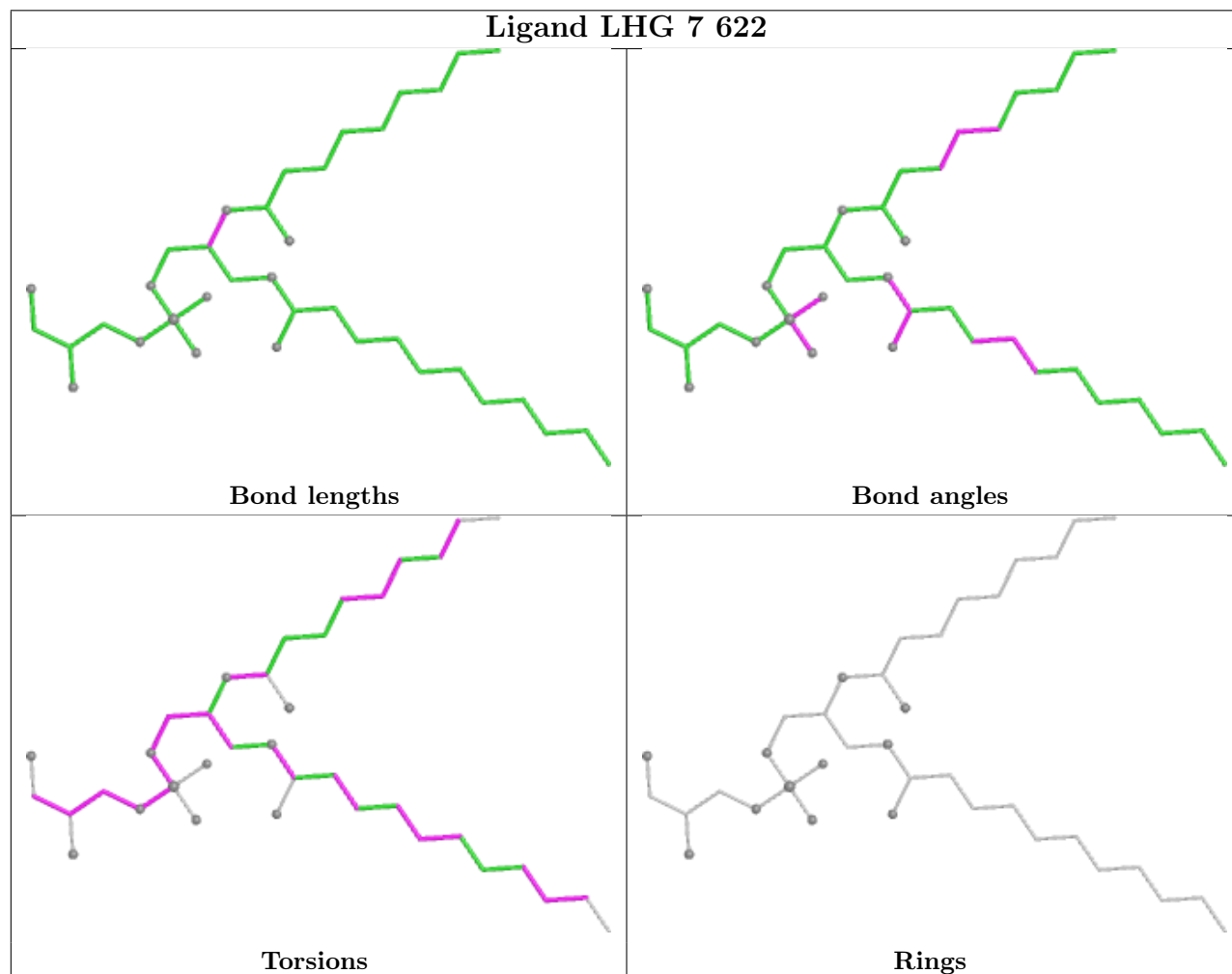
Ligand CLA 4 601

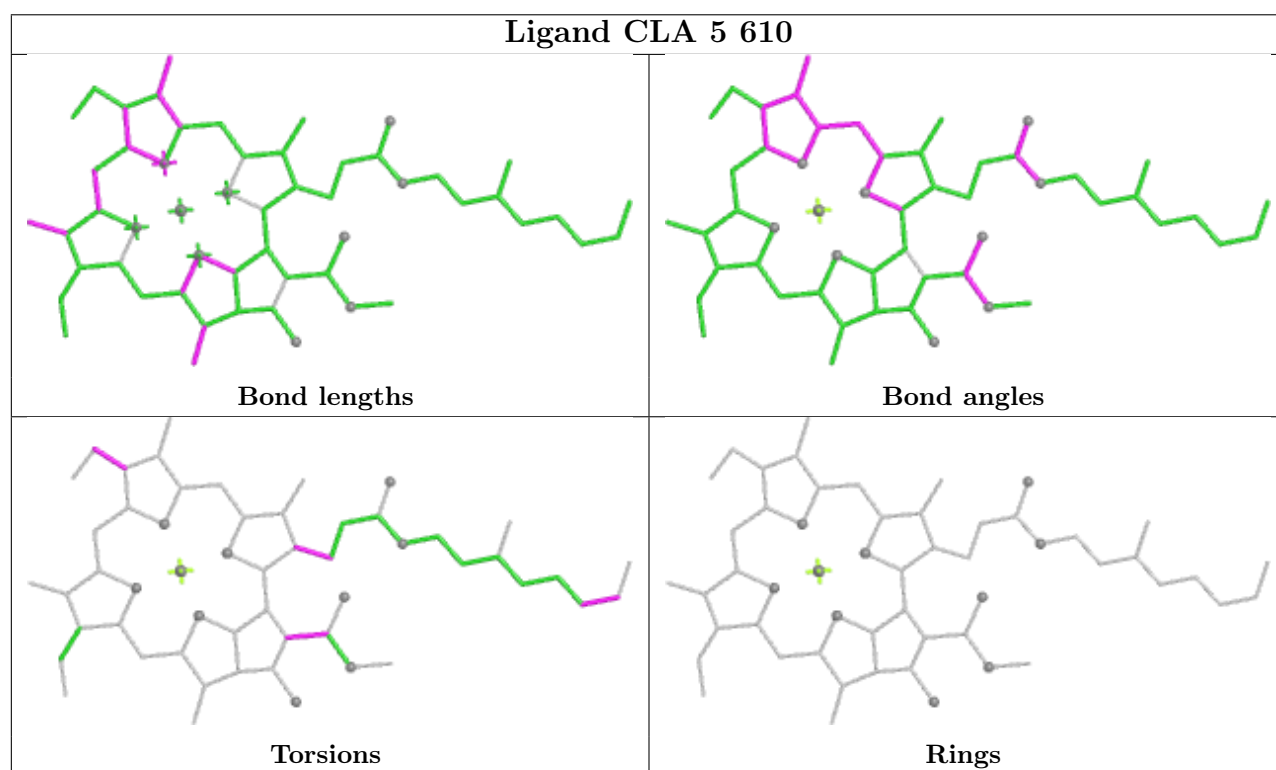
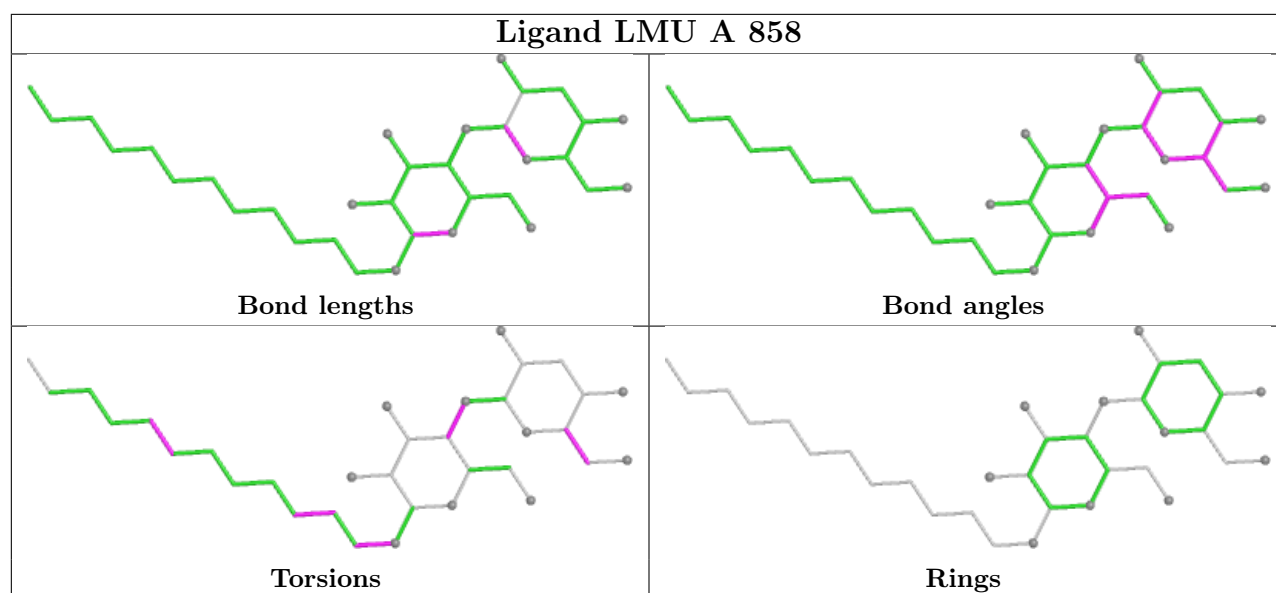


Ligand CLA 8 613

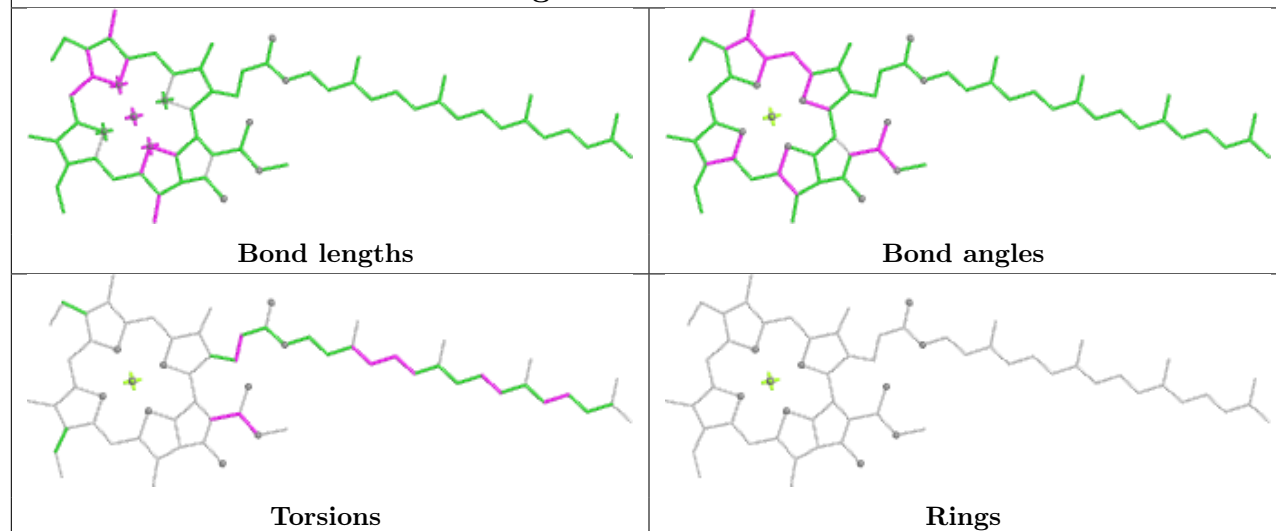


Ligand LHG 7 622

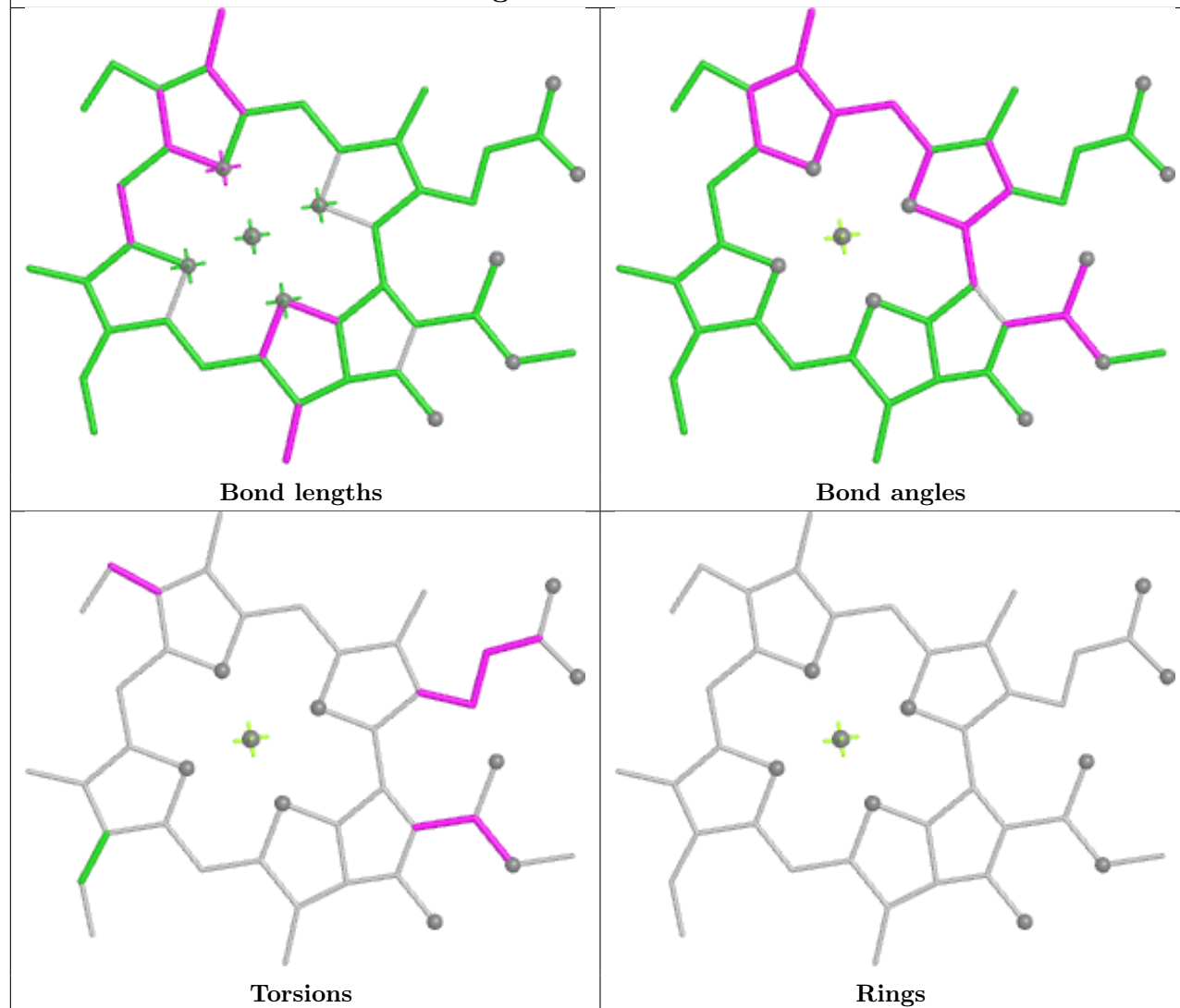




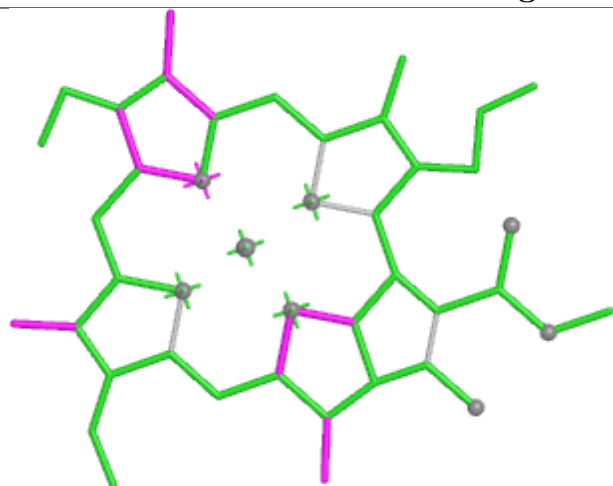
Ligand CLA B 829



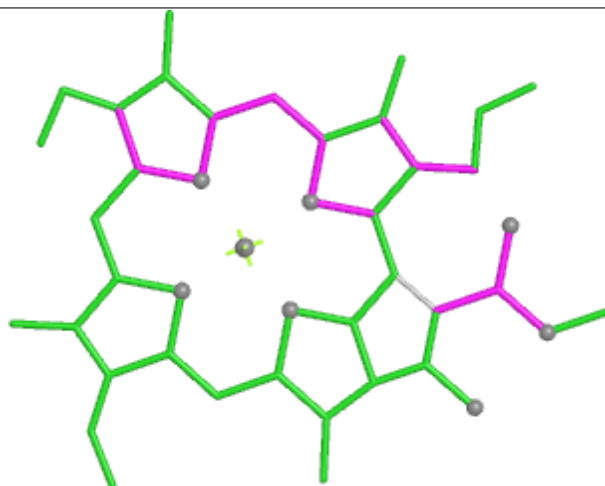
Ligand CLA B 835



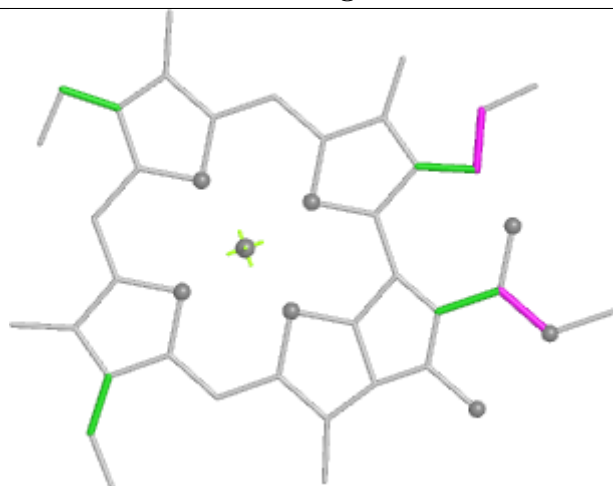
Ligand CLA 3 612



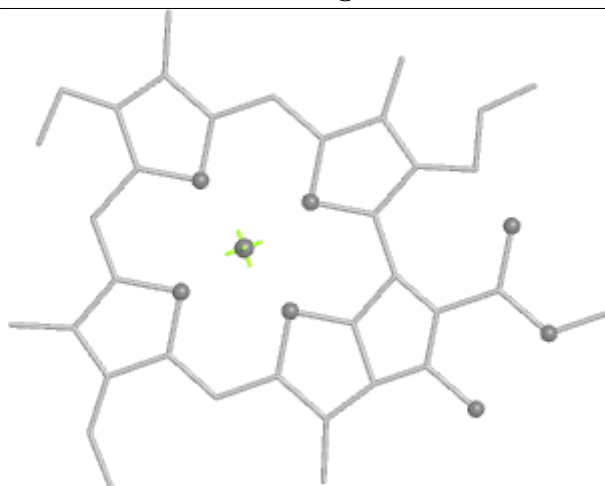
Bond lengths



Bond angles

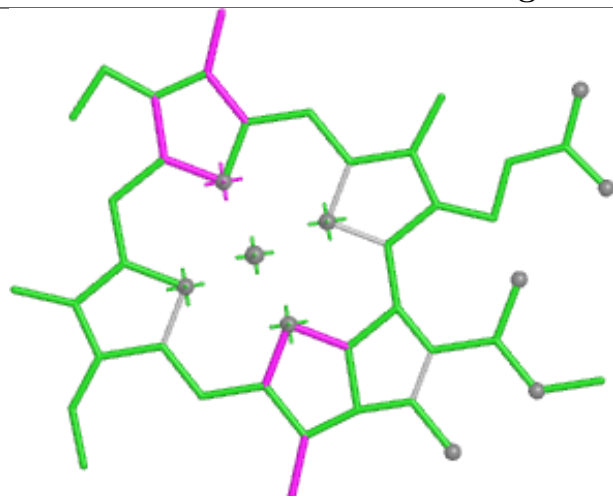


Torsions

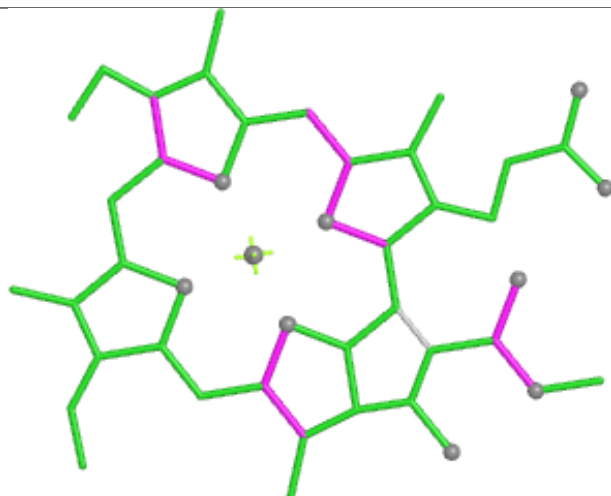


Rings

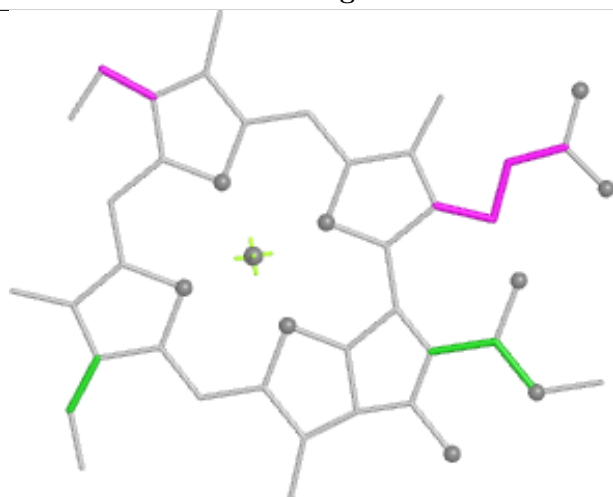
Ligand CLA a 616



Bond lengths



Bond angles

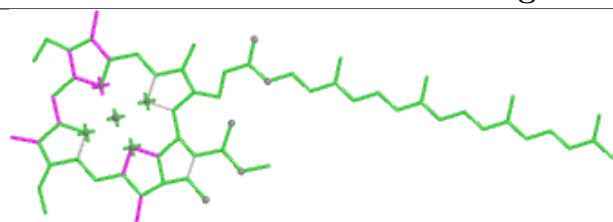


Torsions

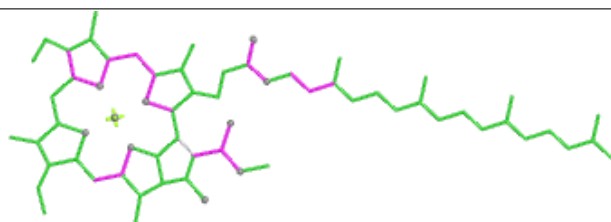


Rings

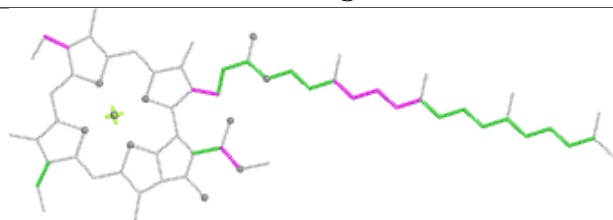
Ligand CLA 7 610



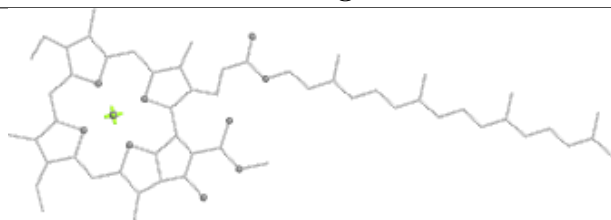
Bond lengths



Bond angles

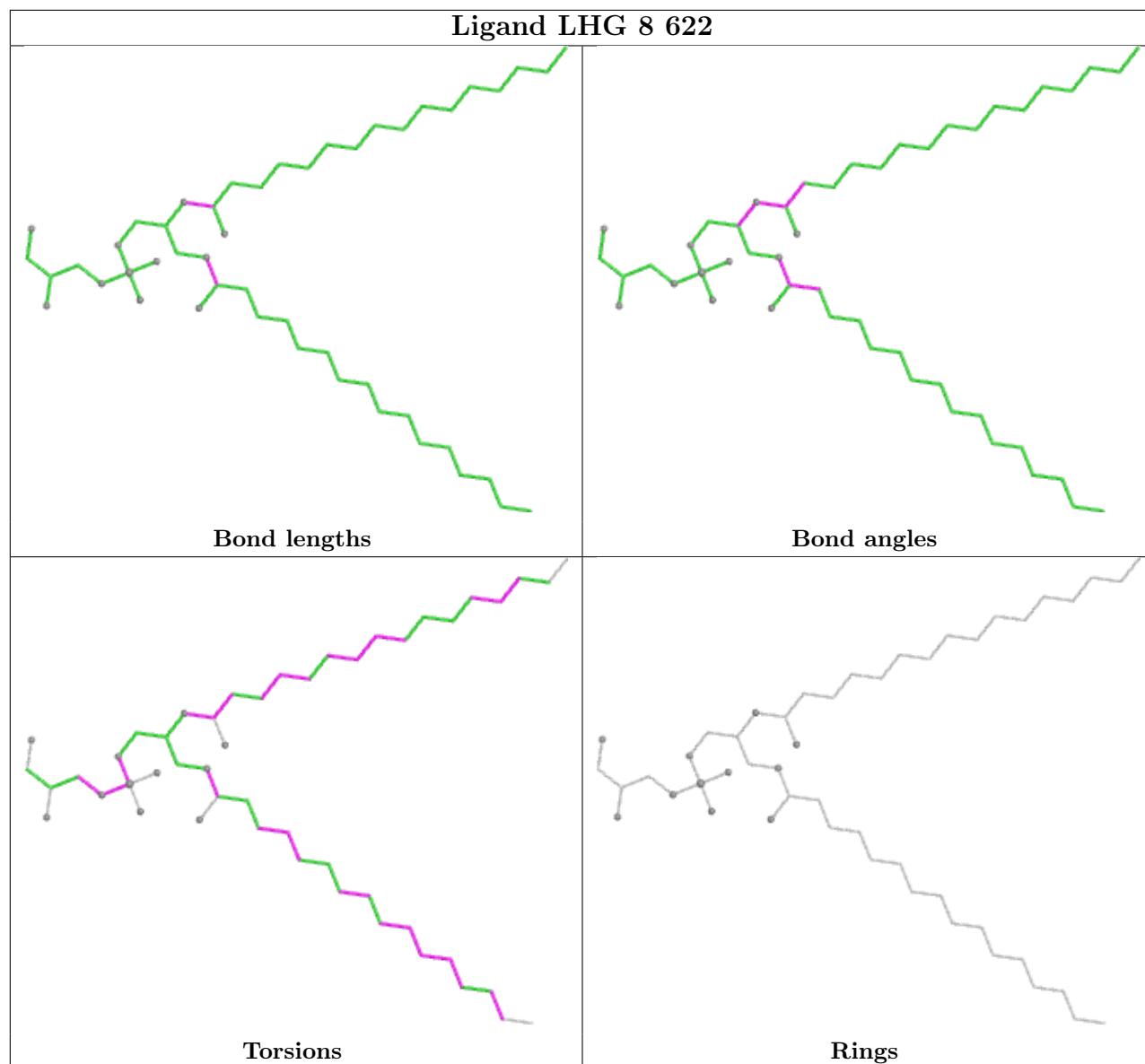


Torsions

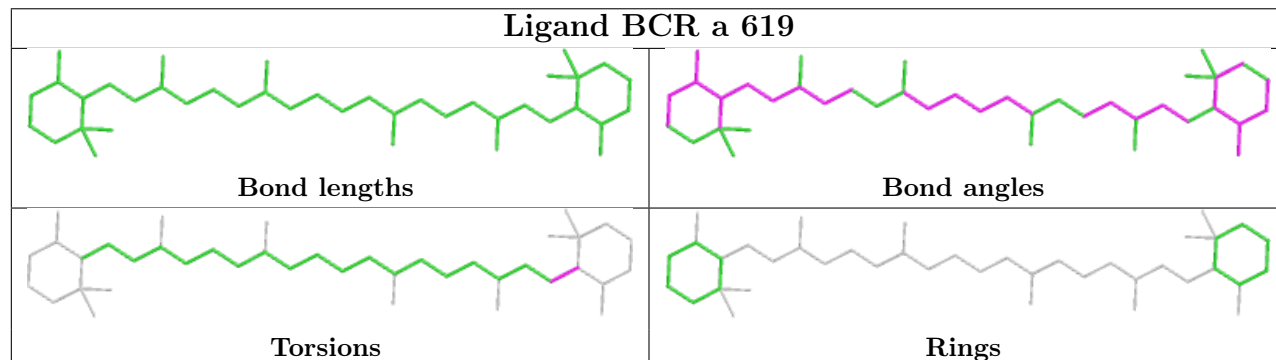


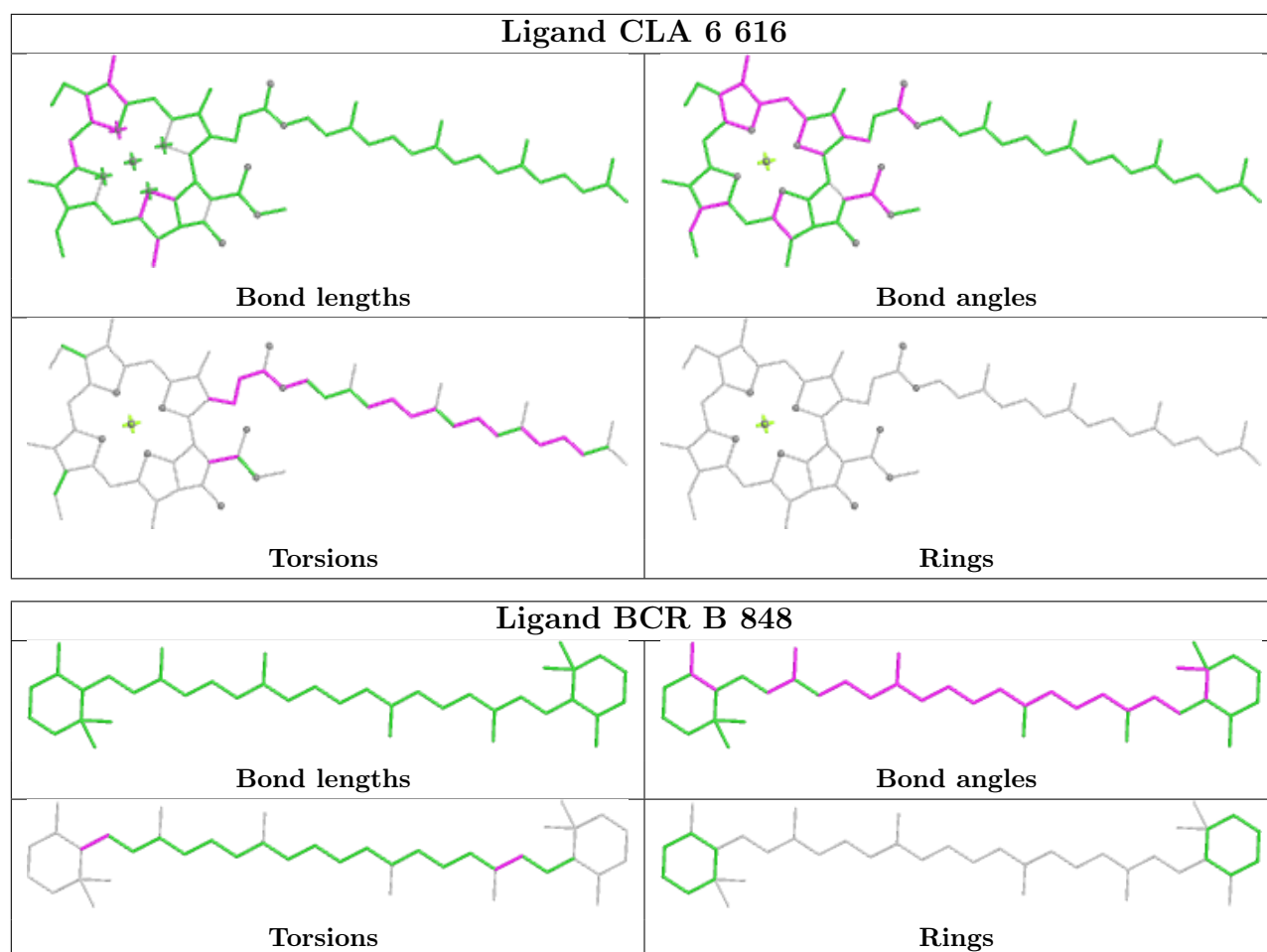
Rings

Ligand LHG 8 622

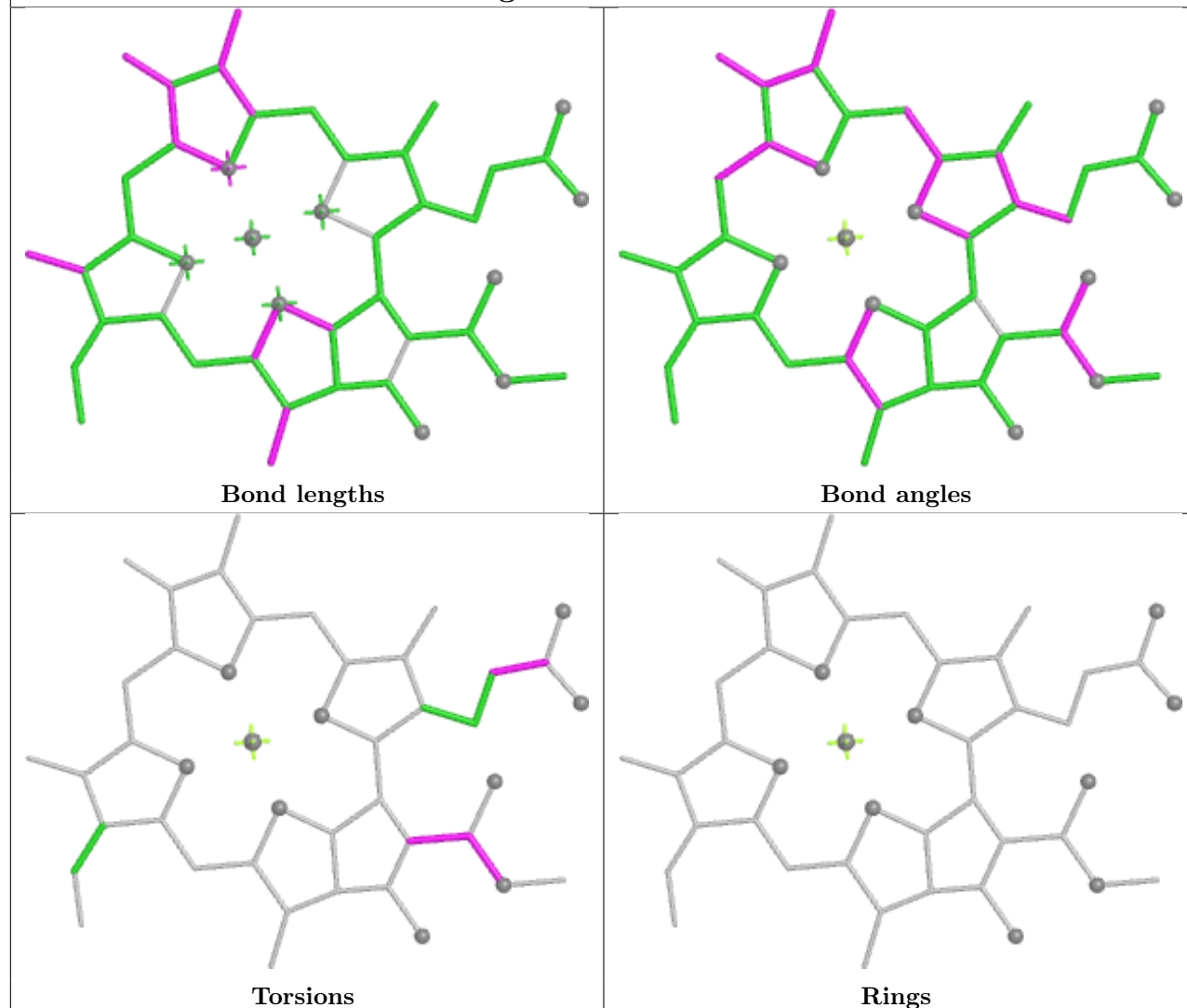


Ligand BCR a 619

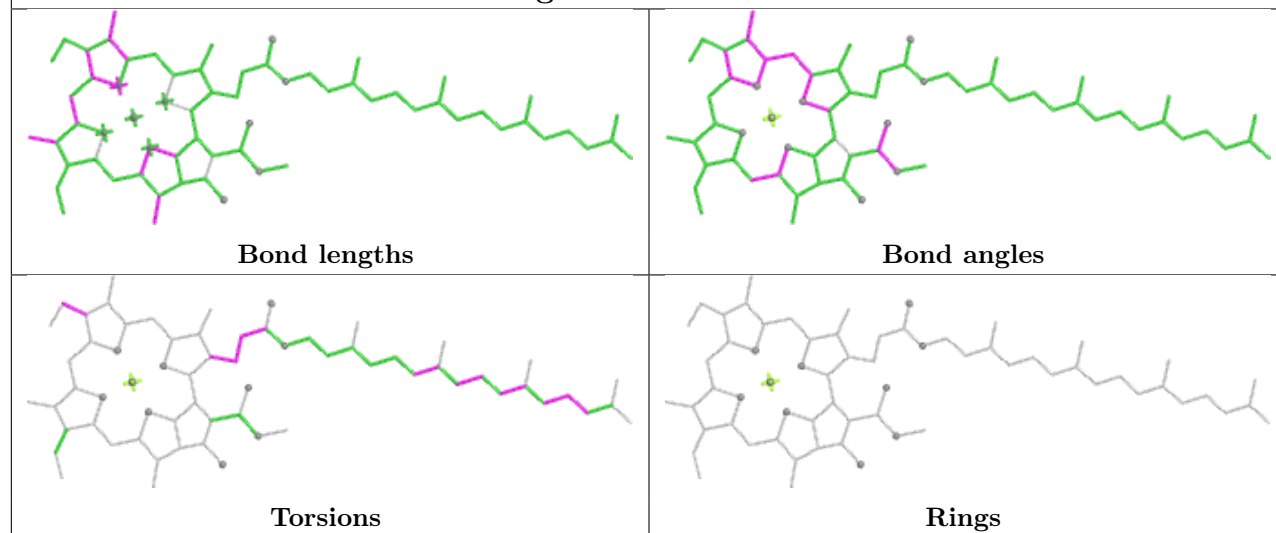




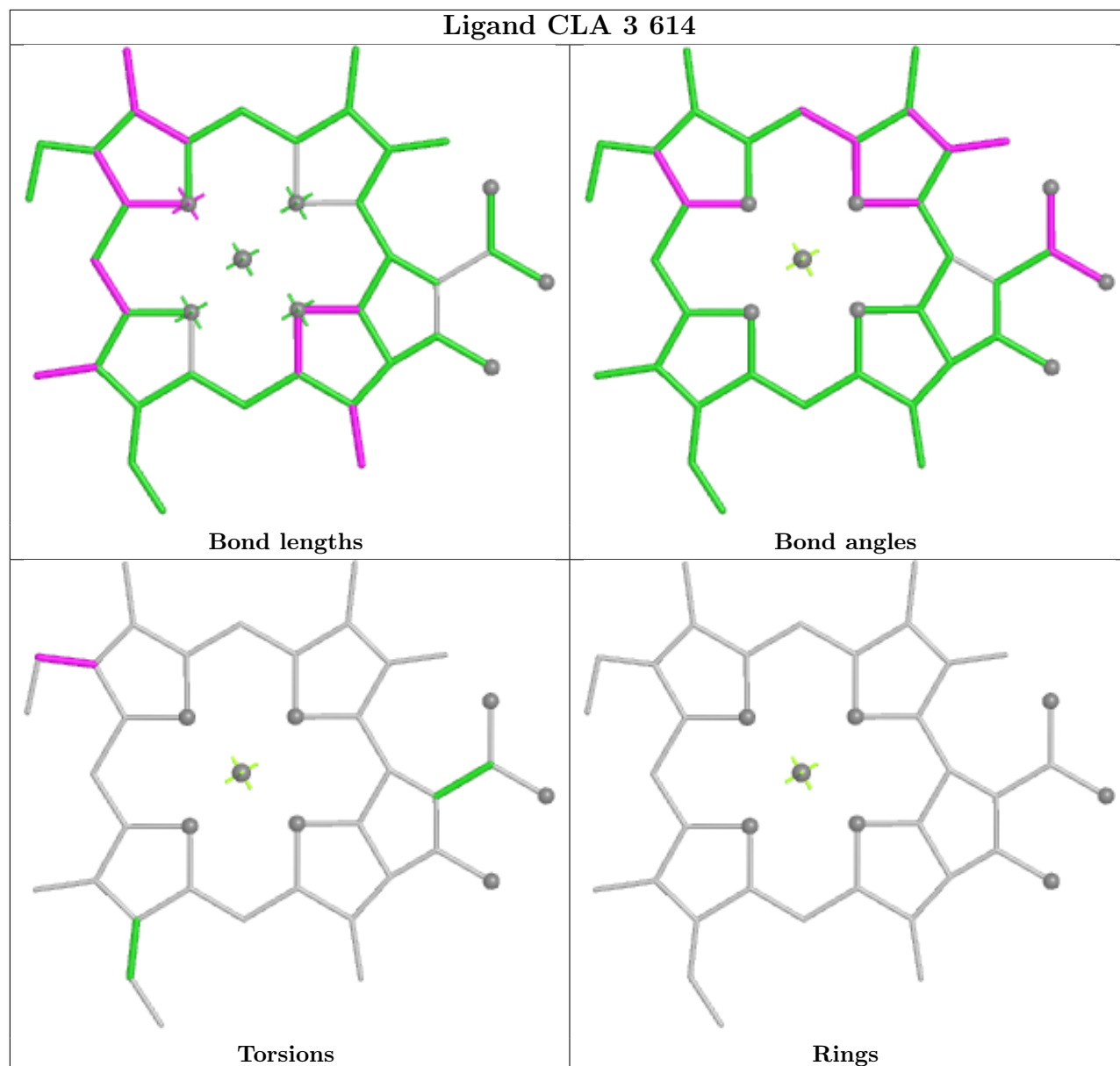
Ligand CLA 4 603



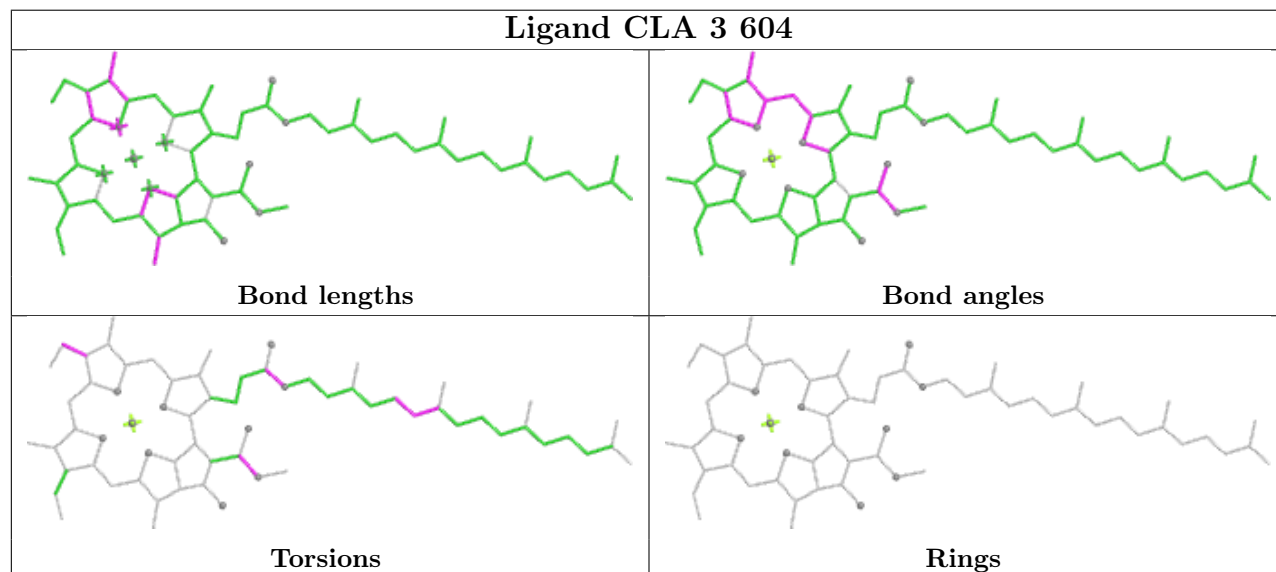
Ligand CLA 6 610



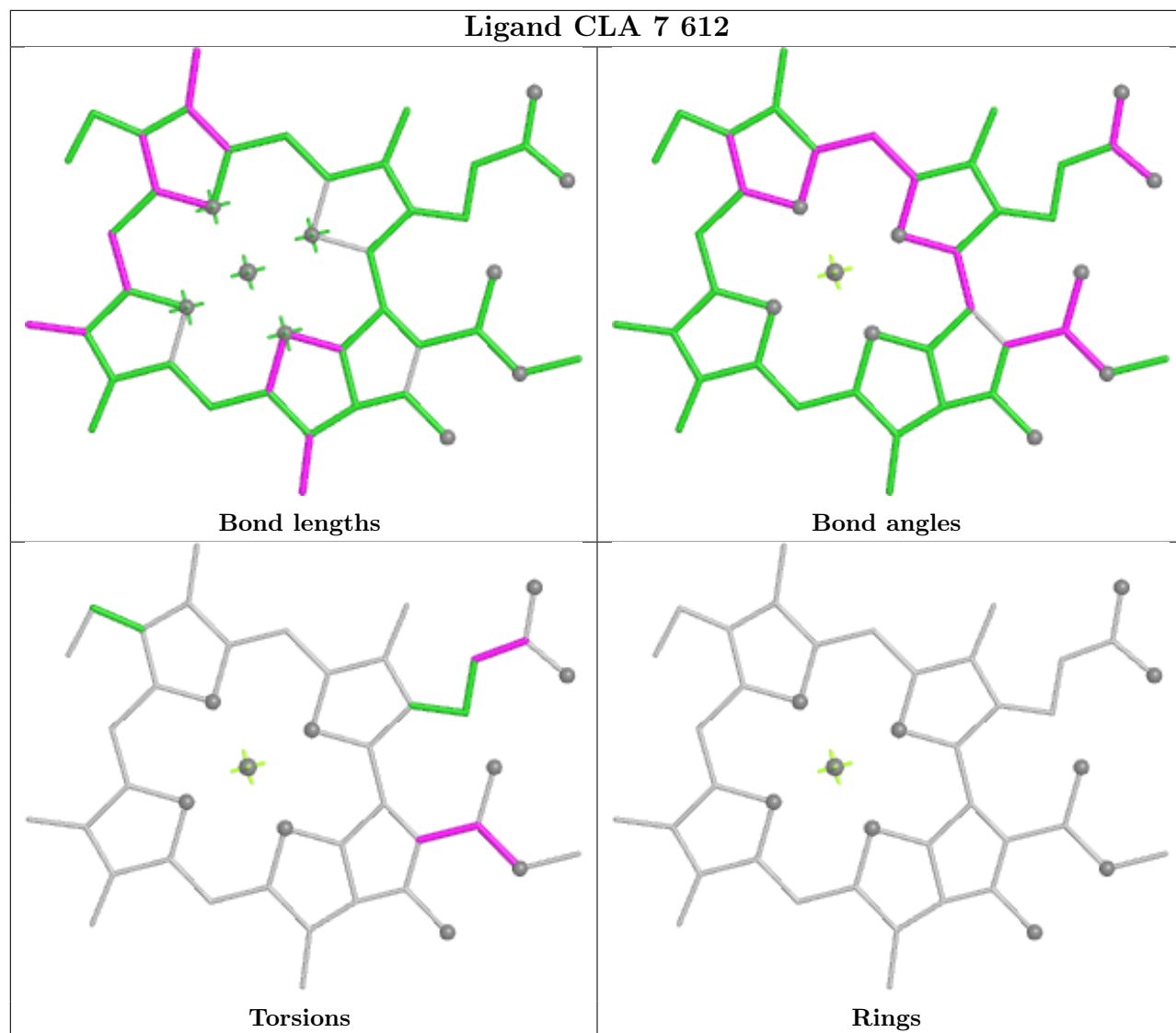
Ligand CLA 3 614



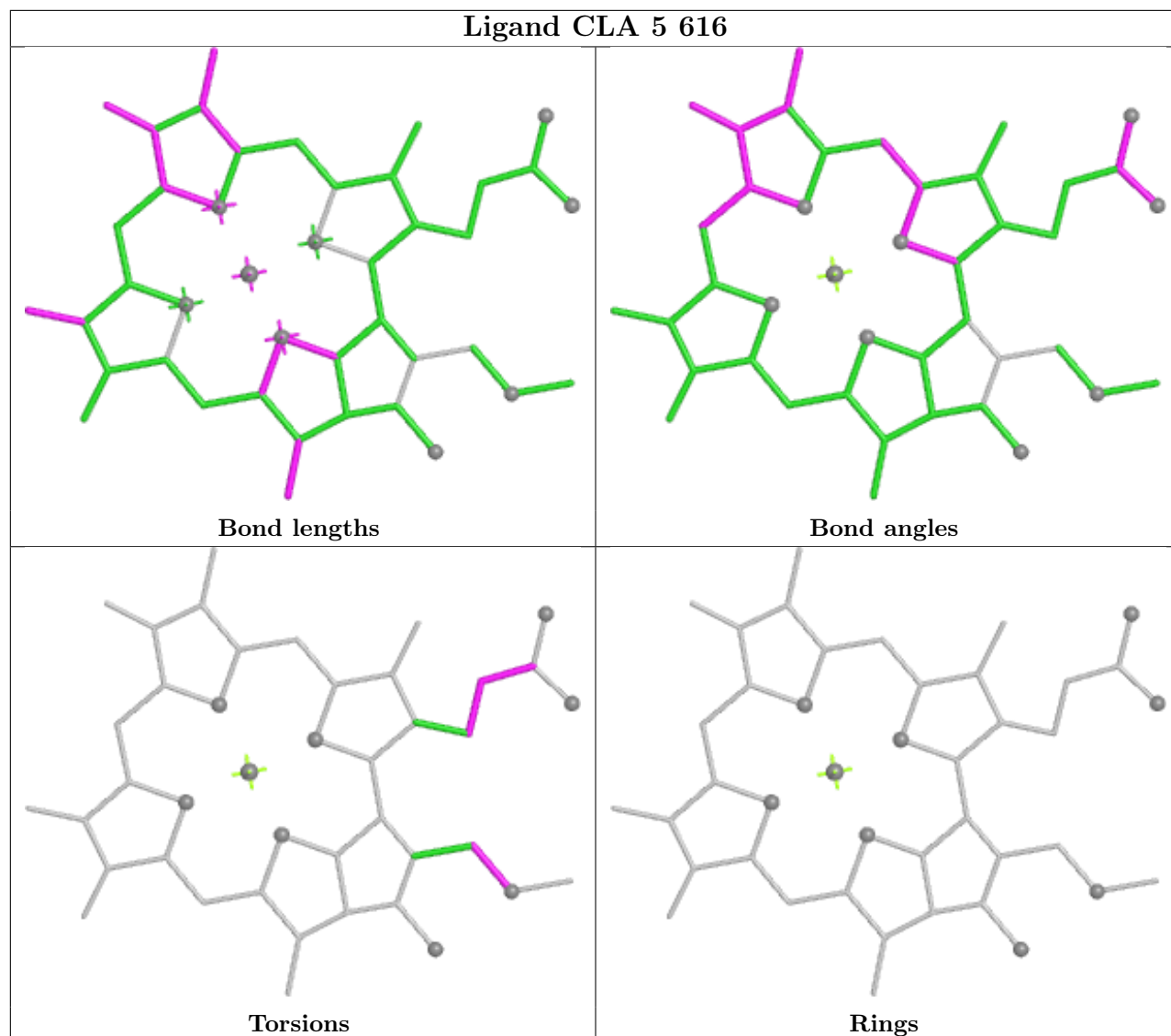
Ligand CLA 3 604



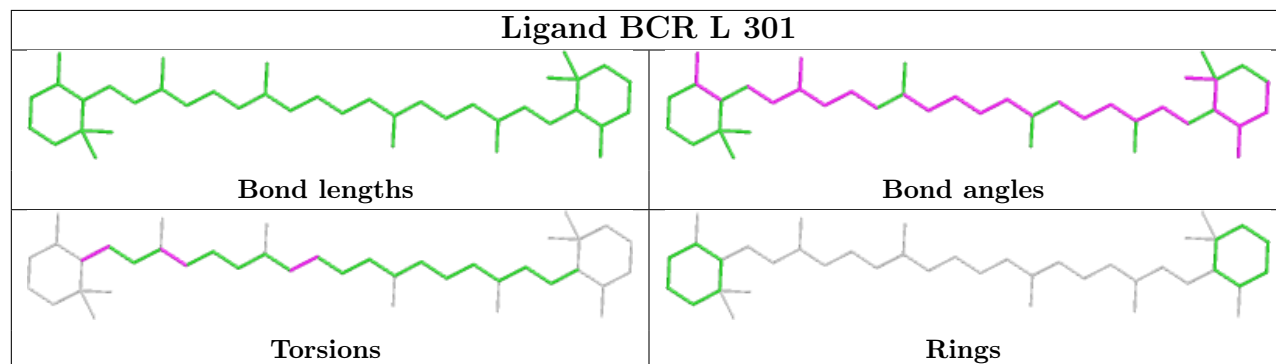
Ligand CLA 7 612



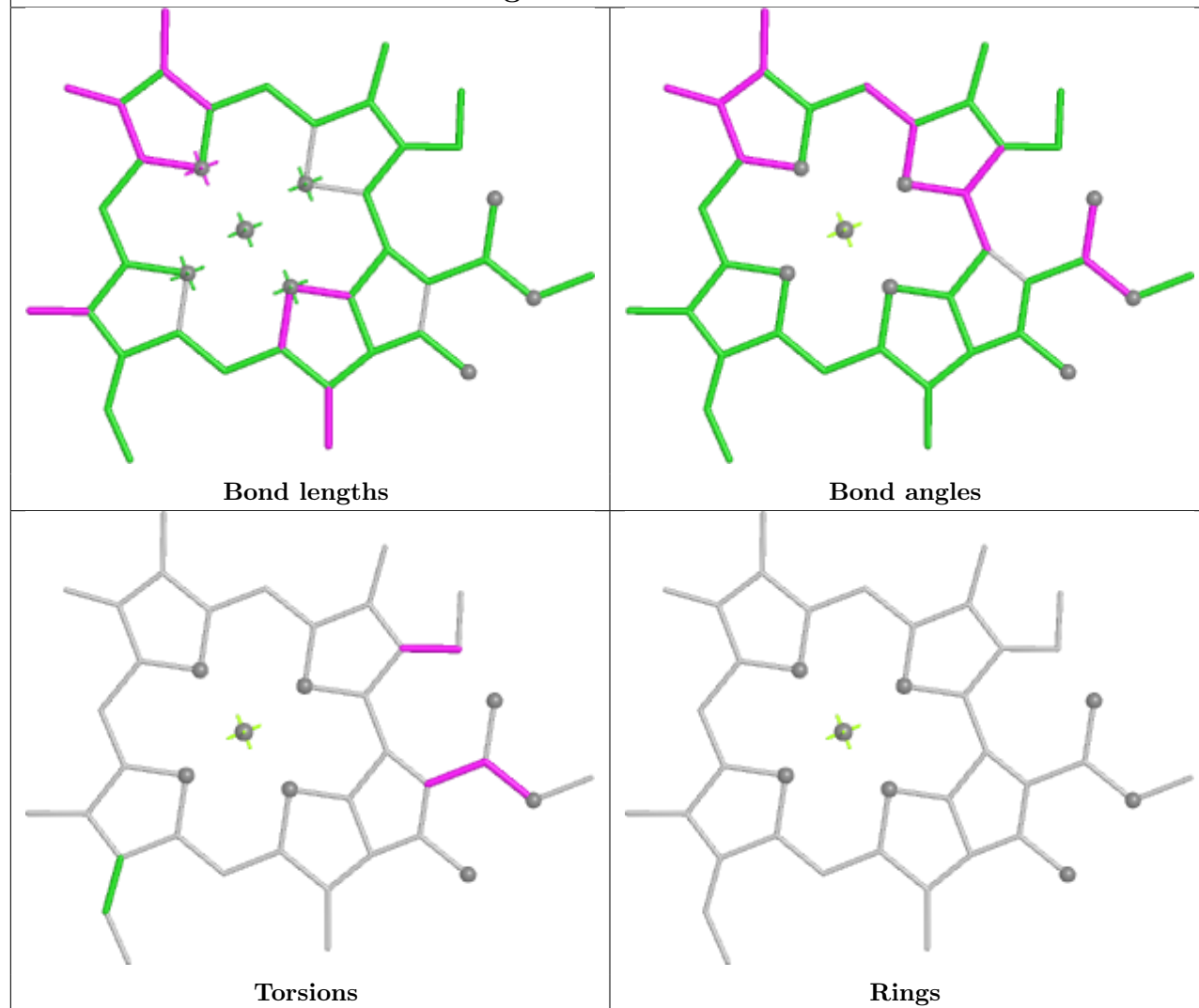
Ligand CLA 5 616



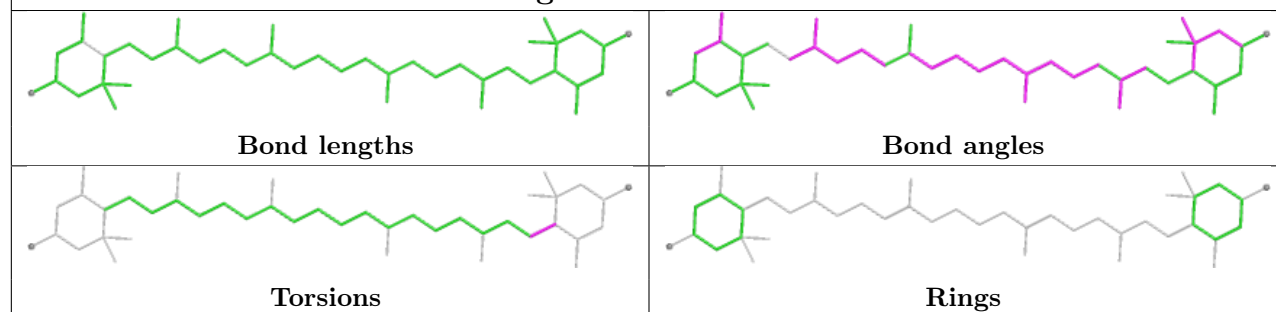
Ligand BCR L 301

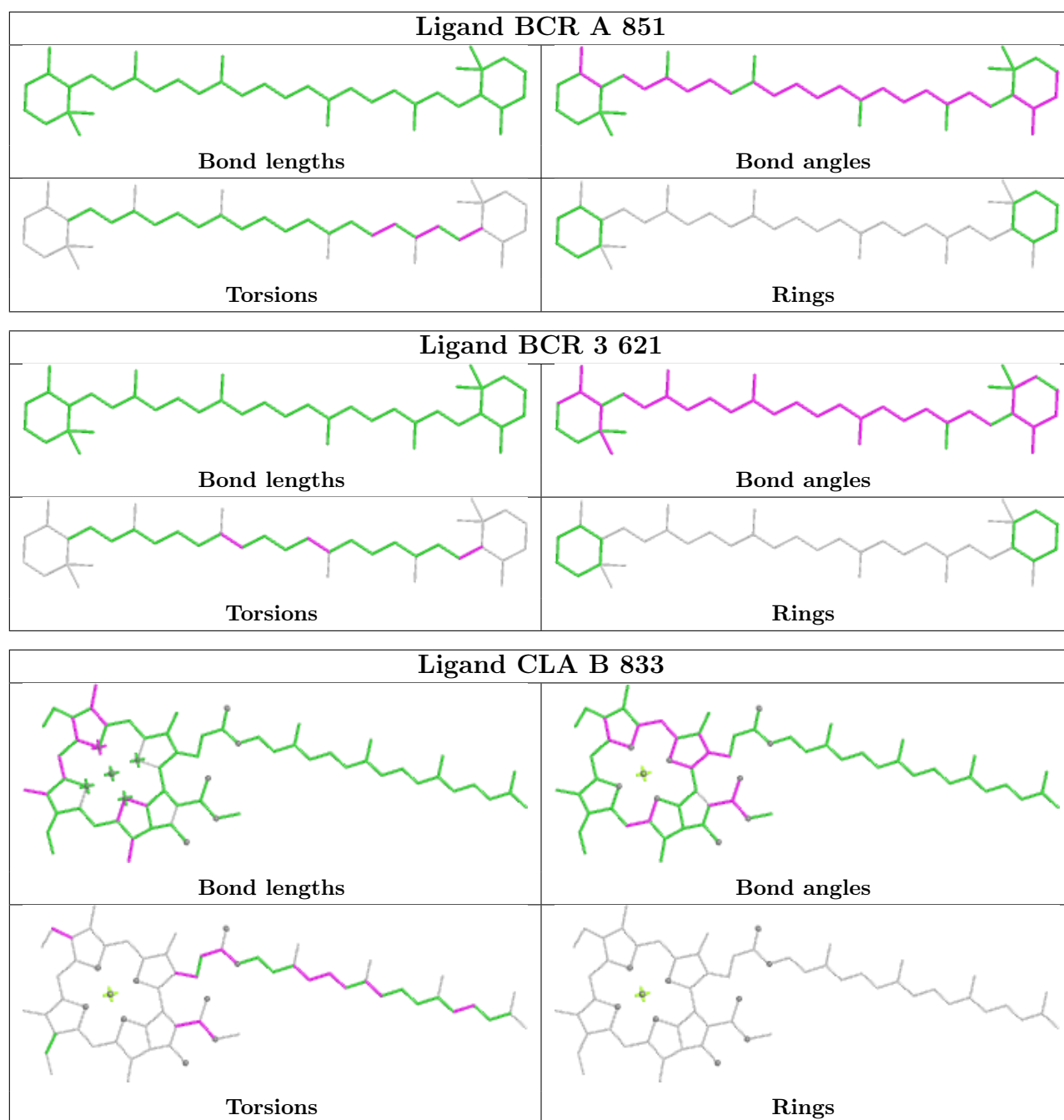


Ligand CLA 8 607

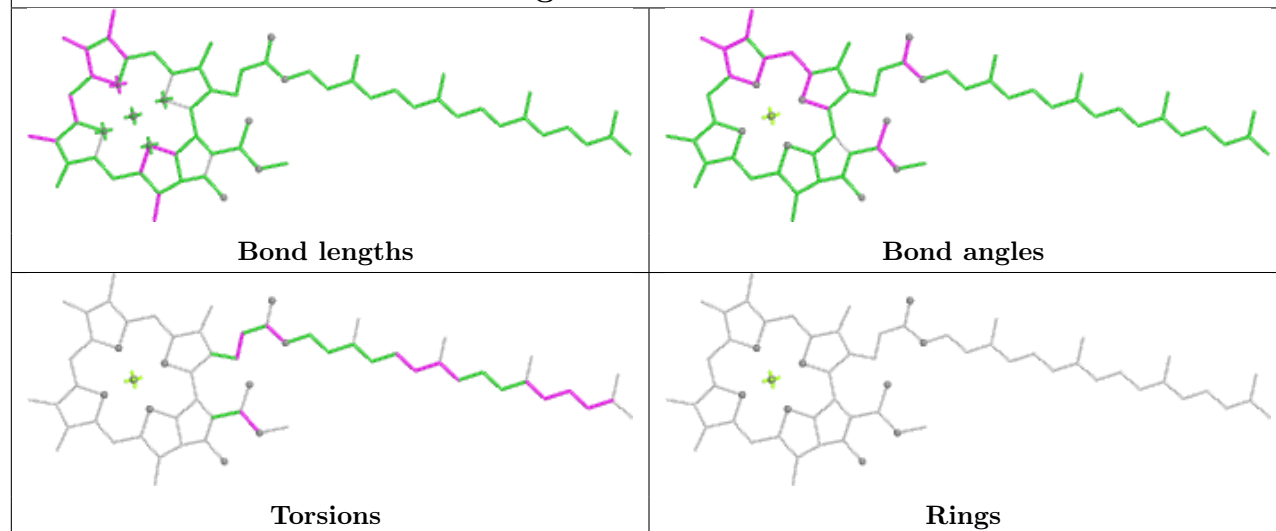


Ligand LUT 6 619

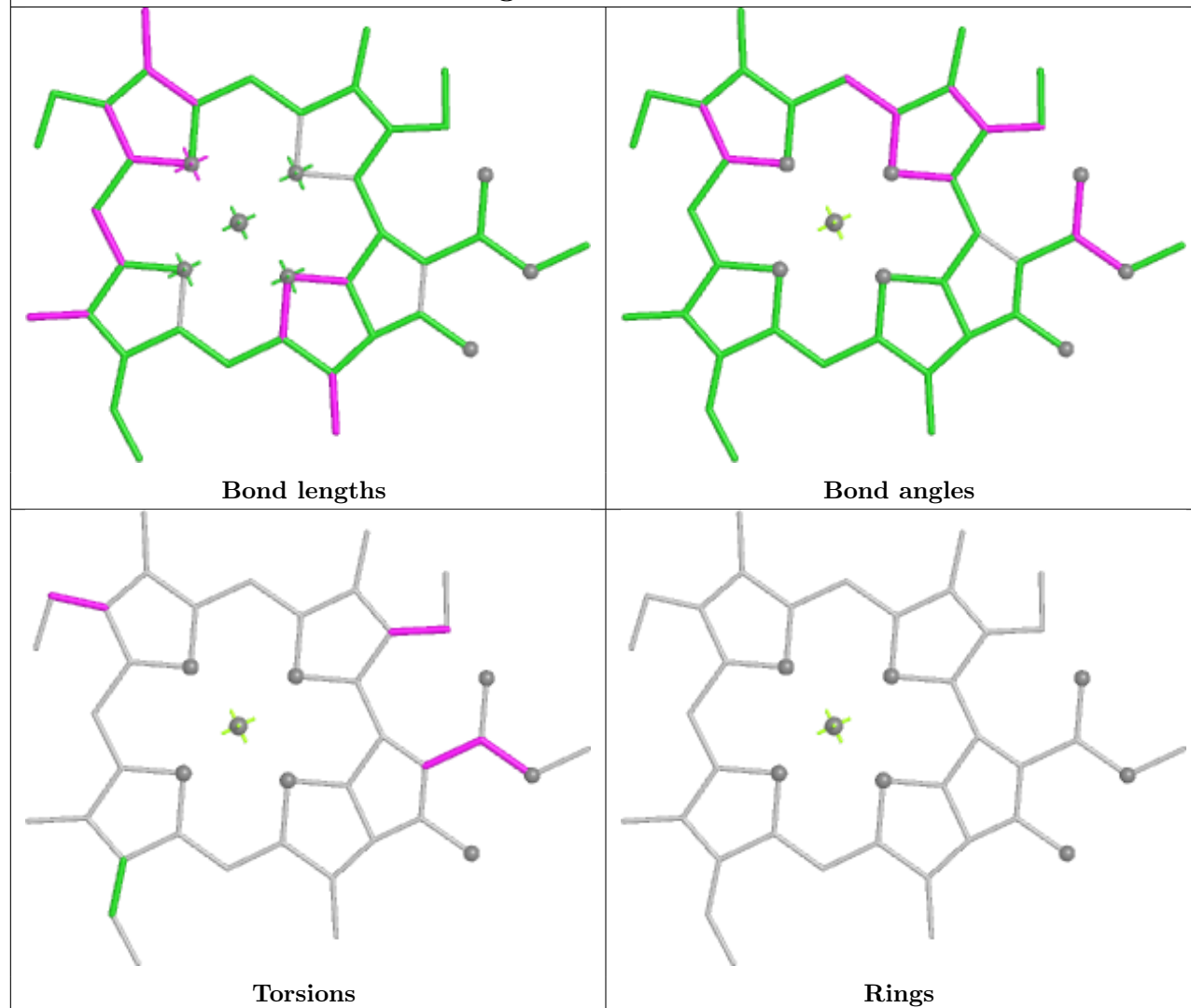




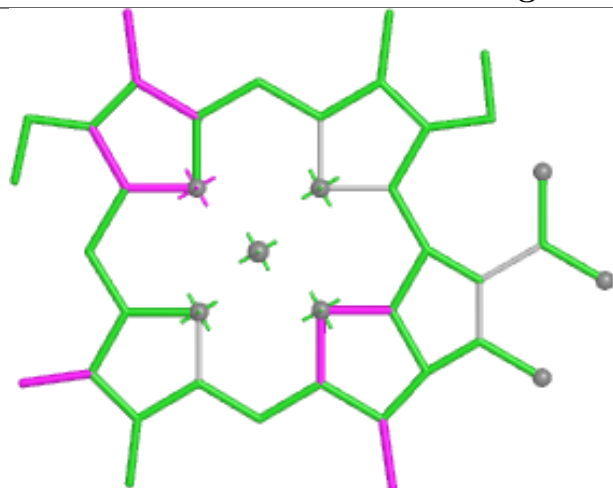
Ligand CLA 5 604



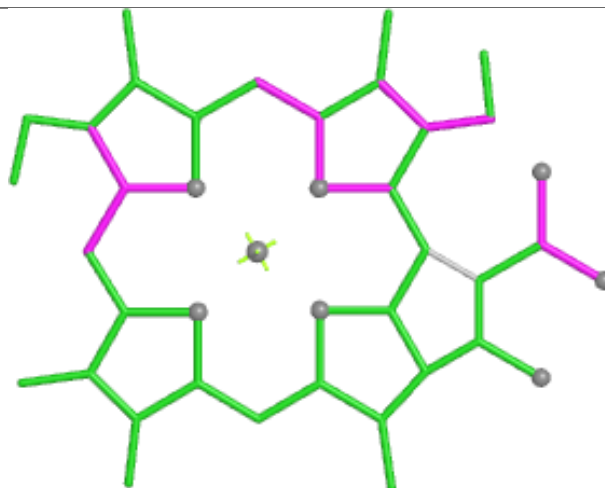
Ligand CLA F 303



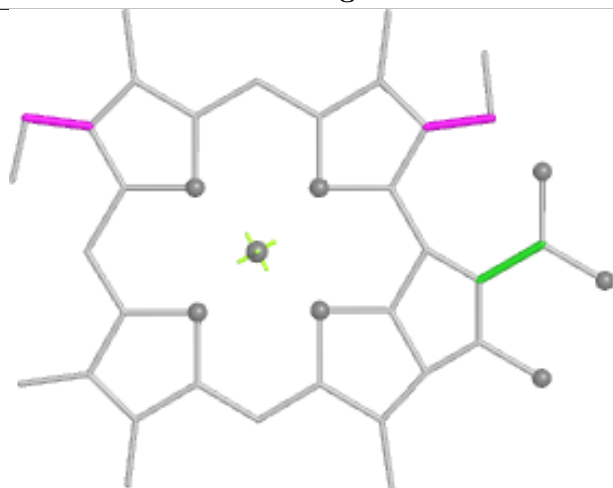
Ligand CLA 3 615



Bond lengths



Bond angles

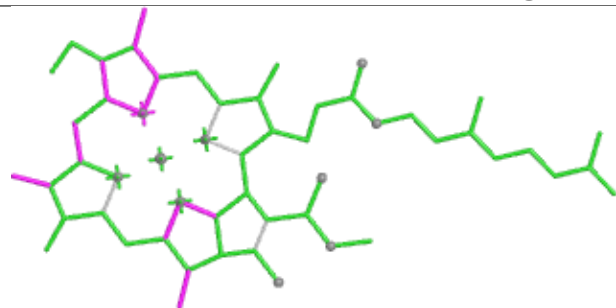


Torsions

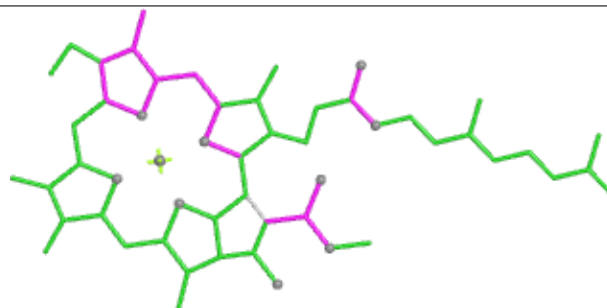


Rings

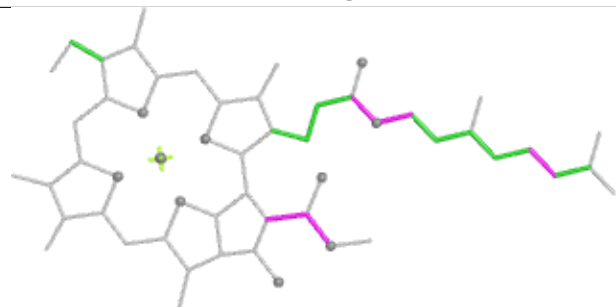
Ligand CLA 7 604



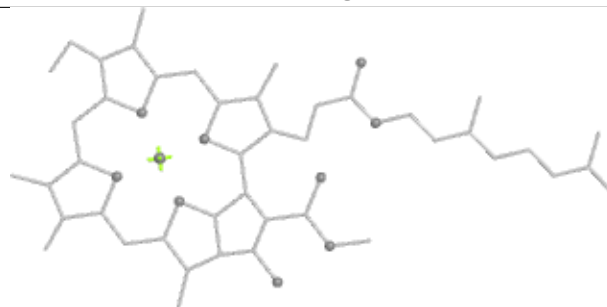
Bond lengths



Bond angles

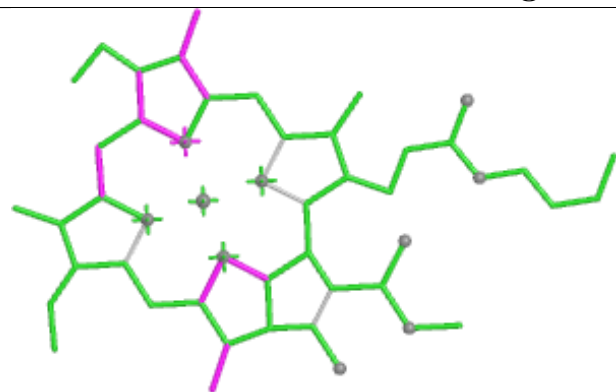


Torsions

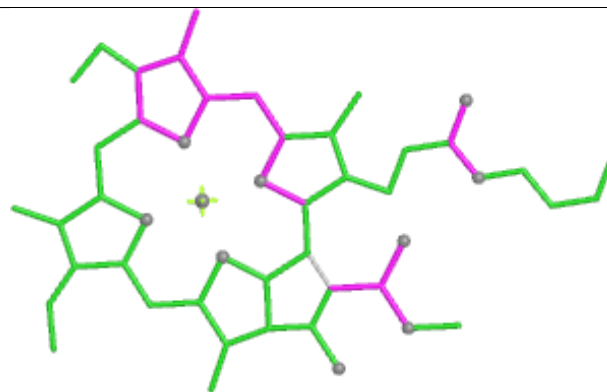


Rings

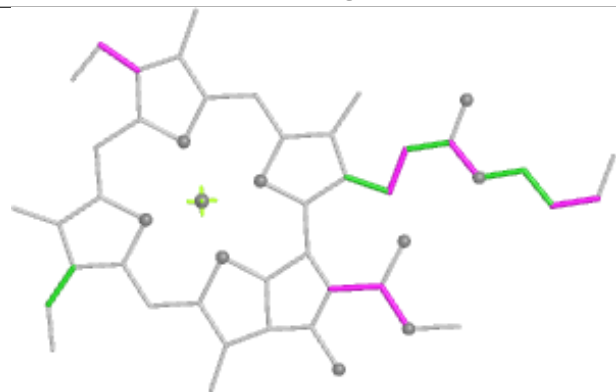
Ligand CLA 1 604



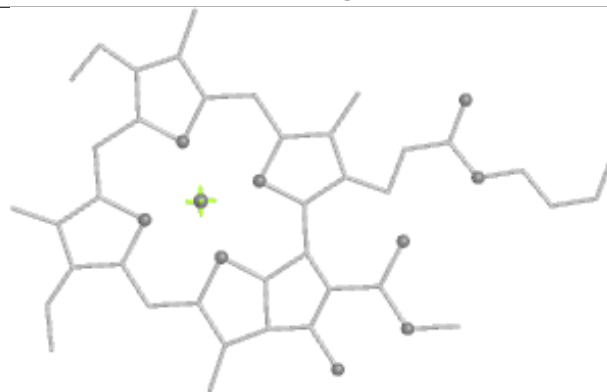
Bond lengths



Bond angles

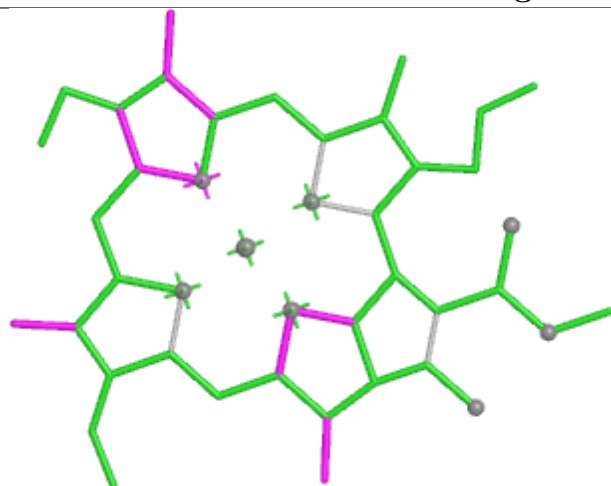


Torsions

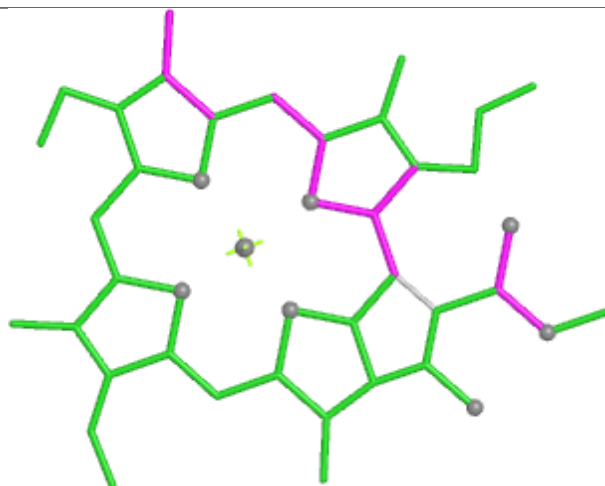


Rings

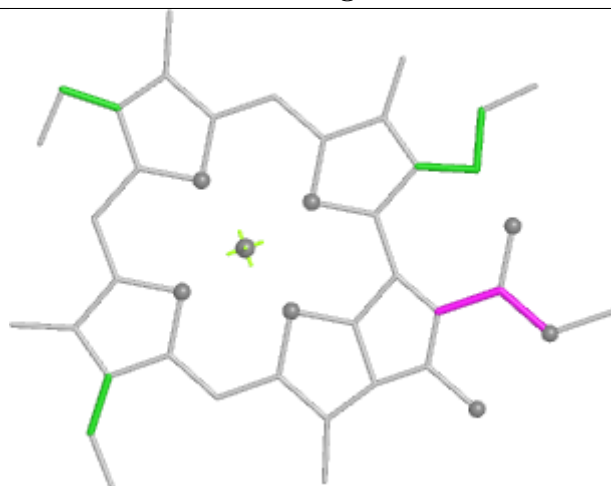
Ligand CLA B 815



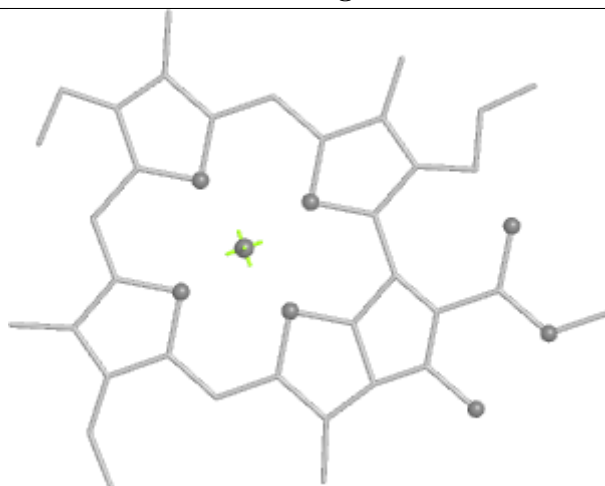
Bond lengths



Bond angles

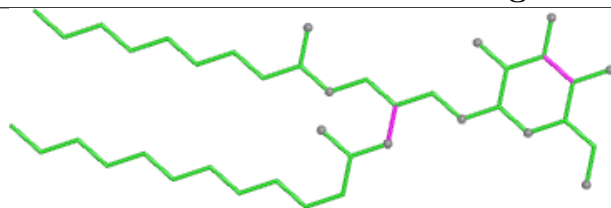


Torsions

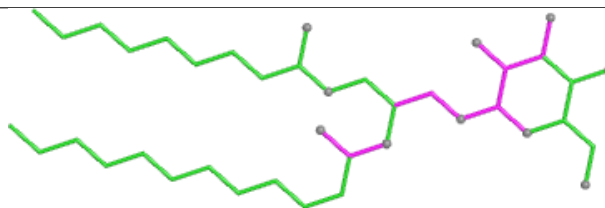


Rings

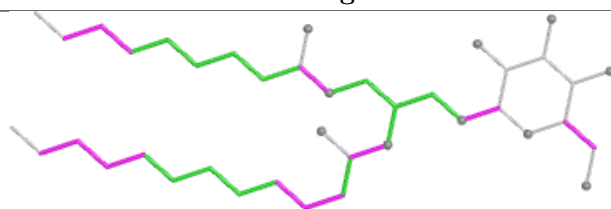
Ligand LMG A 860



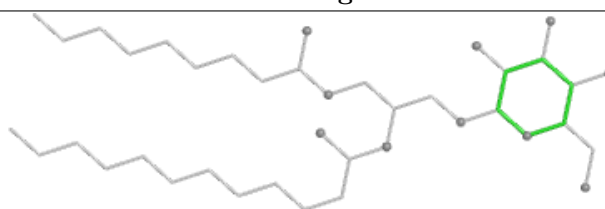
Bond lengths



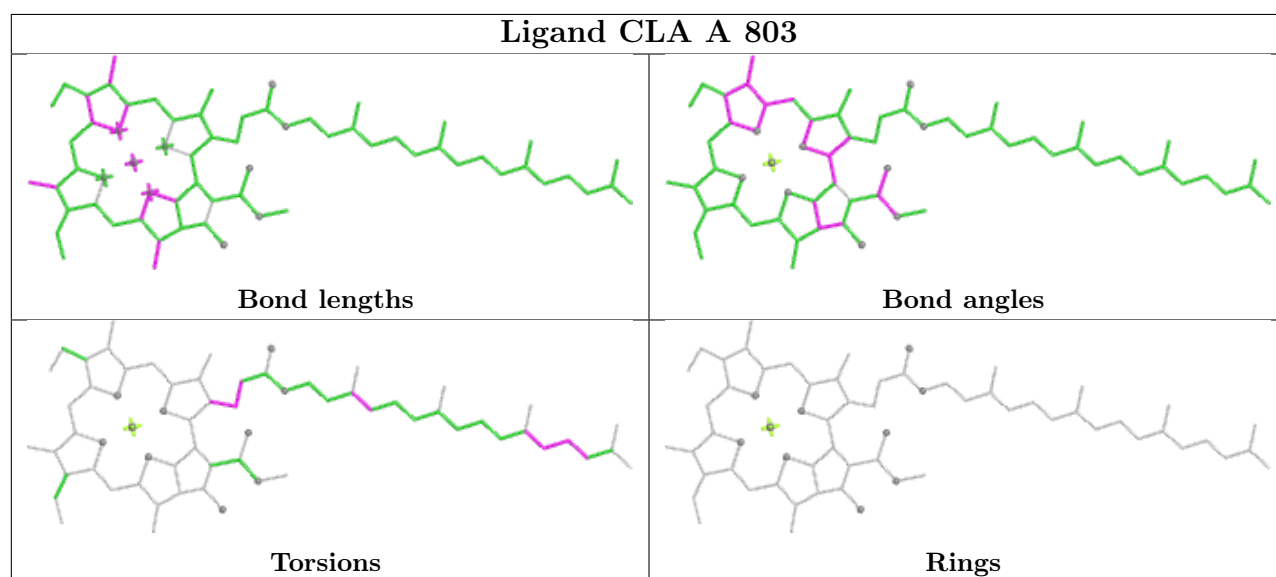
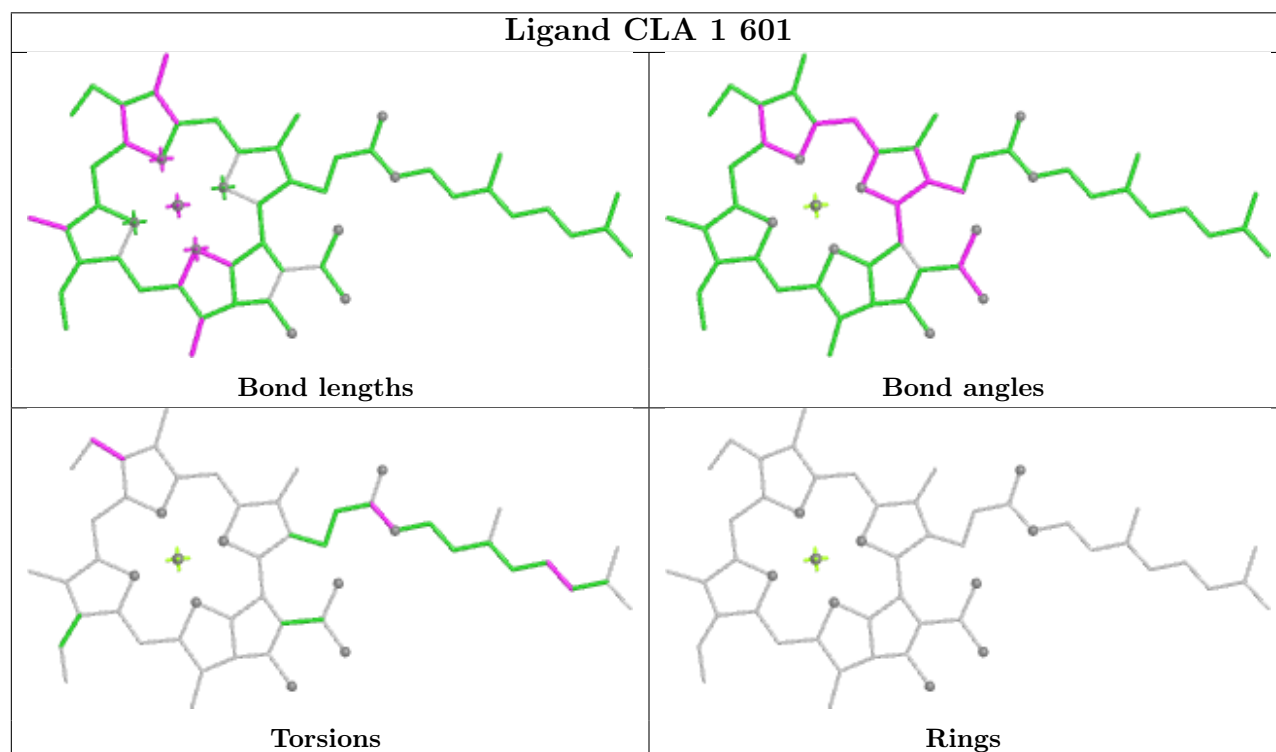
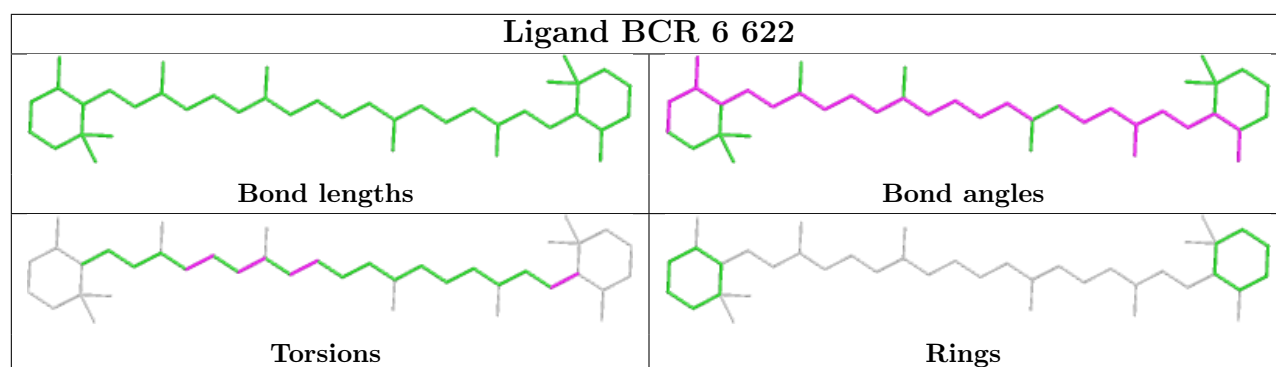
Bond angles

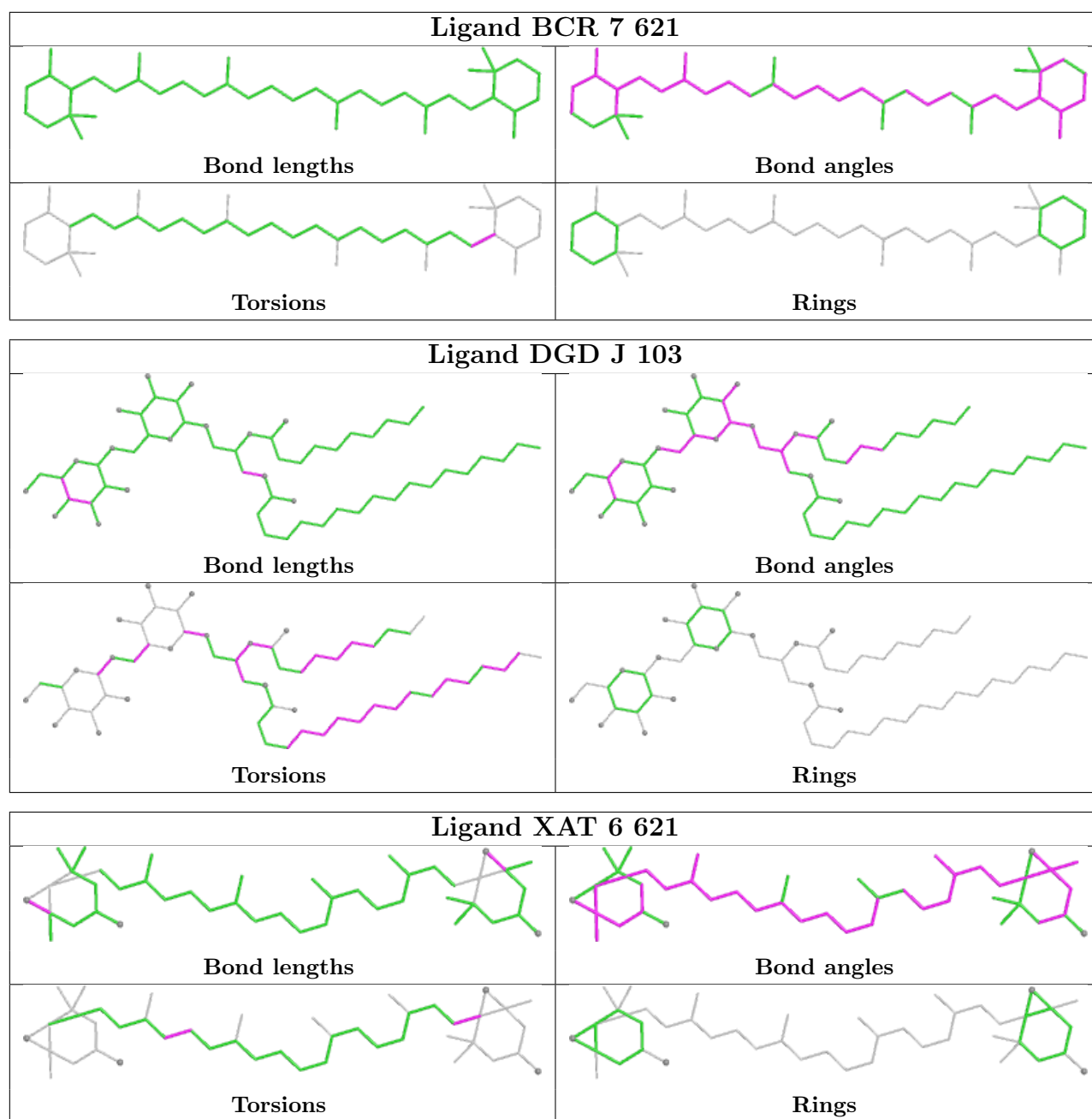


Torsions

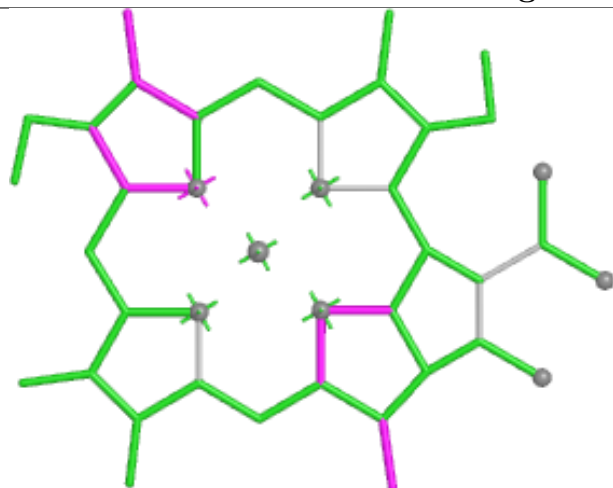


Rings

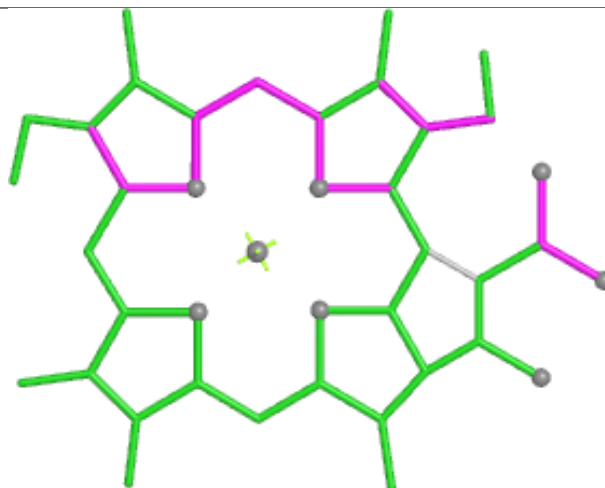




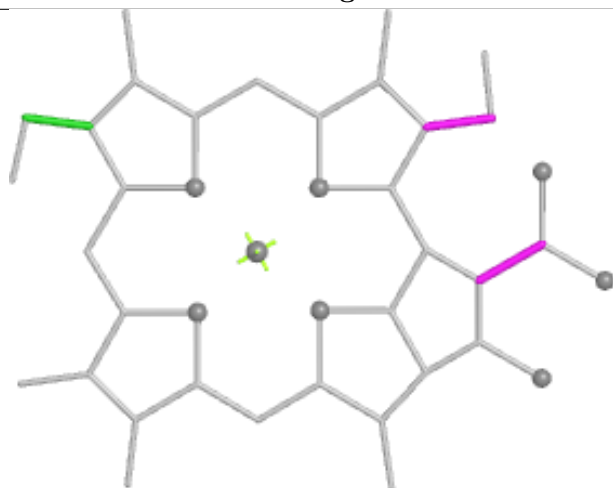
Ligand CLA 5 606



Bond lengths



Bond angles

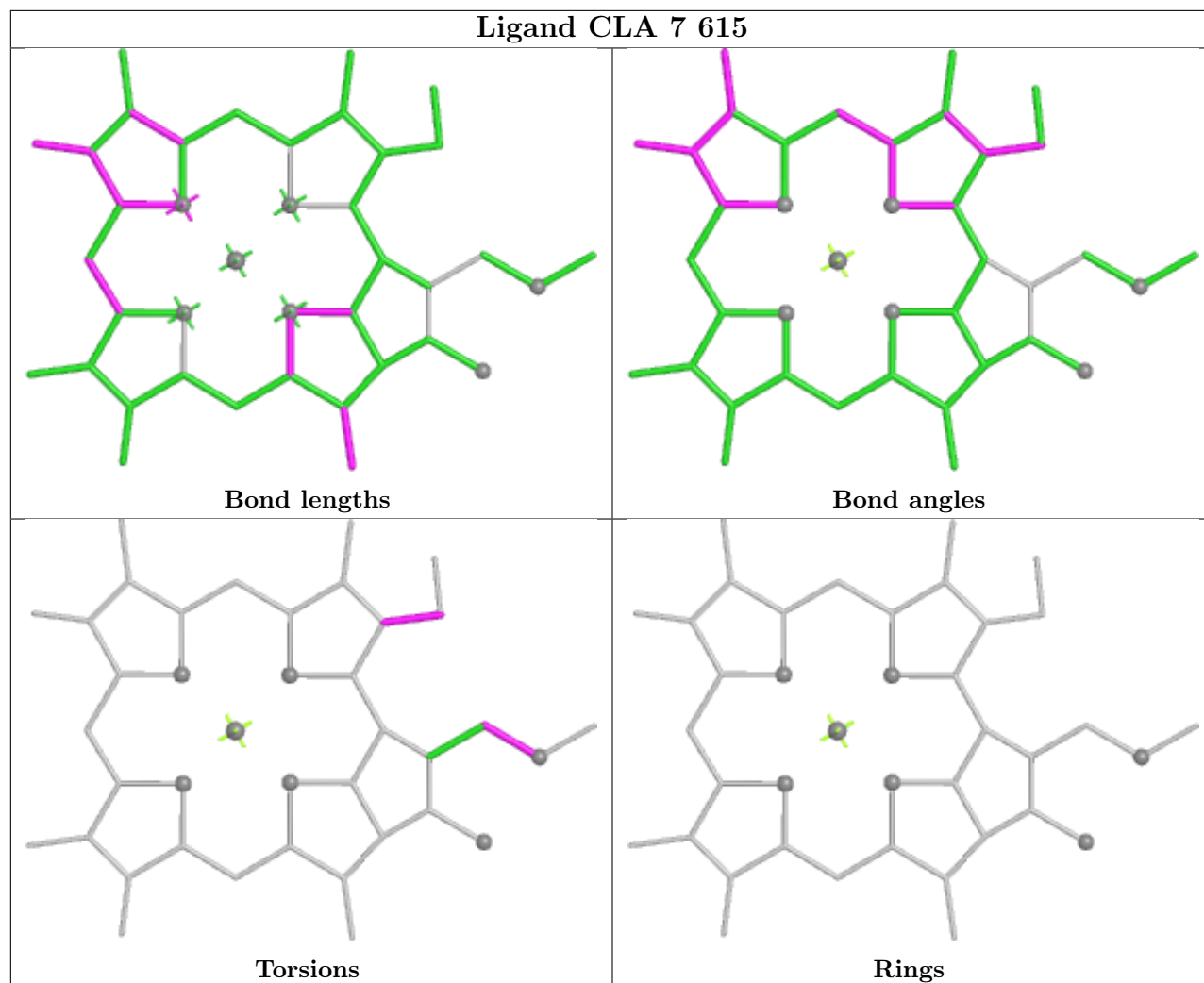


Torsions

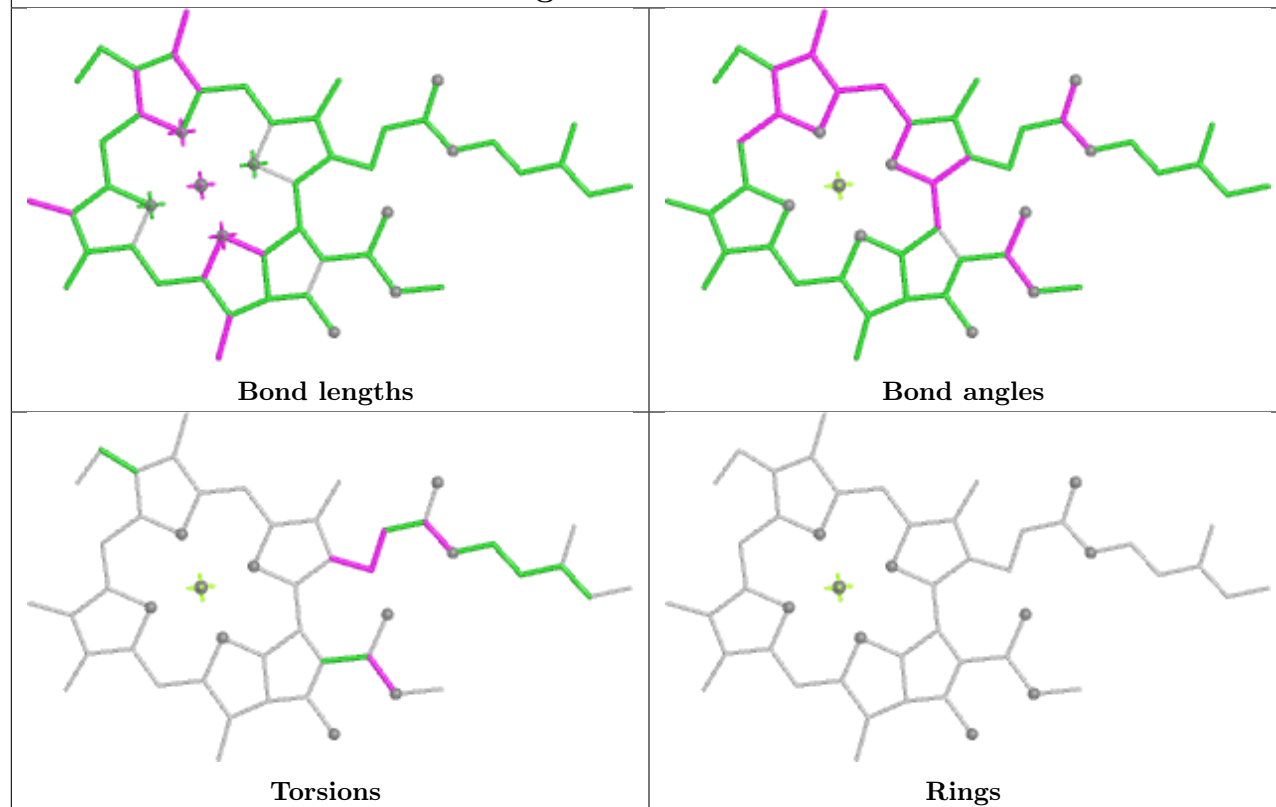


Rings

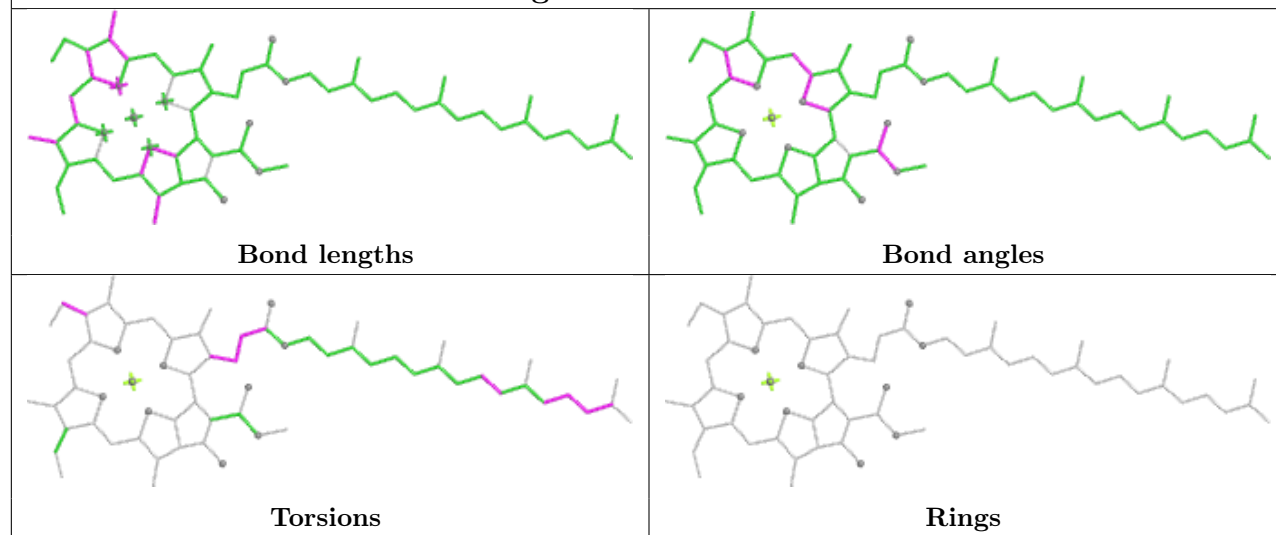
Ligand CLA 7 615



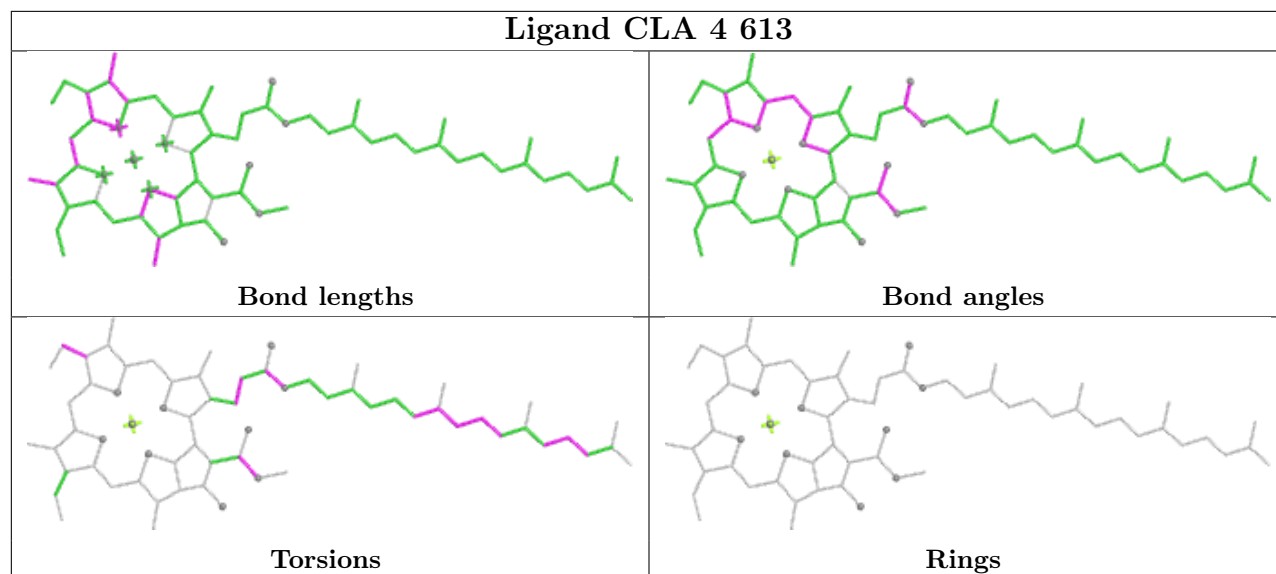
Ligand CLA 5 608



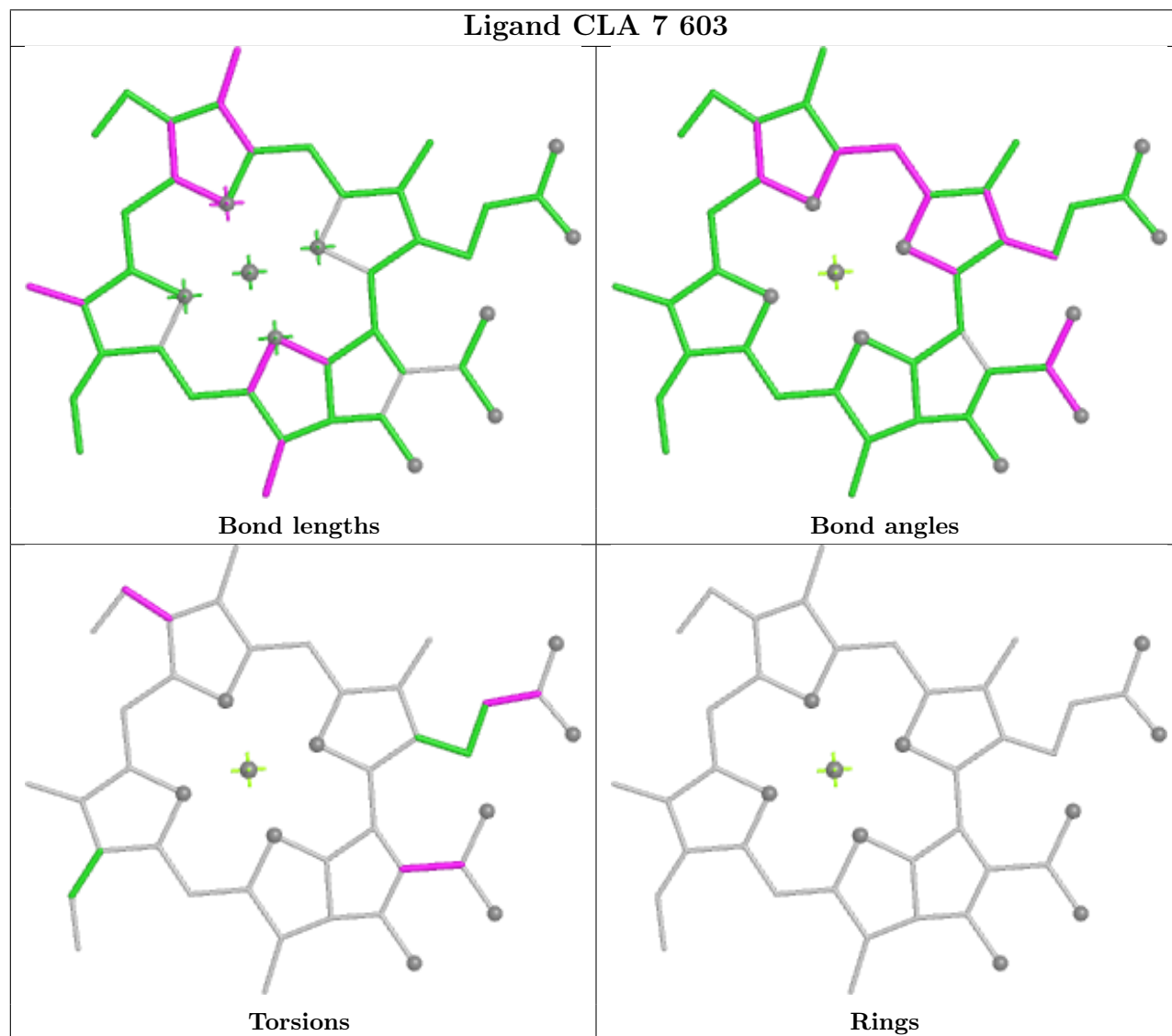
Ligand CLA A 842

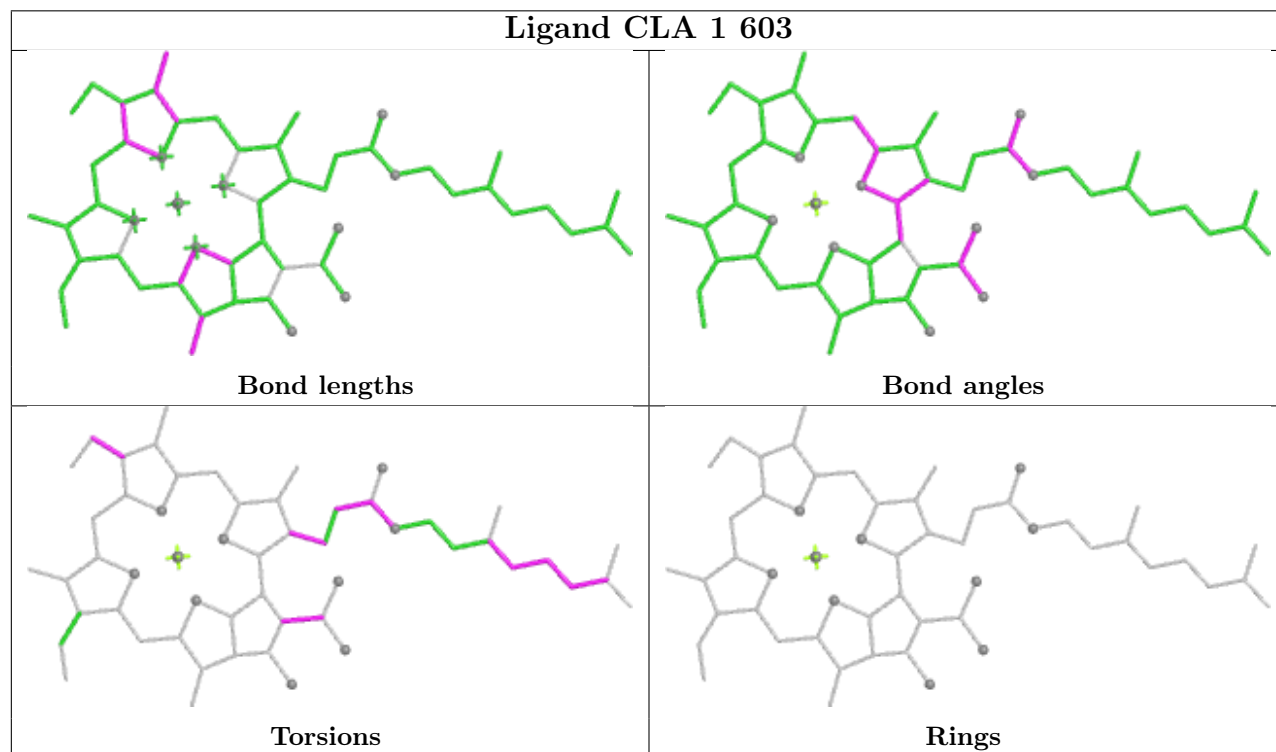
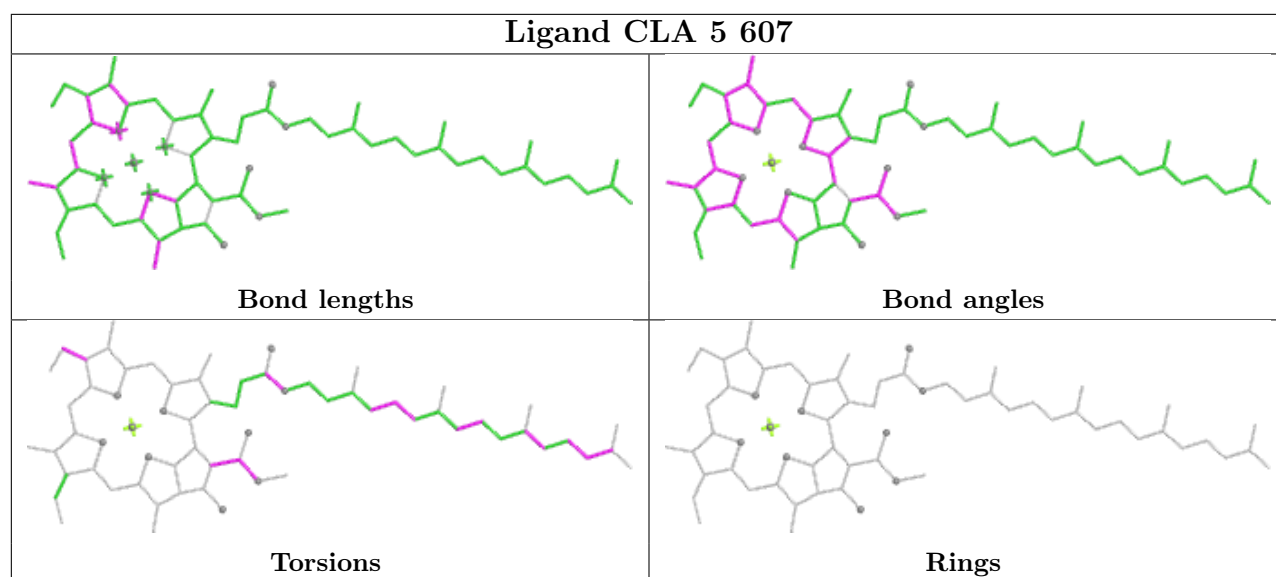


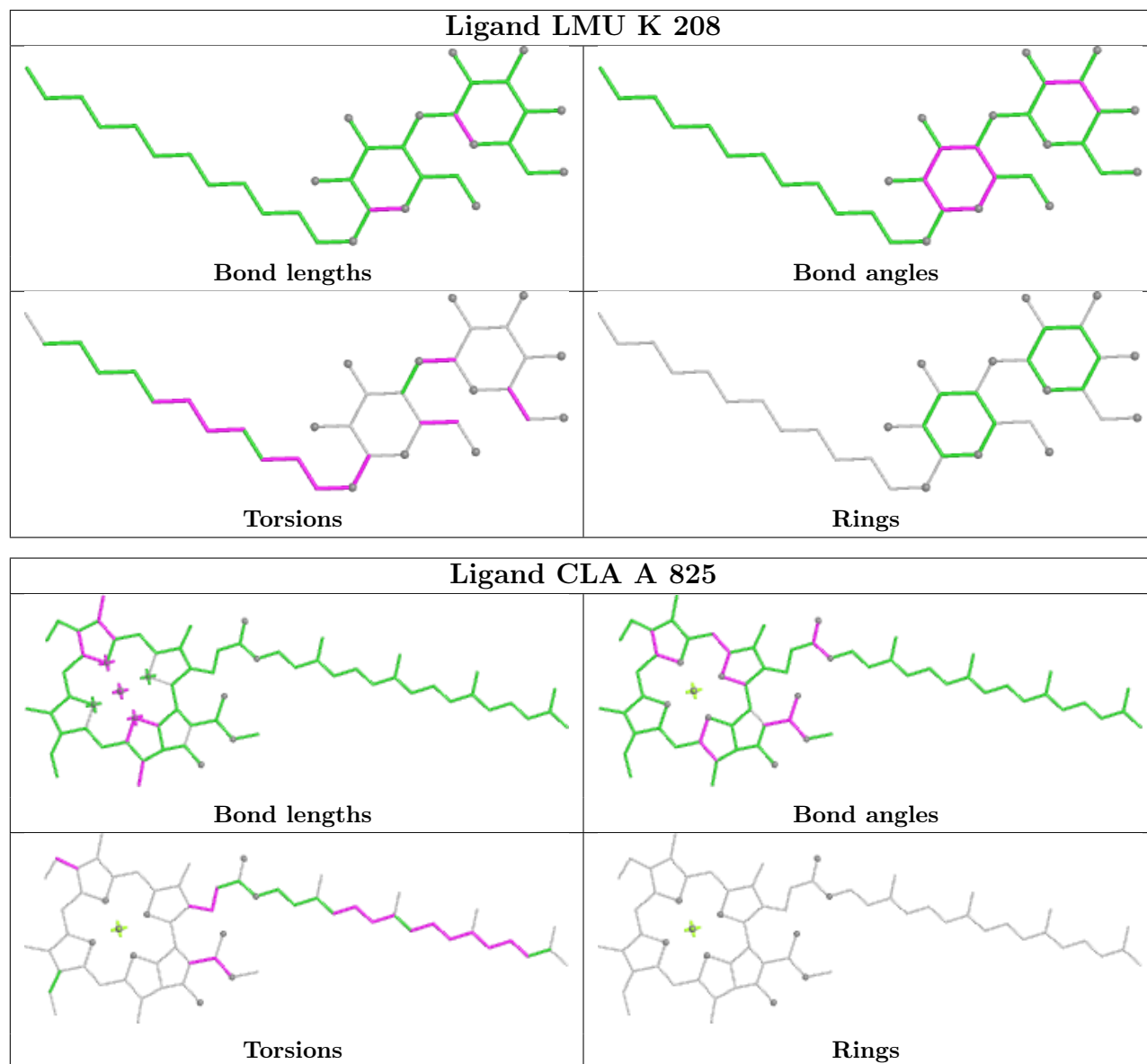
Ligand CLA 4 613



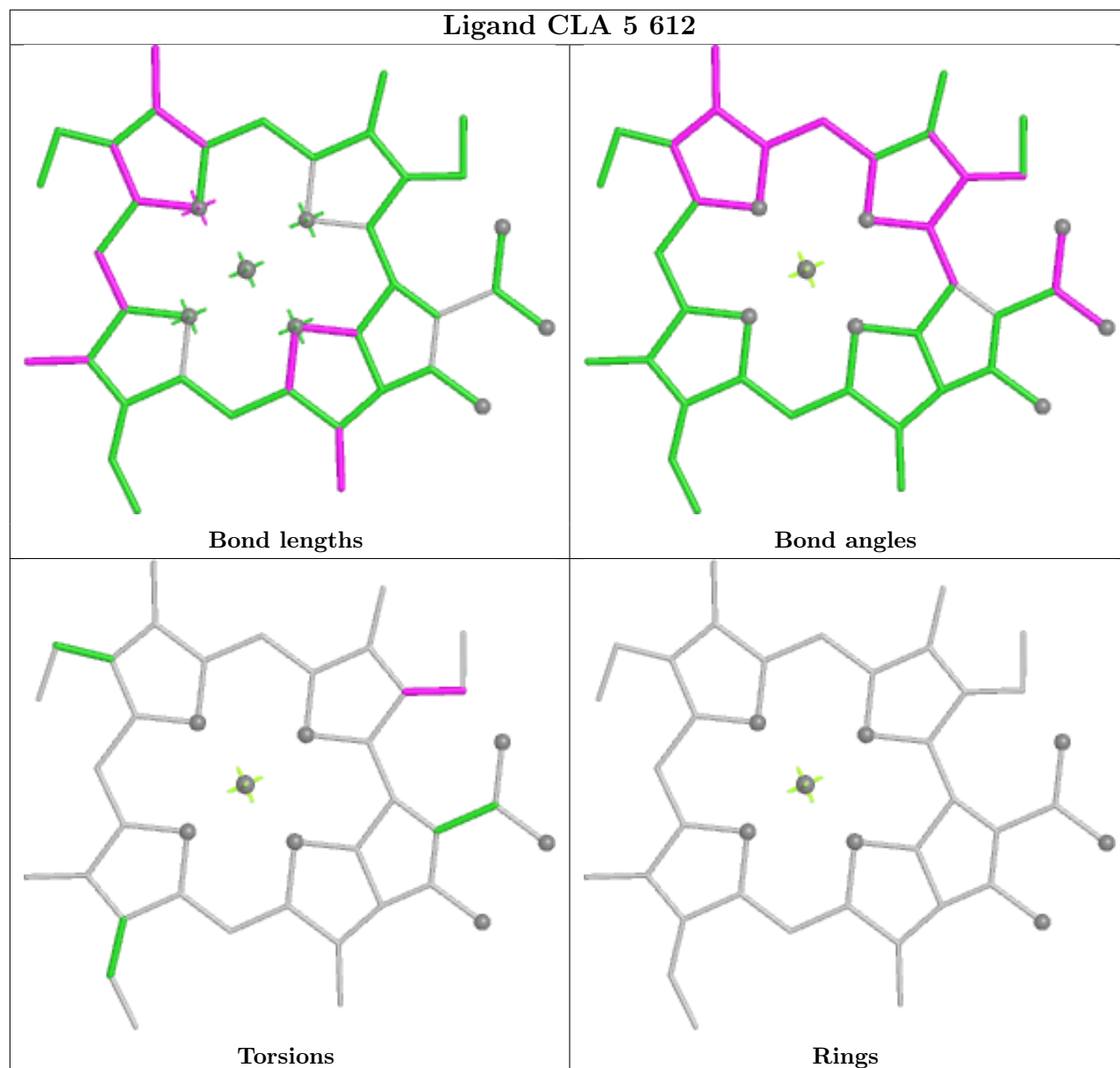
Ligand CLA 7 603



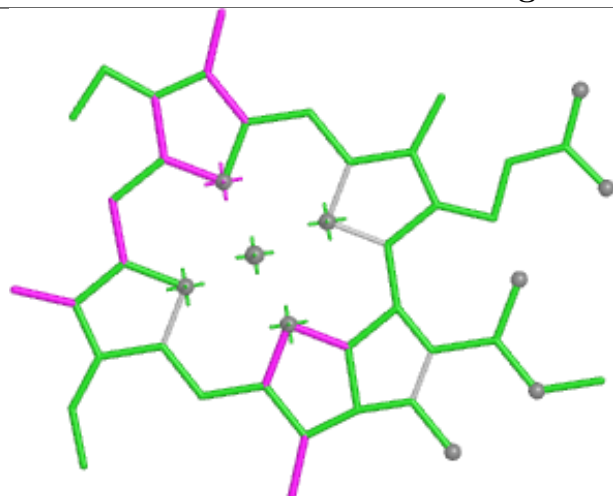




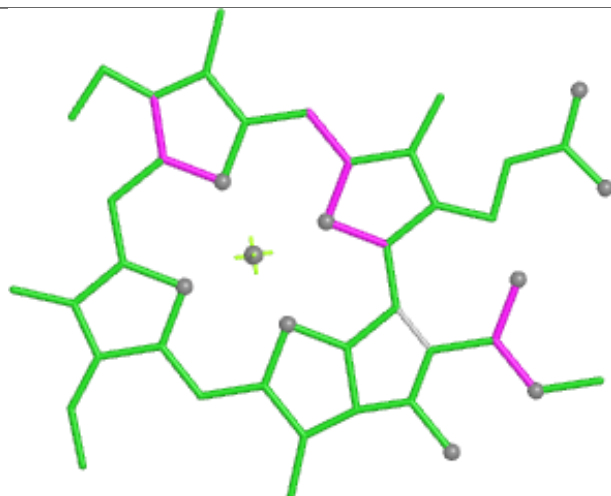
Ligand CLA 5 612



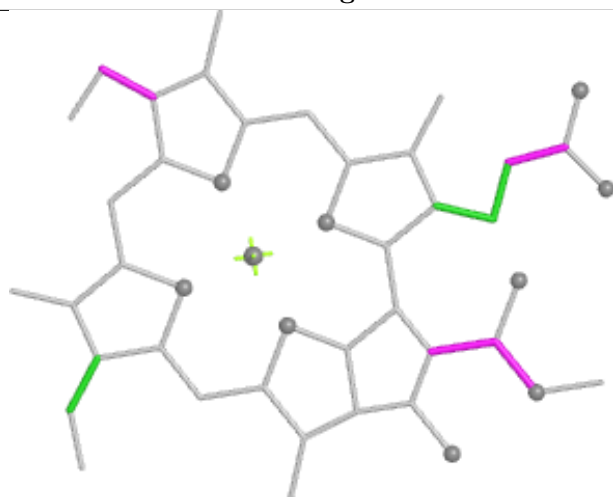
Ligand CLA 6 617



Bond lengths



Bond angles

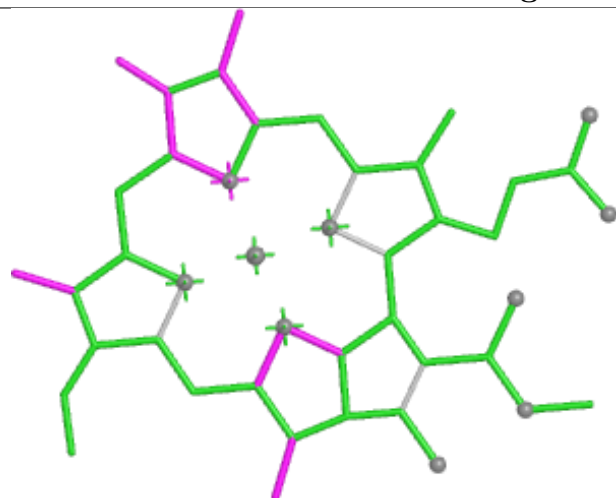


Torsions

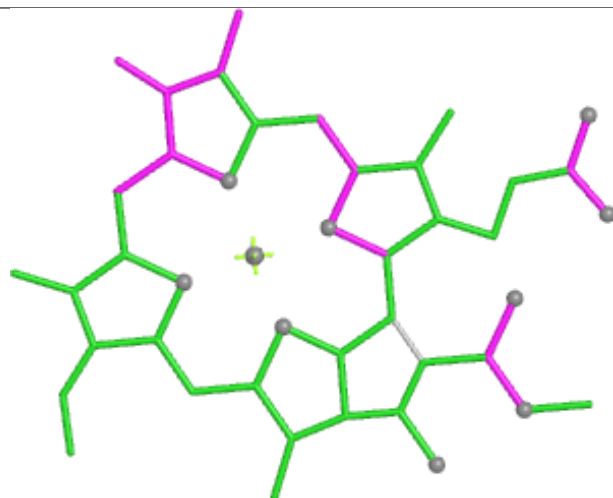


Rings

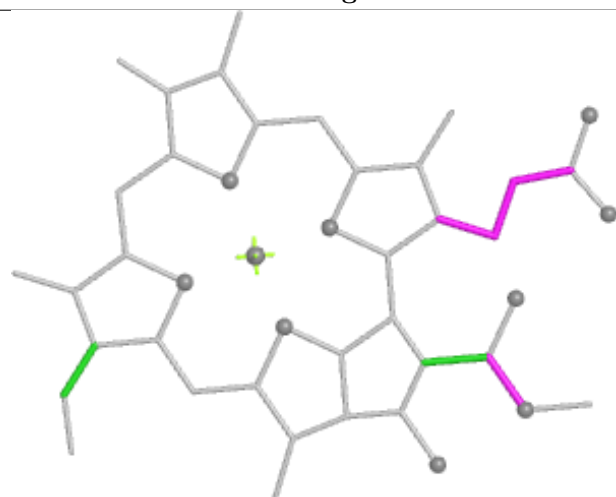
Ligand CLA 8 603



Bond lengths



Bond angles

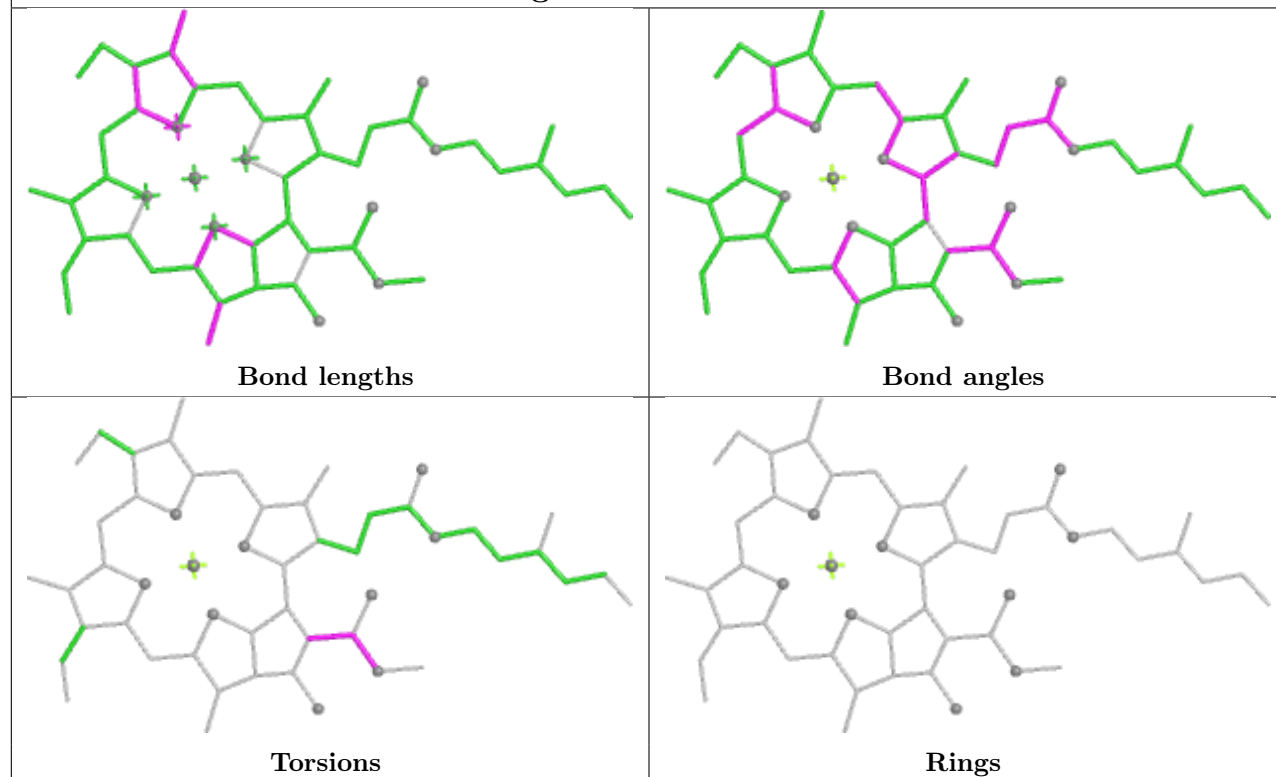


Torsions

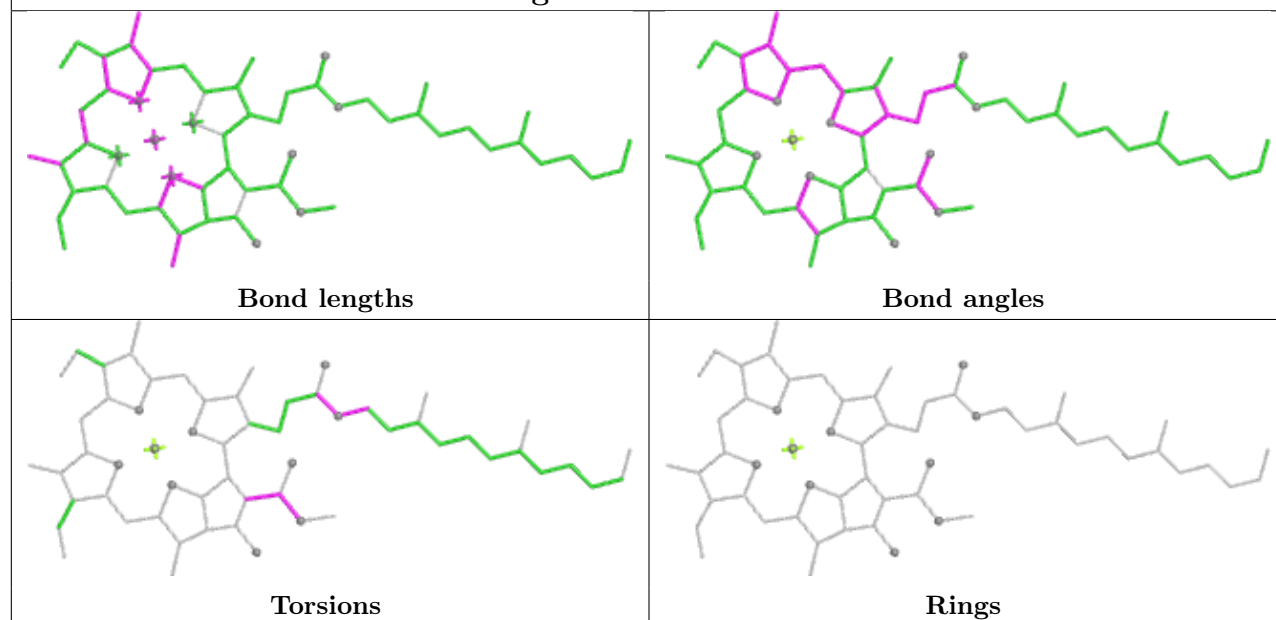


Rings

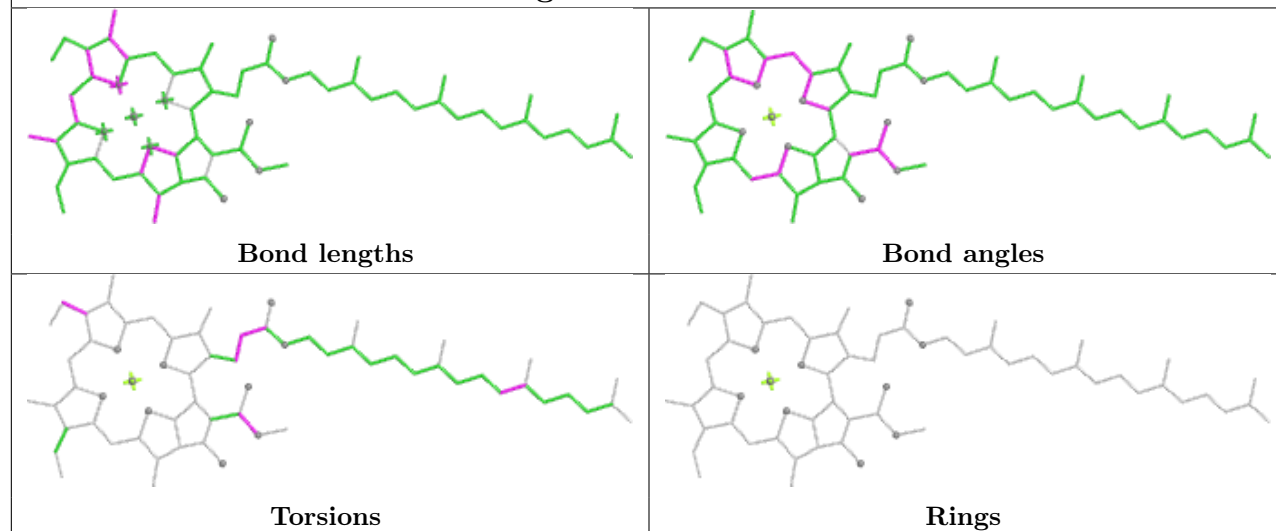
Ligand CLA A 840



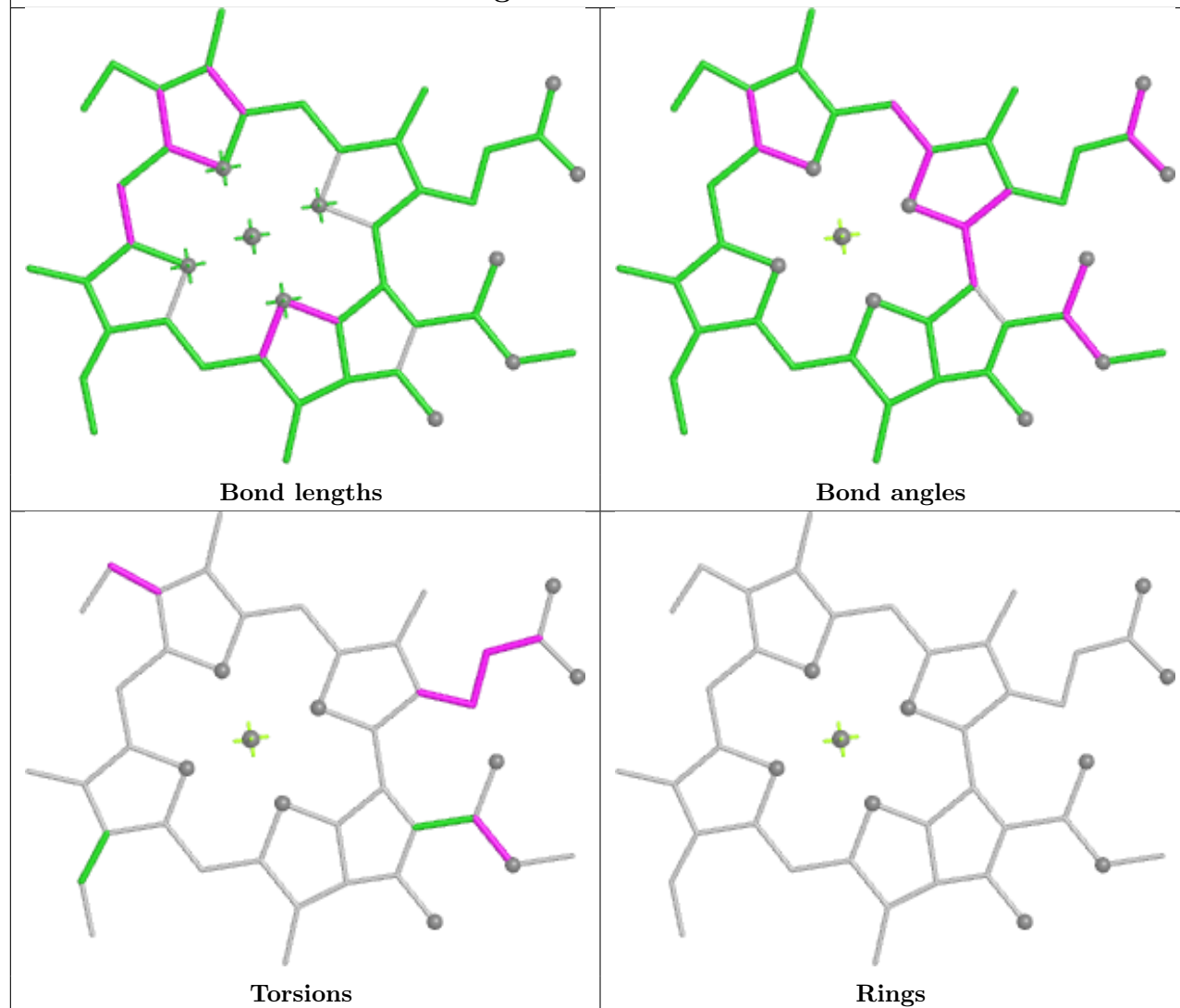
Ligand CLA A 827

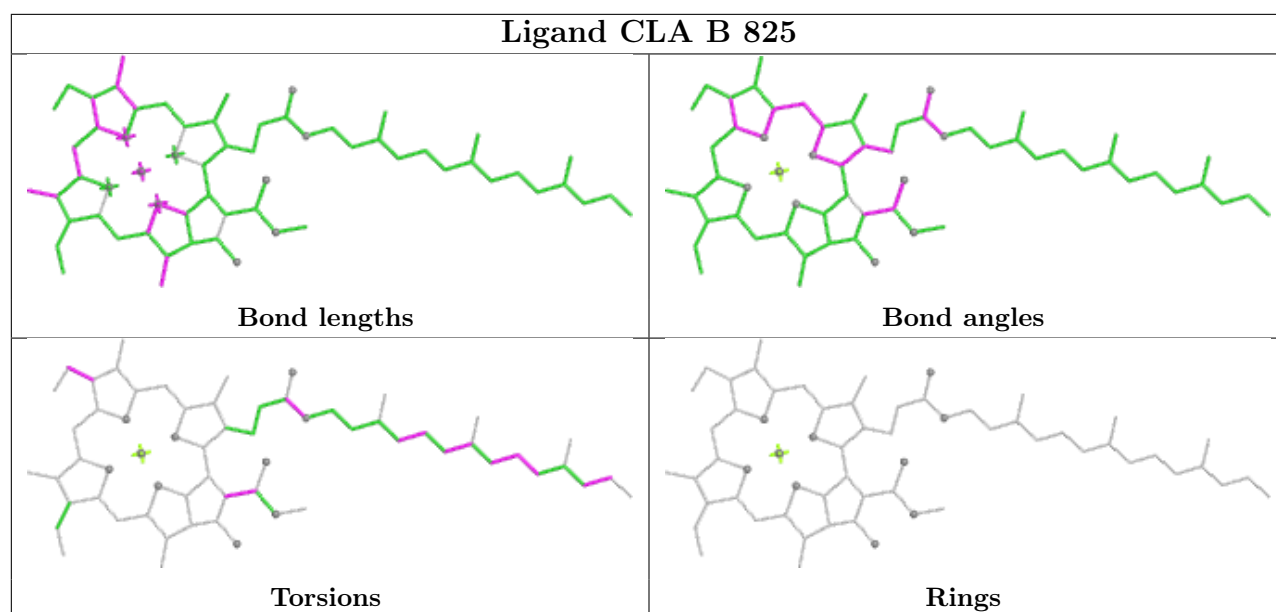


Ligand CLA 6 602

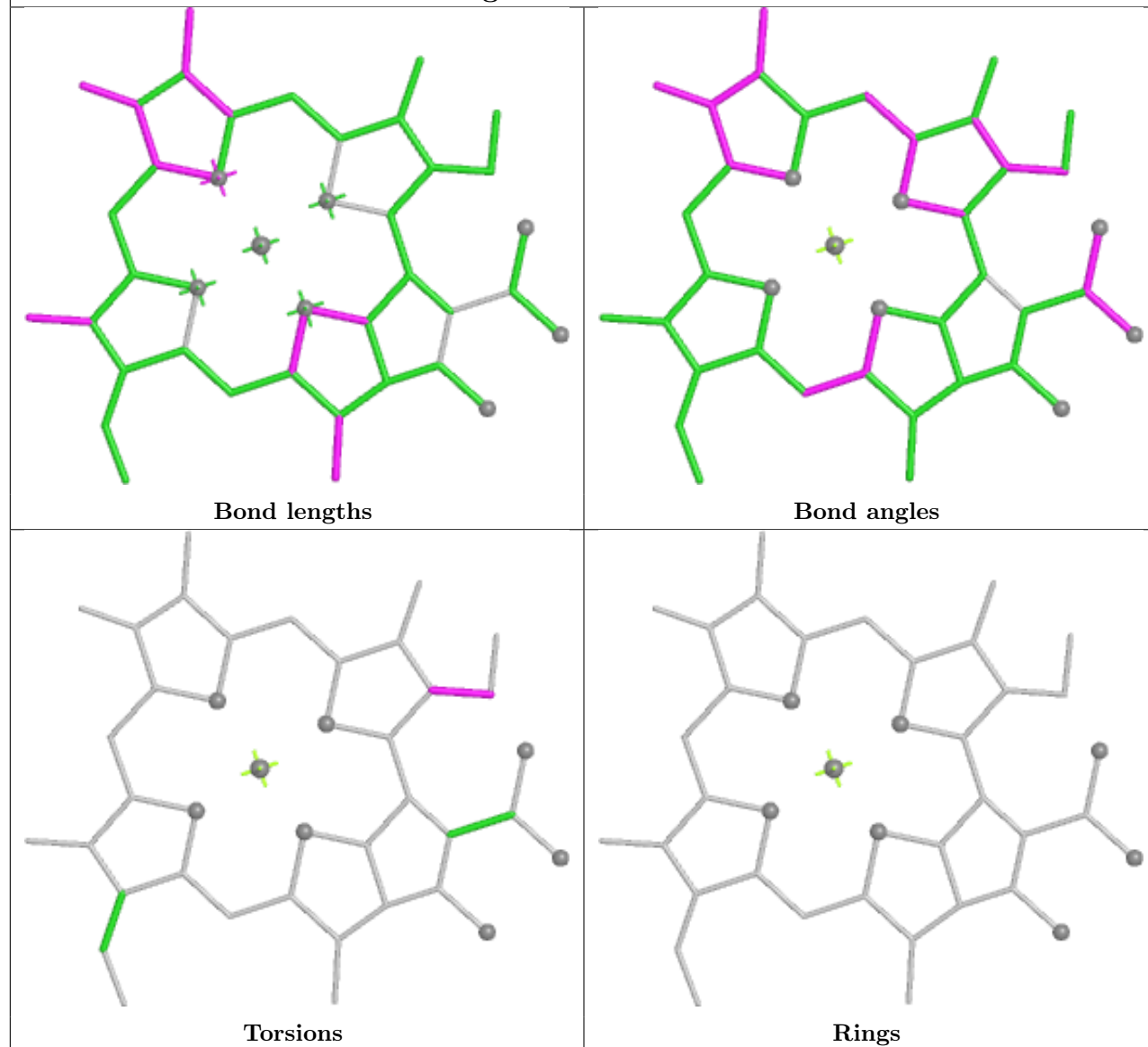


Ligand CLA L 302

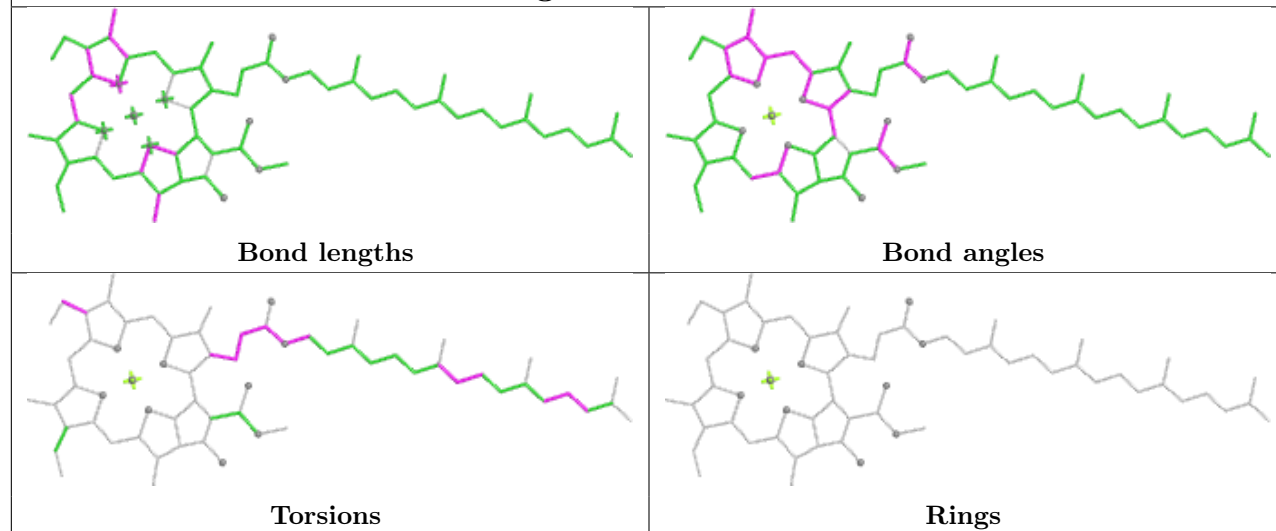


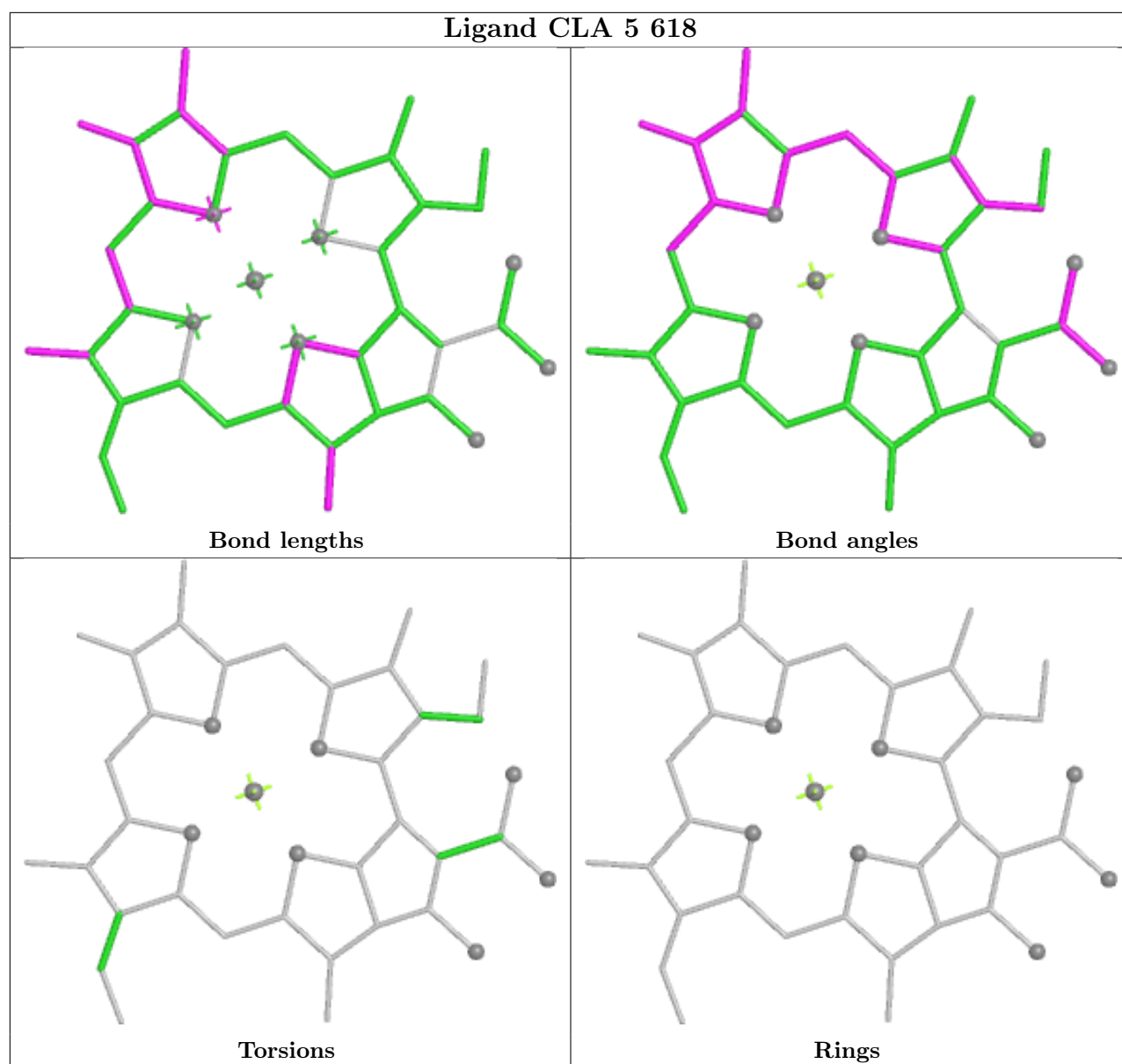


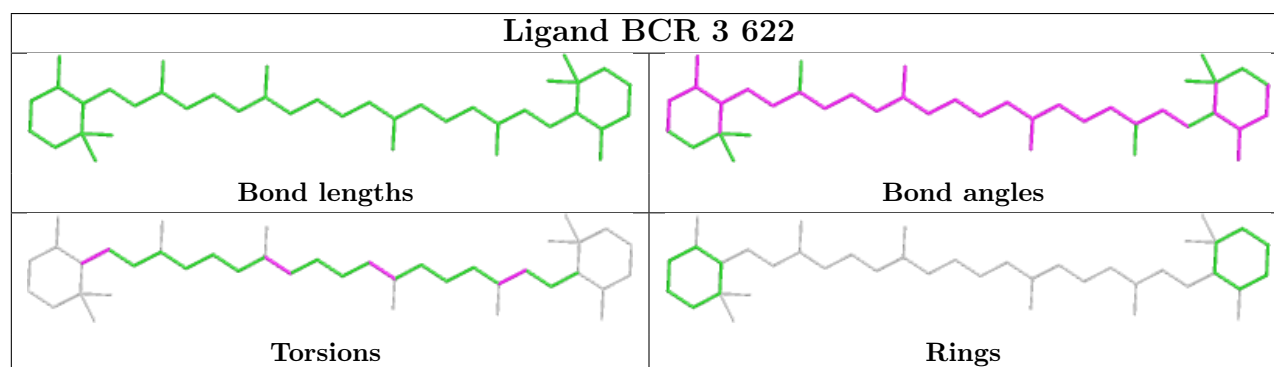
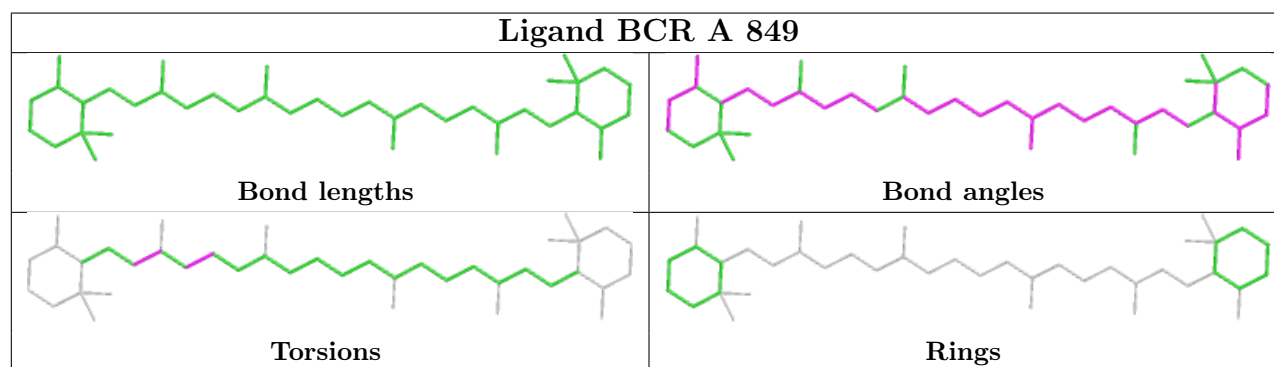
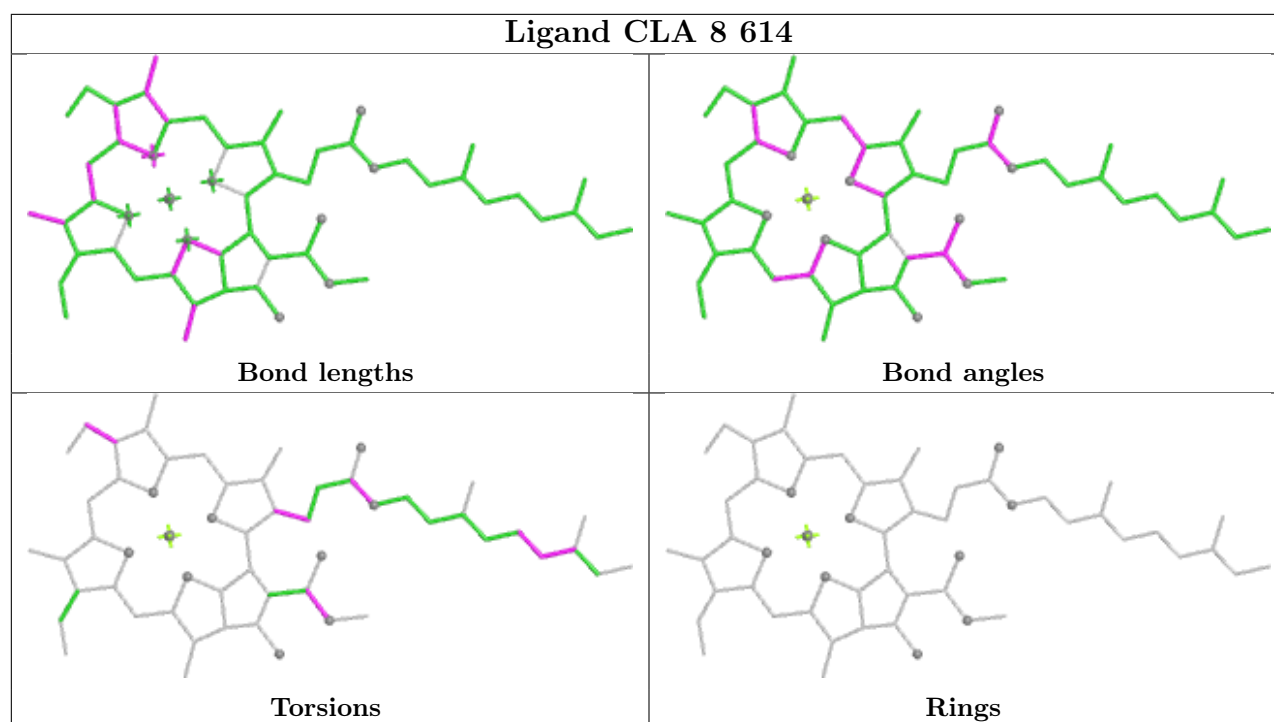
Ligand CLA 4 618

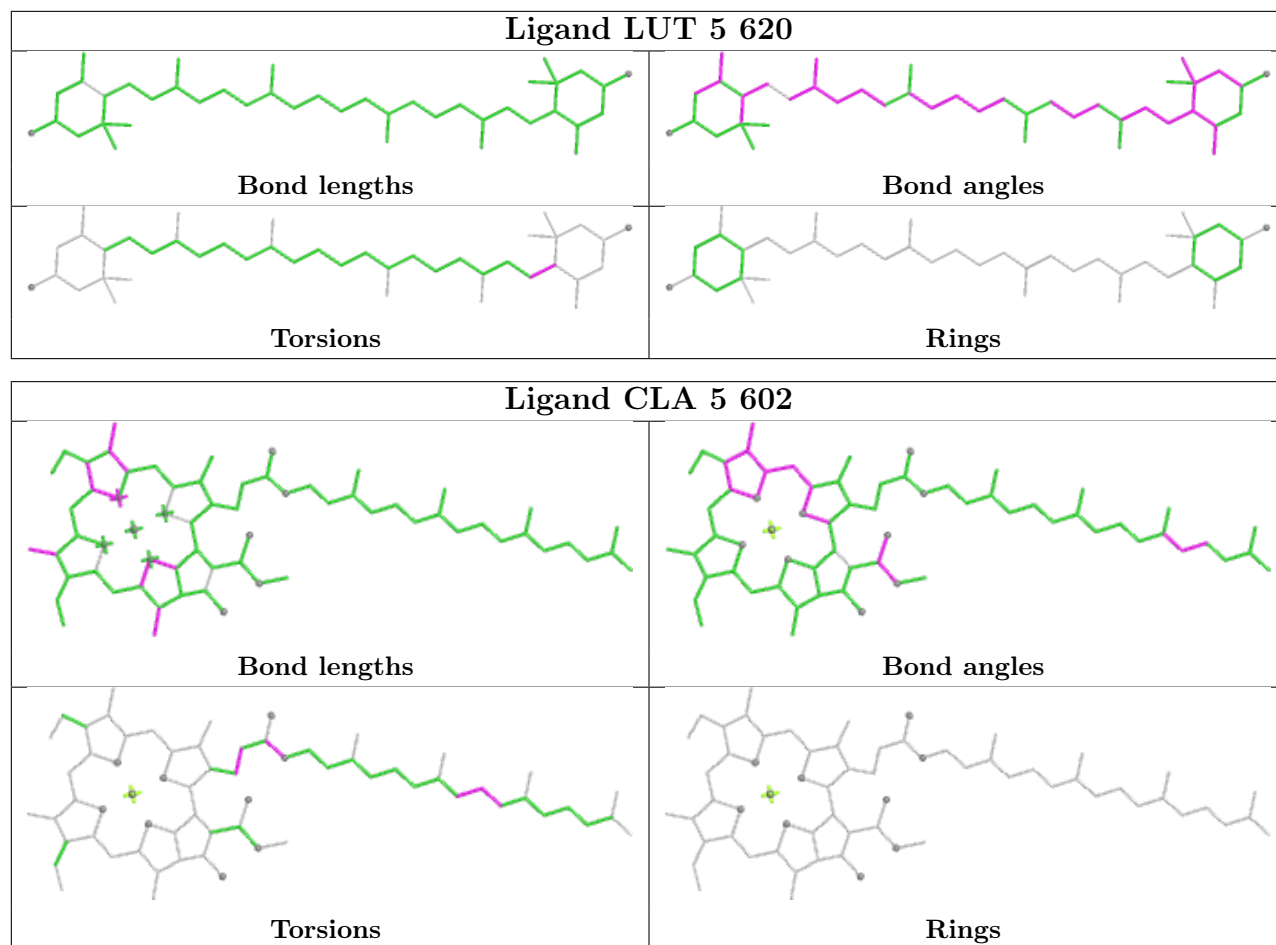


Ligand CLA 5 609

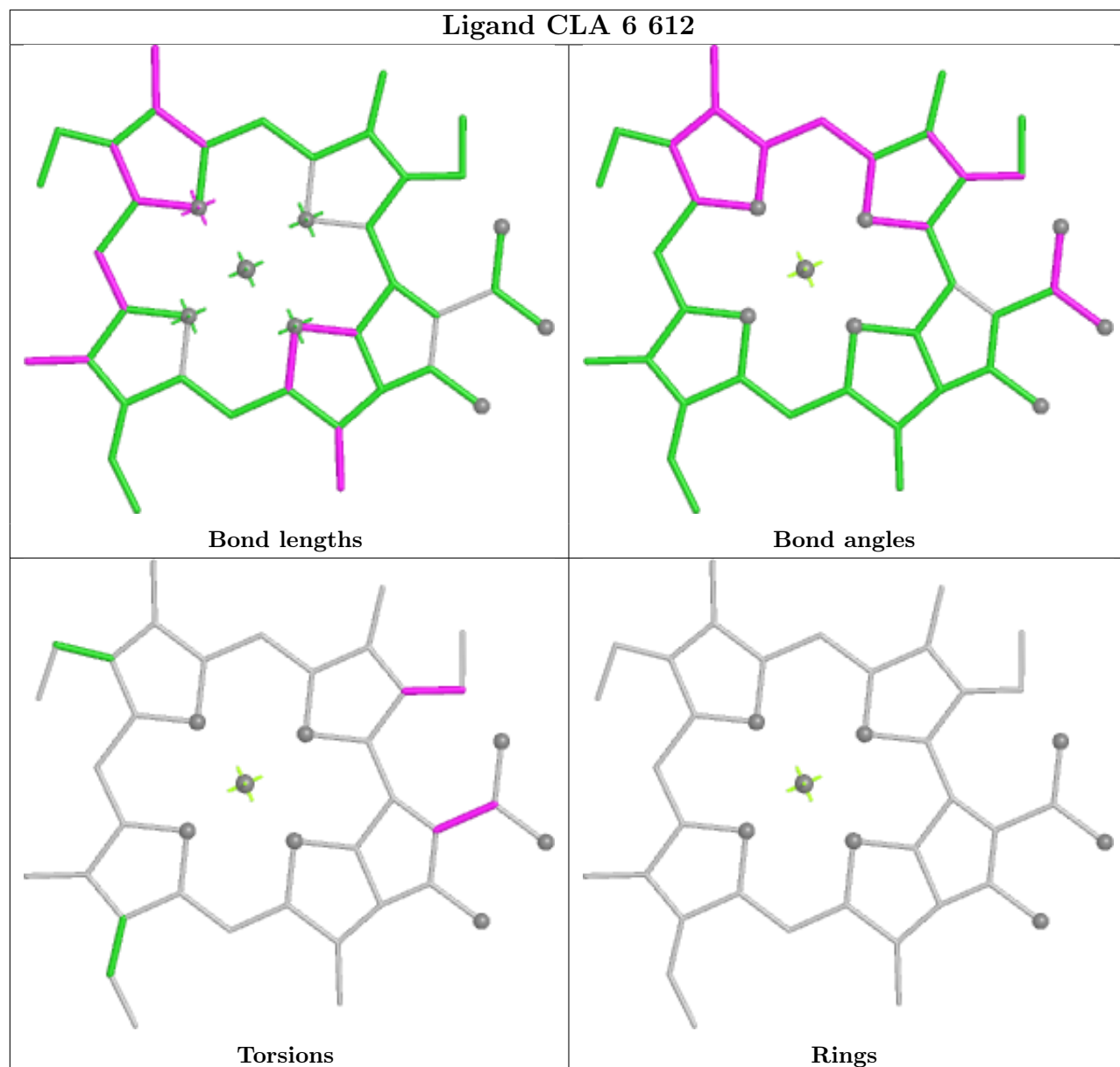


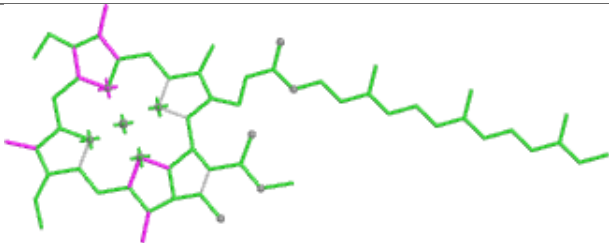
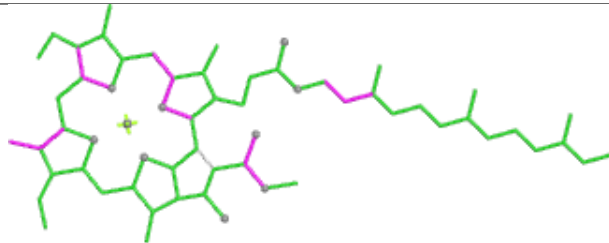
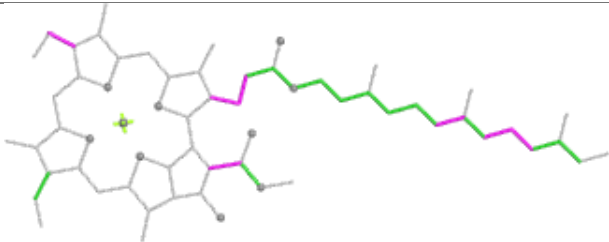
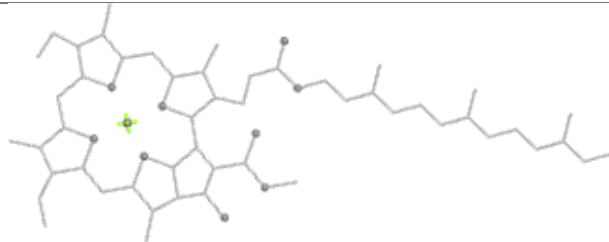


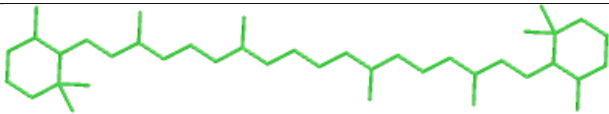
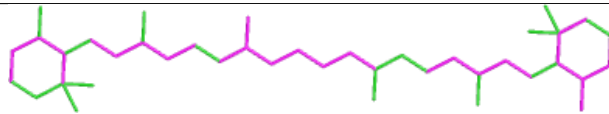
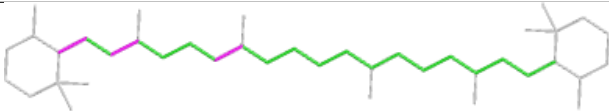
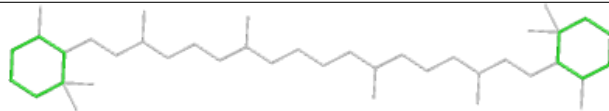


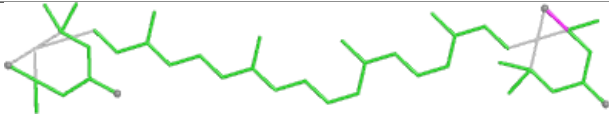
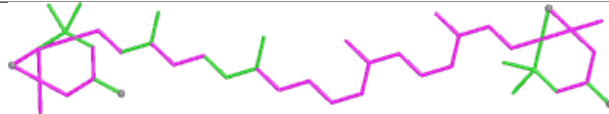
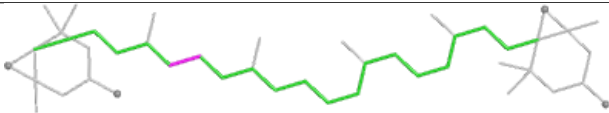
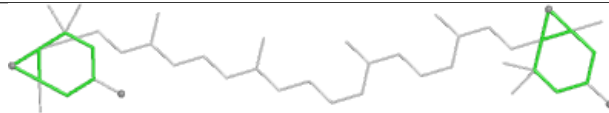


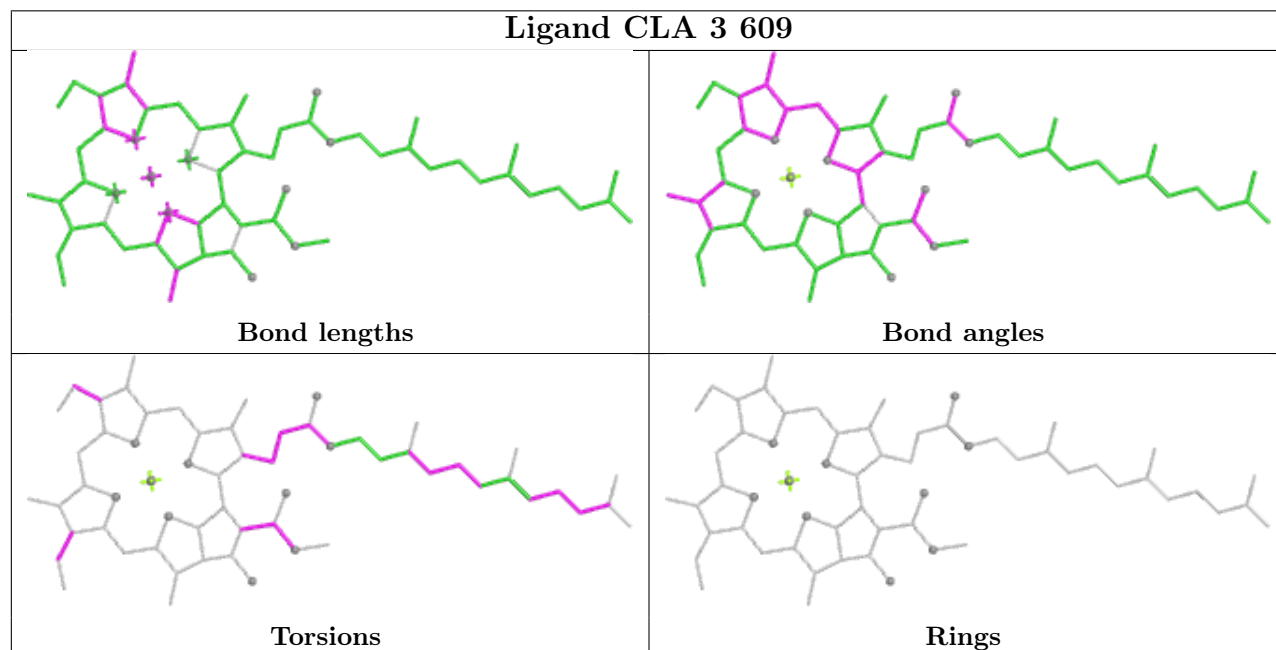
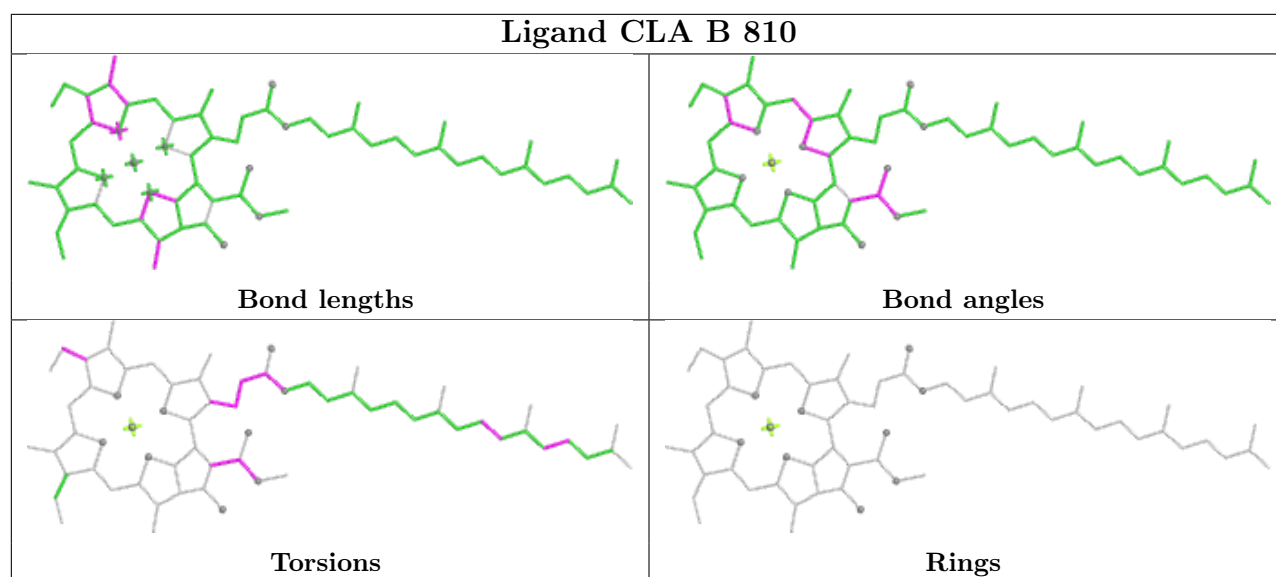
Ligand CLA 6 612

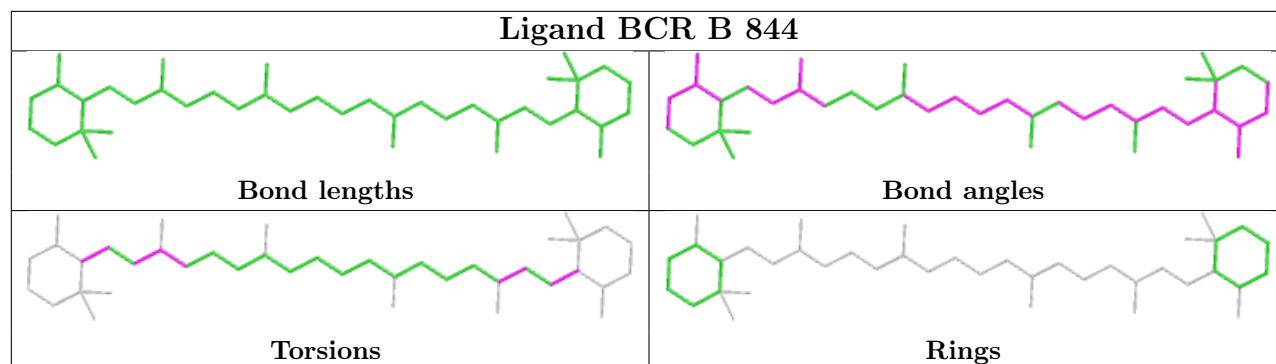
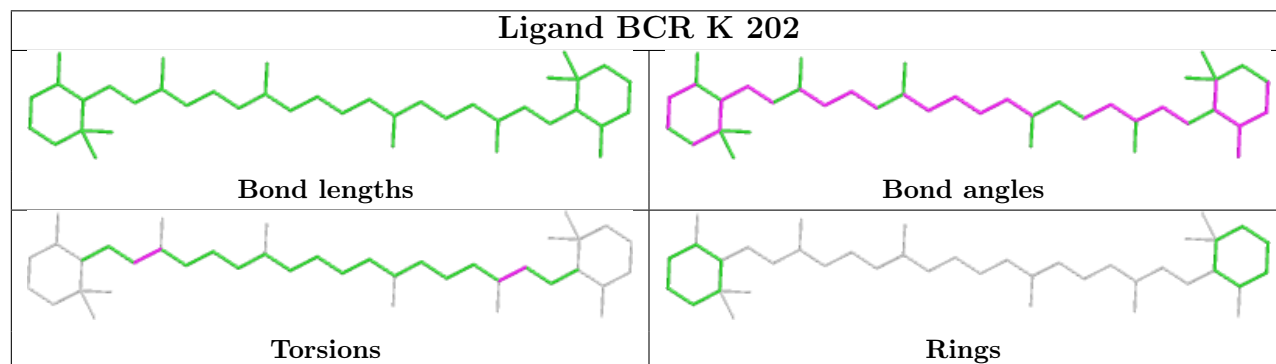
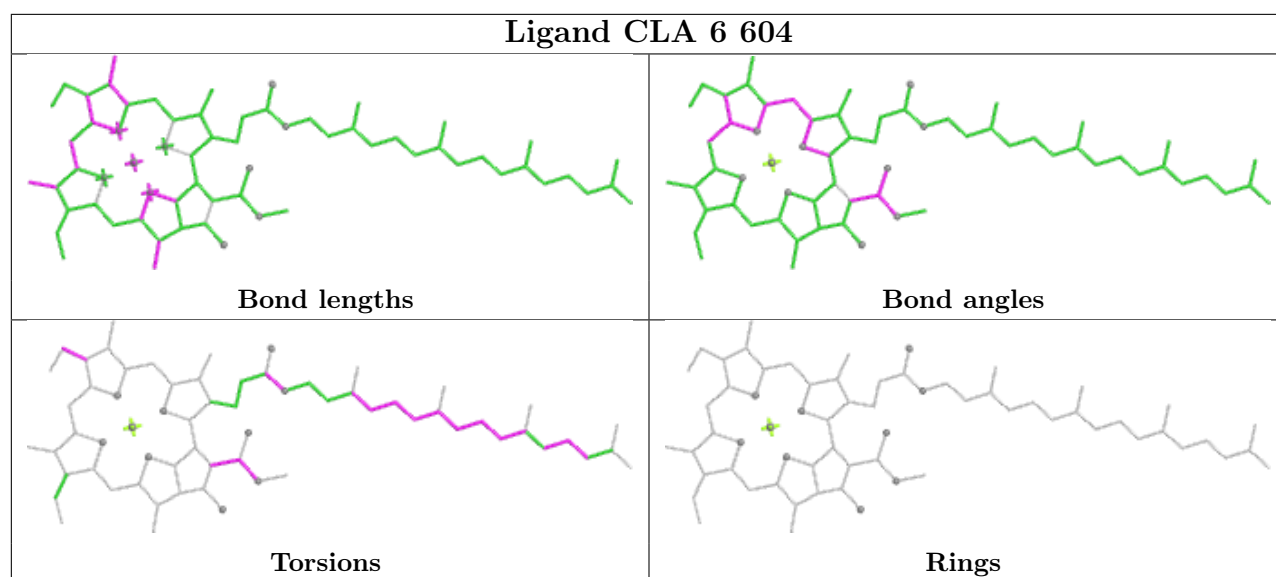


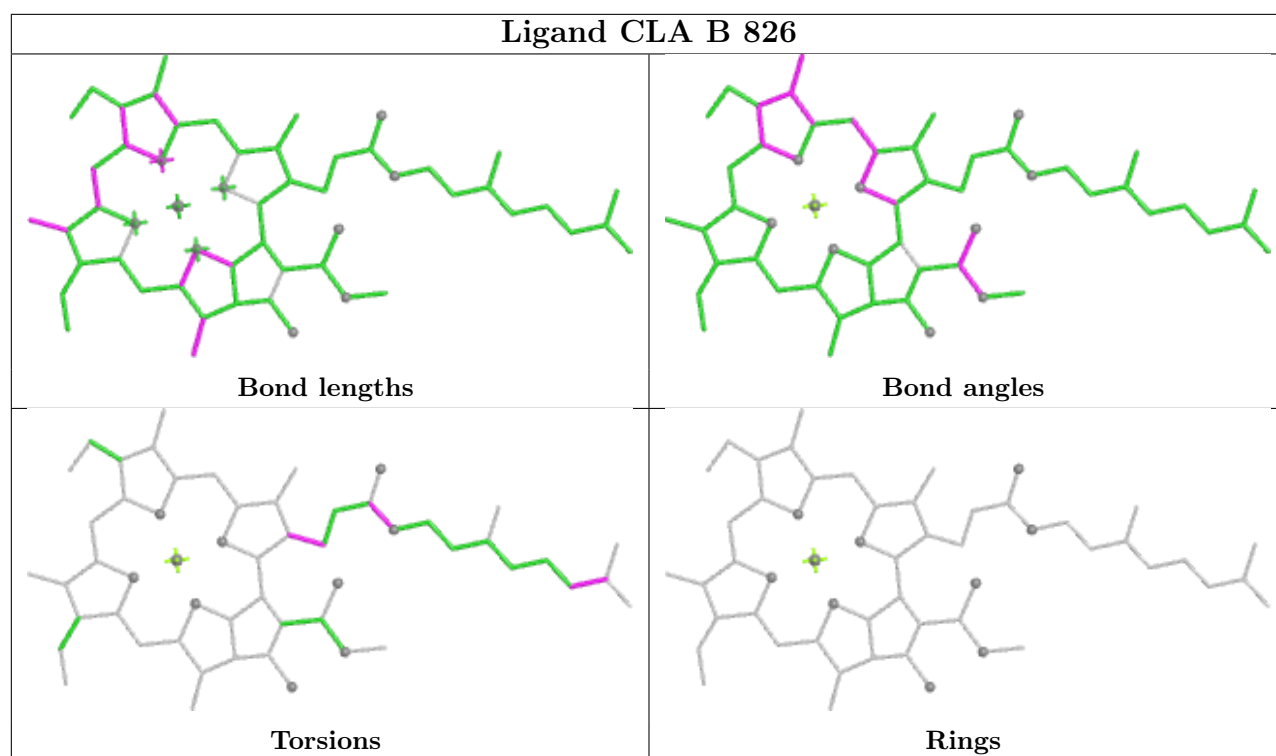
Ligand CLA 4 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

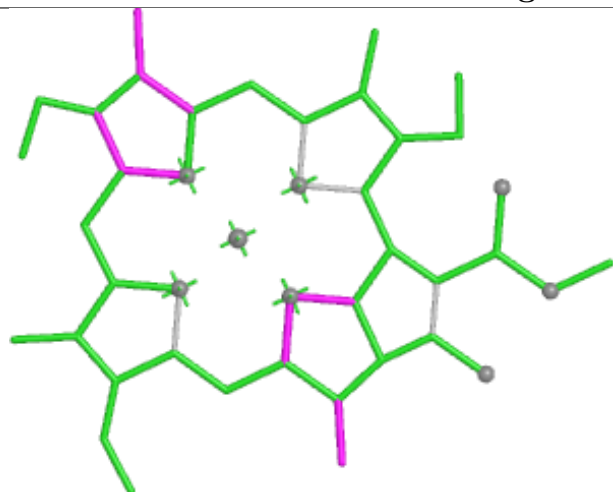
Ligand XAT a 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



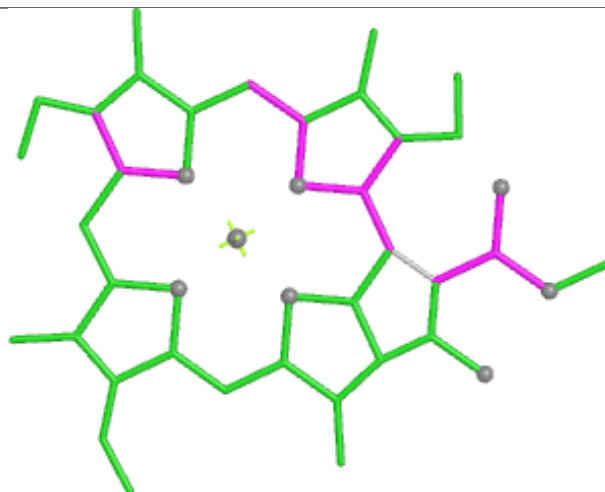




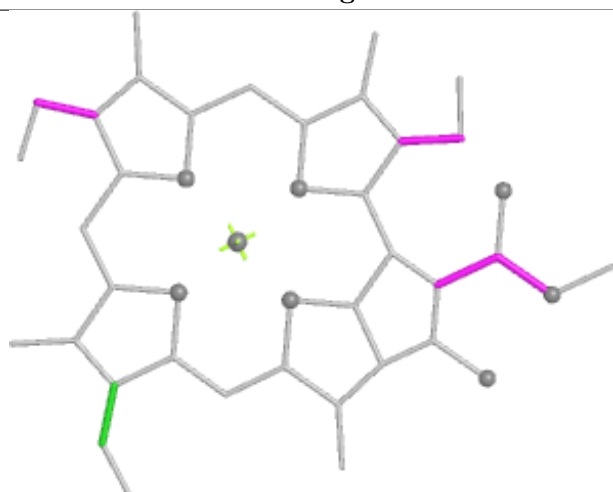
Ligand CLA J 101



Bond lengths



Bond angles

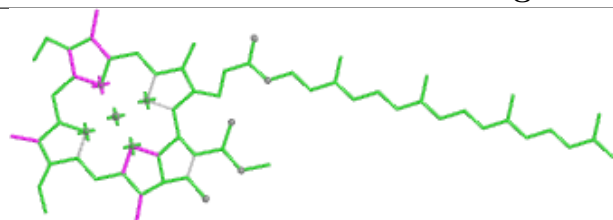


Torsions

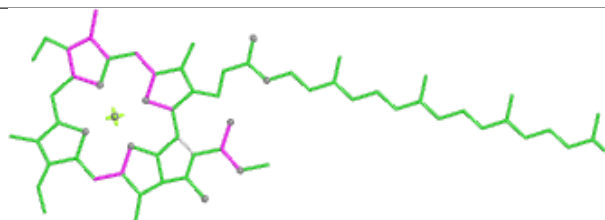


Rings

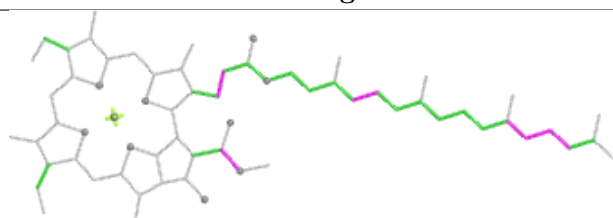
Ligand CLA A 829



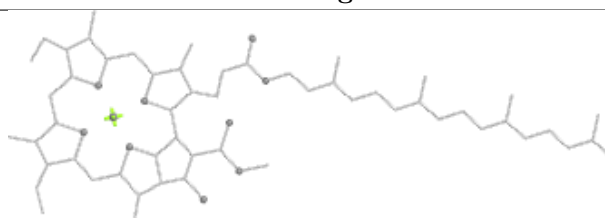
Bond lengths



Bond angles

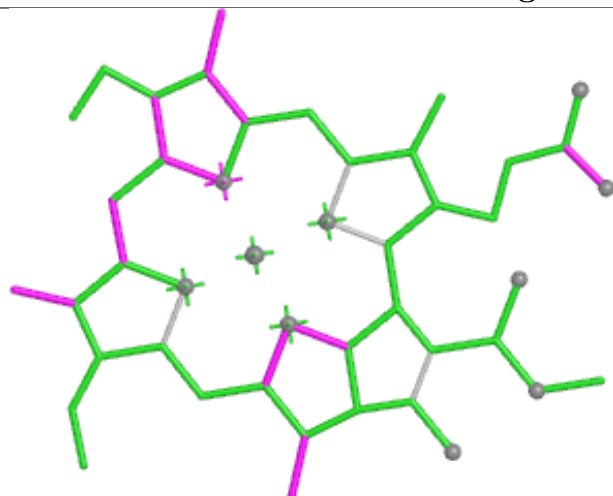


Torsions

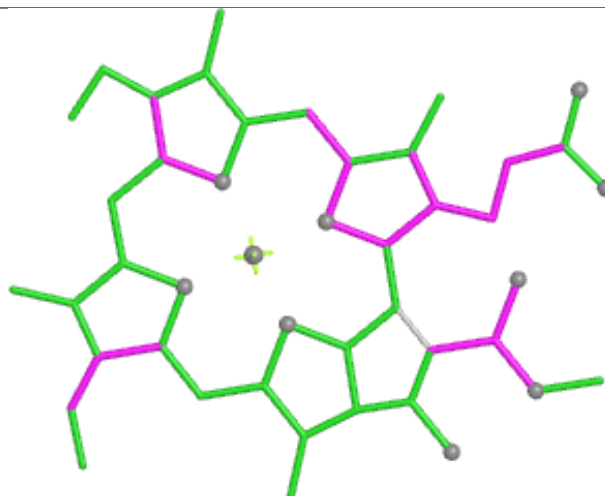


Rings

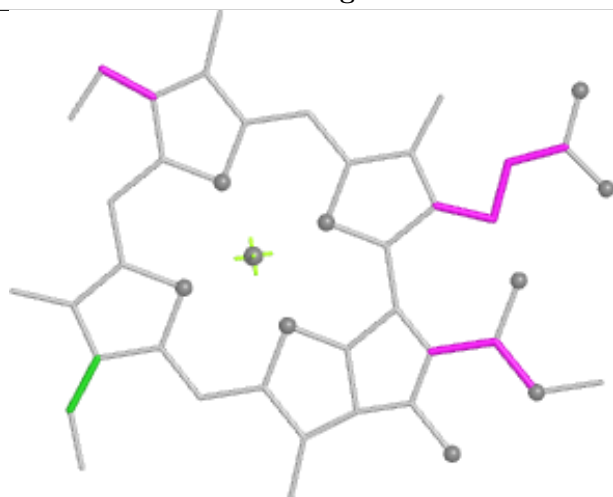
Ligand CLA 6 620



Bond lengths



Bond angles

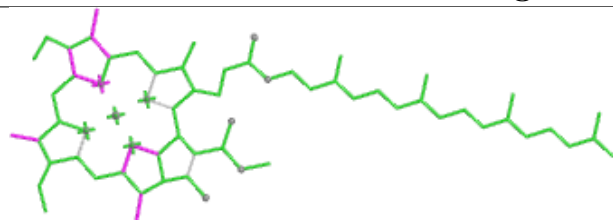


Torsions

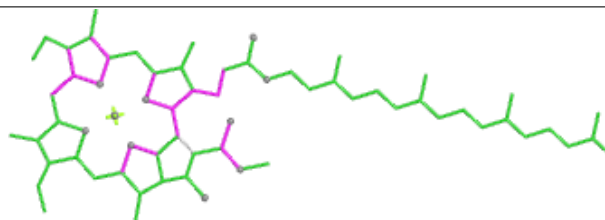


Rings

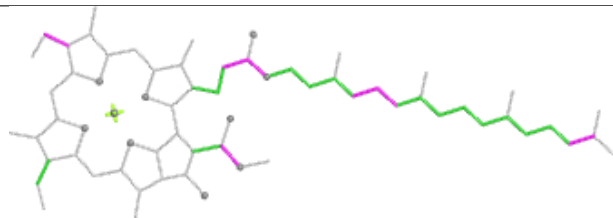
Ligand CLA A 801



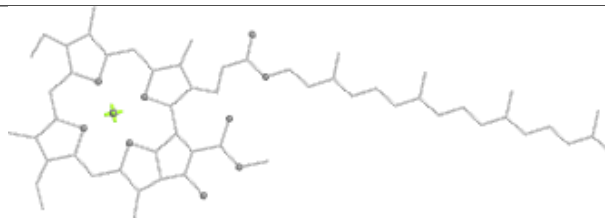
Bond lengths



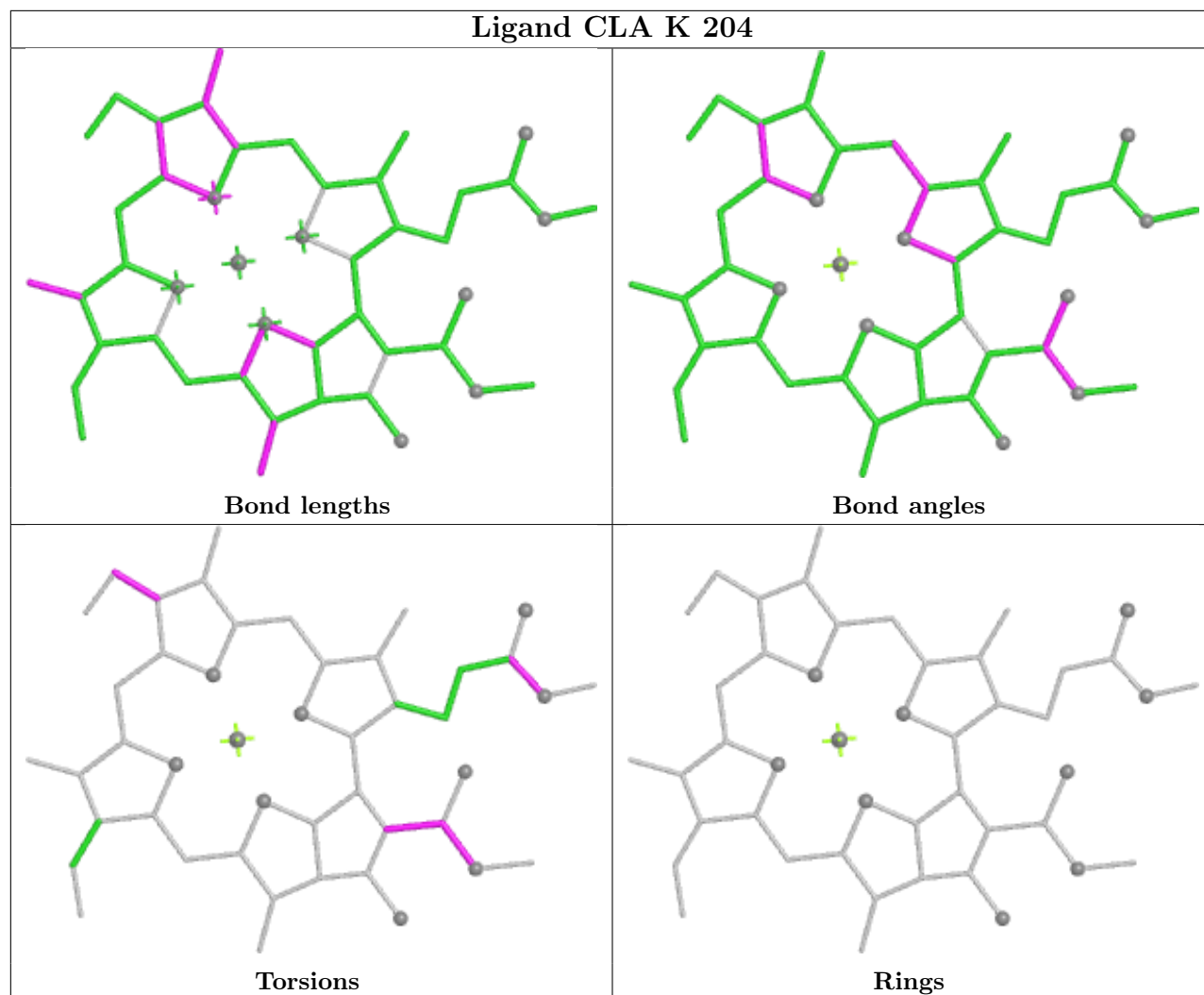
Bond angles



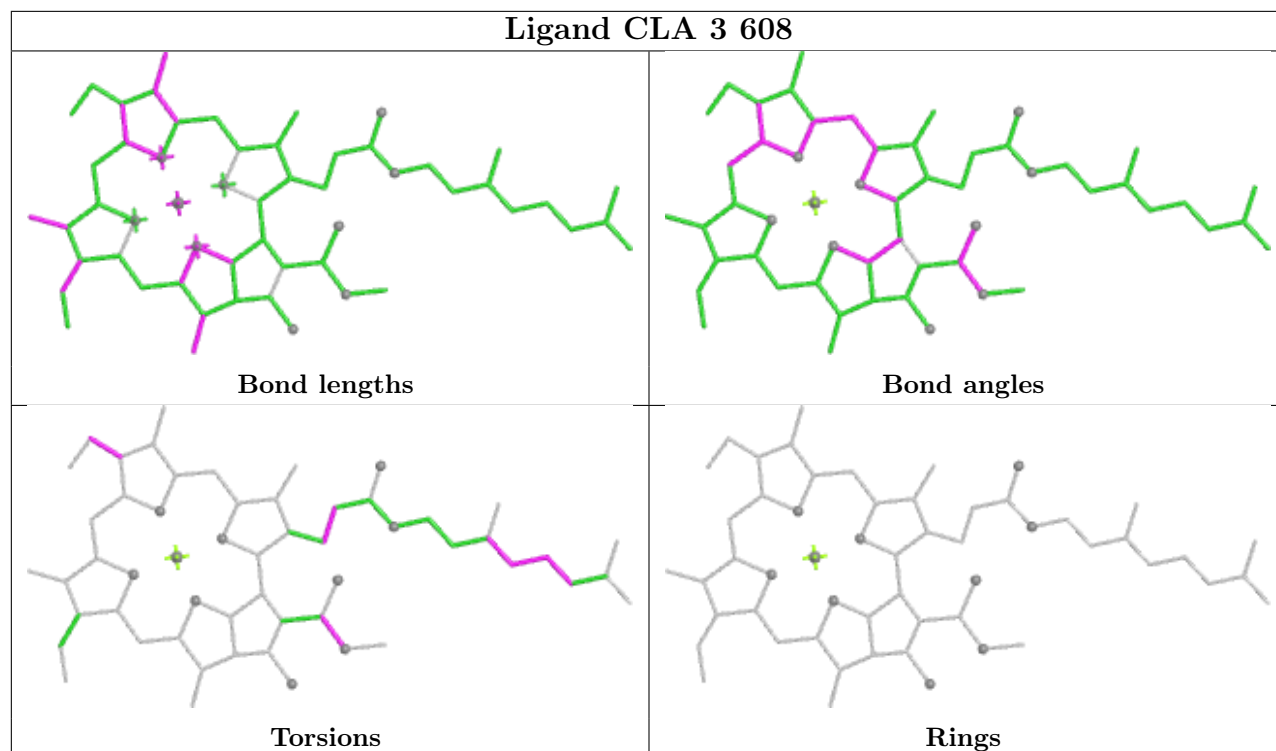
Torsions



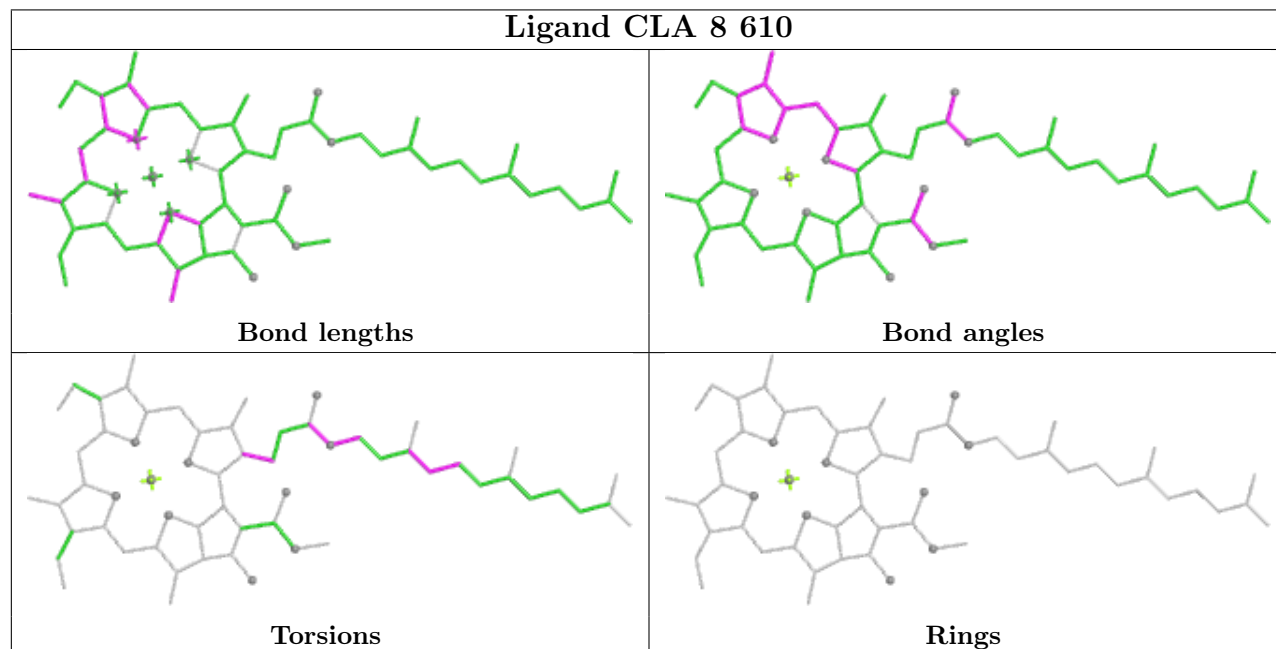
Rings

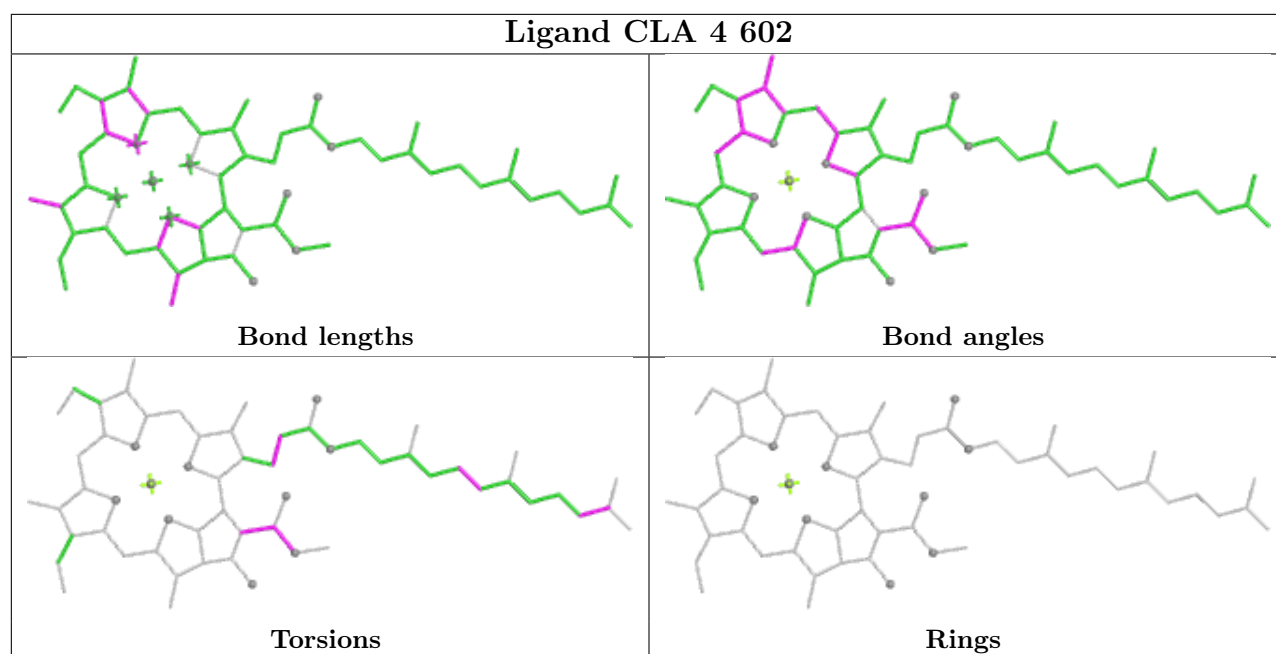


Ligand CLA 3 608

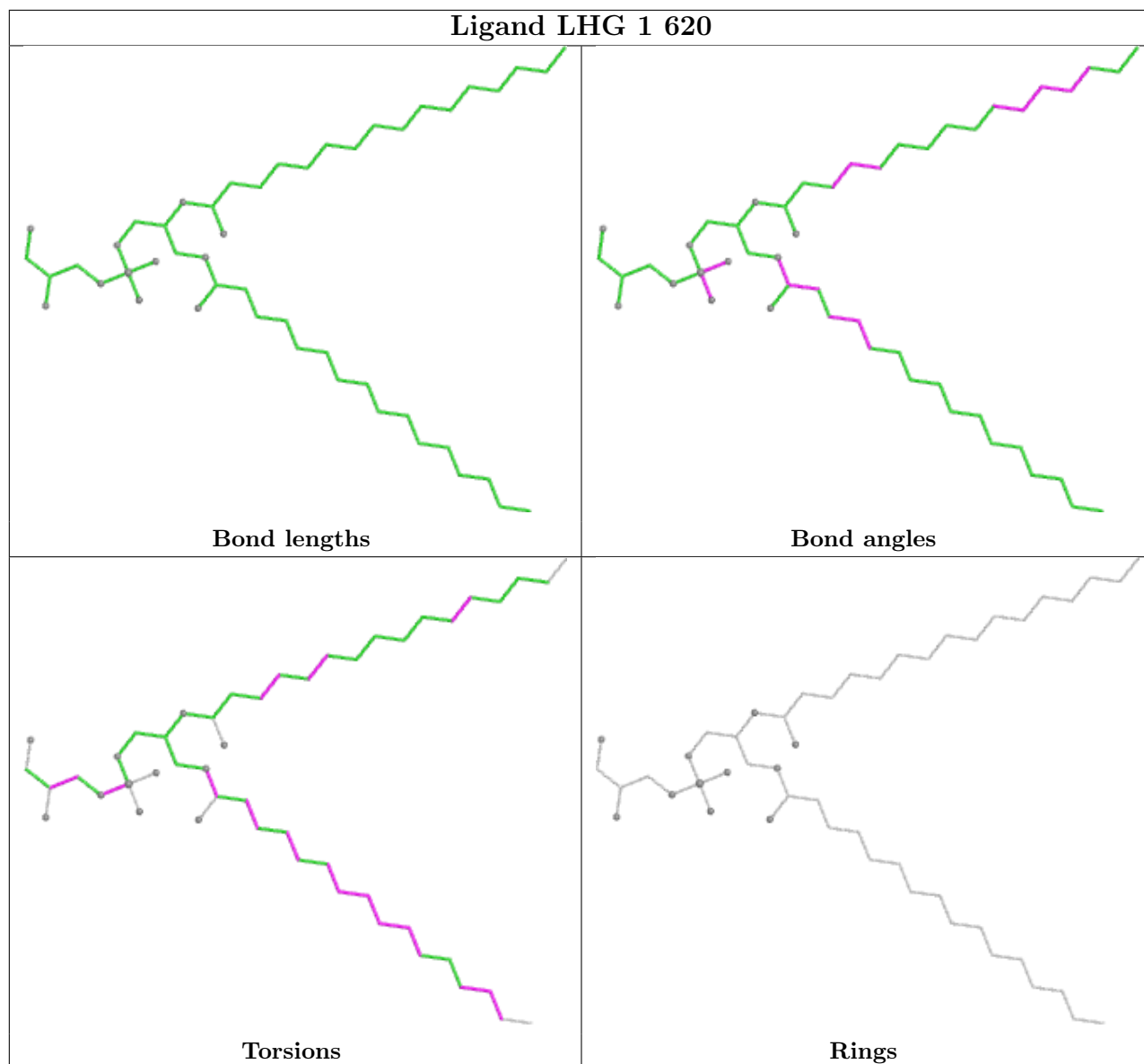


Ligand CLA 8 610

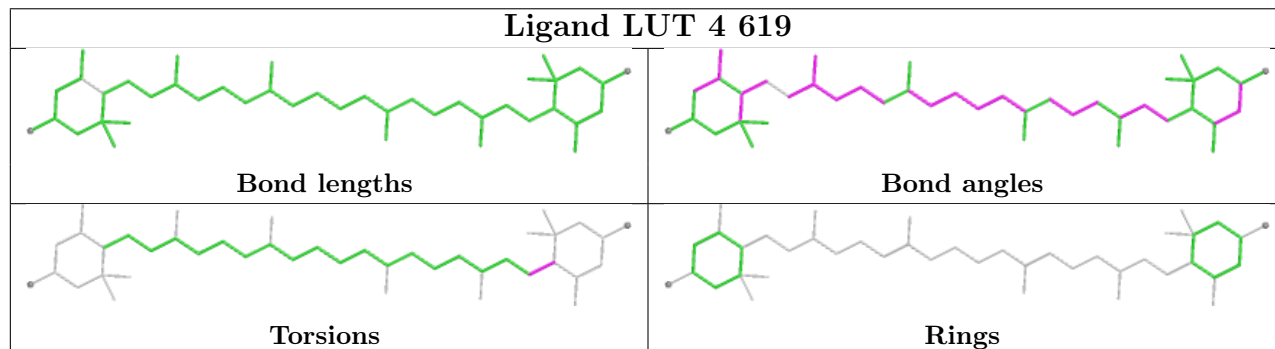


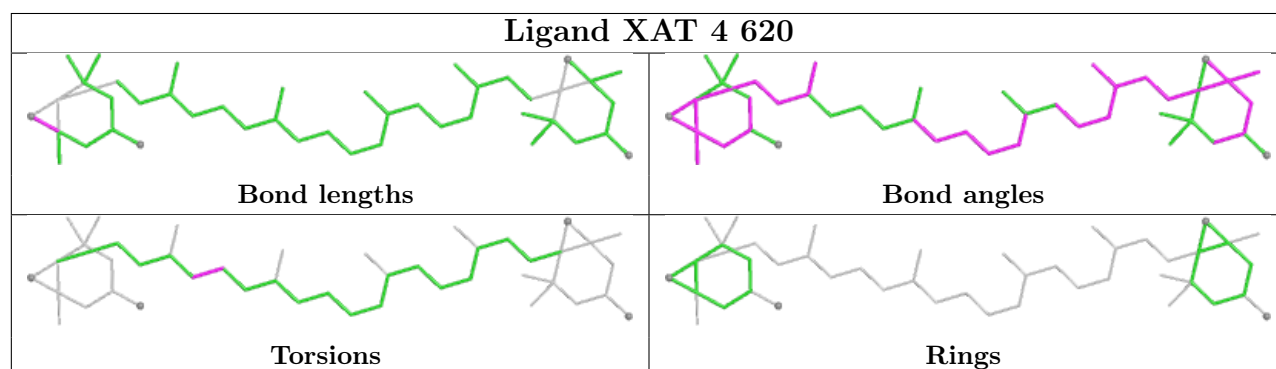
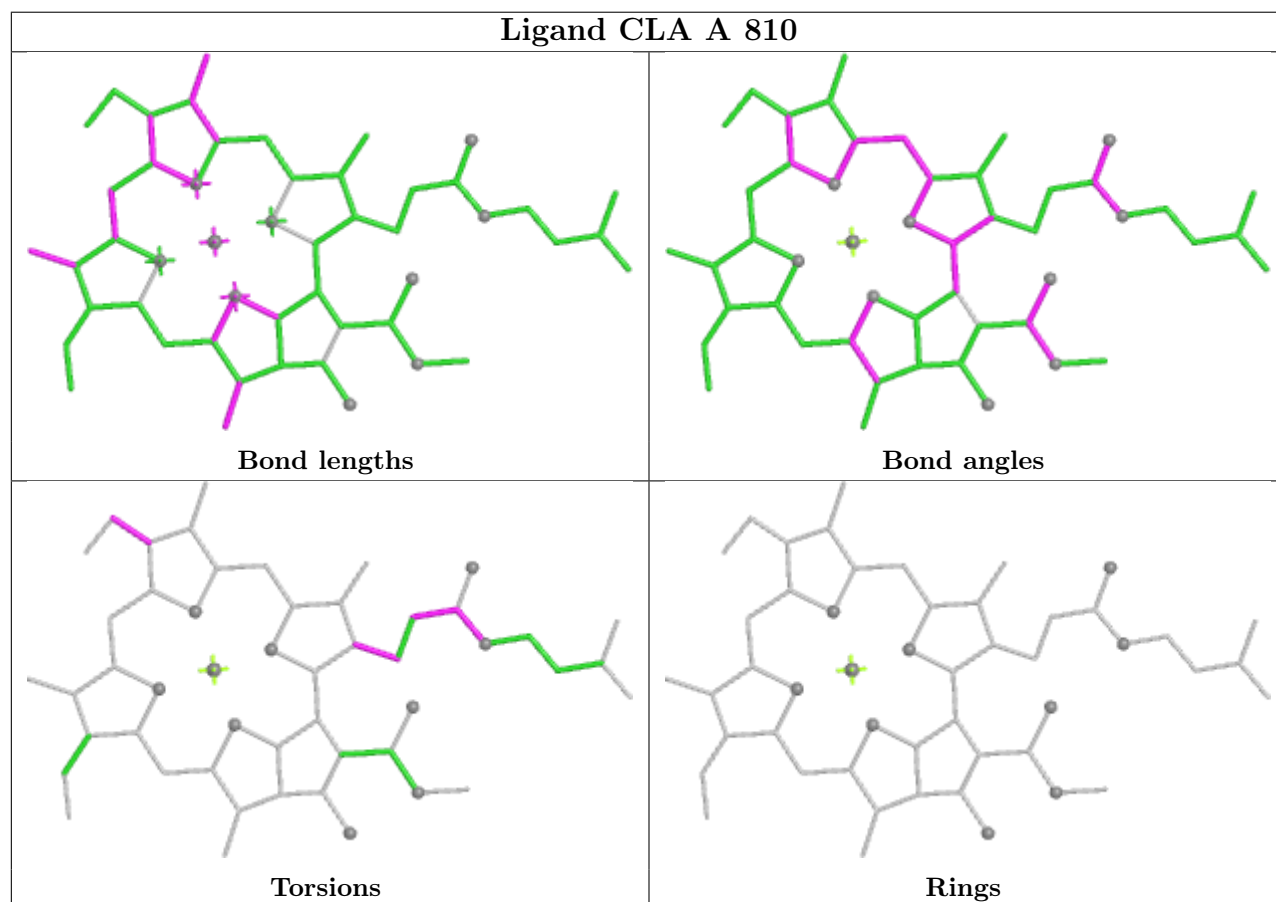
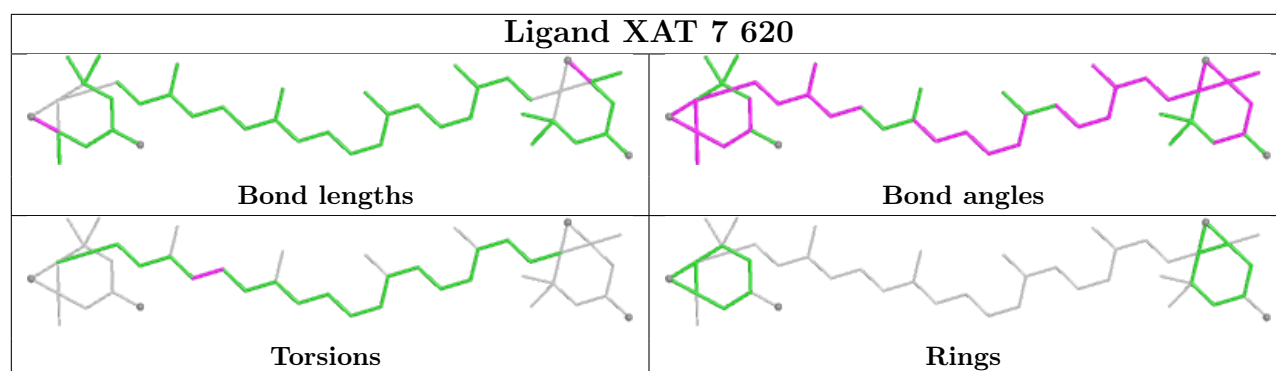


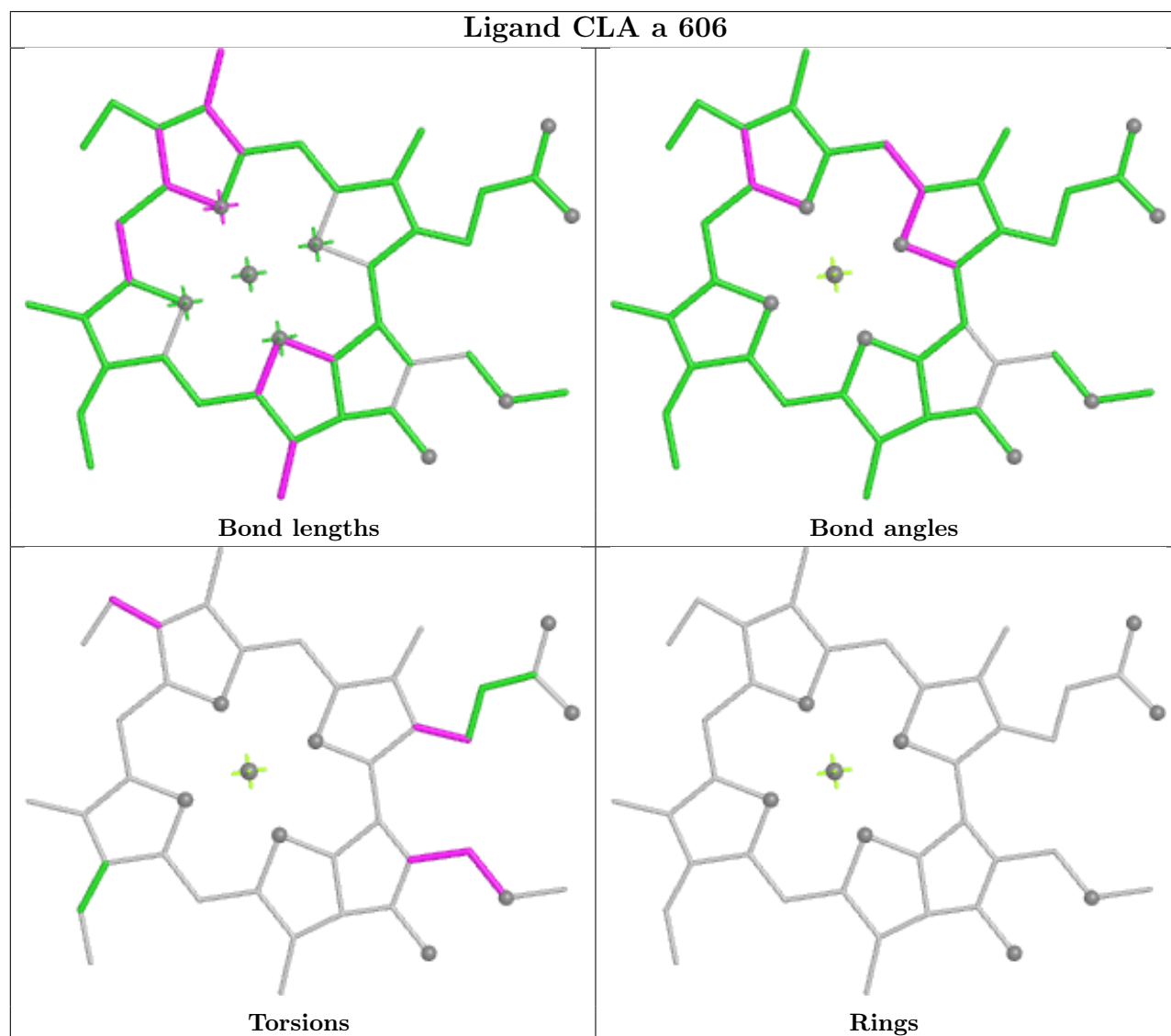
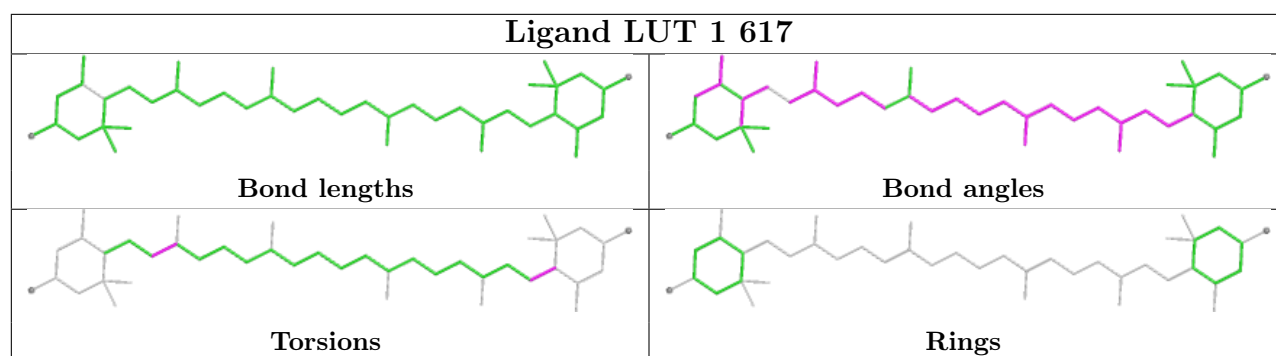
Ligand LHG 1 620



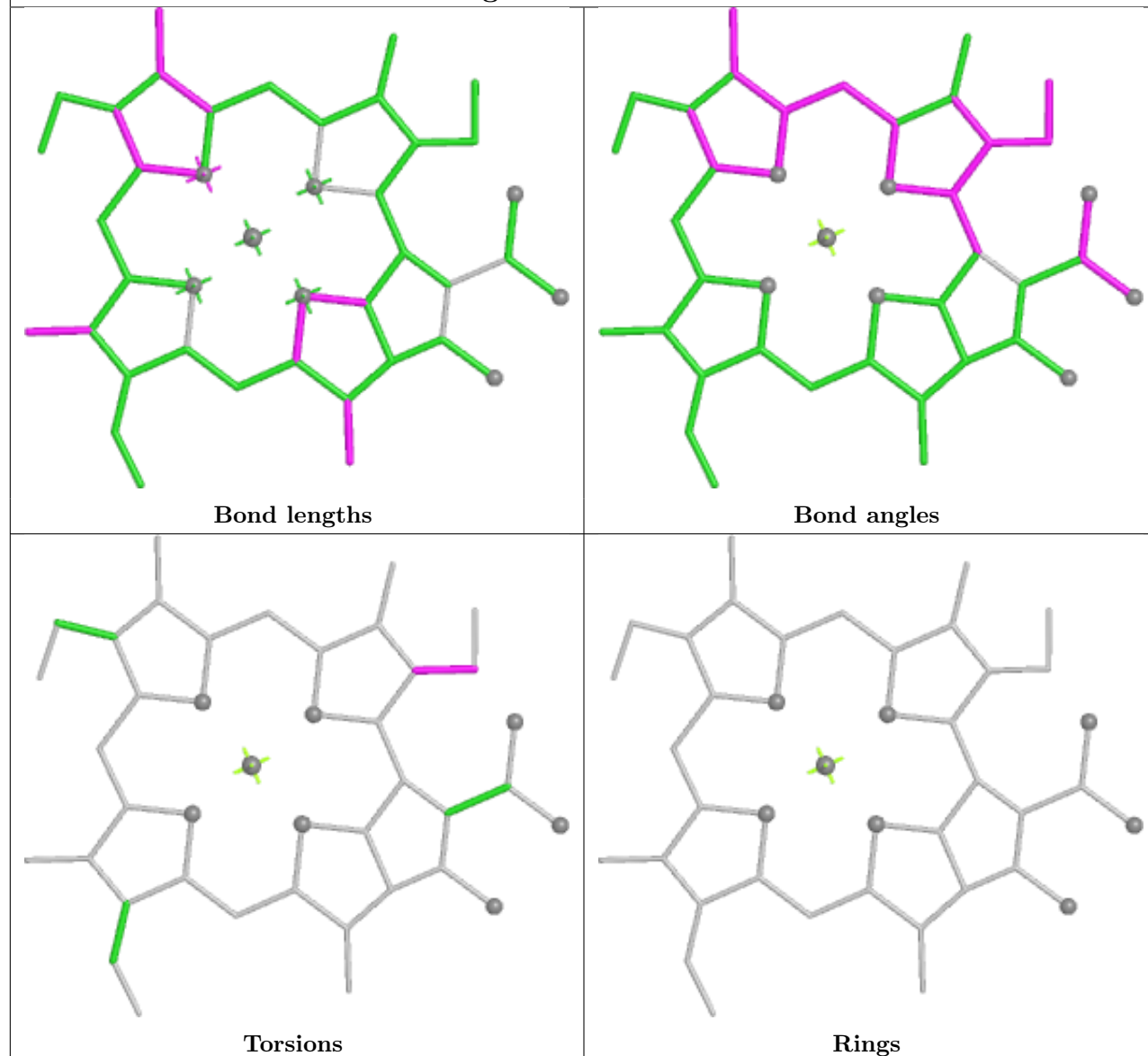
Ligand LUT 4 619



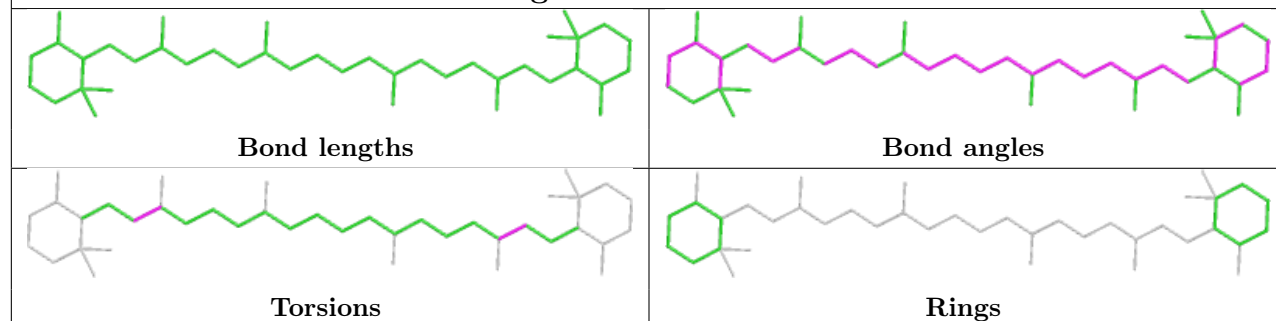


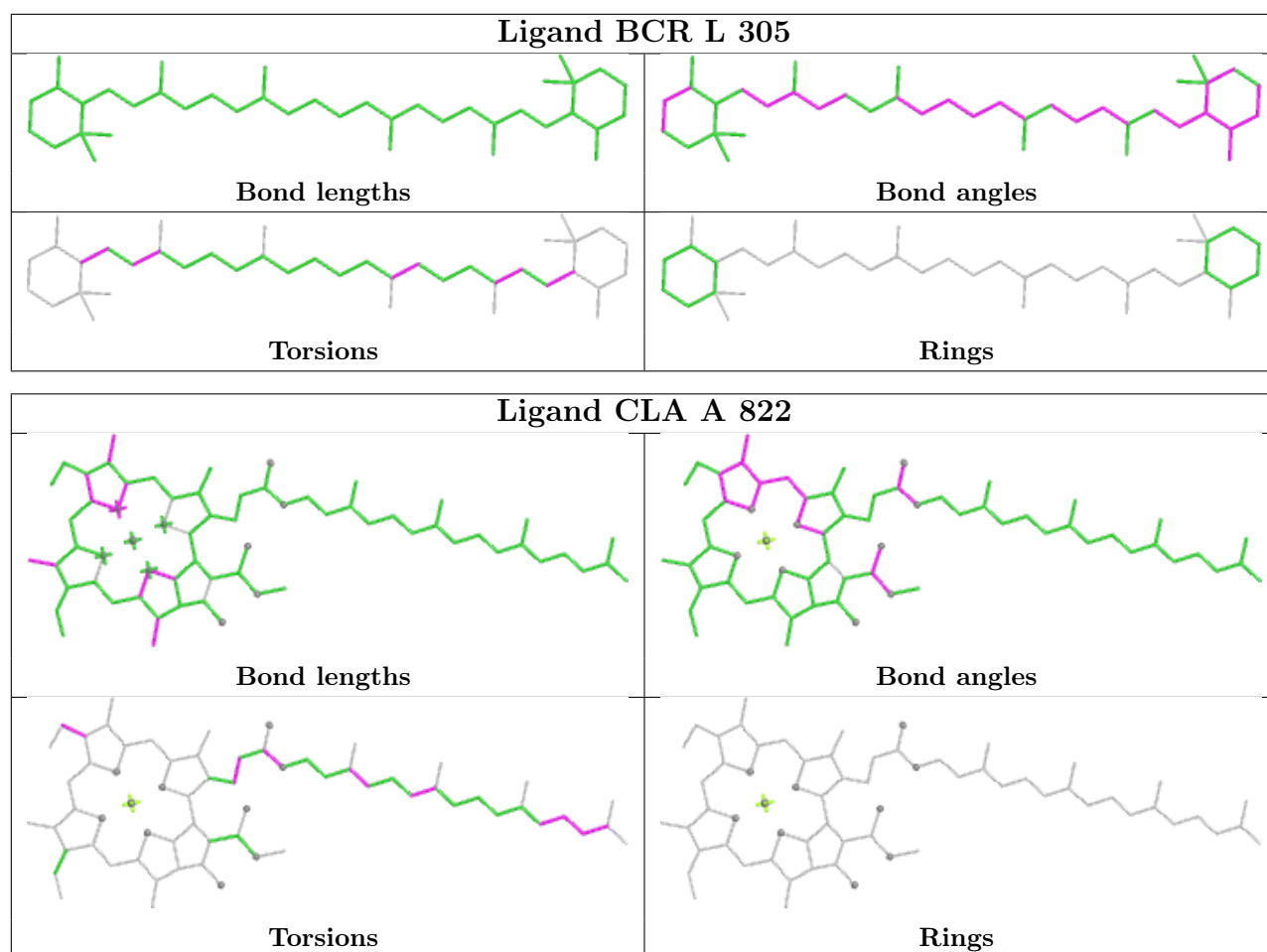


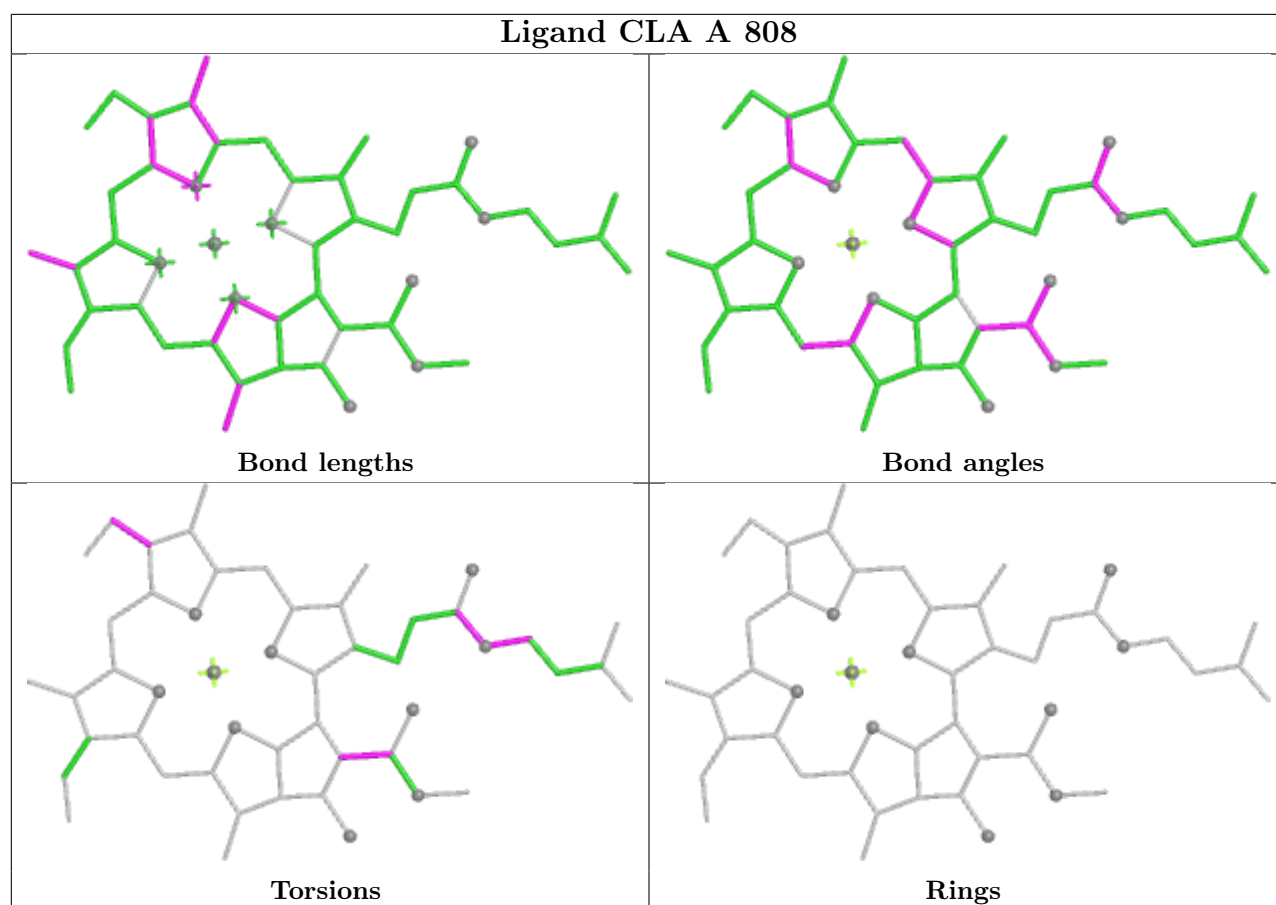
Ligand CLA 8 612



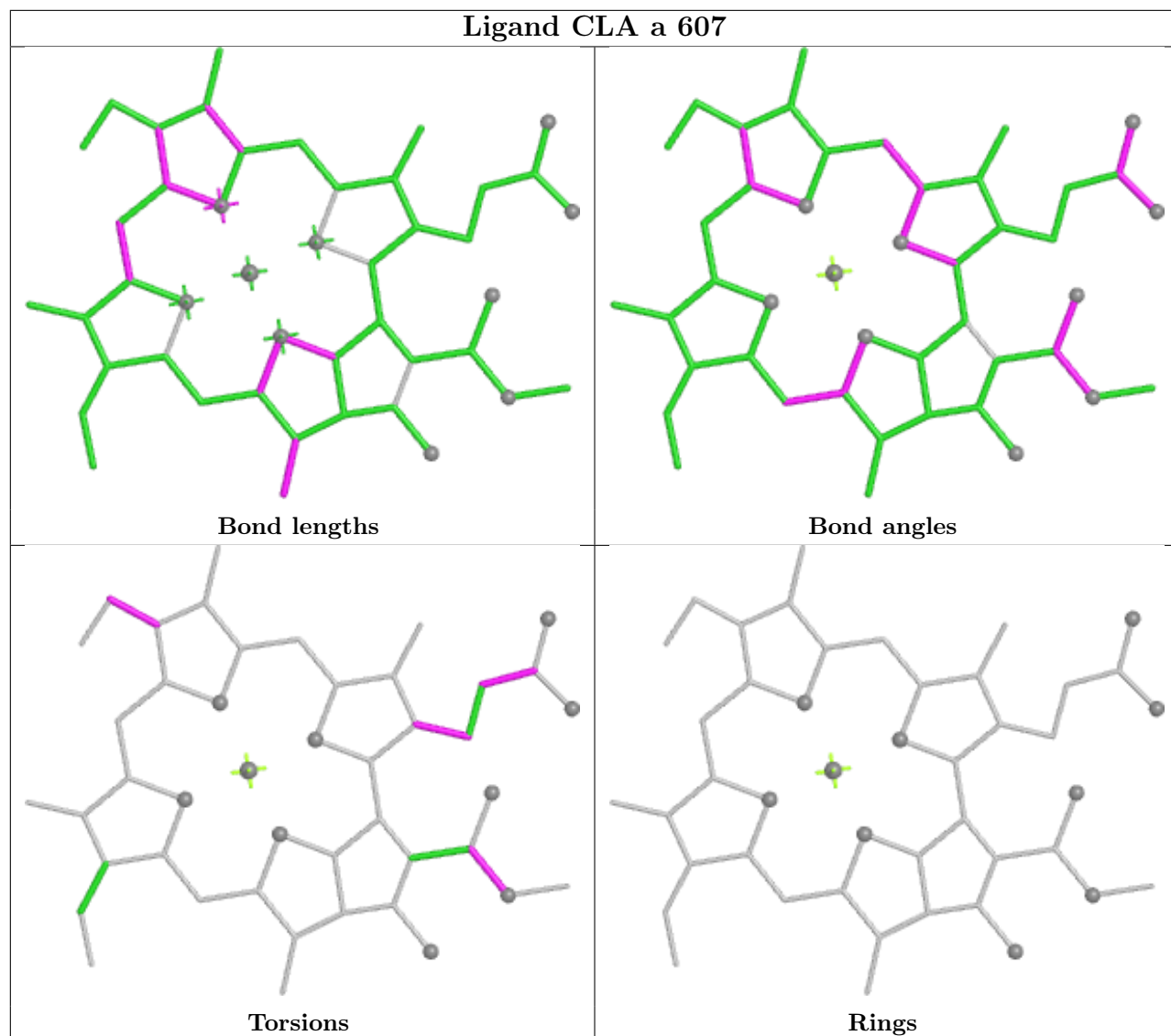
Ligand BCR B 801

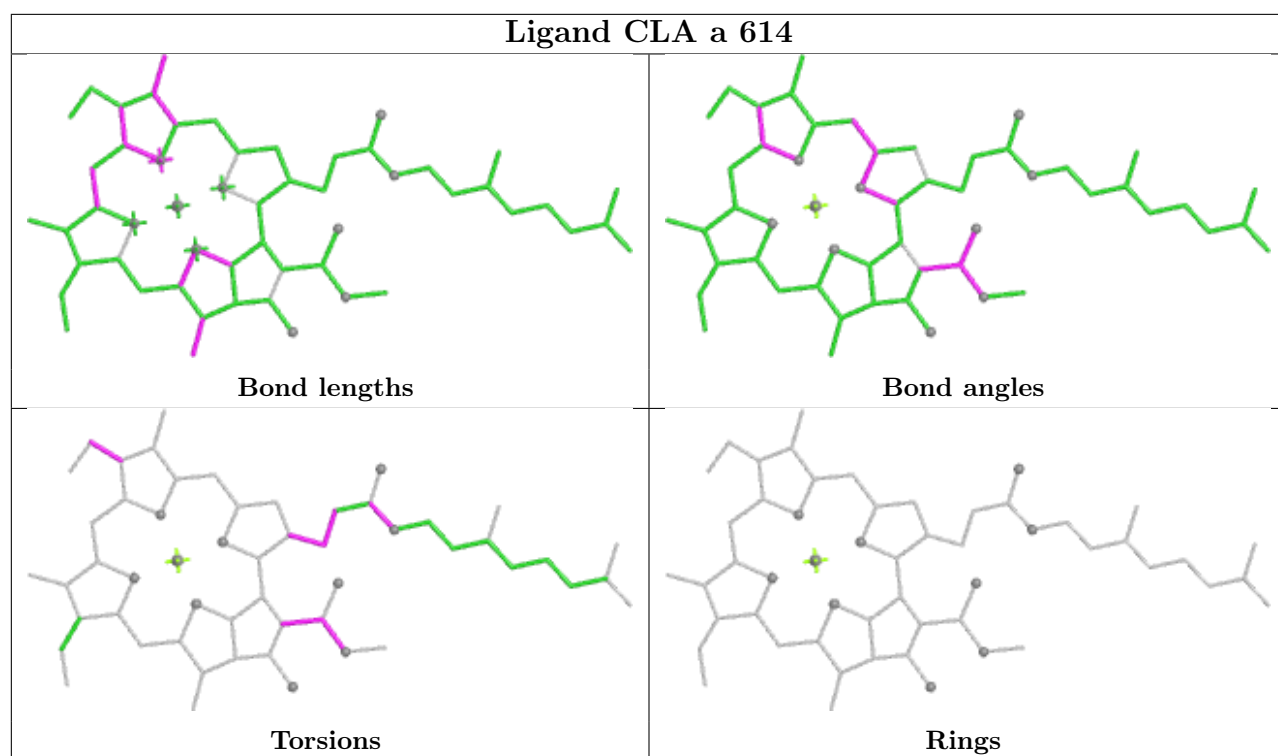




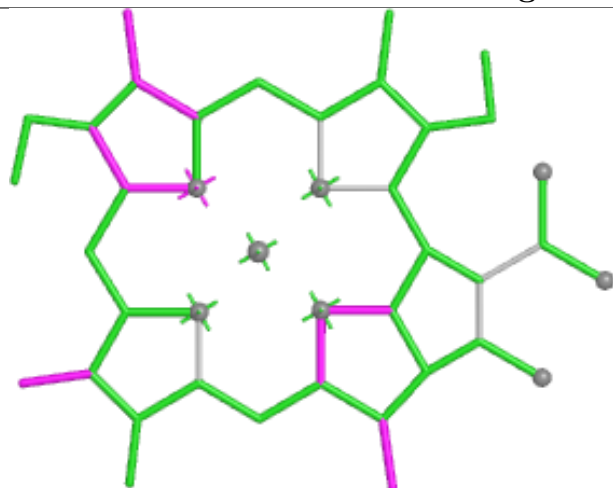


Ligand CLA a 607

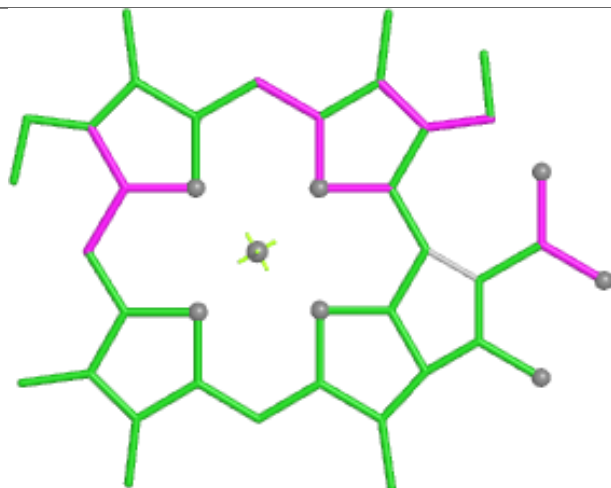




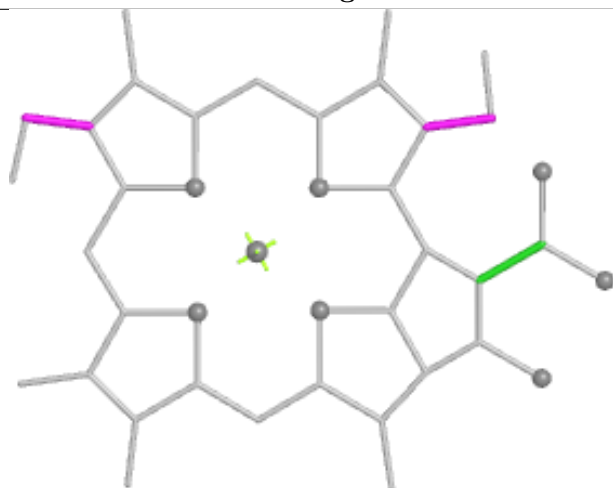
Ligand CLA 4 606



Bond lengths



Bond angles

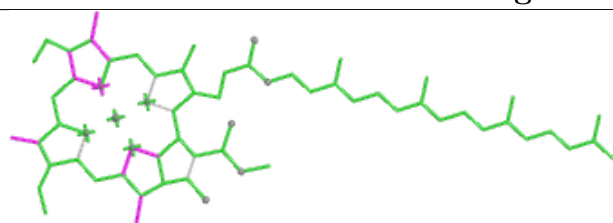


Torsions

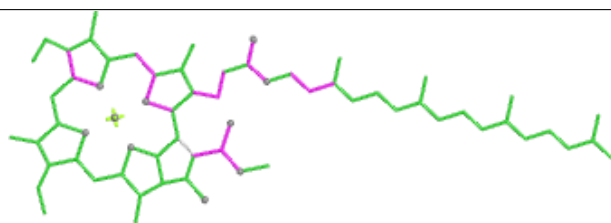


Rings

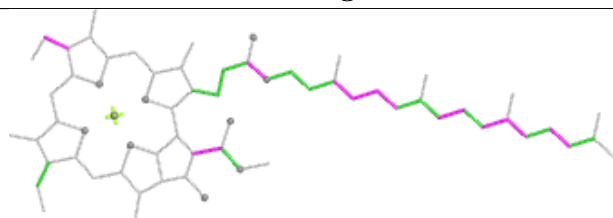
Ligand CLA B 808



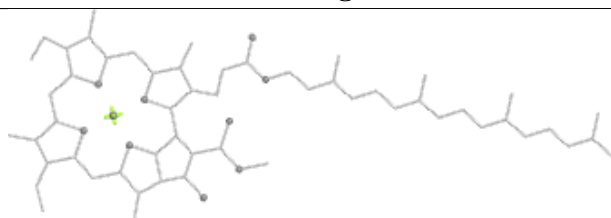
Bond lengths



Bond angles

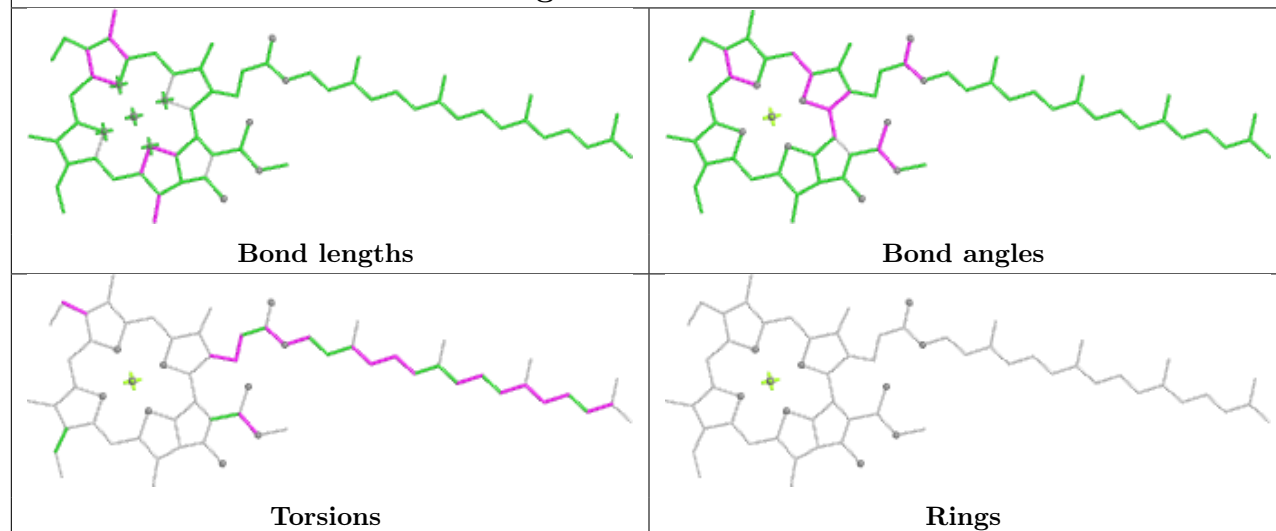


Torsions

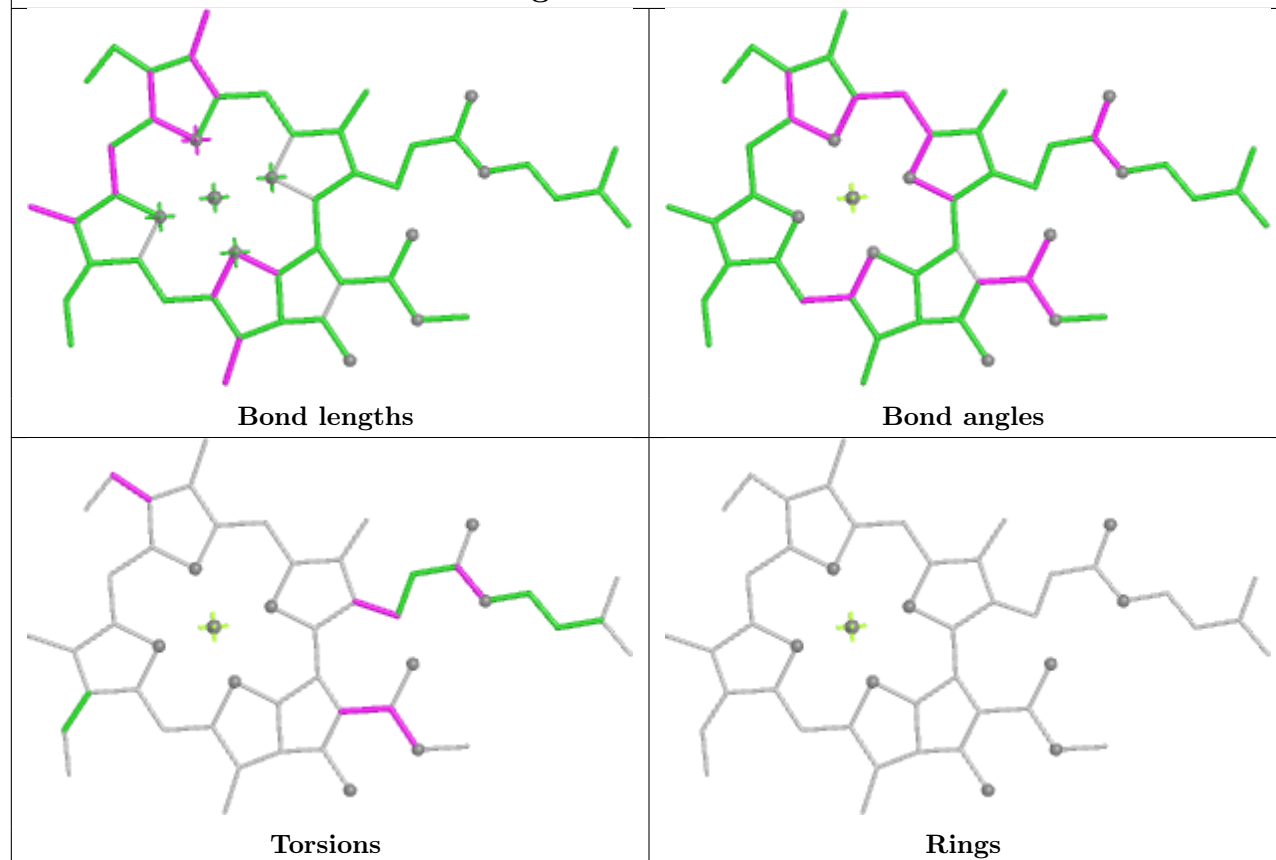


Rings

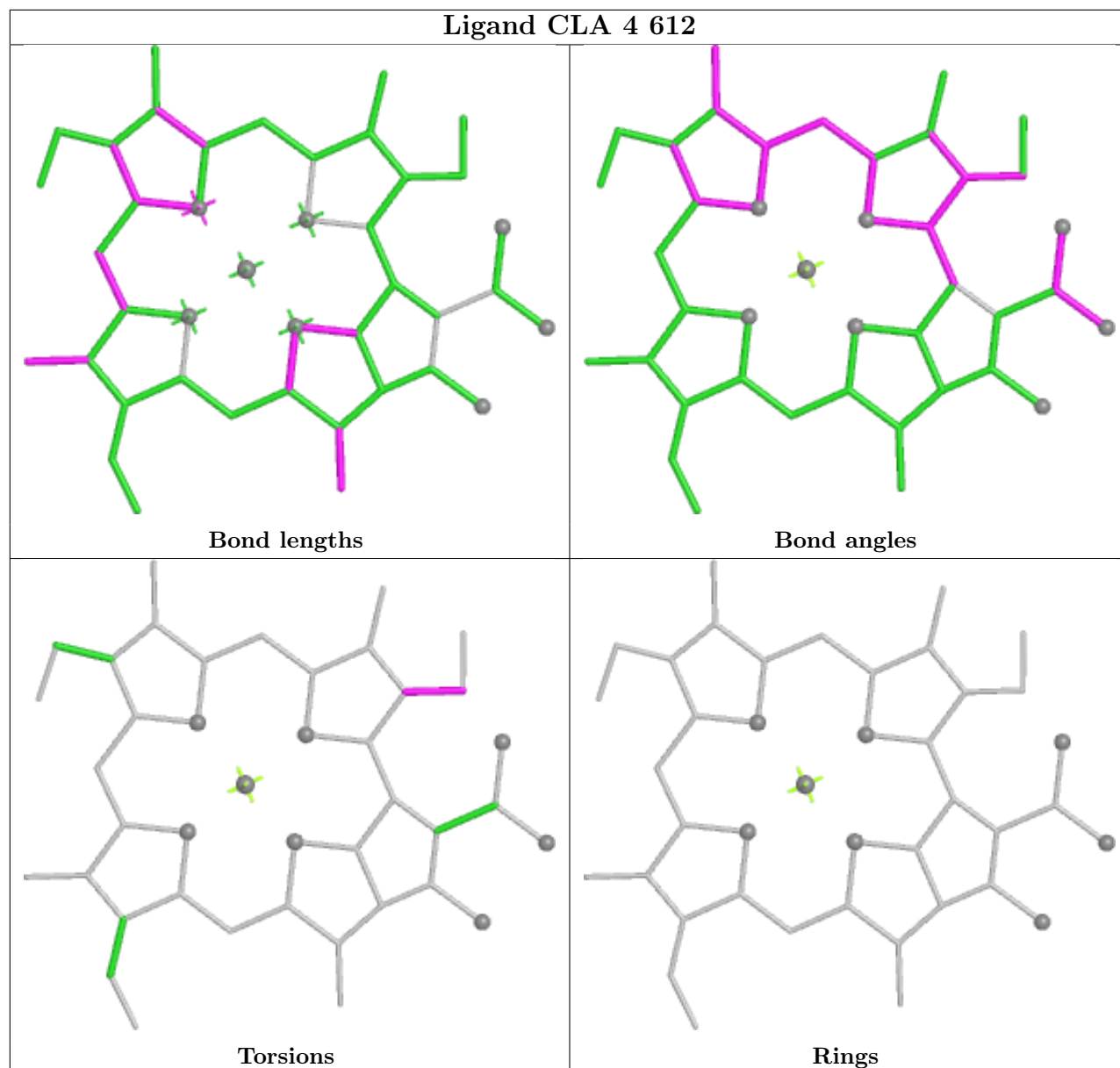
Ligand CLA a 609

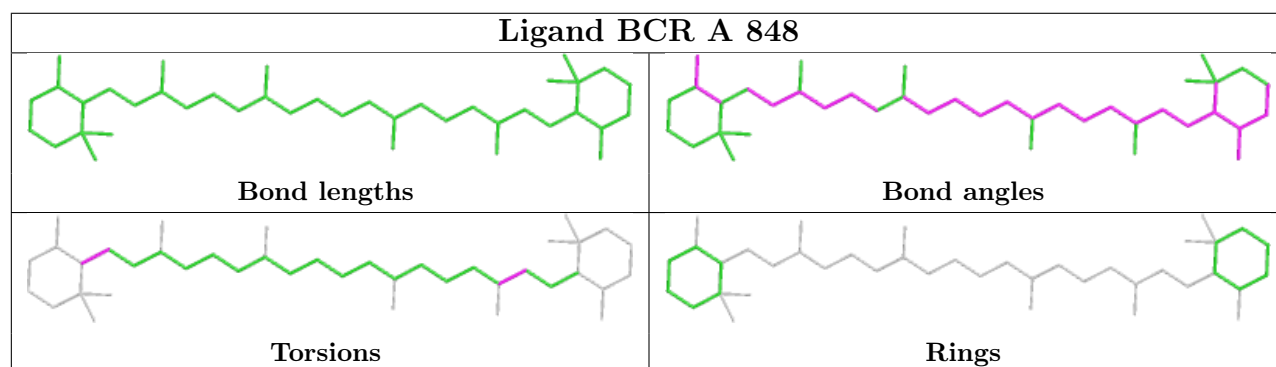
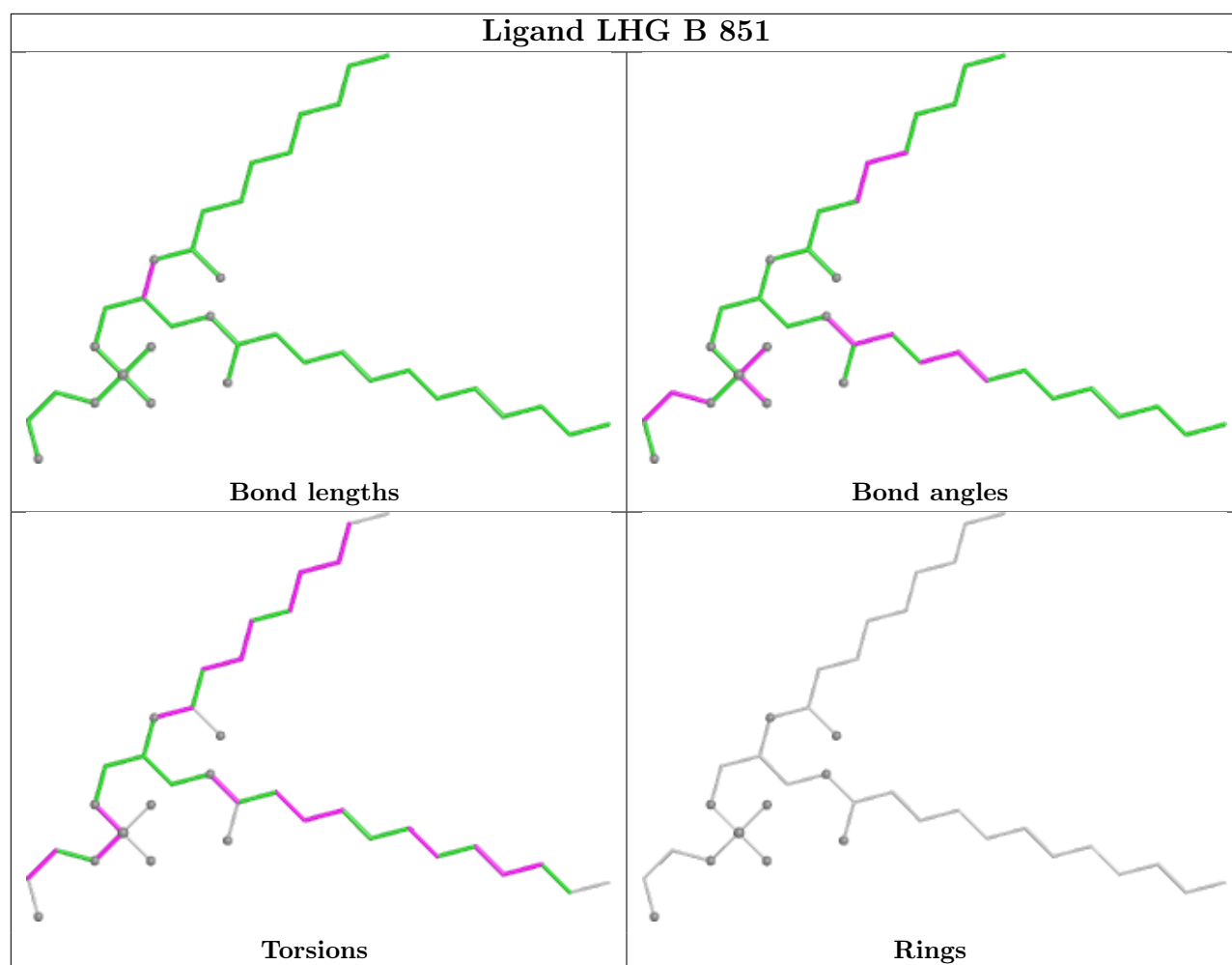


Ligand CLA A 815

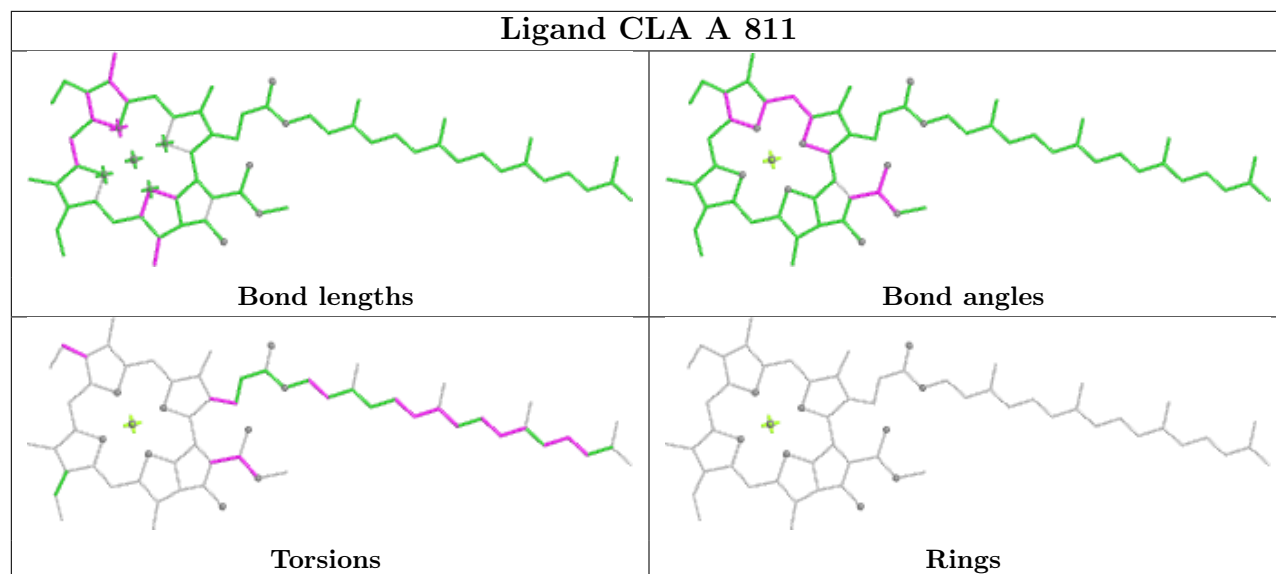


Ligand CLA 4 612

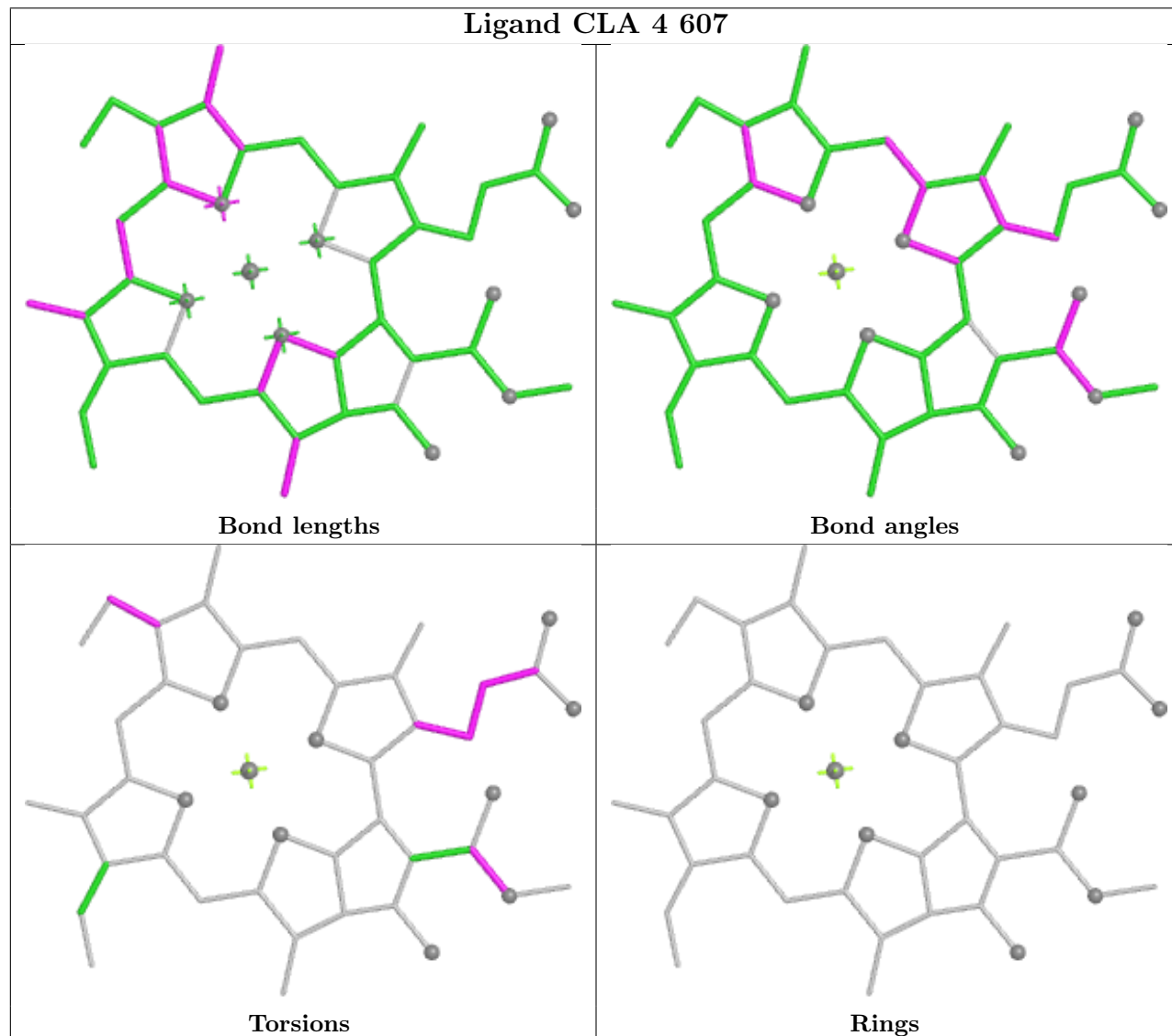


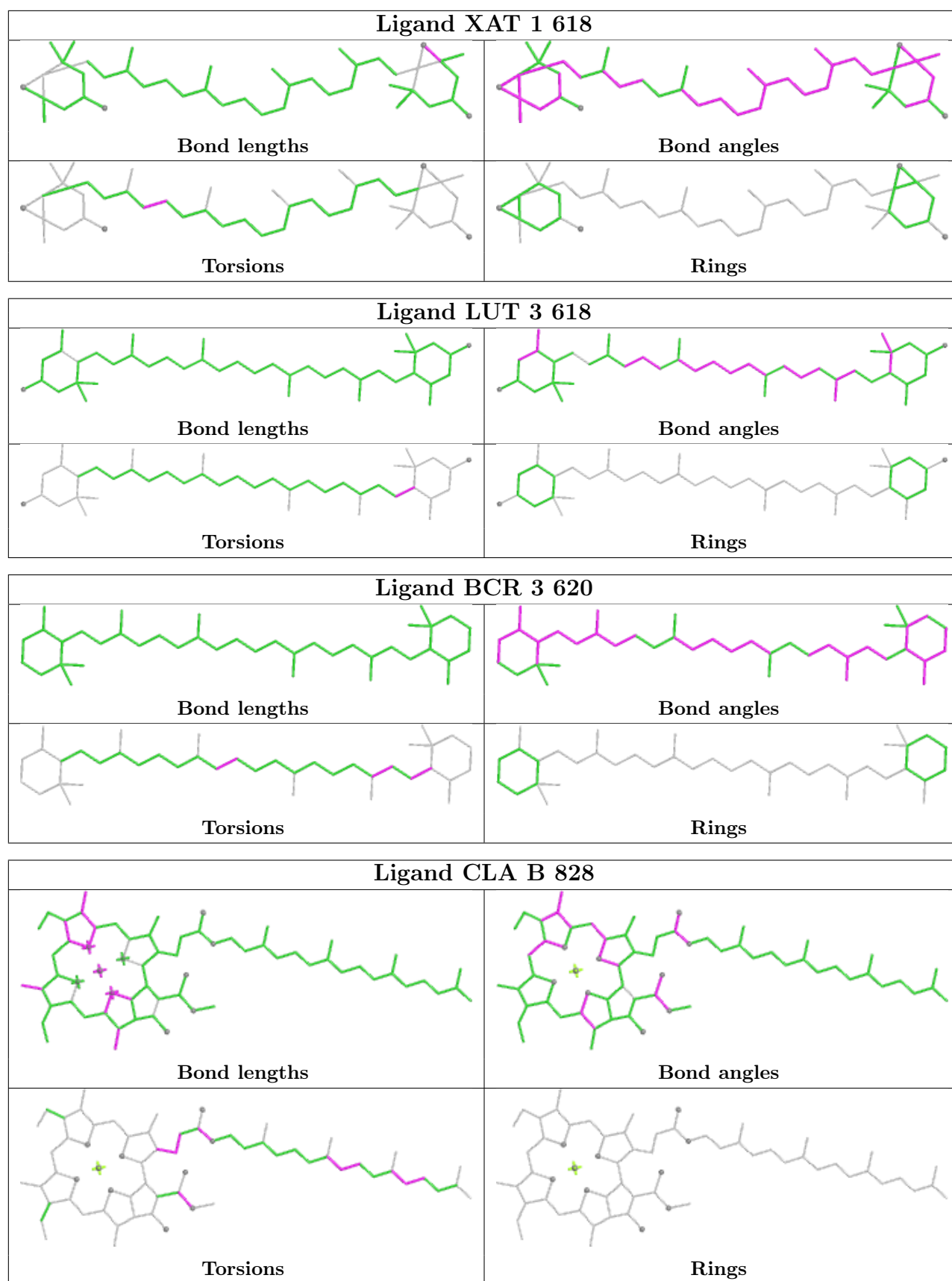


Ligand CLA A 811

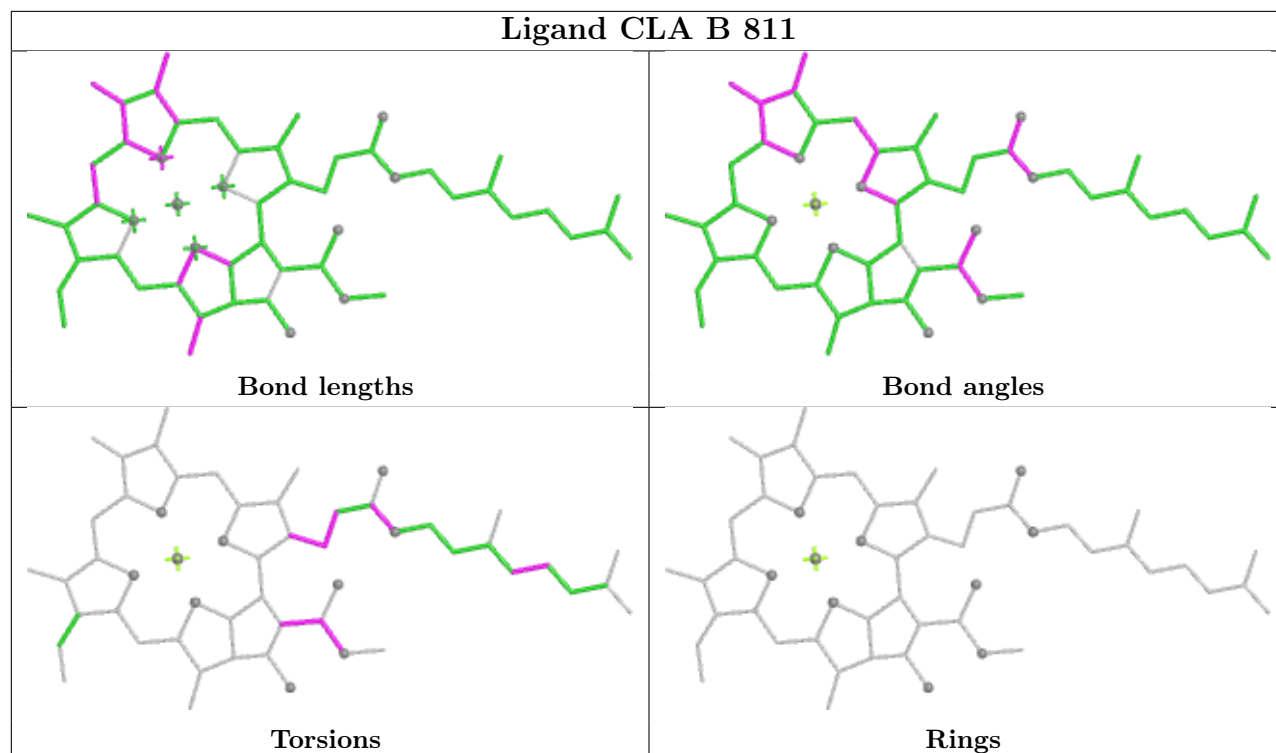


Ligand CLA 4 607

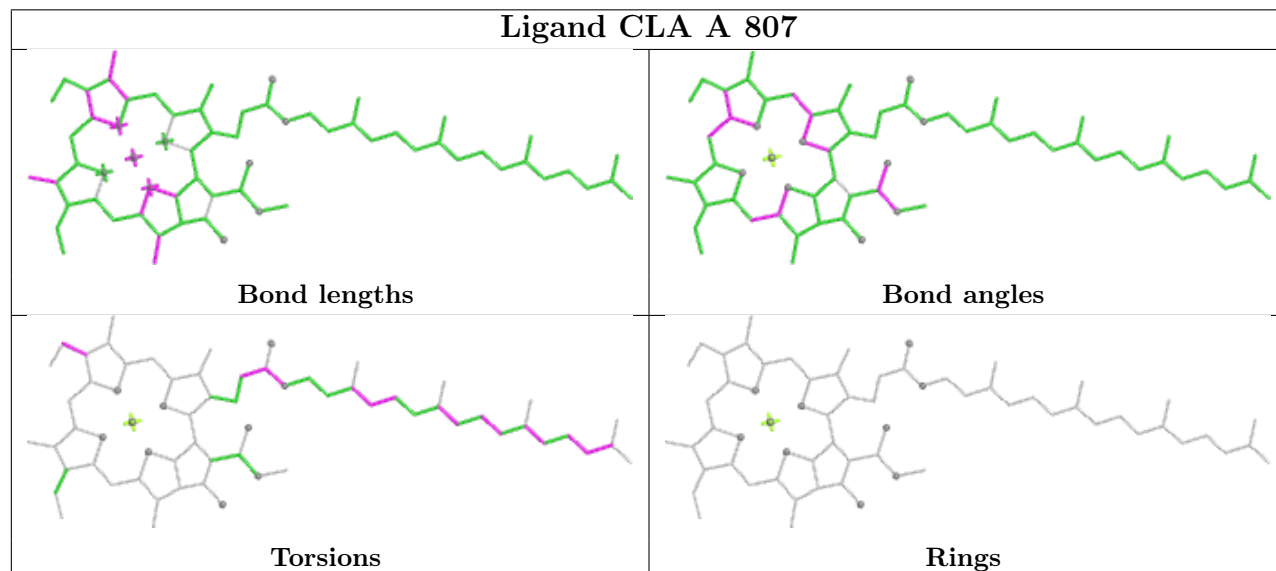




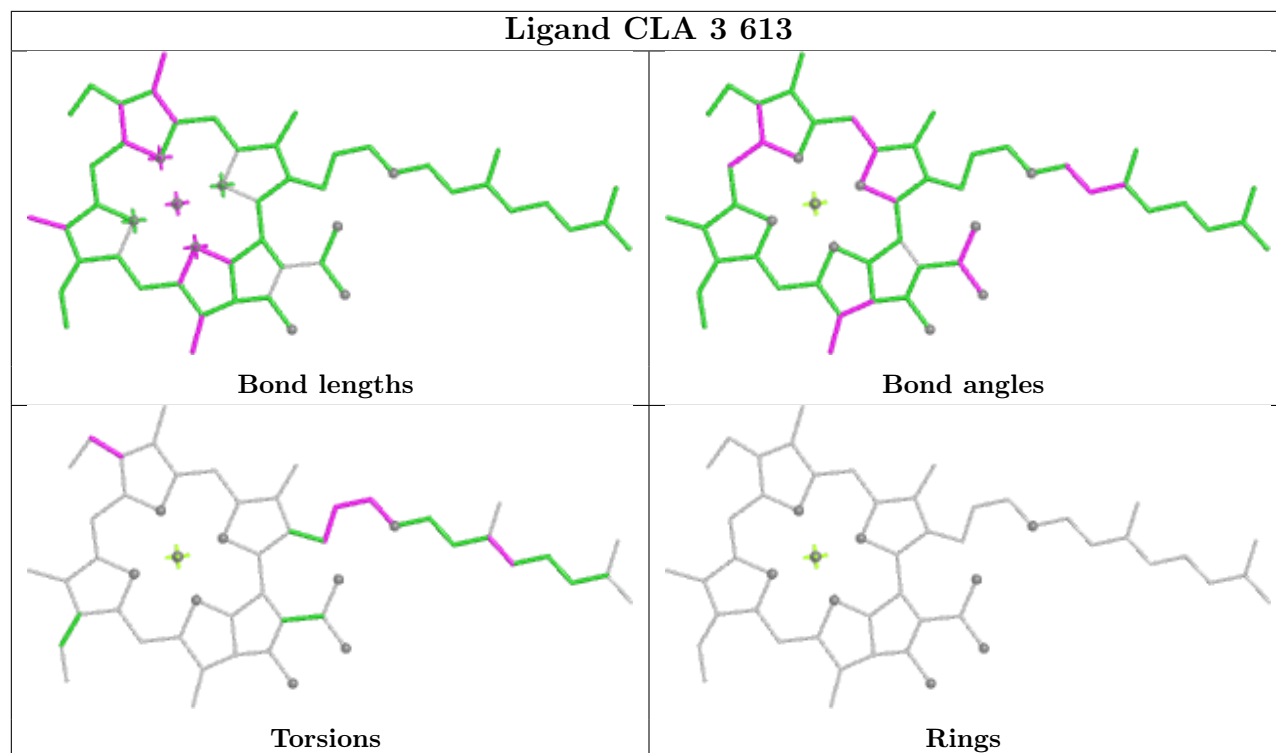
Ligand CLA B 811



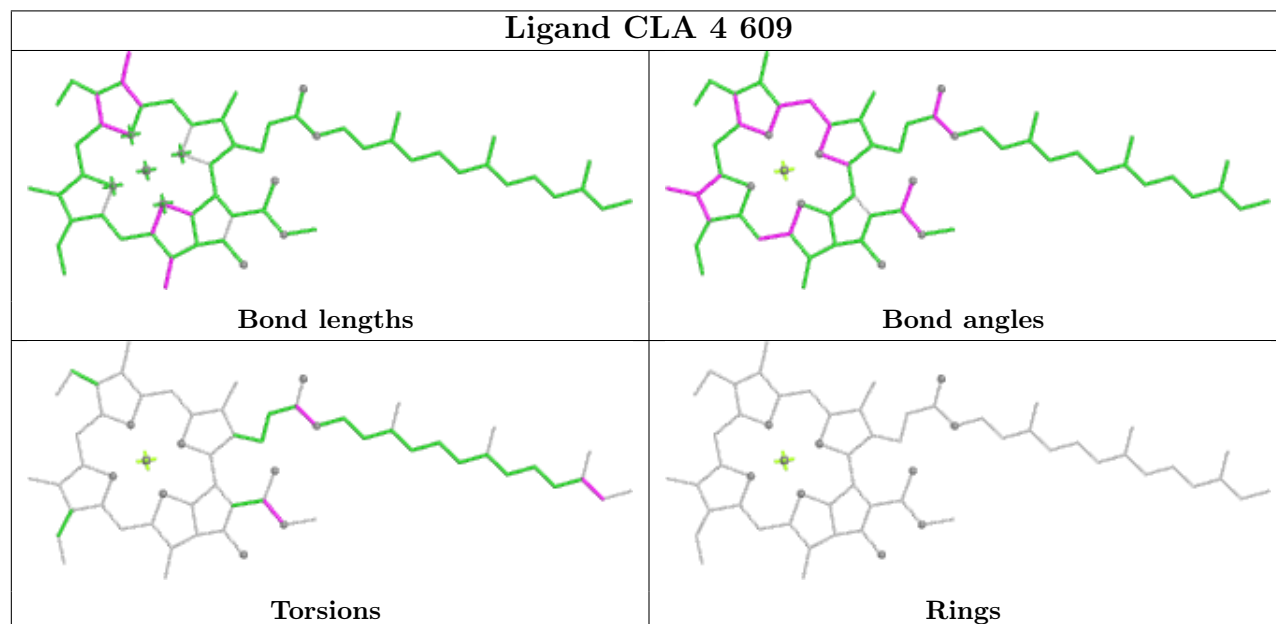
Ligand CLA A 807

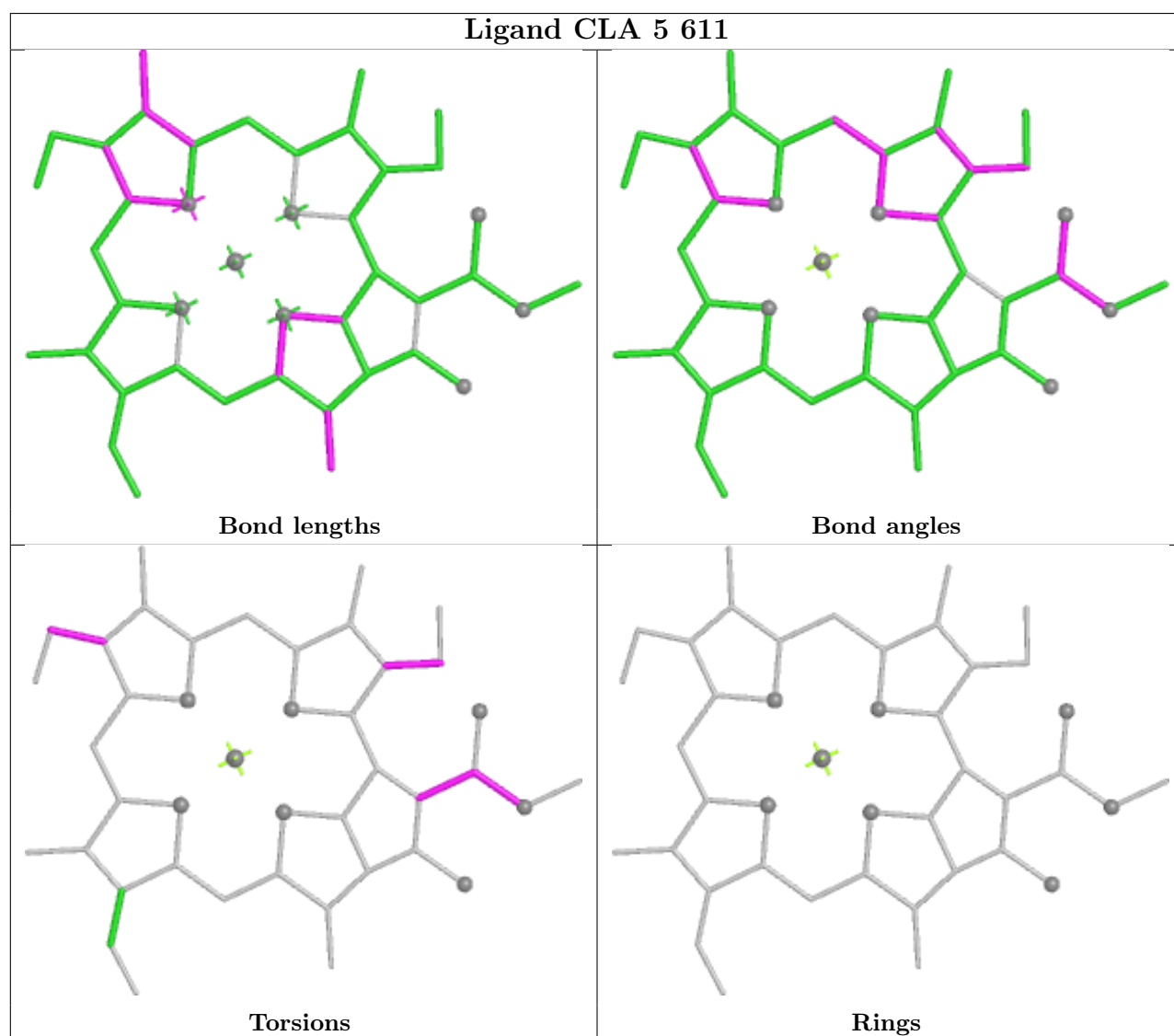
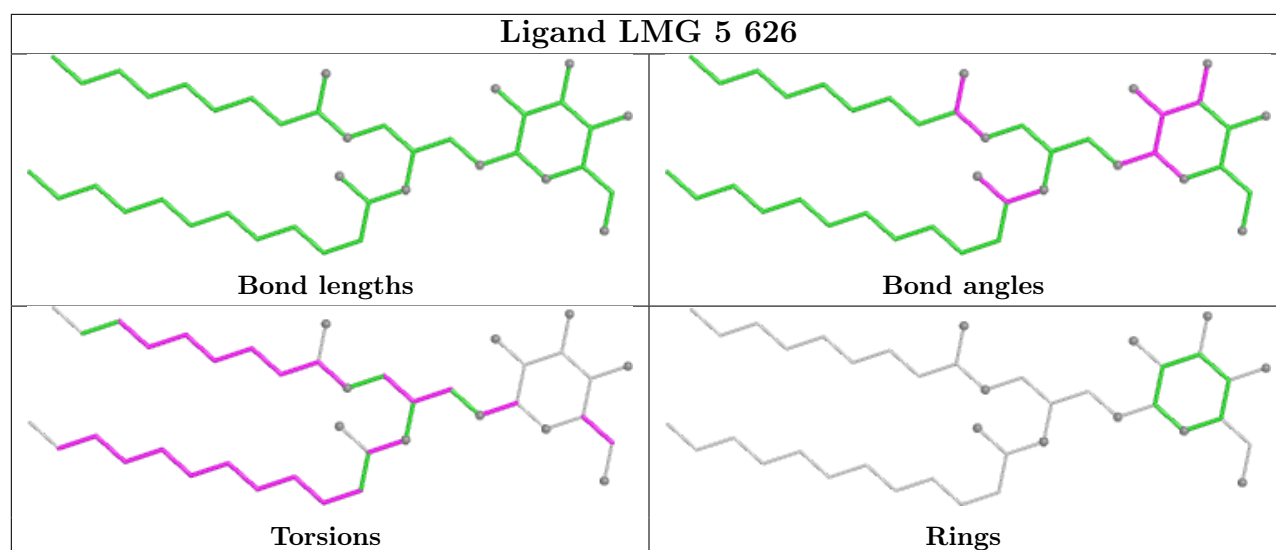


Ligand CLA 3 613

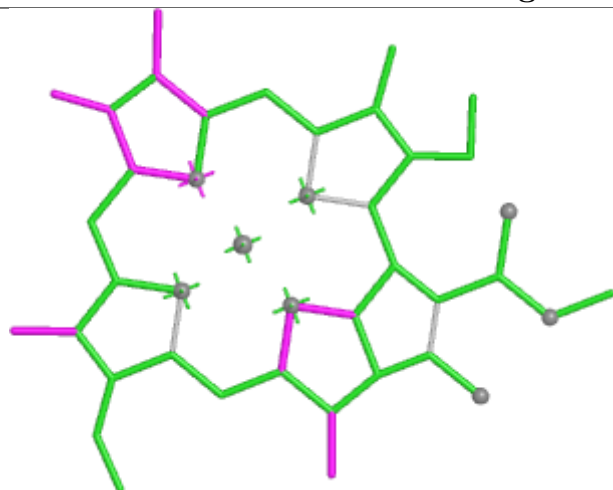


Ligand CLA 4 609

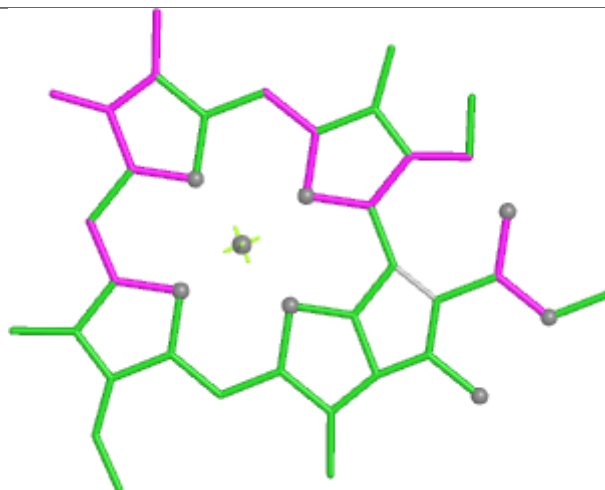




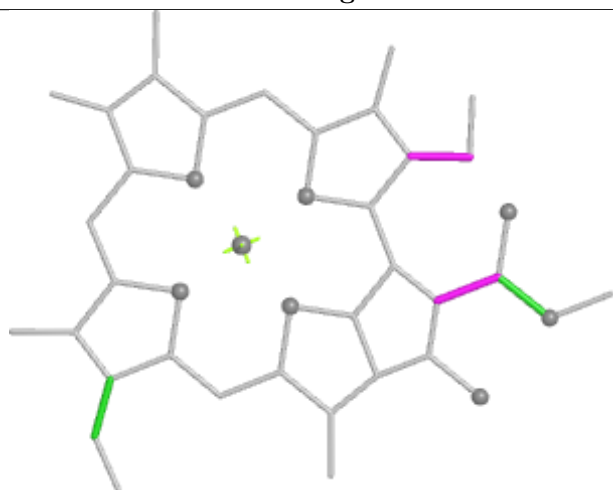
Ligand CLA 6 607



Bond lengths



Bond angles

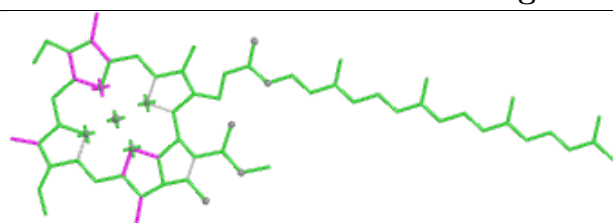


Torsions



Rings

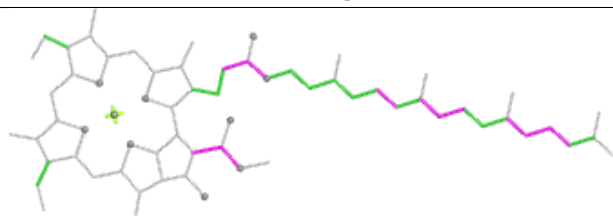
Ligand CLA 6 601



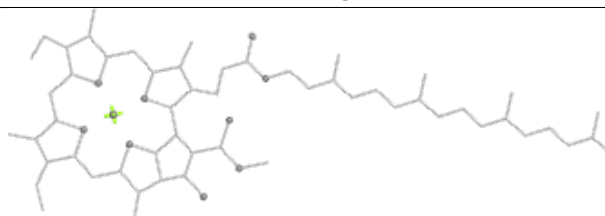
Bond lengths



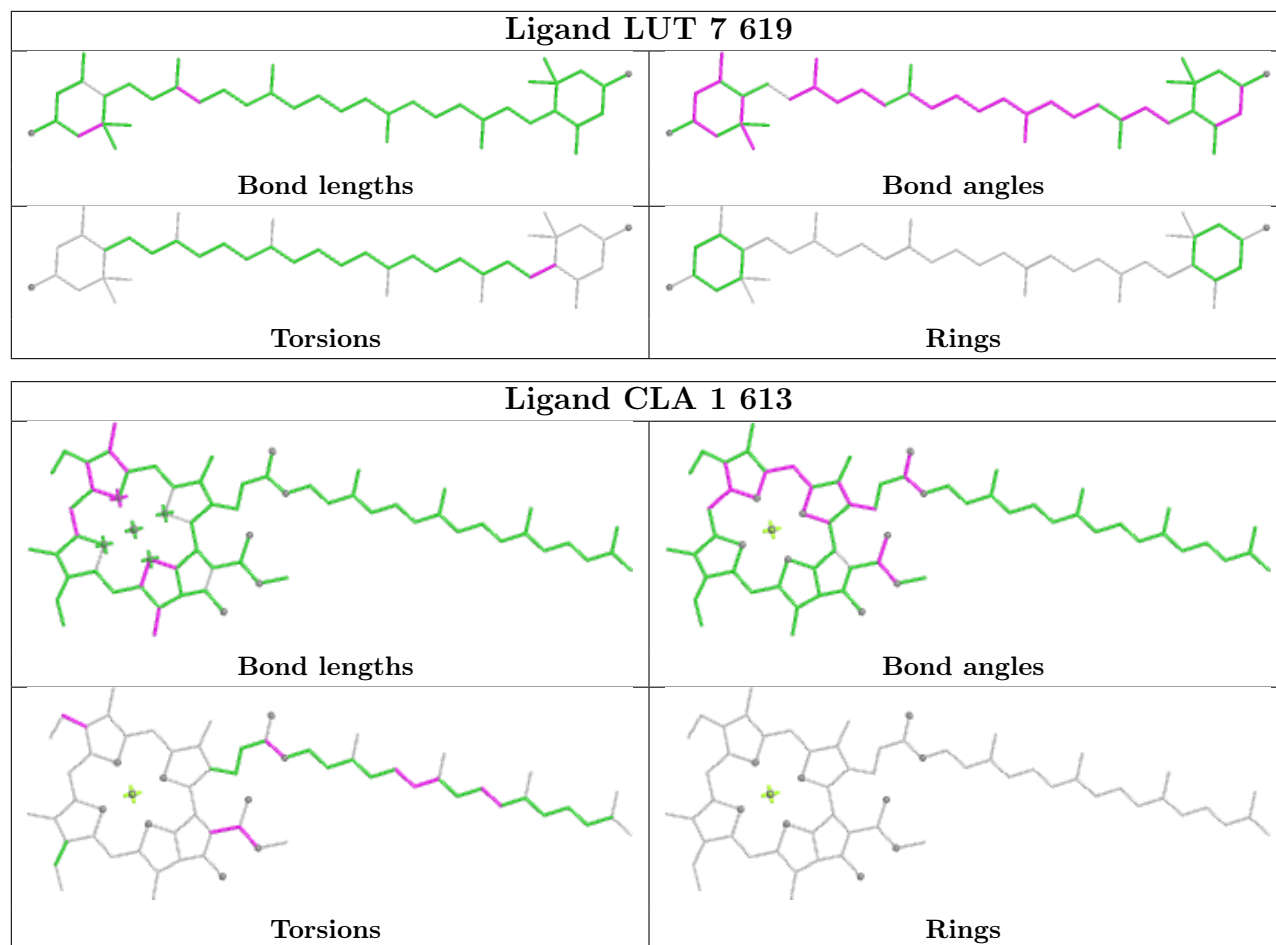
Bond angles



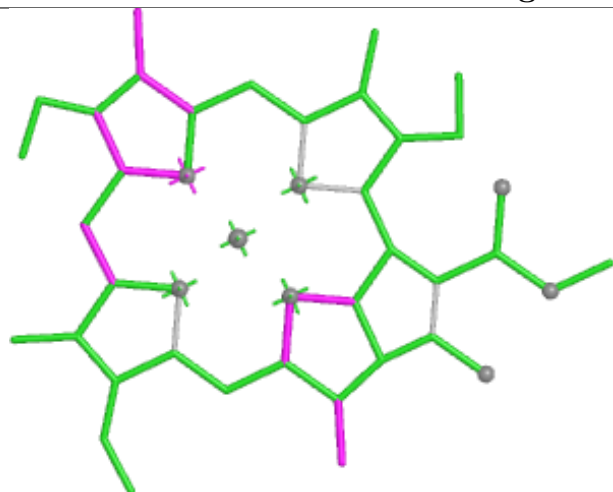
Torsions



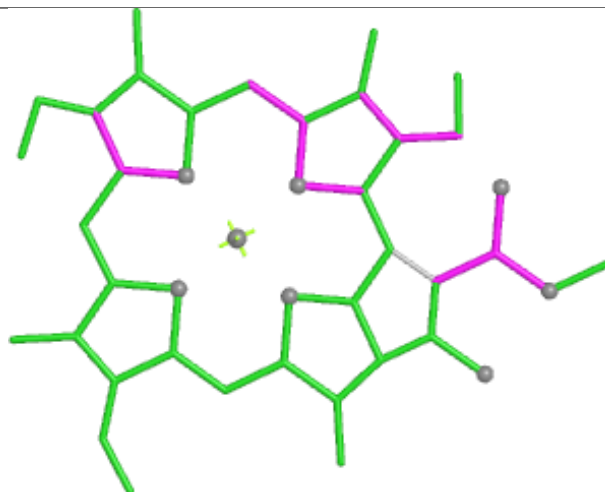
Rings



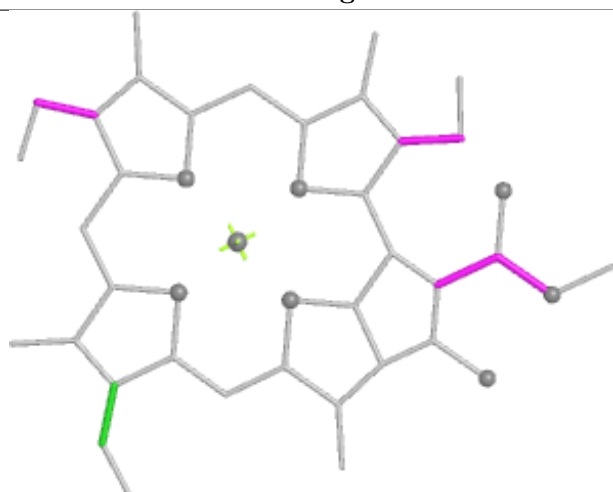
Ligand CLA 7 614



Bond lengths



Bond angles

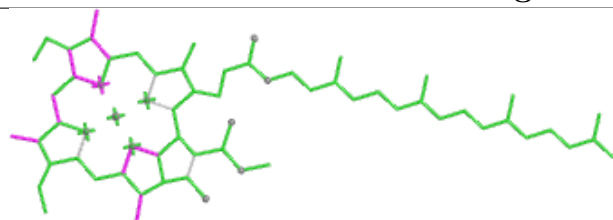


Torsions

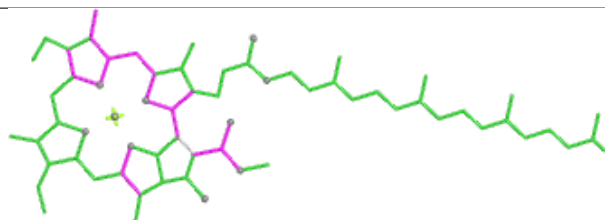


Rings

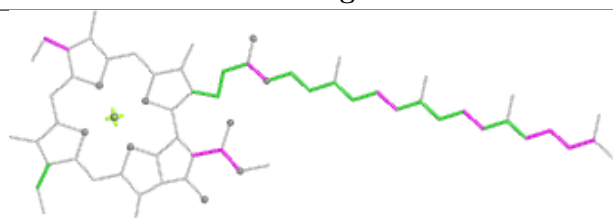
Ligand CLA B 824



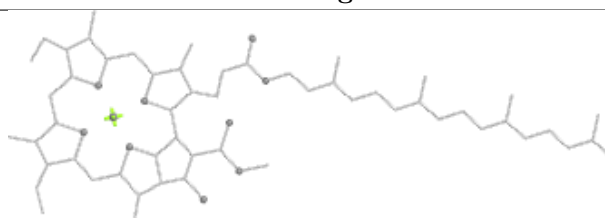
Bond lengths



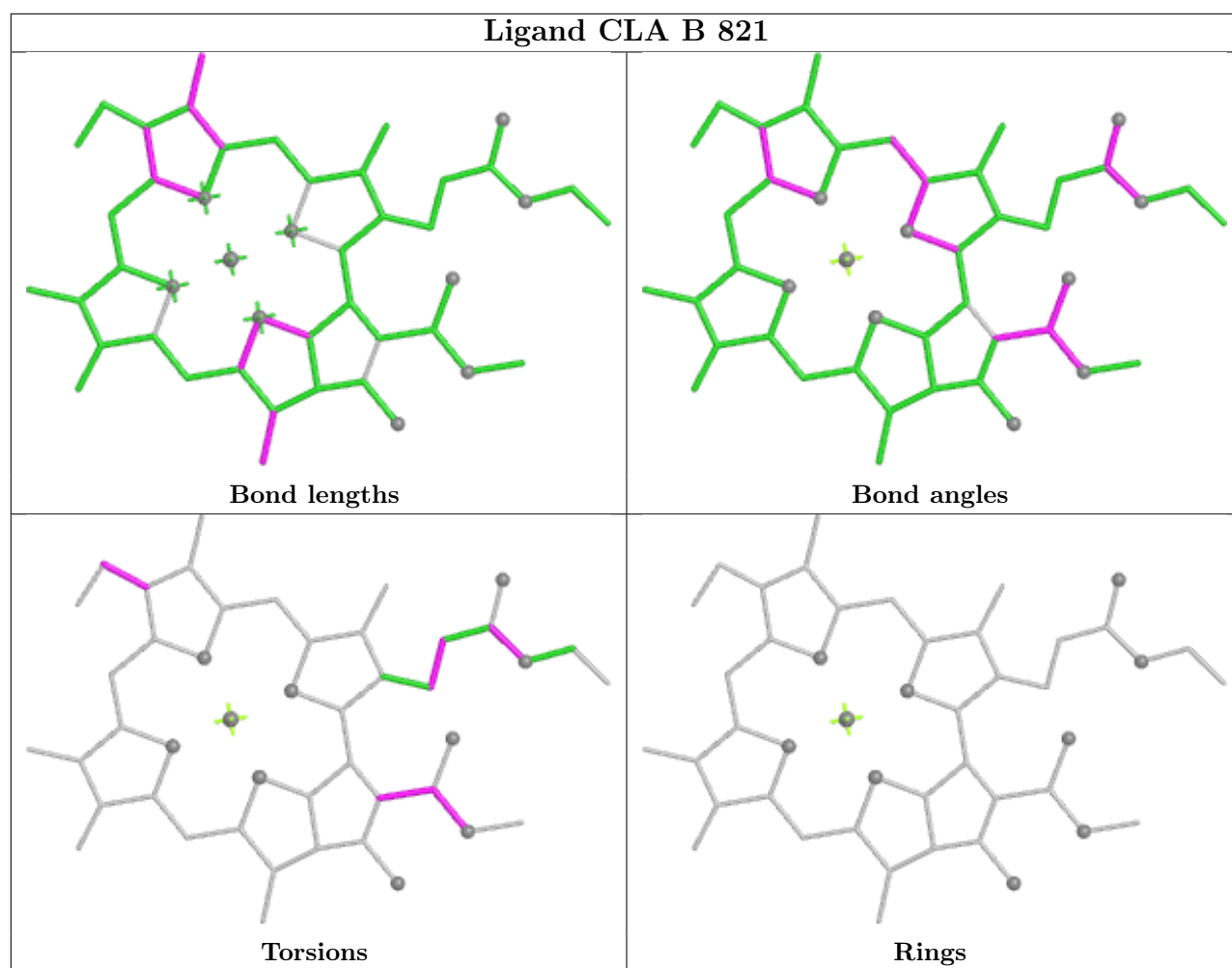
Bond angles

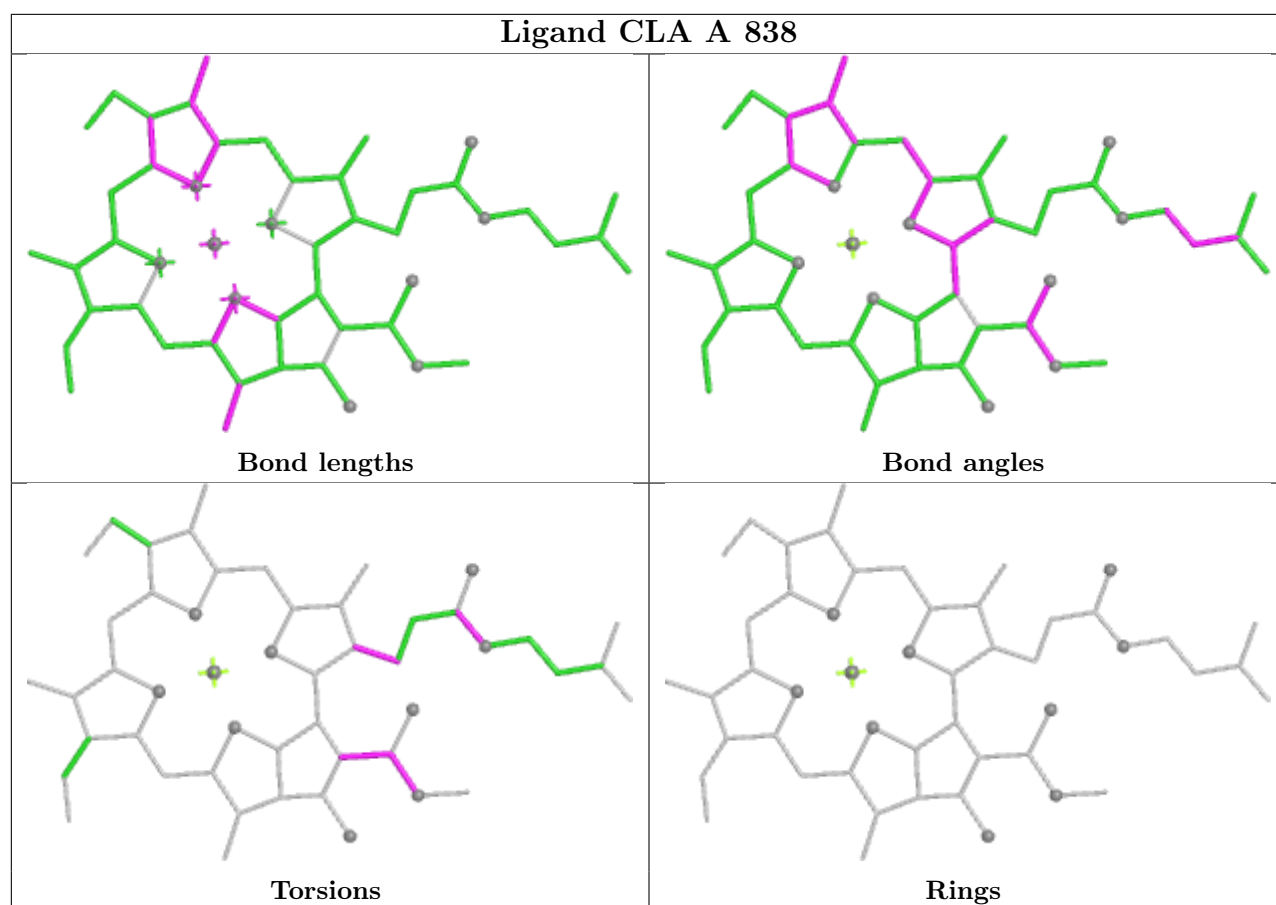


Torsions

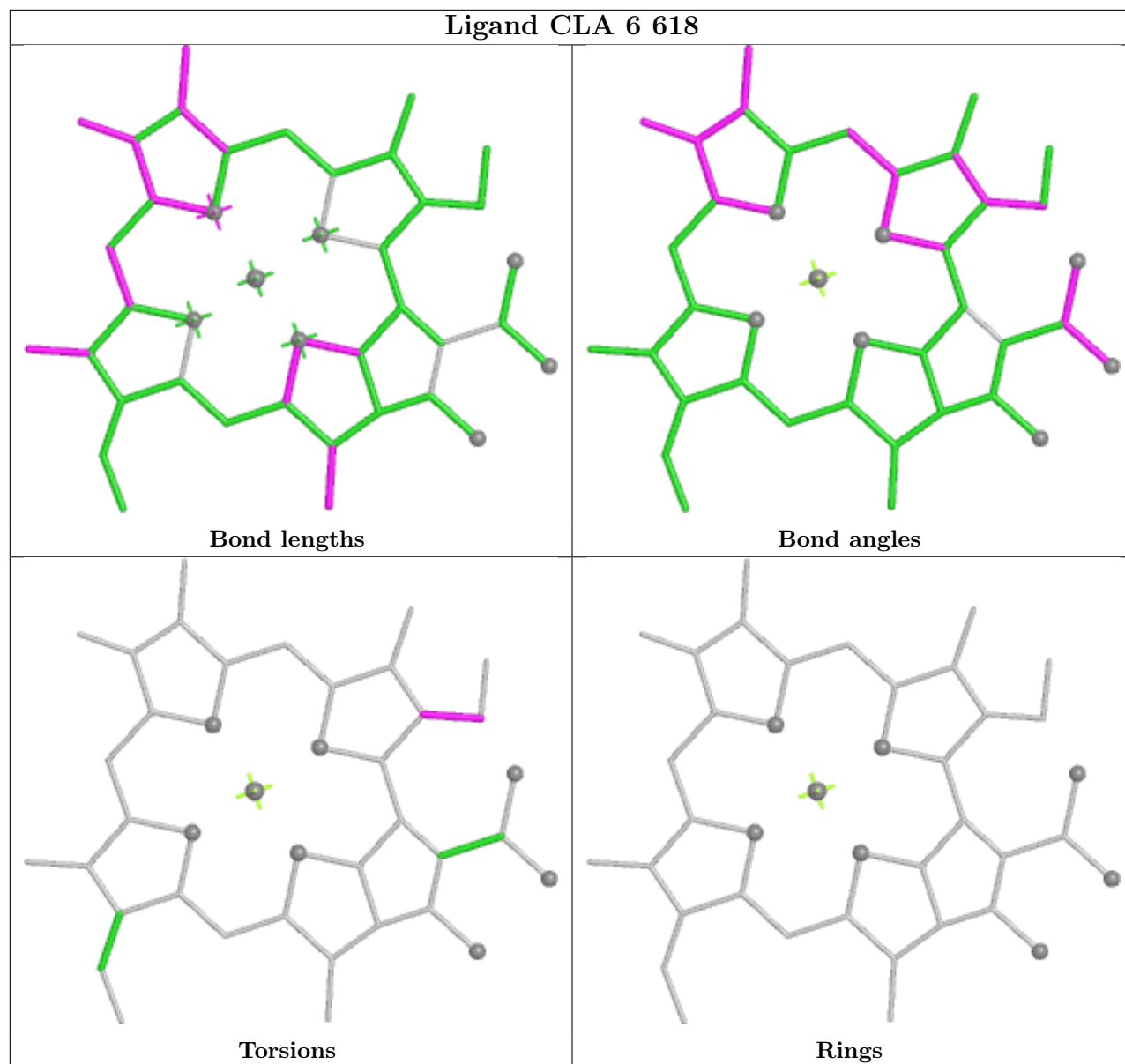


Rings

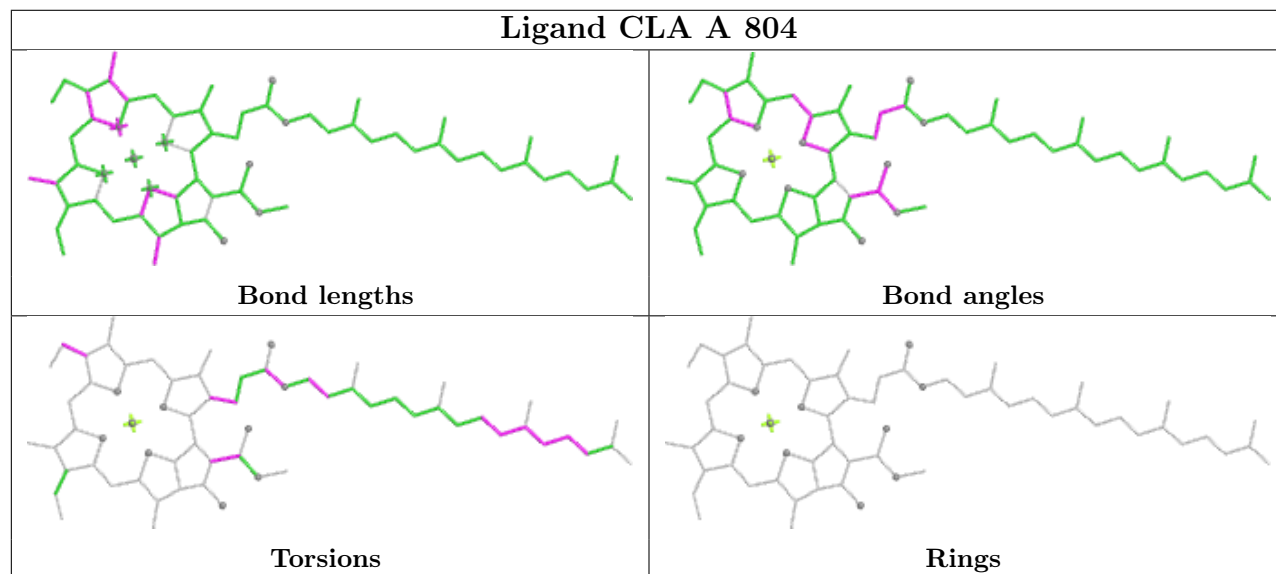




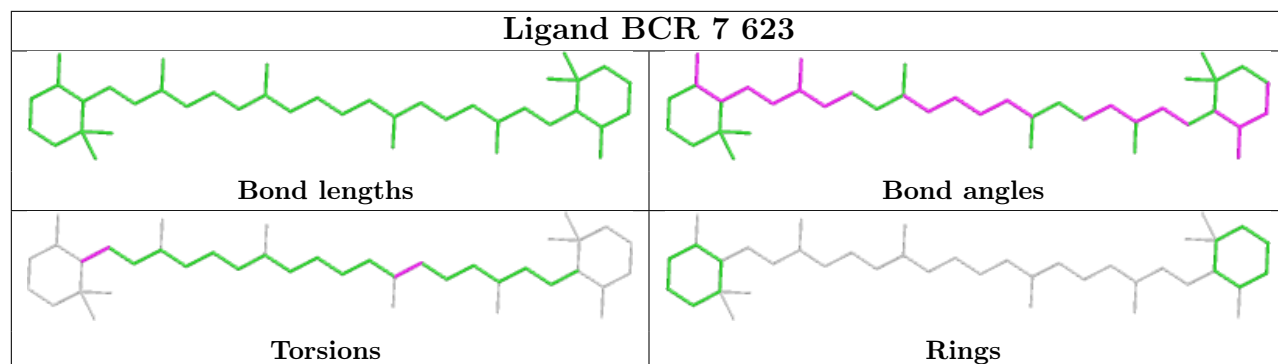
Ligand CLA 6 618



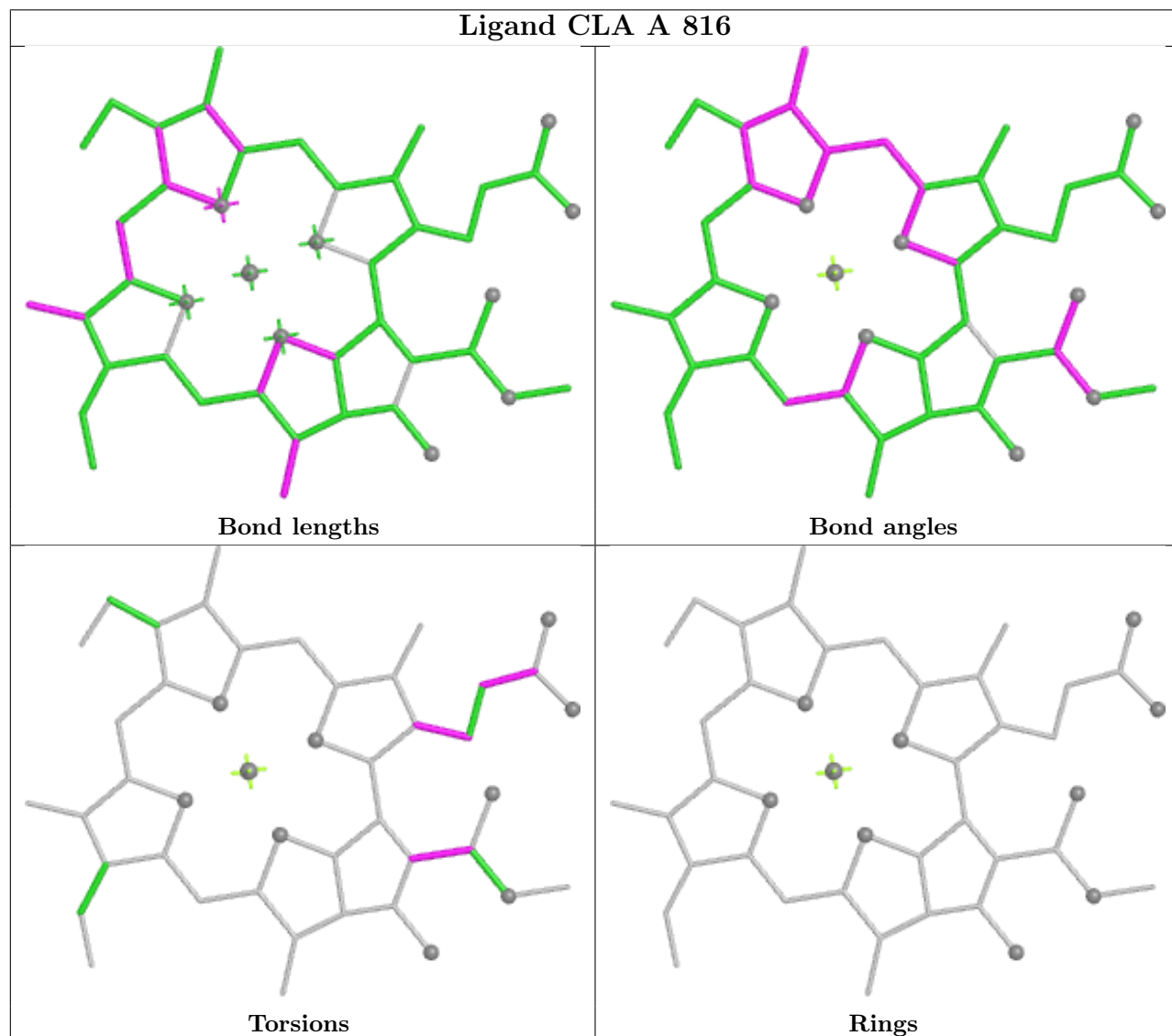
Ligand CLA A 804

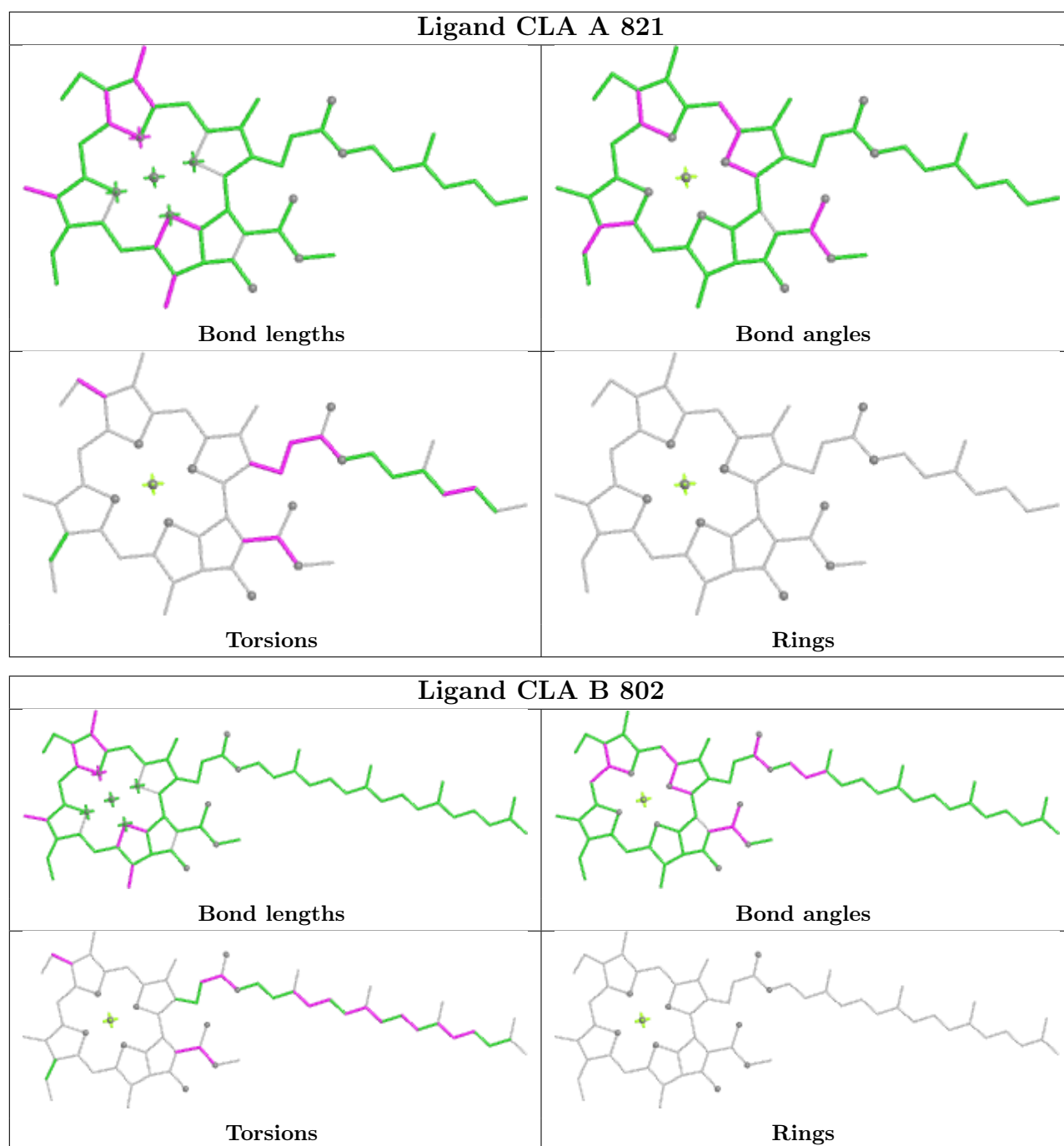


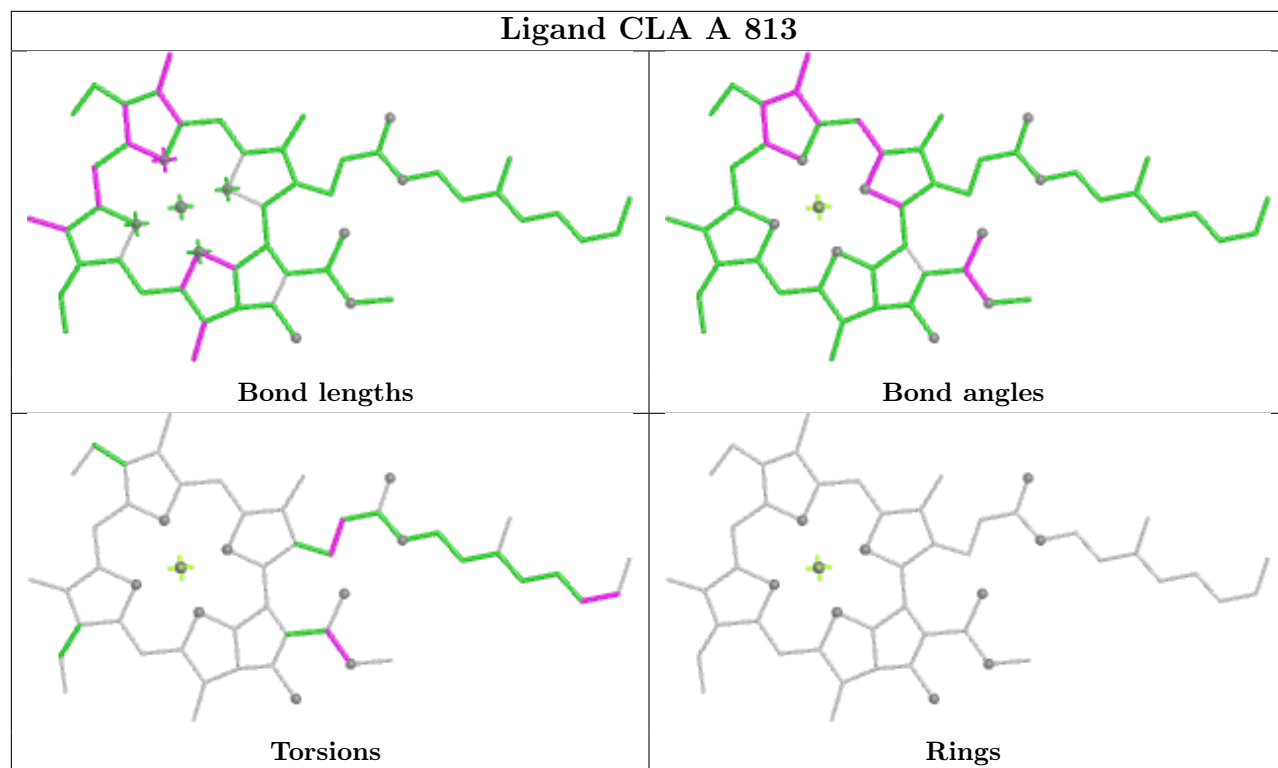
Ligand BCR 7 623

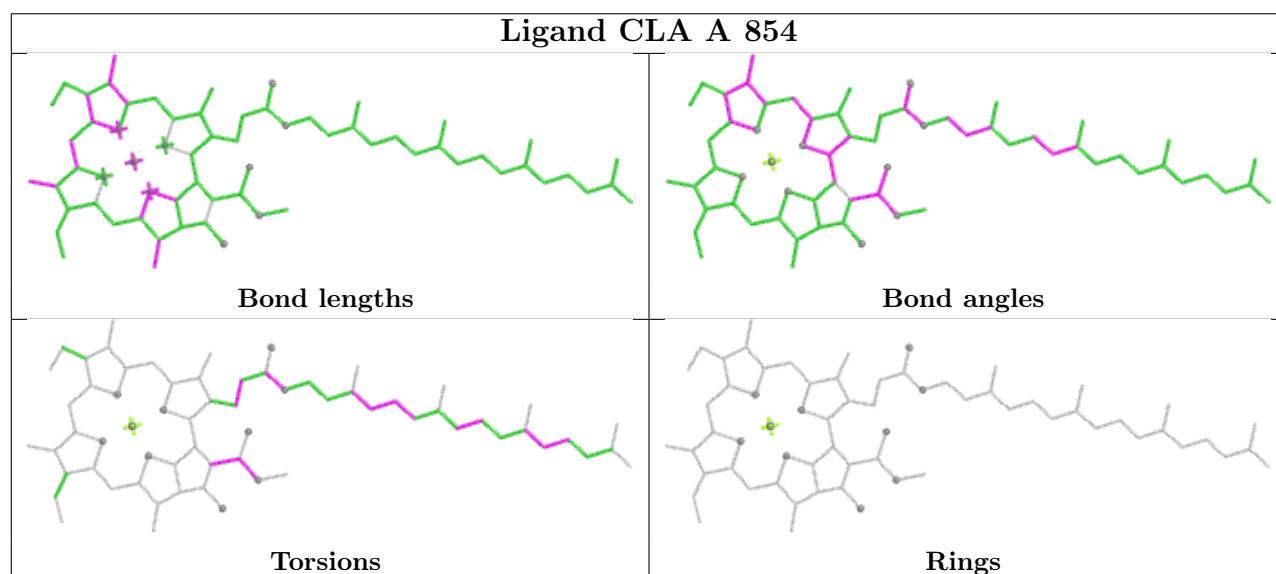
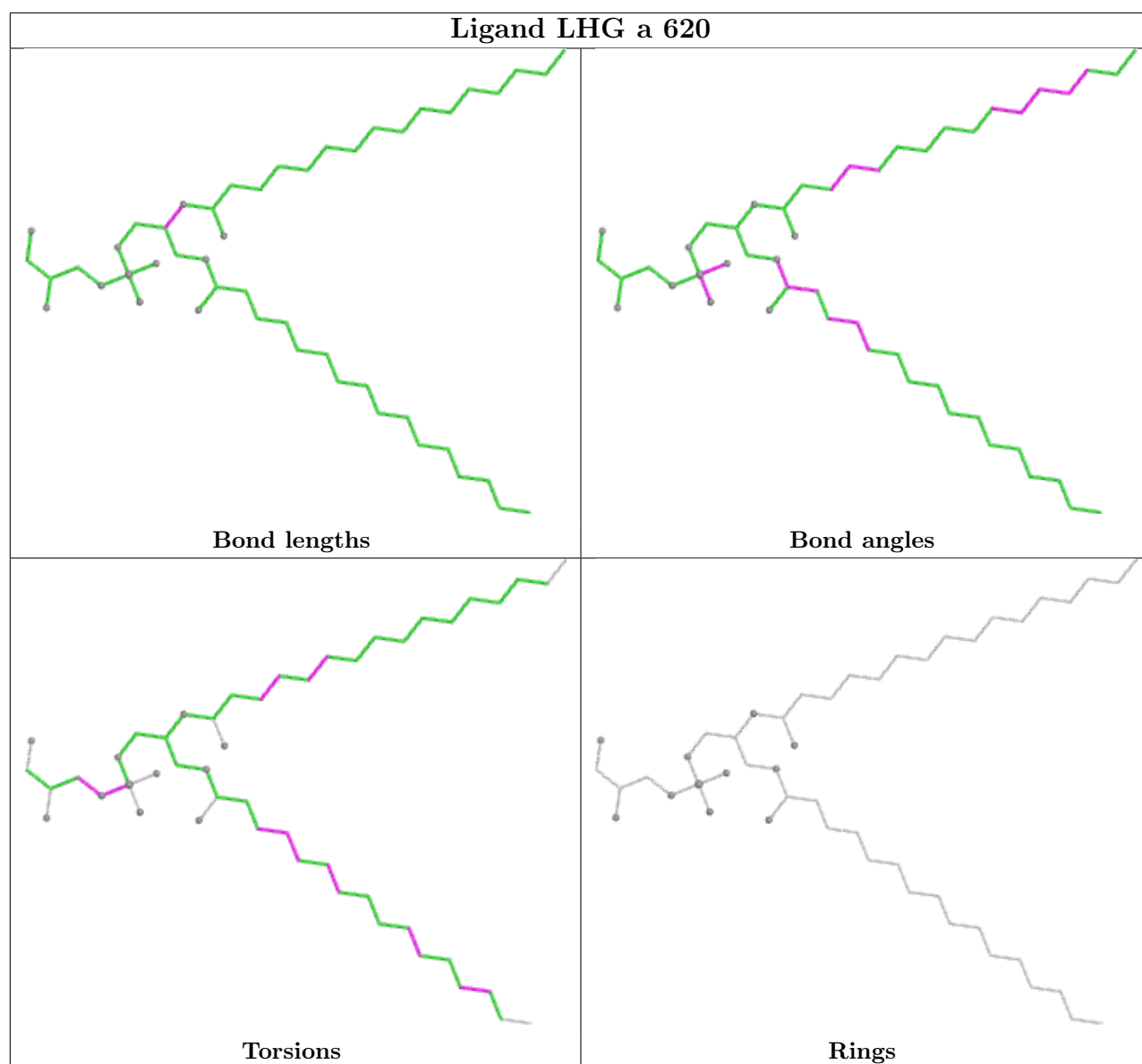


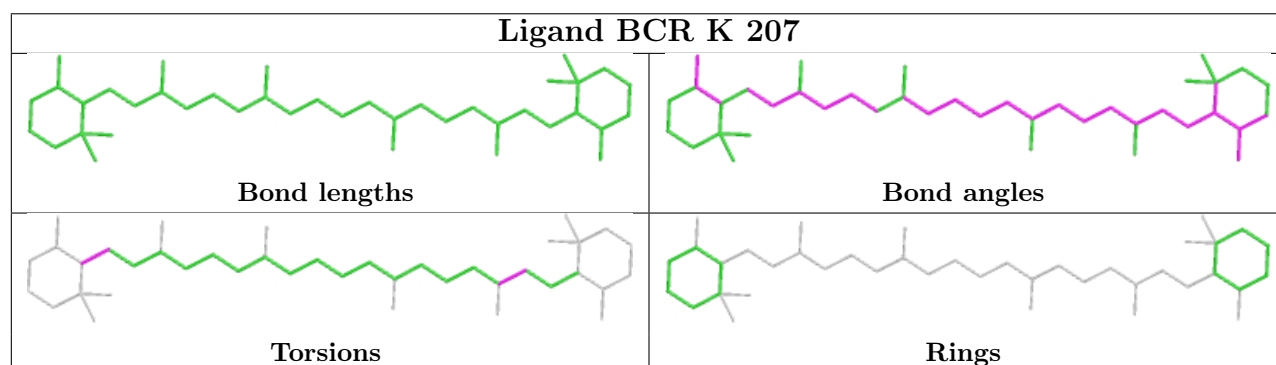
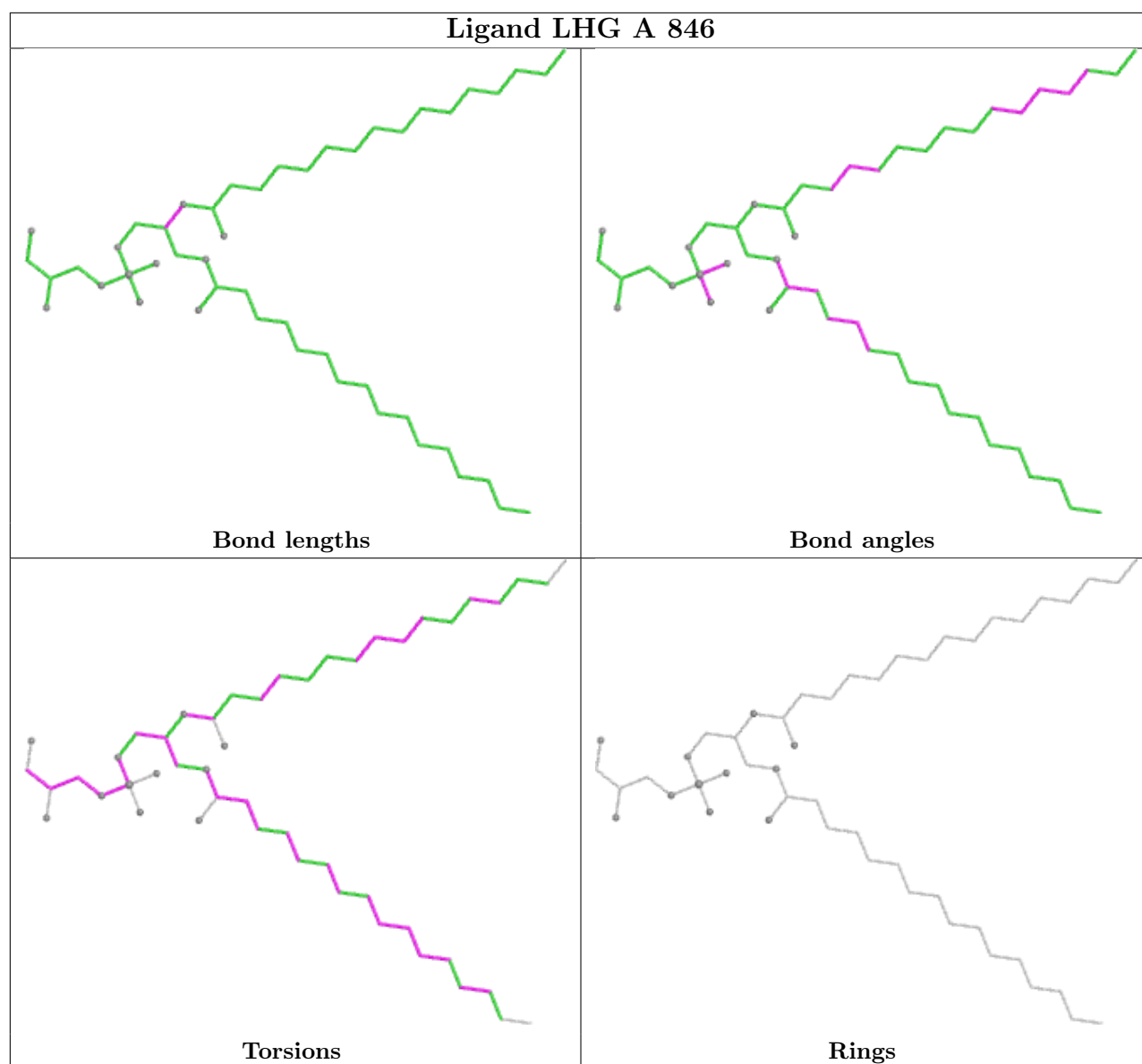
Ligand CLA A 816



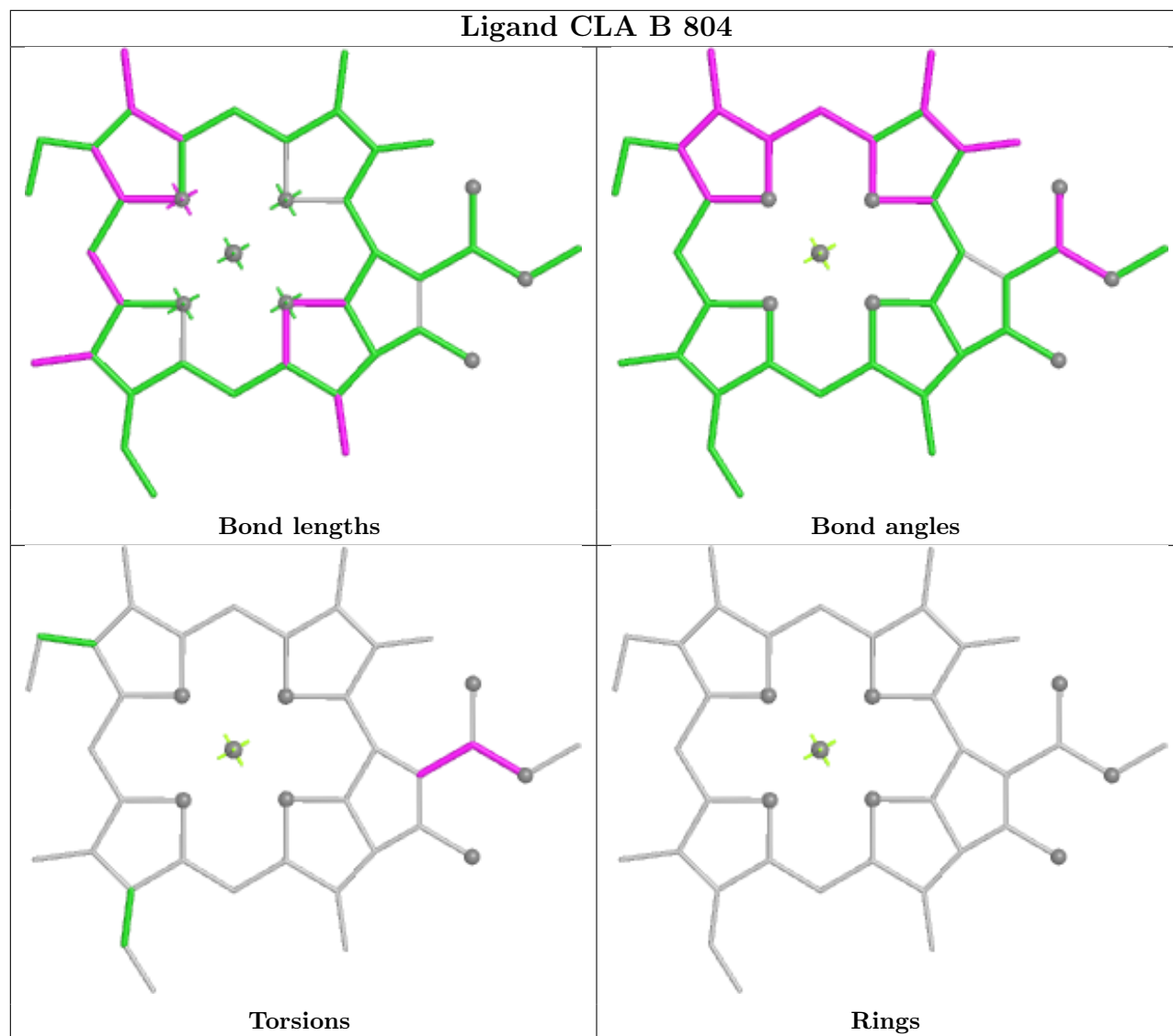




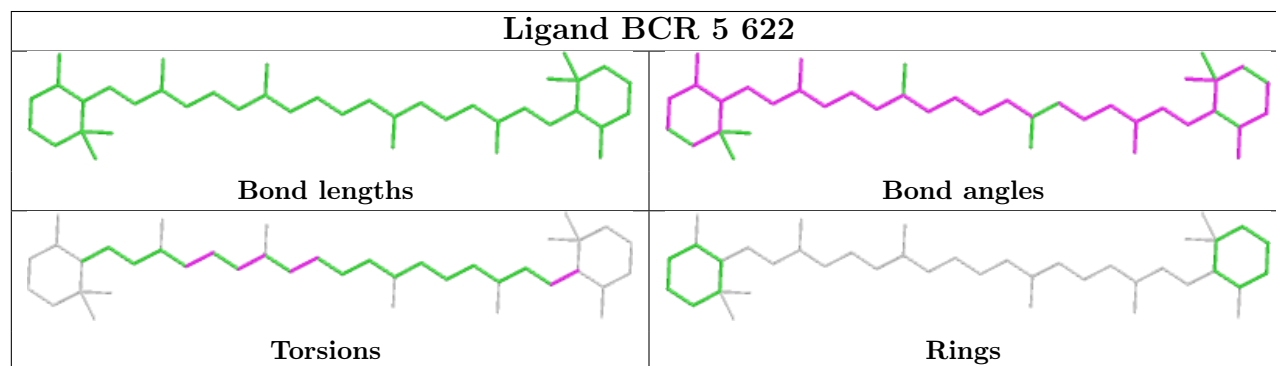


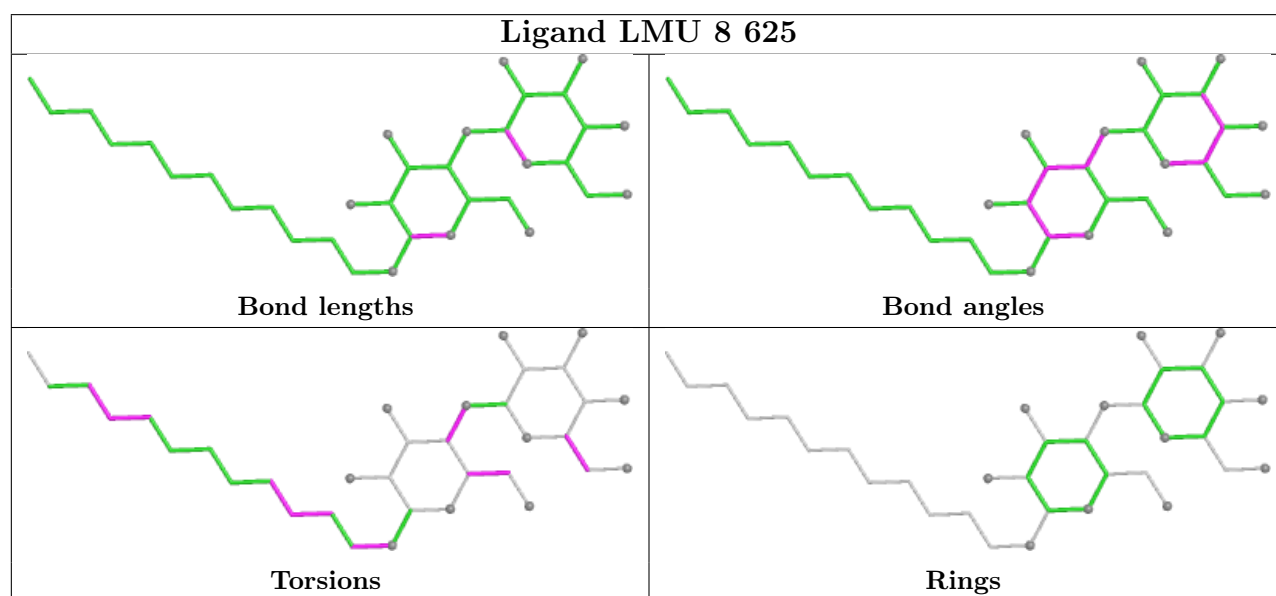
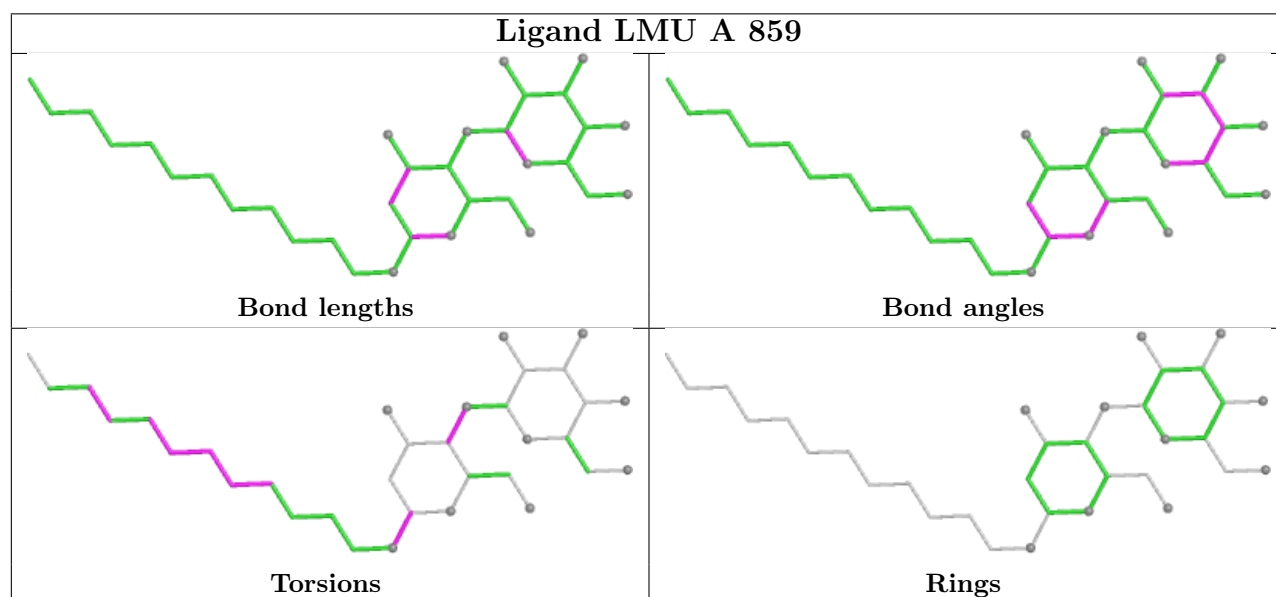
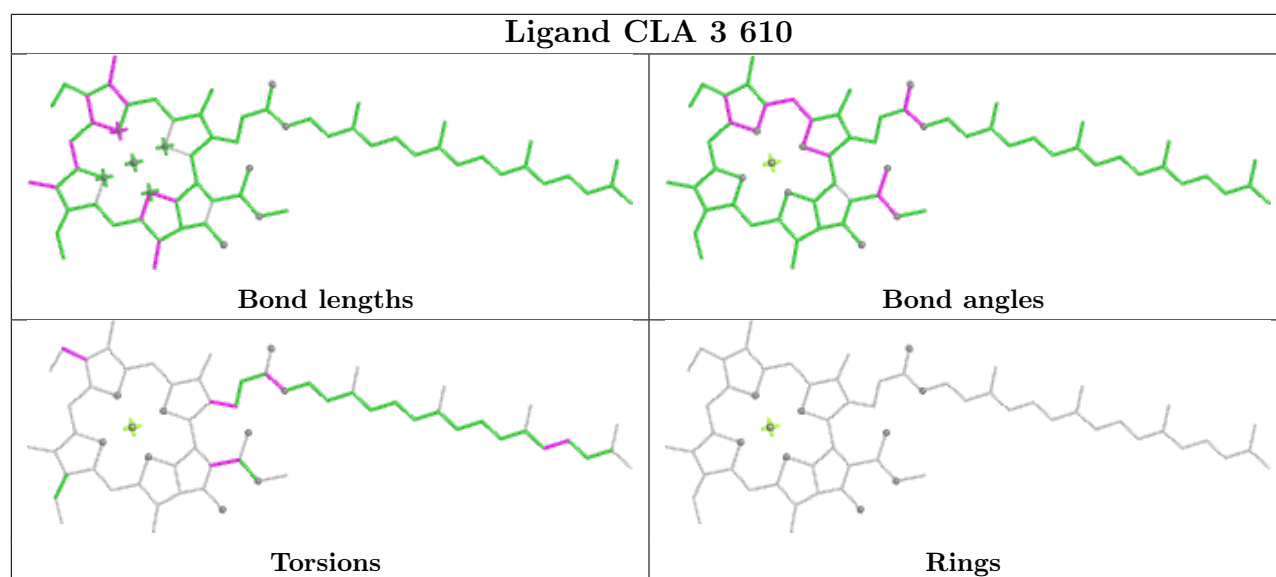


Ligand CLA B 804

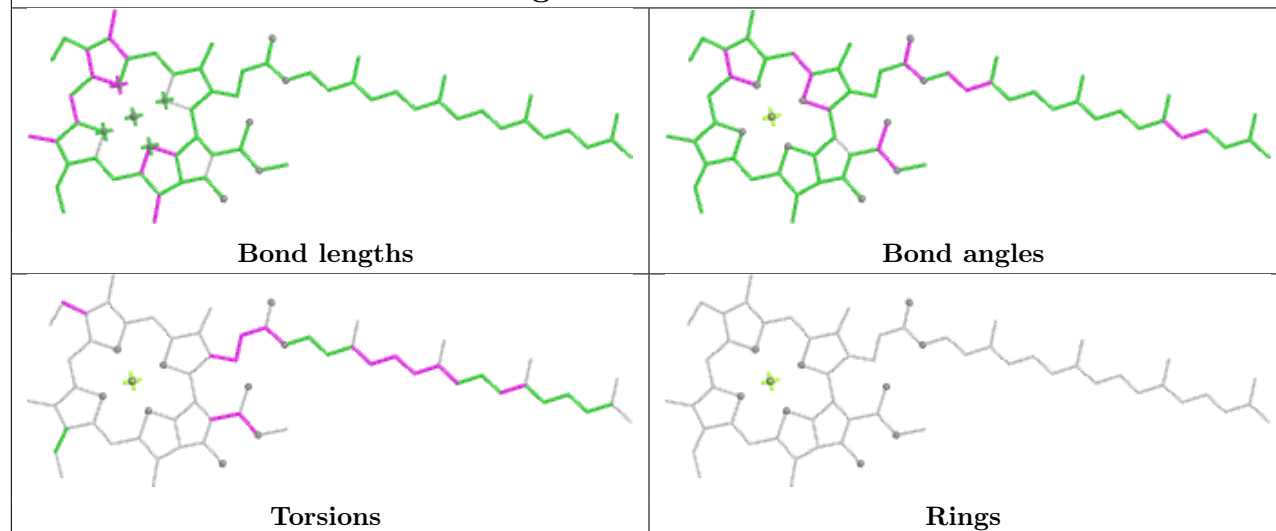


Ligand BCR 5 622

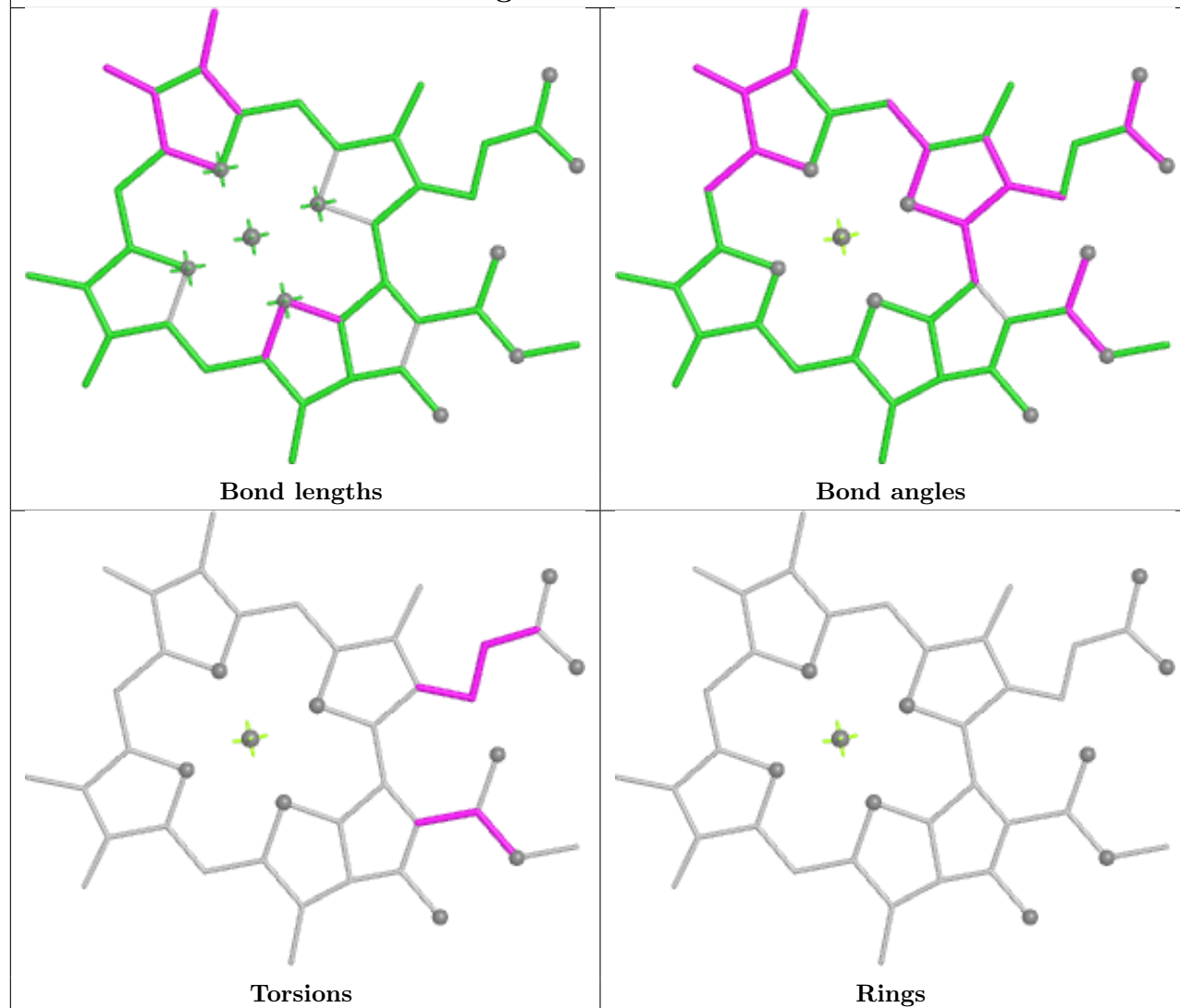




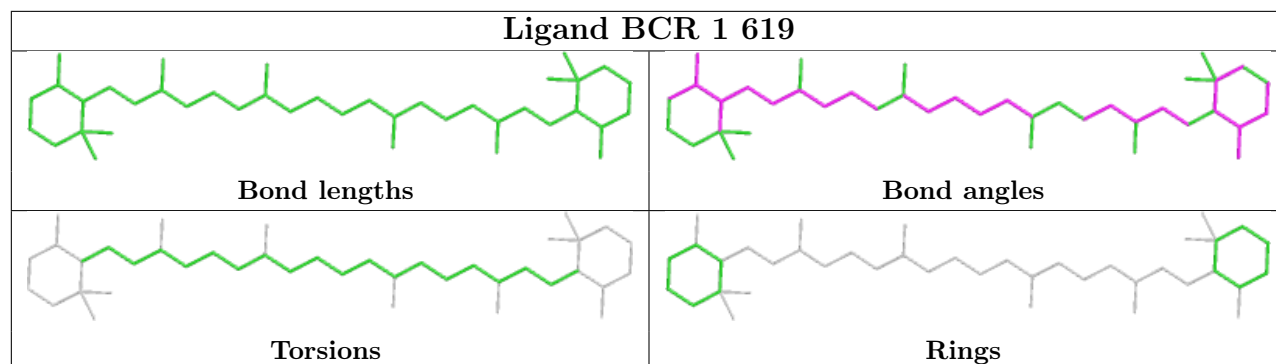
Ligand CLA B 813



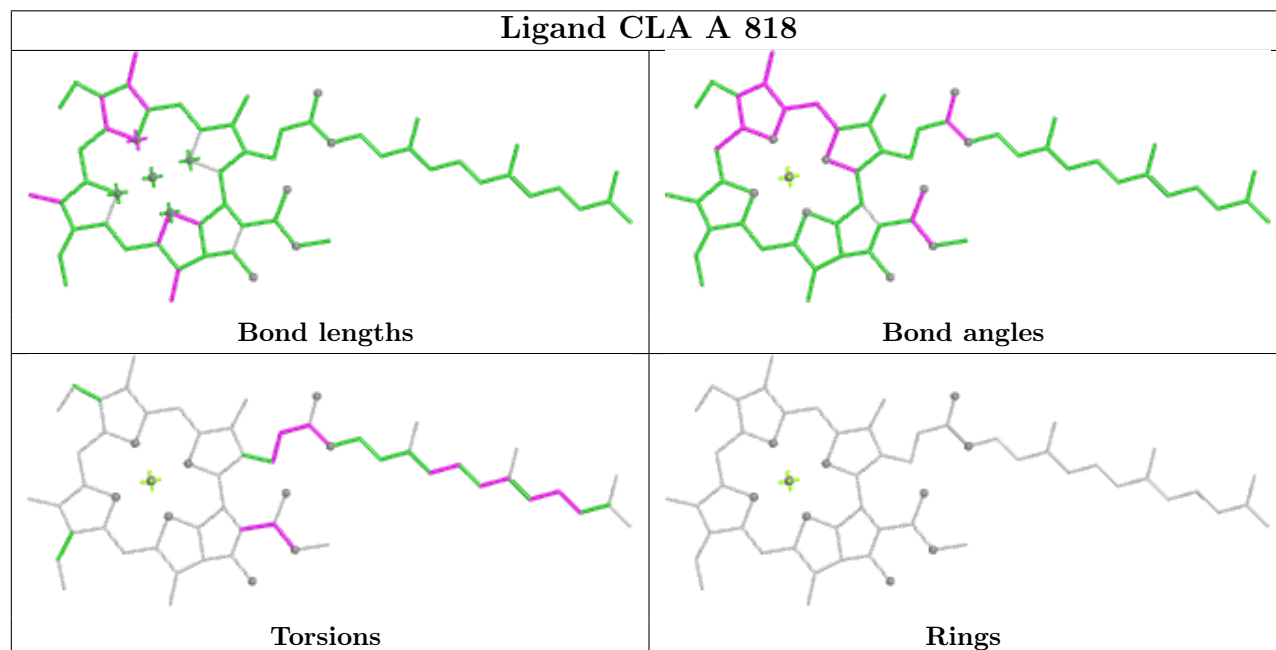
Ligand CLA 8 616



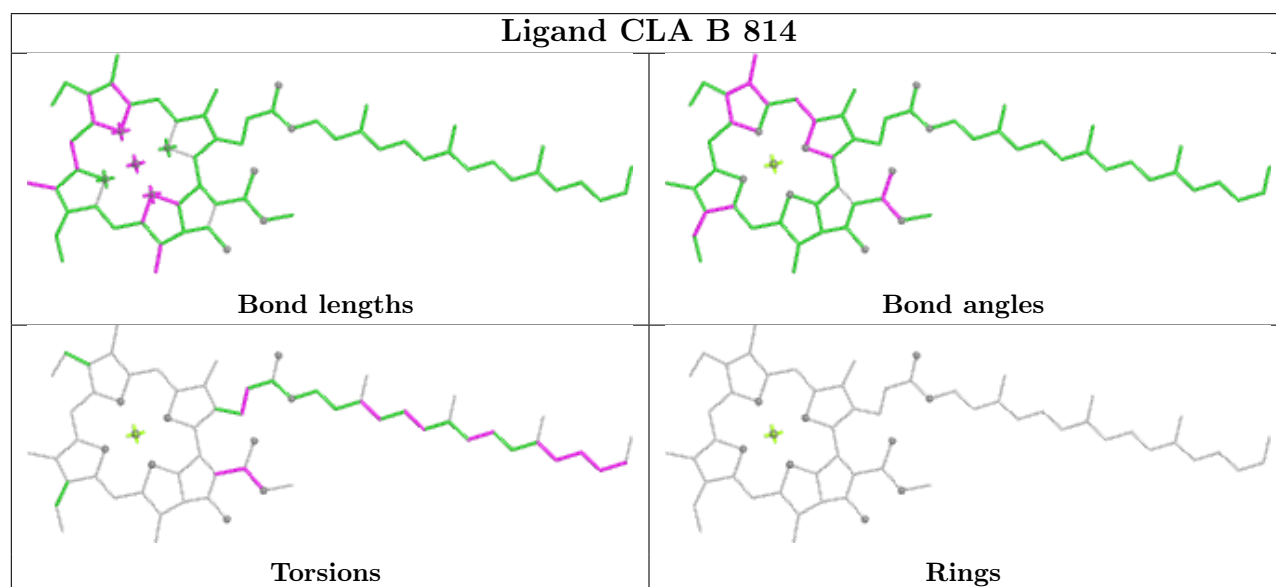
Ligand BCR 1 619

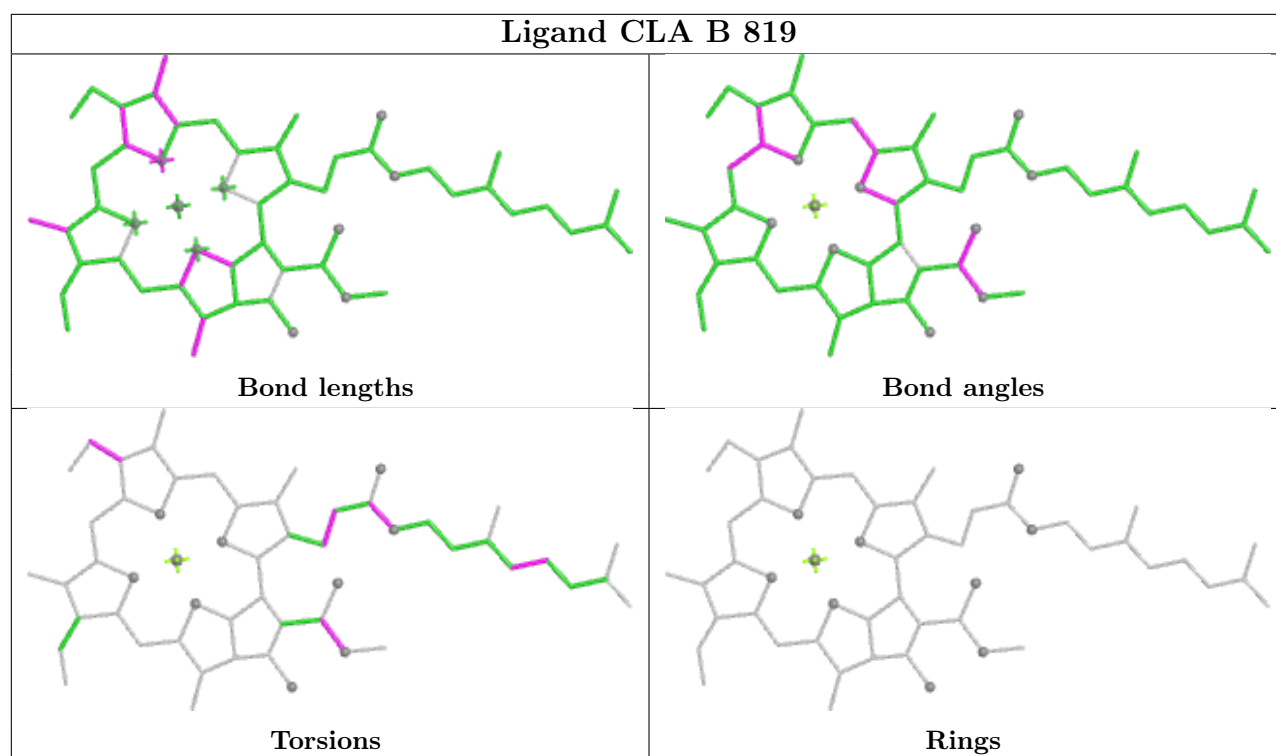


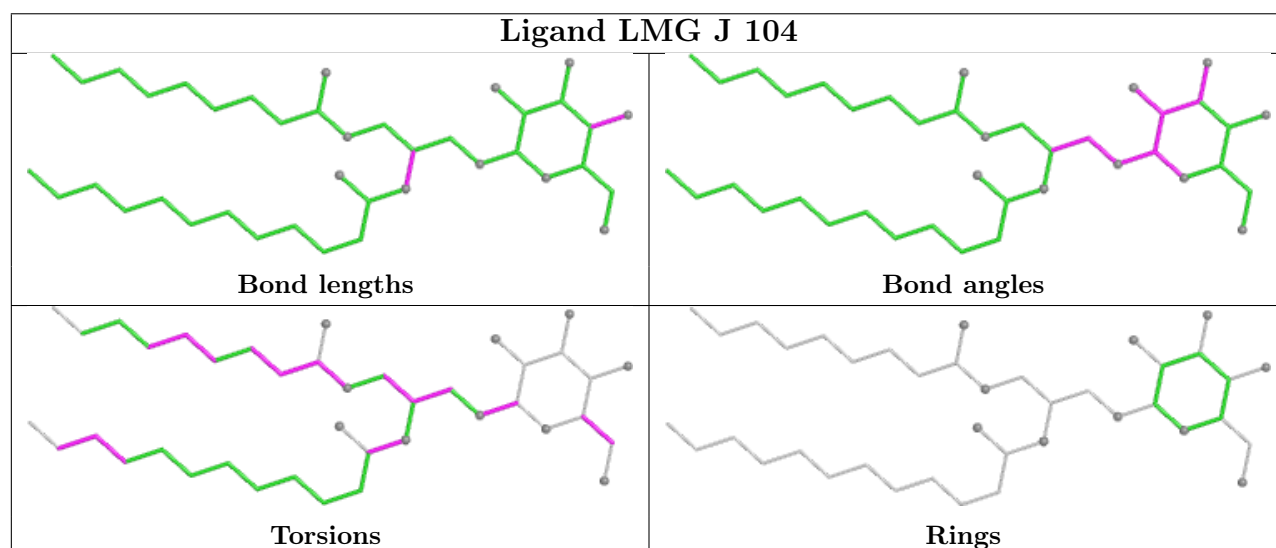
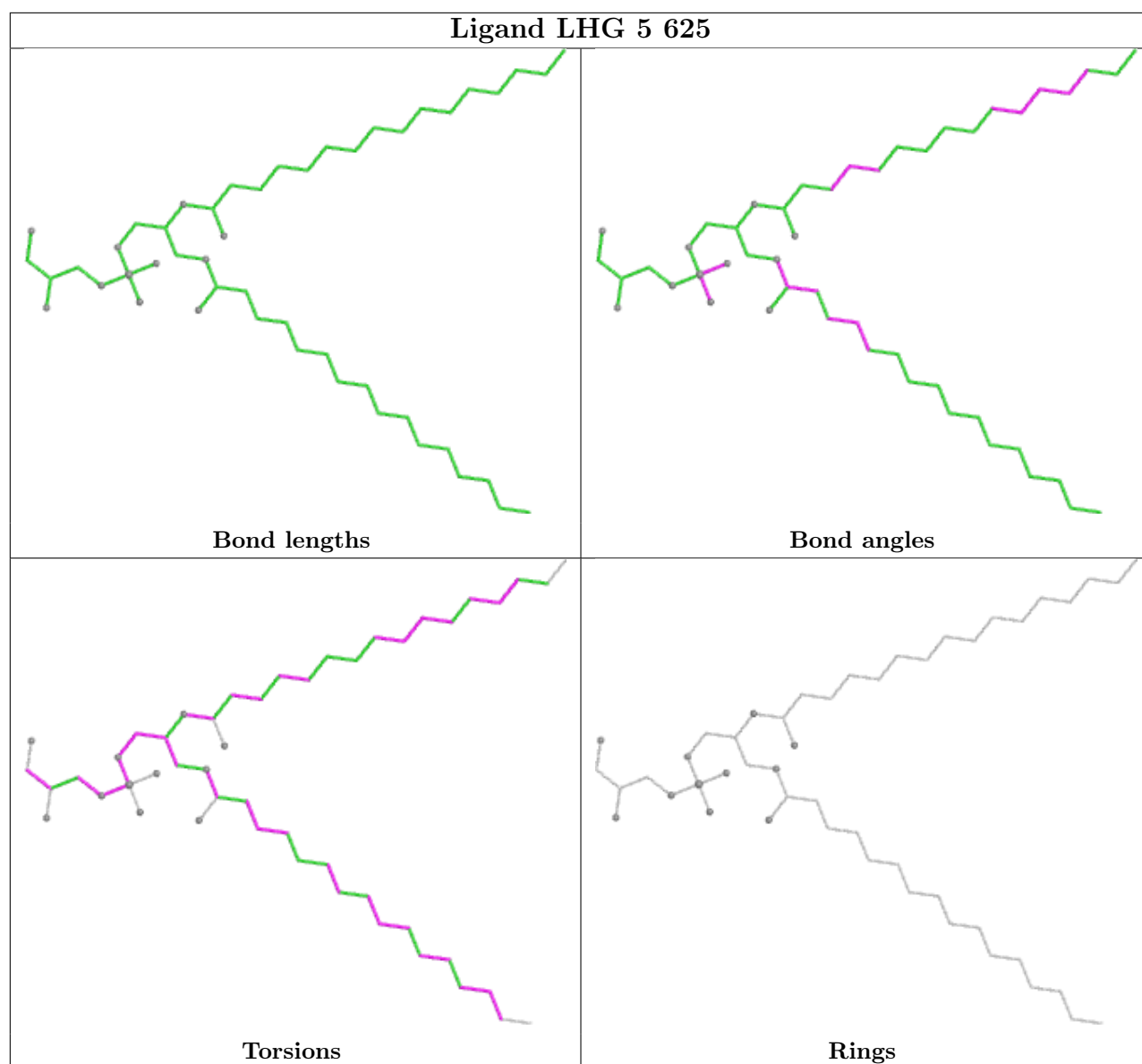
Ligand CLA A 818

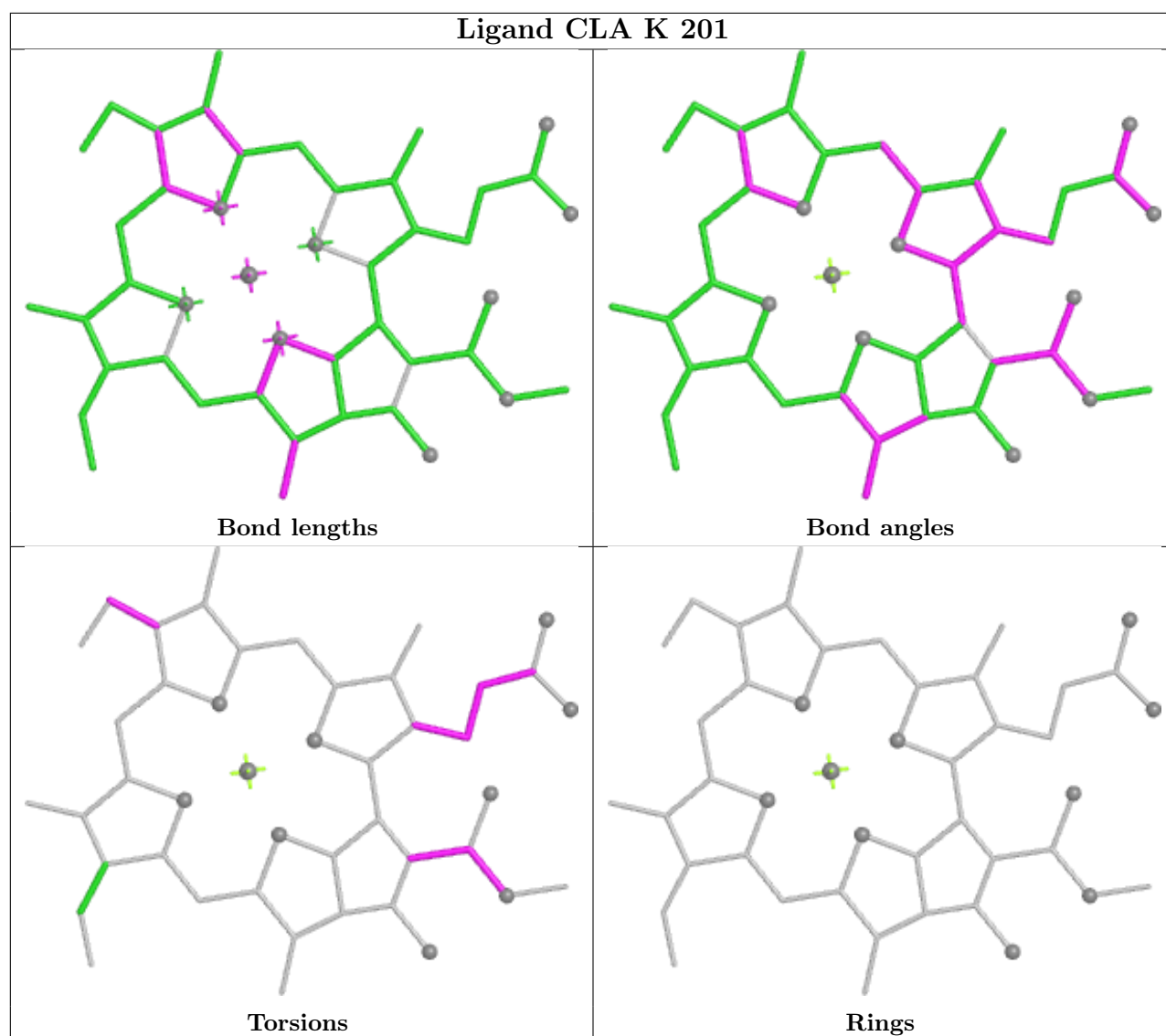


Ligand CLA B 814

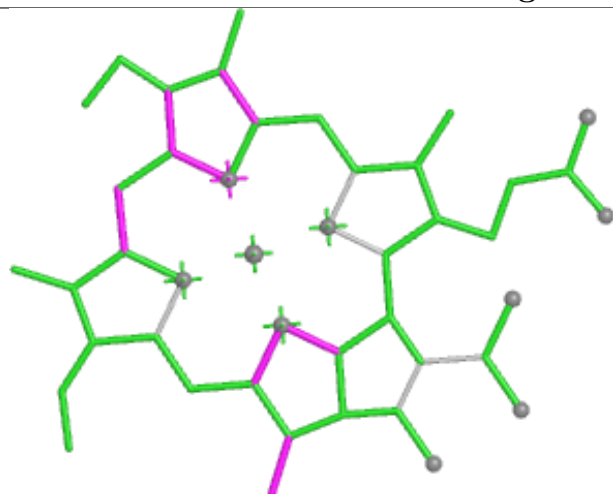








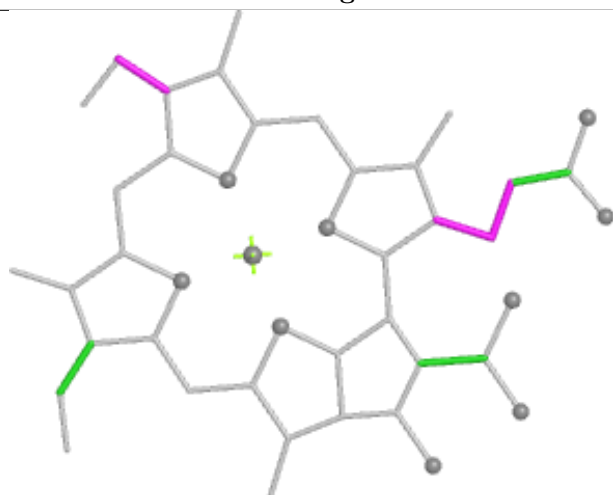
Ligand CLA a 608



Bond lengths



Bond angles

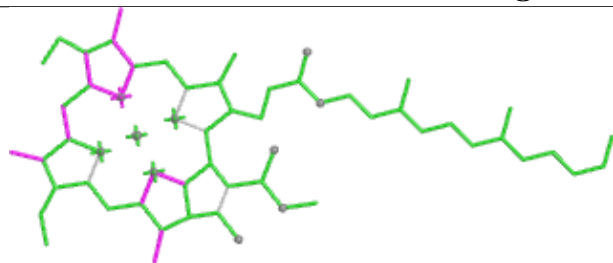


Torsions

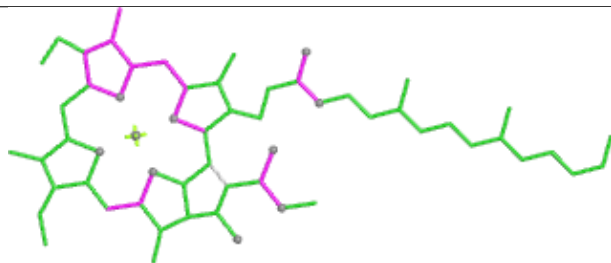


Rings

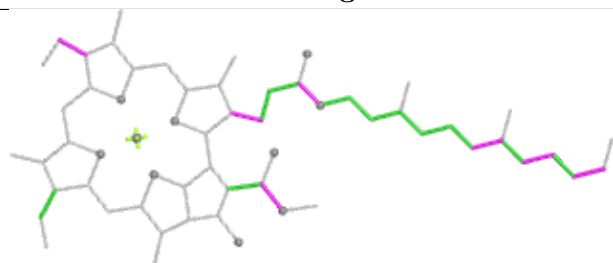
Ligand CLA B 817



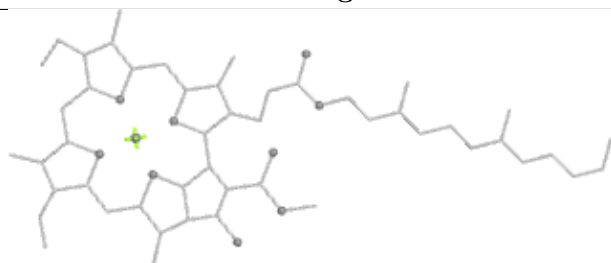
Bond lengths



Bond angles

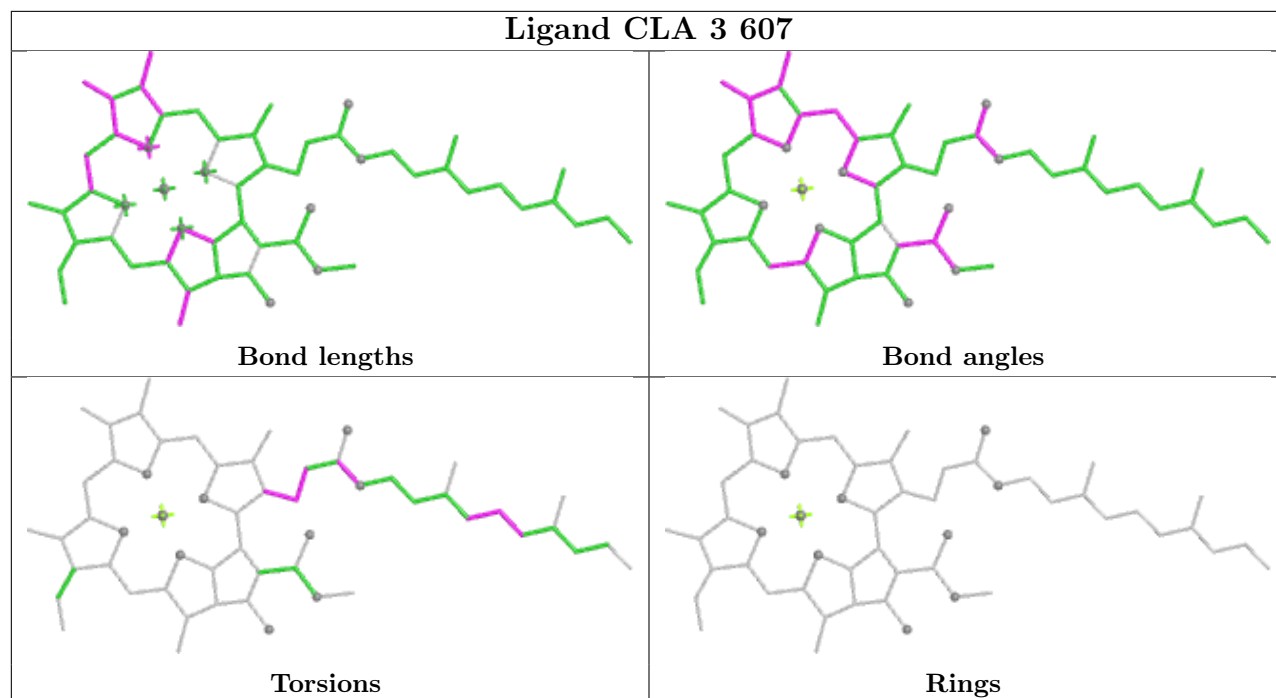


Torsions

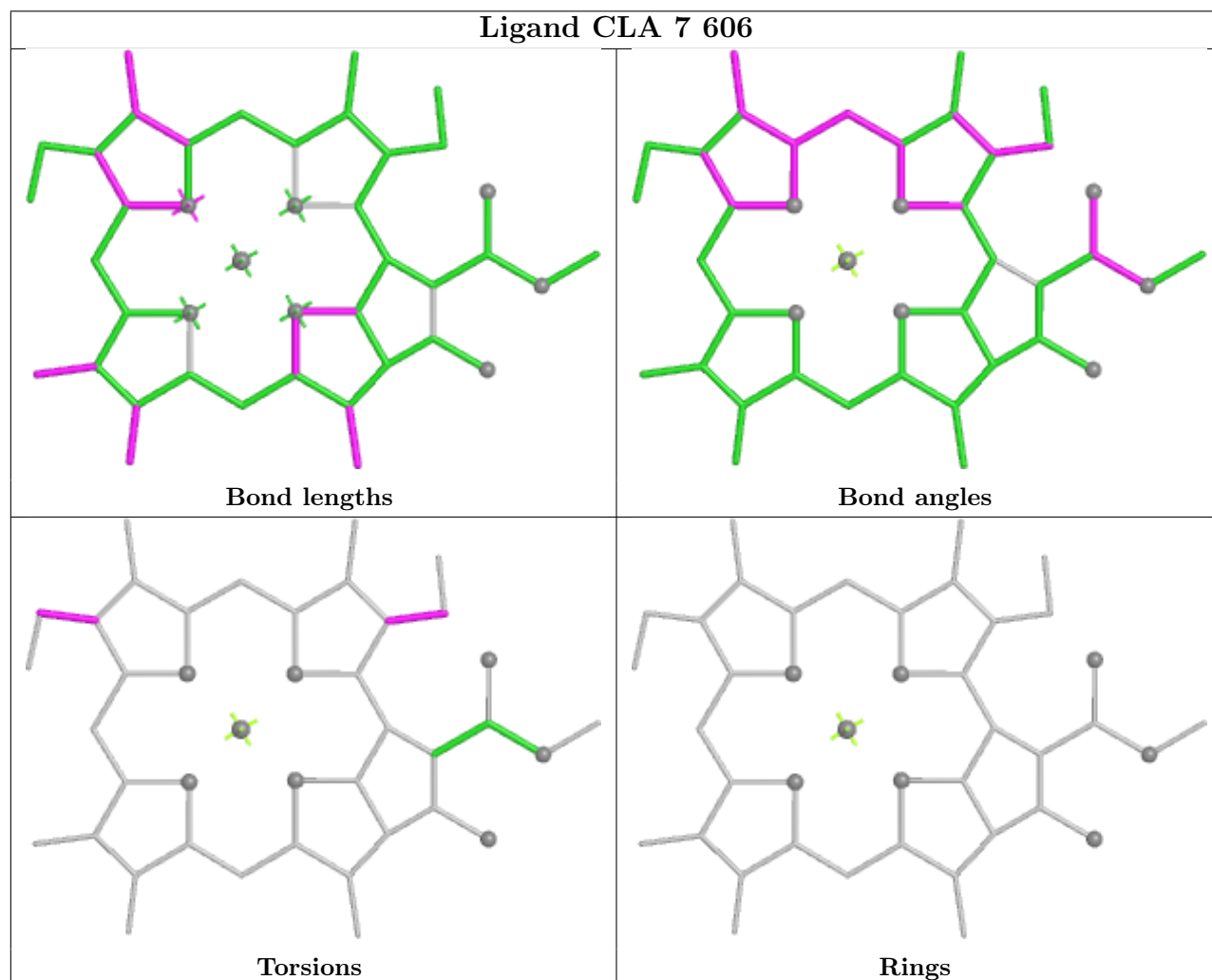


Rings

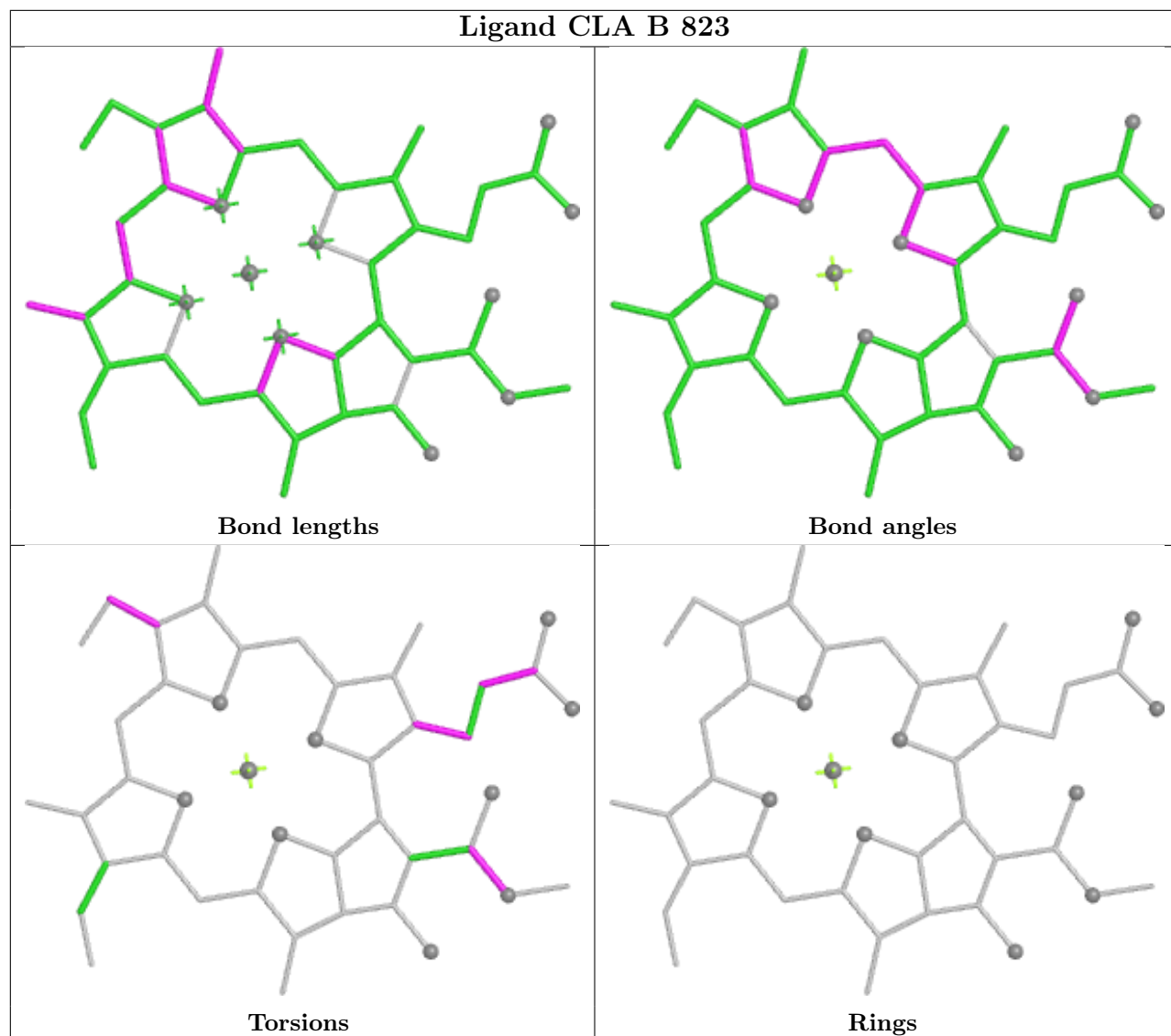
Ligand CLA 3 607



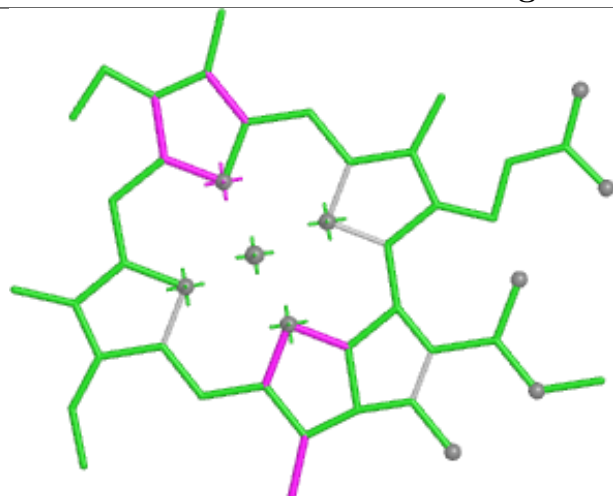
Ligand CLA 7 606



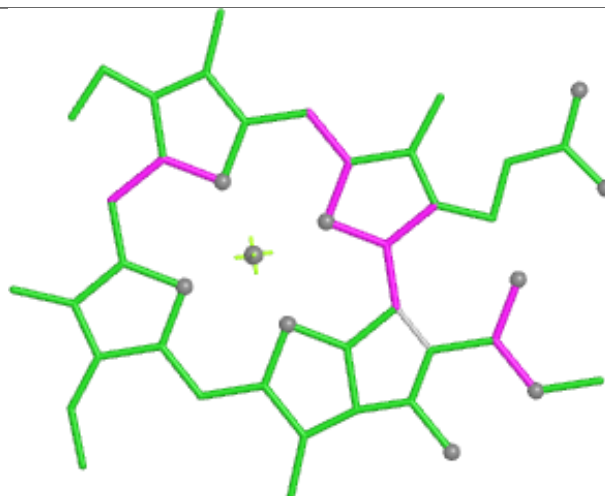
Ligand CLA B 823



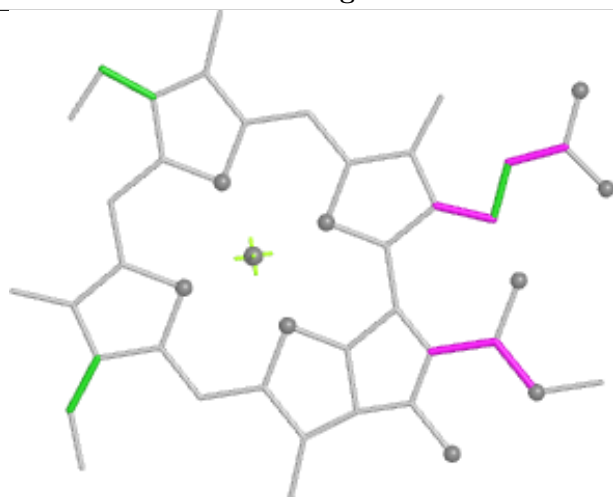
Ligand CLA 1 612



Bond lengths



Bond angles

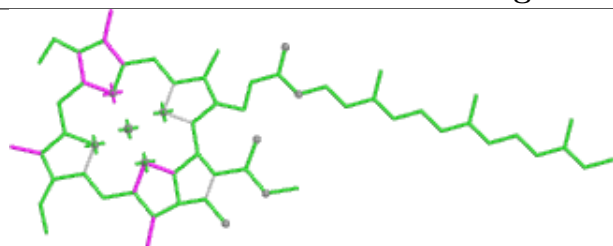


Torsions

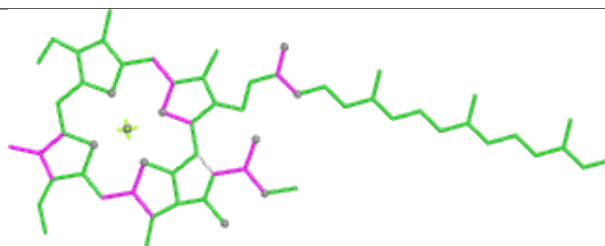


Rings

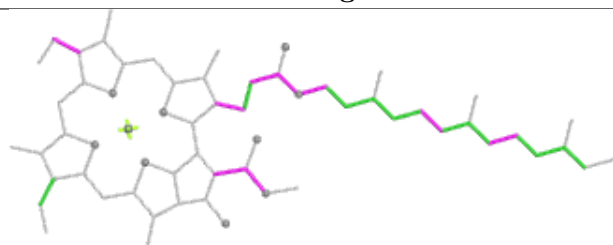
Ligand CLA A 835



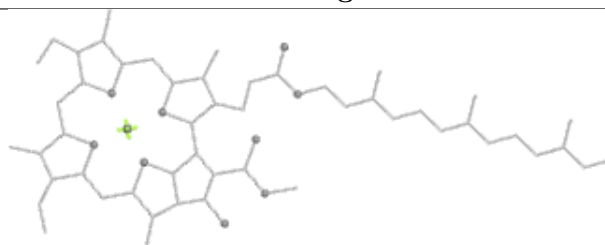
Bond lengths



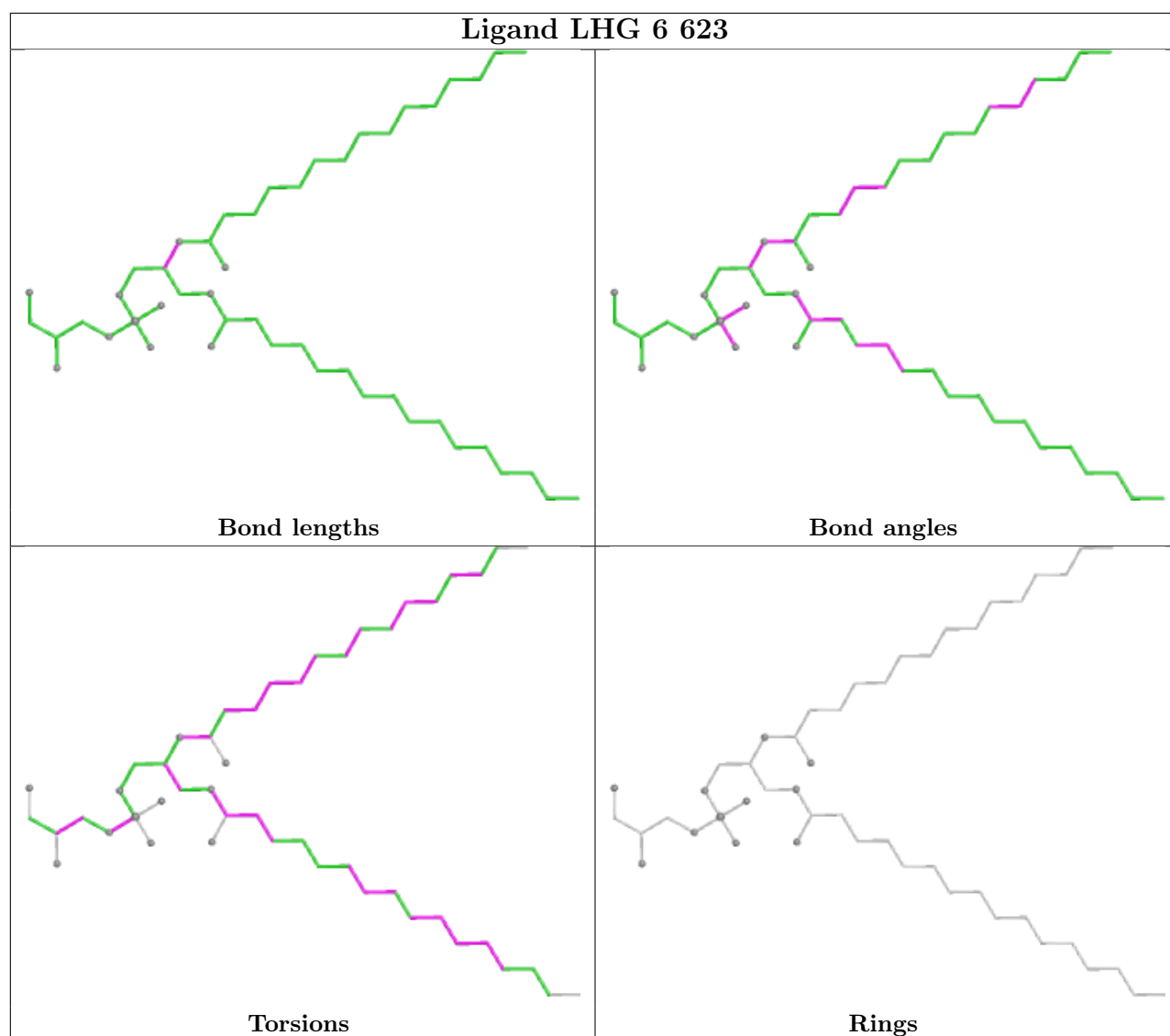
Bond angles

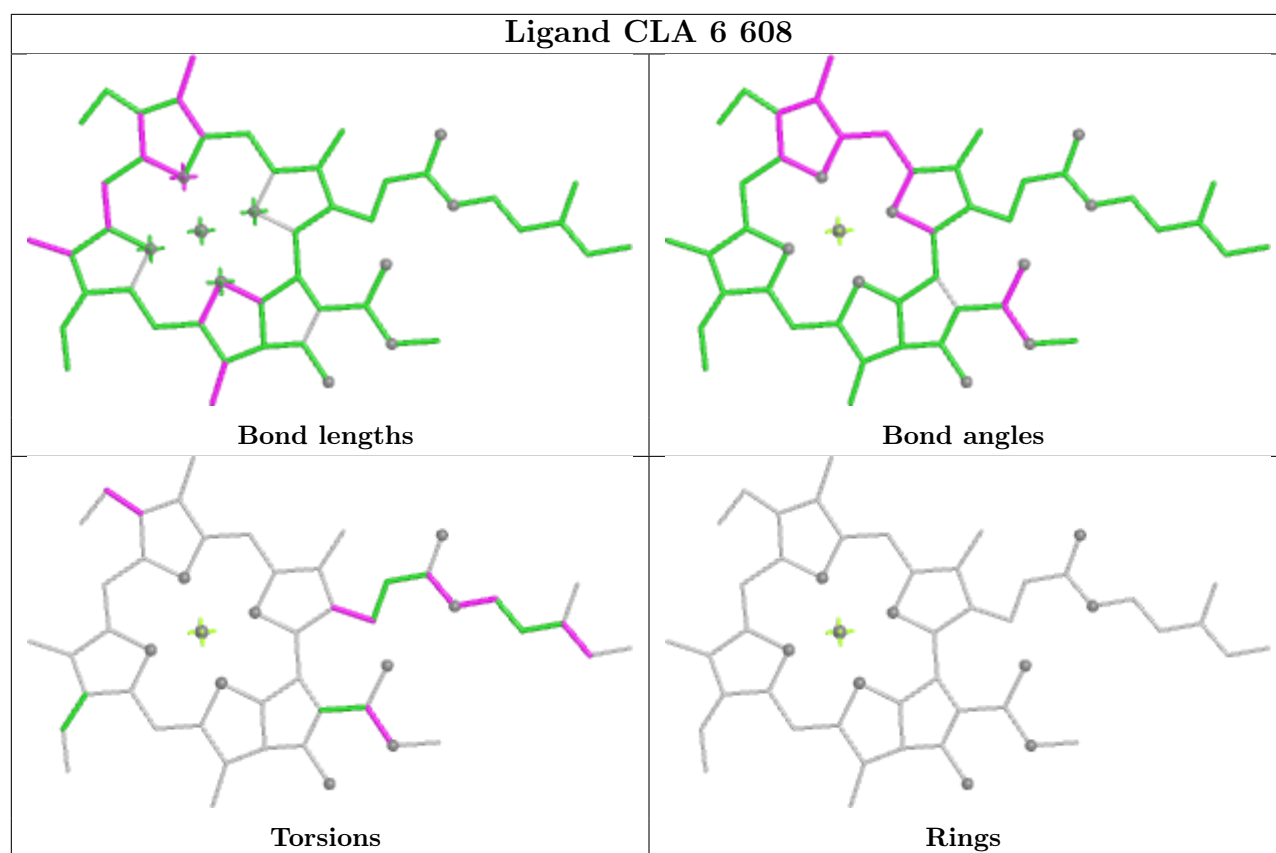


Torsions

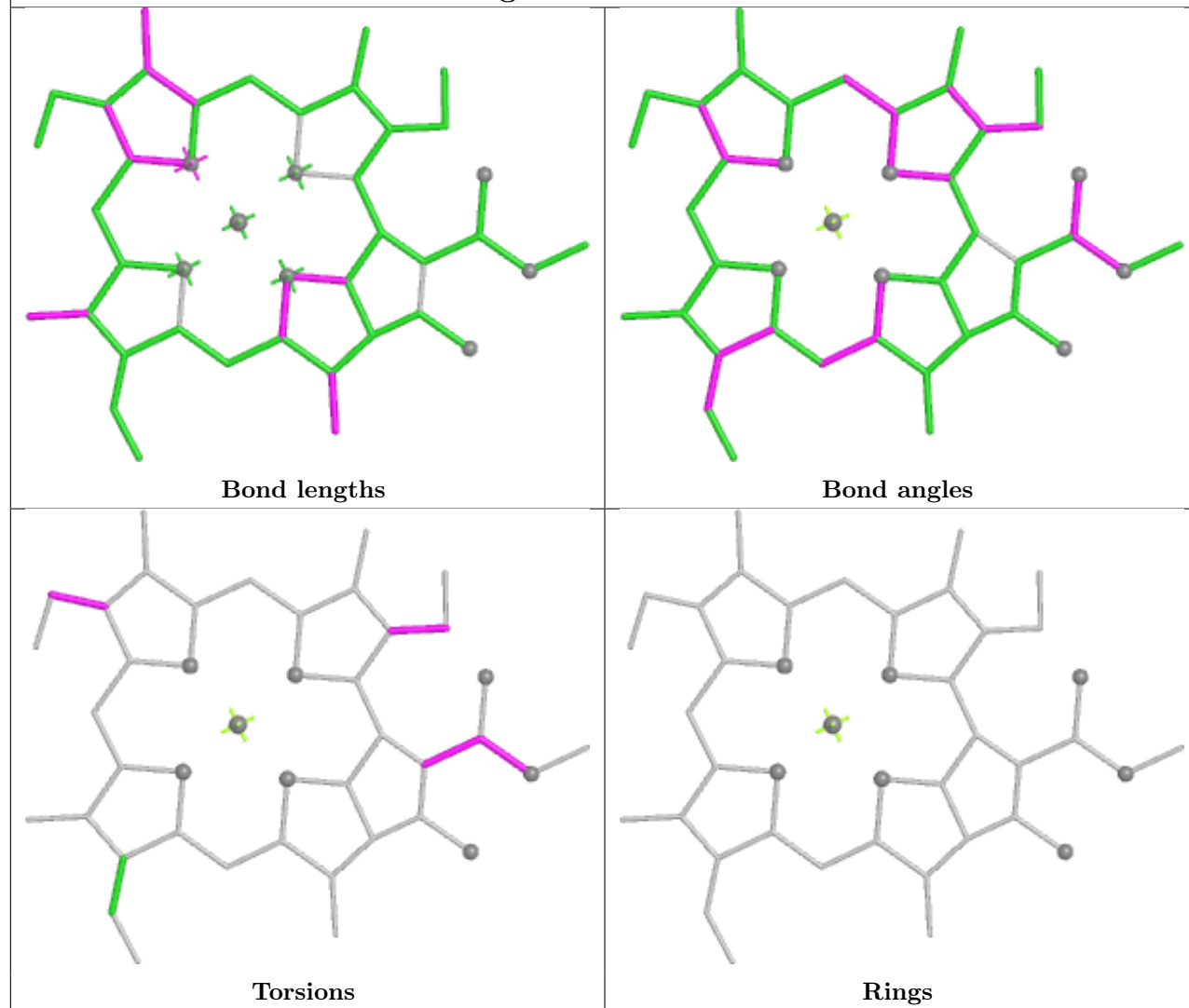


Rings

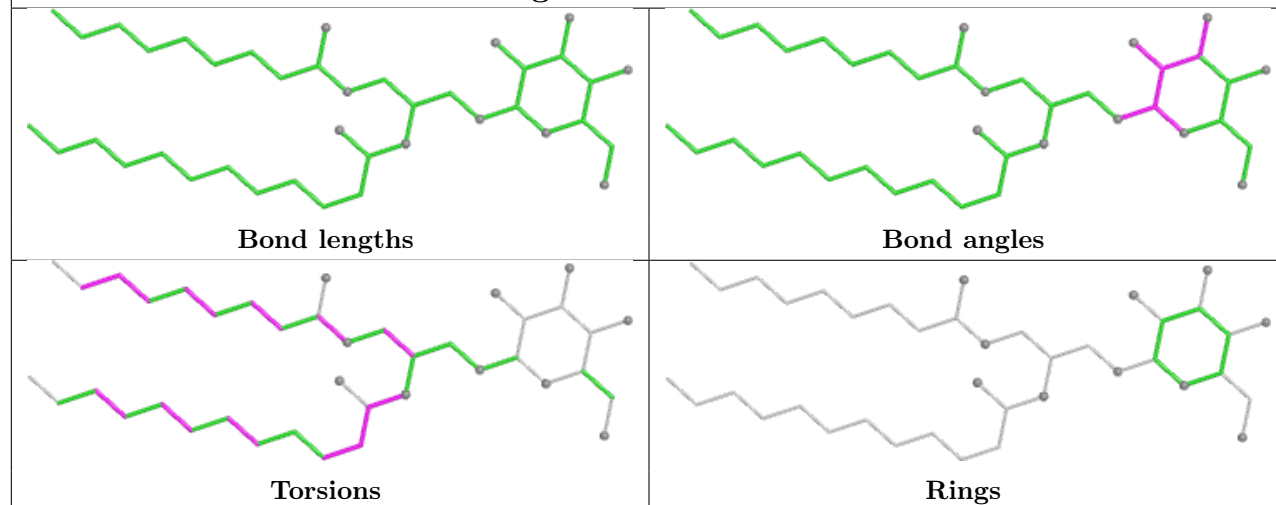




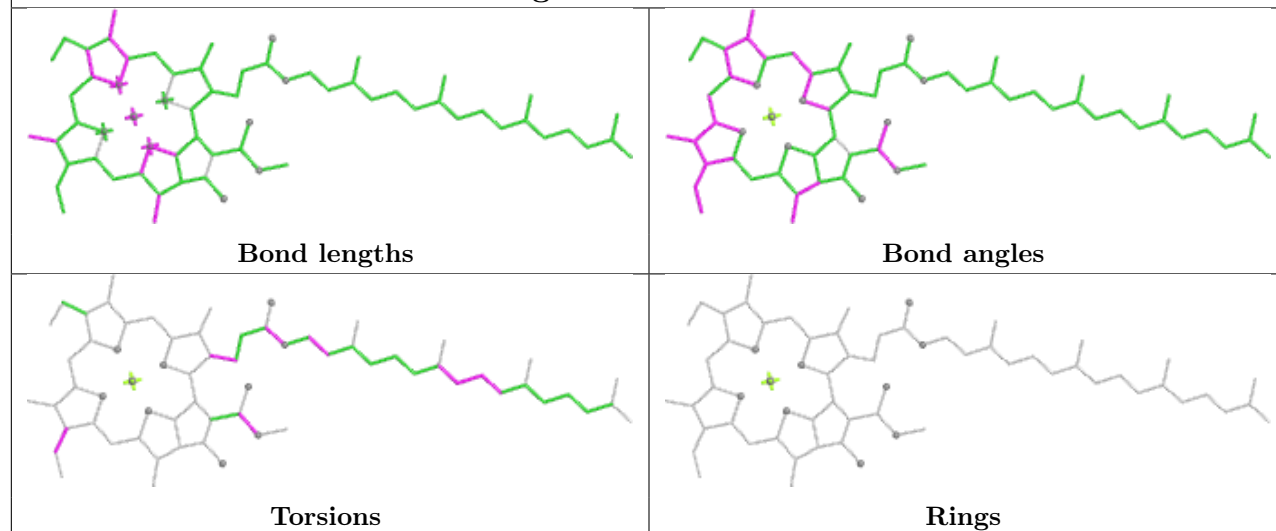
Ligand CLA 7 607



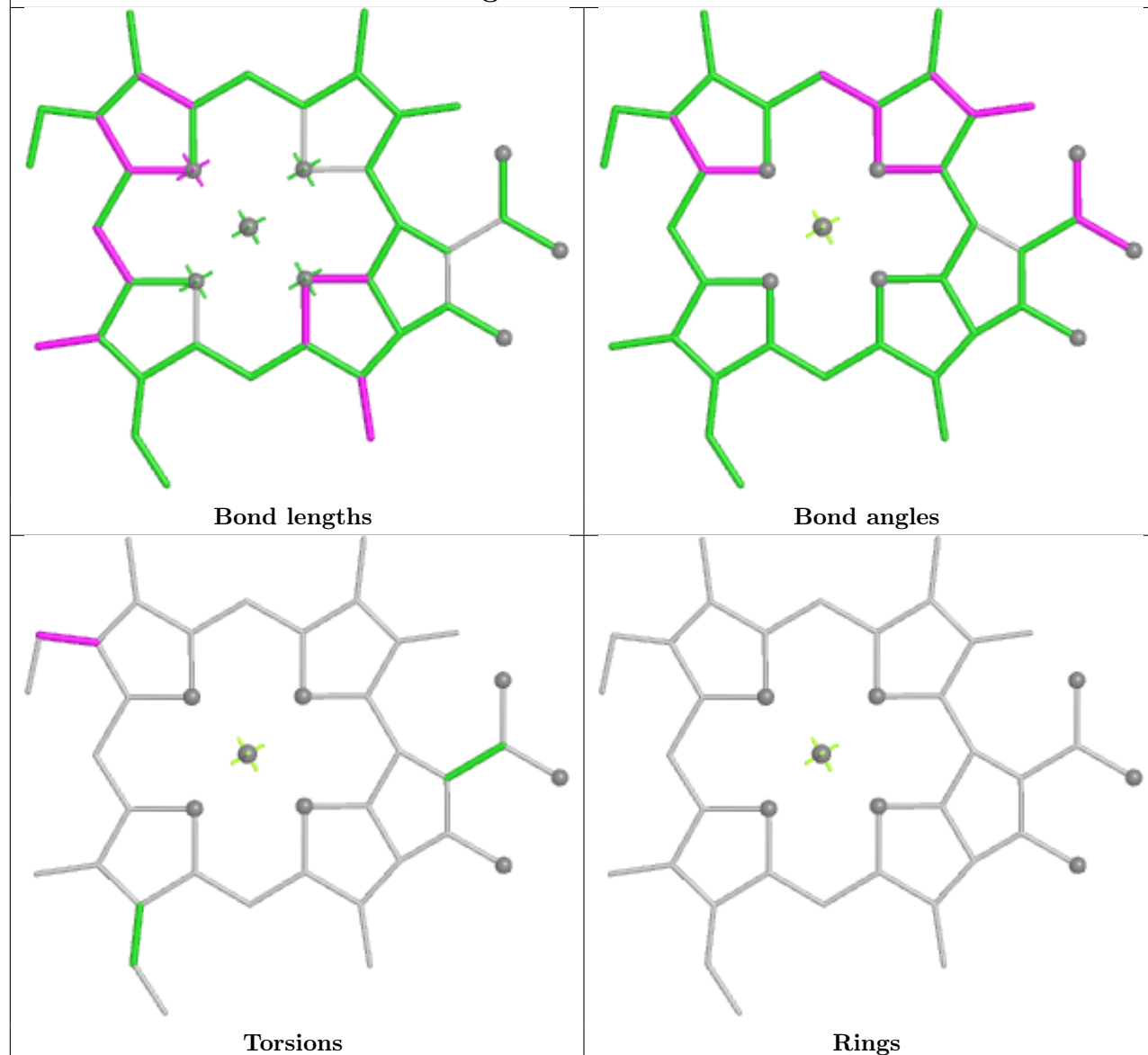
Ligand LMG 5 627



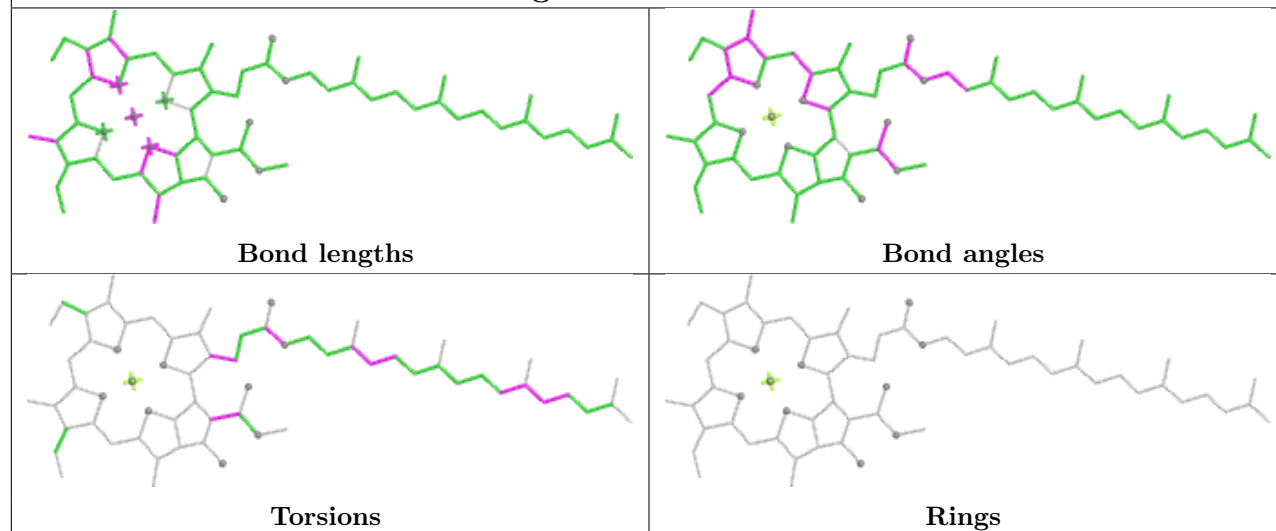
Ligand CLA B 803



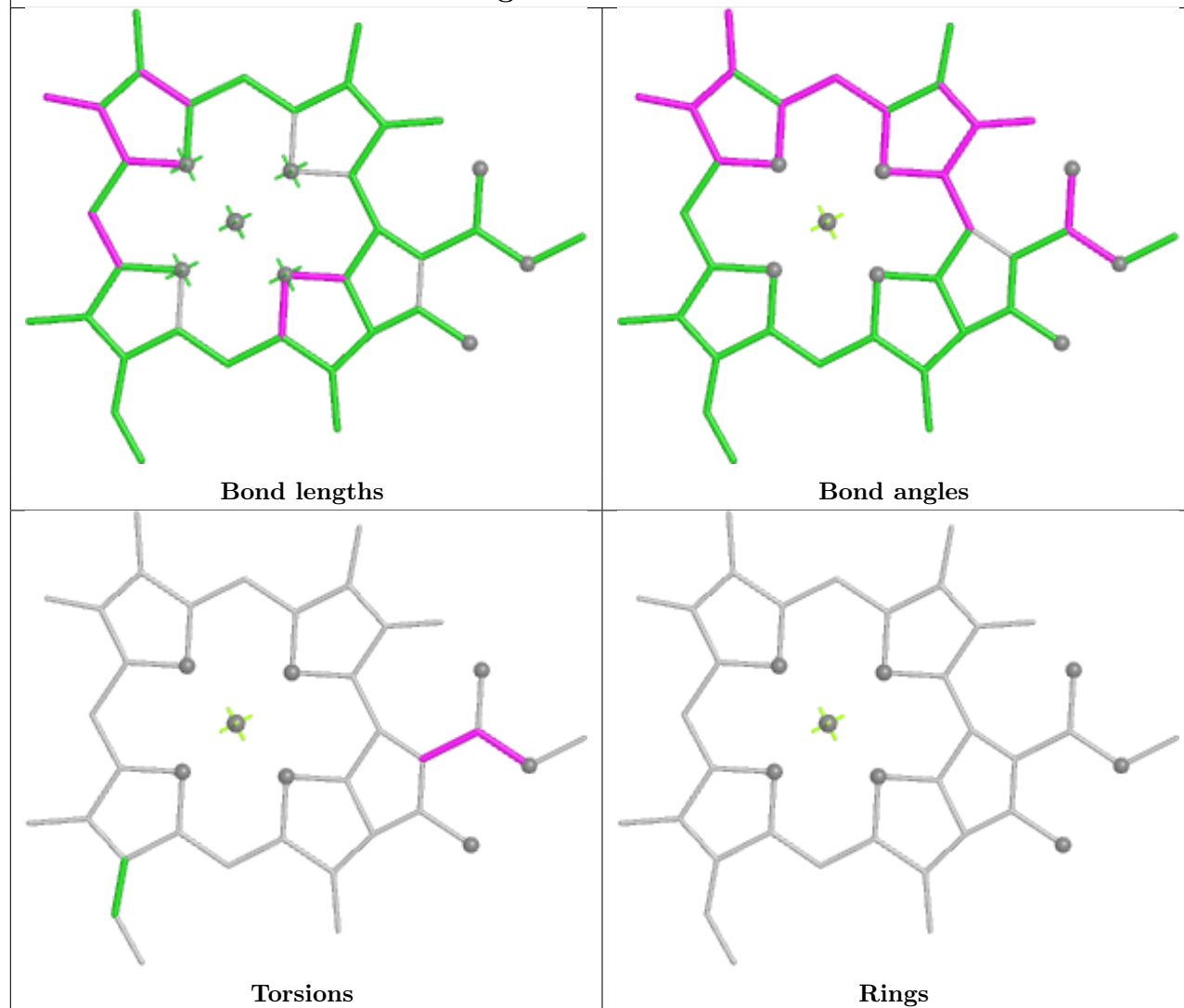
Ligand CLA 1 607

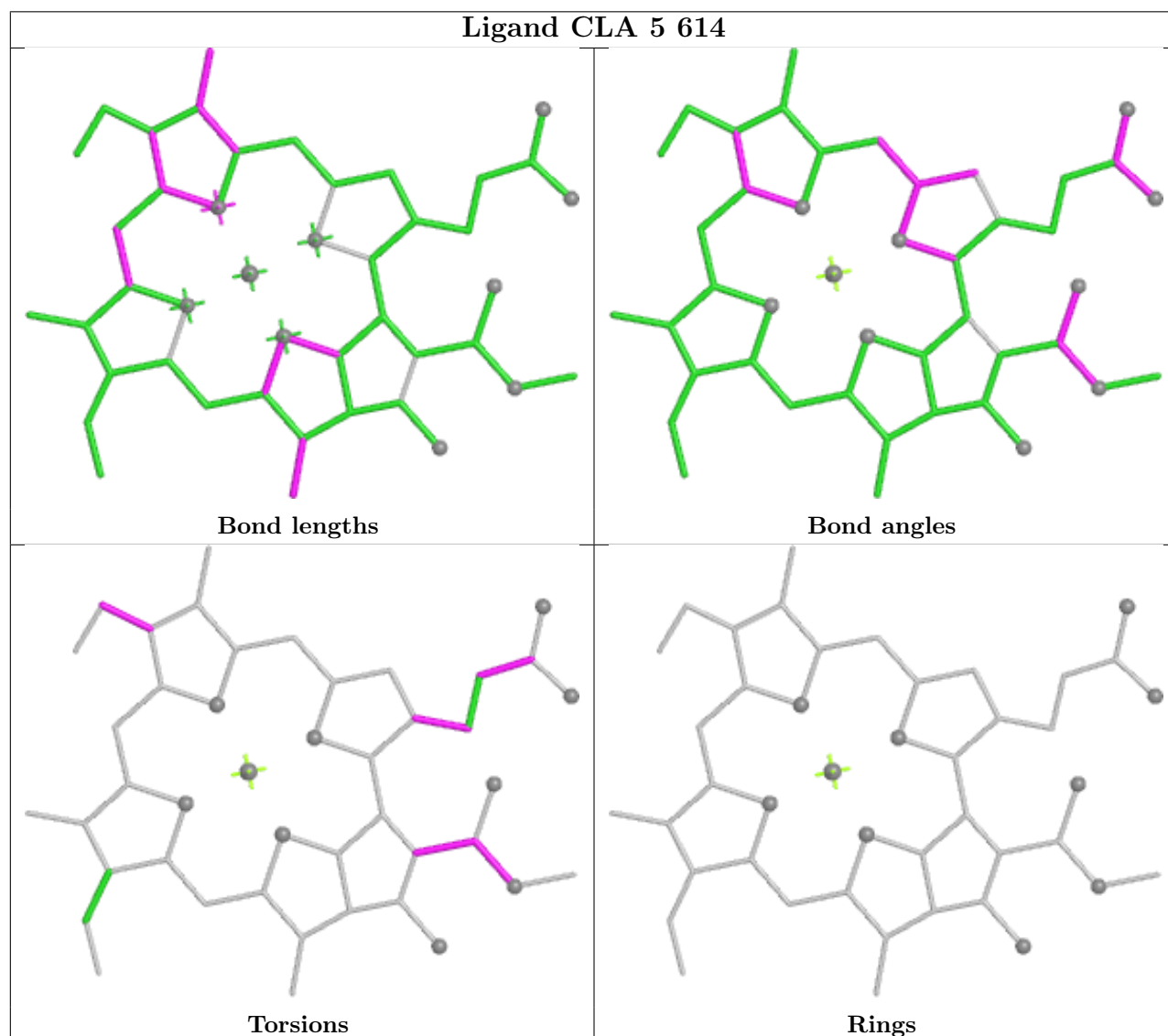
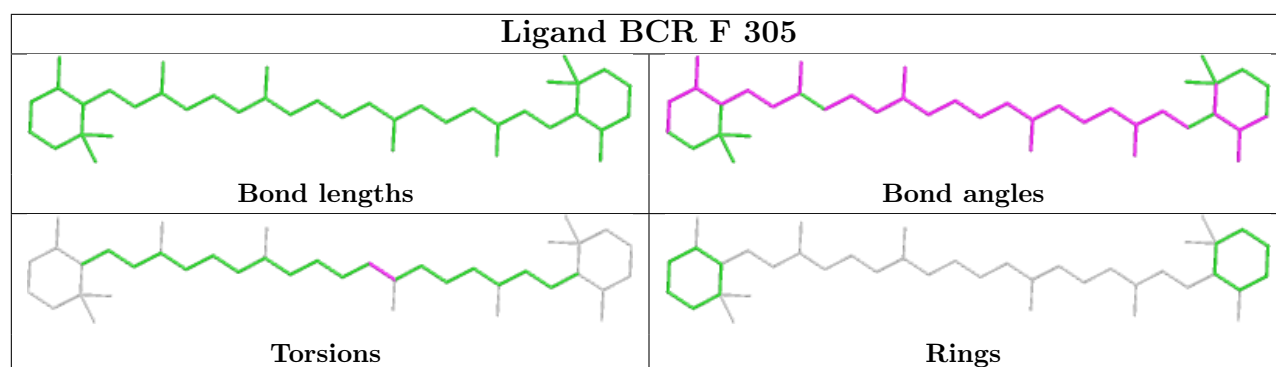


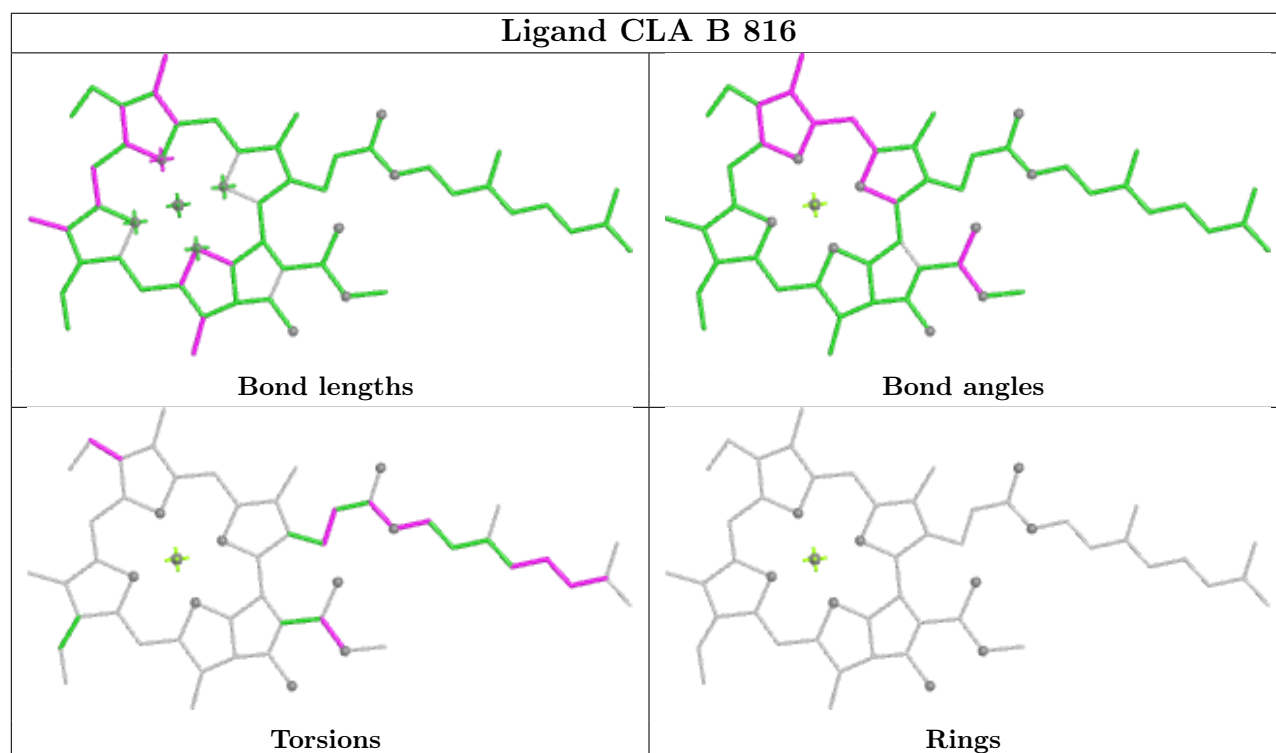
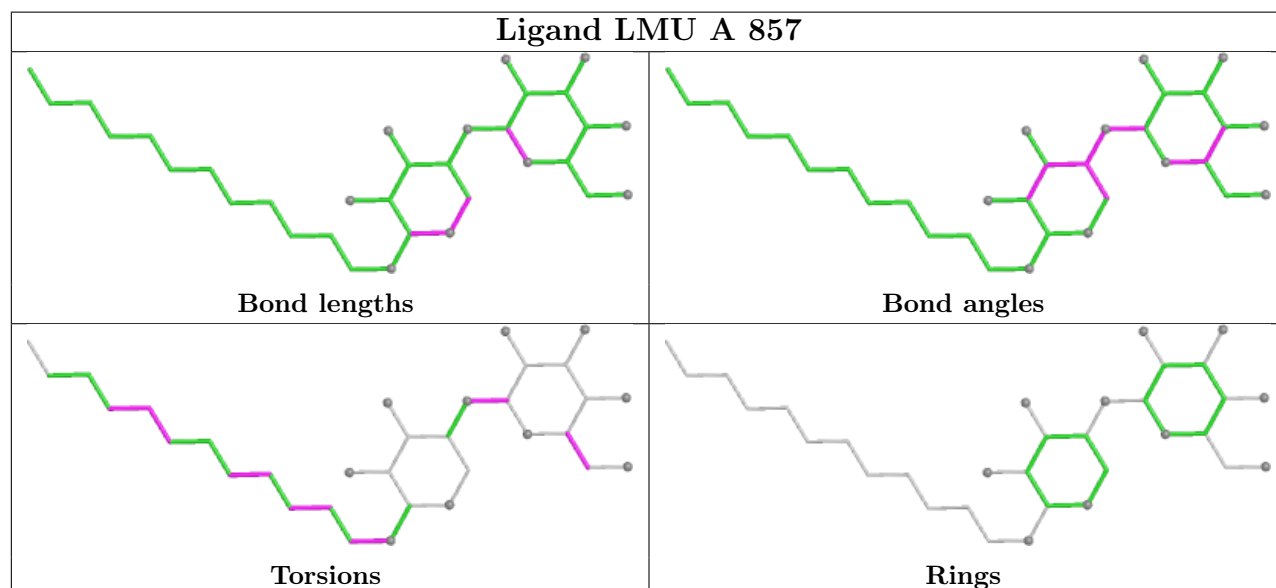
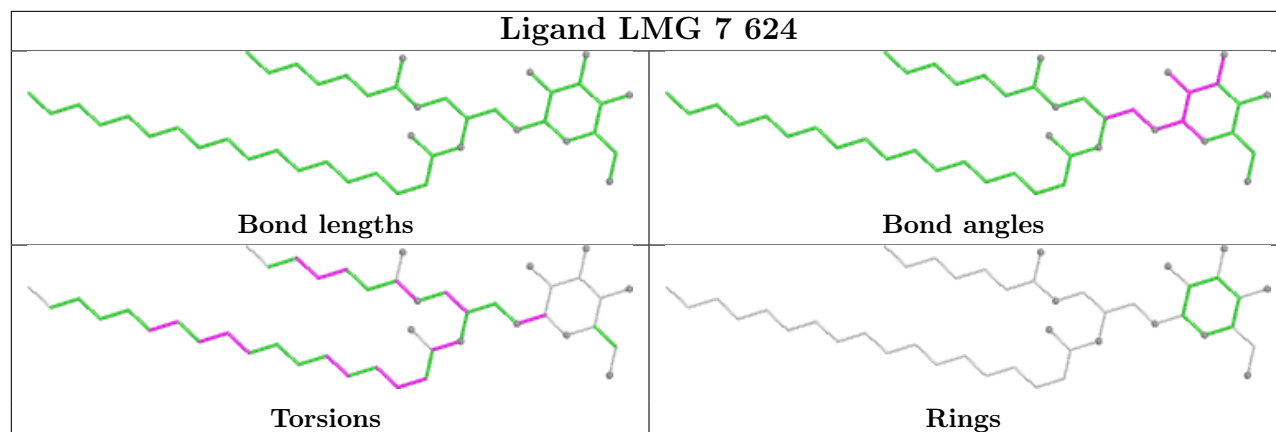
Ligand CLA B 805

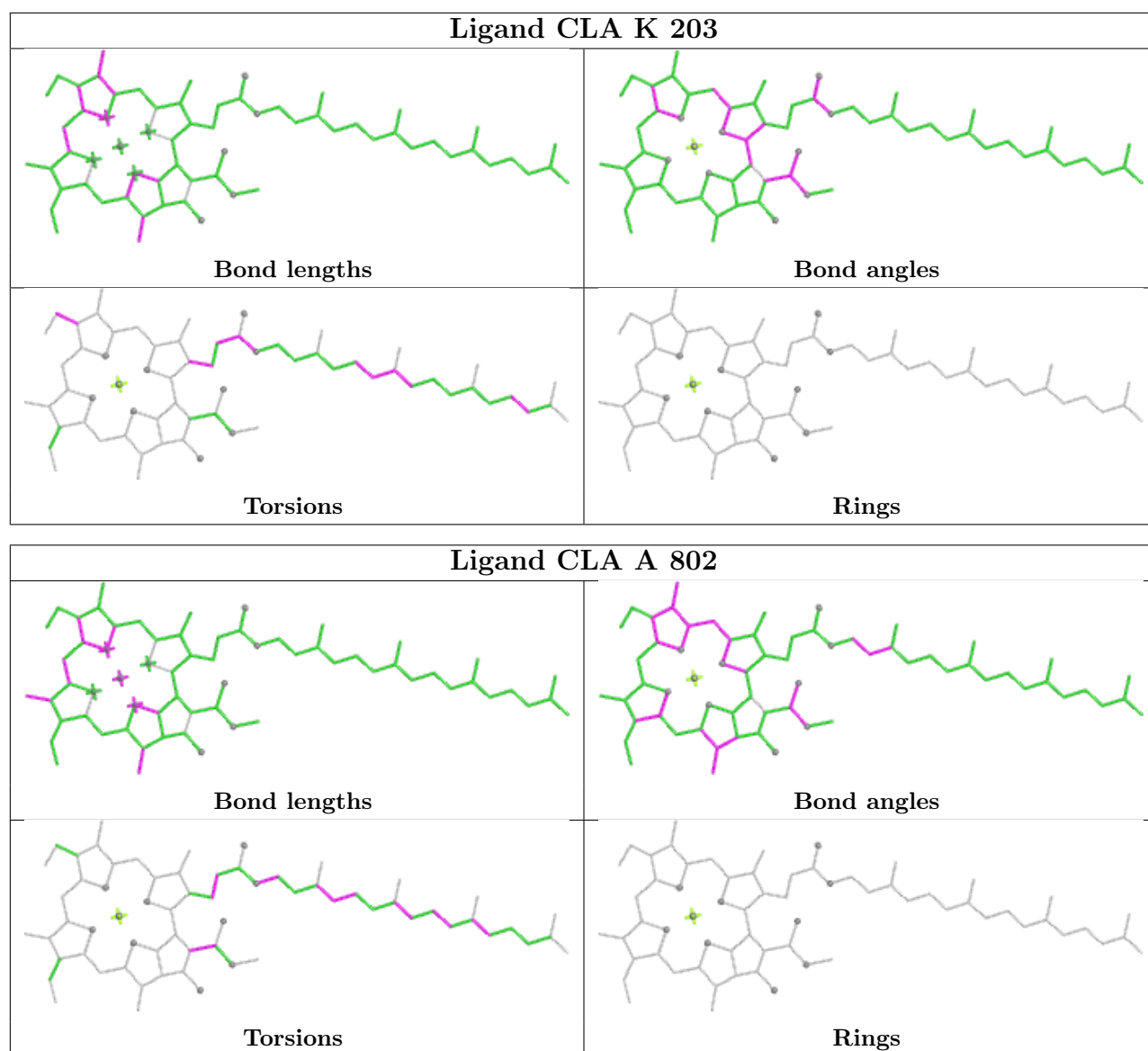


Ligand CLA 1 609

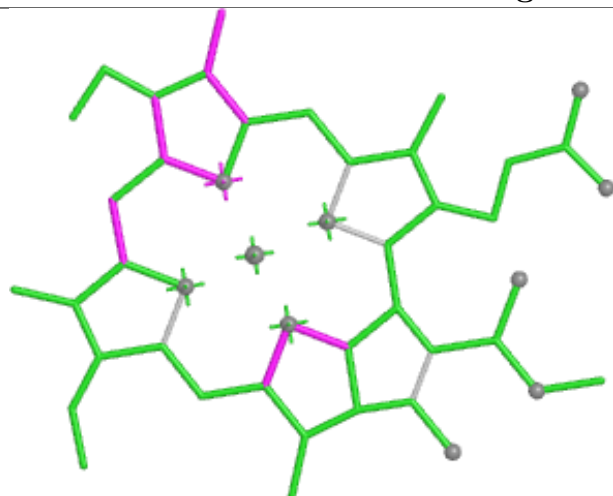




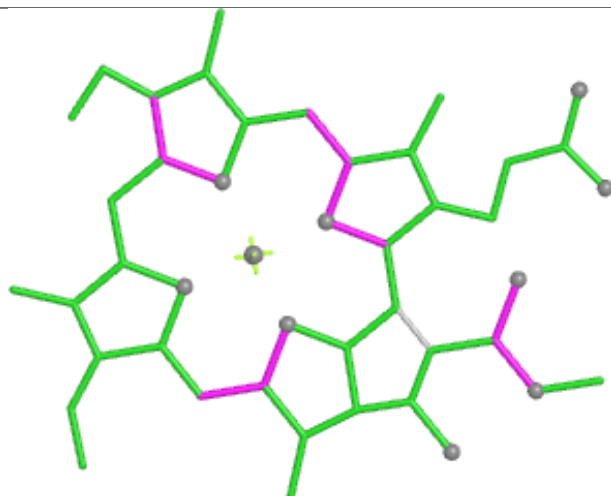




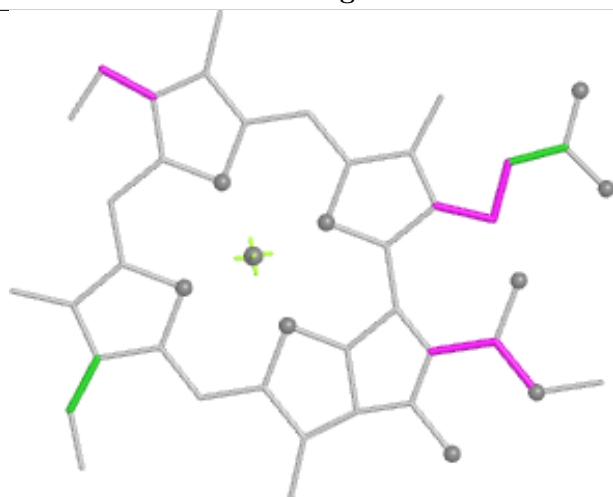
Ligand CLA L 303



Bond lengths



Bond angles

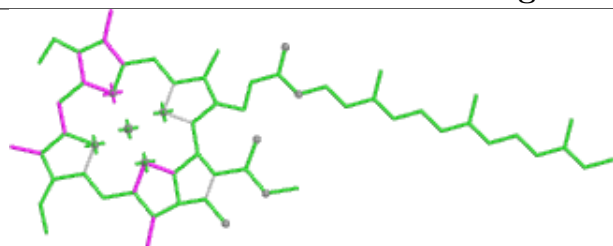


Torsions

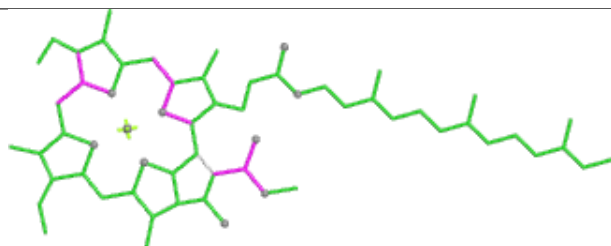


Rings

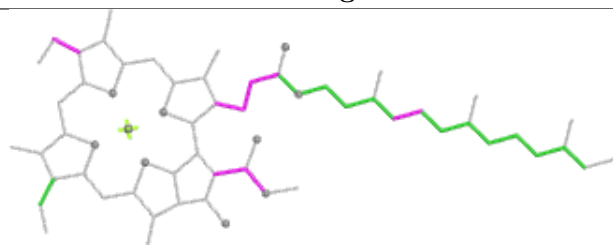
Ligand CLA 1 602



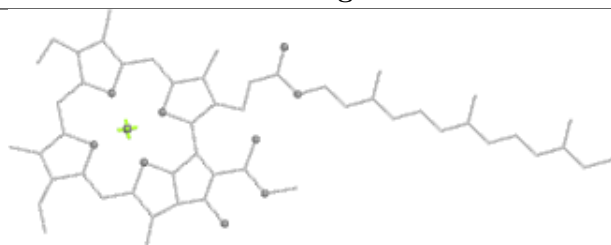
Bond lengths



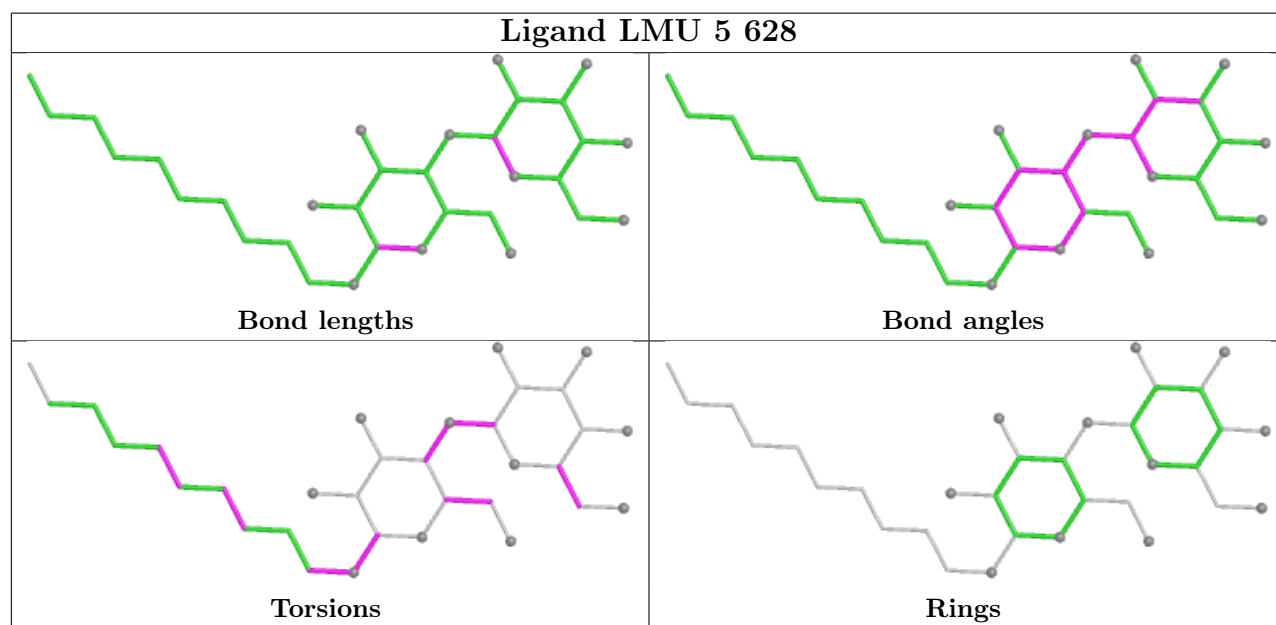
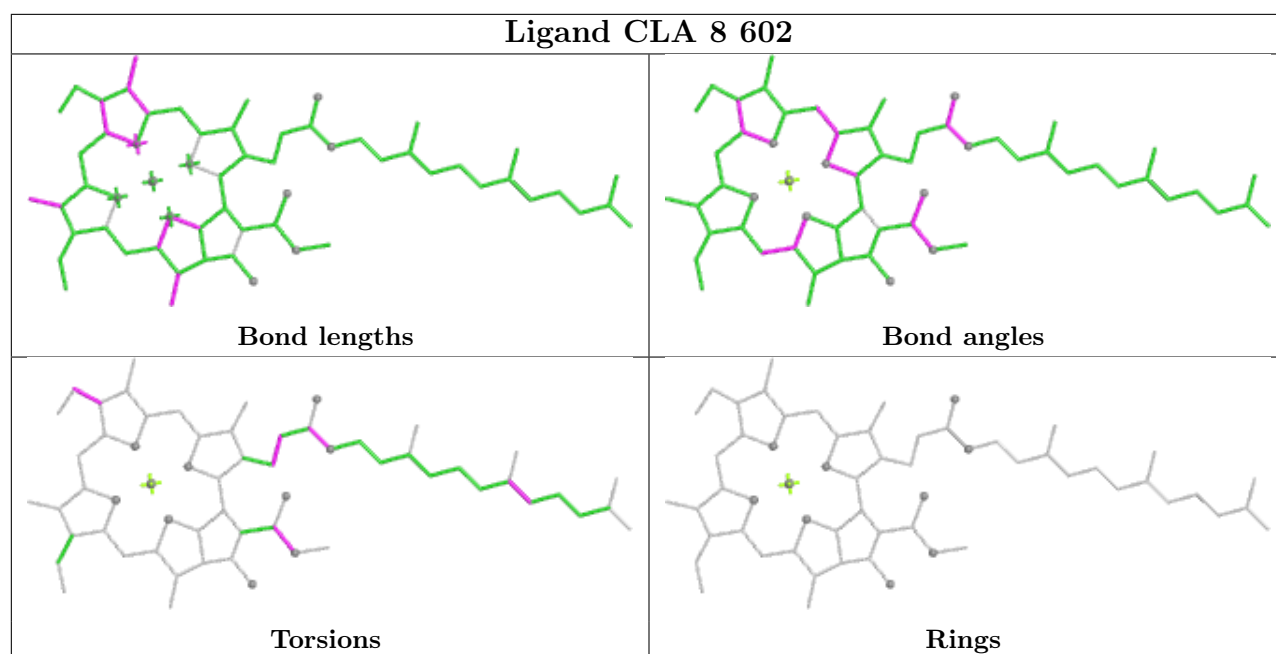
Bond angles

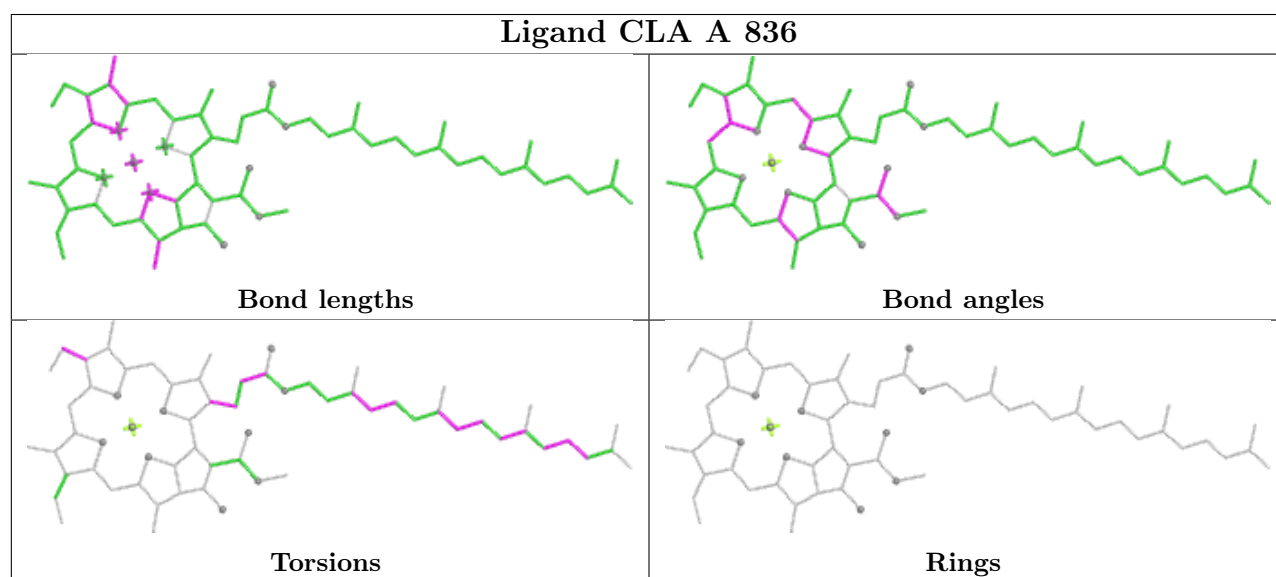
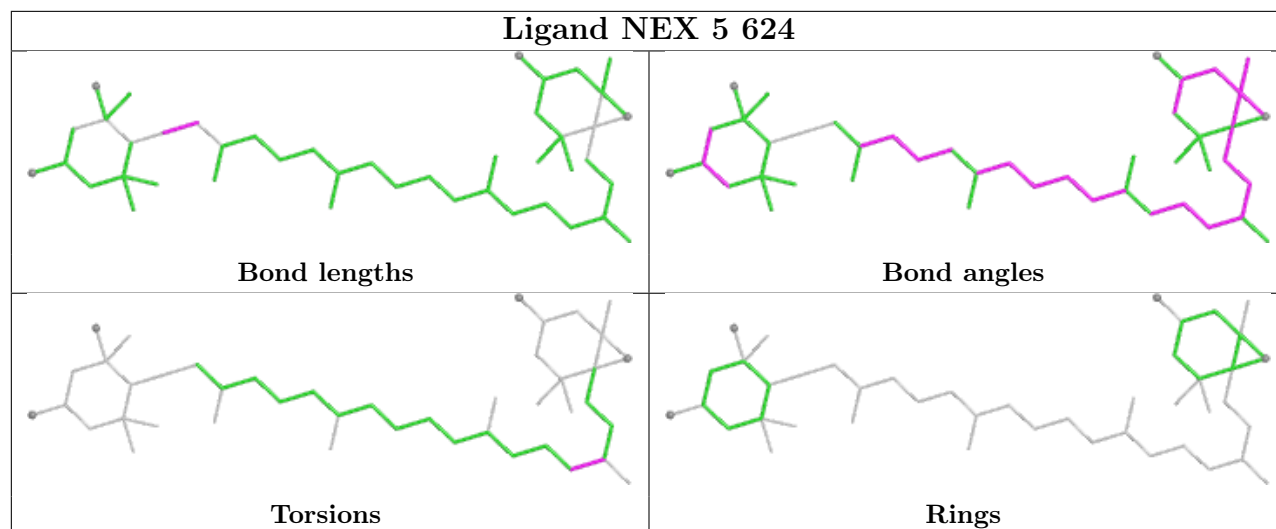


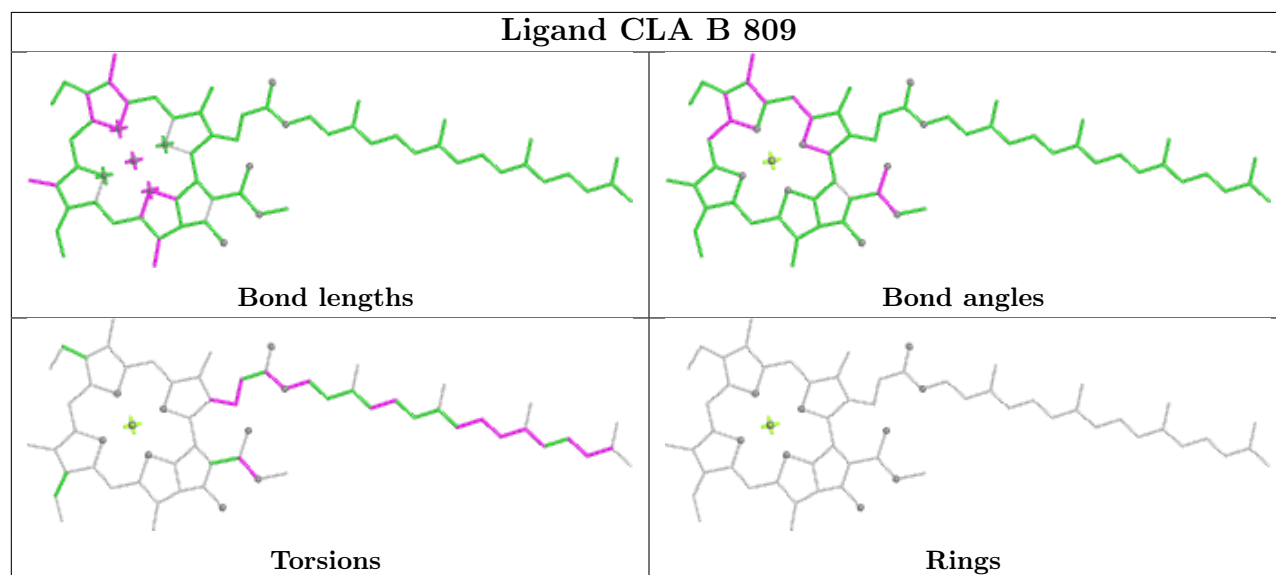
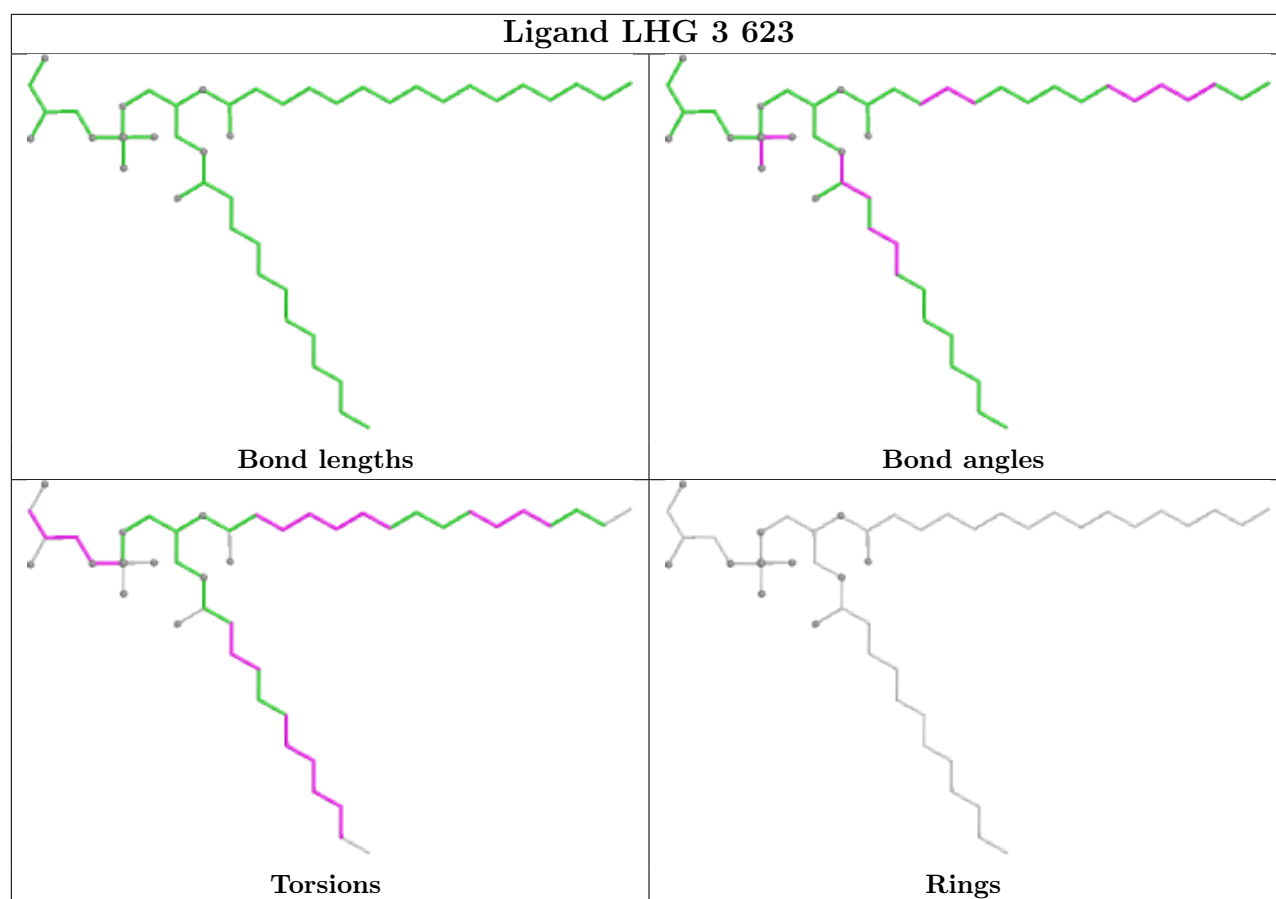
Torsions



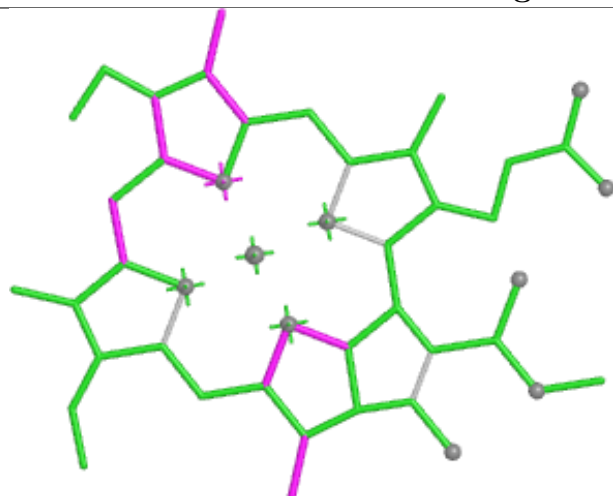
Rings



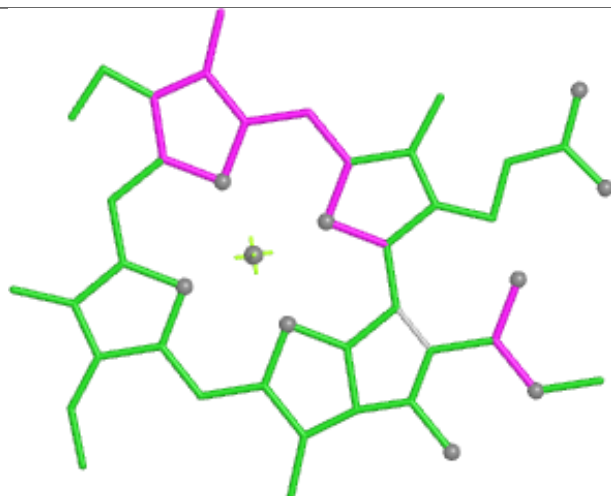




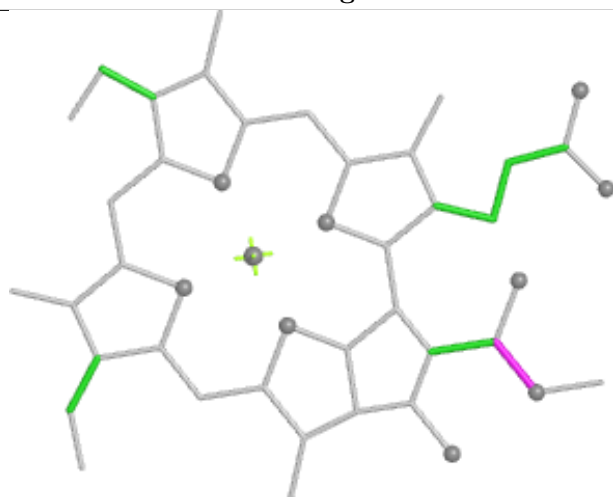
Ligand CLA A 833



Bond lengths



Bond angles

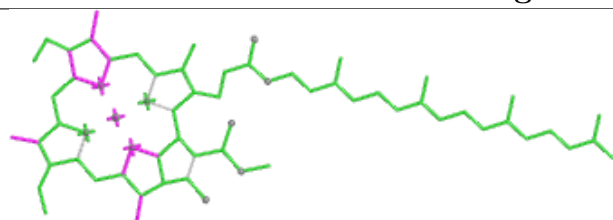


Torsions

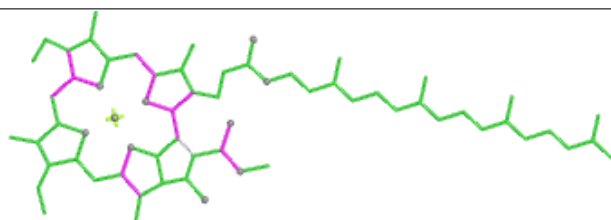


Rings

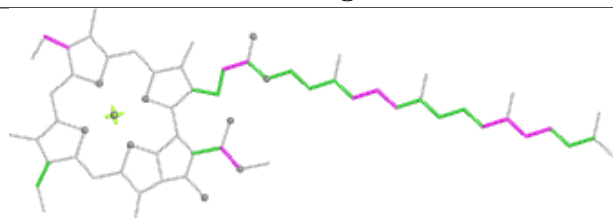
Ligand CLA B 806



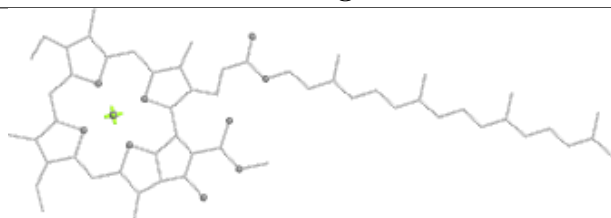
Bond lengths



Bond angles

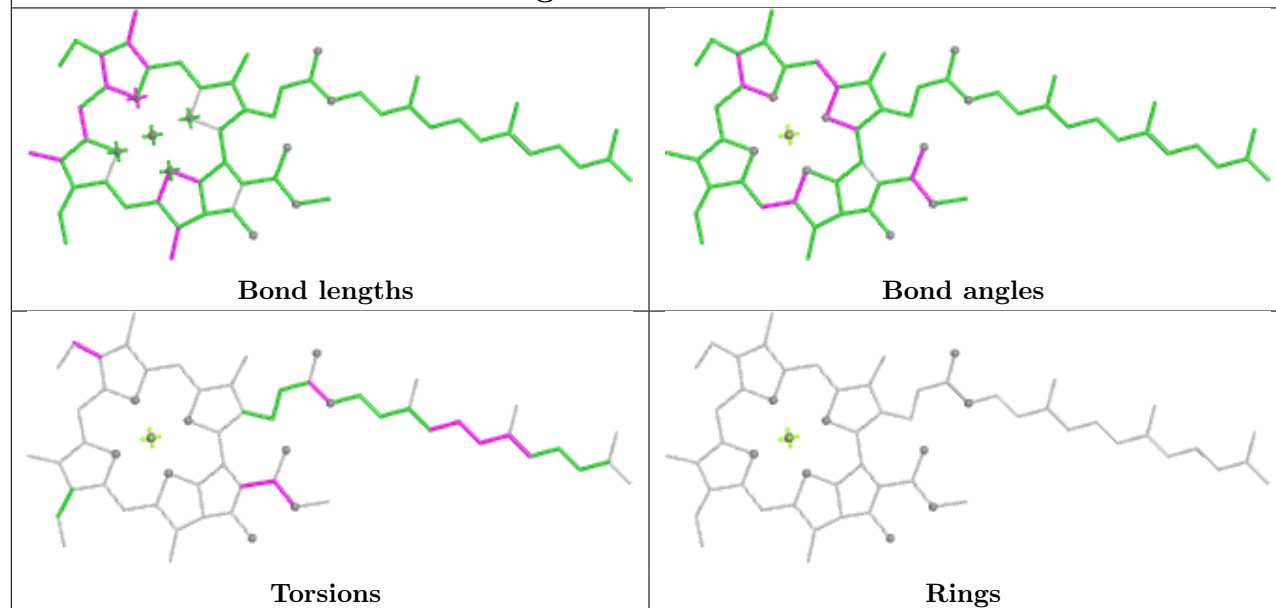


Torsions

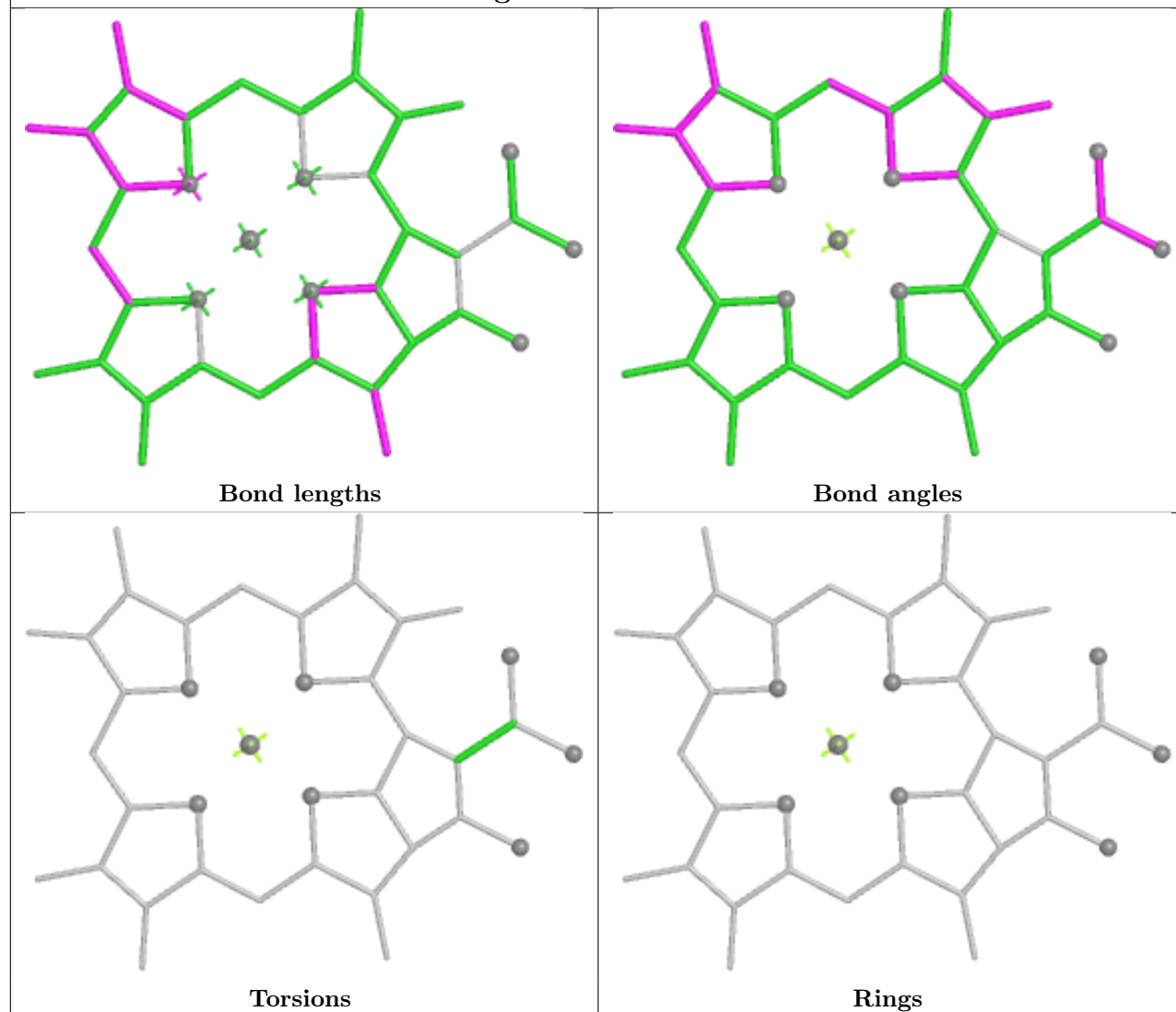


Rings

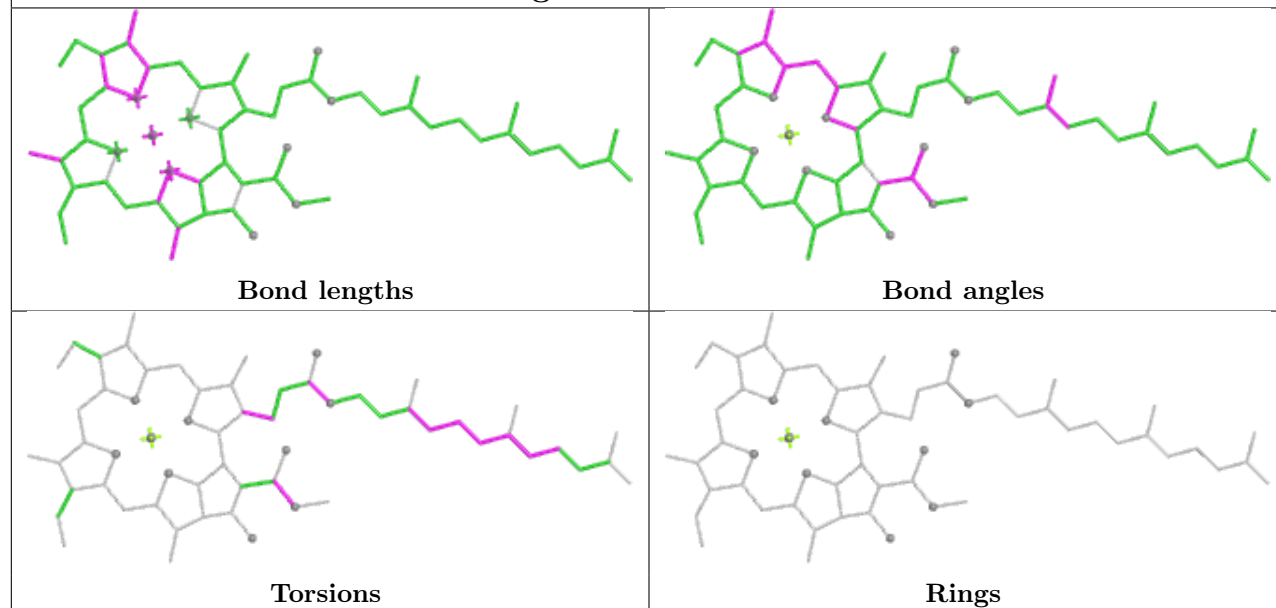
Ligand CLA 6 614



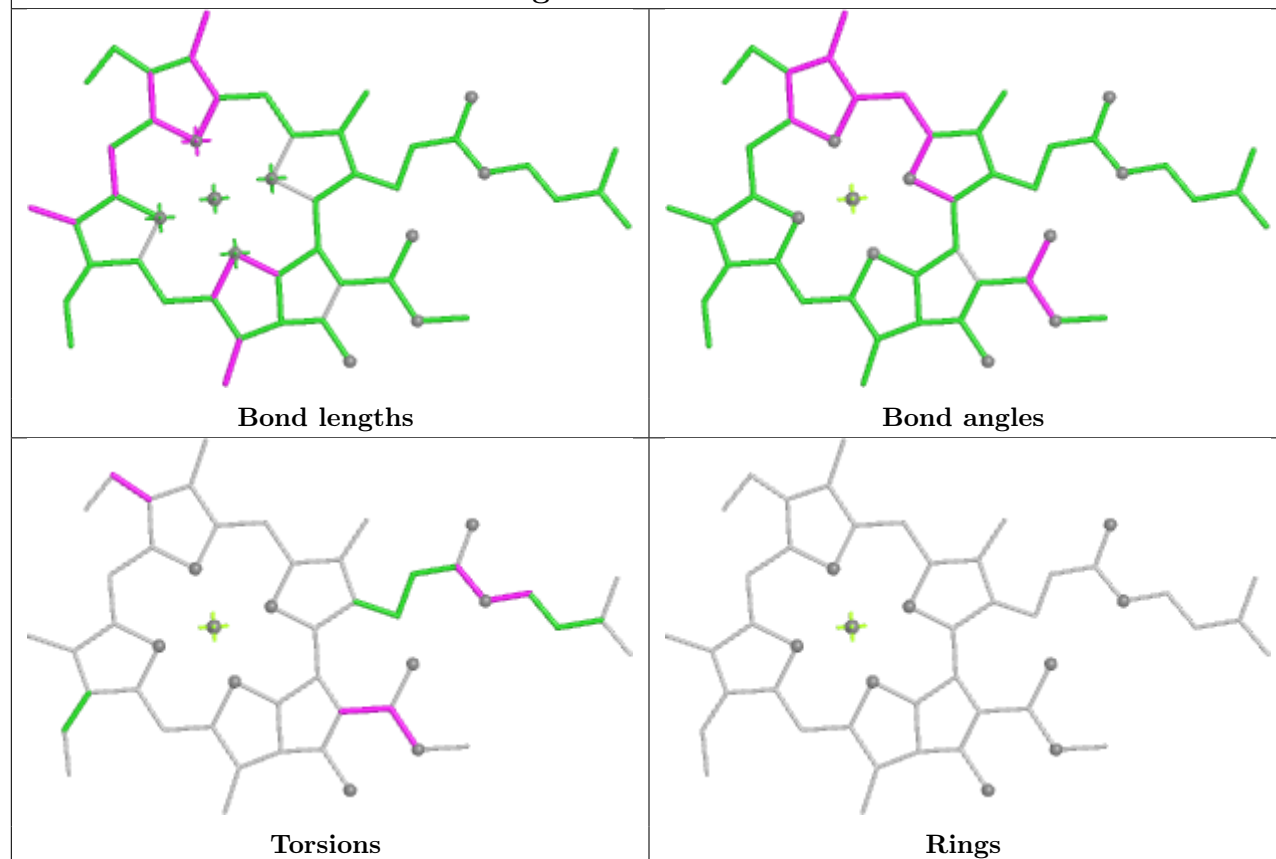
Ligand CLA a 611



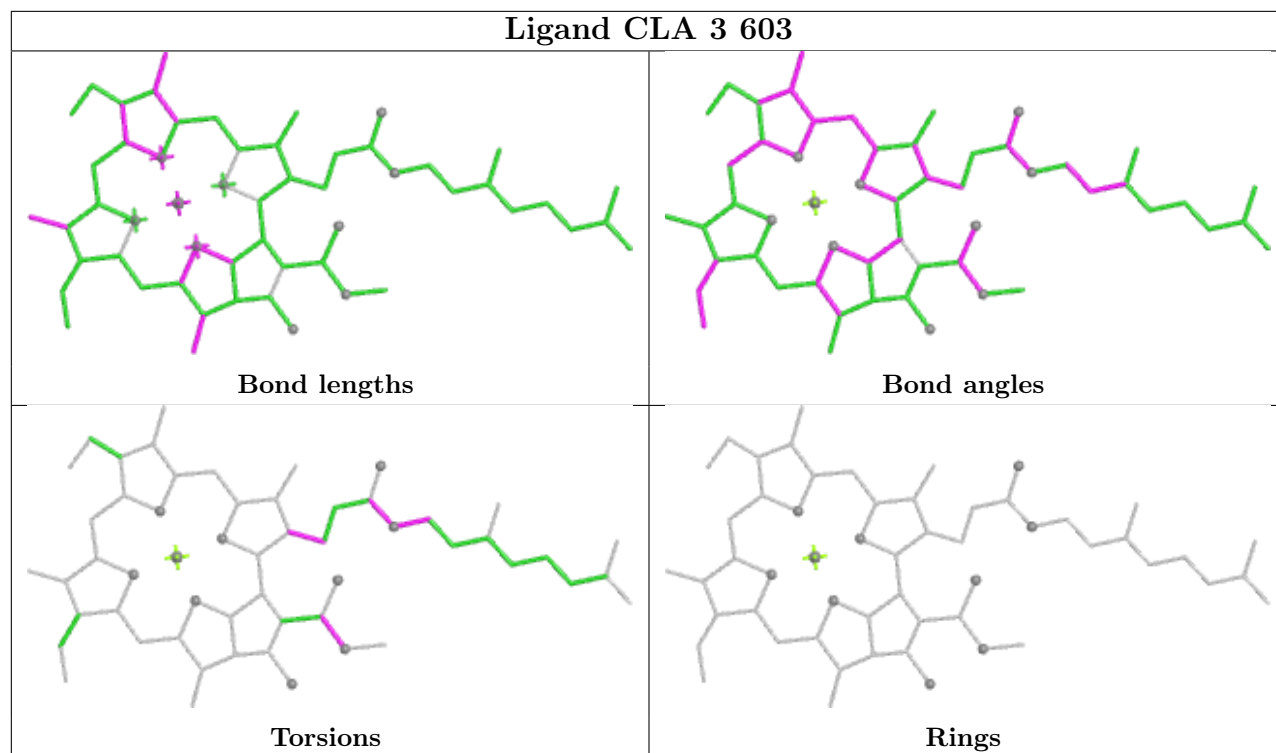
Ligand CLA B 818



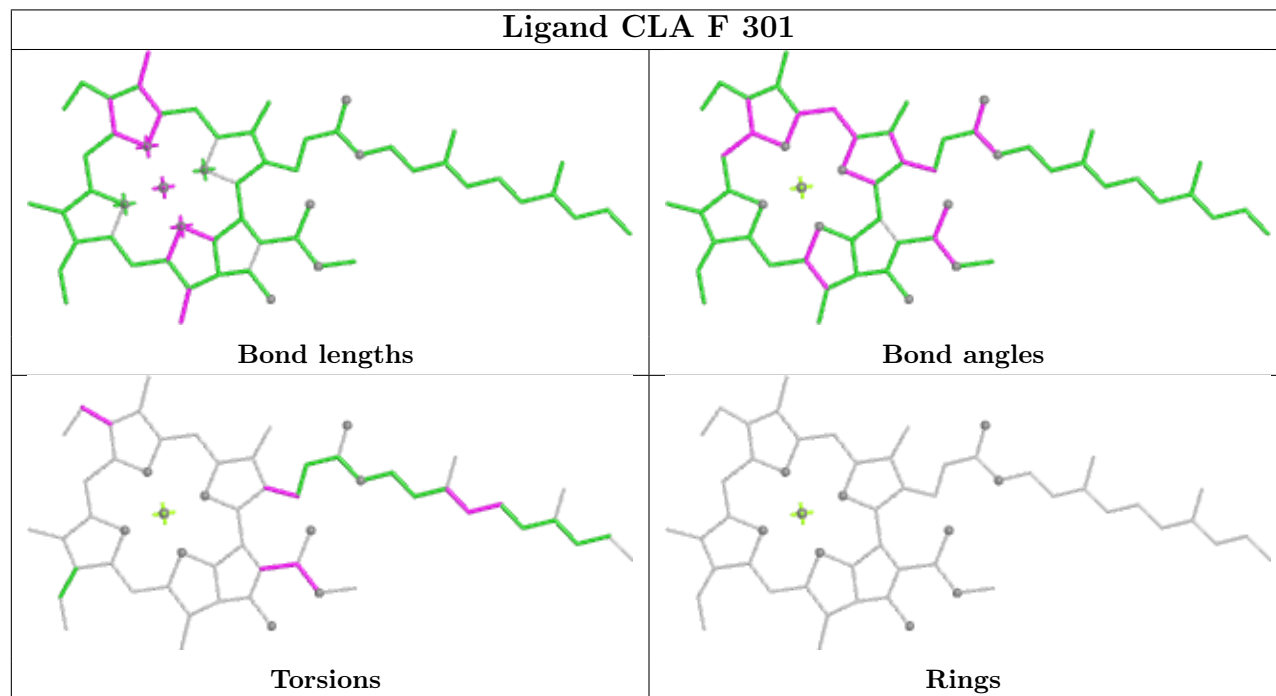
Ligand CLA B 836



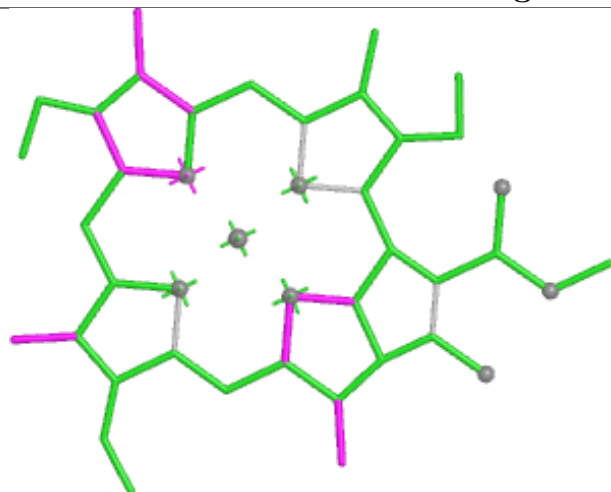
Ligand CLA 3 603



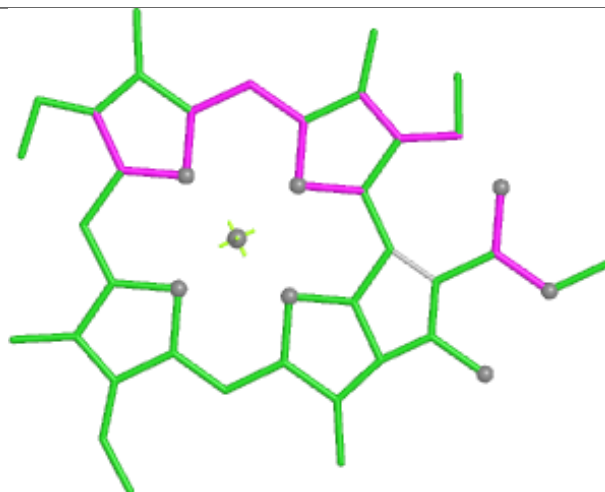
Ligand CLA F 301



Ligand CLA A 823



Bond lengths



Bond angles

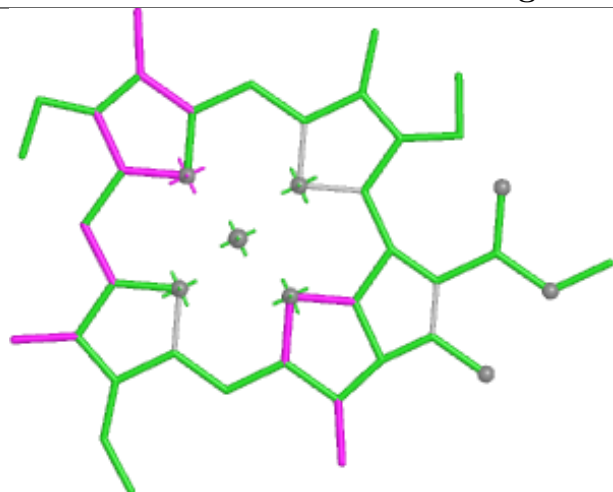


Torsions

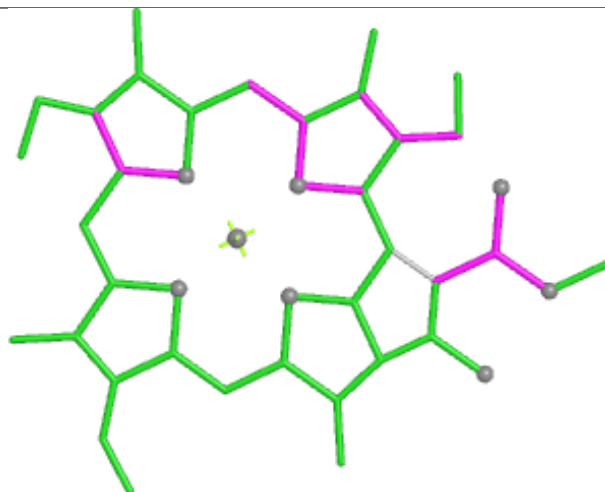


Rings

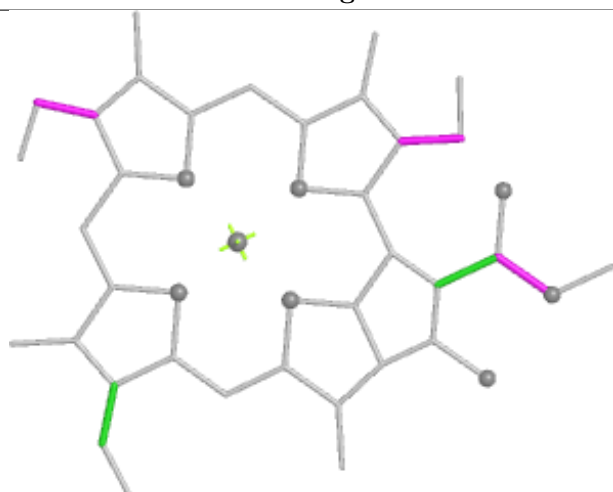
Ligand CLA 4 611



Bond lengths



Bond angles

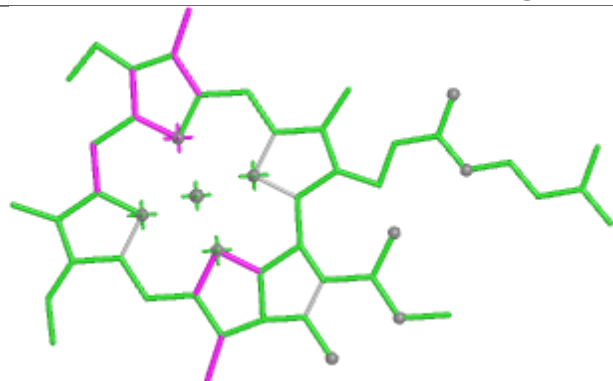


Torsions

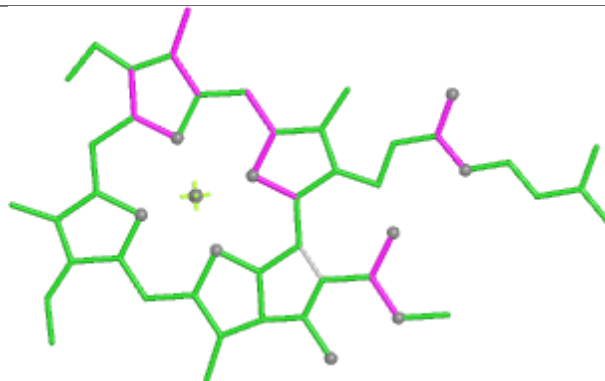


Rings

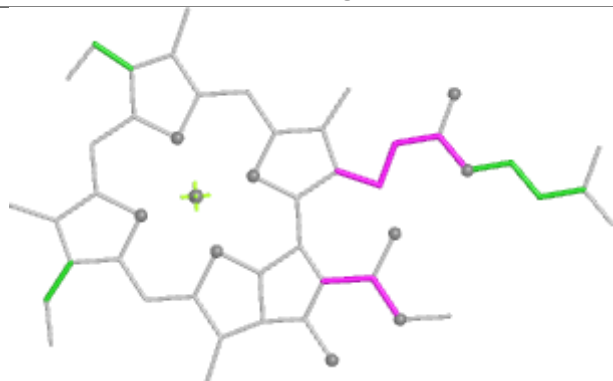
Ligand CLA 8 604



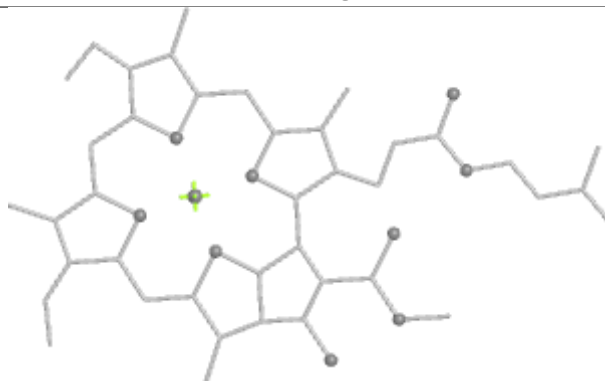
Bond lengths



Bond angles

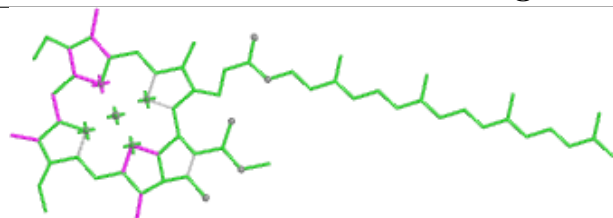


Torsions

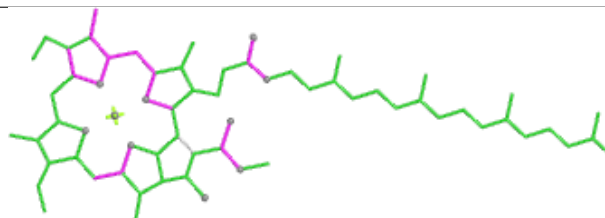


Rings

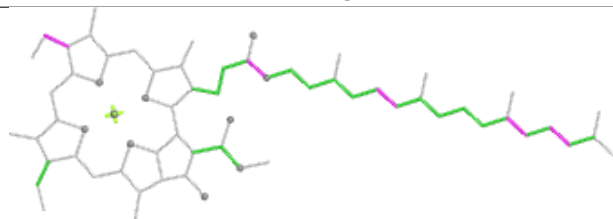
Ligand CLA B 837



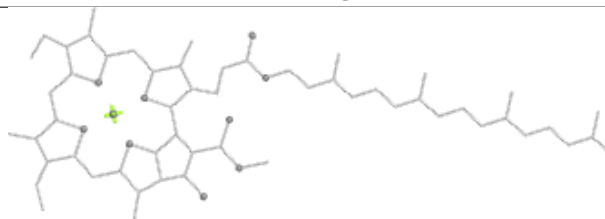
Bond lengths



Bond angles

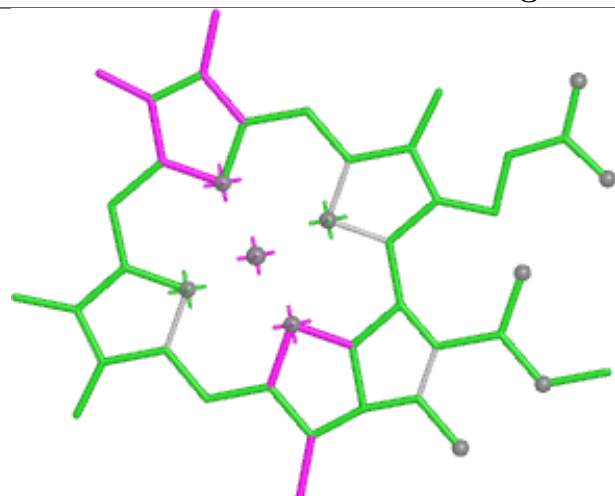


Torsions

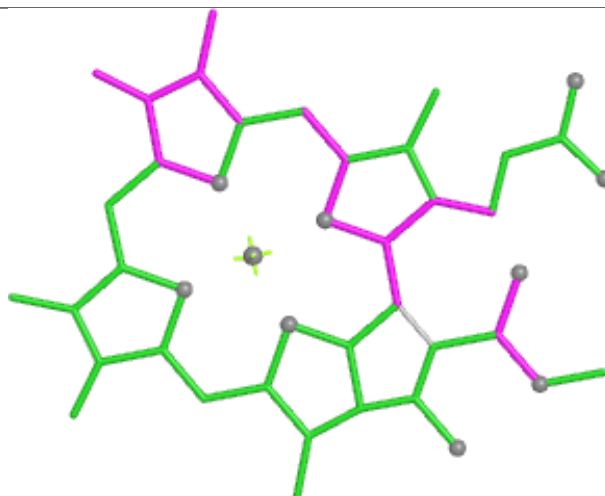


Rings

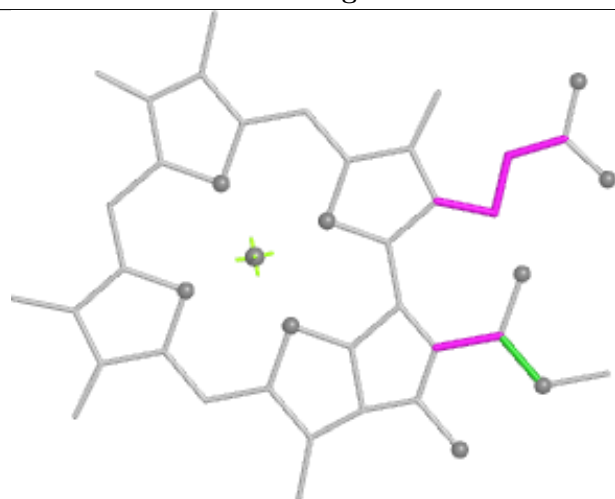
Ligand CLA 5 619



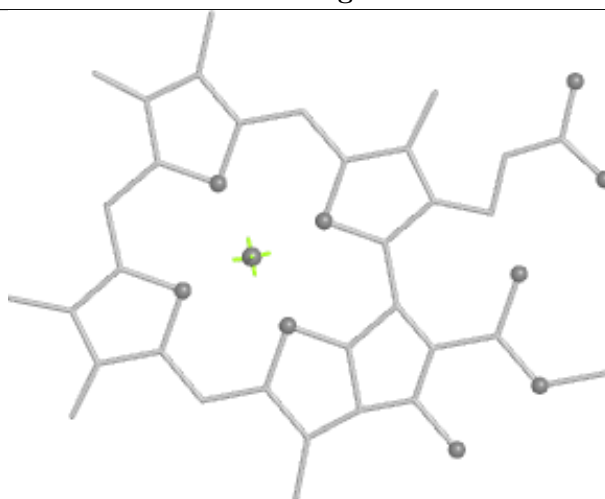
Bond lengths



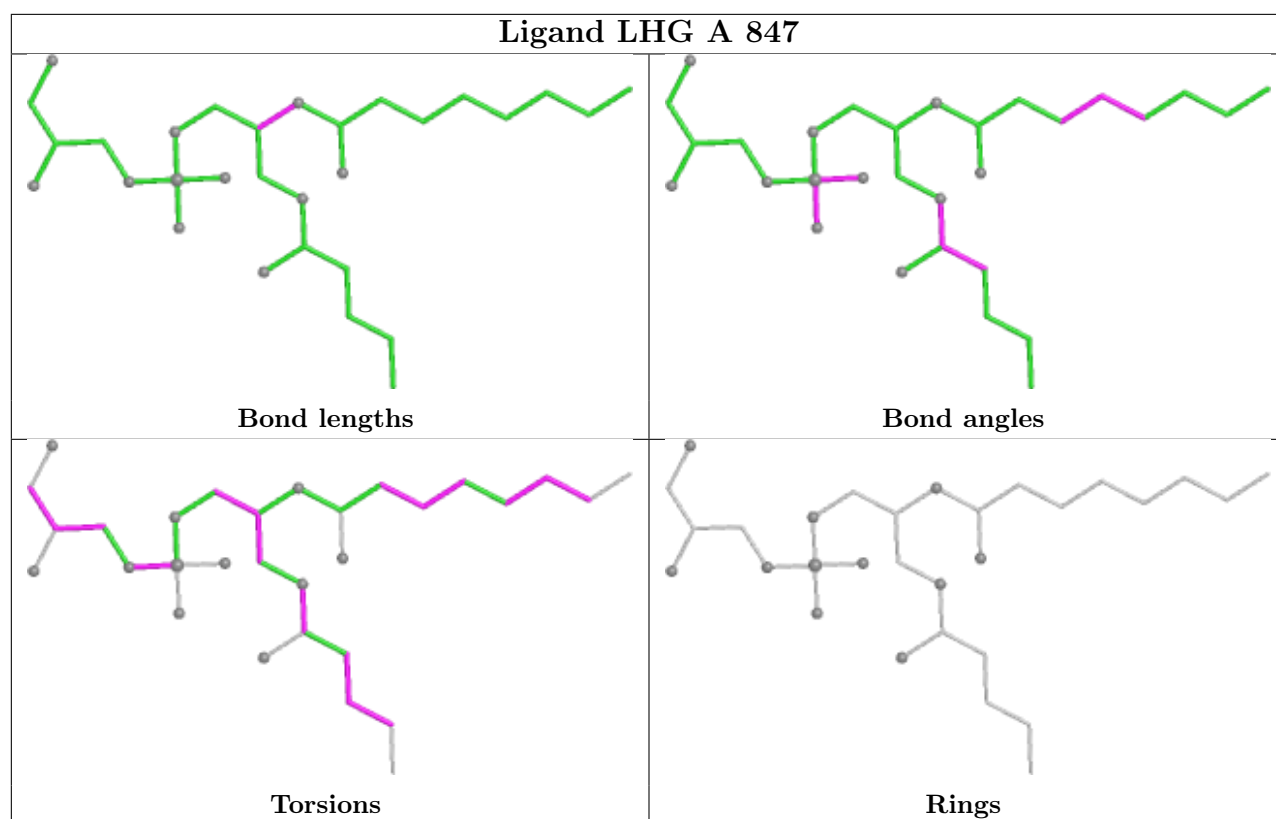
Bond angles



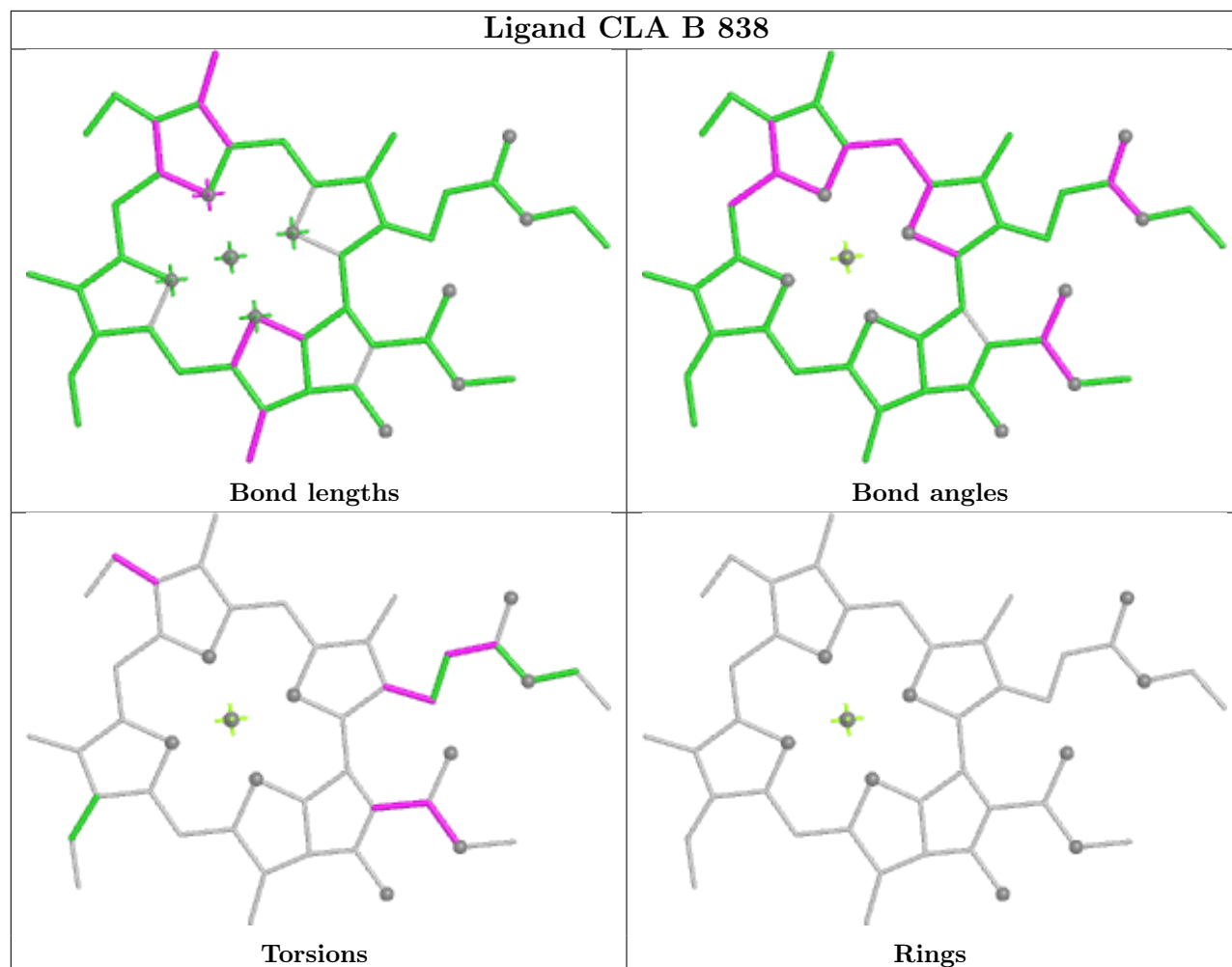
Torsions



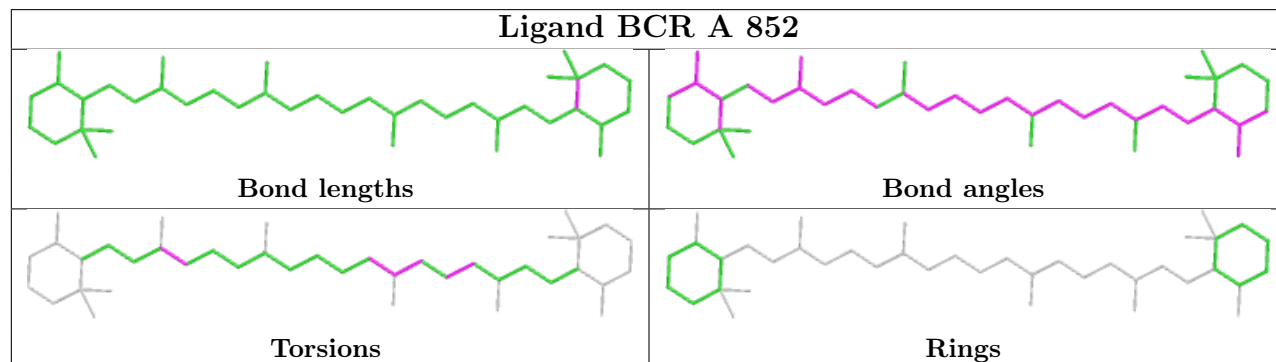
Rings

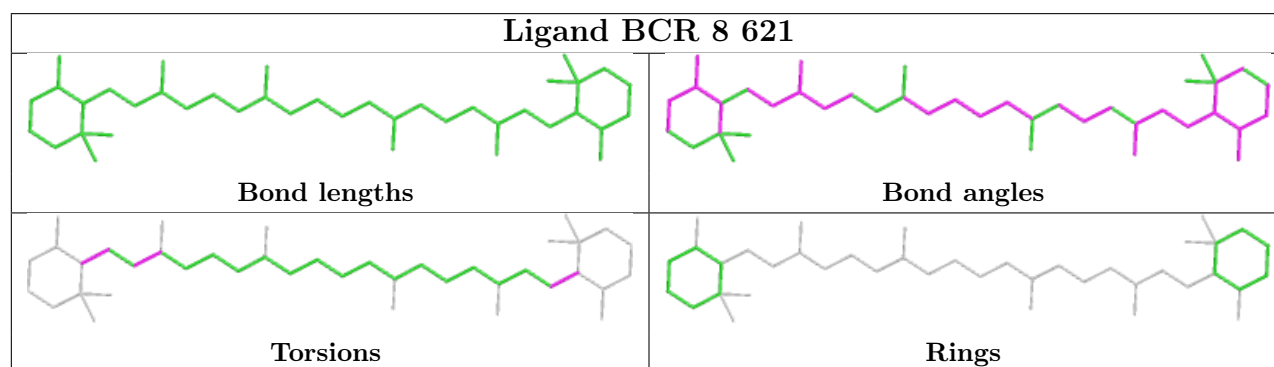
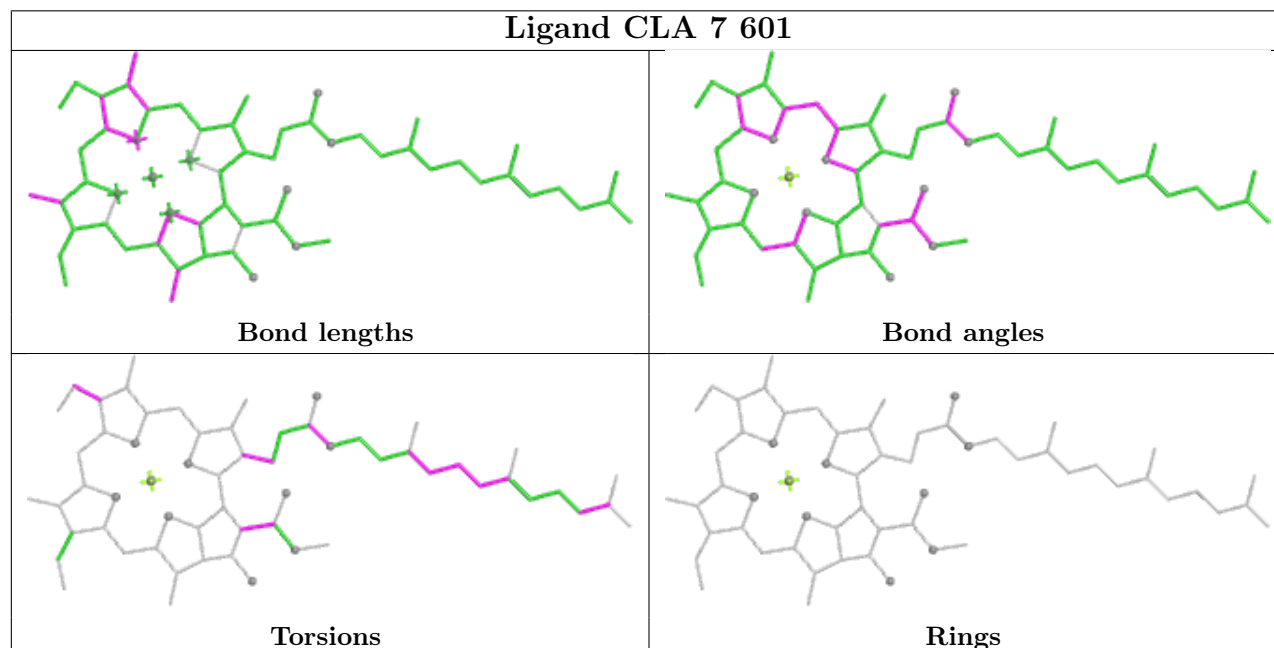
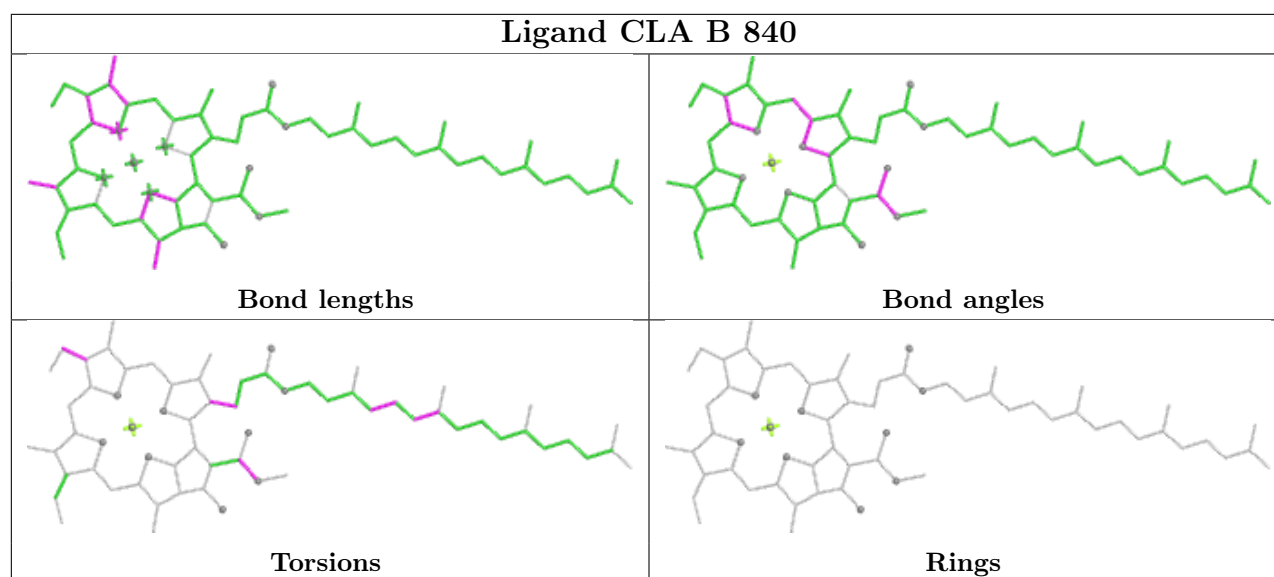


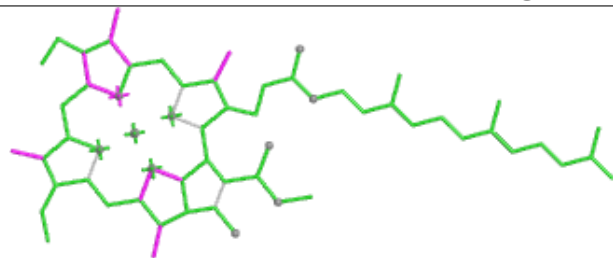
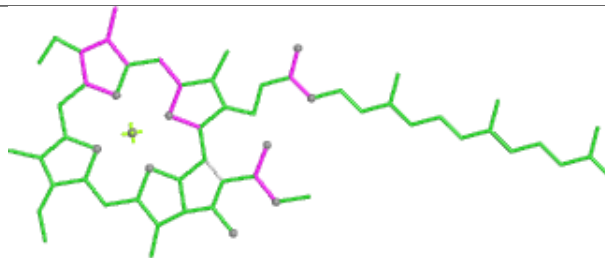
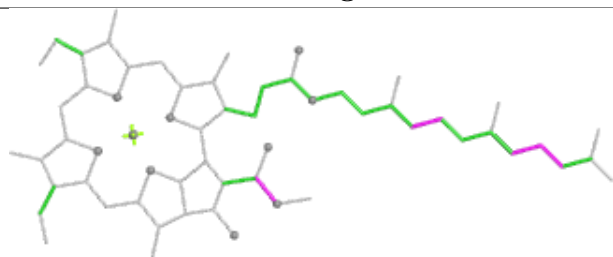
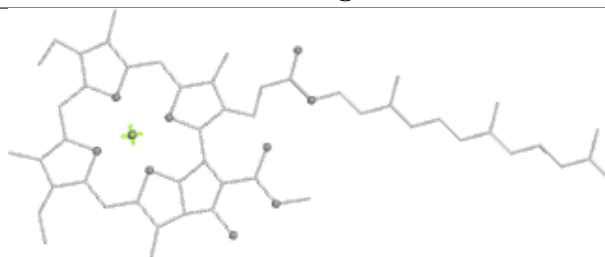
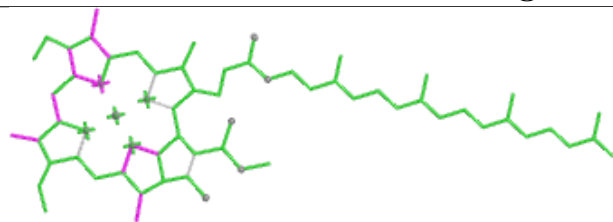
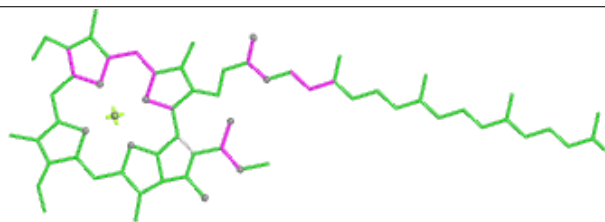
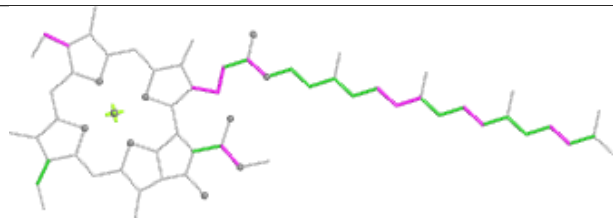
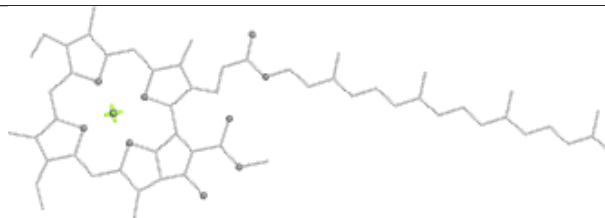
Ligand CLA B 838



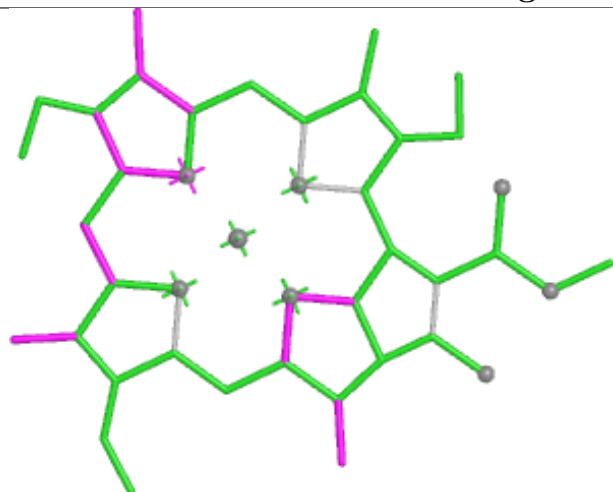
Ligand BCR A 852



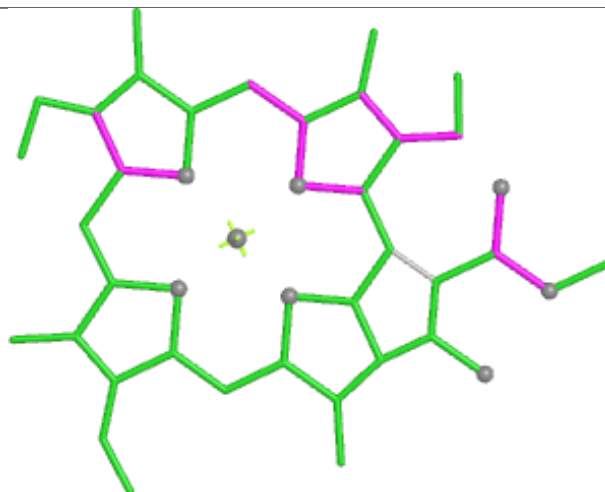


Ligand CLA 3 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 613****Bond lengths****Bond angles****Torsions****Rings**

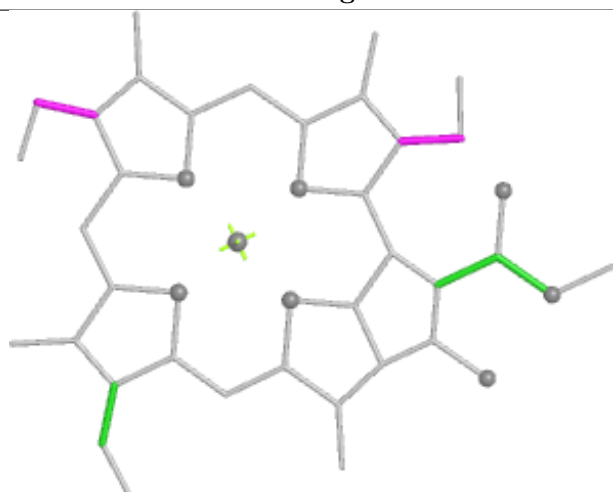
Ligand CLA 6 611



Bond lengths



Bond angles

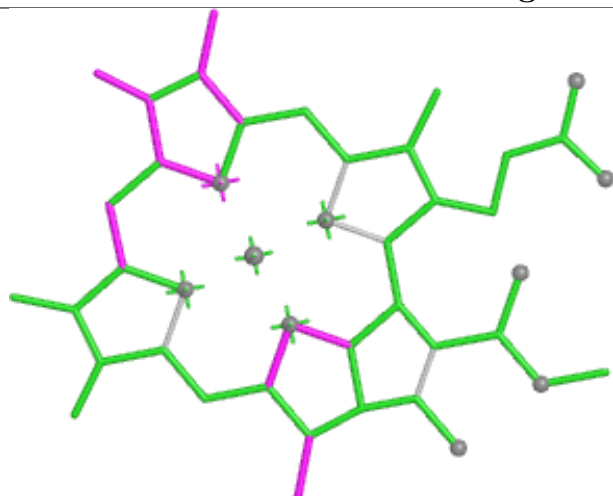


Torsions

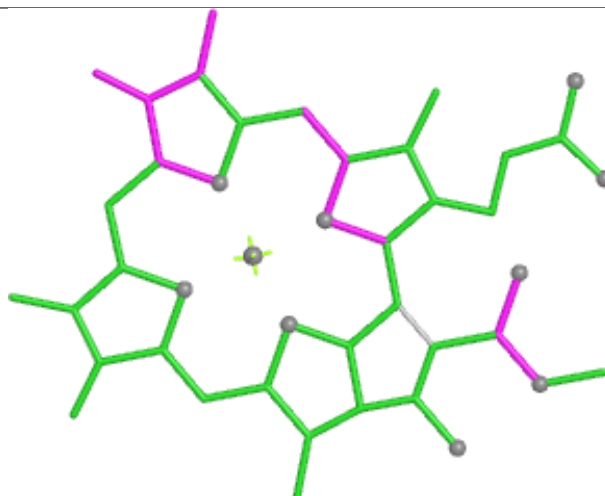


Rings

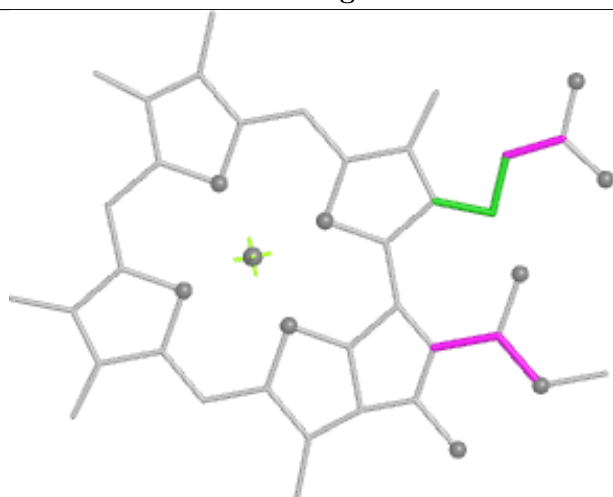
Ligand CLA 7 616



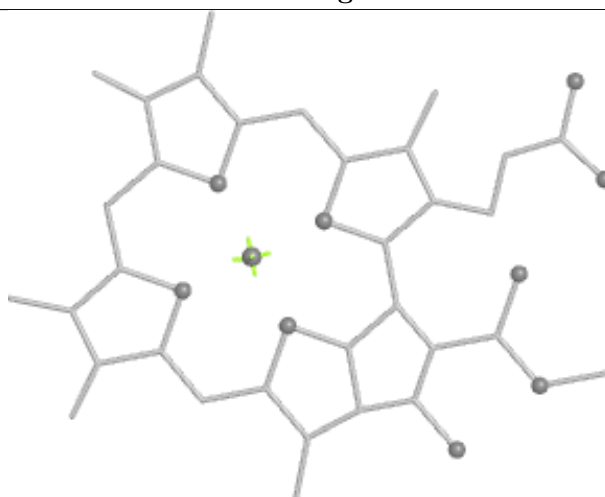
Bond lengths



Bond angles

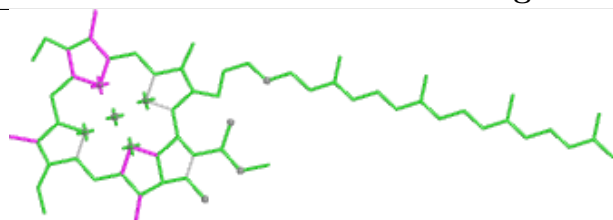


Torsions

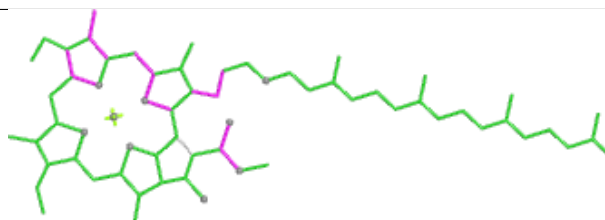


Rings

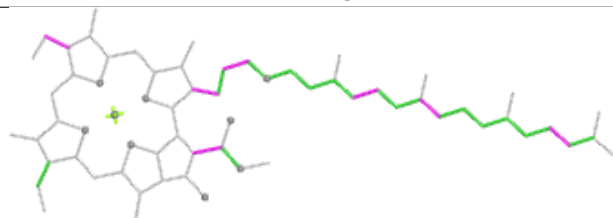
Ligand CLA A 828



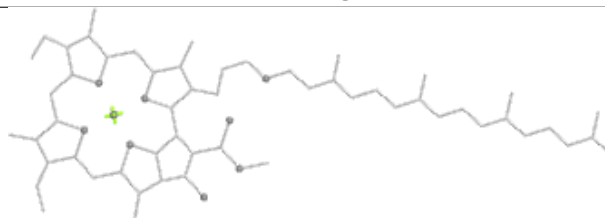
Bond lengths



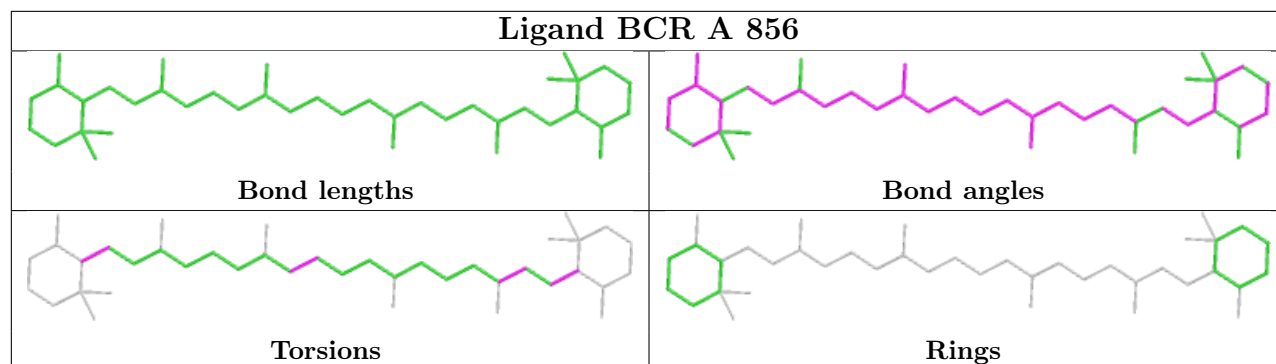
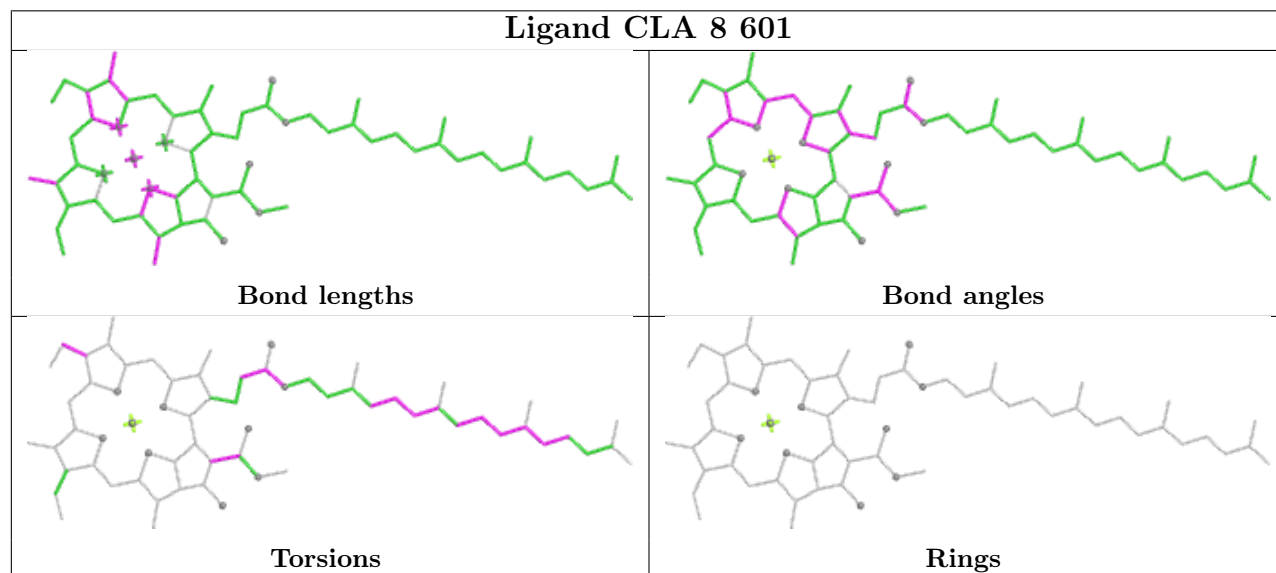
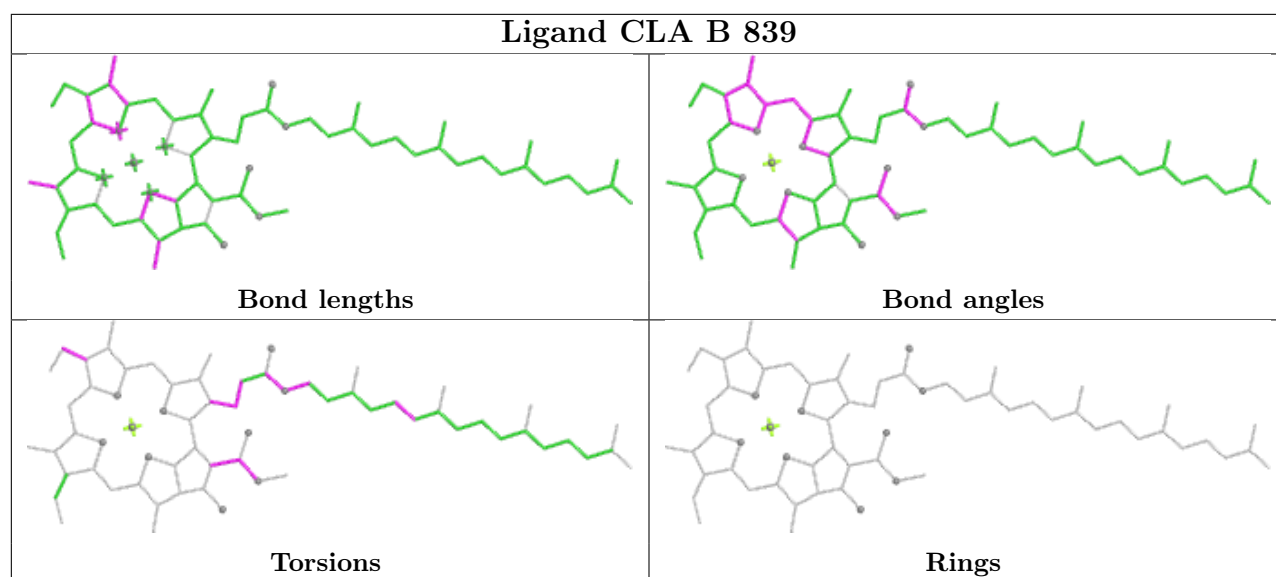
Bond angles

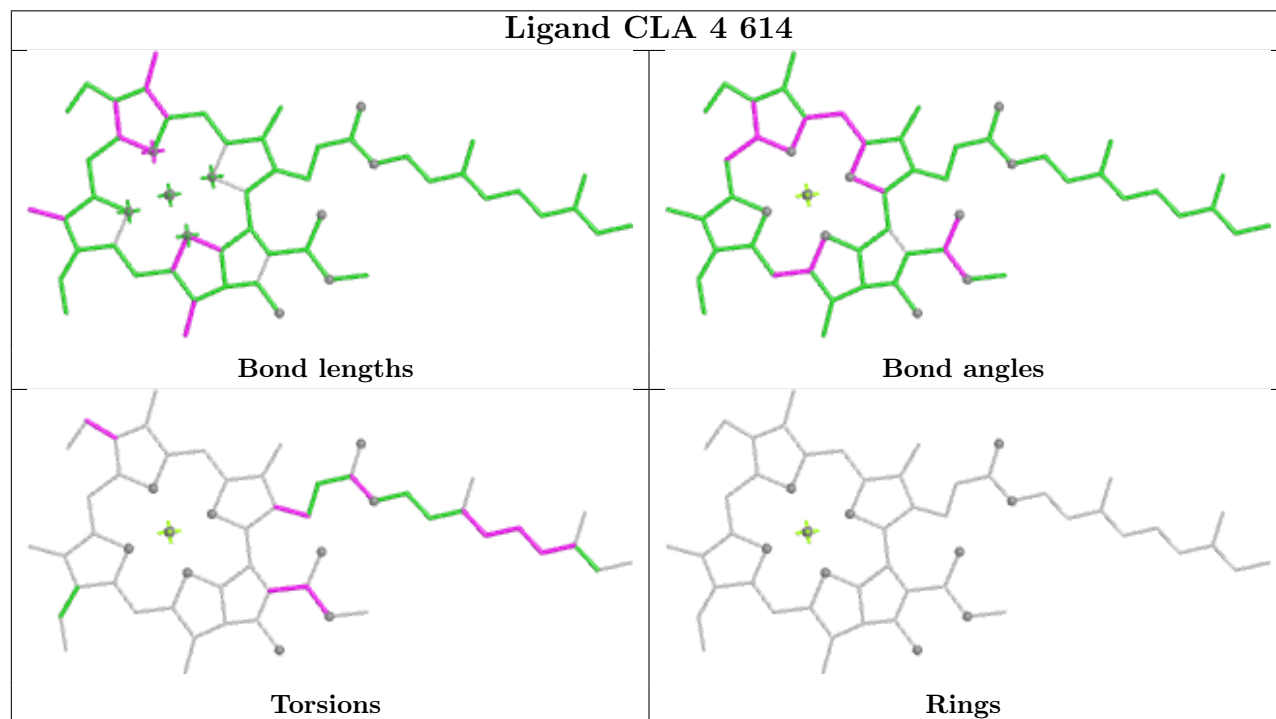
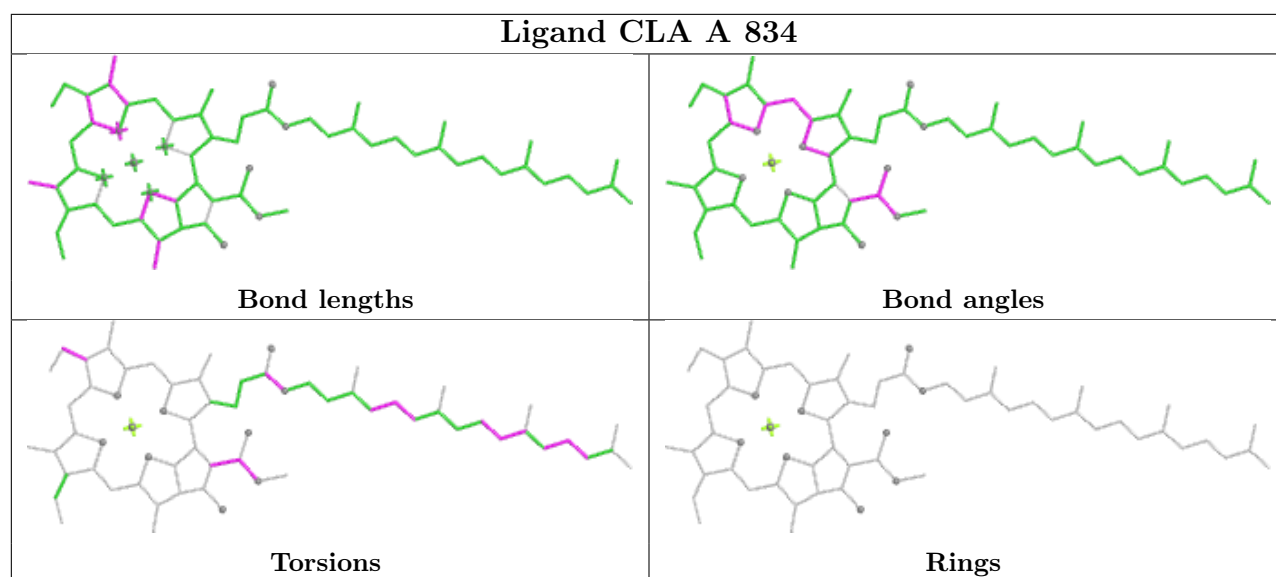


Torsions

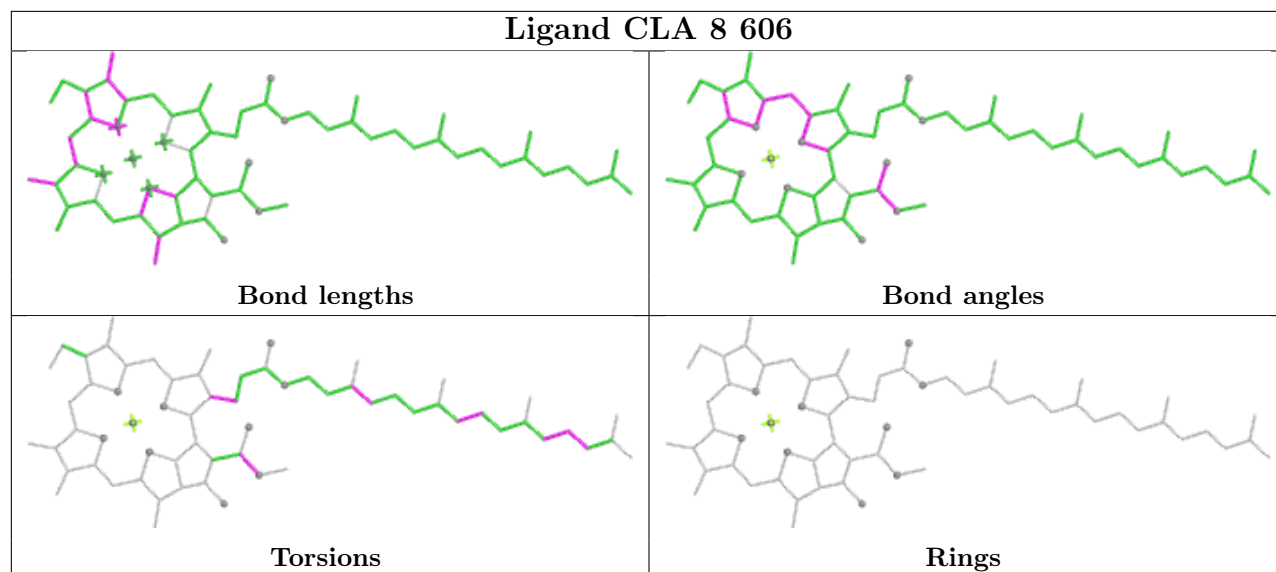


Rings

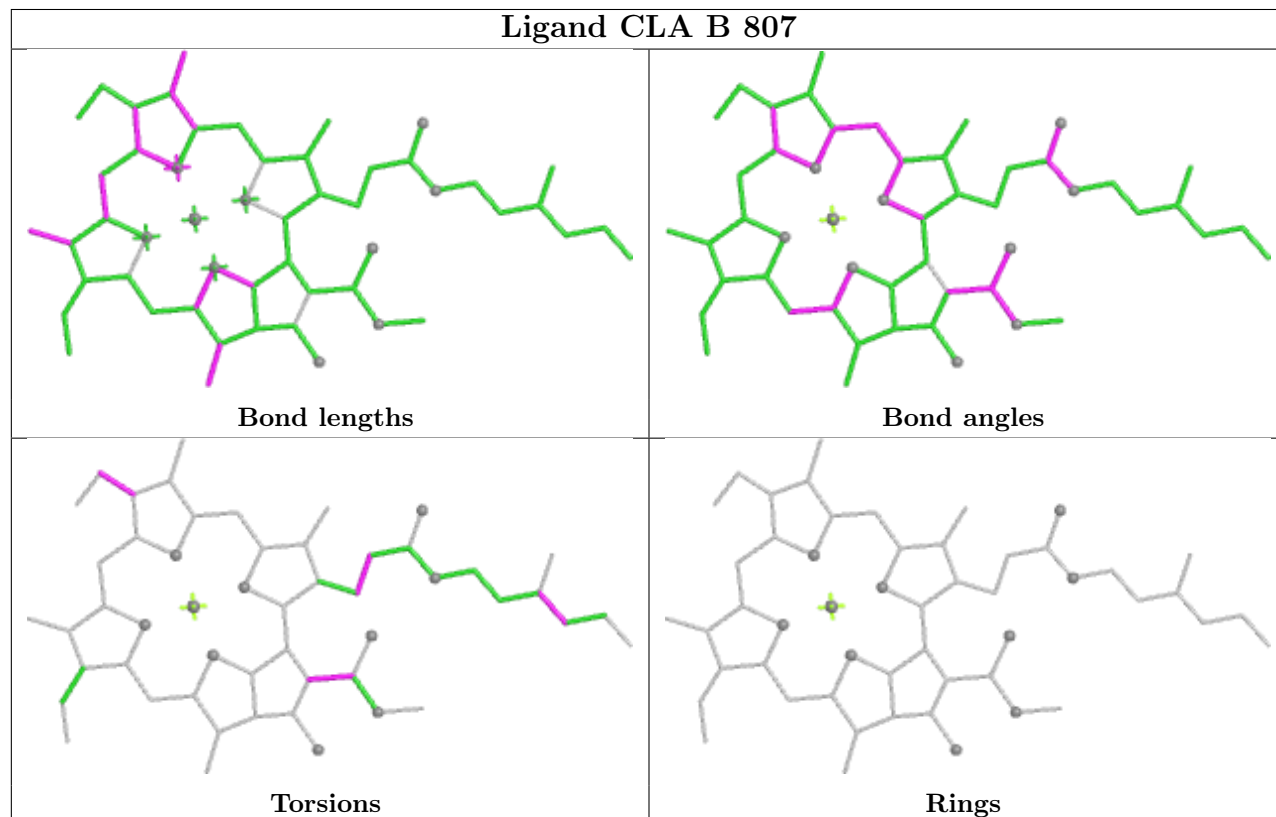


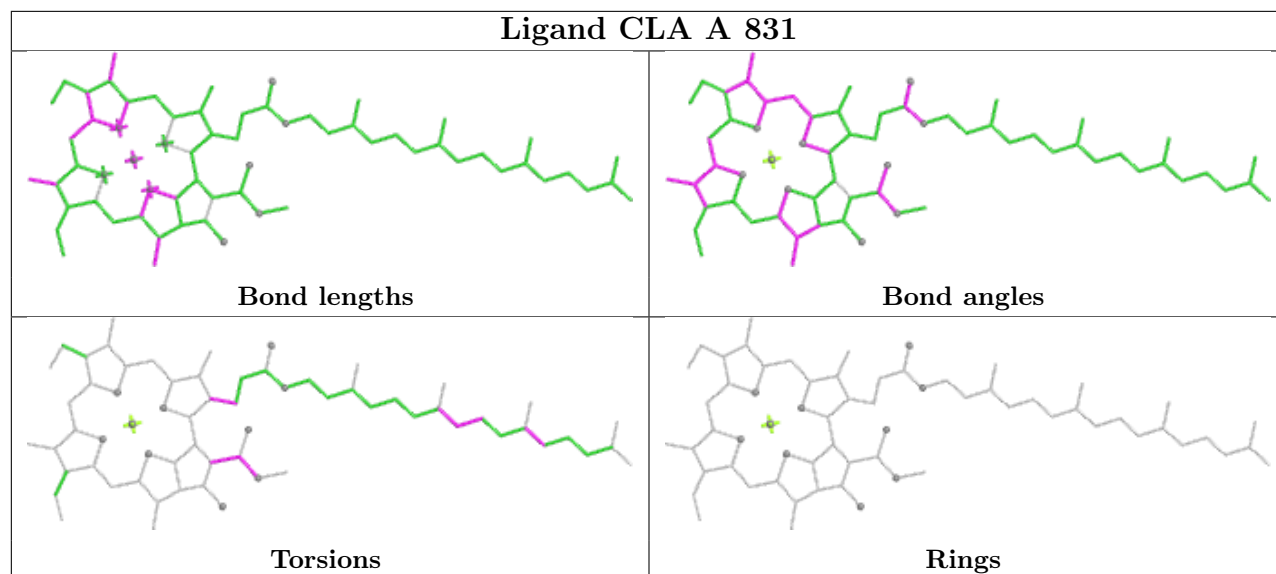
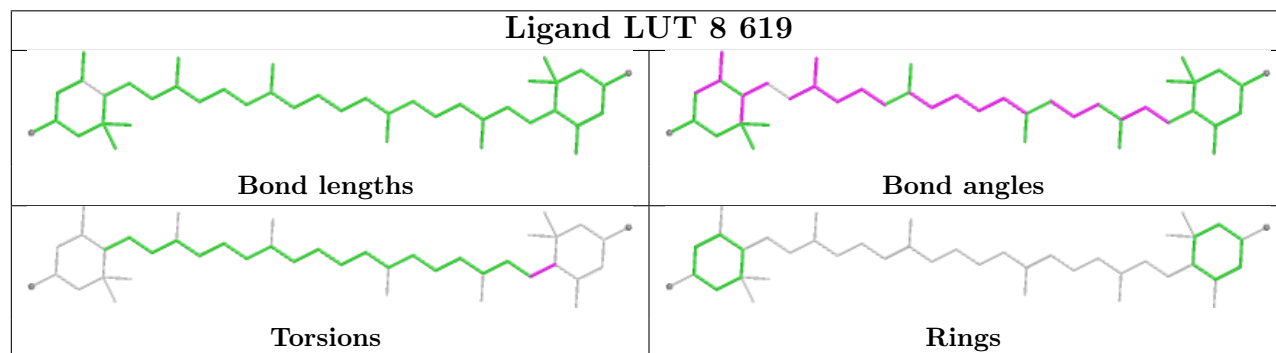
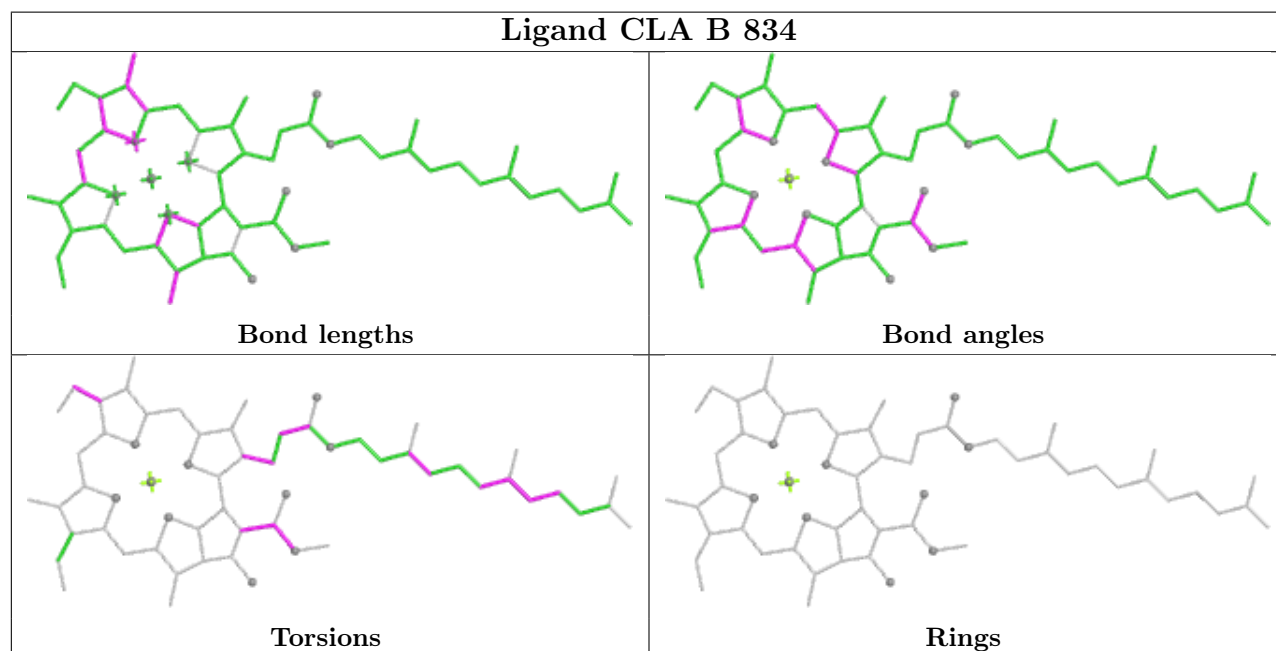


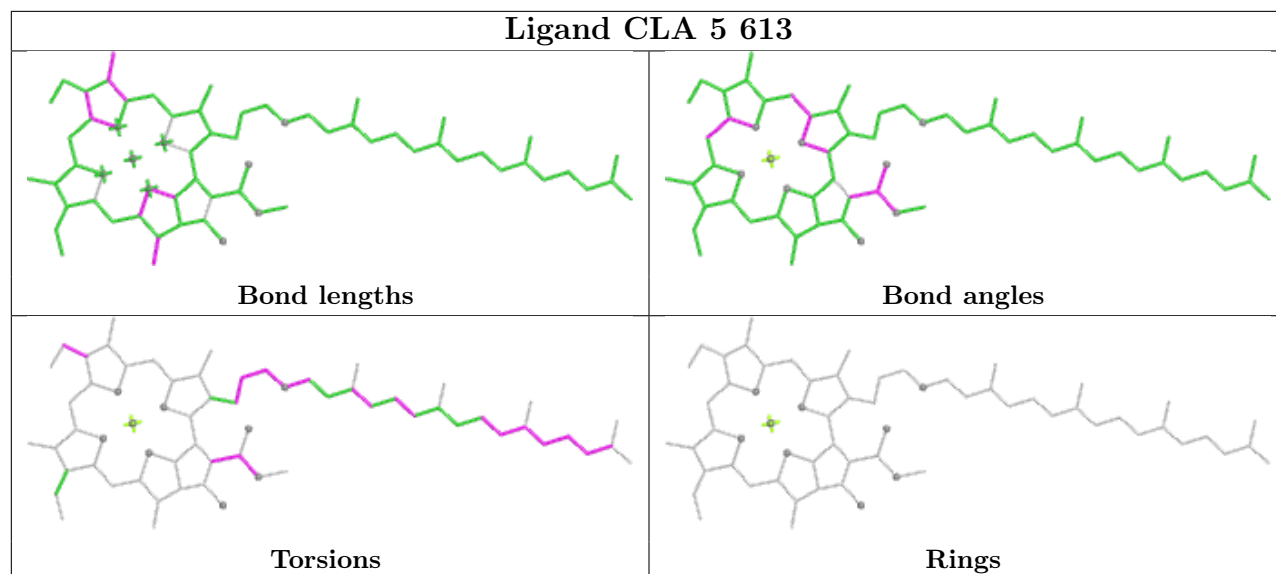
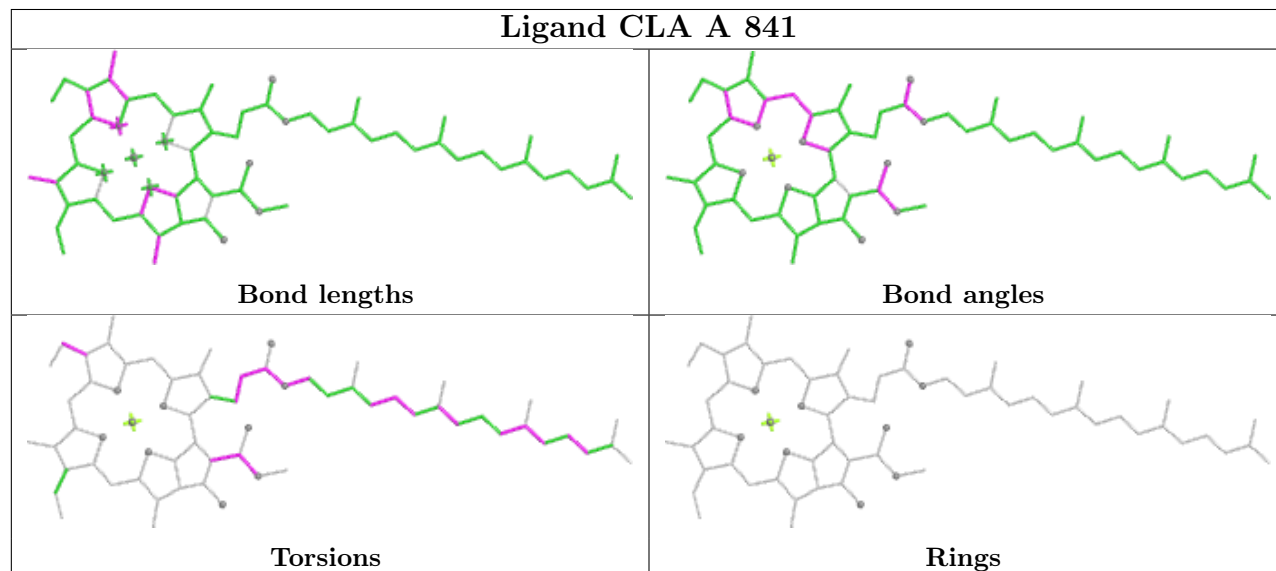
Ligand CLA 8 606



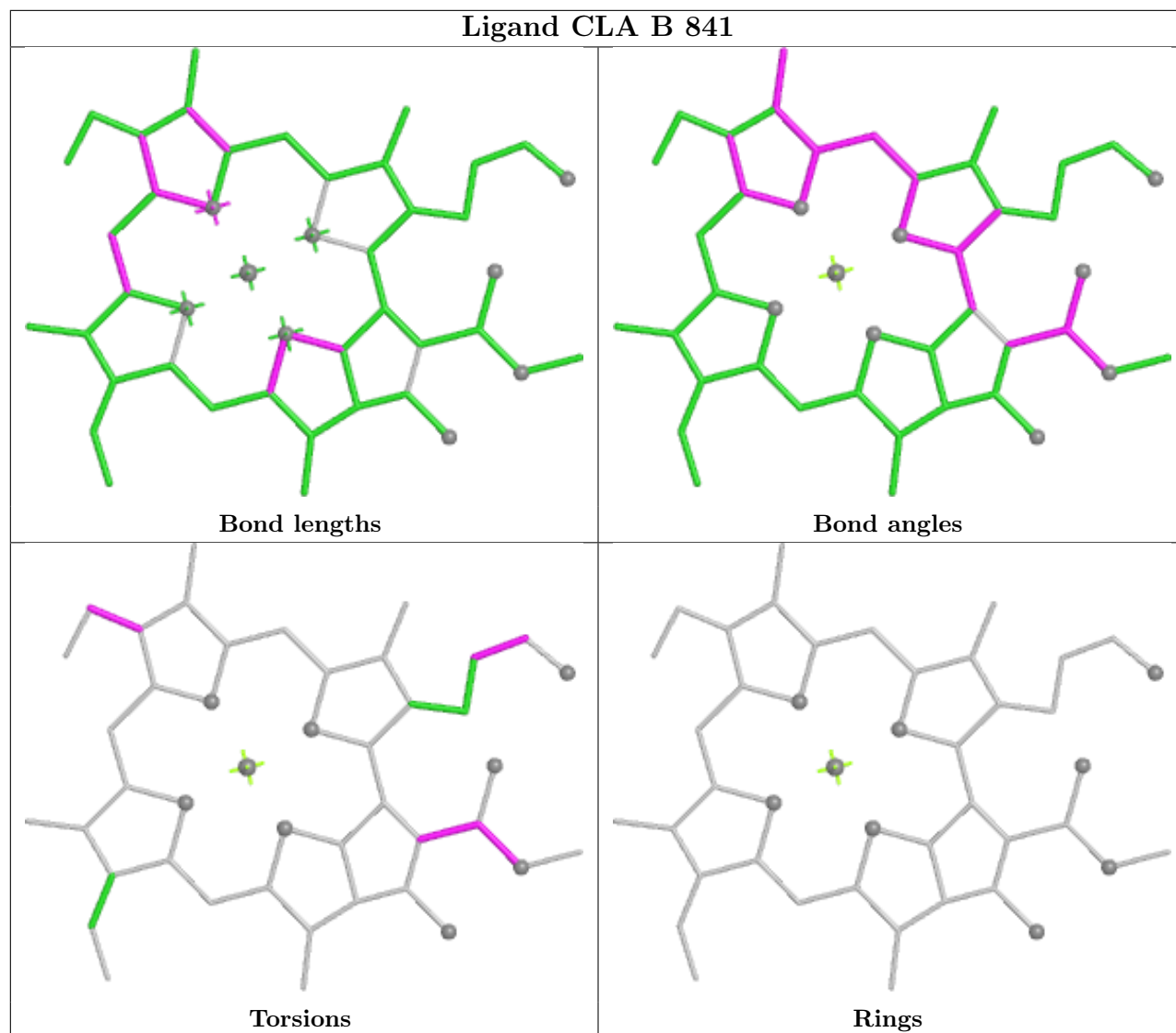
Ligand CLA B 807

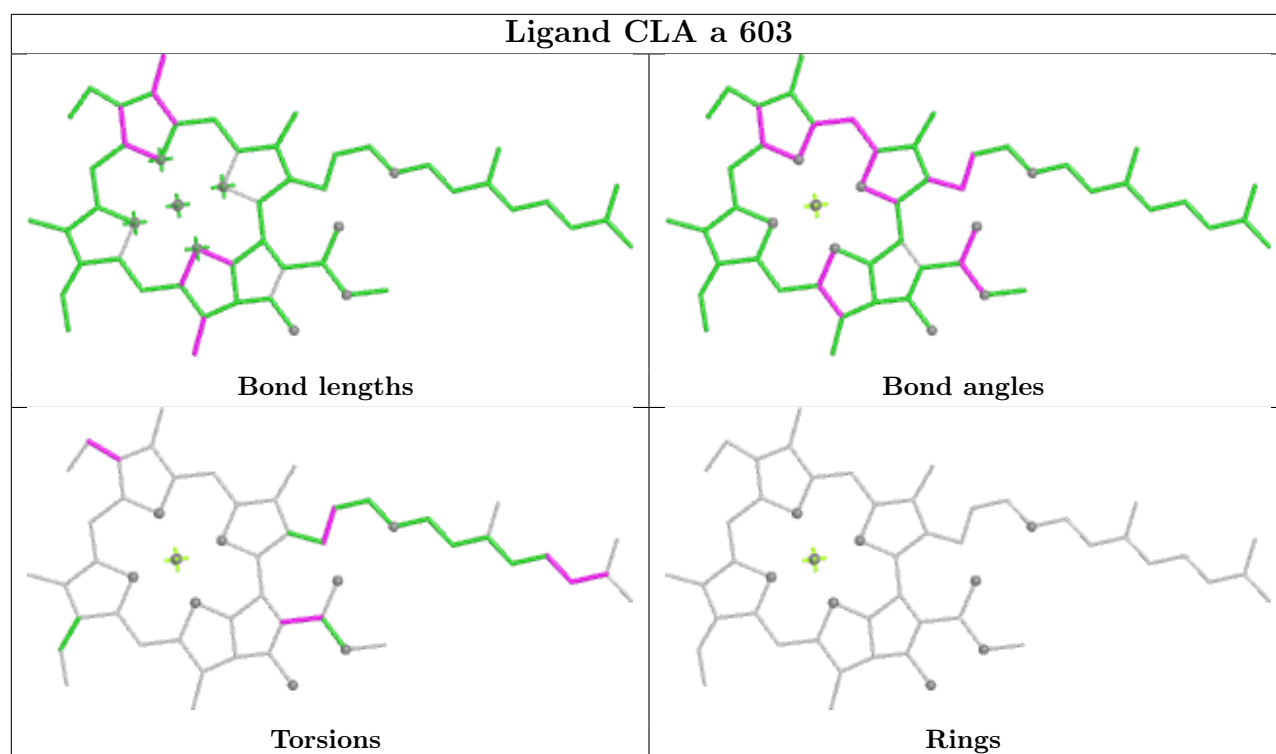


Ligand CLA A 831**Ligand LUT 8 619****Ligand CLA B 834**

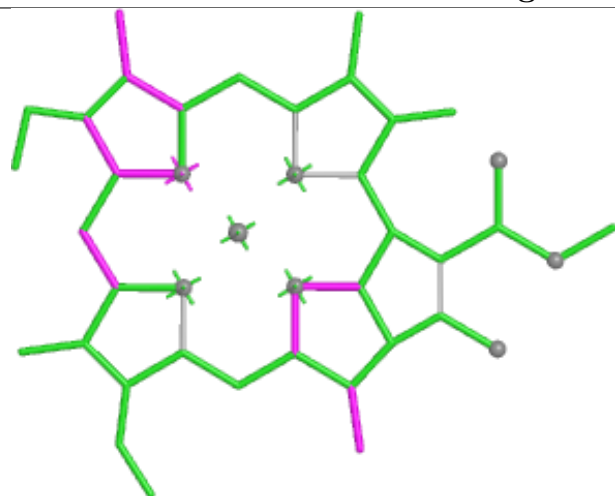
Ligand CLA 5 613**Ligand CLA A 841**

Ligand CLA B 841





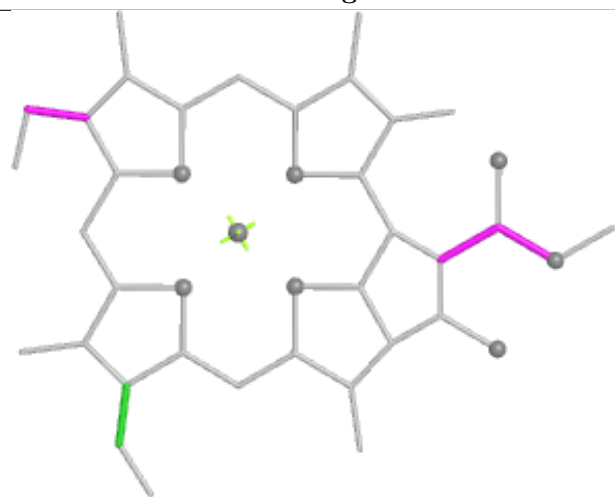
Ligand CLA F 304



Bond lengths



Bond angles

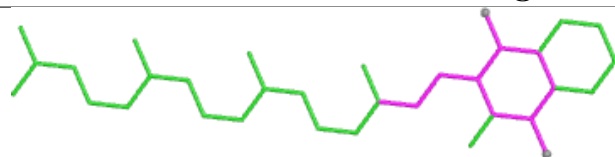


Torsions

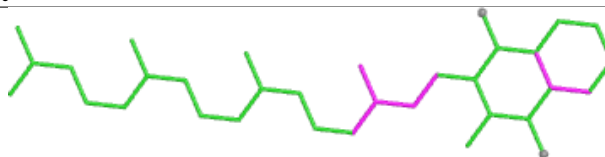


Rings

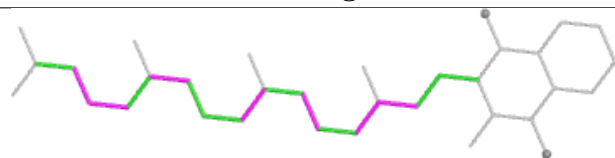
Ligand PQN B 842



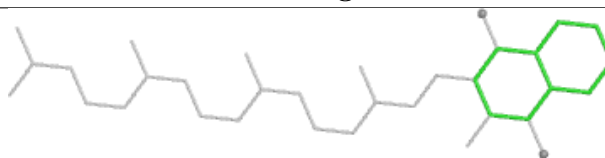
Bond lengths



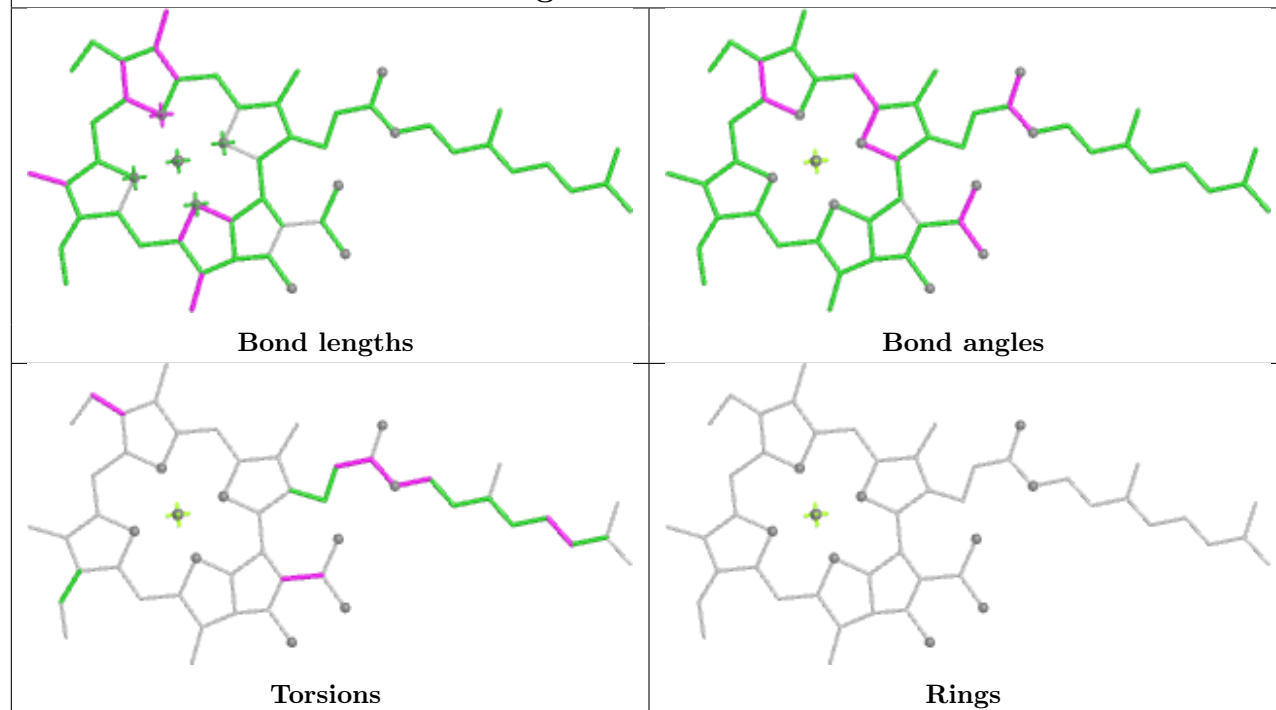
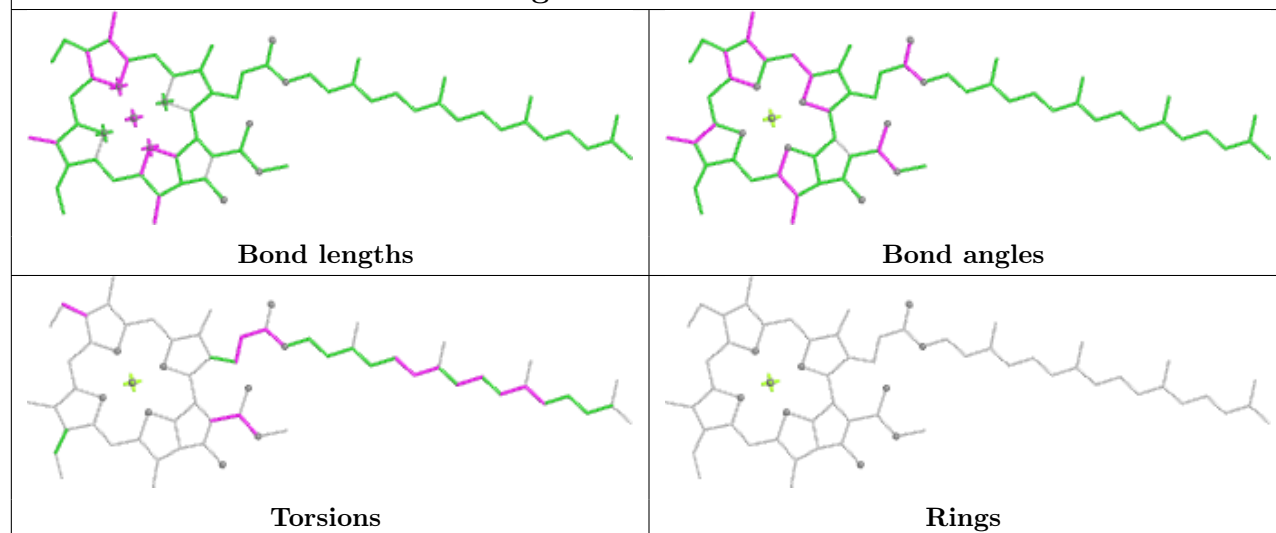
Bond angles



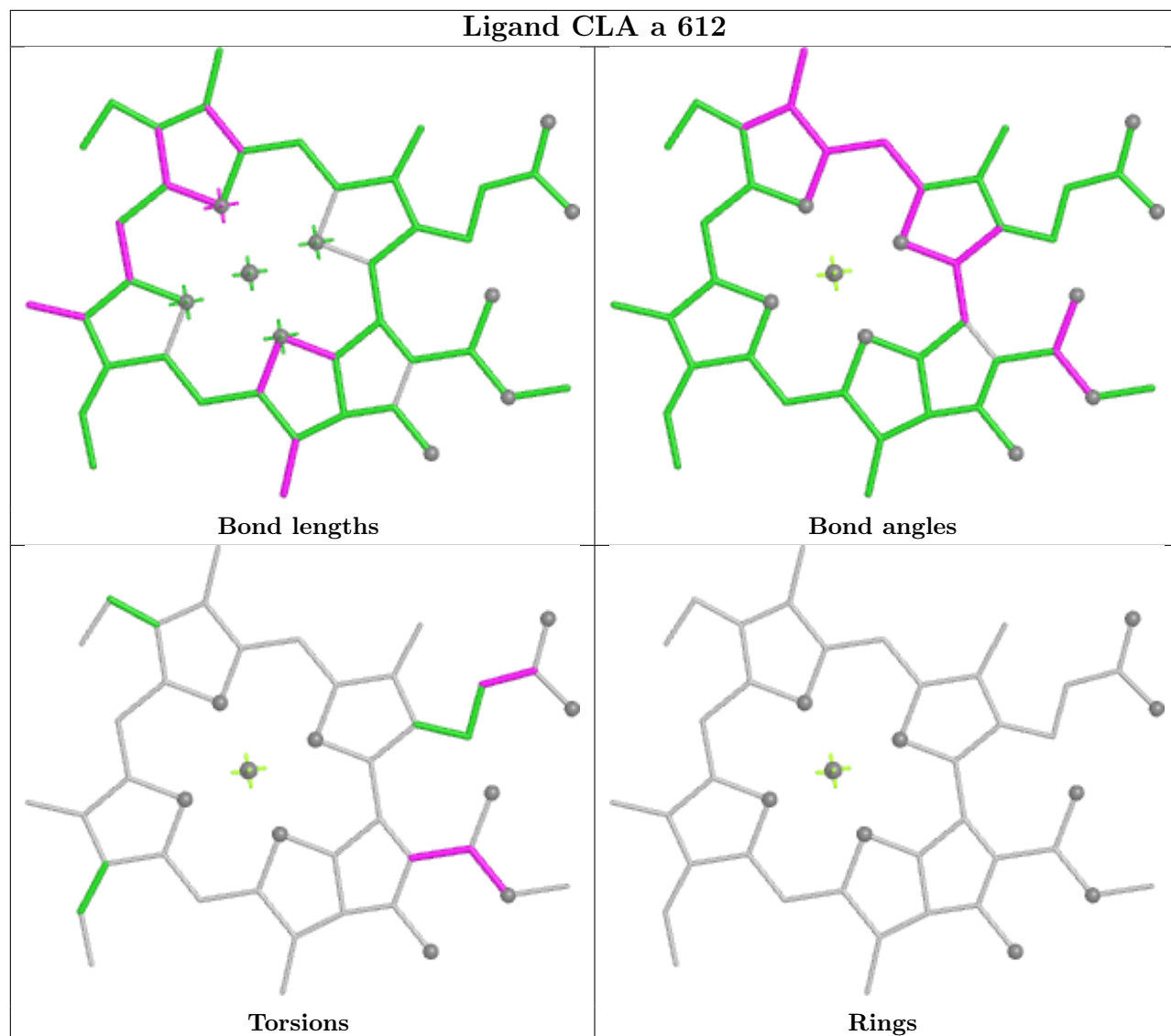
Torsions



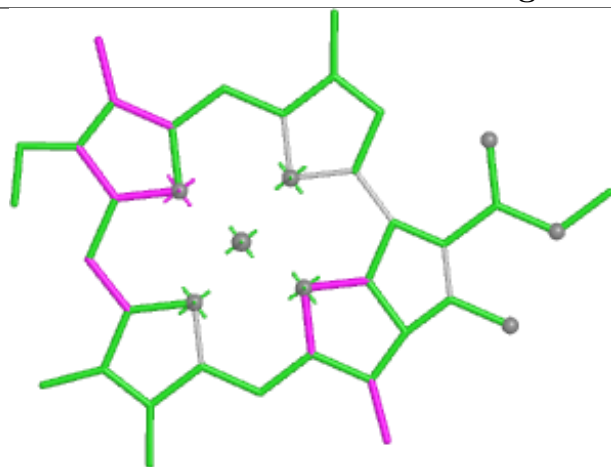
Rings

Ligand CLA 3 606**Ligand CLA A 830**

Ligand CLA a 612



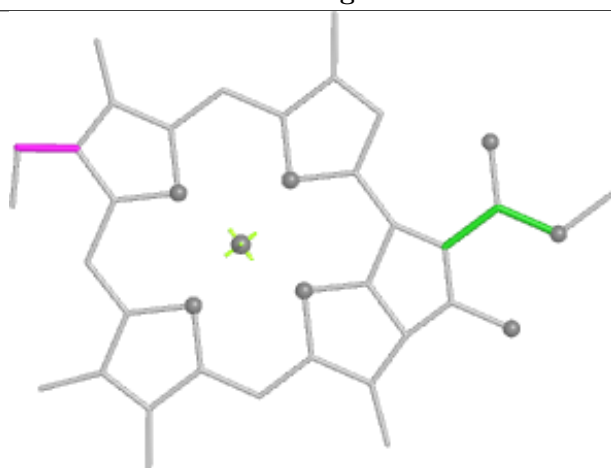
Ligand CLA 1 610



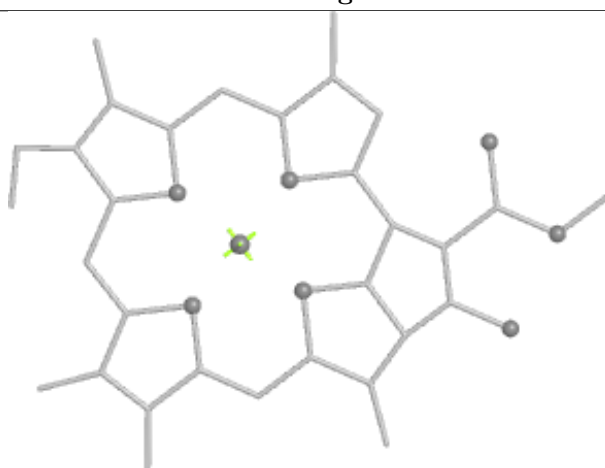
Bond lengths



Bond angles

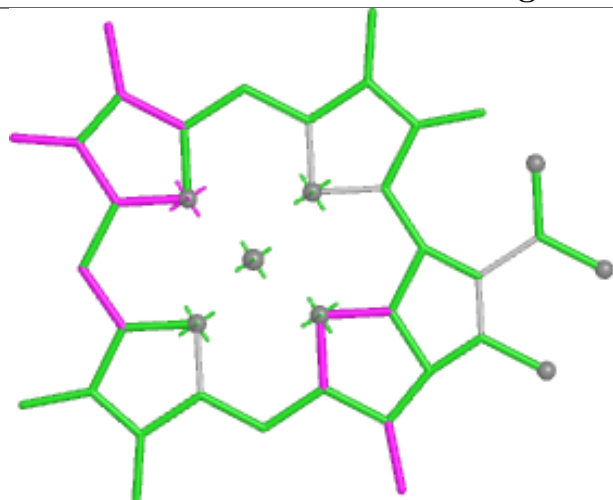


Torsions

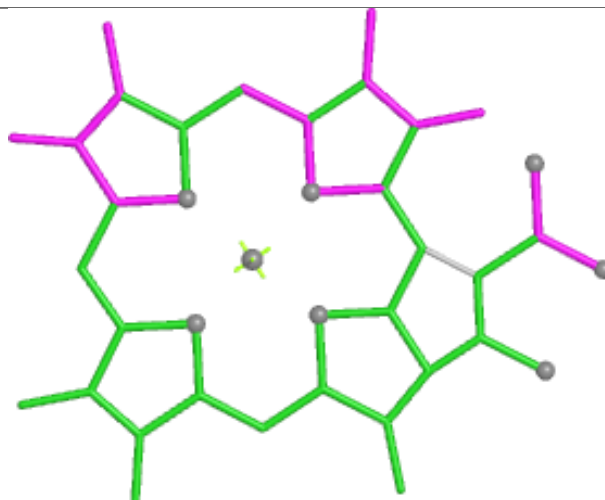


Rings

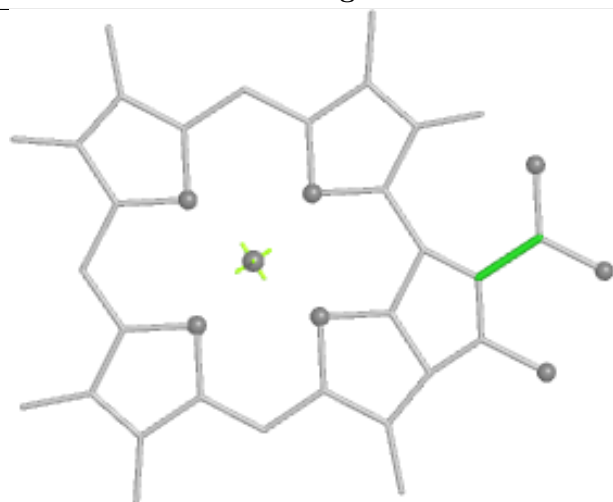
Ligand CLA 3 611



Bond lengths



Bond angles

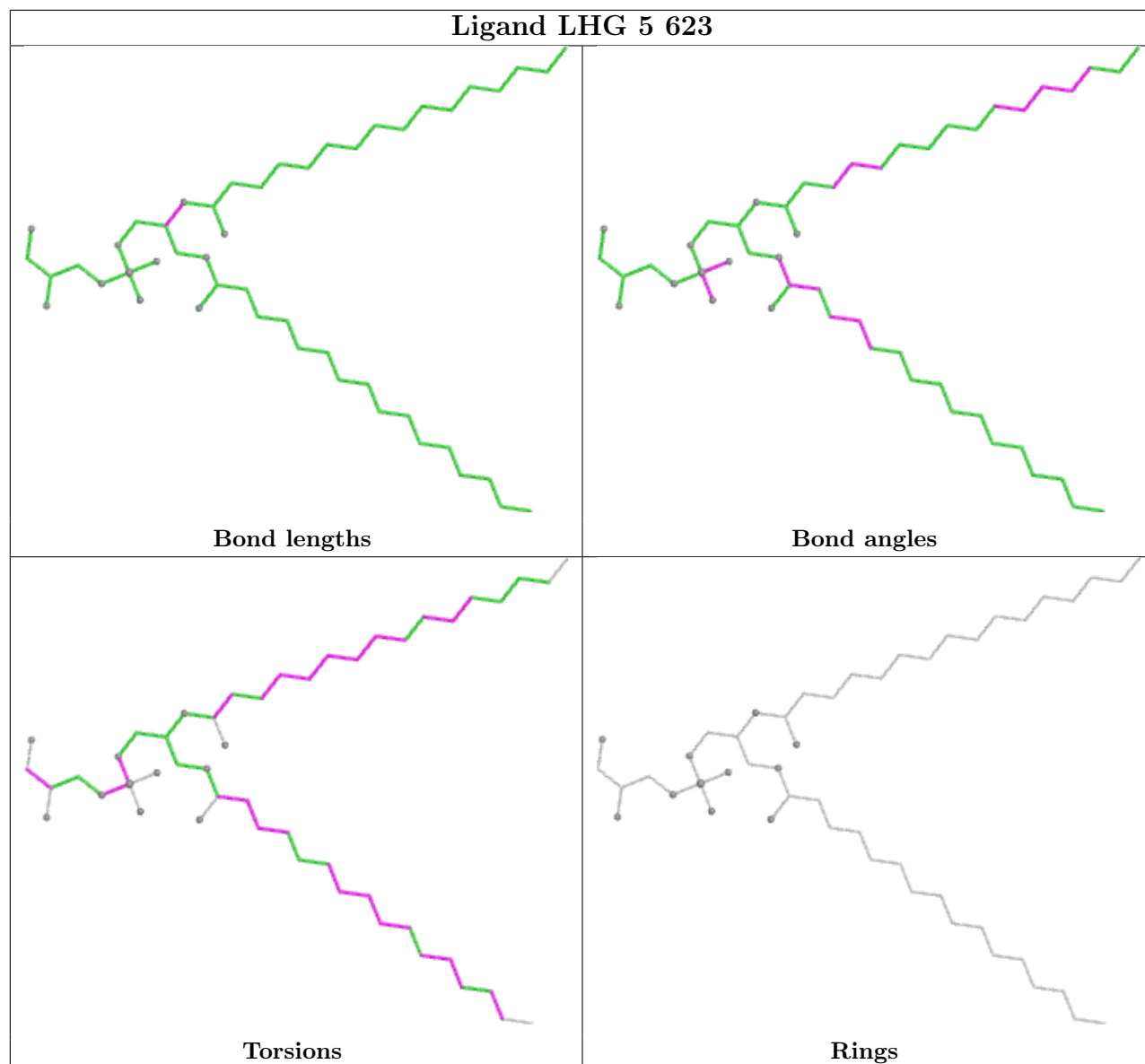


Torsions

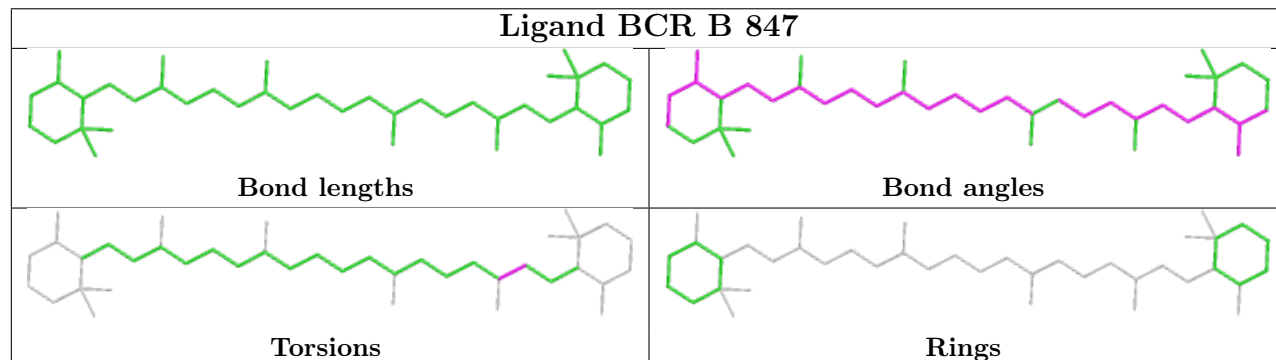


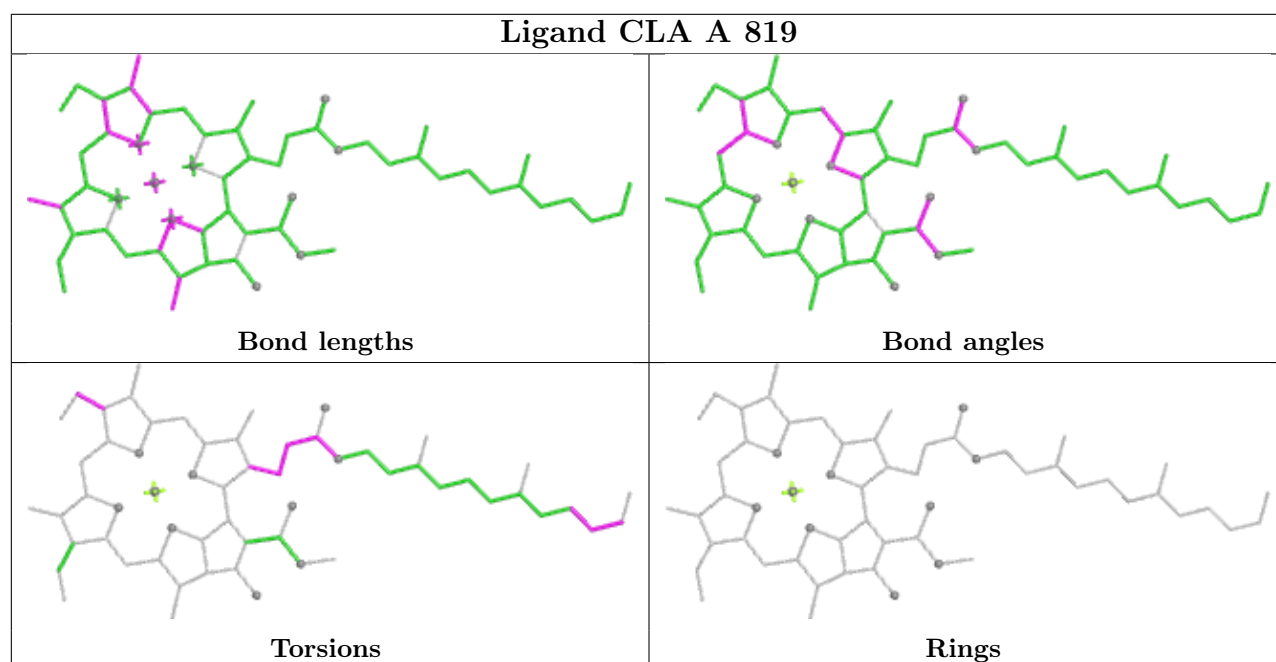
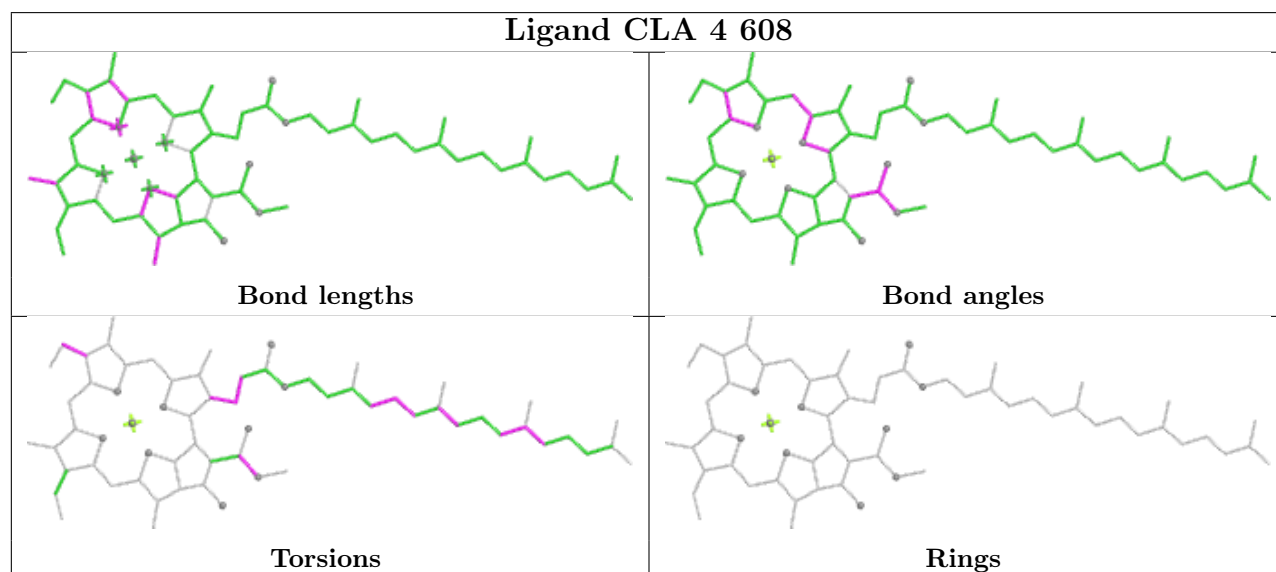
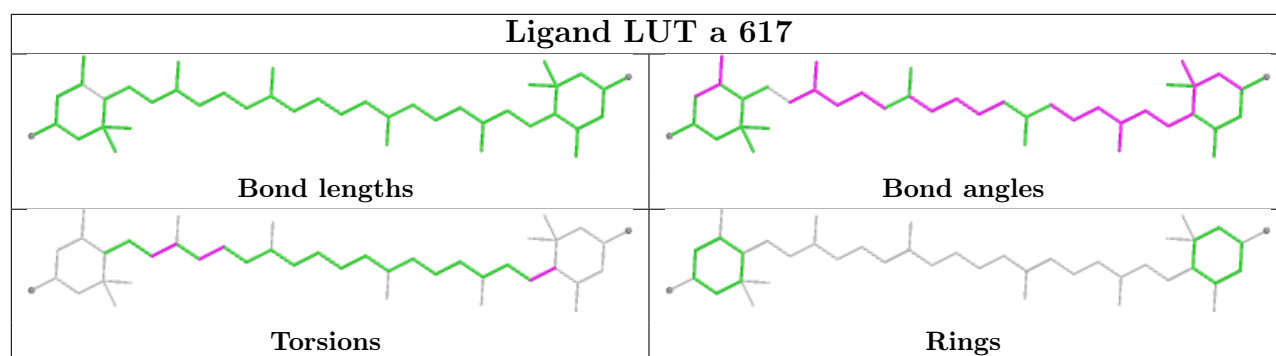
Rings

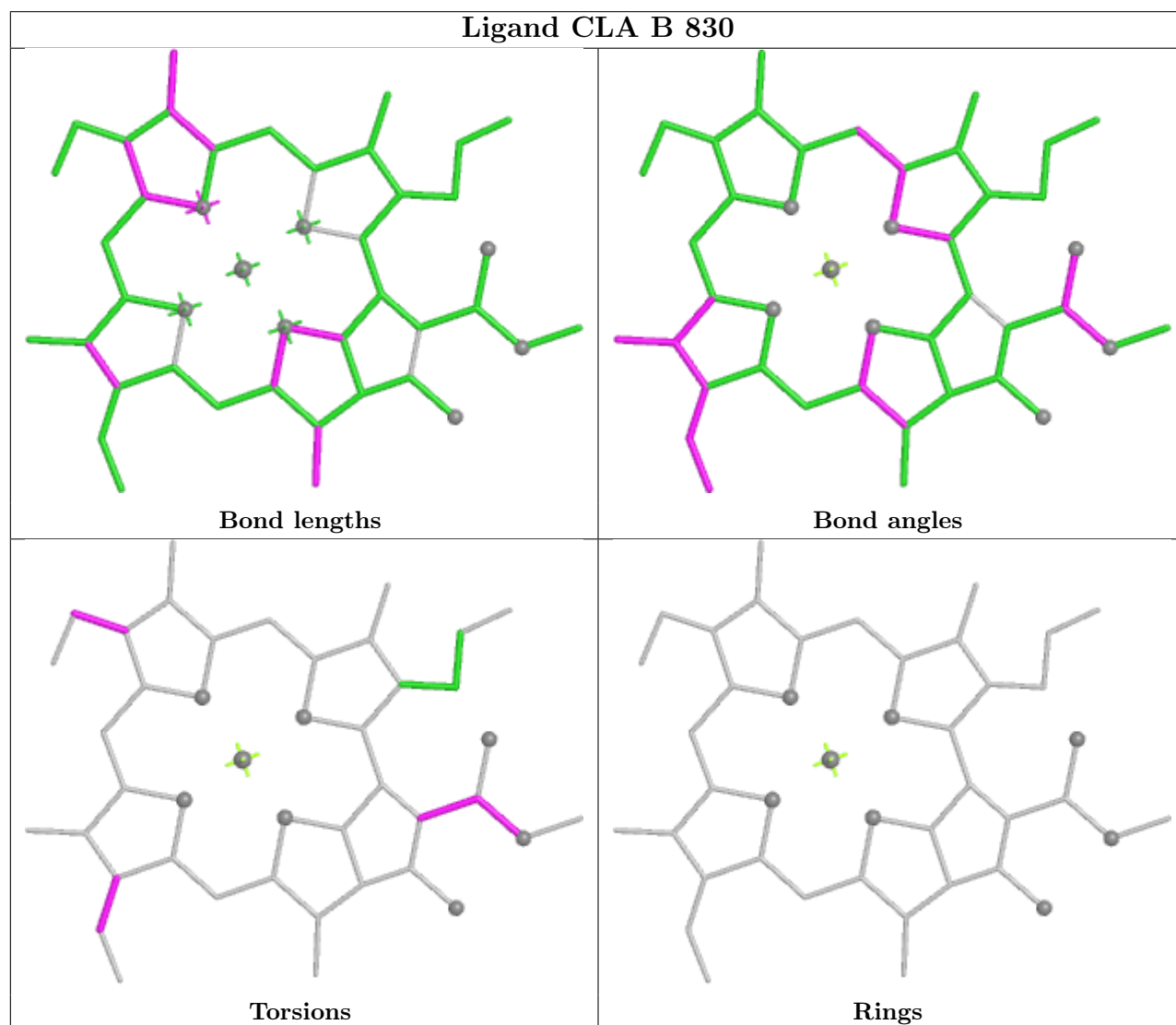
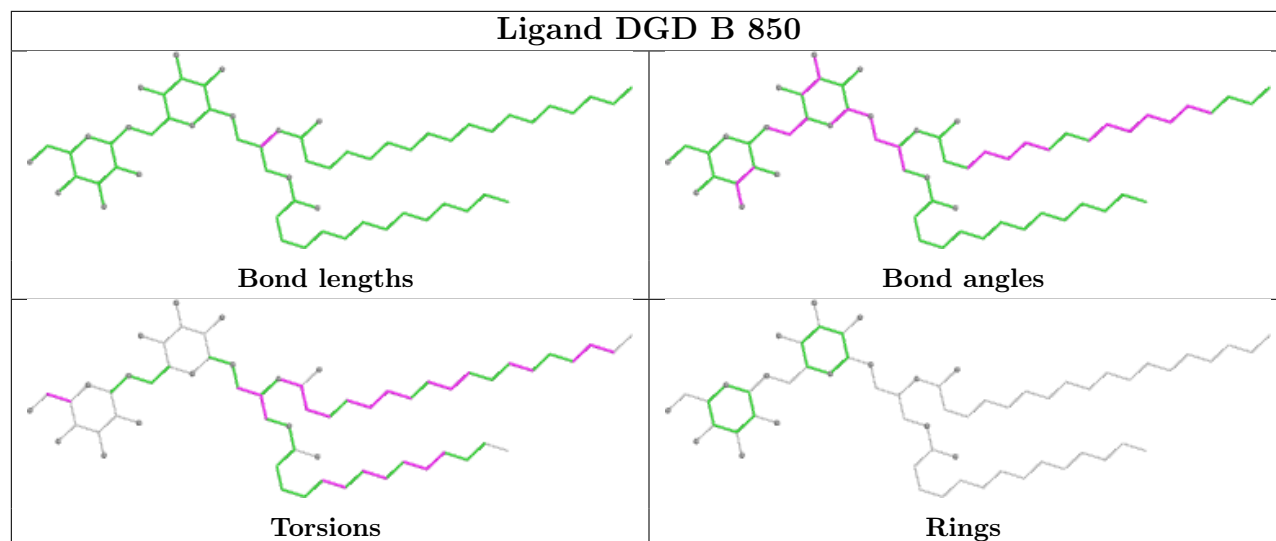
Ligand LHG 5 623

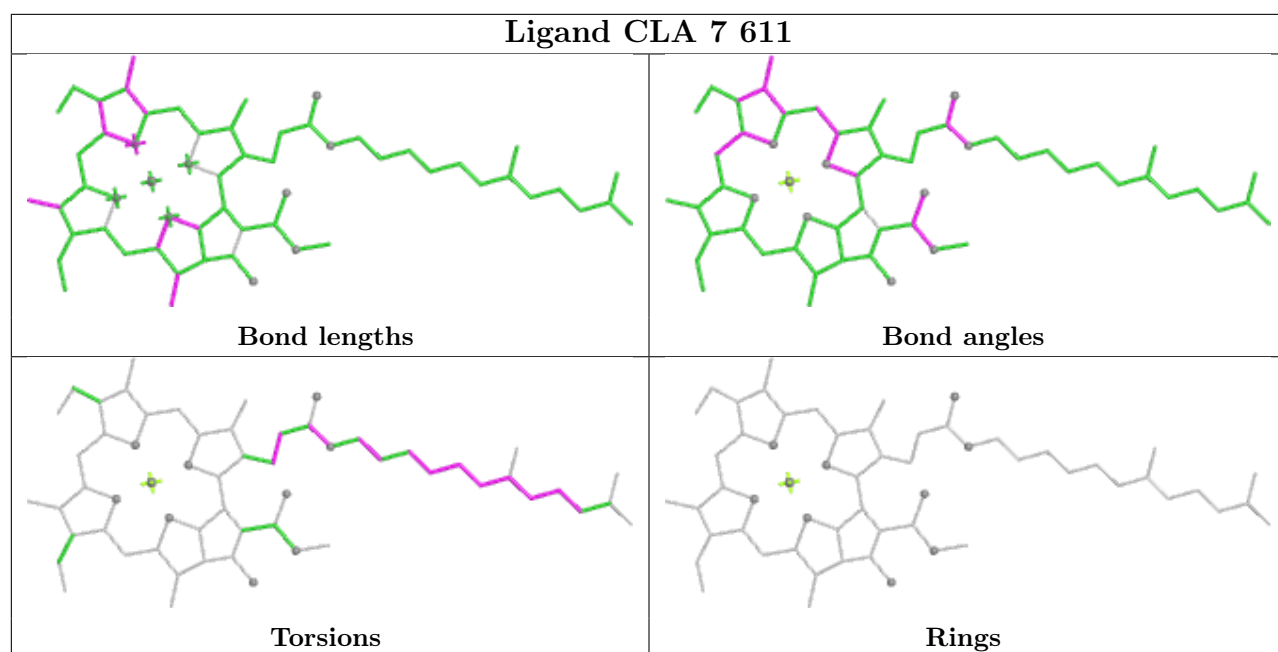


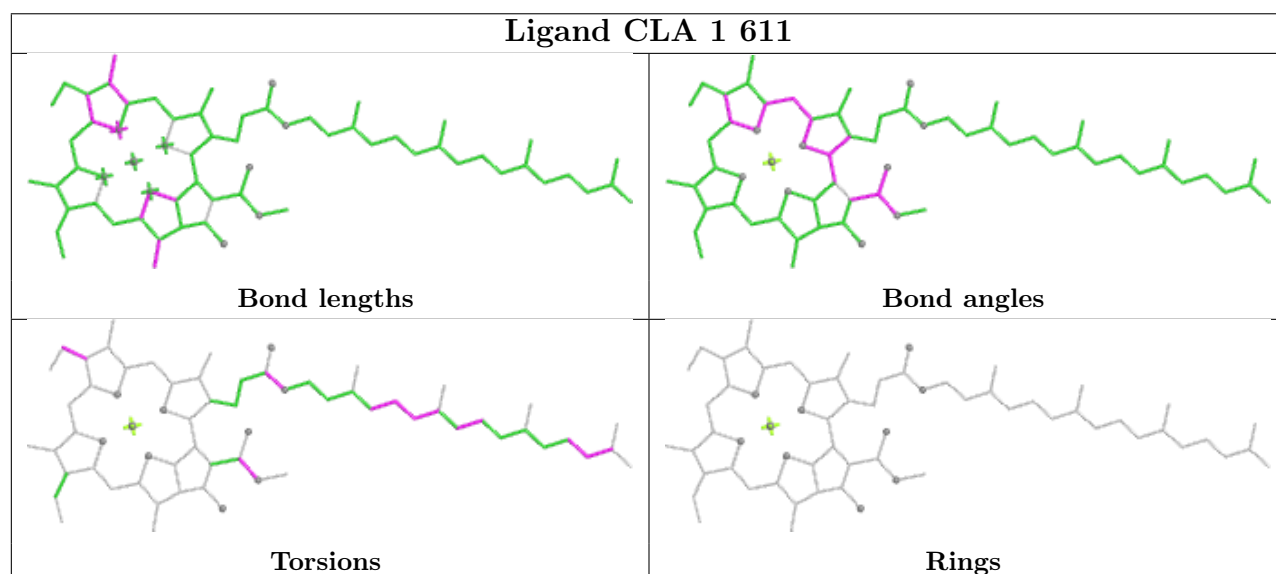
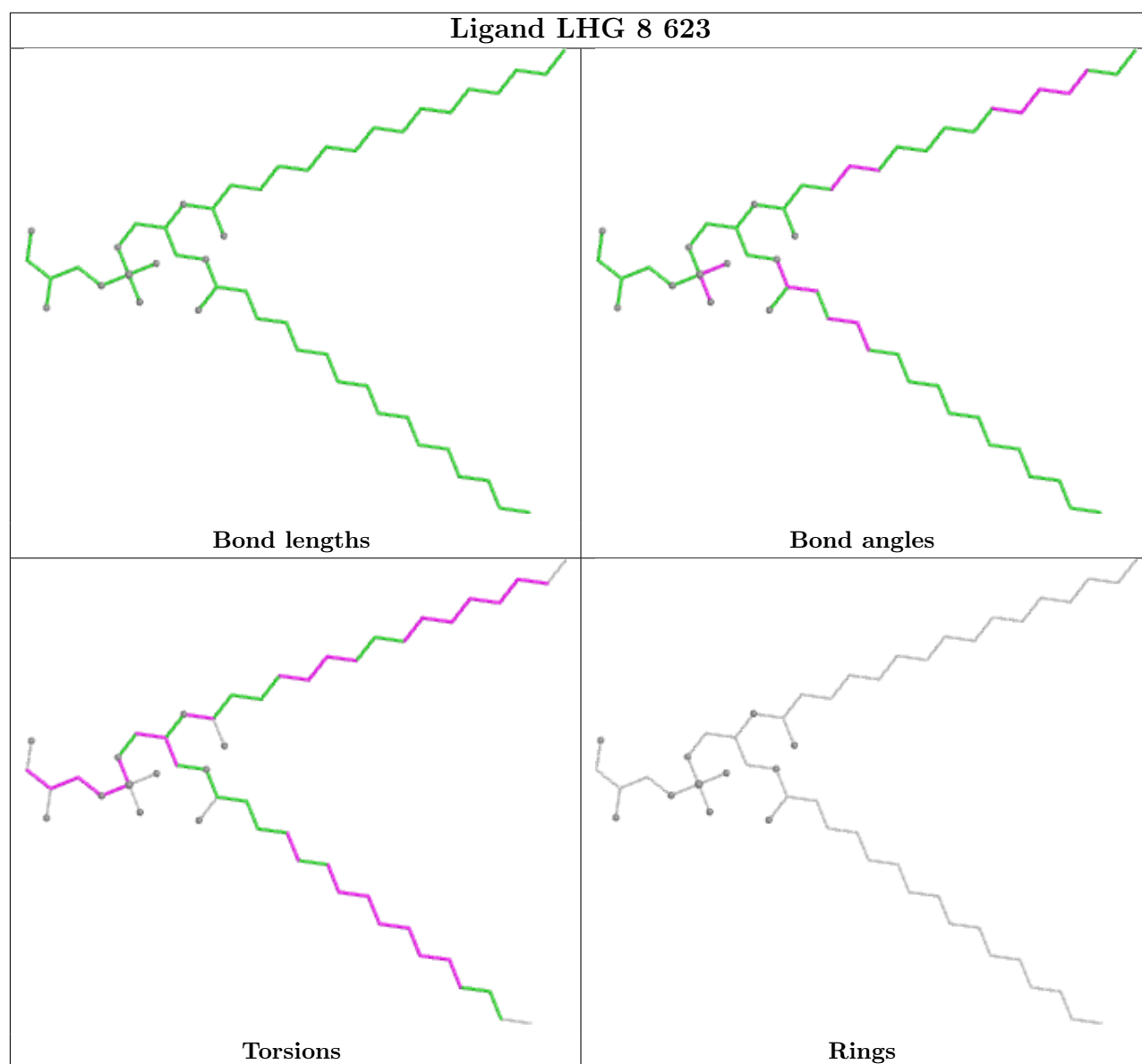
Ligand BCR B 847

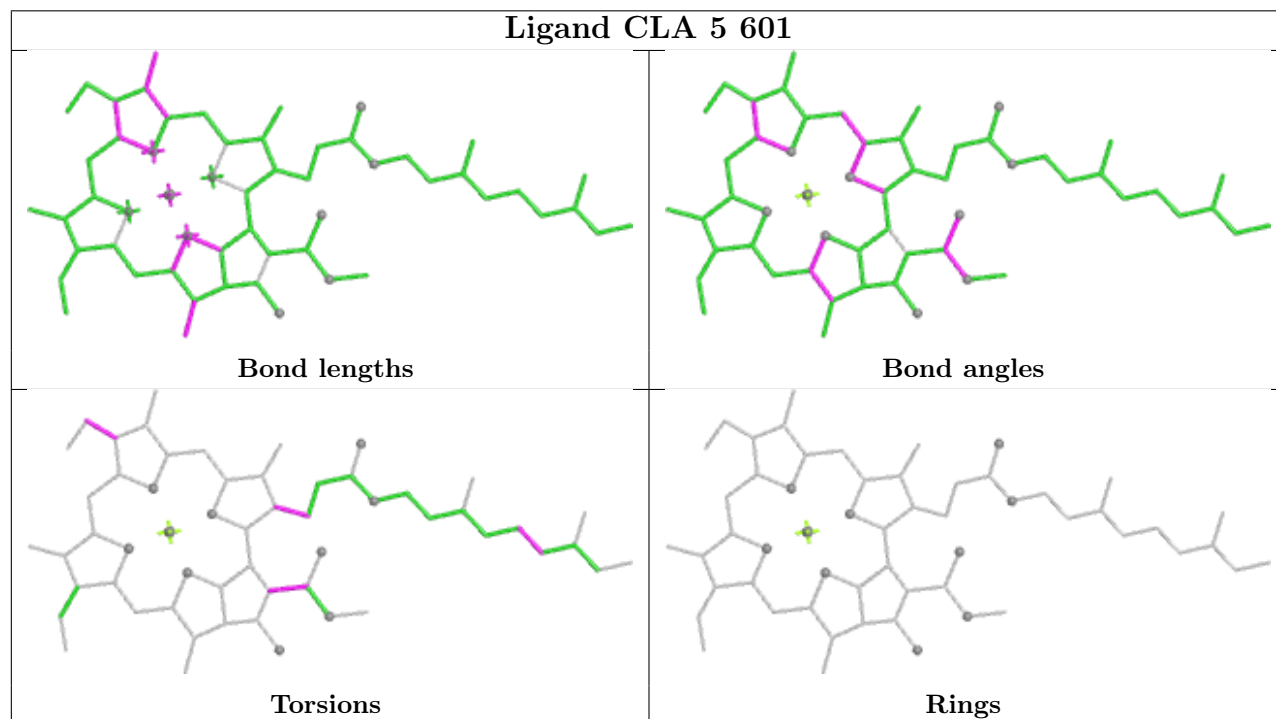
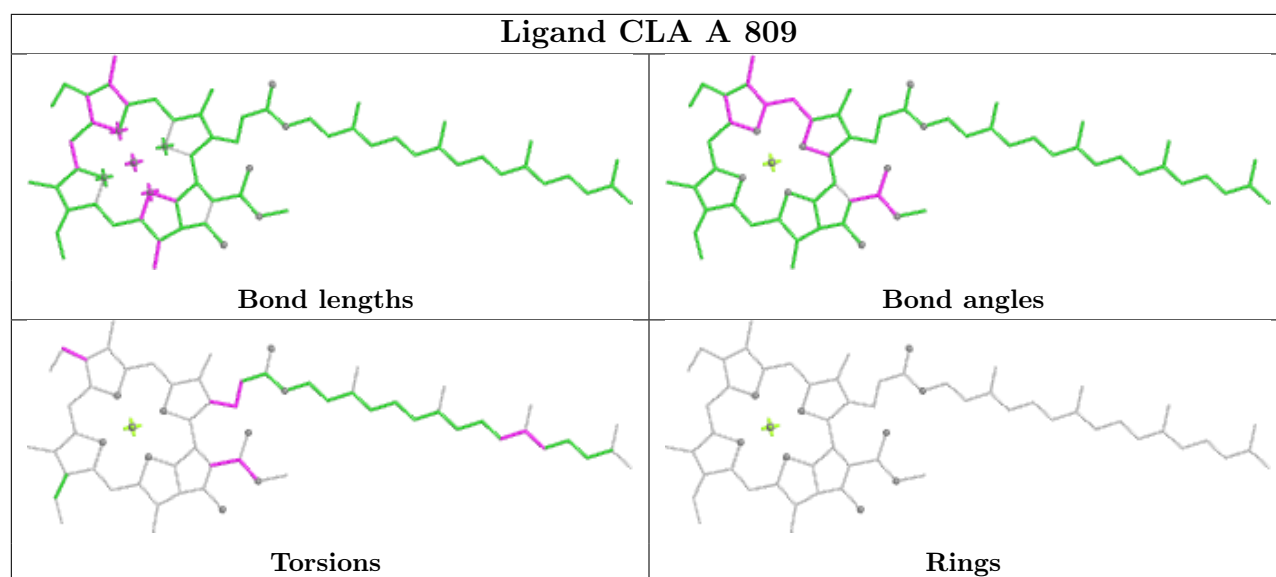




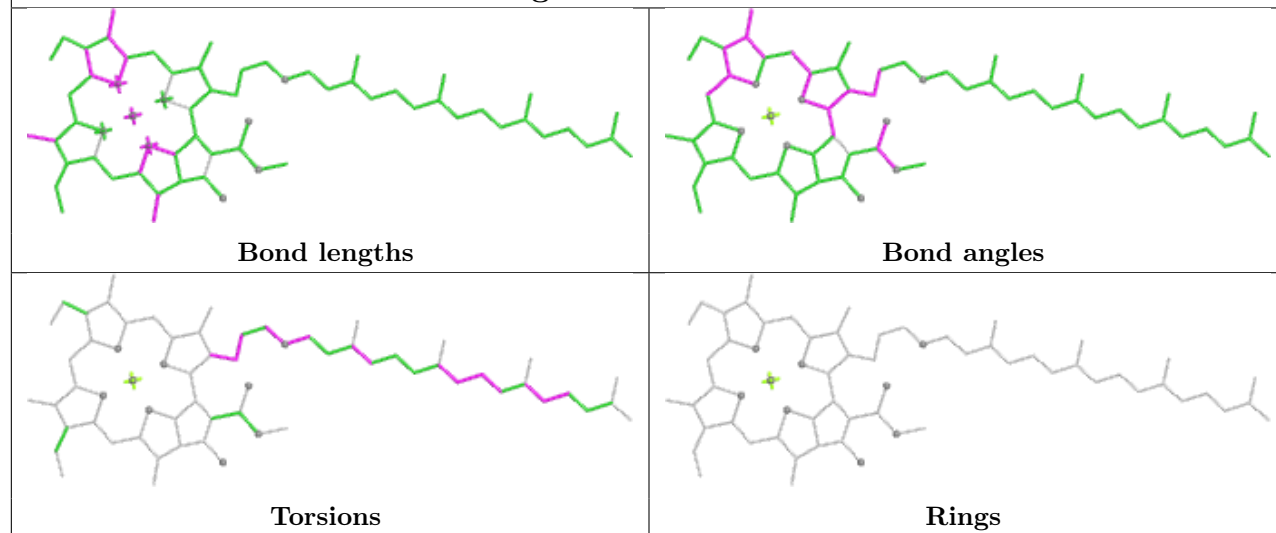




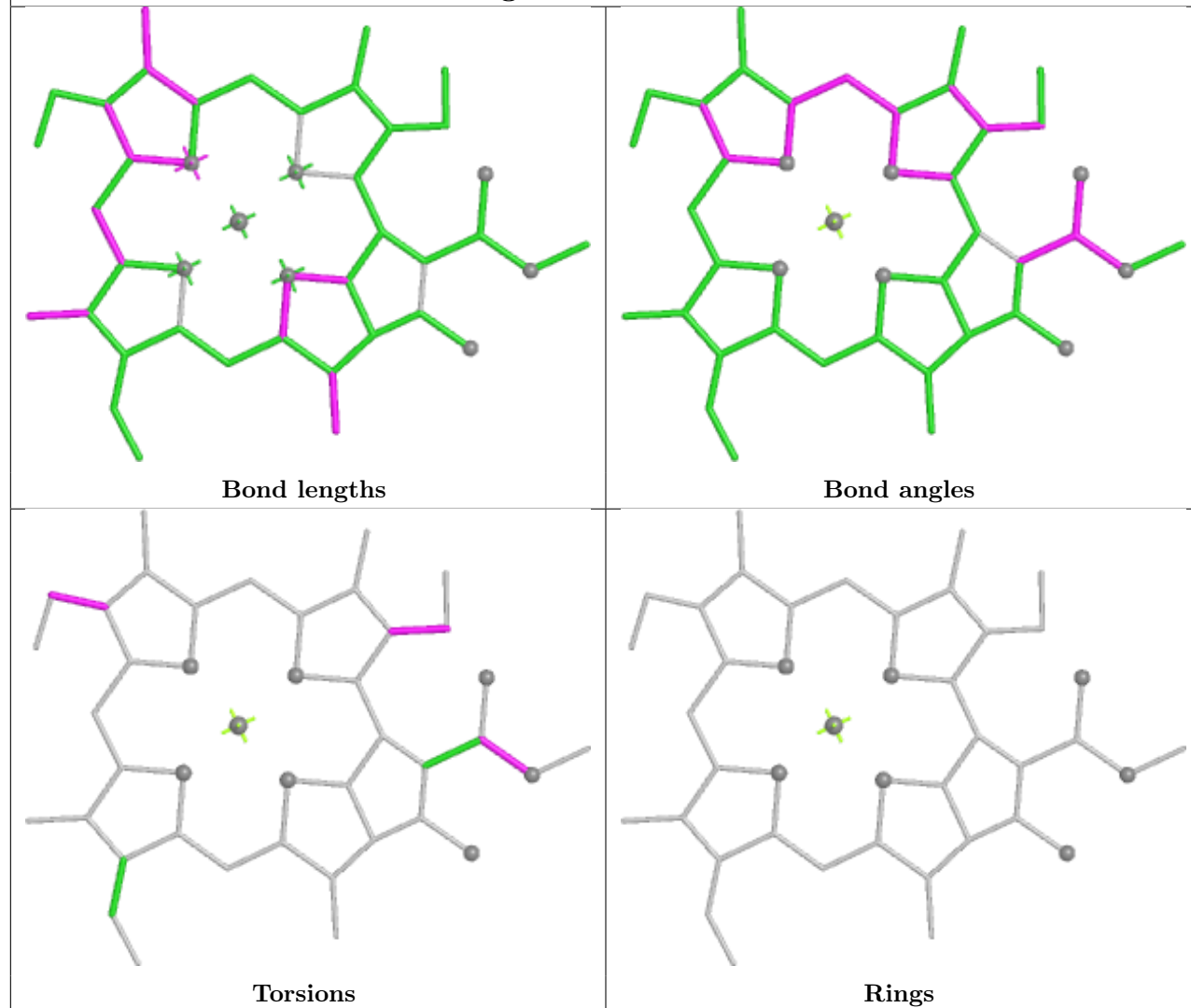




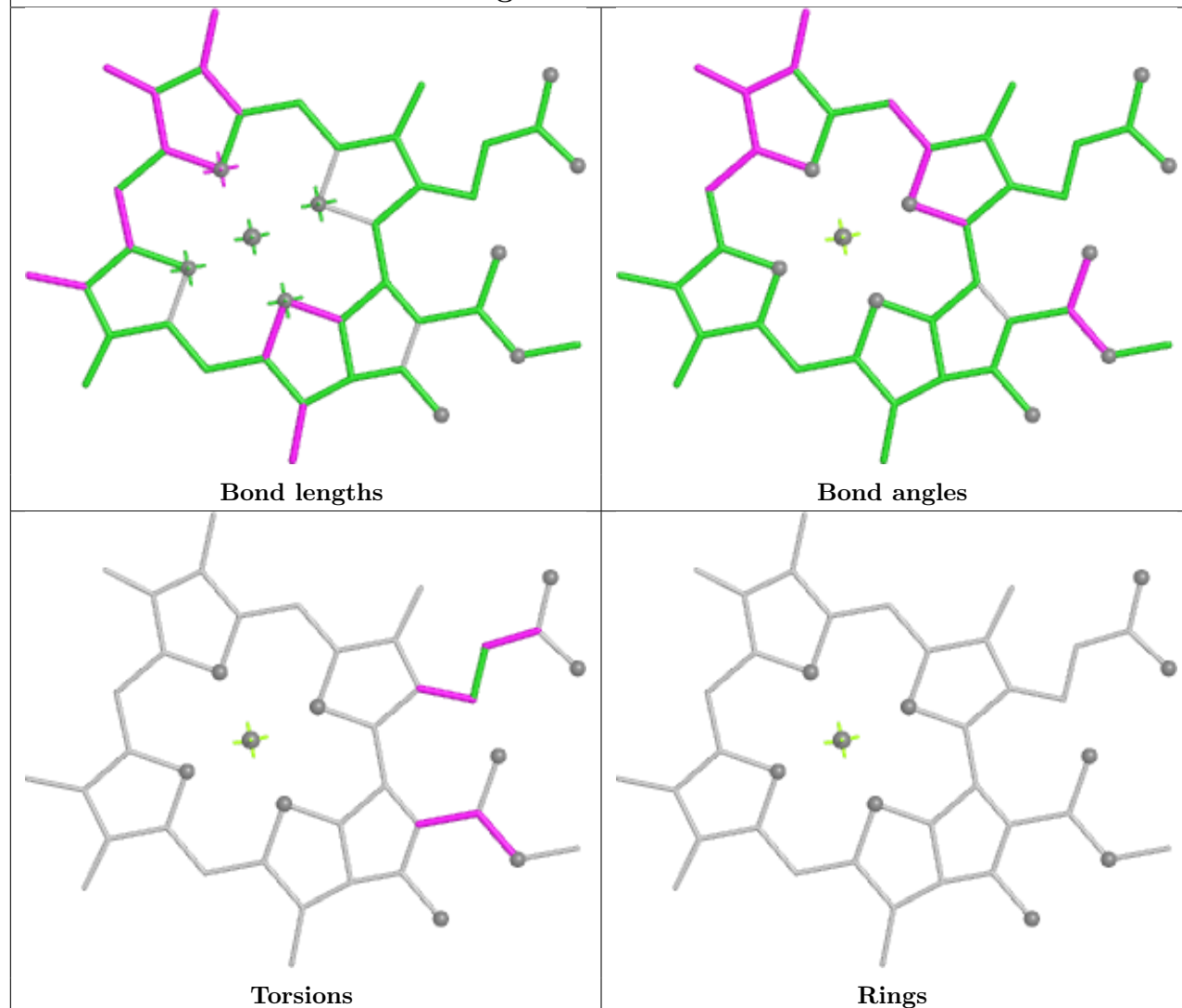
Ligand CLA A 826



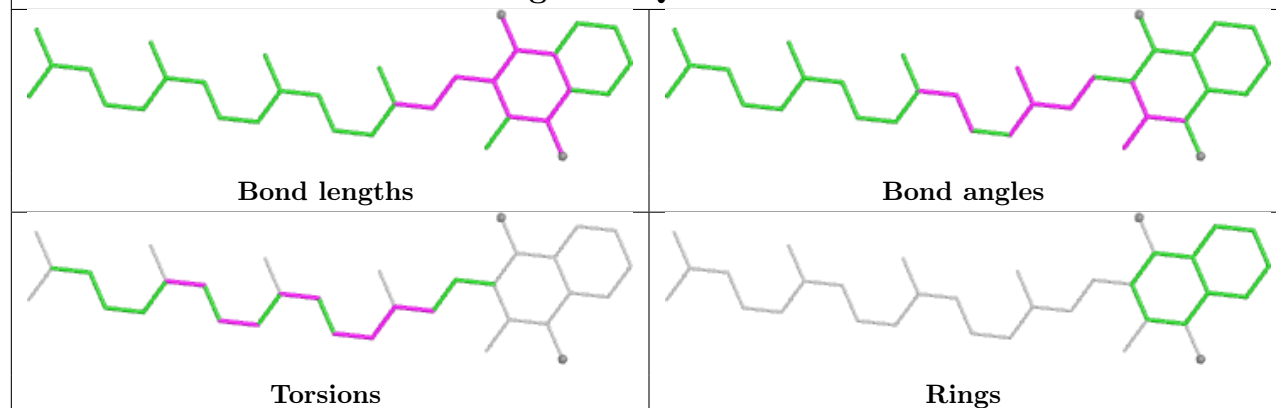
Ligand CLA 8 611

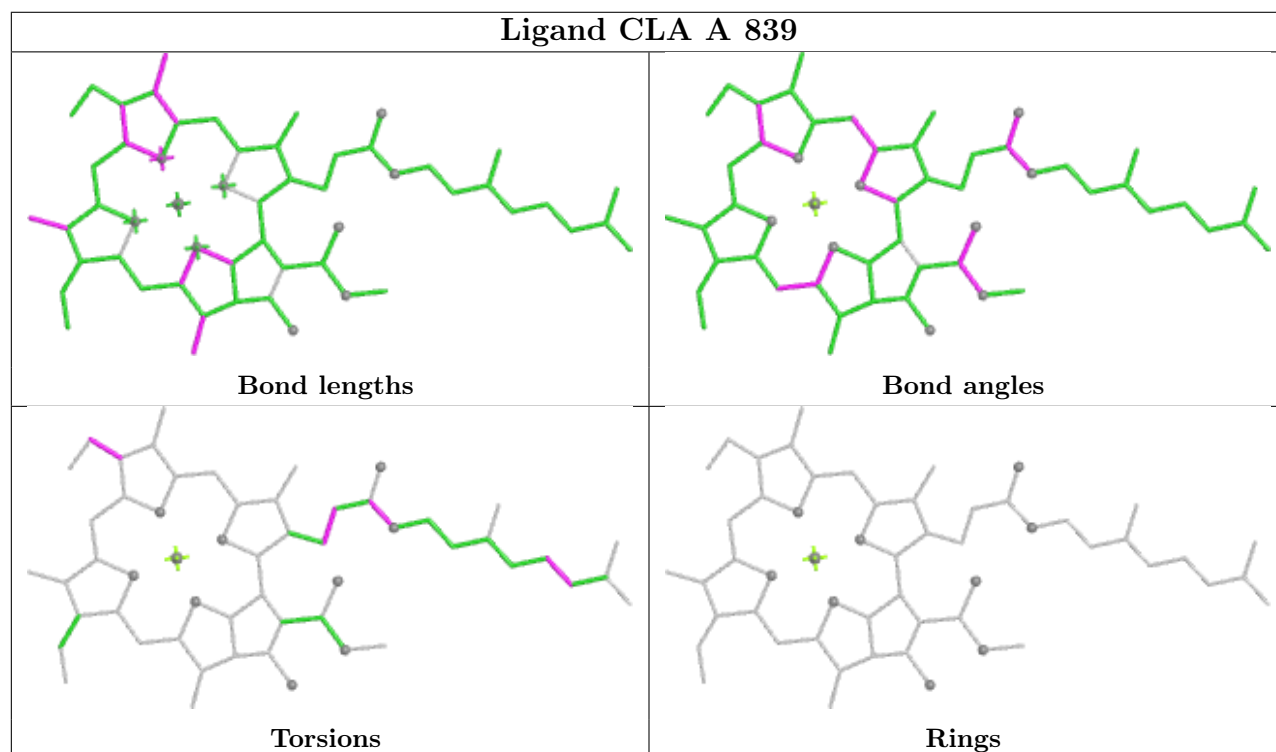
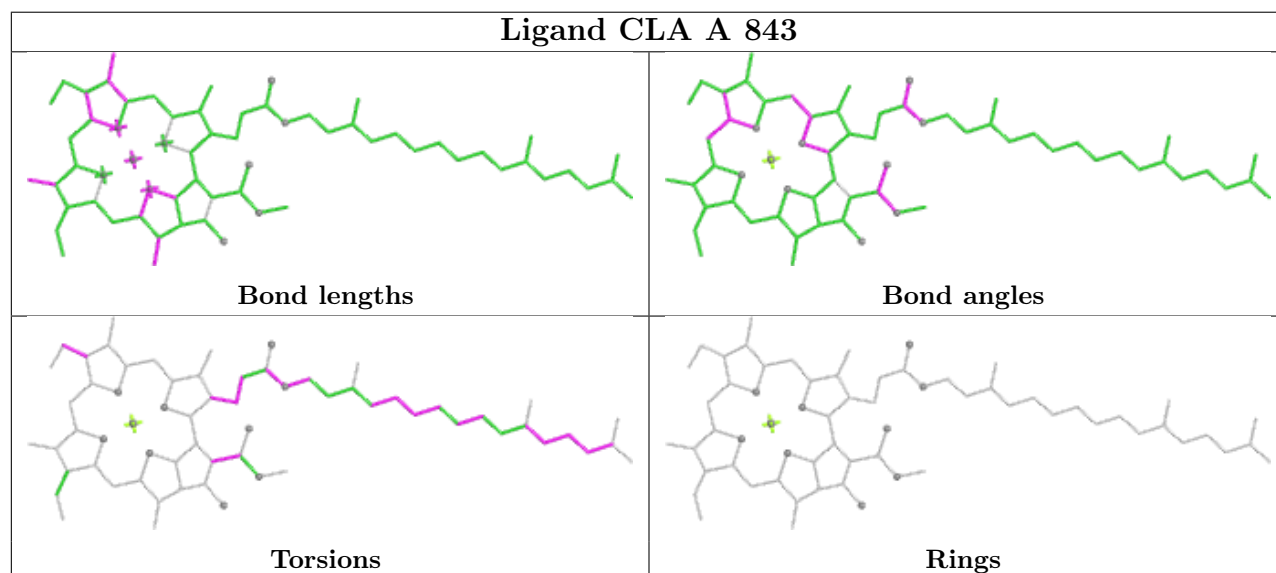
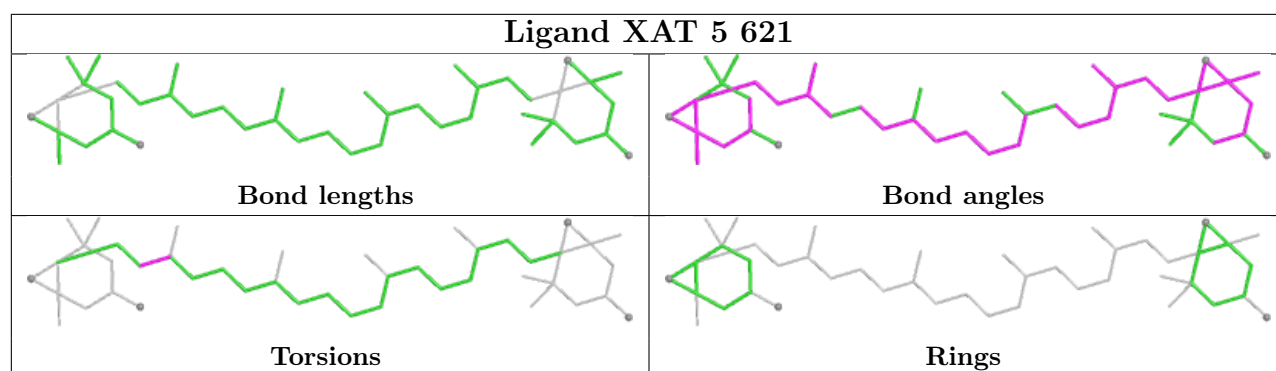


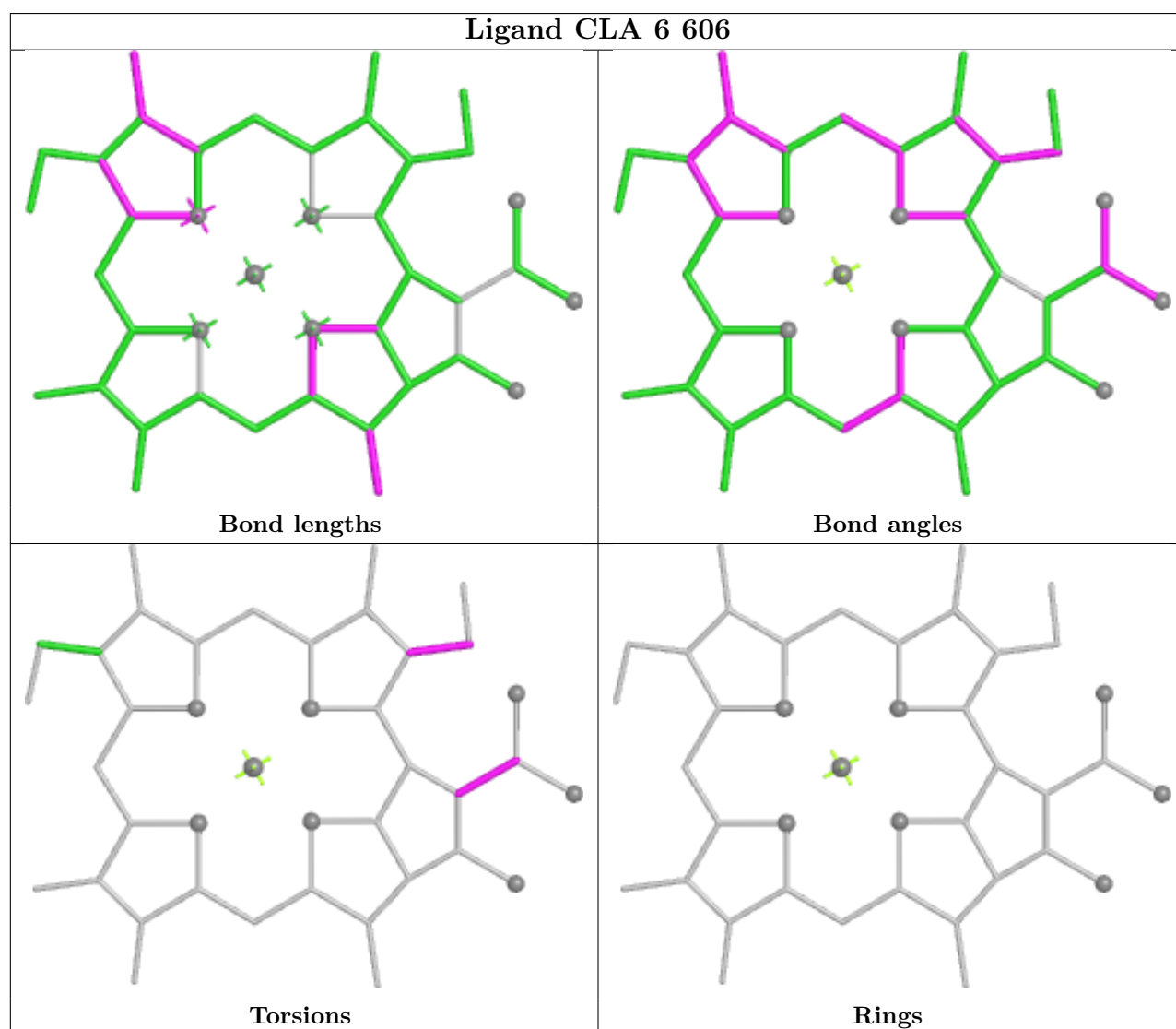
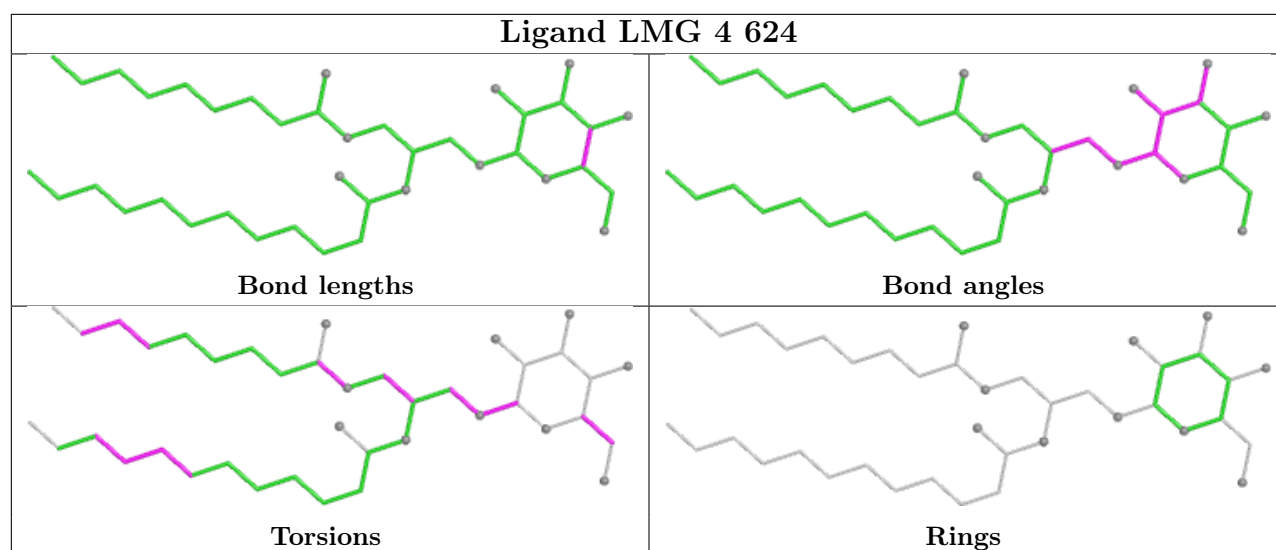
Ligand CLA 4 616

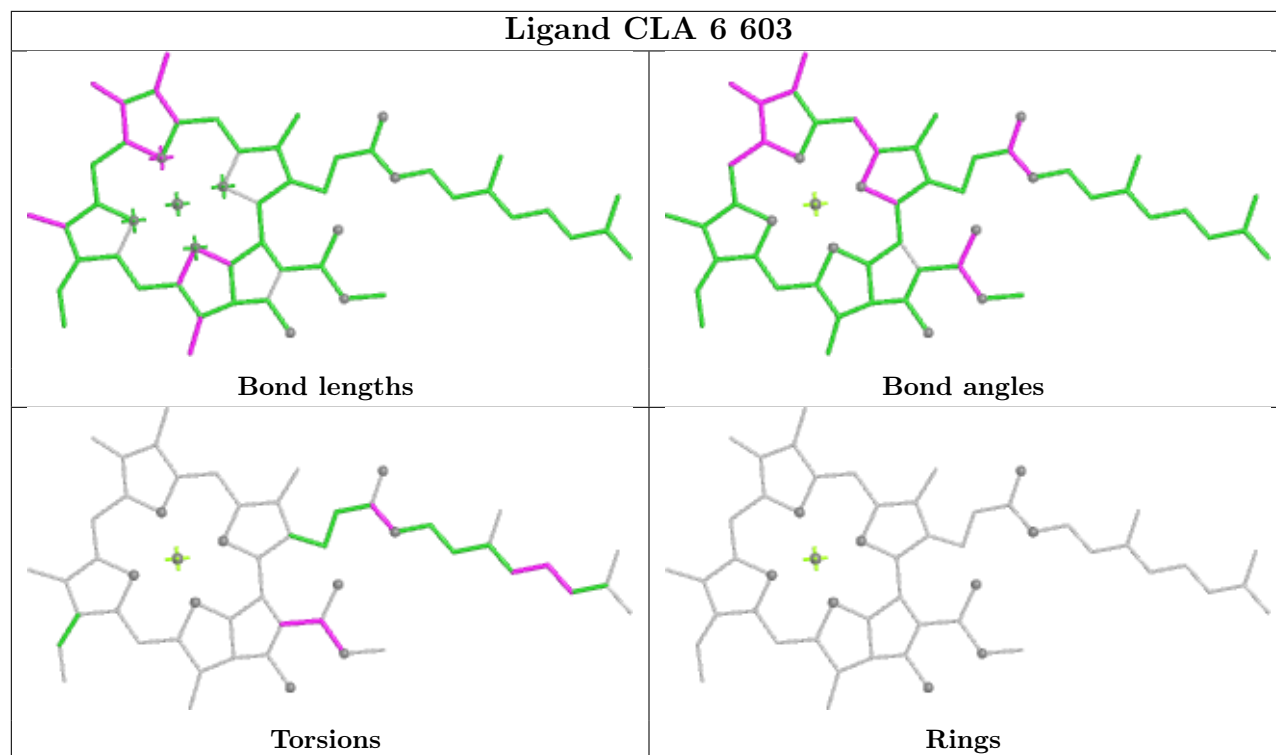
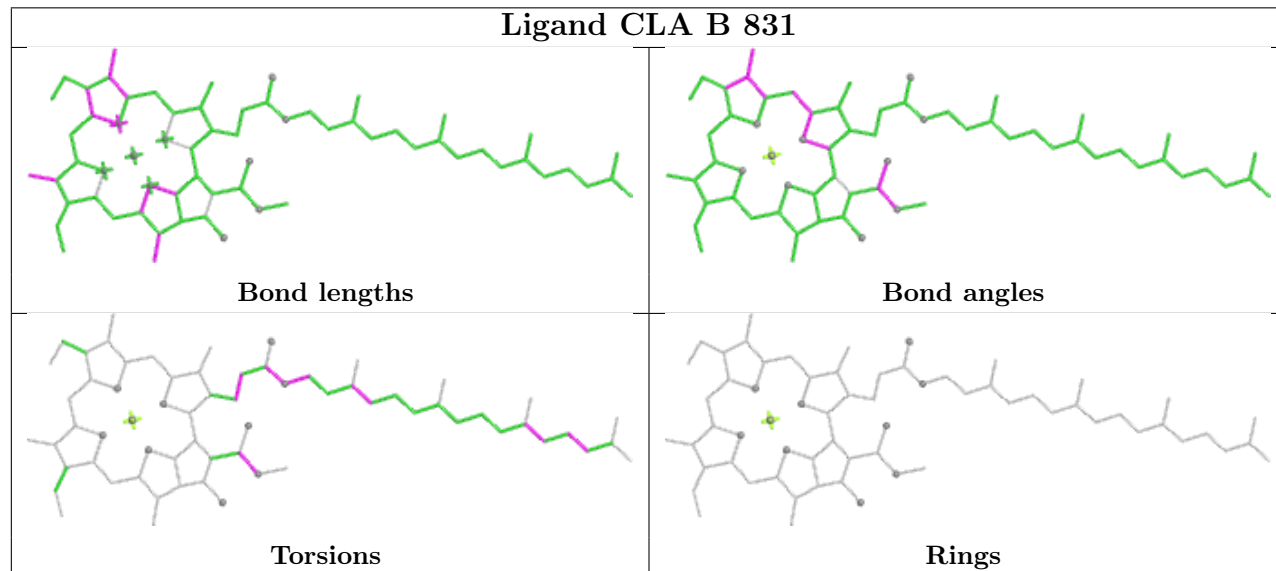


Ligand PQN A 844

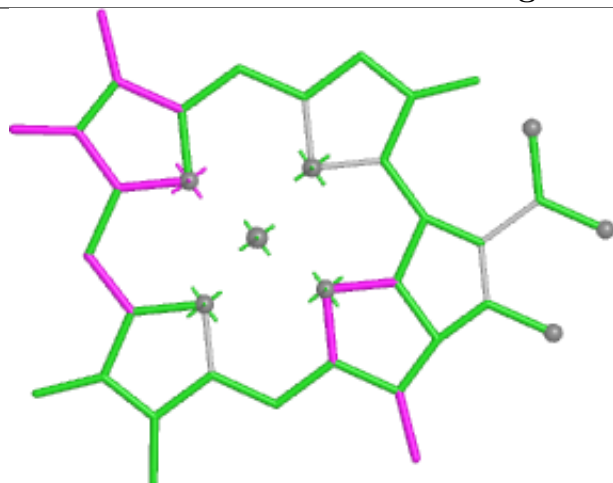




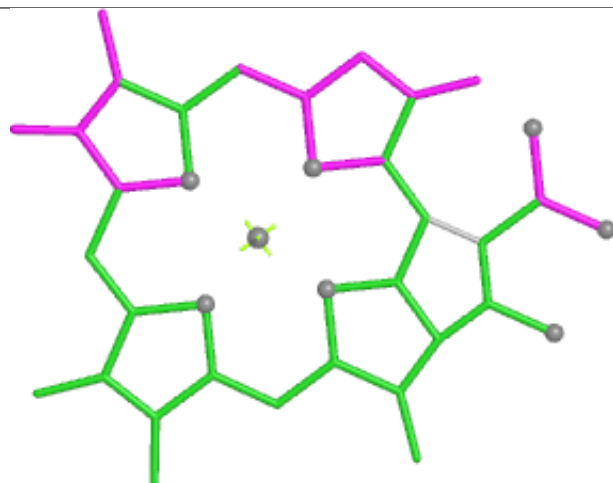


Ligand CLA 6 603**Ligand CLA B 831**

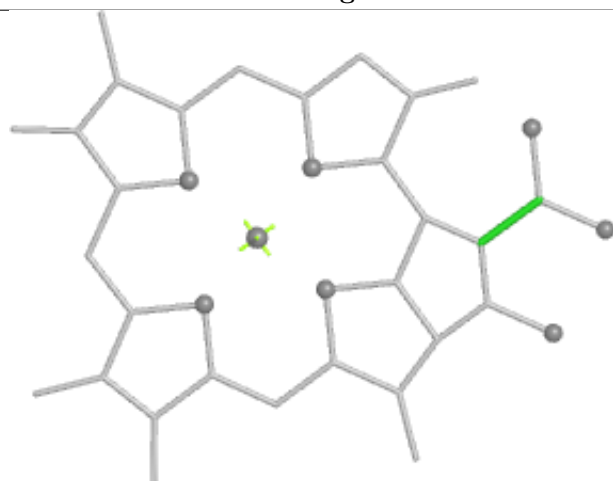
Ligand CLA 1 614



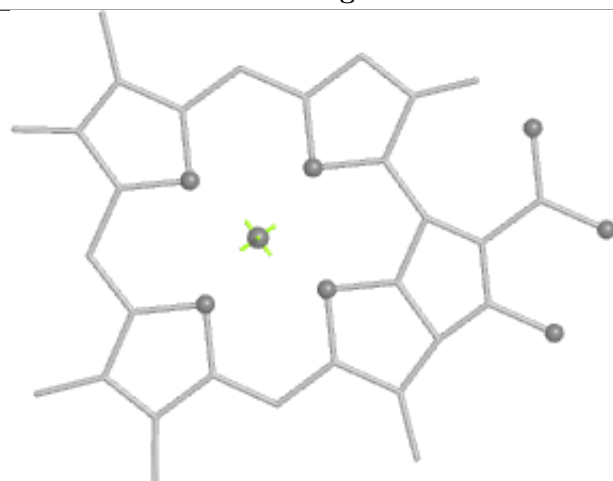
Bond lengths



Bond angles

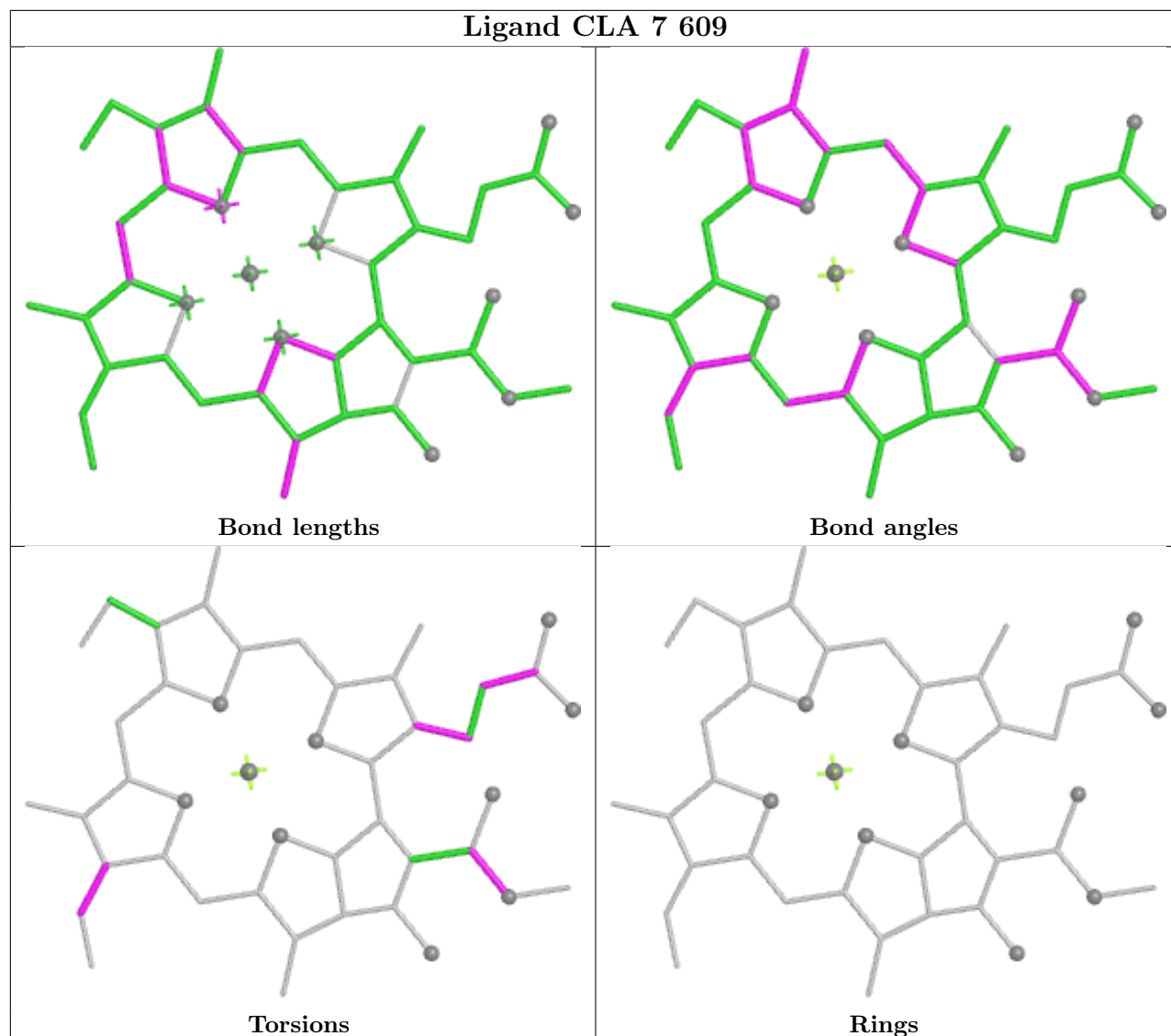


Torsions

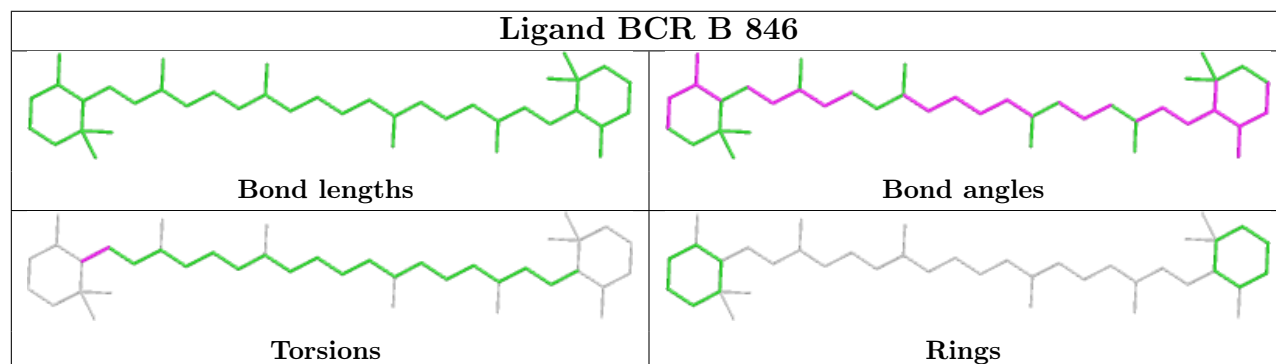


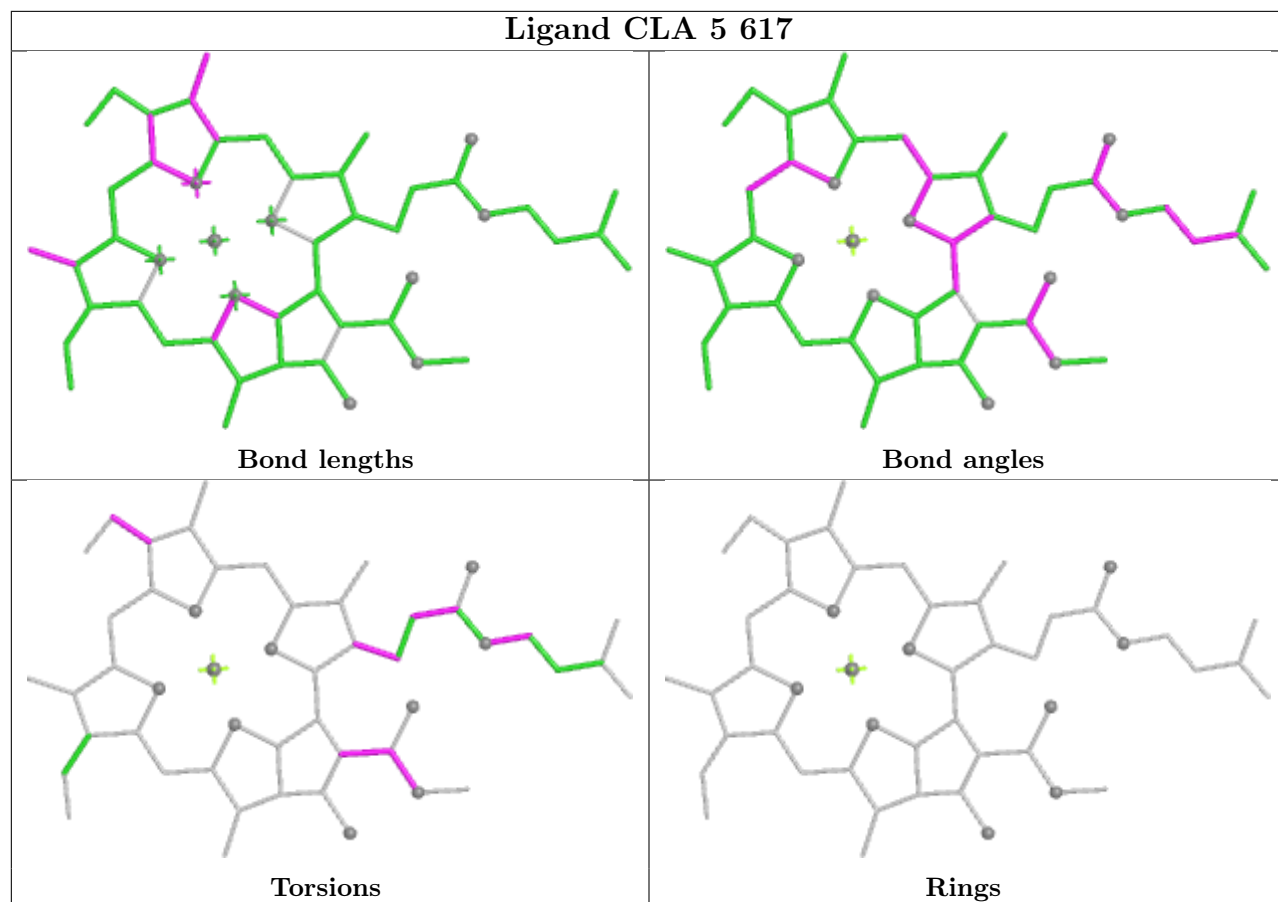
Rings

Ligand CLA 7 609

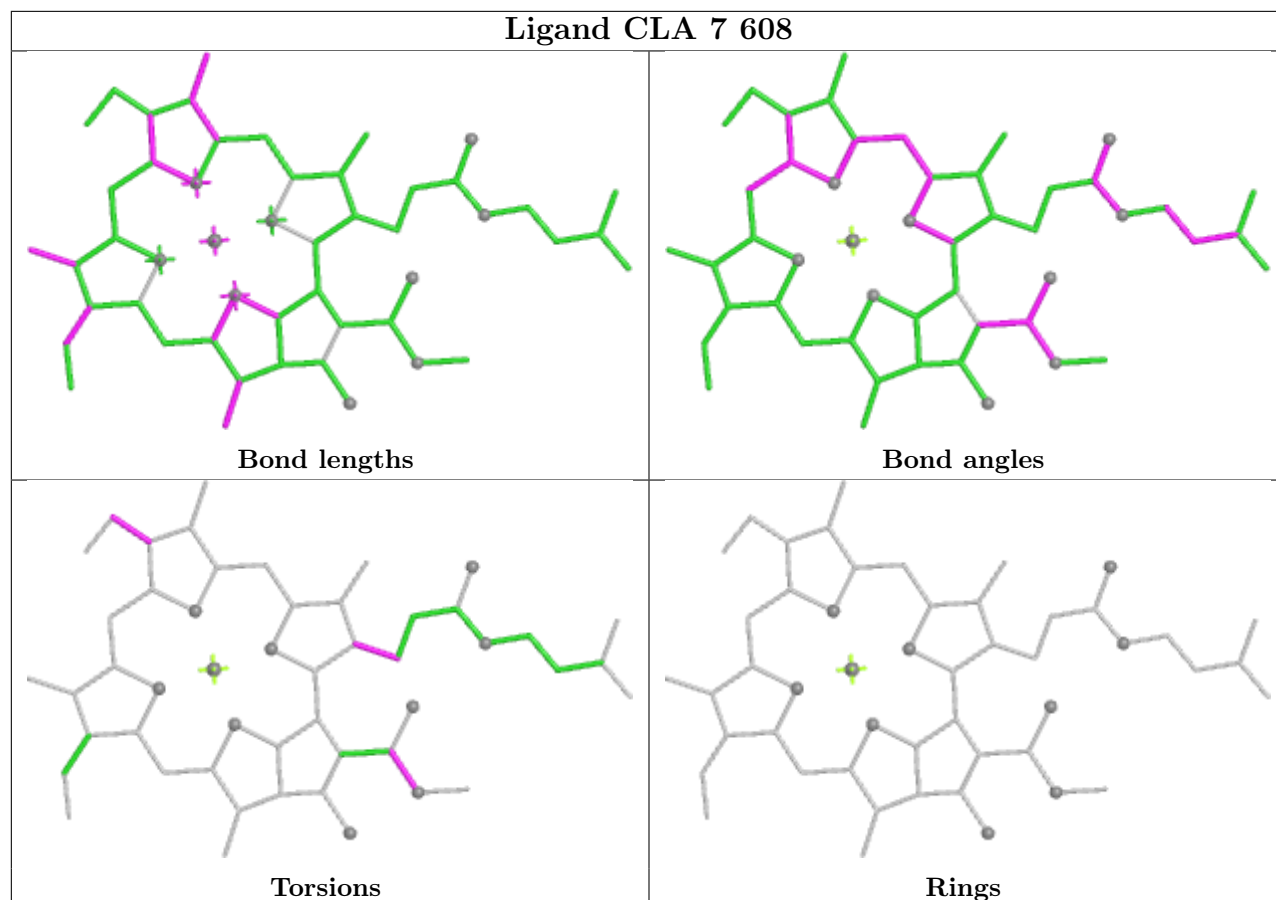


Ligand BCR B 846

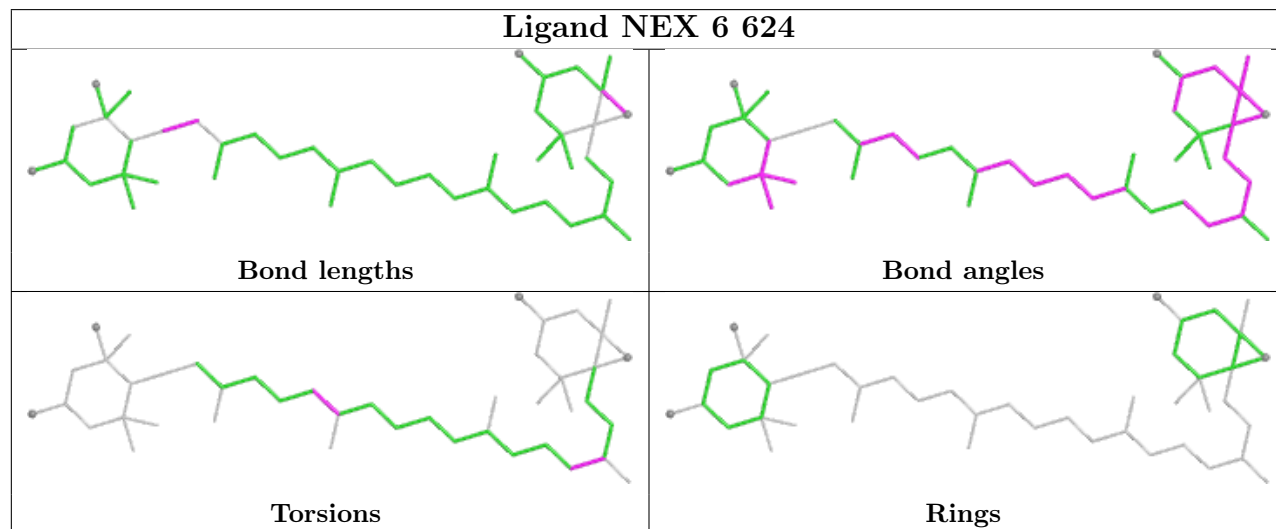


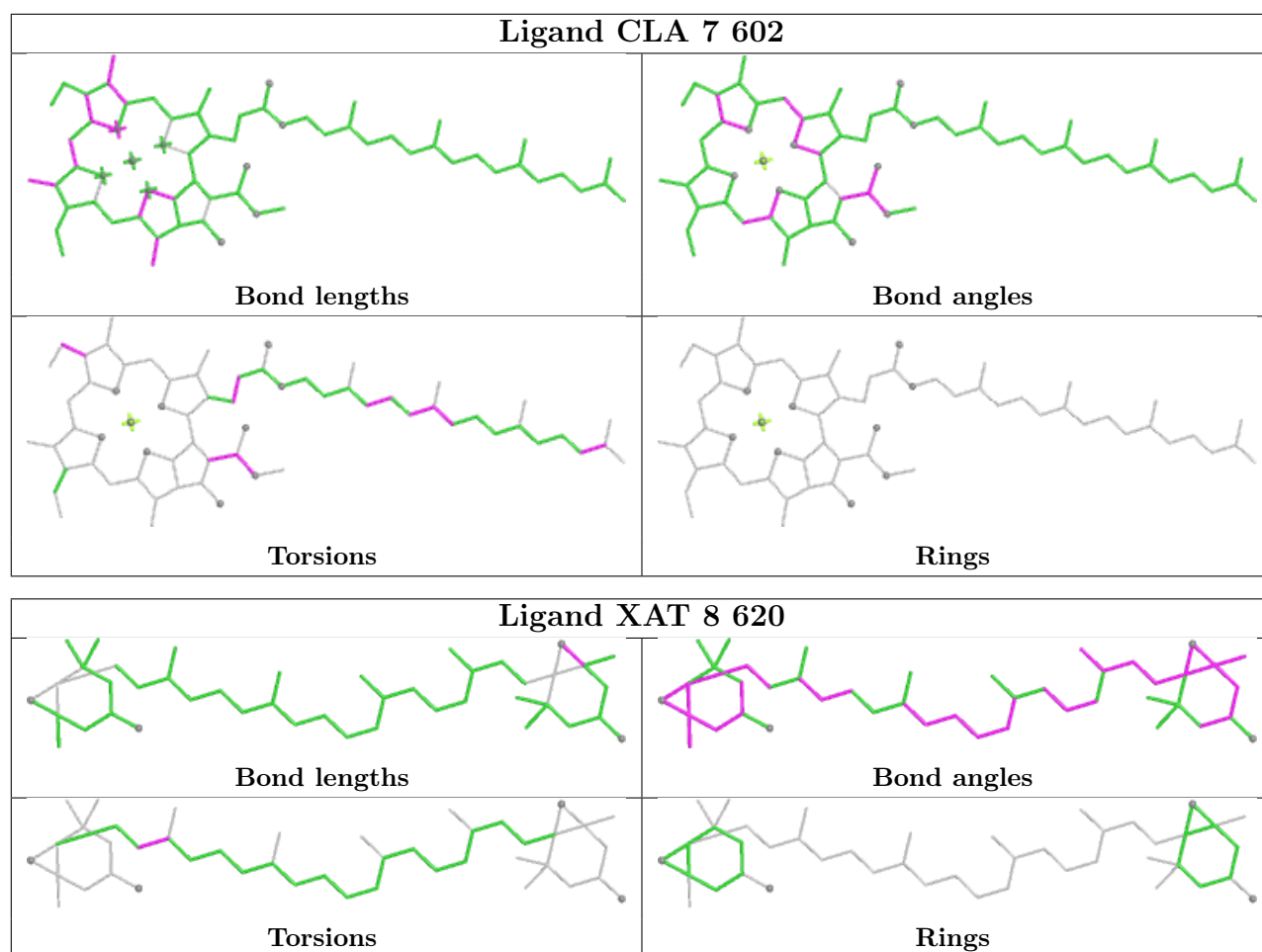


Ligand CLA 7 608

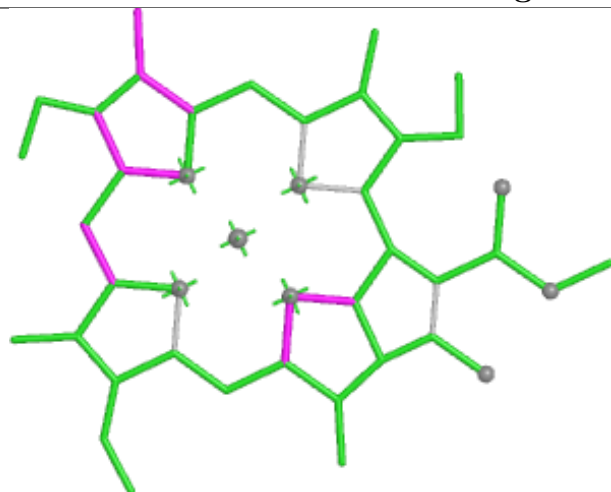


Ligand NEX 6 624

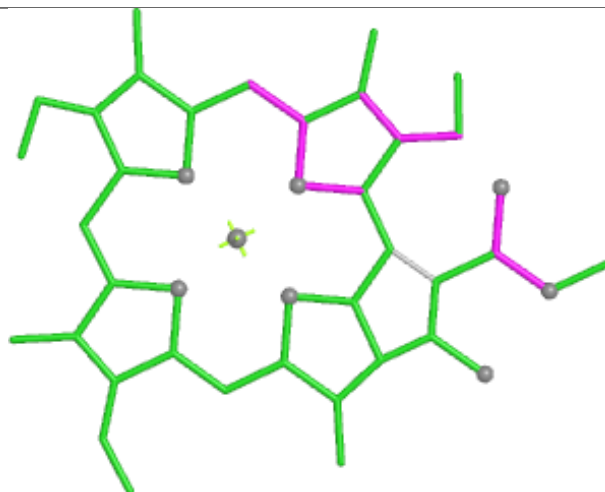




Ligand CLA B 822



Bond lengths



Bond angles

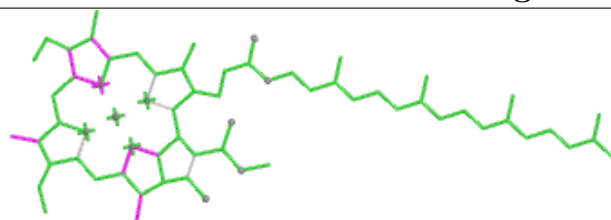


Torsions

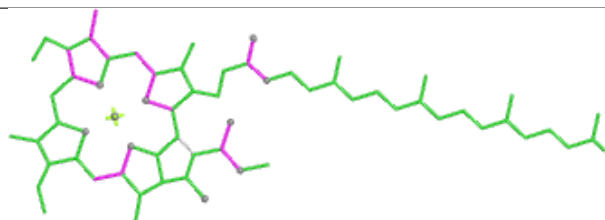


Rings

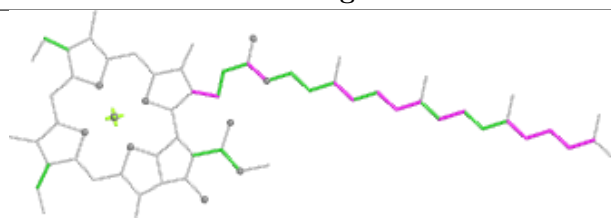
Ligand CLA A 812



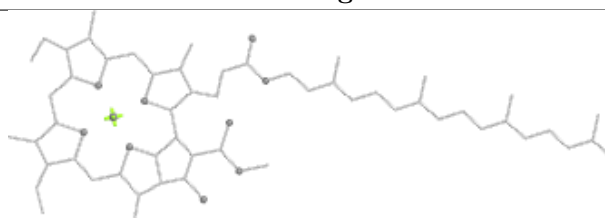
Bond lengths



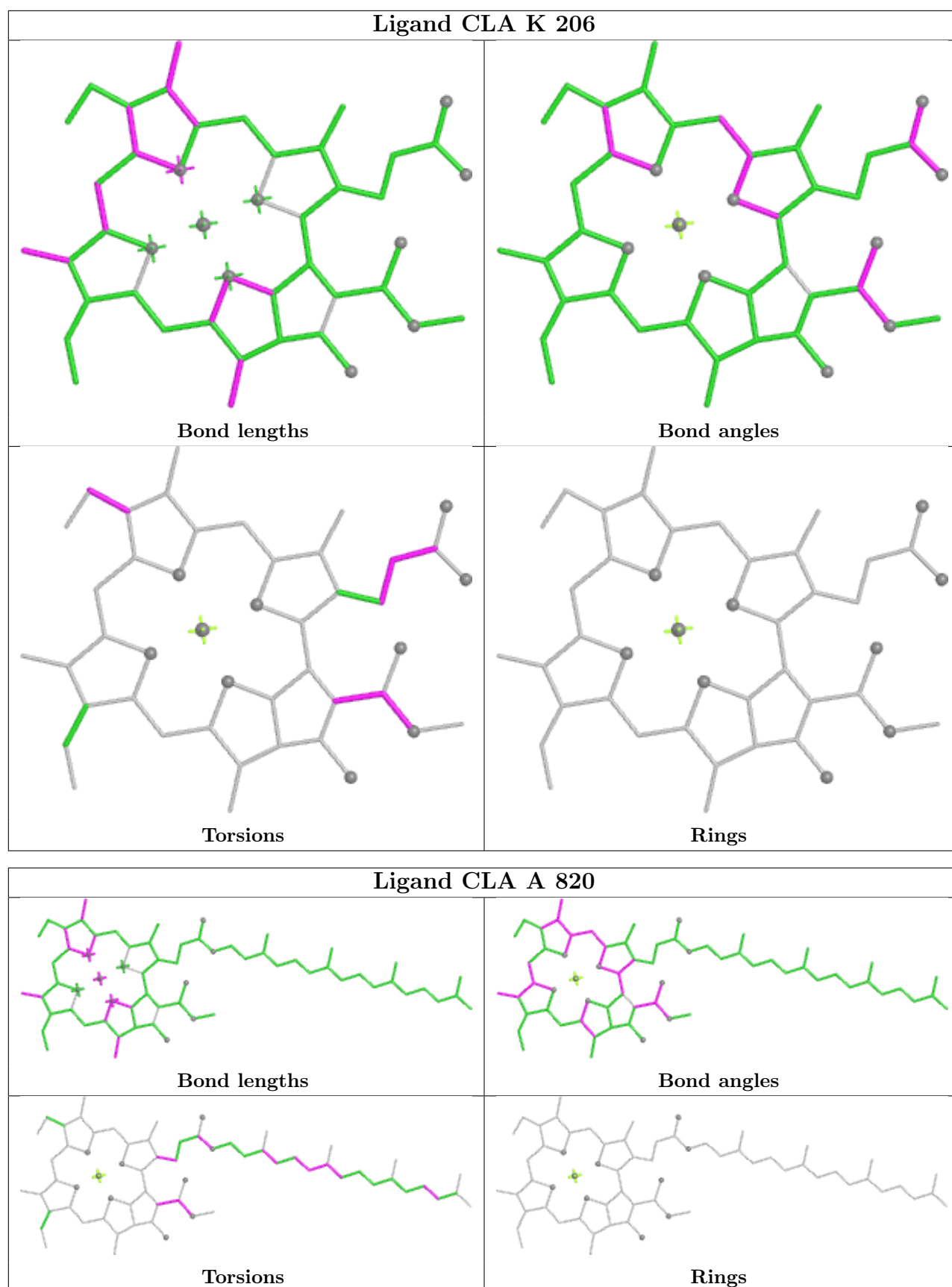
Bond angles

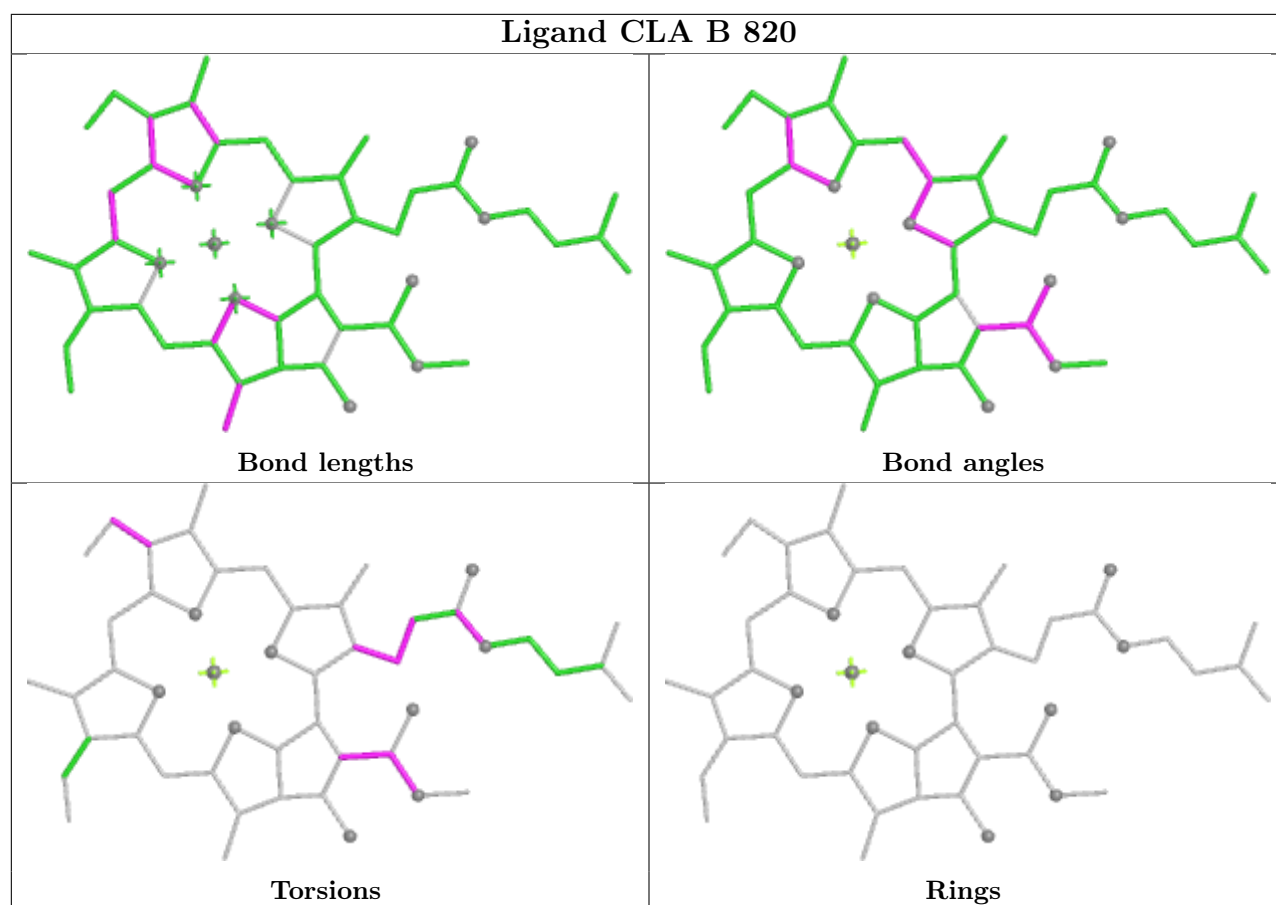


Torsions



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.

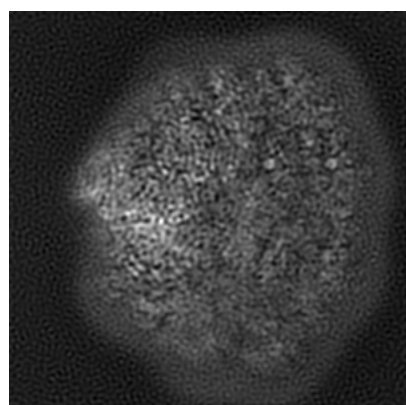
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9678. These allow visual inspection of the internal detail of the map and identification of artifacts.

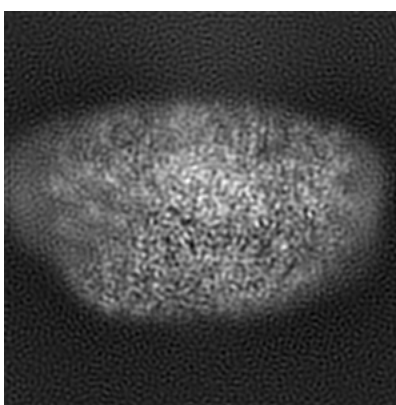
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

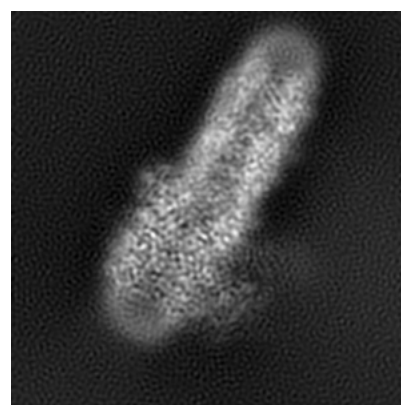
6.1.1 Primary map



X



Y

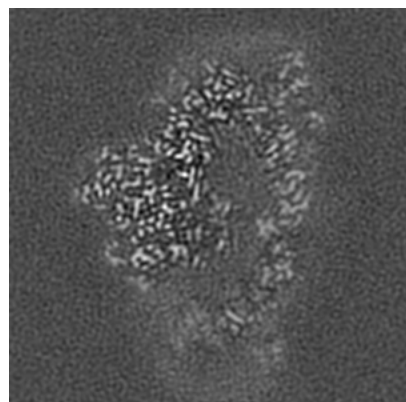


Z

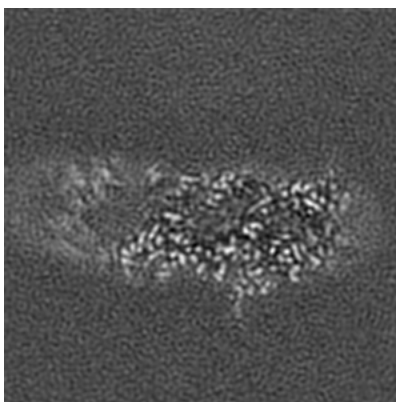
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

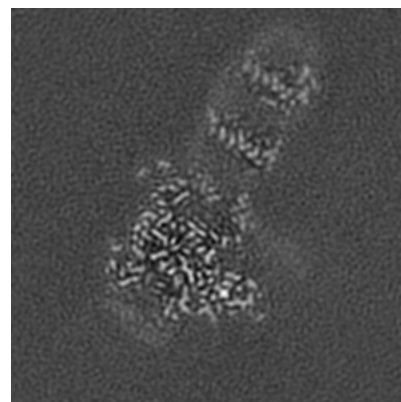
6.2.1 Primary map



X Index: 100



Y Index: 100

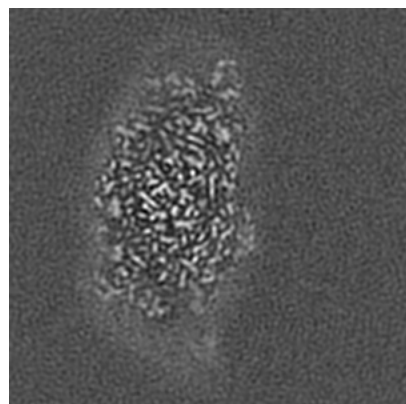


Z Index: 100

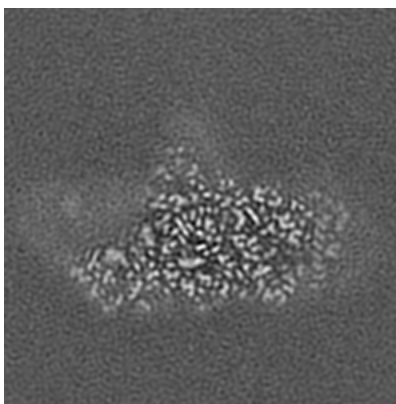
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

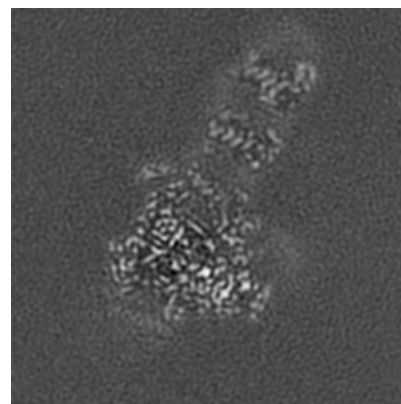
6.3.1 Primary map



X Index: 80



Y Index: 82

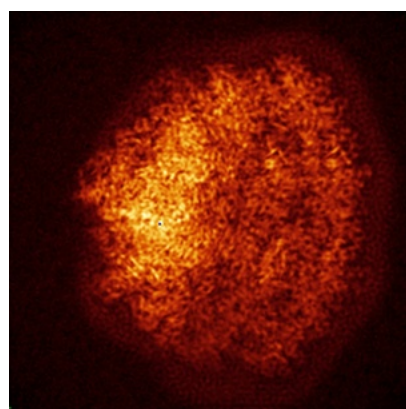


Z Index: 98

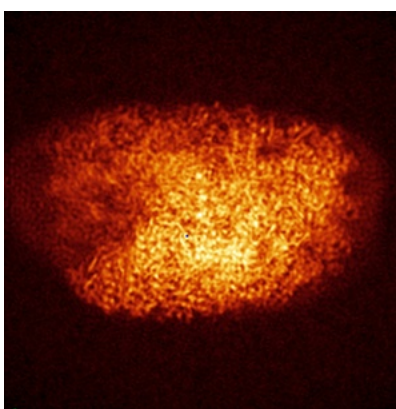
The images above show the largest variance slices of the map in three orthogonal directions.

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

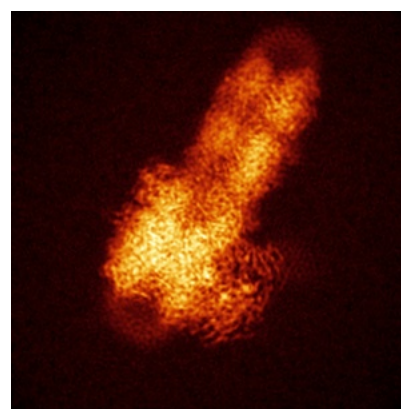
6.4.1 Primary map



X



Y

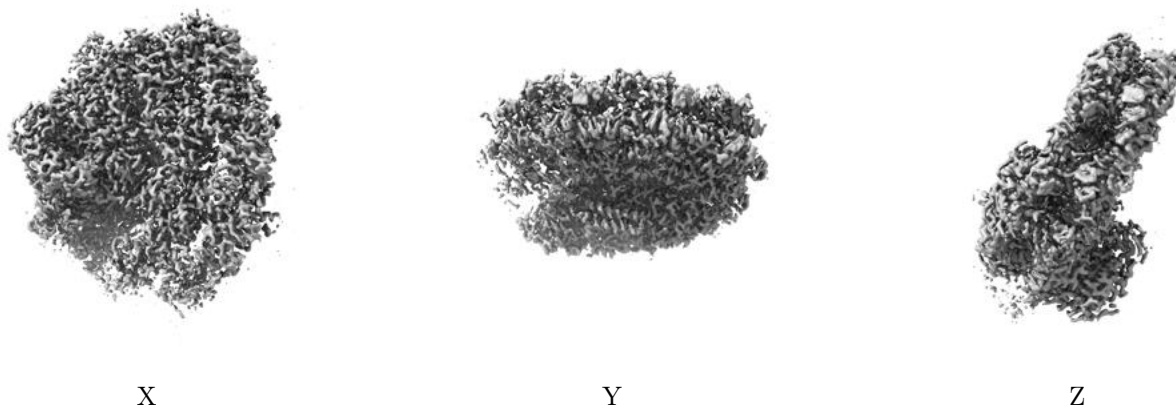


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

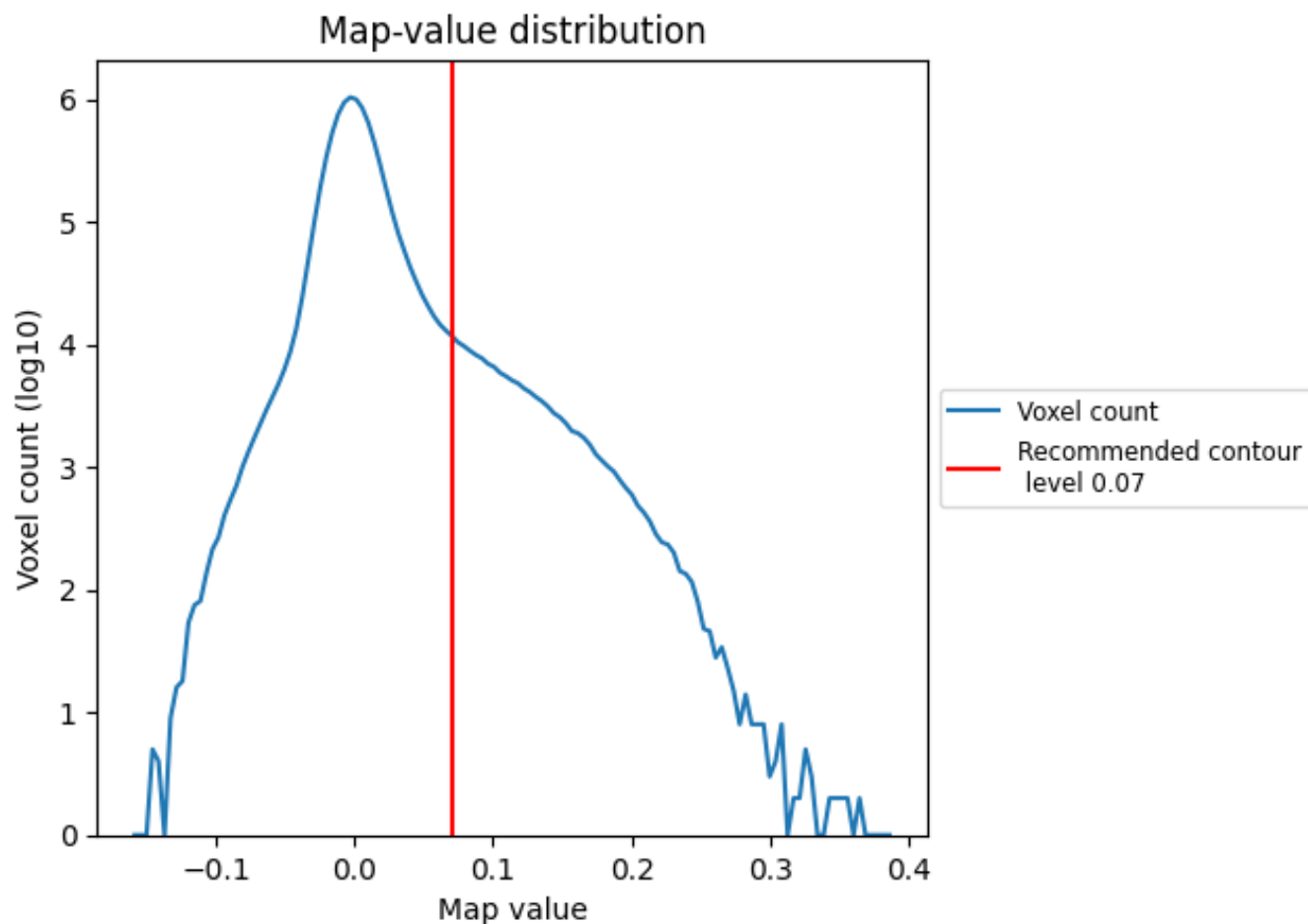
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

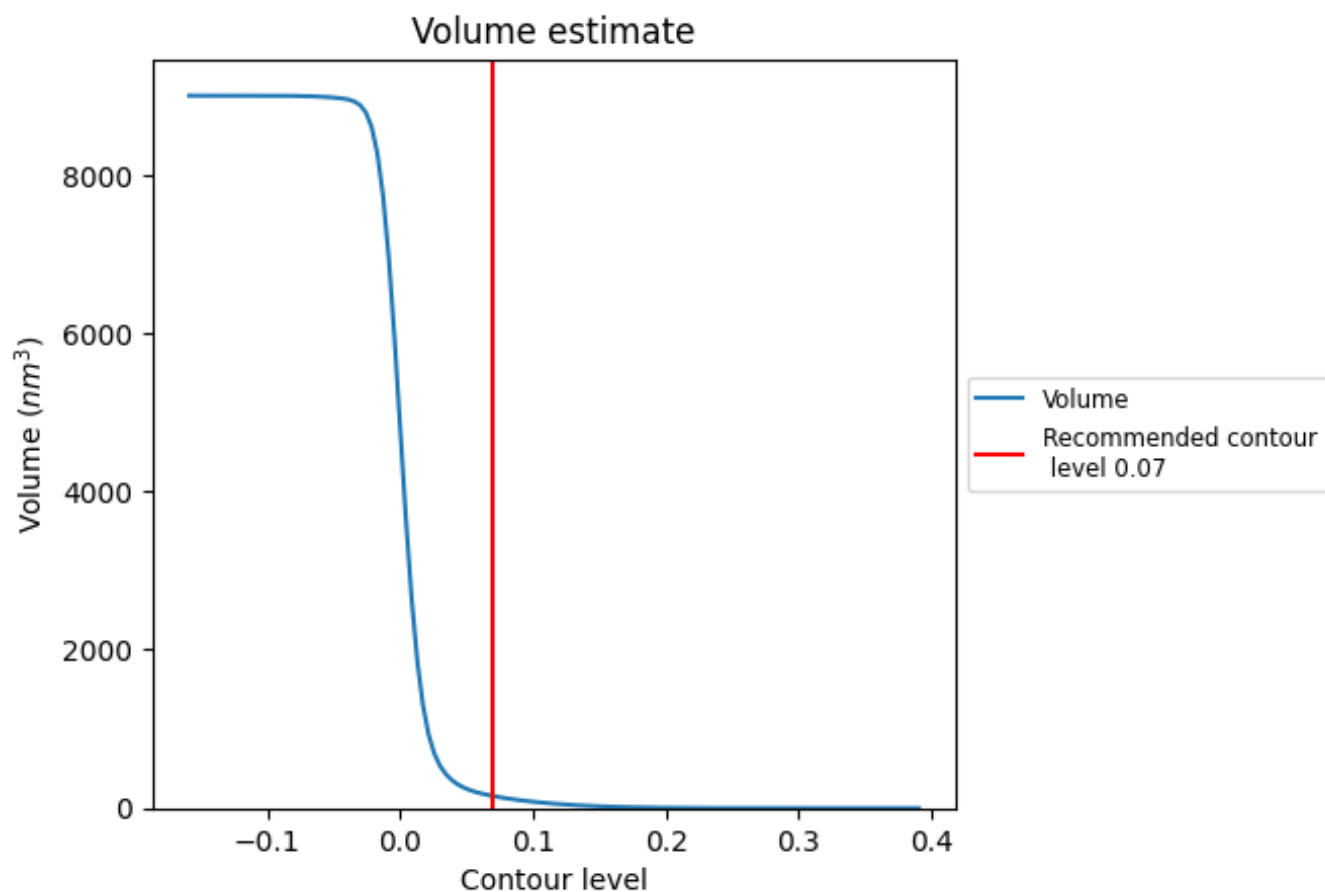
This section contains the results of statistical analysis of the map.

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.

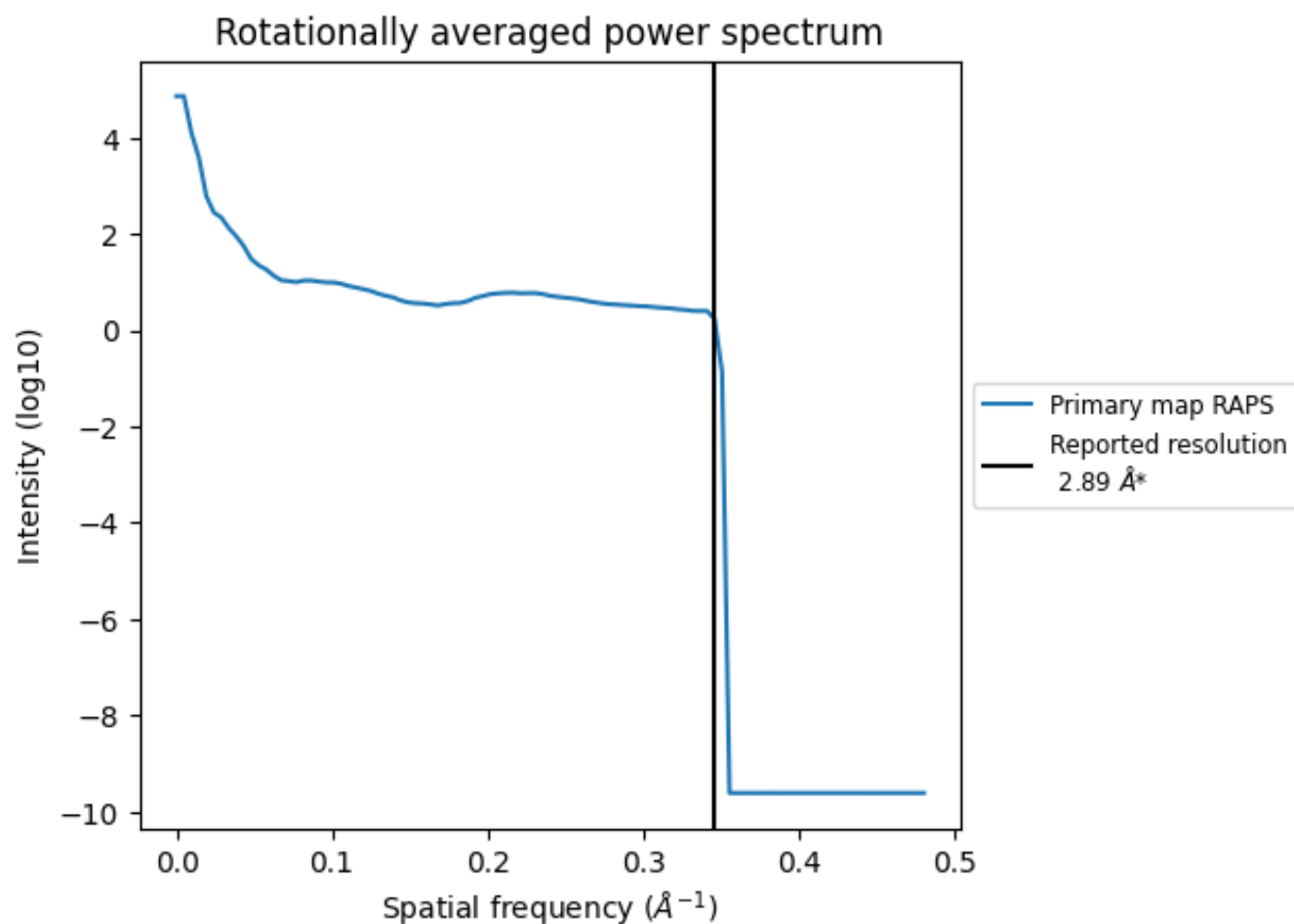
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; this corresponds to an approximate mass of 138 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 0.346 $\text{\AA}^{-1}$

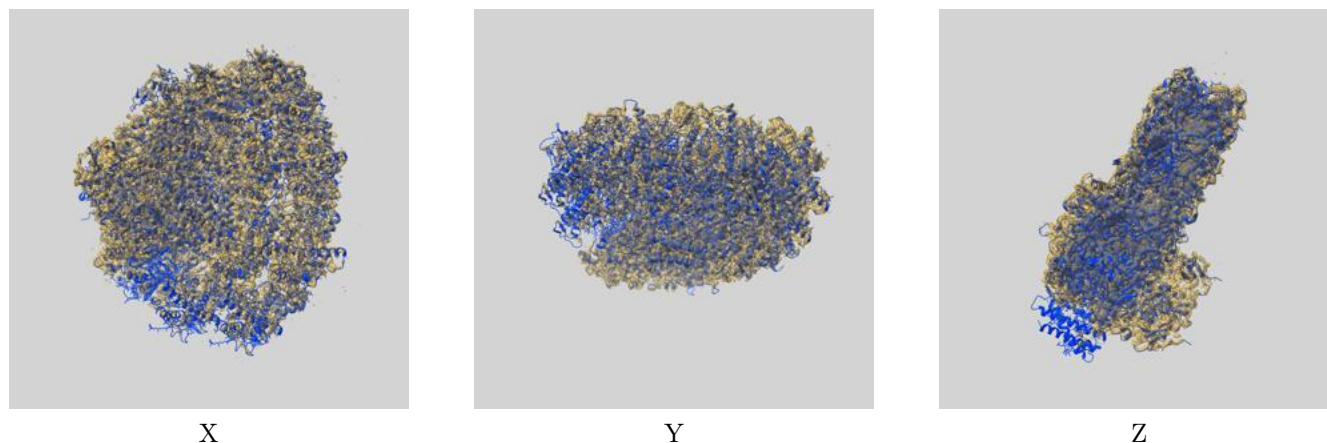
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

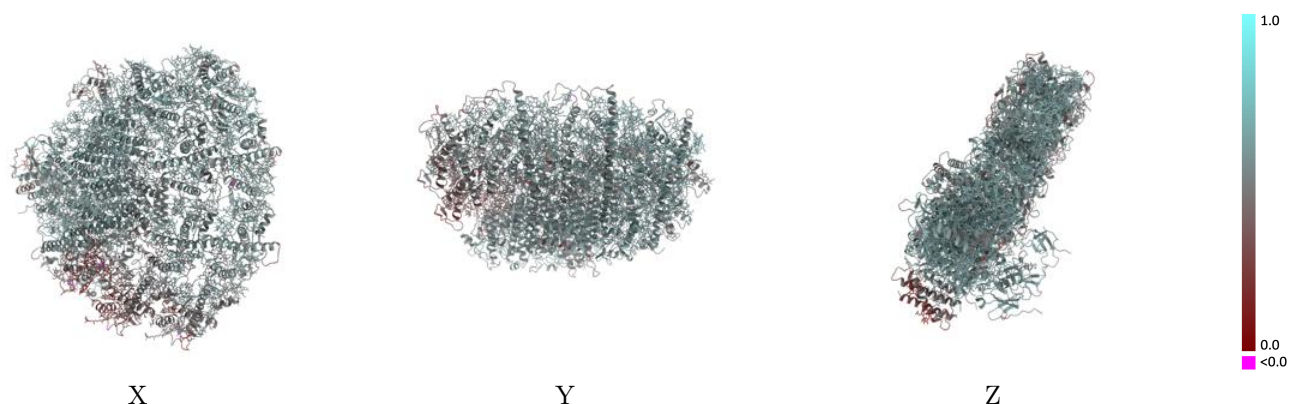
This section contains information regarding the fit between EMDB map EMD-9678 and PDB model 6IJJ. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



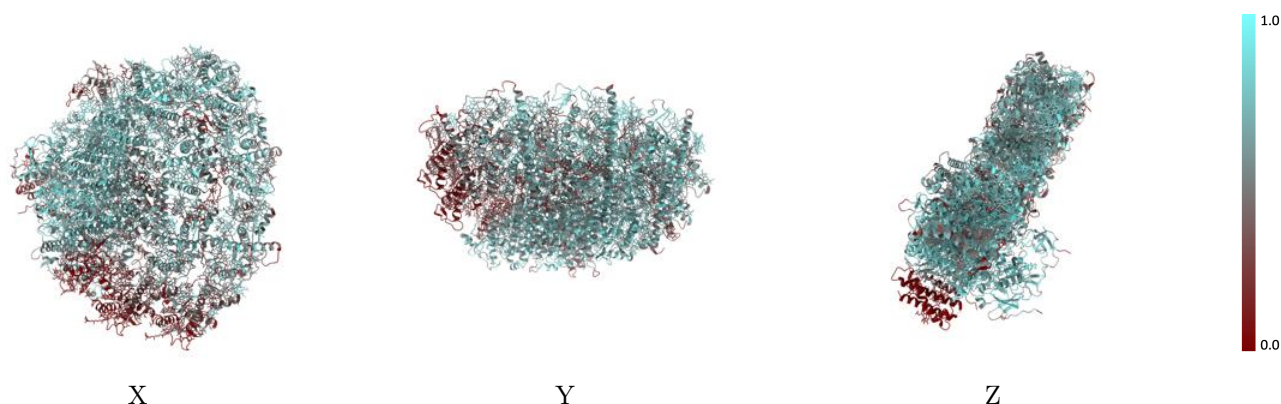
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



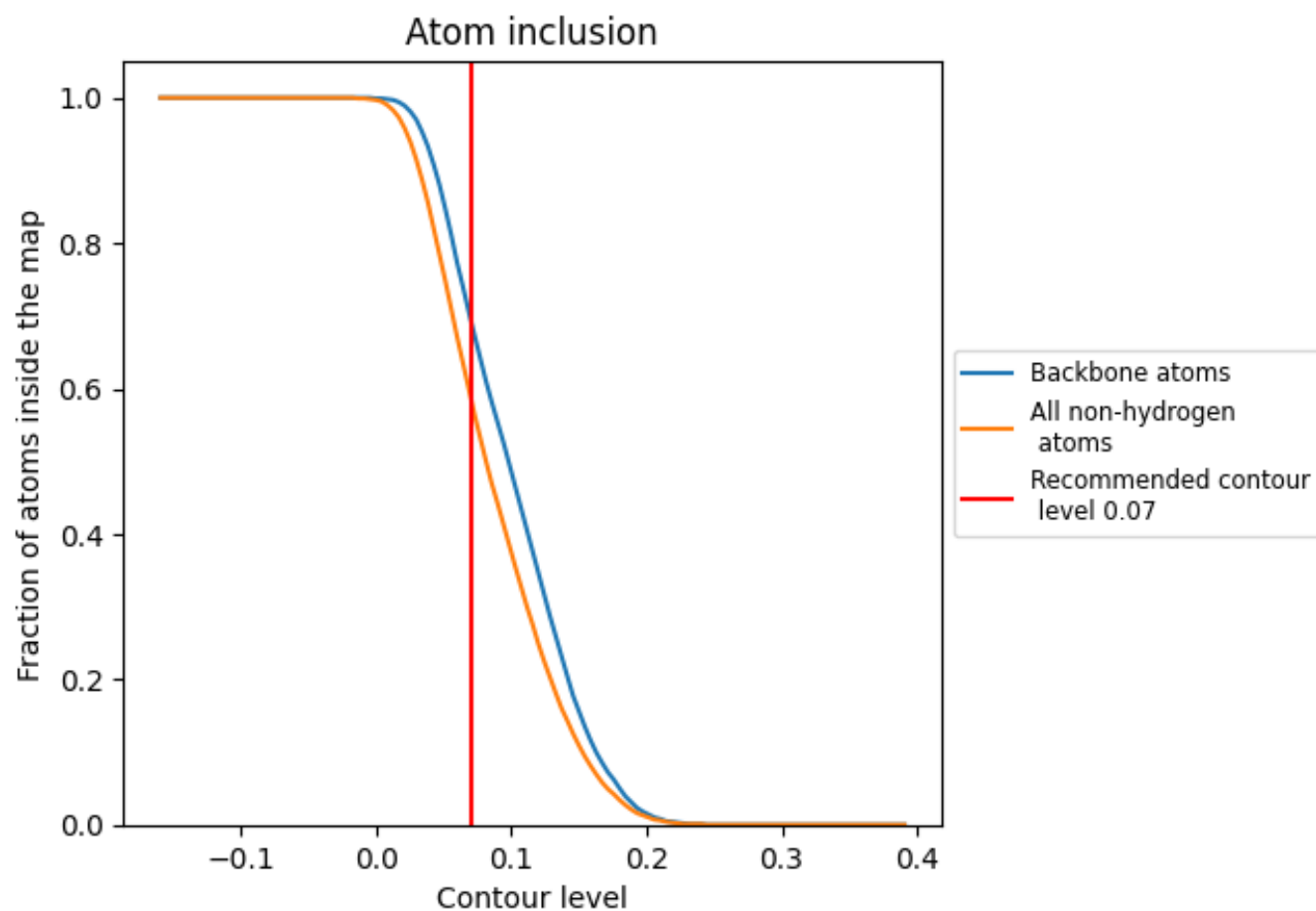
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.5370
1	0.2230	0.3740
3	0.6650	0.5730
4	0.5480	0.5270
5	0.5940	0.5430
6	0.6170	0.5440
7	0.6350	0.5530
8	0.5860	0.5300
A	0.7670	0.6020
B	0.6290	0.5440
C	0.7910	0.5640
D	0.6830	0.5550
E	0.6790	0.5520
F	0.5240	0.5090
I	0.2080	0.4660
J	0.3890	0.5120
K	0.3660	0.5030
L	0.0220	0.3540
a	0.3300	0.4660

